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Sensitivity analysis with dependent random variables: Estimation of the Shapley effects for unknown input distribution and linear Gaussian models

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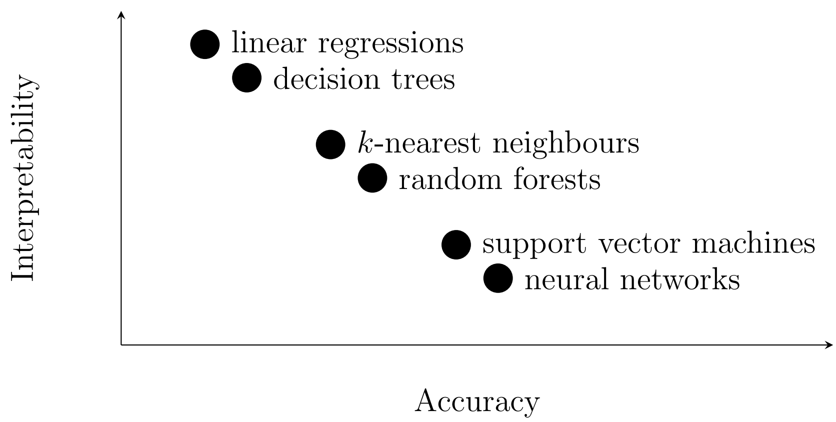
Contents

Introduction

Introduction to sensitivity analysis

Mathematical models are useful tools to the understanding of complex phenomena. A large number of data-driven models have been proposed, ranging from linear models to more and more complicated models, such as random forests and neural networks. The increase of the size of training data and the performance of computers enable the handling of *black-box* models, that require the tuning of many parameters. These kinds of models are widely used in modern engineering and their precision is confirmed in data science challenges. Since important decisions are increasingly delegated to mathematical models (such as driving different means of transport), the question of the reliability of these models arises naturally [RSG16]. It turns out that, the more a model is complex, the less it is inherently easy to interpret, and so to trust.



To increase the reliability of mathematical models, [Sam41] suggests: "In order for the analysis to be useful it must provide information concerning the way in which our equilibrium quantities will change as a result of changes in the parameters". Andrea Saltelli defines in [Sal02b] sensitivity analysis as " the study of how uncertainty in the output of a model (numerical or otherwise) can be apportioned to different sources of uncertainty in the model input". A sensitivity analysis enables to distinguish the input variables that have a large impact on the output uncertainty, and the less impacting input variables.

Sensitivity analysis is also an important tool for the use of computer codes, that simulate a physical quantity of interest. Since the inputs of the computer codes are uncertain physical quantities, sensitivity analysis explain how the uncertainties of the inputs impact the output of the computer code. This knowledge improves the understanding of the physical phenomenon and helps to prioritize efforts on the accuracy of the inputs.

Sensitivity analysis methods can be divided into two groups: local and global.

Local methods consist in the study of the impact of small variations of the inputs around one (of several) nominal value(s) of interest. They are the first sensitivity analysis methods suggested in the literature and rely on the partial derivatives of the model [Har90, Hel93]. Different methods are discussed in [BP16]. However, local sensitivity analysis is no longer relevant for non linear models when considering "large variations" of the inputs, or when the model input is uncertain.

To overcome the disadvantages of the local approach, global sensitivity analysis considers the variation of the inputs on their whole set of definition (see [IL15] for a review of this topic). Global sensitivity analysis improves the interpretability of the model in the following ways:

- We know if the variation of a specific input variable can lead to an important variation of the output or not.

- The non-influential input variables can be fixed to a nominal value to simplify the model.

We can gather global sensitivity methods in two classes: the screening methods and the probabilistic sensitivity methods.

Screening methods use a design of experiments to give a qualitative importance of the inputs. These techniques are particularly used for models with a large number of inputs since they are computationally very cheap. The first aim is to identify the least important inputs to reduce the dimension. For example, in Morris screening method [Mor91], we compute the mean of the squared variations of the model changing only one parameter at a time (this method is also called "One-at-a-time").

Finally, in probabilistic sensitivity analysis, the inputs are assumed to be random variables. For example, the input distribution can model the uncertainty on the inputs. That makes the output a random variable, with some output distribution representing its uncertainty. Hence, the variations of the inputs are not chosen arbitrarily as in local sensitivity analysis, but are defined by the input distribution.

The probabilistic sensitivity analysis methods are more accurate, and most of them aim to associate to each input variable (or each group of input variables) an index that quantify its impact on the output. These indices are called "sensitivity indices".

The first suggested sensitivity indices are defined for linear regression [SM90, Hel93]. Then, several researchers [Sob93, IH90, Wag95] defined similar sensitivity indices almost simultaneously but in different fields. These sensitivity indices are now called "Sobol indices". They are based on the analysis of variance. Although they remain very popular, other sensitivity indices have been proposed in the literature since then (see for example [PBS13, Bor07, Cha13, FKR16, LSA+15]), and we can find in [BHP16] a general framework for defining sensitivity indices based on variances, on densities, or on distributions. These sensitivity indices are very useful in many applications, for example in physics or in the industry. However, many of them suffer from a lack of interpretation when the input variables are dependent.

Recently, Owen defined new sensitivity indices in [Owe14] called "Shapley effects" that have beneficial properties and that are easy to interpret, even in the dependent case. The main advantages of these sensitivity indices compared to the Sobol indices (and their variants) are: they remain positive, their sum is equal to one and there is exactly one index for each input (there are no indices for groups of variables). The Shapley effects are based on the notion of "Shapley value", that originates from game theory in [Sha53]. The Shapley value has been widely studied ([CBSV16], [FWJ08]) and applied in different fields (see for example [MvLG+08] or [HI03]). However, only few articles focus on the Shapley effects in sensitivity analysis (see [Owe14, SNS16, OP17, IP19, BEDC19]). Song et al. suggested an algorithm to estimate the Shapley effects in [SNS16] that is implemented in the R package "`sensitivity`". However, this algorithm requires to be able to generate with the conditional distribution of the input vector.

In this context, the estimation of the Shapley effects has not been enough developed to enable a broad framework of application in the industry. The aim this thesis is to expand this estimation to make the Shapley effects easier to use in the industry and in particular for the "Commissariat à l'énergie atomique et aux énergies alternatives" (CEA). The example of data from CEA in the field of nuclear safety will be treated.

Contributions of the thesis

For real data, the independence assumption of the input variables is not realistic, and so we focus on the computation of the Shapley effects. The contribution is twofold.

First, we focus in the general setting. We suggest new estimators of the Shapley effects in the same framework as the one suggested in [SNS16] with lower variances. Then we extend these estimators to the case where we only observe an i.i.d. sample on the inputs and we obtain rates of convergence for them.

Secondly, we focus on the Shapley effects in the linear Gaussian framework. We suggest an algorithm to compute them when the parameters (input covariance matrix and regression coefficients) are known. Then, we improve the efficiency of the algorithm in high dimension when the covariance matrix is block-diagonal. We give another algorithm to estimate the Shapley effects when the parameters are unknown, particularly in high dimension. We also give guaranties when using the Gaussian linear framework while the model is not linear but the covariance matrix converges to 0.

During the PhD, we also worked on a different topic, namely on kernels defined on the symmetric group. Illustrated by numerical applications, our work on kernels on the symmetric group and on partial ranking enables to handle complex data.

We provide families of kernels and we prove their positive definiteness to use them as covariance functions for Gaussian processes. Based on the works of [Bac14], we prove asymptotic results on the maximum likelihood estimator. We also implemented our kernels to solve optimization problems defined on the symmetric group using the expected improvement strategy. We provide an application to the search of the best Latin Hypercube Design.

We also extend our kernels on partial ranking, with numerical simplifications in some cases. We compare these kernels with a state-of-the-art algorithm on numerical applications, which reveals that our suggested kernels seem to be significantly more efficient.

Organization of the manuscript

The manuscript is organized into three parts.

Part I, contains Chapter 1 on the state-of-the-art of sensitivity analysis and the Shapley effects. First, we define the Sobol indices for independent inputs and we give some estimators. We then give a generalisation of the Sobol indices when the inputs are dependent with a list of other sensitivity indices. Finally, we give the definition of the Shapley effects and the already existing algorithm to estimate them.

Part II, containing Chapter 2, is dedicated to the improvement of the estimation of the Shapley effects in the general case. It is based on [BBD20]. We reduce the variance of the estimates of the Shapley effects and extend them when we only observe an i.i.d. sample of the inputs.

Part III focuses on the Shapley effects in the linear Gaussian framework.

In Chapter 3, we provide an algorithm to compute the Shapley effects using the covariance matrix and the vector of the linear model. It comes from a part of [BBDM19].

Chapter 4 highlights the problem of computing the Shapley effects in the Gaussian linear framework when the number of input variables is large. We give theoretical results on sensitivity indices in a general setting, when the inputs form independent groups of variables. Then we derive an algorithm that computes the Shapley effects in the high-dimensional Gaussian linear framework with a block-diagonal covariance matrix. Chapter 4 is based on the rest of [BBDM19].

In Chapter 5, from [BBCM20], we estimate the Shapley effects in the Gaussian linear setting with a block-diagonal covariance matrix when the parameters are unknown, with a focus on the high-dimensional framework.

In Chapter 6, we aim to approximate a general setting by a Gaussian linear model, when the uncertainties are small, to estimate the Shapley effects using our previous algorithm. Firstly, we focus on the linear approximation of the function and the corresponding Shapley effects, under the Gaussian assumption. Secondly, we study the asymptotic behaviour of the empirical mean of the non Gaussian inputs to approximate it by a Gaussian vector with a covariance matrix that goes to 0. This chapter is based on [BBDM20].

The proofs are given in the appendix. Chapter V in the appendix contains our independent work from [BBGL20] on kernels defined on the symmetric group.

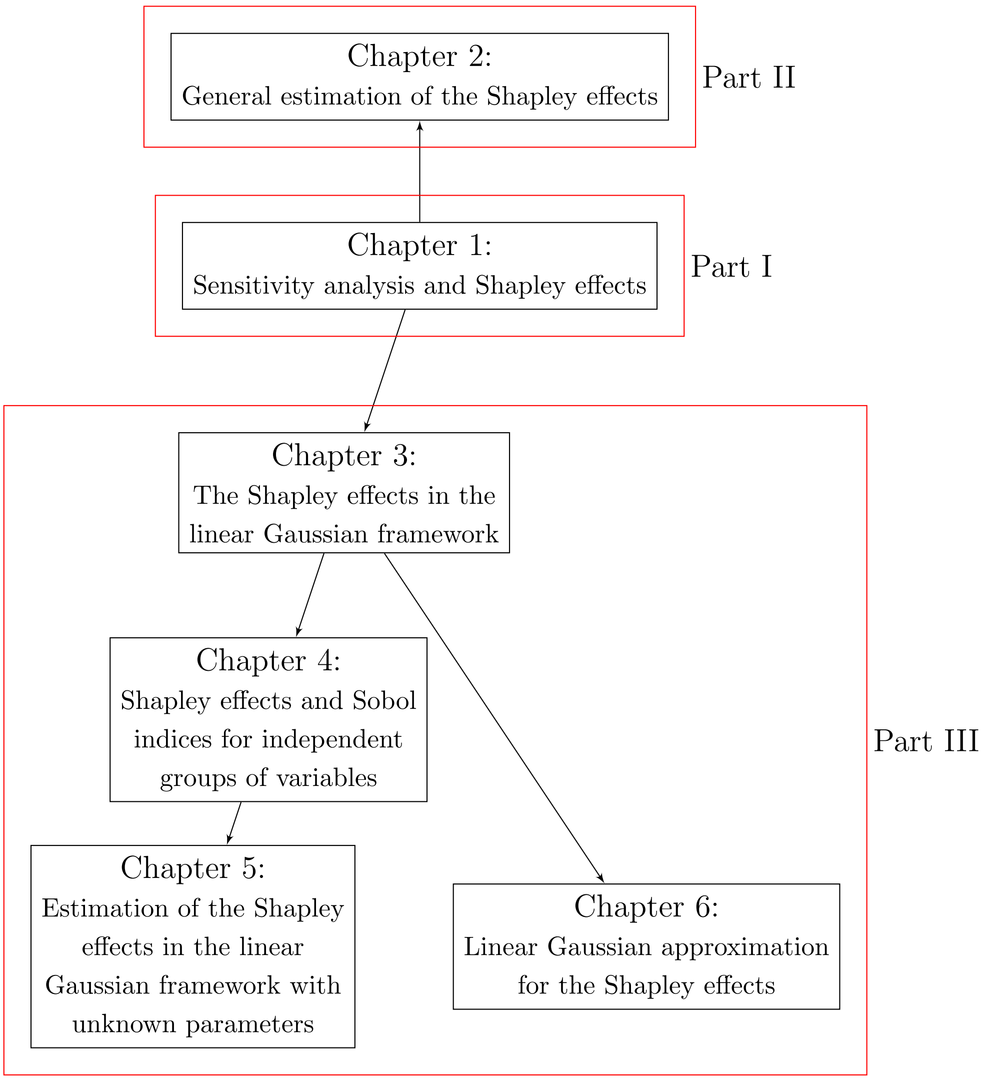


Figure 1: Dependency diagram.

Part I

State of the art

Chapter 1

Sensitivity analysis and Shapley effects

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a probability space, $\mathcal{X} = \prod_{i=1}^{p} \mathcal{X}_i$ be endowed by the product σ-algebra $\mathcal{E} = \otimes_{i=1}^{p} \mathcal{E}_i$ and X be a random variable from Ω to $\mathcal{X}$ with distribution $\mathbb{P}_X$.
If $u \subset [1:p] = \{1, 2, \cdots, p\}$, we define $x_u := (x_i)_{i \in u}$, $\mathcal{X}_u := \prod_{i \in u} \mathcal{X}_i$ and $|u|$ the cardinality of u.

To simplify the notation, let $L^2 := L^2(\mathcal{X}, \mathbb{R}, \mathbb{P}_X)$ be the Hilbert space of the set of squared integrable functions. For orthogonal linear subspaces V_1 and V_2, we will write $V_1 \perp V_2$. If V is a subspace of L^2, let $V^\perp$ be the orthogonal complement of V. We will use the symbol "$\bigoplus$" for the direct sum in L^2 and "$\overset{\perp}{\bigoplus}$" for the orthogonal direct sum in L^2.

Finally, let $f \in L^2$ and $Y = f(X)$. We call X the "input variables" and Y the "output variable". In practice, the random vector X correspond to the uncertain inputs, the function f to the model and the random variable Y to the uncertain output. This setting will be valid throughout the entire manuscript (except for Chapter V in the appendix).

The aim of the sensitivity indices is to quantify the impact of a variable X_i (or of a group of variables X_u) on the output variable Y.

A Sobol indices for independent inputs

In Section A, we assume that the random variables $(X_i)_{i \in [1:p]}$ are independent.

A.1 Definition of the Sobol indices

When the input variables are independent, the variance decomposition into Sobol indices comes from the unique writing of the function f into $f(x) = \sum_{u\subset[1:p]} f_u(x_u)$ where the f_u are not correlated and satisfy further technical conditions. A way to describe this decomposition is defining the subspaces $(H_u^0)_{u\subset[1:p]}$ of L^2 on which we will project the function f onto. Here, we begin to define the subspaces H_u (which are easy to interpret) and the related closed Sobol indices. Then we deduce the more complicated subspaces H_u^0 of the Hoeffding decomposition and the related Sobol indices.

A.1.i) Closed Sobol indices

If u is a subset of $[1:p]$, the first way to assess the impact of the group of variable X_u on $f(X)$ is to project find the closest function of X_u from $f(X)$. Let $\sigma(X_u)$ be the σ-algebra generated by X_u. If a random variable Z is measurable with respect to $\sigma(X_u)$, we will write $Z \in \sigma(X_u)$.

Definition 1. *For all $u \subset [1:p]$, let H_u be the closed linear subset of L^2 defined by:*

$$H_u := \{h_u \in L^2 \mid h_u(X) \in \sigma(X_u)\}.$$

The space H_u is the set of function h_u such that $h_u(X)$ is a function of X_u. Hence, the projection of f on H_u gives the best approximation (in L^2) of f which is a function a X_u. This projection is $x \longmapsto \mathrm{E}(Y|X_u = x_u)$. Now, taking the variance and dividing by $\mathrm{Var}(Y)$, we obtain some sensitivity index called the closed Sobol index (see [IP19]).

Definition 2 (Closed Sobol indices)**.** *For all $u \subset [1:p]$, the quantity S_u^{cl}, defined by*

$$S_u^{cl} := \frac{\mathrm{Var}(\mathrm{E}(Y|X_u))}{\mathrm{Var}(Y)} \tag{1.1}$$

is called the "closed Sobol index" of the group of variables X_u, where we write, by convention $\mathrm{E}(Y|X_\emptyset) = \mathrm{E}(Y)$.

We remark the $S_\emptyset^{cl} = 0$, $S_{[1:p]}^{cl} = 1$ and, for all $u \subset [1:p]$, $S_u^{cl} \in [0,1]$. The Sobol index S_u^{cl} can easily be interpreted as the part of the impact of X_u on the variance of Y. However, the sum over $u \subset [1:p]$ of the closed Sobol indices is not equal to 1 in general, which is an issue for interpretation. In order to define indices which sum is one, we now introduce new linear subspaces of L^2 on which we will project onto.

A.1.ii) Hoeffding decomposition

Definition 3. *Let $H_\emptyset^0$ be the space of functions that are constant $\mathbb{P}_X$ almost everywhere.*
For all $u \subset [1:p]$, $u \neq \emptyset$, we write:

$$H_u^0 := \{h_u \in H_u,\ \forall v \subsetneq u,\ \mathrm{E}(h_u(X_u)|X_v) = 0\}. \tag{1.2}$$

Abusing notation, for $h_u \in H_u$, we write indifferently $h_u(X_u)$ or $h_u(X)$.

These linear subspace have interesting immediate properties.

Lemma 1. *For all $u \subset [1:p]$, the linear subspaces H_u and H_u^0 are closed in L^2, and*

$$\forall u \neq v,\ H_u^0 \perp H_v^0. \tag{1.3}$$

The closeness of H_u^0 comes from the fact that it is the kernel of a continuous linear map. Thus, we can define the orthogonal projection $P_{H_u^0}$ on H_u^0. The next proposition now gives an explicit formula of this projection, and shows that L^2 is actually the orthogonal direct sum of the linear subspaces H_u^0, for $u \subset [1:p]$.

Proposition 1. *For all $g \in L^2$ and for all $u \subset [1:p]$,*

$$P_{H_u^0}(g)(X) = \sum_{v \subset u} (-1)^{|u|-|v|} \mathrm{E}(g(X)|X_v). \tag{1.4}$$

Moreover,

$$\forall u \subset [1:p],\ H_u = \overset{\perp}{\bigoplus_{v \subset u}} H_v^0. \tag{1.5}$$

In particular,

$$L^2 = \overset{\perp}{\bigoplus_{u \subset [1:p]}} H_u^0. \tag{1.6}$$

We can find the proof of Proposition 1 in [Vaa98]. This proposition ensures that there exists an unique decomposition $f = \sum_{u \subset [1:p]} f_u$, called "the Hoeffding decomposition of f" such that $f_u \in H_u^0$ for all $u \subset [1:p]$, where

$$f_u(X) = \sum_{v \subset u} (-1)^{|u|-|v|} \mathrm{E}(f(X)|X_v). \tag{1.7}$$

A.1.iii) Sobol indices

Since the functions $(f_u)_{u\subset[1:p]}$ of the Hoeffding decomposition are orthogonal, we have

$$\mathrm{Var}(f(X)) = \sum_{u\subset[1:p]} \mathrm{Var}(f_u(X_u)).$$

Hence, the decomposition of the function f matches with a decomposition of the variance of $f(X)$. Now, dividing the previous equation by $\mathrm{Var}(Y)$, we obtain

$$\sum_{u\subset[1:p]} \frac{\mathrm{Var}(f_u(X_u))}{\mathrm{Var}(Y)} = 1.$$

So, the quantity $\mathrm{Var}(f_u(X_u))/\mathrm{Var}(Y)$ can be interpreted as the part of the variance of $f(X)$ from the interaction of the group of variable X_u.

Definition 4 (Sobol indices, independent case)**.** *For all $u \subset [1:p]$, the quantity S_u defined by*

$$S_u := \frac{\mathrm{Var}(f_u(X_u))}{\mathrm{Var}(Y)}$$

is called the "Sobol index" of the group of variables X_u.

Since the sum of the Sobol indices is equal to one and they are in $[0,1]$, we interpret them as the following:

- if $u = \{i\}$, $S_i := S_{\{i\}}$ quantifies the impact of the input variable X_i;
- if $u = \{i_1, \cdots, i_k\}$, S_u quantifies the impact of the interaction between the input variables $X_{i_1}, \cdots, X_{i_k}$.

A.1.iv) Comparison of the closed Sobol indices with the Sobol indices

By Equation (1.5), we can easily write the closed Sobol indices using Sobol indices.

Proposition 2. *For all $u \subset [1:p]$, we have*

$$S_u^{cl} = \sum_{v\subset u} S_v.$$

Thus,

$$S_u = S_u^{cl} - \sum_{v\subsetneq u} S_v.$$

Proposition 2 strengthens the idea that the closed Sobol index S_u^{cl} represents the whole impact of the group of variable X_u, and that the Sobol index S_u only represents the impact of the interactions between the variables $(X_i)_{i\in u}$ that are not expressed by subsets of variables $(X_i)_{i\in v}$ for $v \subsetneq u$.

Example 1. *If $X_1, \cdots, X_p$ are zero-mean independent variables with variance 1, and if*

$$f(X) = \sum_{u\subset[1:p]} a_u \prod_{i\in u} X_i,$$

then, for all $\emptyset \subsetneq u \subset [1:p]$

$$S_u = \frac{a_u^2}{\sum_{\emptyset\subsetneq v\subset[1:p]} a_v^2}, \quad S_u^{cl} = \frac{\sum_{\emptyset\subsetneq v\subset u} a_v^2}{\sum_{\emptyset\subsetneq v\subset[1:p]} a_v^2}.$$

Conversely, we can write the Sobol indices with the closed Sobol indices (similarly than the projection of f on the $(H_u^0)_{u\subset[1:p]}$ with the projection of f on the $(H_u)_{u\subset[1:p]}$, see Equation (1.7)).

Proposition 3. *For all $u \subset [1:p]$, we have*

$$S_u = \sum_{v\subset u} (-1)^{|u|-|v|} S_u^{cl}. \tag{1.8}$$

A.1.v) First order Sobol indices and total Sobol indices

When $u = \{i\}$, $S_i = S_i^{cl}$ is called the i-th Sobol index of order one. It measures the influence of X_i on Y without its interactions with other variables. In some cases, the i-th Sobol index is not sufficient to assess the impact of X_i on Y (see Section B.1.iii)). In order to measure the impact of X_i with all its interactions, [HS96] introduced the total Sobol indices, defined, for all $i \in [1:p]$ by:

$$ST_i := \sum_{\substack{u\in[1:p],\\ i\in u}} S_u,$$

and one can easily see that

$$ST_i = 1 - S_{-i}^{cl} = \frac{\mathrm{E}(\mathrm{Var}(Y|X_{-i}))}{\mathrm{Var}(Y)}, \tag{1.9}$$

where we write $-i = [1:p] \setminus \{i\}$.

Remark 1. *The sum of the Sobol indices of order one can be strictly less than* 1*, since we do not take into account all the Sobol indices of higher order. The sum of the total Sobol indices can be strictly larger than* 1*, since the Sobol indices of higher order are counted several times. Indeed,*

$$\sum_{i=1}^{p} ST_i = \sum_{i=1}^{p} \sum_{\substack{u\in[1:p],\\ i\in u}} S_u = \sum_{u\subset[1:p]} |u| S_u \geq \sum_{u\subset[1:p]} S_u = 1. \tag{1.10}$$

A.2 Estimation of the Sobol indices

The estimation of the sensitivity indices is an important subject in global sensitivity analysis. The estimation of the Sobol indices has been studied in different frameworks:

- We only observe a sample $(X^{(n)}, f(X^{(n)}))_{n\in[1:N]}$;
- We observe a sample $(X^{(n)})_{n\in[1:N]}$ and we have the computer code of f (that is to say, we are able to compute $f(x)$ for any input x);
- We know the distributions of the inputs and we have the computer code of f.

Moreover, some estimators require a large number of evaluations of f and so a computationally cheap computer code of f, whereas some researches focus on the estimation with a costly computer code of f.

A.2.i) Pick-and-Freeze estimators of the Sobol indices

The quantities the most difficult to estimate in the Sobol indices and the closed Sobol indices are the $\mathrm{Var}(\mathrm{E}(Y|X_u))$, for $u \subset [1:p]$, and in particular $\mathrm{E}(\mathrm{E}(Y|X_u)^2)$. In general, the estimation of the function $x_u \longmapsto \mathrm{E}(Y|X_u = x_u)$ is a difficult non-parametric problem. Hence, to estimate the quantity $\mathrm{E}(\mathrm{E}(Y|X_u)^2)$ easily, the "Pick-and-Freeze" estimators have been introduced in [HS96]. Since then, they have been widely used and studied by mathematicians. The idea of the Pick-and-Freeze estimator is based on the following proposition, that arises from Fubini Theorem. For $x^{(1)}, x^{(2)} \in \mathcal{X}$ and for $\emptyset \subsetneq u \subsetneq [1:p]$, we let $(x_u^{(1)}, x_{-u}^{(2)})$ be the element $v \in \mathcal{X}$ such that $v_u = x_u^{(1)}$ and $v_{-u} = x_{-u}^{(2)}$, and we let $f(x_u^{(1)}, x_{-u}^{(2)}) := f(v)$. We use this notation throughout the manuscript.

Proposition 4 ([HS96], [JKLR+14])**.** *For $\emptyset \subsetneq u \subsetneq [1:p]$, let X and X' be independent with distribution $\mathbb{P}_X$. Let $X^u := (X_u, X'_{-u})$. Then :*

$$\mathrm{E}(\mathrm{E}(Y|X_u)^2) = \mathrm{E}(f(X)f(X^u)). \tag{1.11}$$

This proposition enables us to write a double expectation as a single expectation, that we can estimation by Monte-Carlo. If we observe an i.i.d. sample $(X^{(n)})_{n\in[1:2N]}$ of X, we can create an i.i.d. sample $(X^{(n)}, X_u^{(n)}, X_{-u}^{(n+N)})_{n\in[1:N]}$ of (X, X^u). Then, we can estimate $\mathrm{E}(f(X)f(X^u))$ by

$$\frac{1}{N}\sum_{n=1}^{N} f(X^{(n)})f(X_u^{(n)}, X_{-u}^{(n+N)}) \underset{N\to+\infty}{\xrightarrow{a.s.}} \mathrm{E}(f(X)f(X^u)).$$

Based on this idea, many different versions of Pick-and-Freeze estimators have been suggested. We can find a list of such estimators in the R package `sensitivity` [IAP20] and in [BBD+16]. For example, in [BBD+16], Martinez estimator enables to write the Sobol index S_u^{cl} as the correlation coefficient $\rho(f(X), f(X^u))$ and to obtain asymptotic confidence intervals using Fisher transformation. There also exist many theoretical results on concentration inequalities, asymptotic distribution, and efficiency of Pick-and-Freeze estimators (see for example [GJK+16, GJKL14, JKLR+14]).

To estimate a Sobol index S_u, we have to estimate the $2^{|u|}-1$ closed Sobol indices $(S_v^{cl})_{\emptyset\subsetneq v\subsetneq u}$ and to use Equation (1.8). Remark that the estimation of the total Sobol index ST_i only requires the estimation of S_{-i}^{cl}, using Equation (1.9).

Remark 2. *Notice that the Pick-and-Freeze estimators require to have the computer of code of f. If the computer code of f is not available, or if it is too costly, one can use a metamodel of f (for example using Gaussian process [SWNW03]). Then, the estimation error of the Pick-and-Freeze estimators comes from the metamodel error and the sampling error, as it is detailed in [JNP14].*

To conclude, Pick-and-Freeze estimators are consistent estimators of the Sobol indices and easy to compute. Many versions are already implemented and their efficiency have been proven theoretically. Moreover, they can be used in any general framework and they only require a sample of X and the computer code of f (or a metamodel).

A.2.ii) Other estimators of the Sobol indices

When the input distribution is known, one can estimate the Sobol indices by different estimators that can be more efficient than the Pick-and-Freeze estimators. Many estimators use an orthonormal basis of L^2 that matches with the subspaces H_u^0 defined in Section A.1.ii). Then, it is easy to write the Hoeffding decomposition of f (and thus the Sobol indices) with the coordinates of f into this orthonormal basis. To estimate the Sobol indices, the sums over the infinite orthonormal basis are remplaced by sums over the first elements of the orthonormal basis, and each coordinate of f is estimated.

The polynomial chaos estimators (see [BS10b, CLMM09]) are based on a polynomial orthonormal basis of L^2. These estimators are implemented in the Scilab package `NISP` [BM10]. For all $i \in\in [1:p]$, we define $(\psi^i)_{n\in\mathbb{N}}$ a polynomial orthonormal basis of $L^2(\mathbb{R}, \mathbb{R}, \mathbb{P}_{X_i})$. Hence, a polynomial orthonormal basis of L^2 is given by $(\psi_{n_1,\cdots,n_p})_{n_1,\cdots,n_p\in\mathbb{N}^p}$, where $\psi_{n_1,\cdots,n_p}(x) := \psi^1_{n_1}(x_1)\cdots\psi^p_{n_p}(x_p)$. From this orthonormal basis, one can easily extract an orthonormal basis of H_u and thus of H_u^0.

The FAST estimators [CFS+73] are based of the Fourier orthonormal basis of L^2. They are implemented in the R package `sensitivity`. To estimate the coordinates of f in the Fourier Basis, the multidimensional integrals are estimated by one-dimensional integrals using the function $x^* : \mathbb{R} \longrightarrow [-1,1]^p$ defined for all $i \in [1:p]$ by

$$x_i^*(s) = G_i(\sin(\omega_i s)),$$

where $(G_i)_{i\in[1:p]}$ are particular functions and $(\omega_i)_{i\in[1:p]}$ is a set of incommensurate frequencies (see [CFS+73, STC99] for details).

There exists a large number of other estimators of the Sobol indices and many of them have similarities with the FAST algorithm. One can cite for example the extended FAST [STC99], random balance designs [TGM06], the works of [Sal02a], of [TGKM07] and of [Pli10]. Note that the estimator suggested is [Pli10] only requires a sample of the inputs-outputs.

B Sensitivity indices for dependent inputs

B.1 Sobol indices for dependent inputs

B.1.i) Closed Sobol indices and Sobol indices

When the input variables are dependent, the Hoeffding decomposition of f does not hold. Hence, we can not define the Sobol indices by Definition 4 anymore. However, Definition 2 of the closed Sobol indices does not require the independence of the inputs. Moreover, we have seen in Proposition 3 how to compute the Sobol indices from the closed Sobol indices in the independent case. Thus, we can extend the definition of the Sobol indices in the dependent case as the following:

Definition 5 (Sobol indices, dependent case). *For all $u \subset [1:p]$, let*

$$S_u = \sum_{v\subset u} (-1)^{|u|-|v|} S_u^{cl}, \tag{1.12}$$

be the Sobol index of X_u*.*

The advantage of the Sobol indices compared to the closed Sobol indices is that their sum is equal to one (because it is equal to $S^{cl}_{[1:p]}$). However, as the Hoeffding decomposition does not hold, the Sobol indices S_u are no longer equal to a ratio of variances, that guarantees the non-negativity of the Sobol indices in the independent case. Thus, when $|u| \geq 2$, we can get negative Sobol indices.

Example 2. *Let* X_1 *and* X_2 *be standard normal random variables with correlation* $\rho > 0$*, and let* $Y = X_1 + X_2$*. We have* $\mathrm{Var}(Y) = 2(1+\rho)$*. Then,*

$$\mathrm{E}(Y|X_1) = X_1 + \rho X_1,$$

and

$$S_1 = S_2 = \frac{(1+\rho)^2}{2(1+\rho)} = \frac{1+\rho}{2}.$$

Now,

$$S_{\{1,2\}} = 1 - S_1 - S_2 = -\rho < 0.$$

To conclude, when the inputs are dependent, the closed Sobol indices are still available but their sum is not equal to one (as in the independent case). We also can extend the Sobol indices but they are no longer non-negative for order larger than 2. In both cases, there are thus interpretation issues with these indices.

B.1.ii) Estimation

When the inputs are dependent, Proposition 4 does not hold and the Pick-and-Freeze estimators given in Section A.2.i) do not converge to the Sobol indices. Hence, different articles focus on the estimation of Sobol indices with dependent inputs.

[GDA16] suggests estimators of the Sobol indices for dependent inputs based on the Pick-and-Freeze estimators. The idea is to transform the inputs variables into two independent groups of variables to use Proposition 4. However, this input transformation requires the conditional cumulative functions of the inputs (which is rarely available), and [GDA16] does not provide convergence results.

The authors of [VG13] suggest a consistent estimator, with rates of convergence, of the first-order Sobol indices for continuous inputs variables, when we only observe an i.i.d. sample and when the input variables can be dependent.
The idea is to write $\mathrm{Var}(\mathrm{E}(Y|X_i))$ as a function $T(f_{X_i,Y})$ of the density $f_{X_i,Y}$ of (X_i, Y). Then, they estimate $f_{X_i,Y}$ by $\widehat{f}_{X_i,Y}$ (for example, in their numerical

application, they use a kernel density estimator). Finally, using a Taylor expansion of

$$F : u \longrightarrow T\left(u f_{X_i,Y} + (1-u)\widehat{f}_{X_i,Y}\right)$$

they compute the bias of $T(\widehat{f}_{X_i,Y})$. This bias is decomposed into two parts: a linear function of the density (which is estimated replacing $f_{X_i,Y}$ by $\widehat{f}_{X_i,Y}$ and using a Monte-Carlo estimation) and a more complicated term, denoted θ. They give an efficient estimator of θ to deduce an efficient estimator of $T(f_{X_i,Y}) = \mathrm{Var}(\mathrm{E}(Y|X_i))$. However, one of the limitation of the method suggested in [VG13] is that the estimator requires an estimator of the density $f_{X_i,Y}$.

B.1.iii) Limits of the Sobol indices

When the input variables are dependent, the Sobol indices can be defined as in Section B.1.i). However, the interpretation of high-order indices is difficult since they can take negative values.

A first idea is to focus only on the first-order Sobol indices, which remain in $[0,1]$. However, these first-order indices do not always allow to know the influence of the inputs. For example, in many cases, some of these indices S_i are equal to 0 even if the output Y depends on the input X_i. [PBS13] gives a setting when first-order Sobol indices are equal to 0.

Proposition 5 ([PBS13])**.** *If there exists $i_0 \in [1:p]$, $I \subset [1:p]$, $J \subset [1:p]$ such that*

1. $[1:p] = I \sqcup J \sqcup \{i_0\}$,
2. $f(x) = a(x_I)g(x_{i_0}) + b(x_J)$,
3. X_{i_0}, X_I *and* X_J *are independent,*
4. $\mathrm{E}(g(X_{i_0})) = 0$,

then $\forall i \in I,\ S_i = 0$.

This proposition generalizes the case of the Ishigami model, defined by

$$f(x_1, x_2, x_3) = \sin(x_1) + a\sin^2(x_2) + b\, x_3^4 \sin(x_1) = (1 + b\, x_3^4)\sin(x_1) + a\sin^2(x_2),$$

with the inputs variables $(X_i)_{i\in[1:3]}$ are i.i.d. with distribution $\mathcal{U}([-\pi,\pi])$. In this example, we obtain $S_3 = 0$ whereas [PBS13] shows that the probability density function of Y is different from the probability density function of Y conditionally to $X_3 = x_3$. Hence, the first order Sobol index S_3 does not give enough information on the impact of X_3 on Y, and one could use the total Sobol index ST_3 which is strictly positive.

Another way to deal with dependent inputs is to group together the inputs variables into independent groups, and to consider each group as an input variable [JLD06]. However, this method only provides information of the groups of variables, without detail on the impact of each variable.

Hence, with dependent inputs, one needs to define new sensitivity indices, as it will be done in the rest of Section B.

B.2 Generalized Sobol indices

B.2.i) Definition of the generalized Sobol indices

The generalized Sobol indices are introduced in [Cha13] and are based on the works of [Sto92]. A generalized Hoeffding decomposition is suggested, from which one can deduce the generalized Sobol indices.

For all $i \in [1 : p]$, let μ_i be a σ-finite measure on $(\mathcal{X}_i, \mathcal{E}_i)$ and we define $\mu = \bigotimes_{i=1}^p \mu_i$. Assume that $\mathbb{P}_X$ is absolutely continuous with respect to μ and let p_X be its density. If $u \subset [1 : p]$, we define $\mu_u = \bigotimes_{i \in u} \mu_i$ and p_{X_u} be the marginal density of X_u with respect to μ_u. Moreover, we make the following assumption:

Assumption 1. *We have*

$$\exists M \in]0, 1[, \ \forall u \subset [1 : p], \ p_X \geq M p_{X_u} p_{X_{-u}}. \tag{1.13}$$

Remark 3. *In order that Assumption 1 holds, it suffices that* $\exists M_1 > 0$, $\exists M_2 > 0$ *such that* $M_1 \leq p_X \leq M_2$.

Let us now define the linear subspaces on which we will project onto. For all $u \subset [1 : p]$, let:

$$H_u^0 \ := \ \{h_u \in H_u, \ \langle h_u, h_v \rangle = 0, \ \forall v \subsetneq u, \ \forall h_v \in H_v\} = H_u \cap \bigcap_{v \subsetneq u} H_v^{\perp} \tag{1.14}$$

Remark 4. *These subspaces are closed. Indeed,* H_u^0 *is closed as the intersection of* H_u *(which is closed) with an intersection of orthogonal complements.*

Remark 5. *The definition of* H_u^0 *defined in Equation (1.14) generalizes the definition given in Equation (1.2) for independent input variables.*

Remark 6. *In [Cha13], the subspace H_u^0 is defined by $H_u \cap \bigcap_{v \subsetneq u} (H_u^0)^\perp$. However, in order to prove Theorem 1, it seems that one needs to define H_u^0 by Equation (1.14).*

We now give the central theorem of [Cha13] to define the generalized Hoeffding decomposition.

Theorem 1 ([Cha13])**.** *Under Assumption 1, for all $g \in L^2$, there exists an unique decomposition*

$$g = \sum_{u \subset [1:p]} g_u \tag{1.15}$$

such that $\forall u \subset [1:p]$, $g_u \in H_u^0$. In other words:

$$L^2 = \bigoplus_{u \subset [1:p]} H_u^0. \tag{1.16}$$

As in the independent case, the linear space L^2 is the direct sum of the linear subspaces H_u^0, for $u \subset [1:p]$. However, these subspaces are no longer orthogonal with dependent inputs. Moreover, we do not have explicit formula for the projection of a function $g \in L^2$ onto these subspaces.

Definition 6. *Let $(f_u)_{u \subset [1:p]}$ be the component of f on H_u^0 defined by Equation (1.14). That is,*

$$f = \sum_{u \subset [1:p]} f_u,$$

where $f_u \in H_u^0$ for all $u \subset [1:p]$. In the particular case where the inputs are independent, f_u is defined by Equation (1.7).

Remark 7. *Theorem 1 requires Assumption 1. However, it is mentioned in [OP17] that this assumption is strong. Actually, if there exists $u \subset [1:p]$ and $(R_u, R_{-u}) \in \mathcal{E}_u \times \mathcal{E}_{-u}$ such that $\mathbb{P}_X(R_u \times R_{-u}) = 0$, $\mathbb{P}_{X_u}(R_u) > 0$ and $\mathbb{P}_{X_{-u}}(R_{-u}) > 0$, then Assumption 1 does not hold (for example, when X has the uniform distribution on the triangle $\{(x_1, x_2) \in [0,1]^2,\ x_1 \leq x_2\}$ or the distribution $p\delta_{(1,0)} + (1-p)\delta_{(0,1)}$).*

Remark 8. *Using Theorem 1, we now can prove that, for all $u \subset [1:p]$, $H_u^0 = H_u \cap \bigcap_{v \subsetneq u} (H_v^0)^\perp$, as defined by [Cha13].*

As in the independent case, we derive the generalized Sobol indices from the generalized Hoeffding decomposition.

Definition 7 ([Cha13])**.** *Under Assumption 1, for all $u \subset [1:p]$, we define S_u^{gen}, the generalized Sobol index of X_u, by:*

$$S_u^{gen} := \frac{\mathrm{Var}(f_u(X_u)) + \sum_{v, s.t.\ u \cap v \notin \{u,v\}} \mathrm{cov}(f_u(X_u), f_v(X_v))}{\mathrm{Var}(Y)} \tag{1.17}$$

Definition 7 of the generalized Sobol indices S_u^{gen} is another extension of the Sobol indices for dependent inputs, different from the one given in Definition 5. Indeed, when the inputs are independent, we have $\forall u \neq v$, $\mathrm{cov}(f_u(X_u), f_v(X_v)) = 0$.

[Cha13] suggests to decompose the sensitivity index S_u^{gen} into two terms:

- $\mathrm{Var}(f_u(X_u))/\mathrm{Var}(Y) \in [0,1]$ corresponding to the direct contribution of X_u on the variance of Y,
- $\displaystyle\sum_{v, s.t.\ u\cap v\notin\{u,v\}} \mathrm{cov}(f_u(X_u), f_v(X_v))/\mathrm{Var}(Y)$ corresponding to the contribution of Y from the dependence of X_i on the other variables.

Even in the dependent case, we have the following proposition:

Proposition 6 ([Cha13])**.** *We have:*

$$\sum_{u\subset[1:p]} S_u^{gen} = 1. \tag{1.18}$$

Example 3. *Let X_1 and X_2 be standard normal random variables with correlation $\rho > 0$, and let $Y = X_1 + X_2$. We have $\mathrm{Var}(Y) = 2(1+\rho)$. Remark that $f_\emptyset = 0$, $f_1(X_1) = X_1$, $f_2(X_2) = X_2$, $f_{\{1,2\}}(X) = 0$ is the unique generalized Hoeffding decomposition of f. Indeed, we have in this case, $f_\emptyset \in H_\emptyset^0$, $f_i \in H_i^0$, $f_{\{1,2\}}^0 \in H_{\{1,2\}}^0$ and $f = f_\emptyset + f_1 + f_2 + f_{\{1,2\}}$. Then, we have*

$$\begin{cases} S_1^g = \frac{\mathrm{Var}(X_1)+\mathrm{cov}(X_1,X_2)}{\mathrm{Var}(Y)} = \frac{1}{2} \\ S_2^g = \frac{\mathrm{Var}(X_2)+\mathrm{cov}(X_1,X_2)}{\mathrm{Var}(Y)} = \frac{1}{2} \\ S_{\{1,2\}}^g = 0, \end{cases}$$

which seems more intuitive than the Sobol indices given in Section B.1.i) (see Example 2).

Example 4. *Now assume that $Y = X_1 + X_2$ and X has the distribution $\mathcal{N}\left(0, \begin{pmatrix} 2 & \alpha \\ \alpha & 1 \end{pmatrix}\right)$. Then, for all $\alpha \in]-\sqrt{2}, -1[$, we have $\mathrm{Var}(X_2) + \mathrm{cov}(X_1, X_2) < 0$ and $S_2 < 0$.*

To conclude, the generalized Sobol indices given in [Cha13] can have advantages on the generalization of the Sobol indices for dependent inputs defined in Section B.1.i), as it is highlighted in Example 3. However, the interpretation of these Sobol indices is still problematic because they can take negative values, including the first order generalized Sobol indices (see Example 4).

B.2.ii) Estimation of the generalized Sobol indices

An estimator of the generalized Sobol indices has been suggested in [Cha13] and [CCGP15].

The main problem to estimate these sensitivity indices comes from the fact that they rely on an unknown decomposition $(f_u)_{u\subset[1:p]}$ of f. Moreover, to simplify computations, we assume that, for $|u|>d$, we have $f_u=0$, and we choose for example $d=2$ (but this can be generalized for any $d\in[3:p]$). The idea is to approximate the subspaces $(H_u^0)_{|u|\leq 2}$ by finite dimensional subspaces $(H_u^{0,L})_{|u|\leq 2}$.

For all $i\in[1:p]$, let $(\psi_l^i)_{l\in\mathbb{N}}$ an orthonormal basis of $L^2(\mathcal{X}_i,\mathcal{E}_i,\mathbb{P}_{X_i})$ such that $\psi_0^i(x_i)=1$ for all $x_i\in\mathcal{X}_i$. Then for all $(i,j)\in[1:p]$, $(\phi_l^i\otimes\psi_{l'}^j)_{(l,l')\in\mathbb{N}^2}$ is an orthonormal basis of

$$L^2(\mathcal{X}_i,\mathcal{E}_i,\mathbb{P}_{X_i})\otimes L^2(\mathcal{X}_j,\mathcal{E}_j,\mathbb{P}_{X_j})=L^2(\mathcal{X}_i\times\mathcal{X}_j,\mathcal{E}_i\otimes\mathcal{E}_j,\mathbb{P}_{X_i}\otimes\mathbb{P}_{X_j}).$$

Moreover, thanks to Assumption 1, we have

$$L^2(\mathcal{X}_i\times\mathcal{X}_j,\mathcal{E}_i\otimes\mathcal{E}_j,\mathbb{P}_{X_{\{i,j\}}})\subset L^2(\mathcal{X}_i\times\mathcal{X}_j,\mathcal{E}_i\otimes\mathcal{E}_j,\mathbb{P}_{X_i}\otimes\mathbb{P}_{X_j}).$$

Hence, any element of $H_{\{i,j\}}=L^2(E_i\times E_j,\mathcal{E}_i\otimes\mathcal{E}_j,\mathbb{P}_{X_{\{i,j\}}})$ is the limit (in $L^2(\mathcal{X}_i\times\mathcal{X}_j,\mathcal{E}_i\otimes\mathcal{E}_j,\mathbb{P}_{X_i}\otimes\mathbb{P}_{X_j})$) of linear combinations of $(\phi_l^i\otimes\psi_{l'}^j)_{(l,l')\in\mathbb{N}^2}$.

Then, for a fixed $L\in\mathbb{N}^*$, we approximate $H_{\{i,j\}}$ by $H_{\{i,j\}}^L$ the linear span of $(\phi_l^i\otimes\psi_{l'}^j)_{(l,l')\in[0,L]^2}$ and H_i by H_i^L the linear span of $(\psi_l^i)_{l\in[0:L]}$, and we let $H_\emptyset^L=H_\emptyset$ be the subset of the constant functions. Thanks to Assumption 1, $(\phi_l^i\otimes\psi_{l'}^j)_{(l,l')\in[0,L]^2}$ is linearly independent in $L^2(\mathcal{X}_i\times\mathcal{X}_j,\mathcal{E}_i\otimes\mathcal{E}_j,\mathbb{P}_{X_{\{i,j\}}})$.

Then, for all $|u|\leq 2$, to approximate H_u^0, we define

$$H_u^{L,0}:=\{h_u\in H_u^L,\ \forall v\subsetneq u,\ \forall h_v\in H_v^{0,L},\ \langle h_u,h_v\rangle=0\}.$$

We need to define an orthonormal basis $(\phi_l^u)_{l\in L_u}$ of the finite spaces $(H_u^{L,0})_{|u|\leq 2}$ in $L^2(\mathcal{X}_i\times\mathcal{X}_j,\mathcal{E}_i\otimes\mathcal{E}_j,\mathbb{P}_{X_{\{i,j\}}})$. For $u=\emptyset$, let $L_\emptyset=\{0\}$ and $\phi_\emptyset^0=1$. For $u=\{i\}$, let $L_{\{i\}}=[1:L]$ and for all $l\in[1:L]$, let $\phi_l^i=\psi_l^i$. For $u=\{i,j\}$, let $L_u=[1:L]^2$ and remark that $(\psi_{l_i}^i\otimes\psi_{l_j}^j)_{(l_i,l_j)\in[1:L]^2}$ is orthonormal in $L^2(\mathcal{X}_i\times\mathcal{X}_j,\mathcal{E}_i\otimes\mathcal{E}_j,\mathbb{P}_{X_i}\otimes\mathbb{P}_{X_j})$ but is not orthonormal in $L^2(\mathcal{X}_i\times\mathcal{X}_j,\mathcal{E}_i\otimes\mathcal{E}_j,\mathbb{P}_{X_{\{i,j\}}})$. Thus, for any $(l_i,l_j)\in[1:L]^2$, we define

$$\phi_{l_i,l_j}^{i,j}=\psi_{l_i}^i\otimes\psi_{l_j}^j+\sum_{k=1}^L\lambda_{k,l_i,l_j}^i\psi_k^i+\sum_{k=1}^L\lambda_{k,l_i,l_j}^j\psi_k^j+C_{l_i,l_j}$$

for some constants $(\lambda_{k,l_i,l_j}^i,\lambda_{k,l_i,l_j}^j,C_{l_i,l_j})_{(l_i,l_j,k)\in[1:L]^3}$ that make $(\phi_{l_i,l_j}^{i,j})_{(l_i,l_j)\in[0:L]^2}$ orthonormal (see [Cha13] for more details on these constants). These constants are estimated using the empirical distribution of $\mathbb{P}_{X_{\{i,j\}}}$ with an i.i.d. sample $(X^{(l)})_{l\in[1:n_1]}$. We obtain estimates $(\widehat{\phi}^{i,j}_{l_i,l_j})_{(l_i,l_j)\in[0:L]^2}$ of $(\phi^{i,j}_{l_i,l_j})_{(l_i,l_j)\in[0:L]^2}$. One can find in [CCGP15] theoretical results on the rate of convergence of these estimates.

Then, if $(X^{(l)},Y^{(l)})_{l\in[1:n_2]}$ is a new i.i.d. sample of (X,Y), we estimate f by

$$\widehat{f} := \sum_{|u|\leq 2}\sum_{l_u\in L_u} \widehat{\beta}^u_{l_u}\widehat{\phi}^u_{l_u,n_1},$$

with

$$(\widehat{\beta}^u_{l_u})_{u,l_u} = \underset{(\beta^u_{l_u})_{u,l_u}}{\arg\min}\frac{1}{n_2}\sum_{l=1}^{n_2}\left(Y^{(l)} - \sum_{|u|\leq d}\sum_{l_u\in L_u}\beta^u_{l_u}\widehat{\phi}^u_{l_u,n_1}(X^{(l)})\right) + \lambda\,\mathrm{pen}\left((\beta^{l_u}_u)_{u,l_u}\right),$$

and where $\lambda J\left((\beta^{l_u}_u)_{u,l_u}\right)$ is a penalisation term. An algorithm has been suggested in [CCGP15] to estimate these $(\widehat{\beta}^u_{l_u})_{u,l_u}$ with theoretical results.

Now that the generalized Hoeffding decomposition is estimated, the generalized Sobol indices are estimated by Monte-Carlo in the following way. Let $(X^{(l)},Y^{(l)})_{l\in[1:n_3]}$ be another i.i.d. sample of (X,Y) and let

$$\begin{aligned}
\widehat{\mathrm{Var}}(Y) &= \frac{1}{n_3-1}\sum_{l=1}^{n_3}(Y^{(l)}-\overline{Y})^2,\\
\widehat{\mathrm{Var}}(f_u(X)) &= \frac{1}{n_3-1}\sum_{l=1}^{n_3}\widehat{f}_u(X^{(l)})^2,\quad 1\leq |u|\leq 2,\\
\widehat{\mathrm{cov}}(f_u(X_u),f_v(X_v)) &= \frac{1}{n_3-1}\sum_{l=1}^{n_3}\widehat{f}_u(X^{(l)})\widehat{f}_v(X^{(l)}),\quad u\neq v,\ 1\leq |u|,|v|\leq 2.
\end{aligned}$$

Then, we use Definition 7 to obtain estimates of the generalized Sobol indices.

These estimators of the generalized Sobol indices have been implemented in [CCGP15] with numerical experiments.

B.3 The δ-indices

The δ-indices have been introduced in [Bor07] and quantify the impact of the observation of an input variable on the density function of the output.

Definition 8 (First-order δ-indices [Bor07])**.** *Assume that, for all $i\subset[1:p]$, the distribution of Y conditionally to X_i exists and is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}$. Let*

$$\delta_i := \frac{1}{2}\mathrm{E}\left(\int |f_Y(y)-f_{Y|X_i}(y)|dy\right) \tag{1.19}$$

be the "moment independent sensitivity indicator of parameter X_i with respect to output Y".

Remark that the coefficient $1/2$ enables to bound δ_i by 1.

[PBS13] noticed that δ_i depends on the total variation distance between $\mathbb{P}_Y$ and $\mathbb{P}_{Y|X_i}$. Thus, one can extend the definition of the δ-indices to the case where the distribution of Y conditionally to X_i exists and to groups of variables X_u.

Definition 9 (δ-indices [PBS13])**.** *Assume that, for all $u \subset [1:p]$, the distribution of Y conditionally to X_u exists. Let $\mathcal{B}$ be the set of Borel sets of $\mathbb{R}$. Let*

$$\delta_u := \mathrm{E}\left(\sup_{B \in \mathcal{B}} |\mathbb{P}_Y(B) - \mathbb{P}_{Y|X_u}(B)| \right) \tag{1.20}$$

be the δ-index of the group of variable X_u.

As the closed Sobol indices, the δ-indices satisfy the following properties:

Properties 1 ([Bor07])**.**

- $\forall u, \ \delta_u \in [0,1]$;
- $Y \perp\!\!\!\perp X_u \implies \delta_u = 0$;
- $u \subset v \implies \delta_u \leq \delta_v$;
- $\delta_\emptyset = 0$;
- $\delta_{[1:p]} = 1$.

The authors of [PBS13] studied these global sensitivity indices and proved that, $\delta_u = 0$ if, and only if, Y is independent on X_u.

Moreover, they give an estimator of the first order indices δ_i in the case where the inputs are continuous.

First, they divide the input space $\mathcal{X}_i$ into a partition $\mathcal{P} = (\mathcal{C}_m)_{m \in [1:M]}$. Thus, they can approximate the expectation on X_i in Equation (1.19) by

$$\delta_i^{\mathcal{P}} = \frac{1}{2} \sum_{m=1}^{M} \int_{\mathbb{R}} |f_Y(y) - f_{Y|X_i \in \mathcal{C}_m}(y)| dy \, \mathbb{P}(X_i \in \mathcal{C}_m)$$

Secondly, they estimate f_Y and $f_{Y|X_i \in \mathcal{C}_m}$ with kernel-density estimators, with bandwidths α and α_m respectively. They obtain an estimator $\widehat{\delta_i}$ that only requires an i.i.d. sample $(X^{(l)}, Y^{(l)})_{l \in [1:n]}$ and they give theoretical guaranties.

B.4 Full Sobol indices and independent Sobol indices

The idea of the full Sobol indices and independent Sobol indices, introduced in [MTA15], is to transform the dependent input variables into independent input variables and to compute the related Sobol indices. Moreover, [MTA15] suggests different ways to transform the dependent input variables into independent input variables. Each manner provides different Sobol indices, such as the full Sobol indices and the independent Sobol indices.

Assume that X is a continuous random vector of $\mathbb{R}^p$. For all $i \in [1:p]$, let U^i be the Rosenblatt transformation T_i [Ros52] of $X^i := (X_i, X_{i+1}, \cdots, X_p, X_1, \cdots, X_{i-1})$, which is uniformly distributed on $[0,1]^p$. That is, $U_1^i = F_{X_1^i}(X_1^i) = F_{X_i}(X_i)$ and, for all $k \in [2:p]$,

$$U_k^i = F_{X_k^i | X_{[1:k-1]}^i}(X_k^i),$$

where F is the cumulative distribution function.

Now, let $T^{-1} : [0,1]^p \longrightarrow \mathbb{R}^p$ defined by $(T_i^{-1}(u))_1 = F_{X_1^i}^{-1}(u_1)$ and, for all $k \in [2:p]$,

$$(T_i^{-1}(u))_k = F^{-1}_{X_k^i | X^i_{[1:k-1]} = (T_i^{-1}(u))_{[1:k-1]}}(u_k),$$

where F^{-1} is the generalized inverse distribution function. Remark that, almost everywhere, $X^i = T^{-1}(U^i)$. Thus, there exists $g_i : [0,1]^p \longrightarrow \mathbb{R}$ such that, almost everywhere, $Y = g_i(U^i)$. Now, Y is a function of the independent input variables $(U_1^i, \cdots, U_p^i)$, and thus we can define its Sobol indices $(S_u^i)_{u \subset [1:p]}$ and the total Sobol indices $(ST_j^i)_{j \in [1:p]}$ as in Section A.1.

If we want to assess the impact of the variable X_i with all its dependencies on the other variables, we define the "full Sobol indices" as:

$$S_i^{full} := S_1^i, \quad ST_i^{full} := ST_1^i.$$

See [MTA15, BEDC19] for an interpretation of S_i^{full}.

Remark 9. *We have, $S_i^{full} = S_i^{cl} = S_i$ where the definitions of S_i^{cl} and S_i are given in Section B.1.i). Indeed, using that $U_1^i = F_{X_i}(X_i)$ and then that $X_i = F_{X_i}^{-1}(U_1^i)$, we have:* $\mathrm{Var}(\mathrm{E}(Y|X_i)) \geq \mathrm{Var}(\mathrm{E}(Y|U_1^i)) \geq \mathrm{Var}(\mathrm{E}(Y|X_i))$.

Now, if we want to asses the impact of the variable X_i without its dependencies on the other variables, we define the "independent Sobol indices" as:

$$S_i^{ind} := S_p^{i+1}, \; ST_i^{ind} := ST_p^{i+1}.$$

See [BEDC19] for an estimation procedure of these indices.

To conclude, [MTA15] defines two Sobol indices when the input variables are dependent. The full Sobol indices take into account the dependencies on the other variables. The independent Sobol indices do not take into account the dependencies on the other variables. A particularity of these indices is that, for each input variable, there exist 4 indices that measure different quantities. However, these various choices of sensitivity indices can become a problem when we seek for simplicity.

C Shapley effects

C.1 Definition and properties

C.1.i) Shapley value

The Shapley effects, which are suggested in [Owe14], are based on a concept derived from game theory, called "Shapley value" [Sha53]. The Shapley value enables to asses, in a team game, the part of the winnings due to a particular player. This concept will lead to define the part of the variance of Y due to a particular input X_i. We consider a set of p player, numbered from 1 to p, playing a game. Let $c : \mathcal{P}([1:p]) \longrightarrow \mathbb{R}$ be such that $c(\emptyset) = 0$ and representing the score attained by the subsets of players playing the game.

Definition 10 (Shapley value [Sha53])**.** *The Shapley value of the player i with respect to c is defined by*

$$\phi_i = \frac{1}{p} \sum_{u \subset -i} \binom{p-1}{|u|}^{-1} (c(u \cup \{i\}) - c(u)), \tag{1.21}$$

where $-i := [1:p] \setminus \{i\}$.

The Shapley value ϕ_i is a convex combination of $(c(u \cup \{i\}) - c(u))_{u \subset -i}$. Thus, it represents some average over $u \subset -i$ of the incremental score of including player i in set u. The coefficients of the convex combination only depend on $|u|$ and their sum over the subsets of cardinal k is still equal to $1/p$, for $k = 0, \cdots, p-1$.

At the end of [Sha53], Shapley noticed that the Shapley value can be written in the following way.

Let $\mathcal{S}_p$ be the set of permutations of $[1:p]$. An element $\sigma \in \mathcal{S}_p$ is a bijective function from $[1:p]$ to $[1:p]$. An element $\sigma \in \mathcal{S}_p$ represents an order of the p players, where $\sigma(i)$ is the rank of the player i. Then, let $T_i(\sigma)$ be the set of players preceding i in the order σ, that is

$$T_i(\sigma) := \{j \in [1:p] \mid \sigma(j) \in [1:\sigma(i)-1]\}.$$

Example 5. *If* $p = 5$, $\sigma(1) = 3$, $\sigma(2) = 5$, $\sigma(3) = 4, \sigma(4) = 2$, $\sigma(5) = 1$, *which can also be written as the cycle* $\sigma = (1\ 3\ 4\ 2\ 5)$ *or, writing players ranked by preference (as in [FKS03] for example),* $\sigma = (5; 4; 1; 3; 2)$, *we have* $T_1(\sigma) = \{5, 4\}, T_2(\sigma) = \{5, 4, 1, 3\}$, $T_3(\sigma) = \{5, 4, 1\}$, $T_4(\sigma) = \{5\}$, $T_5(\sigma) = \emptyset$.

Then,

$$\phi_i = \frac{1}{p!} \sum_{\sigma \in \mathcal{S}_p} (c(T_i(\sigma) \cup \{i\}) - c(T_i(\sigma))). \tag{1.22}$$

Hence, the Shapley value ϕ can be computed by two different ways: using Equation (1.21) or using Equation (1.22).

The Shapley values satisfy the following properties:

Properties 2. *We have:*

- $\sum_{i=1}^p \phi_i = c((1 : p])$;
- $c(u \cup \{i\}) = c(u \cup \{j\})\ \forall u \subset [1 : p] \setminus \{i, j\} \implies \phi_i = \phi_j$;
- $c(u \cup \{i\}) = c(u)\ \forall u \subset -i \implies \phi_i = 0$;
- $(\phi_i)_{i \in [1:p]}$ *is linear with respect to* c.

C.1.ii) Shapley effects

In [Owe14], Owen suggests to use the Shapley value with the score function $c(u) = S_u^{cl}$ to obtain sensitivity indices.

Definition 11 (Shapley effects [Owe14])**.** *For all* $i \in [1 : p]$, *we define* η_i, *the Shapley effect of* X_i *as:*

$$\eta_i = \frac{1}{p} \sum_{u \subset -i} \binom{p-1}{|u|}^{-1} (S_{u \cup \{i\}}^{cl} - S_u^{cl}).$$

Remark 10. *In [Owe14], Owen uses the score function* $c(u) = \mathrm{Var}(\mathrm{E}(Y|X_u))$. *In Definition 11, we divide by the variance to normalize the Shapley values.*

The Shapley effects are linear combinations of the closed Sobol indices (and thus of the Sobol indices defined in Definition 5). An interesting particularity of the Shapley effects is that there exists only one index per input variable, which evaluates the impact of the variable taken alone and of all its interactions with the other input variables on the output.

Remark that different convex combinations of $(c(u \cup \{i\}) - c(u))_{u \subset -i}$ in Definition 10 can lead to the first Sobol index S_i or the total Sobol index ST_i when using the score function $u :\longrightarrow S_u^{cl}$.

[SNS16] noticed that, using the law of total variance, the score function $u \longrightarrow \mathrm{E}(\mathrm{Var}(Y|X_{-u}))$ also leads to the Shapley effects. Thus, for all $u \subset [1:p]$, we define:

$$V_u := \mathrm{Var}(\mathrm{E}(Y|X_u)) \tag{1.23}$$

and

$$E_u := \mathrm{E}(\mathrm{Var}(Y|X_{-u})). \tag{1.24}$$

We let by convention $\mathrm{E}(Y|X_\emptyset) = \mathrm{E}(Y)$ and $\mathrm{Var}(Y|X_\emptyset) = \mathrm{Var}(Y)$. We define the "conditional elements" $(W_u)_{u\subset[1:p]}$ as being either $(V_u)_{u\subset[1:p]}$ or $(E_u)_{u\subset[1:p]}$. Then, for all $i \in [1:p]$, the Shapley effect η_i is equal to:

$$\eta_i := \frac{1}{p\mathrm{Var}(Y)} \sum_{u\subset -i} \binom{p-1}{|u|}^{-1} (W_{u\cup\{i\}} - W_u). \tag{1.25}$$

C.1.iii) Properties of the Shapley effects

The Shapley effects have interesting properties, derived from the properties of the closed Sobol indices and the Shapley values.

Properties 3. *We have:*

- $\forall i \in [1:p],\ \eta_i \in [0,1]$;
- $\sum_{i=1}^p \eta_i = 1$;
- $X_i \perp\!\!\!\perp (Y, X_{-i}) \implies \eta_i = 0$.

Thus, even when the inputs are dependent, all the Shapley effects are positive and their sum is equal to one. Both properties are not satisfied with the sensitivity indices given in the previous sections with dependent inputs.

Proposition 7 ([Owe14]). *When the input variables are independent, we have, for all $i \in [1:p]$,*

$$\eta_i = \sum_{u\in -i} \frac{S_{u\cup\{i\}}}{|u\cup\{i\}|}.$$

Hence, we have in this case

$$S_i \leq \eta_i \leq ST_i.$$

The previous proposition shows that, in the independent case, the Shapley effect η_i is between the Sobol index S_i (which the sum over i is in general less than 1) and ST_i (which the sum over i is in general larger than 1). [IP19] provides on numerical experiments the values of η_i, S_i and ST_i. We can remark on these experiments that, even for dependent cases, the Shapley effect η_i is still between $\min(S_i, ST_i)$ and $\max(S_i, ST_i)$, even if ST_i is smaller than S_i. Hence the Shapley effect η_i appears to be a trade-off between the Sobol index S_i and the total Sobol index ST_i.

C.1.iv) Gaussian linear framework

Theorem 2 ([OP17]). *If $f : x \longmapsto \beta_0 + \beta^T x$ and if $X \sim \mathcal{N}(\mu, \Sigma)$, with $\Sigma \in S_p^{++}(\mathbb{R})$ (where $S_p^{++}(\mathbb{R})$ is the set of the symmetric positive definite matrices of size $p \times p$), then, for all $i \in [1:p]$:*

$$\eta_i = \frac{1}{p\mathrm{Var}(Y)} \sum_{u \in -i} \binom{p-1}{|u|}^{-1} \frac{\mathrm{cov}(X_i, X_{-u}^T \beta_{-u} | X_u)}{\mathrm{Var}(X_j | X_u)}.$$

Thus, in the linear Gaussian framework, [OP17] gives another expression of the Shapley effects. To prove this result, [OP17] uses Equation (1.25) where the conditional elements are equal to $(E_u)_{u \subset [1:p]}$. Then, for all subset $u \subset [1:p]$, we have

$$E_u = \mathrm{Var}(\beta_u^T X_u | X_{-u}) = \beta_u^T (\Sigma_{u,u} - \Sigma_{u,-u} \Sigma_{-u,-u}^{-1} \Sigma_{-u,u}) \beta_u, \tag{1.26}$$

where $\beta_u := (\beta_i)_{i \in u}$ and $\Sigma_{u,v} := (\Sigma_{i,j})_{i \in u, j \in v}$. These conditional variances are constant so they are equal to their expectation.

As in [IP19], we can use Equation (1.26) to compute numerically the Shapley effects in the linear Gaussian framework.

Remark 11. *If the matrix Σ is not invertible, there exist subsets u such that $\Sigma_{u,u}$ is not invertible. However, Equation (1.26) still holds if we replace $\Sigma_{u,u}^{-1}$ by the generalized inverse (for symmetric matrices) of $\Sigma_{u,u}$.*

Remark 12. *One can show a similar result than Equation (1.26) when X follows an asymmetric Laplace distribution $AL_p(m, \Sigma)$. However, the conditional variances are not constant in this case and their expectations must be estimated, for instance by Monte-Carlo.*

Remark 13. *Equation (1.26) can be used to compute closed Sobol indices or Sobol indices, using that*

$$S_u^{cl} = 1 - \frac{\mathrm{E}(\mathrm{Var}(Y|X_u))}{\mathrm{Var}(Y)}, \quad S_u = -\sum_{v \subset u} (-1)^{|u|-|v|} \frac{\mathrm{E}(\mathrm{Var}(Y|X_v))}{\mathrm{Var}(Y)}. \tag{1.27}$$

The value of the Shapley effects in the Gaussian linear framework are equal to the LMG measures of variable importance (the first definition is given in [LMG80] but is also has been defined in [Bud93]). This measure of importance is the average over all the subset of input variables of the improvement of the R^2 when adding the variable X_i to the multiple regression, divided by the variance of the whole regression.

C.2 Estimation of the Shapley effects

An algorithm is suggested in [SNS16] to estimate the Shapley effects. This algorithm uses the form given in Equation (1.22) for the Shapley values. We have

$$\eta_i = \frac{1}{p!}\sum_{\sigma \in \mathcal{S}_p} (E_{T_i(\sigma)\cup\{i\}} - E_{T_i(\sigma)}) = \frac{1}{p!}\sum_{\pi \in \mathcal{S}_p} (E_{T_i(\pi^{-1})\cup\{i\}} - E_{T_i(\pi^{-1})}),$$

where π^{-1} is the inverse function of π. Then, writing $P_i(\sigma) := T_i(\sigma^{-1})$, that is

$$P_i(\sigma) = \{j \in [1:p] \mid \sigma^{-1}(j) \in [1:\sigma^{-1}(i)-1]\} = \{\sigma(j) \mid j \in [1:\sigma^{-1}(i)-1]\},$$

we have:

$$\eta_i = \frac{1}{p!}\sum_{\sigma \in \mathcal{S}_p} (E_{P_i(\sigma)\cup\{i\}} - E_{P_i(\sigma)}). \tag{1.28}$$

Since the number of permutations is $p!$, the sum over $\sigma \in \mathcal{S}_p$ is no longer tractable for large values of p. Thus, on could estimate η_i by

$$\widehat{\eta}_i = \frac{1}{M}\sum_{m=1}^{M} (E_{P_i(\sigma_m)\cup\{i\}} - E_{P_i(\sigma_m)}), \tag{1.29}$$

where $M \in \mathbb{N}^*$ is a parameter and $(\sigma_m)_{m\in[1:M]}$ are i.i.d. with distribution $\mathcal{U}(\mathcal{S}_p)$.

Remark 14. *We have seen that, to compute the Shapley effects, one can use two different ways: summing over the subsets (as in Equation* (1.25)*) or summing over permutations (as in Equation* (1.28) *for example). The advantage of the sum over the permutations is that the summands have the same coefficient, and it can be estimated by Monte-Carlo as in Equation* (1.29)*, generating permutations with uniform distribution.*

Hence, a first algorithm would be to make a loop over $i \in [1:p]$, a loop over $m \in [1:M]$, and to estimate $E_{P_i(\sigma_m)\cup\{i\}}$ and $E_{P_i(\sigma_m)}$.

However, the authors of [SNS16] use a trick to divide the computation cost by 2. They notice that for $1 \le i < p$, for any permutation $\sigma \in \mathcal{S}_p$, we have

$$P_{\sigma(i+1)}(\sigma) = P_{\sigma(i)}(\sigma) \cup \{\sigma(i)\}. \tag{1.30}$$

Remark 15. *In [SNS16], the definition of $P_i(\sigma)$ is not explicitly written, but the authors of [SNS16] provide the interpretation of P_i. They say that $P_i(\sigma)$ is the set of players that precede player i in σ, which was in fact our interpretation of $T_i(\sigma)$. This is due to the interpretation of a permutation. In general (see for example [Dia88, JV17, KB10]) and in this manuscript, i denotes a player (or an item) and $\sigma(i)$ denotes his rank. In [SNS16], i denotes a rank and $\sigma(i)$ denotes the player with rank i.*

We know that we give the same definition of $P_i(\sigma)$ as the authors of [SNS16] because they use Equation (1.30) which is satisfied by P but not by T.

Notice that T satisfies a similar equation as Equation (1.30): for $1 \leq i < p$ and for any $\sigma \in \mathcal{S}_p$, we have

$$T_{\sigma^{-1}(i)}(\sigma) \cup \{\sigma^{-1}(i)\} = T_{\sigma^{-1}(i+1)}(\sigma).$$

Hence, [SNS16] provides the following algorithm:

Algorithm 1 ([SNS16])

(1) Choose M, N_V, N_0 and N_I; set $\widehat{\eta}_i = 0$ for $i = 1, 2, \cdots, p$

(2) For $l = 1, 2, \cdots, N_V$

  (I) Sample $X^{(l)}$ with distribution X

  (II) Evaluate $Y^{(l)} = f(X^{(l)})$

(3) Calculate $\overline{Y} = N_V^{-1} \sum_{l=1}^{N_V} Y^{(l)}$ and $\widehat{\mathrm{Var}}(Y) = (N_V - 1)^{-1} \sum_{l=1}^{N_V} (Y^{(l)} - \overline{Y})^2$

(4) For $m = 1, \cdots, M$

  (I) Generate σ_m uniformly on $\mathcal{S}_p$

  (II) Set $prevC = 0$

  (III) For $j = 1, 2, \cdots, p$

    (A) If $j = p$, $\widehat{E}_{P_{\sigma_m(j)}(\sigma_m) \cup \{\sigma_m(j)\}} = \widehat{\mathrm{Var}}(Y)$

    (B) Else

      (i) For $l = 1, 2, \cdots, N_0$

        (a) Sample $X^{(l)}_{-P_{\sigma_m(j+1)}(\sigma_m)}$ with distribution $X_{-P_{\sigma_m(j+1)}(\sigma_m)}$

        (b) For $h = 1, 2, \cdots, N_I$

          (1) Sample $X^{(l,h)}_{P_{\sigma_m(j+1)}(\sigma_m)}$ with distribution $X_{P_{\sigma_m(j+1)}(\sigma_m)}$ conditionally to $X_{-P_{\sigma_m(j+1)}(\sigma_m)} = X^{(l)}_{-P_{\sigma_m(j+1)}(\sigma_m)}$

          (2) Evaluate $Y^{(l,h)} = f\left(X^{(l,h)}_{P_{\sigma_m(j+1)}(\sigma_m)}, X^{(l)}_{-P_{\sigma_m(j+1)}(\sigma_m)}\right)$

(c) Calculate $\overline{Y}^{(l)} = N_I^{-1} \sum_{h=1}^{N_I} Y^{(l,h)}$

(d) Calculate $\widehat{\mathrm{Var}}\left(Y \middle| X^{(l)}_{-P_{\sigma_m(j+1)}(\sigma_m)}\right) = (N_I - 1)^{-1} \sum_{h=1}^{N_O} (Y^{(l,h)} - \overline{Y}^{(l)})^2$

(ii) Calculate $\widehat{E}_{P_{\sigma_m(j+1)}(\sigma_m)} = N_O^{-1} \sum_{l=1}^{N_O} \widehat{\mathrm{Var}}\left(Y \middle| X^{(l)}_{-P_{\sigma_m(j+1)}(\sigma_m)}\right)$

(C) Calculate $\widehat{\Delta}_{\sigma_m(j)} = \widehat{E}_{P_{\sigma_m(j+1)}(\sigma_m)} - prevC$

(D) Update $\widehat{\eta}_{\sigma_m(j)} = \widehat{\eta}_{\sigma_m(j)} + \widehat{\Delta}_{\sigma_m(j)}$

(E) Set $prevC = \widehat{E}_{P_{\sigma_m(j+1)}(\sigma_m)}$

(5) $\widehat{\eta}_i = \widehat{\eta}_i / p$ for $i = 1, 2, \cdots, p$

Algorithm 1 has been implemented in the R package `sensitivity` as the function "shapleyPermRand".

The authors of [SNS16] suggest to take $N_O = 1$, $N_I = 3$ and M as large as possible, with theoretical arguments. They also suggest, when p is small, to let the complete sum over the permutations instead of estimate it by Monte-Carlo (that is to say, using Equation (1.28) instead of Equation (1.29)). The corresponding R function is called "shapleyPermEx".

Notice that Algorithm 1 requires to be able to sample with the conditional distributions of the inputs in Step (4) (III) (B) (i) (b) (1), which is a very restrictive condition. [IP19] provides numerical experiments when the inputs are Gaussian, and when the parameters of the Gaussian distribution are known, which is almost the only case where it is feasible to sample with the conditional distributions for dependent input variables.

Remark that in Step (2) (II) and in Step (4) (III) (B) (i) (b) (2), Algorithm 1 needs to evaluate f at new points. When the computational code of f is expensive, [IP19] suggests to replace f by a metamodel (as in Section A.2.i)), and they make numerical experiments with Gaussian processes.

[SNS16] provides an upper-bound to the variance of the estimates of the Shapley effects provided by Algorithm 1 if $E_{P_{\sigma_m(j+1)}(\sigma_m)}$ in Step (4) (III) (ii) were known. Finally, to get confidence intervals of this estimator, [IP19] suggests to use the Central Limit Theorem and [BEDC19] suggest to use a bootstrap method.

To conclude, [SNS16] suggests an algorithm to estimate the Shapley effects.

However, the setting of this algorithm is very restrictive since it requires to be able to sample with the conditional distributions on the inputs. Moreover, no theoretical result is provided on Algorithm 1 in [SNS16]. Algorithm 1 will be studied in details in Chapter 2.

Part II

Estimation of the Shapley effects in the general framework

Chapter 2

General estimation of the Shapley effects

A Introduction

In this chapter, we aim at extending the works of [SNS16] on the estimation of the Shapley effects (see Algorithm 1 in Chapter 1). We divide this estimation into two parts. The first part is the estimation of quantities that we call the "conditional elements", on which the Shapley effects depend. The second part consists in aggregating the estimates of the conditional elements in order to obtain estimates of the Shapley effects. We call this part the W-aggregation procedure. We refer to Sections B and C for more details on these two parts.

First, we focus on the estimation of the conditional elements with two different estimators: the double Monte-Carlo estimator (used in Algorithm 1 suggested by [SNS16]) and the Pick-and-Freeze estimator (see Chapter 1 Section A.2.i) for the independent case) that we extend to the case where the inputs are dependent. We present the two estimators when it is possible to sample from the conditional distributions of the input vector. Then we suggest a new W-aggregation procedure, based on the subsets of $[1:p]$, to estimate all the Shapley effects (for all the input variables) at the same time. We choose the best parameters to minimize the sum of the variances of all the Shapley effects estimators. The algorithm of [SNS16] uses a W-aggregation procedure based on permutations of $[1:p]$. We study this W-aggregation procedure and explain how it minimizes the variance of the estimates of the Shapley effects. Our suggested W-aggregation procedure provides an improved accuracy, compared to the W-aggregation procedure in [SNS16], using all the estimates of the conditional elements for all the estimates of the Shapley effects. The comparison between the two W-aggregation procedures is illustrated with numerical experiments. These experiments also show that the double Monte-

Carlo estimator provides better results than the Pick-and-Freeze estimator.

Then, we extend the estimators of the conditional elements (the double Monte-Carlo estimator and the Pick-and-Freeze estimator) to the case where we only observe an i.i.d. sample from the input variables. The extension relies on nearest-neighbour techniques, which are widely used for many non-parametric estimation problems [BS19, BSY19]. To the best of our knowledge, the estimators we suggest are the first that do not require exact samples from the conditional distributions of the input variables. One of our main results is the consistency of these estimators under some mild assumptions, and their rate of convergence under additional regularity assumptions. We then give the consistency of the estimators of the Shapley effects with the two W-aggregation procedures and using the double Monte-Carlo estimator or the Pick-and-Freeze estimator. We observe, in numerical experiments, that the estimators of the Shapley effects have a similar accuracy as when it is possible to sample from the conditional distributions. We also apply one of these estimators on meteorological data, more specifically on the output of three different metamodels predicting the ozone concentration in function of nine input variables (with some categorical variables and some continuous variables). This application enables to study the influence of the inputs variables on black-box machine learning procedures.

This chapter is organized as follows. In the rest of Section A, we recall some notation with two different ways to write the Shapley effects. In Section B, we assume that the input distribution is known and we present the two methods to estimate the conditional elements. In Section C, we suggest a new W-aggregation procedure and we study the W-aggregation procedure used by the algorithm of [SNS16]. In Section D, we summarize the four estimators of the Shapley effects, give their consistency and we illustrate them with numerical applications. In Section E, we assume that the input distribution is unknown and that we just observe a sample of the input vector. We give consistent estimators of the conditional elements and thus consistent estimators of the Shapley effects in this case, and we illustrate this with numerical experiments. In Section F, we apply one of our estimators to a real data set. We conclude in Section G.

Recall that $X = (X_1, ..., X_p)$ is the input random vector on the input domain $\mathcal{X} = \mathcal{X}_1 \times ... \times \mathcal{X}_p$ with distribution $\mathbb{P}_X$ and $Y = f(X)$, with $f \in L^2$. Recall that for all $u \subset [1:p]$, we define:

$$V_u := \mathrm{Var}(\mathrm{E}(Y|X_u)), \tag{2.1}$$

$$E_u := \mathrm{E}(\mathrm{Var}(Y|X_{-u})), \tag{2.2}$$

and the conditional elements $(W_u)_{u\subset[1:p]}$ are either $(V_u)_{u\subset[1:p]}$ or $(E_u)_{u\subset[1:p]}$. For all

$i \in [1:p]$, recall that the Shapley effect η_i is defined by:

$$\eta_i := \frac{1}{p\mathrm{Var}(Y)} \sum_{u \subset -i} \binom{p-1}{|u|}^{-1} (W_{u\cup\{i\}} - W_u), \tag{2.3}$$

Remark 16. *The quantities $W_\emptyset$ and $W_{[1:p]}$ are equal to 0 and $\mathrm{Var}(Y)$ respectively. The variance of Y is easy to estimate, so we assume without loss of generality that we know the theoretical value $\mathrm{Var}(Y)$.*

We can notice that the Shapley effects are a sum over the subsets $u \subset -i$. We have seen in Chapter 1 Section C.2 another classical way to compute the Shapley effects, summing over the permutations of $[1:p]$. Recall that, for $i \in [1:p]$ and $\sigma \in \mathcal{S}_p$, we let $P_i(\sigma) := \{\sigma(j) |\ j \in [1 : \sigma^{-1}(i) - 1]\}$.

Proposition 8. *[Equation (11) in [SNS16], Section 4.1] We have*

$$\eta_i = \frac{1}{p!\mathrm{Var}(Y)} \sum_{\sigma \in \mathcal{S}_p} (W_{P_i(\sigma)\cup\{i\}} - W_{P_i(\sigma)}). \tag{2.4}$$

Our aim is to estimate the Shapley effects. We have seen two different ways to compute the Shapley effects, given by Equation (2.3) (with a sum over the subsets) and Equation (2.4) (with a sum over the permutations). These two equations will correspond to two different W-aggregation procedures of the Shapley effects.

B Estimation of the conditional elements

We explain now how to estimate these $(W_u)_{\emptyset \subsetneq u \subsetneq [1:p]}$ in a restricted setting (recall that $W_\emptyset = 0$ and $W_{[1:p]} = \mathrm{Var}(Y)$ are known). The restricted setting is the following: as in [SNS16], we will assume that for any $\emptyset \subsetneq u \subsetneq [1:p]$ and $x_u \in \mathcal{X}_u$, it is feasible to generate an i.i.d. sample from the distribution of X_{-u} conditionally to $X_u = x_u$. Moreover, we assume that we have access to the computer code of f.

To estimate W_u, we suggest two different estimators. The first one consists in a double Monte-Carlo procedure to estimate E_u, and it is the estimator used in the algorithm of [SNS16]. The other one is the well-known Pick-and-Freeze estimator (see [HS96] for the first definition, [GJKL14, GJK+16] for theoretical studies) for V_u, that we extend to the case where the input variables $(X_i)_{i\in[1:p]}$ are not independent.

Finally, we assume that each evaluation of f is costly, so we define the cost of each estimator $\widehat{W}_u$ as the number of evaluations of f.

B.1 Double Monte-Carlo

A first way to estimate $E_u = \mathrm{E}(\mathrm{Var}(Y|X_{-u}))$ is using double Monte-Carlo: a first Monte-Carlo step of size N_I for the conditional variance, another one of size N_u for the expectation. Thus, the estimator of E_u suggested in [SNS16] is

$$\widehat{E}_{u,MC}^{known} := \frac{1}{N_u}\sum_{n=1}^{N_u}\frac{1}{N_I-1}\sum_{k=1}^{N_I}\left(f(X_{-u}^{(n)},X_u^{(n,k)}) - \overline{f(X_{-u}^{(n)})}\right)^2, \tag{2.5}$$

where for $n = 1, ..., N_u$, $\overline{f(X_{-u}^{(n)})} := N_I^{-1}\sum_{k=1}^{N_I} f(X_{-u}^{(n)}, X_u^{(n,k)})$, $(X_{-u}^{(n)})_{n\in[1:N_u]}$ is an i.i.d. sample with the distribution of X_{-u} and $(X_u^{(n,k)})_{k\in[1:N_I]}$ conditionally to $X_{-u}^{(n)}$ is i.i.d. with the distribution of X_u conditionally to $X_{-u} = X_{-u}^{(n)}$. In Equation (2.5), the exponent "known" means that the distribution of X is known, that is, we are able to sample with the conditional distribution.

For all $n \in [1 : N_u]$, the computation of

$$\frac{1}{N_I-1}\sum_{k=1}^{N_I}\left(f(X_{-u}^{(n)},X_u^{(n,k)}) - \overline{f(X_{-u}^{(n)})}\right)^2$$

requires the values of $\left(f(X_{-u}^{(n)}, X_u^{(n,k)})\right)_{k\in[1:N_I]}$. We will take $N_I = 3$, as suggested in [SNS16]. Thus, the double Monte-Carlo estimator given in Equation (2.5) has a cost (number of evaluations of f) of $3N_u$.

Remark 17. *The estimator of Equation (2.5) is an unbiased estimator of $E_u = \mathrm{E}(\mathrm{Var}(Y|X_{-u}))$.*

B.2 Pick-and-freeze

We now provide a second estimator of W_u: the Pick-and-Freeze estimator for V_u. We have

$$V_u = \mathrm{Var}(\mathrm{E}(Y|X_u)) = \mathrm{E}(\mathrm{E}(Y|X_u)^2) - \mathrm{E}(Y)^2.$$

Remark that $\mathrm{E}(Y)$ is easy to estimate so we assume without loss of generality that we know the value of $\mathrm{E}(Y)$ (for the numerical applications, we will take the empirical mean). It remains to estimate $\mathrm{E}(\mathrm{E}(Y|X_u)^2)$, which seems to be complicated. We prove the following proposition that enables to simplify the formulation of this quantity.

Proposition 9. *Let $X = (X_u, X_{-u})$ and $X^u = (X_u, X'_{-u})$ of distribution $\mathbb{P}_X$ such that, a.s. $\mathbb{P}_{(X_{-u},X'_{-u})|X_u=x_u} = \mathbb{P}_{X_{-u}|X_u=x_u}\otimes\mathbb{P}_{X_{-u}|X_u=x_u}$. We have*

$$\mathrm{E}(\mathrm{E}(Y|X_u)^2) = \mathrm{E}(f(X)f(X^u)). \tag{2.6}$$

Remark that Proposition 9 enables to write a double expectation as one single expectation, that we estimate by a simple Monte-Carlo. Thus, we suggest the Pick-and-Freeze estimator, for $\emptyset \subsetneq u \subsetneq [1:p]$,

$$\widehat{V}_{u,PF}^{known} := \frac{1}{N_u}\sum_{n=1}^{N_u} f\left(X_u^{(n)}, X_{-u}^{(n,1)}\right) f\left(X_u^{(n)}, X_{-u}^{(n,2)}\right) - \mathrm{E}(Y)^2, \tag{2.7}$$

where $(X_u^{(n)})_{n\in[1:N_u]}$ is an i.i.d. sample with the distribution of X_u and where $X_{-u}^{(n,1)}$ and $X_{-u}^{(n,2)}$ conditionally to $X_u^{(n)}$ are independent with the distribution of X_{-u} conditionally to $X_u = X_u^{(n)}$. This estimator has a cost of $2N_u$.

C W-aggregation procedures

As we can see in Equation (2.3) or in Equation (2.4), the Shapley effects are functions of the conditional elements $(W_u)_{u\subset[1:p]}$. In Section B, we have seen how to estimate these conditional elements when it is possible to sample from the conditional distributions of the input vector. In this section, we assume that we have estimators $(\widehat{W}_u)_{u\subset[1:p]}$. From Remark 16, we let $\widehat{W}_\emptyset = W_\emptyset = 0$ and $\widehat{W}_{[1:p]} = W_{[1:p]} = \mathrm{Var}(Y)$. We also add the following assumption that will be needed for the theoretical results that we will prove.

Assumption 2. *For all $\emptyset \subsetneq u \subsetneq [1:p]$, $\widehat{W}_u$ is computed with a cost κN_u by $\widehat{W}_u = \frac{1}{N_u}\sum_{n=1}^{N_u}\widehat{W}_u^{(n)}$ where the $(\widehat{W}_u^{(n)})_{n\in[1:N_u]}$ are independent and identically distributed. The $(\widehat{W}_u)_{u\subset[1:p]}$ are independent. The integer $\kappa \in \mathbb{N}^*$ is the number of evaluations of the computer code f (i.e. the cost) for each $\widehat{W}_u^{(n)}$.*

Assumption 2 means that we estimate the $(W_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$ by Monte-Carlo, independently and with different costs $(\kappa N_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$. The accuracy N_u corresponds to computing N_u independent and identically distributed estimators $\widehat{W}_u^{(1)}, ..., \widehat{W}_u^{(N_u)}$ that are averaged. We have seen in Section B two estimators that satisfy Assumption 2: the double Monte-Carlo estimator (with $\kappa = 3$) and the Pick-and-Freeze estimator (with $\kappa = 2$).

We call "W-aggregation procedure" an algorithm that estimates the Shapley effects from the estimates $(\widehat{W}_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$ and that selects the values of the accuracies $(N_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$. We first suggest a new W-aggregation procedure. Then we obtain a theoretical insight on the W-aggregation procedure of [SNS16].

C.1 The subset procedure

In this section, we suggest a new W-aggregation procedure for the Shapley effects. This procedure consists in computing once for all the estimates $\widehat{W}_u$ for all $u \subset [1:$

$p]$, and to store them. Then, we use these estimates to estimate all the Shapley effects.

C.1.i) The W-aggregation procedure

We suggest to estimate the Shapley effects $(\eta_i)_{i\in[1:p]}$ by using the following W-aggregation procedure:

Procedure (subset W-aggregation procedure)

1. For all $u \subset [1:p]$, compute $\widehat{W}_u$.
2. For all $i \in [1:p]$, estimate η_i by

$$\widehat{\eta}_i := \frac{1}{p\mathrm{Var}(Y)} \sum_{u\subset -i} \binom{p-1}{|u|}^{-1} (\widehat{W}_{u\cup\{i\}} - \widehat{W}_u). \tag{2.8}$$

We can note that each estimate $\widehat{W}_u$ is used for all the estimates $(\widehat{\eta}_i)_{i\in[1:p]}$. It remains to choose the values of the accuracies $(N_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$.

C.1.ii) Choice of the accuracy of each $\widehat{W}_u$

In this section, we explain how to choose the values of the accuracies $(N_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$. In the following proposition, we give the best choice of the accuracies $(N_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$ to minimize $\sum_{i=1}^p \mathrm{Var}(\widehat{\eta}_i)$ for a fixed total cost $\kappa\sum_{\emptyset\subsetneq u\subsetneq[1:p]} N_u$.

Proposition 10. *Let a total cost $N_{tot}\in\mathbb{N}$ be fixed. Under Assumption 2, if the Shapley effects are estimated with the subset W-aggregation procedure, the solution of the relaxed program (i.e. the problem without the constraint of letting the $(N_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$ be integers)*

$$\min_{(N_u)_{\emptyset\subsetneq u\subsetneq[1:p]}\in(0,+\infty)^{2^p-2}} \sum_{i=1}^p \mathrm{Var}(\widehat{\eta}_i) \quad \textit{subject to} \quad \kappa \sum_{\emptyset\subsetneq u\subsetneq[1:p]} N_u = N_{tot} \tag{2.9}$$

is $(N_u^*)_{\emptyset\subsetneq u\subsetneq[1:p]}$ with for all $\emptyset\subsetneq u\subsetneq[1:p]$

$$N_u^* = \frac{N_{tot}}{\kappa}\frac{\sqrt{(p-|u|)!|u|!(p-|u|-1)!(|u|-1)!\mathrm{Var}(\widehat{W}_u^{(1)})}}{\sum_{\emptyset\subsetneq v\subsetneq[1:p]}\sqrt{(p-|v|)!|v|!(p-|v|-1)!(|v|-1)!\mathrm{Var}(\widehat{W}_v^{(1)})}}.$$

Usually, we do not know the values of $\mathrm{Var}(\widehat{W}_u^{(1)})$ for $\emptyset \subsetneq u \subsetneq [1:p]$, but we need them to compute the value of N_u^*. In practice, we will assume that these values are equal in order to compute N_u^*. Furthermore, the sum over the subsets v such that $\emptyset \subsetneq v \subsetneq [1:p]$ can be too costly to compute. Hence, we make the following approximations in practice:

$$N_u^* \approx \frac{\frac{N_{tot}}{\kappa}\binom{p}{|u|}^{-\frac{1}{2}}\binom{p}{|u|-1}^{-\frac{1}{2}}}{\sum_{\emptyset\subsetneq v\subsetneq[1:p]}\binom{p}{|v|}^{-\frac{1}{2}}\binom{p}{|v|-1}^{-\frac{1}{2}}} \approx \frac{\frac{N_{tot}}{\kappa}\binom{p}{|u|}^{-1}}{\sum_{\emptyset\subsetneq v\subsetneq[1:p]}\binom{p}{|v|}^{-1}} = \frac{N_{tot}}{\kappa}\frac{\binom{p}{|u|}^{-1}}{p-1}. \tag{2.10}$$

Hence, when implementing the subset W-aggregation procedure, we will choose N_u^* as

$$N_u^* := \mathrm{Round}\left(N_{tot}\kappa^{-1}\binom{p}{|u|}^{-1}(p-1)^{-1}\right) \tag{2.11}$$

for $\emptyset \subsetneq u \subsetneq [1:p]$, where Round is the nearest integer function. In this way, for a fixed total cost, we take the accuracies $(N_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$ near the optimal choice that minimizes $\sum_{i=1}^p \mathrm{Var}(\widehat{\eta}_i)$. Hence, the parameter N_{tot} is now the only parameter left to choose. In practice, this parameter is often imposed as a global budget constraint.

Remark 18. *With the approximation discussed above, the real total cost* $\kappa\sum_{\emptyset\subsetneq u\subsetneq[1:p]} N_u$ *can be different from the* N_{tot} *chosen (because of the approximations and the choice of the closest integer). In this case, we suggest to adapt the value of* N_{tot} *in order to make the total cost* $\kappa\sum_{\emptyset\subsetneq u\subsetneq[1:p]} N_u^*$ *take the desired value.*

Remark 19. *In order to compute the* $(N_u^*)_{\emptyset\subsetneq u\subsetneq[1:p]}$ *in practice, we assume that the values of* $\mathrm{Var}(\widehat{W}_u^{(1)})$*, for* $\emptyset \subsetneq u \subsetneq [1:p]$*, are equal. We can see on unreported numerical experiments that this choice of* N_u *gives much better results than if we choose the same value of* N_u *for all* $\emptyset \subsetneq u \subsetneq [1:p]$*. However, it seems difficult to obtain theoretical results on the values of* $\mathrm{Var}(\widehat{W}_u^{(1)})$*, as they depend on the conditional distributions of* X *in a complicated way.*

Hence, this assumption is more a convenient heuristic to compute the best accuracies $(N_u^*)_{\emptyset\subsetneq u\subsetneq[1:p]}$ *than a real property satisfied in many cases. Proposition 10 and the heuristic in Equation (2.10) justify the choice of* $(N_u^*)_{\emptyset\subsetneq u\subsetneq[1:p]}$ *given in Equation (2.11), and we make this choice even if the assumption of equal values of the* $(\mathrm{Var}(\widehat{W}_u^{(1)}))_{\emptyset\subsetneq u\subsetneq[1:p]}$ *is not satisfied.*

Remark 20. *By Equation (2.11), if* $|u|$ *is close to* 0 *or* p *and if* $|v|$ *is close to* $p/2$*, the value of* N_u^* *is larger than the value of* N_v^**. Hence, the estimate of* W_u *is more* *accurate than the estimate of W_v. This is not surprising since, in the computation of the Shapley effects given by Equation (2.3), the coefficient associated with the quantity W_u is larger than the one associated with W_v (hence, the estimate of W_v does not need to be as accurate as the estimate of W_u).*

C.1.iii) Consistency

A straightforward consequence of the subset W-aggregation procedure and Equation (2.8) is that the consistency of $(\widehat{W}_u)_{u\subset[1:p]}$ implies the consistency of $(\widehat{\eta}_i)_{i\in[1:p]}$ (Assumption 2 is not necessary).

Proposition 11. *Assume that for all $\emptyset \subsetneq u \subsetneq [1:p]$, we have estimators $\widehat{W}_u$ that converge to W_u in probability (resp. almost surely) when N_u goes to $+\infty$, where κN_u is the cost of $\widehat{W}_u$. If we use the subset W-aggregation procedure with the choice of $(N_u^*)_{\emptyset\subsetneq u\subsetneq[1:p]}$ given by Equation (2.11), the estimators of the Shapley effects converge to the Shapley effects in probability (resp. almost surely) when N_{tot} goes to $+\infty$ (where N_{tot} is the total cost of the subset W-aggregation procedure).*

C.2 The random-permutation procedure

In this section, we present and study the "random-permutation W-aggregation procedure" suggested in [SNS16].

C.2.i) The W-aggregation procedure

The W-aggregation procedure of the algorithm of [SNS16] is based on Equation (2.4). Because of the equation, one could estimate η_i by

$$\widehat{\eta}_i = \frac{1}{p!\mathrm{Var}(Y)} \sum_{\sigma\in\mathcal{S}_p} \left(\widehat{W}_{P_i(\sigma)\cup\{i\}} - \widehat{W}_{P_i(\sigma)}\right), \tag{2.12}$$

for $i \in [1:p]$. In Equation (2.12), informally, $(\widehat{W}_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$ are estimators. However, as the number of permutations is $p!$, there are too many summands and [SNS16] suggests to replace the sum over all the $p!$ permutations by the sum over M ($M < p!$) random uniformly distributed permutations. Thus, for a fixed $i \in [1:p]$, the estimator of η_i suggested in [SNS16] is

$$\widehat{\eta}_i = \frac{1}{M\mathrm{Var}(Y)} \sum_{m=1}^{M} \left(\widehat{W}_{P_i(\sigma_m)\cup\{i\}}(m) - \widehat{W}_{P_i(\sigma_m)}(m)\right), \tag{2.13}$$

where $(\sigma_m)_{m\in[1:M]}$ are independent and uniformly distributed on $\mathcal{S}_p$. If $m, m' \in [1:M]$ with $m \neq m'$ and $P_i(\sigma_m) = P_i(\sigma_{m'}) =: u$, [SNS16] estimates twice the same

W_u. To formalize these different estimations, we write $\widehat{W}_u(m)$ the estimation of W_u at step m in Equation (2.13).

Finally, [SNS16] reduces the computation cost using the following idea. The authors of [SNS16] notice that for $1 \leq i < p$, for any permutation $\sigma \in \mathcal{S}_p$ and for $i \in [1:p]$, we have $P_{\sigma(i+1)}(\sigma) = P_{\sigma(i)}(\sigma) \cup \{\sigma(i)\}$. Thus, the algorithm of [SNS16] uses every estimate $\widehat{W}_{P_{\sigma_m(i)}(\sigma_m)\cup\{\sigma_m(i)\}}(m)$ for $\widehat{\eta}_{\sigma_m(i)}$ (as an estimator of $W_{P_{\sigma_m(i)}(\sigma_m)\cup\{\sigma_m(i)\}}$) and for $\widehat{\eta}_{\sigma_m(i+1)}$ (as an estimator of $W_{P_{\sigma_m(i+1)}(\sigma_m)}$). With this improvement, the number of estimations of W_u (for $\emptyset \subsetneq u \subsetneq [1:p]$) is divided by two when estimating all the Shapley effects $\eta_1, ..., \eta_p$.

Procedure (random-permutation W-aggregation procedure)

1. Let $\widehat{\eta}_1 = ... = \widehat{\eta}_p = 0$.
2. For all $m = 1, 2, ..., M$
   (a) Generate σ_m uniformly distributed on $\mathcal{S}_p$.
   (b) Let $prevC = 0$.
   (c) For all $i = 1, 2, ..., p$
      i. Let $u = P_{\sigma_m(i)}(\sigma_m)$.
      ii. Compute $\widehat{W}_{u\cup\{\sigma_m(i)\}}(m)$.
      iii. Compute $\widehat{\Delta} = \widehat{W}_{u\cup\{\sigma_m(i)\}}(m) - prevC$.
      iv. Update $\widehat{\eta}_{\sigma_m(i)} = \widehat{\eta}_{\sigma_m(i)} + \widehat{\Delta}$.
      v. Set $prevC = \widehat{W}_{P_{\sigma_m(i+1)}(\sigma_m)}$.
3. Let $\widehat{\eta}_i = \widehat{\eta}_i / (\mathrm{Var}(Y)M)$ for all $i = 1, ..., p$.

Remark 21. *Recall that in the subset W-aggregation procedure, each estimation of W_u was used for the estimation of all the $(\eta_i)_{i\in[1:p]}$ (and not only for two of them). Thus the subset W-aggregation procedure seems to be more efficient.*

Remark 22. *When the number of inputs p is small, [SNS16] suggests to take all the permutations of $[1:p]$ instead of choosing random permutations in Step 2a of the random-permutation W-aggregation procedure. However, this algorithm requires small values of p and the total cost is a multiple of $p!$ (so there are very restricted possible values). Furthermore, this method still remains very costly due to the computation of $(p-1)!$ conditional variances. For example, in the linear Gaussian framework with $p = 10$ (where the computation of the conditional elements is* *immediate) it spends more than ten minutes computing the Shapley effects. Hence, the algorithm with all the permutations is not explicitly detailed in [SNS16].*

C.2.ii) Choice of the accuracy of each $\widehat{W}_u$

As in Section C.1.ii), we suggest a choice of the accuracies $(N_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$.

In order to avoid a random total cost, we require for all $\emptyset \subsetneq u \subsetneq [1:p]$ that the accuracy N_u of the $\left(\widehat{W}_u(m)\right)_m$ depends only on $|u|$, and we write $N_{|u|} := N_u$. In this case, the total cost of the random-permutation W-aggregation procedure is equal to $N_{tot} = \kappa M \sum_{k=1}^{p-1} N_k$. Moreover, we assume that the total cost $N_{tot} = \kappa M \sum_{k=1}^{p-1} N_k$ is proportional to $(p-1)$, and thus can be written $N_{tot} = \kappa M N_O(p-1)$ for some fixed $N_O \in \mathbb{N}^*$. As the permutations $(\sigma_m)_{m\in[1:M]}$ are random, we choose to minimize $\mathrm{E}\left[\sum_{i=1}^p \mathrm{Var}\left(\widehat{\eta}_i | (\sigma_m)_{m\in[1:M]}\right)\right]$.

To compute the optimal values of $(N_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$, we introduce the following assumption.

Assumption 3. *For all $\emptyset \subsetneq u \subsetneq [1:p]$ and all $m \in [1:M]$, $\widehat{W}_u(m)$ is computed with a cost $\kappa N_{|u|}$ by $\widehat{W}_u(m) = \frac{1}{N_{|u|}} \sum_{n=1}^{N_{|u|}} \widehat{W}_u^{(n)}(m)$ where the $(\widehat{W}_u^{(n)}(m))_{n\in[1:N_u]}$ are independent and identically distributed. The $(\widehat{W}_u(m))_{\emptyset\subsetneq u\subsetneq[1:p],\, m\in[1:M]}$ are independent.*

When it is possible to sample from the conditional distributions of the input vector, we can generate i.i.d. double Monte-Carlo estimators $(\widehat{E}_{u,MC}(m))_{m\in[1:M]}$ or Pick-and-Freeze estimators $(\widehat{V}_{u,PF}(m))_{m\in[1:M]}$. Hence, they satisfy Assumption 3 by taking $N_u = N_{|u|}$ for all $\emptyset \subsetneq u \subsetneq [1:p]$.

Proposition 12. *Assume that we estimate the Shapley effects with the random-permutation W-aggregation procedure under Assumption 2 and that the variances $(\mathrm{Var}(\widehat{W}_u^{(1)}(1)))_{\emptyset\subsetneq u\subsetneq[1:p]}$ are equal. Then, the solution of the problem*

$$\min_{(N_k)_{k\in[1:p-1]}\in(0,+\infty)^{p-1}} \mathrm{E}\left[\sum_{i=1}^p \mathrm{Var}\left(\widehat{\eta}_i | (\sigma_m)_{m\in[1:M]}\right)\right] \quad \textit{subject to} \quad \kappa M \sum_{k=1}^{p-1} N_k = \kappa M N_O(p-1)$$

is $(N_k^{**})_{k\in[1:p-1]}$ with for all $k \in [1:p-1]$,

$$N_k^{**} = N_O.$$

Hence, from now on, with the random permutation W-aggregation procedure, we will choose the accuracy $N_u = N_O$ for all subset u.

Remark 23. *As in Remark 19, we assume in Proposition 12 that the variances $(\mathrm{Var}(\widehat{W}_u^{(1)}(1)))_{\emptyset\subsetneq u\subsetneq[1:p]}$ are equal. This assumption is not easy to check, but is required technically to prove Proposition 12.*

Remark 24. *With the exact-permutation W-aggregation procedure (see Remark 22), $N_k^* = N_O p!$ is the solution of the problem $\sum_{i=1}^p \mathrm{Var}(\widehat{\eta}_i)$ subject to $\sum_{k=1}^{p-1} N_k = p! N_O (p-1)$.*

There are now two parameters to choose: the number of permutations M and the accuracy N_O of the estimations of the $(W_u)_{\emptyset \subsetneq u \subsetneq [1:p]}$. Typically, their product MN_O is imposed by budget constraints.

C.2.iii) Choice of N_O

We have seen that for all $\emptyset \subsetneq u \subsetneq [1:p]$, we choose $N_u = N_{|u|}^{**} = N_O$. In this section, we explain why we should choose $N_O = 1$ under Assumption 2 and M as large as possible.

Proposition 13 generalizes the result given in [SNS16], Appendix B. Its proof is given in the supplementary material, which is much simpler than the arguments in [SNS16].

Assumption 4. *Assumption 3 holds and for all $\emptyset \subsetneq u \subsetneq [1:p]$, we have $\mathrm{E}(\widehat{W}_u^{(1)}(1)) = W_u$.*

Assumption 4 ensures that the estimators have a zero bias. Recall that the double Monte-Carlo estimator and the Pick-and-Freeze estimator have a zero bias. Hence, they satisfy Assumption 4 by generating i.i.d. $(\widehat{W}_u(m))_{m \in [1:M]}$ and by taking $N_u = N_{|u|}$ for all $\emptyset \subsetneq u \subsetneq [1:p]$.

Proposition 13. *Let $i \in [1:p]$ be fixed. Under Assumption 4, in order to minimize, over N_O and M, the variance of $\widehat{\eta}_i$ with a fixed cost $\kappa M N_O \times (p-1) = \kappa C \times (p-1)$ (for some $C \in \mathbb{N}^*$), we have to choose $N_O = 1$ and $M = C$.*

From now on, we assume that $N_u = N_O = 1$ when we use the random-permutation W-aggregation procedure and we will let M, the number of random permutations, go to infinity. Then, the total cost N_{tot} of the random-permutation W-aggregation procedure is equal to $N_{tot} = \kappa M(p-1)$, for estimating the p Shapley effects $\eta_1, \dots, \eta_p$. Hence, under Assumption 3 or Assumption 4, $\widehat{W}_u(m) = \widehat{W}_u^{(1)}(m)$ and has now a cost κ.

C.2.iv) Consistency

We give here two sufficient conditions for the consistency of the estimators of the Shapley effects given by the random-permutation W-aggregation procedure. We introduce a general assumption.

Assumption 5. *For all u such that $\emptyset \subsetneq u \subsetneq [1:p]$, $\left(\widehat{W}_u(m)\right)_{m\in[1:M]}$ have a cost κ (since we chose $N_u = 1$) and are identically distributed with a distribution that depends on an integer N such that $\mathrm{E}\left(\widehat{W}_u(1)\right) \underset{N\to+\infty}{\longrightarrow} W_u$. Moreover, for all u such that $\emptyset \subsetneq u \subsetneq [1:p]$, we have*

$$\frac{1}{M^2}\sum_{m,m'=1}^{M} \mathrm{cov}\left(\widehat{W}_u(m), \widehat{W}_u(m')\right) \underset{N,M\to+\infty}{\longrightarrow} 0.$$

Assumption 5 is more general than Assumption 4. Indeed, it enables the estimators to have a bias and a covariance which go to zero. This assumption will be useful to prove the consistency results in Section E.2. Remark that in Assumption 5, for all $\emptyset \subsetneq u \subsetneq [1:p]$, each estimate $\left(\widehat{W}_u(m)\right)_{m\in[1:M]}$ has a cost κ, as in Assumption 4 since we fixed $N_u = N_O = 1$.

Proposition 14. *Assume that we estimate the Shapley effects using the random-permutation W-aggregation procedure. Let $N_{tot} = \kappa M(p-1)$ be the total cost of the random-permutation W-aggregation procedure.*

1. *Under Assumption 4, the estimates of the Shapley effects converge to the Shapley effects in probability when N_{tot} goes to $+\infty$.*
2. *Under Assumption 5, the estimates of the Shapley effects converge to the Shapley effects in probability when N_{tot} and N go to $+\infty$.*

D Estimators of the Shapley effects

D.1 Four consistent estimators of the Shapley effects

Recall that in Section B, we have seen two estimators of the $(W_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$: double Monte-Carlo (used in the algorithm of [SNS16]) and Pick-and-Freeze. In Section C, we have studied two W-aggregation procedures for the Shapley effects using estimators of the $(W_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$: the subset W-aggregation procedure and the random-permutation W-aggregation procedure (used in the algorithm of [SNS16]). To sum up, four estimators of the Shapley effects are available:

- subset W-aggregation procedure with double Monte-Carlo;
- subset W-aggregation procedure with Pick-and-Freeze;
- random-permutation W-aggregation procedure with double Monte-Carlo, which is the already existing algorithm of [SNS16];

- random-permutation W-aggregation procedure with Pick-and-Freeze.

With the random-permutation W-aggregation procedure, we have seen that we need different estimators $(\widehat{W}_u(m))_{m\in[1:M]}$ of the same W_u. In this case, we choose i.i.d. realizations of the estimator of W_u. Moreover, we have seen in Section C.2.iii) that when we use the random-permutation W-aggregation procedure, we choose $N_u = N_O = 1$.

By Propositions 11 and 14, all these four estimators are consistent when the global budget N_{tot} goes to $+\infty$. Indeed, by Proposition 11, the consistency of the $(\widehat{W}_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$ is sufficient for the consistency with the subset procedure and by Proposition 14, unbiased and i.i.d. estimators $(\widehat{W}_u(m))_{m\in[1:M]}$ for all $\emptyset \subsetneq u \subsetneq [1:p]$ provide the consistency with the random-permutation procedure.

D.2 Numerical comparison of the different algorithms

In this section, we carry out numerical experiments on the different algorithms in the restricted framework (where the exact conditional samples are available).

To compare these estimators, we use the linear Gaussian framework: $\mathcal{X} = \mathbb{R}^p$, $X \sim \mathcal{N}(\mu, \Sigma)$ and $Y = \sum_{i=1}^p \beta_i X_i$. In this case, the theoretical values are easily computable (see [OP17, IP19, BBDM19]). We choose $p = 10$, $\beta_i = 1$ for all $i \in [1:p]$ and $\Sigma = A^T A$ where A is a $p\times p$ matrix which components are realisations of p^2 i.i.d. Gaussian variables with zero mean and unit variance. To compare these different estimators, we fix a total cost (number of evaluations of f) of $N_{tot} = 54000$. We compute 1000 realizations of each estimator.

In Figure 2.1, we plot the theoretical values of the Shapley effects together with the boxplots of the 1000 realizations of each estimator.

In Figure 2.2, we plot the sum over $i\in[1:p]$ of the quadratic risks: $\sum_{i=1}^p \mathrm{E}\left((\widehat{\eta}_i - \eta_i)^2\right)$ (estimated with 1000 realizations) of each estimator.

We can see that the subset W-aggregation procedure gives better results than the random-permutation W-aggregation procedure, and that the double Monte-Carlo estimator is better than the Pick-and-Freeze estimator.

Remark 25. *It appears that double Monte-Carlo is numerically more efficient than Pick-and-Freeze for estimating the Shapley effects. Indeed, if we focus only on the estimation of one W_u for a fixed $\emptyset \subsetneq u \subsetneq [1:p]$, we can see numerically that the Pick-and-Freeze estimator has a larger variance than the double Monte-Carlo estimator. This finding appears to be difficult to confirm theoretically in the general case. Nevertheless, we can obtain such a theoretical confirmation in a simple, specific example. Let $X \sim \mathcal{N}(0, I_2)$, $Y = X_1 + X_2$. Remark that, in this example, the variances of $\widehat{W}_u^{(1)}$, $\emptyset \subsetneq u \subsetneq [1:p]$, are equal. In this case, and for $u = \{1\}$, we can easily get $\mathrm{Var}(\widehat{V}_{u,PF}^{known}) = \frac{40}{9}\mathrm{Var}(\widehat{E}_{u,MC}^{known})$ for the same cost*

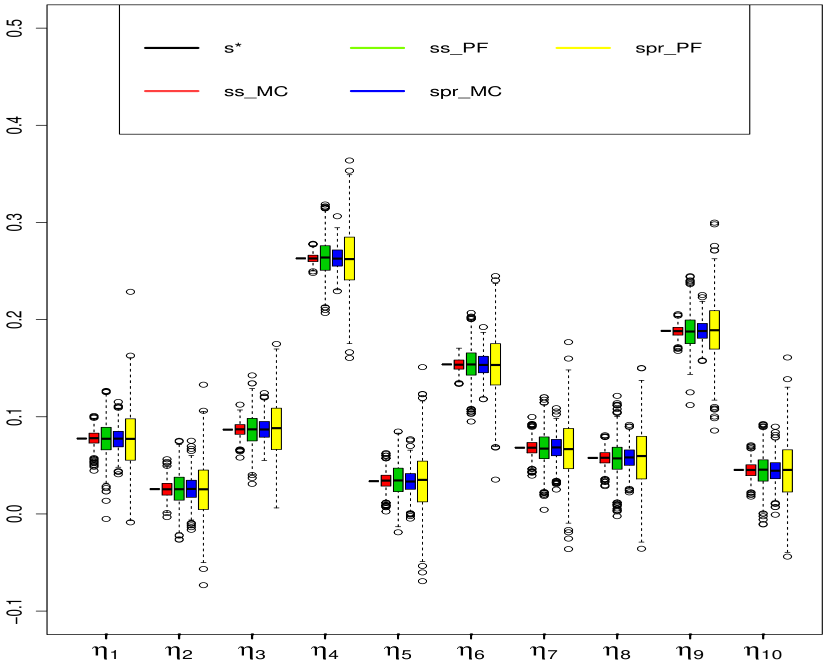


Figure 2.1: Estimation of the Shapley effects in the linear Gaussian framework. In black (s*) we show the theoretical values, in red (ss_MC) the estimates from the subset W-aggregation procedure with the double Monte-Carlo estimator, in green (ss_PF) the estimates from the subset W-aggregation procedure with the Pick-and-Freeze estimator, in blue (spr_MC) the estimates from the random-permutation W-aggregation procedure with the double Monte-Carlo estimator and in yellow (spr_PF) the estimates from the random-permutation W-aggregation procedure with the Pick-and-Freeze estimator.

(number of evaluations of f), and choosing $N_I = 3$ for the double Monte-Carlo estimator. This could be surprising since [JKLR+14] proved that some Pick-and-Freeze estimator is asymptotically efficient in the independent case. However, this result and our finding are not contradictory for two reasons: the authors of [JKLR+14] estimate the variance of Y so their result does not apply here and the double Monte-Carlo estimator is based on different observations from the Pick-and-Freeze estimator.

To conclude, we improved the already existing algorithm of [SNS16] (random-permutation W-aggregation procedure with double Monte-Carlo) by the estimator given by the subset W-aggregation procedure with double Monte-Carlo.

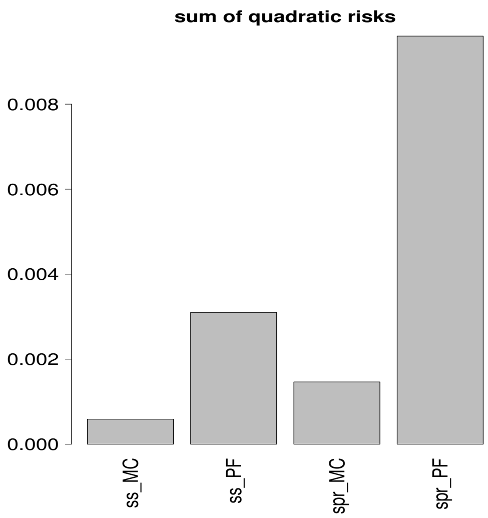


Figure 2.2: Sum over $i \in [1:p]$ of the estimated quadratic risks of the four estimators of the Shapley effects in the linear Gaussian framework.

E Extension when we observe an i.i.d. sample

In Section D, we have considered a restricted framework: we assumed that for all $\emptyset \subsetneq u \subsetneq [1:p]$ and all $x_u \in \mathcal{X}_u$, we could generate an i.i.d. sample from the distribution of X_{-u} conditionally to $X_u = x_u$. However, in many cases, we can not generate this sample, as we only observe an i.i.d. sample of X. In this section, we assume that we only observe an i.i.d. sample $(X^{(n)})_{nin[1:N]}$ of X and that we have access to the computer code f. We extend the double Monte-Carlo and Pick-and-Freeze estimators in this general case and show their consistency and rates of convergence. We then give the consistency of the implied estimators of the Shapley effects (obtained from the W-aggregation procedures studied previously). To the best of our knowledge, these suggested estimators are the first estimators of Shapley effects in this general framework. We conclude giving numerical experiments.

We choose a very general framework to prove the consistency of the estimators. This framework is given in the following assumption.

Assumption 6. *For all $i \in [1:p]$, $(\mathcal{X}_i, d_i)$ is a Polish space with metric d_i and $X = (X_1, ..., X_p)$ has a density f_X with respect to a finite measure $\mu = \bigotimes_{i=1}^p \mu_i$ which is bounded and $\mathbb{P}_X$-almost everywhere continuous.*

This assumption is really general. Actually, it enables to have some continuous variables (with the Euclidean distance), some categorical variables in countable ordered or unordered sets and some variables in separable Hilbert spaces (for example $L^2(\mathbb{R}^d)$, for some $d \in \mathbb{N}^*$). The fact that X has a continuous density f_X with respect to a finite measure $\mu = \bigotimes \mu_i$ means that the distribution of X is smooth. Assumption 6 is satisfied in many realistic cases. The assumption of a bounded density which is $\mathbb{P}_X$-almost everywhere continuous may be less realistic in some cases but is needed in the proofs. It would be interesting to alleviate it in a future work.

To prove rates of convergence, we will need the following stronger assumption.

Assumption 7. *The function f is $\mathcal{C}^1$, $\mathcal{X}$ is compact in $\mathbb{R}^p$, X has a density f_X with respect to the Lebesgue measure λ_p on $\mathcal{X}$ such that λ_p-a.s. on $\mathcal{X}$, we have $0 < C_{\inf} \leq f_X \leq C_{\sup} < +\infty$. Furthermore, f_X is Lipschitz continuous on $\mathcal{X}$.*

Assumption 7 is more restrictive than Assumption 6. It requires all the input variables to be continuous and real-valued. Moreover, their values are restricted to a compact set where the density is lower-bounded. Assumption 7 will be satisfied in some realistic cases (for instance with uniform or truncated Gaussian input random variables). Nevertheless, there also exist realistic cases where the input density is not lower-bounded (for instance with triangular input random variables). We remark that the assumption of a lower-bounded density is common in the field of non-parametric statistics [Gho01]. Here, it enables us to control the order of magnitude of conditional densities.

E.1 Estimators of the conditional elements

As far as we know, only [VG13] suggests a consistent estimator of W_u when we only observe an i.i.d. sample and when the input variables can be dependent, but only for V_u with $|u| = 1$. The estimator suggested in [VG13] is asymptotically efficient but the fact that u has to be a singleton prevents us to use this estimator for the Shapley effects (because we have to estimate W_u for all $\emptyset \subsetneq u \subsetneq [1:p]$). We can find another estimator of the $(V_u)_{u\subset[1:p]}$ in [Pli10] (but no theoretical results on the convergence are given). Finally, note that [PBS13] provides an estimator of different sensitivity indices, with convergence proofs.

In this section we introduce two consistent estimators of $(W_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$ when we observe only an i.i.d. sample of X, and which are easy to implement. These two estimators follow the principle of the double Monte-Carlo and Pick-and-Freeze estimators, but **replacing exact samples from the conditional distributions by approximate ones based on nearest-neighbours methods**.

To that end, we have to introduce some additional notation. Let $N \in \mathbb{N}$ and $(X^{(n)})_{n\in[1:N]}$ be an i.i.d. sample of X. If $\emptyset \subsetneq v \subsetneq [1:p]$, let us write $k_N^v(l,n)$ for the index such that $X_v^{(k_N^v(l,n))}$ is the (or one of the) n-th closest element to $X_v^{(l)}$ in $(X_v^{(i)})_{i\in[1:N]}$, and such that $(k_N^v(l,n))_{n\in[1:N_I]}$ are two by two distinct.

The index $k_N^v(l,n)$ could be not uniquely defined if there exist different observations $X_v^{(i)}$ at equal distance from $X_v^{(l)}$. In this case, we will choose $k_N^v(l,n)$ uniformly over the indices of these observations, with the following independence assumption.

Assumption 8. *Conditionally to $(X_v^{(n)})_{n\in[1:N]}$, $k_N^v(l,i)$ is randomly and uniformly chosen over the indices of all the i-th nearest neighbours of $X_v^{(l)}$ in $(X_v^{(n)})_{n\in[1:N]}$ and the $(k_N^v(l,i))_{i[1:N_I]}$ are two by two distinct. Furthermore, conditionally to $(X_v^{(n)})_{n\in[1:N]}$, for all $l\in[1:N]$, the random vector $(k_N(l,i))_{i\in[1:N_I]}$ is independent on all the other random variables.*

To summarize the idea of Assumption 8, we can say that the nearest neighbours of $X_v^{(l)}$ are chosen uniformly among the possible choices and independently on the other variables. Assumption 8 actually only formalizes the random choice of the nearest neighbours where there can be equalities of the distances and this choice is easy to implement in practice.

When X_v is absolutely continuous with respect to the Lebesgue measure, distance equalities can not happen and $k_N^v(l,n)$ is uniquely defined. Thus, Assumption 8 trivially holds in this case. Assumption 8 is thus specific to the case where some input variables are not continuous.

E.1.i) Double Monte-Carlo

We write $(s(l))_{l\in[1:N_u]}$ a sample of uniformly distributed integers in $[1:N]$ (with or without replacement) independent of the other random variables. Then, we define two slightly different versions of the double Monte-Carlo estimator by

$$\widehat{E}_{u,MC}^{mix}=\frac{1}{N_u}\sum_{l=1}^{N_u}\widehat{E}_{u,s(l),MC}^{mix}, \tag{2.14}$$

and

$$\widehat{E}_{u,MC}^{knn}=\frac{1}{N_u}\sum_{l=1}^{N_u}\widehat{E}_{u,s(l),MC}^{knn}, \tag{2.15}$$

with

$$\widehat{E}_{u,s(l),MC}^{mix}=\frac{1}{N_I-1}\sum_{i=1}^{N_I}\left[f\left(X_{-u}^{(s(l))},X_u^{(k_N^{-u}(s(l),i))}\right)-\frac{1}{N_I}\sum_{h=1}^{N_I}f\left(X_{-u}^{(s(l))},X_u^{(k_N^{-u}(s(l),h))}\right)\right]^2 \tag{2.16}$$

and

$$\widehat{E}_{u,s(l),MC}^{knn}=\frac{1}{N_I-1}\sum_{i=1}^{N_I}\left[f\left(X^{(k_N^{-u}(s(l),i))}\right)-\frac{1}{N_I}\sum_{h=1}^{N_I}f\left(X^{(k_N^{-u}(s(l),h))}\right)\right]^2. \tag{2.17}$$

The double Monte-Carlo estimator has two sums: one of size N_I for the conditional variance, one other of size N_u for the expectation. The integer N_I is also the number of nearest neighbours and it is a fixed parameter to choose. For example, we can choose $N_I = 3$ (as in the case where the conditional samples are available).

Remark 26. *If we observe the sample $(X^{(n)})_{n\in[1:N]}$ and if the values of $(f(X^{(n)}))_{n\in[1:N]}$ have to be assessed, the cost of the estimators $\widehat{E}_{u,MC}^{mix}$ and $\widehat{E}_{u,MC}^{knn}$ remains the number of evaluations of f (which is $N_I N_u$). If we observe the sample $(X^{(n)}, f(X^{(n)}))_{n\in[1:N]}$, the estimator $\widehat{E}_{u,MC}^{knn}$ does not require evaluations of f but the cost remains proportional to N_u (for the search of the nearest neighbours and for the elementary operations).*

Remark 27. *The integer N is the size of the sample of X (that enables us to estimate implicitly its conditional distributions through the nearest neighbours) and the integer N_u is the accuracy of the estimator $\widehat{E}_{u,MC}$ from the estimated distribution of X. Of course, it would be intuitive to take $N_u = N$ and $(s(l))_{l\in[1:N]} = (l)_{l\in[1:N]}$, but this framework would not be general enough for the subset W-aggregation procedure (in which the accuracy N_u of $\widehat{E}_{u,MC}$ depends on u) and for the proof of the consistency when using the random-permutation W-aggregation procedure in Section E.2. Furthermore, we may typically have to take N_u smaller than N.*

Remark that we give two versions of the double Monte-Carlo estimator. The "mix" version seems more accurate but requires to call the computer code of f at new inputs. For the "knn" version, it is sufficient to have an i.i.d. sample $(X^{(n)}, f(X^{(n)}))_{n\in[1:N]}$.

Now that we defined these two versions of the double Monte-Carlo estimator for an unknown input distribution, we give the consistency of these estimators in Theorem 3. We let $\widehat{E}_{u,MC}$ be given by Equation (2.14) or Equation (2.15). In the asymptotic results below, N_I is fixed and N and N_u go to infinity.

Theorem 3. *Assume that Assumption 6 holds and Assumption 8 holds for $v = -u$. If f is bounded, then $\widehat{E}_{u,MC}$ converges to E_u in probability when N and N_u go to $+\infty$.*

Furthermore, with additional regularity assumptions, we can give the rate of convergence of these estimators in Theorem 4 and Corollary1.

Theorem 4. *Under Assumption 7, for all $\varepsilon > 0$, $\varepsilon' > 0$, there exist fixed constants $C_{\sup}^{(1)}(\varepsilon')$ and $C_{\sup}^{(2)}$ such that*

$$\mathbb{P}\left(\left|\widehat{E}_{u,MC} - E_u\right| > \varepsilon\right) \leq \frac{1}{\varepsilon^2}\left(\frac{C_{\sup}^{(1)}(\varepsilon')}{N^{\frac{1}{p-|u|}-\varepsilon'}} + \frac{C_{\sup}^{(2)}}{N_u}\right). \tag{2.18}$$

Corollary 1. *Under Assumption 7, choosing* $N_u \geq CN^{1/(p-|u|)}$ *for some fixed* $0 < C < +\infty$*, we have for all* $\delta > 0$,

$$\left|\widehat{E}_{u,MC} - E_u\right| = o_p\left(\frac{1}{N^{\frac{1}{2(p-|u|)}-\delta}}\right).$$

We remark that for $|u| = p-1$, we nearly obtain a parametric rate of convergence $N^{\frac{1}{2}}$. The rate of convergence decreases when $|u|$ decreases which can be interpreted by the fact that we estimate non-parametrically the function $x_{-u} \mapsto \mathrm{Var}(f(X)|X_{-u} = x_{-u})$. The estimation problem is higher-dimensional when $|u|$ decreases.

E.1.ii) Pick-and-Freeze

We now give similar results for the Pick-and-Freeze estimators. The number N_I of nearest neighbours that we need for the Pick-and-Freeze estimators is equal to 2. Assume that $\mathrm{E}(Y)$ is known and let $(s(l))_{l\in[1:N_u]}$ be as in Section E.1.i). Then, we define two slightly different versions of the Pick-and-Freeze estimator by

$$\widehat{V}_{u,PF}^{mix} = \frac{1}{N_u}\sum_{l=1}^{N_u} \widehat{V}_{u,s(l),PF}^{mix}, \tag{2.19}$$

and

$$\widehat{V}_{u,PF}^{knn} = \frac{1}{N_u}\sum_{l=1}^{N_u} \widehat{V}_{u,s(l),PF}^{knn}, \tag{2.20}$$

with

$$\widehat{V}_{u,s(l),PF}^{mix} = f\left((X^{(k_N^u(s(l),1))}\right) f\left(X_u^{(k_N^u(s(l),1))}, X_{-u}^{(k_N^u(s(l),2))}\right) - \mathrm{E}(Y)^2 \tag{2.21}$$

and

$$\widehat{V}_{u,s(l),PF}^{knn} = f(X^{(k_N^u(s(l),1))})f(X^{(k_N^u(s(l),2))}) - \mathrm{E}(Y)^2. \tag{2.22}$$

As for the double Monte-Carlo estimators, we give the consistency of the Pick-and-Freeze estimators in Theorem 5 and the rate of convergence in Theorem 6 and in Corollary2. We let $\widehat{V}_{u,PF}$ be given by Equation (2.19) or Equation (2.20).

Theorem 5. *Assume that Assumption 6 holds and Assumption 8 holds for* $v = u$ *and* $N_I = 2$*. If* f *is bounded, then* $\widehat{V}_{u,PF}$ *converges to* V_u *in probability when* N *and* N_u *go to* $+\infty$.

Theorem 6. *Under Assumption 7, if* $|u| = 1$*, for all* $\varepsilon > 0$, $\varepsilon' > 0$,

$$\mathbb{P}\left(\left|\widehat{V}_{u,PF} - V_u\right| > \varepsilon\right) \leq \frac{1}{\varepsilon^2}\left(\frac{C_{\sup}^{(1)}(\varepsilon')}{N^{1-\varepsilon'}} + \frac{C_{\sup}^{(2)}}{N_u}\right), \tag{2.23}$$

and if $|u| > 1$*, for all* $\varepsilon > 0$*,*

$$\mathbb{P}\left(\left|\widehat{V}_{u,PF} - V_u\right| > \varepsilon\right) \leq \frac{C_{\sup}^{(3)}}{\varepsilon^2}\left(\frac{1}{N^{\frac{1}{|u|}}} + \frac{1}{N_u}\right), \tag{2.24}$$

with fixed constants $C_{\sup}^{(1)}(\varepsilon') < +\infty$*,* $C_{\sup}^{(2)} < +\infty$ *and* $C_{\sup}^{(3)} < +\infty$*.*

Corollary 2. *Under Assumption 7, choosing* $N_u \geq CN^{1/|u|}$ *for some fixed* $0 < C < +\infty$*, we have*

1. *for all* u *such that* $|u| = 1$*, for all* $\delta > 0$*,*

$$\left|\widehat{V}_{u,PF} - V_u\right| = o_p\left(\frac{1}{N^{\frac{1}{2}-\delta}}\right).$$

2. *for all* u *such that* $|u| > 1$*,*

$$\left|\widehat{V}_{u,PF} - V_u\right| = O_p\left(\frac{1}{N^{\frac{1}{2|u|}}}\right).$$

The interpretation of the rates of convergence is the same as for the double Monte-Carlo estimators.

E.2 Consistency of the Shapley effect estimators

Now that we have constructed estimators of W_u with an unknown input distribution, we can obtain estimators of the Shapley effects using the subset and random-permutation W-aggregation procedures. Note that for each W-aggregation procedure, we need to choose the accuracy N_u of the $(\widehat{W_u})_{\emptyset\subsetneq u\subsetneq[1:p]}$. Although Assumption 2 does not hold with the estimators $\widehat{E}_{u,MC}$ and $\widehat{V}_{u,PF}$ (the summands of these estimators are not independent), we keep choosing $N_u = N_O = 1$ for the random-permutation W-aggregation procedure and N_u as the closest integer to $N_{tot}\kappa^{-1}\binom{p}{|u|}^{-1}(p-1)^{-1}$ with the subset W-aggregation procedure. To unify notation, let $N_I = 2$ when the estimators of the conditional elements $(W_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$ are the Pick-and-freeze estimators (in this way, N_I is the number of nearest neighbours). With the double Monte-Carlo estimators, let N_I be a fixed integer (for example $N_I = 3$).

Finally, recall that for the random-permutation W-aggregation procedure, we need different estimators $(\widehat{W}_u(m))_{m\in[1:M]} = (\widehat{W}_u(m)^{(1)})_{m\in[1:M]}$ of W_u, with the notation of Assumption 3. In this case, we choose i.i.d. realizations of $\widehat{W}_u$ conditionally to $(X^{(n)})_{n\in[1:N]}$. That is $(\widehat{W}_u(m))_{m\in[1:M]} = \left(\widehat{W}_{u,s(m)}\right)_{m\in[1:M]}$, where $\widehat{W}_{u,s(m)}$ is defined by either Equation (2.16), Equation (2.17), Equation (2.21) or Equation (2.22), and $(s(m))_{m\in[1:M]}$ are independent and uniformly distributed on $[1:N]$. This enables to have different estimators with a small covariance using the same sample $(X^{(n)})_{n\in[1:N]}$. Indeed, to prove the consistency in Proposition 15 of the Shapley effects estimator with the random-permutation procedure, we show that Assumption 5 is satisfied.

Proposition 15. *Assume that Assumption 6 holds and Assumption 8 holds for all subset u, $\emptyset \subsetneq u \subsetneq [1:p]$. If f is bounded, then the estimators of the Shapley effects defined by the random-permutation W-aggregation procedure or the subset W-aggregation procedure combined with $\widehat{W}_u = \widehat{E}_{u,MC}$ (resp. $\widehat{W}_u = \widehat{V}_{u,PF}$) converge to the Shapley effects in probability when N and N_{tot} go to $+\infty$.*

Remark 28. *The Sobol indices are functions of the $(W_u)_{u\subset[1:p]}$. Indeed, we can define the Sobol index of a group of variables X_u by either S_u as in [Cha13, BBDM19] or S_u^{cl} as in [IP19], where*

$$S_u := \frac{1}{\mathrm{Var}(Y)} \sum_{v\subset u} (-1)^{|u|-|v|} V_v, \quad S_u^{cl} := \frac{V_u}{\mathrm{Var}(Y)},$$

and where we note that $V_u = \mathrm{Var}(Y) - E_{-u}$ by the law of total variance. Thus, we get consistent estimators of the Sobol indices in the general setting of Assumption 6. Note that the sum over $u \subset [1:p]$ of the Sobol indices S_u^{cl} is not equal to 1, and when the inputs are dependent, the Sobol index S_u can take negatives values.

E.3 Numerical experiments

In this section, we compute numerically the estimators of the Shapley effects with an unknown input distribution. As in Section D.2, we choose the linear Gaussian framework to compute the theoretical values of the Shapley effects.

We now have 8 consistent estimators given by:

- 2 different W-aggregation procedures: subset or random-permutation;
- 2 different estimators of W_u: double Monte-Carlo or Pick-and-Freeze;
- 2 slightly different versions of the estimators of W_u: "mix" or "knn".

We take the same parameters as in Section D.2. The size N of the observed sample $(X^{(n)})_{n\in[1:N]}$ is 10000. In Figure 2.3, we plot the theoretical values of the Shapley effects, together with the boxplots of the 200 realizations of each estimator, and with a total cost $N_{tot} = 54000$ (we assume here that f is a costly computer code and that for all estimators, the cost is the number of evaluations of f). With these parameters, each realization requires around 6 minutes and 30 seconds to be computed on a personal computer.

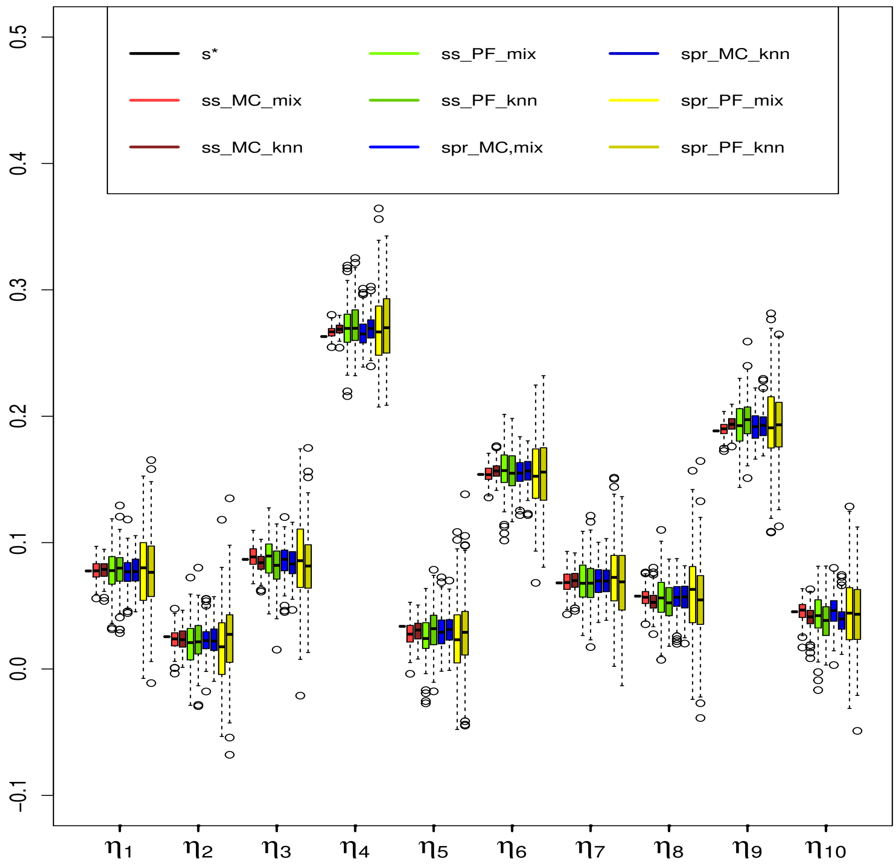


Figure 2.3: Estimation of the Shapley effects in the linear Gaussian framework when we only observe a sample of X. In black (s*) we show the theoretical results, in red the estimates from the subset W-aggregation procedure with the double Monte-Carlo estimator (ss_MC_mix and ss_MC_knn), in green the estimates from the subset W-aggregation procedure with the Pick-and-Freeze estimator (ss_PF_mix and ss_PF_knn), in blue the estimates from the random-permutation W-aggregation procedure with the double Monte-Carlo estimator (spr_MC_mix and spr_MC_knn) and in yellow the estimates from the random-permutation W-aggregation procedure with the Pick-and-Freeze estimator (spr_PF_mix and spr_PF_knn).

Remark 29. *In the linear Gaussian framework, the function f is not bounded and the assumptions of Proposition 15 do not hold. We can thus not guarantee the consistency of the Shapley effects estimators. However, this framework enables*

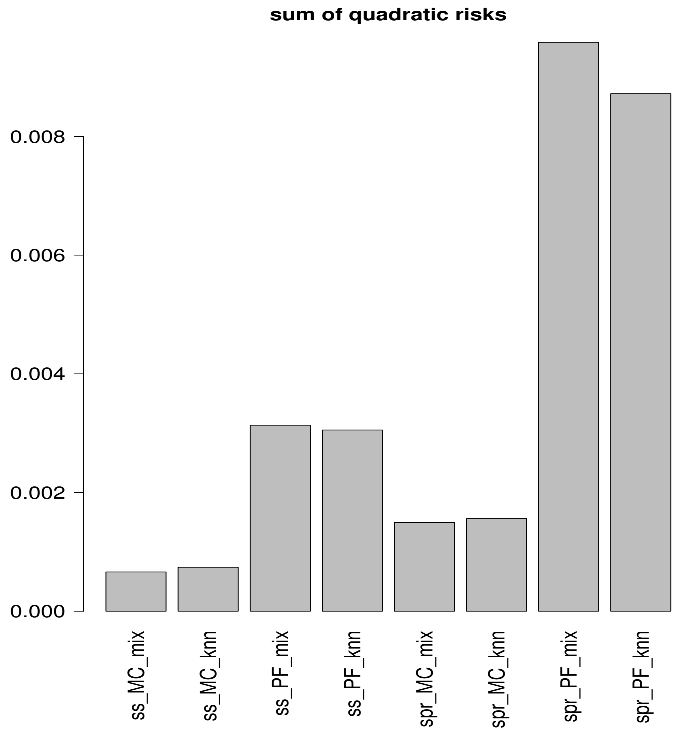


Figure 2.4: Sum over i of the estimated quadratic risks of the eight estimators of the Shapley effects in the linear Gaussian framework when we only observe a sample of X.

to compute the theoretical Shapley effects and we can see numerically that the estimators seem to be consistent.

We show the sums over $i \in [1:p]$ of their quadratic risks (estimated with 200 realizations) in Figure 2.4. As in Section D.2, the subset W-aggregation procedure is better than the random-permutation W-aggregation procedure and double Monte-Carlo is better than Pick-and-Freeze. Furthermore, there are no significant differences between the version "mix" and the version "knn". Recall that, in order to compute the estimators with the "mix" version, we need to call the computer code of f at new inputs whereas "knn" only needs an i.i.d. sample $(X^{(n)}, f(X^{(n)}))_{n\in[1:N]}$.

We now compare the sums over $i \in [1:p]$ of the estimated quadratic risks of the estimators from the subset W-aggregation procedure with double Monte-Carlo when we know the distribution of X (results of Section D.2) and when we just observe a sample of size 10000 (previous results of this section). These values are equal to $5.9\ 10^{-3}$ when we know the distribution of X, to $6.6\ 10^{-3}$ when we only observe the sample with $\widehat{E}_{u,MC}^{mix}$ and to 7.4 10^{-3} when we only observe the sample with $\widehat{E}_{u,MC}^{knn}$. Thus, in this linear Gaussian example in dimension 10, replacing the knowledge of X by a sample of size 10000 does not seem to deteriorate significantly our estimates of the Shapley effects.

F Application to real data

In this section, we apply the estimator of the Shapley effects given by the subset W-aggregation procedure and the double Monte-Carlo estimator $\widehat{E}_{u,MC}^{knn}$ in Equation (2.15) to a real data set. We use the "depSeuil.dat" data, available at `http://www.math.univ-toulouse.fr/~besse/Wikistat/data` from [BMM+07]. This data set contains 10 variables with 1041 sample observations. The variables are:

- JOUR: type of day (holiday: 1, no holiday: 0);
- O3obs: observed ozone concentration;
- MOCAGE: ozone concentration predicted by a fluid mechanics model;
- TEMPE: temperature predicted by the official meteorology service of France;
- RMH2O: humidity ratio;
- NO2: nitrogen dioxide concentration;
- NO: nitrogen oxide concentration;
- STATION: site of observation (5 different sites);
- VentMOD: wind force;
- VentANG: wind direction.

Here, we focus on the ozone concentration O3obs in function of the nine other variables. Hence, let $\tilde{Y}$ be the random variable of the ozone concentration and let X be the random vector containing the nine other random variables. Using the estimator $\widehat{E}_{\emptyset,MC}^{knn}$ of $\mathrm{E}_\emptyset = \mathrm{E}(\mathrm{Var}(\tilde{Y}|X))$ given by Equation (2.15), with $N_I = 3$ and $N_\emptyset = 1000$, we estimate the value of $\mathrm{Var}(\mathrm{E}(\tilde{Y}|X))/\mathrm{Var}(\tilde{Y})$ to 0.57, whereas it would be equal to 1 if $\tilde{Y}$ was a function of X. Thus, it seems that the ozone concentration is not a function of the nine other random variables.

The theory and methodology of this article holds when $\tilde{Y}$ is a deterministic function of X. Hence, we create metamodels of the ozone concentration in function of X, and we write Y the output of the metamodel. In this case, Y is indeed a deterministic function of X and we can compute the Shapley effects, which now quantify the impact of the inputs on the metamodel prediction. In practice, we replace the output column by the fitted values given by the metamodel.

To study the impact of the metamodel on the Shapley effects, we estimate the Shapley effects corresponding to three metamodels:

- XGBoost, from the R package `xgboost`, with optimized parameter by cross-validation;
- generalized linear model (GLM);
- Random Forest, from the R package `randomForest`, which optimizes automatically the parameters by out-of-bag.

Remark 30. *We estimate the value of* $\mathrm{Var}(\mathrm{E}(Y|X))/\mathrm{Var}(Y)$ *to 0.90, 0.93 and 0.90 (see Table 2.1) where* Y *denotes the output of each of the three metamodels XGBoost, GLM and Random Forest respectively. In contrast, the estimated value of* $\mathrm{Var}(\mathrm{E}(\tilde{Y}|X))/\mathrm{Var}(\tilde{Y})$ *is 0.57 when* $\tilde{Y}$ *denotes the original observed ozone concentrations. This shows that the predicted values are different from the initial values of the ozone concentration. Moreover, this shows that the metamodels do not overfit the data, since the estimated values of* $\mathrm{Var}(\mathrm{E}(Y|X))/\mathrm{Var}(Y)$ *are close to 1. Indeed, that means that the fitted values of the ozone concentration are much more explained by* X *and have been smoothed by the metamodels. The values of* $\mathrm{Var}(\mathrm{E}(Y|X))/\mathrm{Var}(Y) = 1 - \mathrm{E}(\mathrm{Var}(Y|X))/\mathrm{Var}(Y)$ *are estimated using the estimator* $\widehat{E}^{knn}_{\emptyset,MC}$ *defined by Equations (2.15) and (2.17) with* $u = \emptyset$ *(that is, the nearest neighbours are chosen with all inputs). Remark that* $\widehat{E}^{knn}_{\emptyset,MC}$ *is essentially a sum of square differences between the images of nearest neighbours through the metamodel. This estimator converges to* 0 *when the number of observations* N *goes to* $+\infty$ *but it is strictly positive for fixed* N *when there are continuous inputs. However, if* $\widehat{E}^{knn}_{\emptyset,MC} > 0$ *significantly, then there exist nearest neighbours such that their images through the metamodel are far from each other, and thus the metamodel is not smooth. Hence, if there is overfitting with the metamodel, the metamodel function will not be smooth, and this can be detected by high values of* $\widehat{E}^{knn}_{\emptyset,MC}$ *and thus by estimated values of* $\mathrm{Var}(\mathrm{E}(Y|X))/\mathrm{Var}(Y)$ *significantly smaller than one.*

In order to assess the quality of the three metamodels, we also give on Table 2.1 the values of the coefficient of determination R^2 *and the estimate of* $\mathrm{Var}(\mathrm{E}(\tilde{Y}|Y))/\mathrm{Var}(\mathrm{E}(\tilde{Y}|X))$*. Remark that, if* $\tilde{Y} = f^*(X) + \varepsilon$*, with* $\varepsilon \perp\!\!\!\perp X$ *and with* $\mathrm{E}(\varepsilon) = 0$*, and if the metamodel is equal to* f^**, then* $\mathrm{E}(\tilde{Y}|X = x) = \mathrm{E}(f^*(x) + \varepsilon)$ *is equal to* $\mathrm{E}(\tilde{Y}|Y = f^*(x))$*. Thus, composing by* X *and taking the variance, we have* $\mathrm{Var}(\mathrm{E}(\tilde{Y}|Y))/\mathrm{Var}(\mathrm{E}(\tilde{Y}|X)) = 1$*. This shows that values of* $\mathrm{Var}(\mathrm{E}(\tilde{Y}|Y))/\mathrm{Var}(\mathrm{E}(\tilde{Y}|X))$ *close to one indicate that the metamodel function is close to* $f^\star$ *and thus indicate*

	XGBoost	GLM	Random Forest
$\mathrm{Var}(\mathrm{E}(Y\|X))/\mathrm{Var}(Y)$	0.90	0.93	0.90
$\mathrm{Var}(\mathrm{E}(\tilde{Y}\|Y))/\mathrm{Var}(\mathrm{E}(\tilde{Y}\|X))$	1.23	0.99	1.05
R^2	0.69	0.54	0.62

Table 2.1: Estimates of three features for the three metamodels.

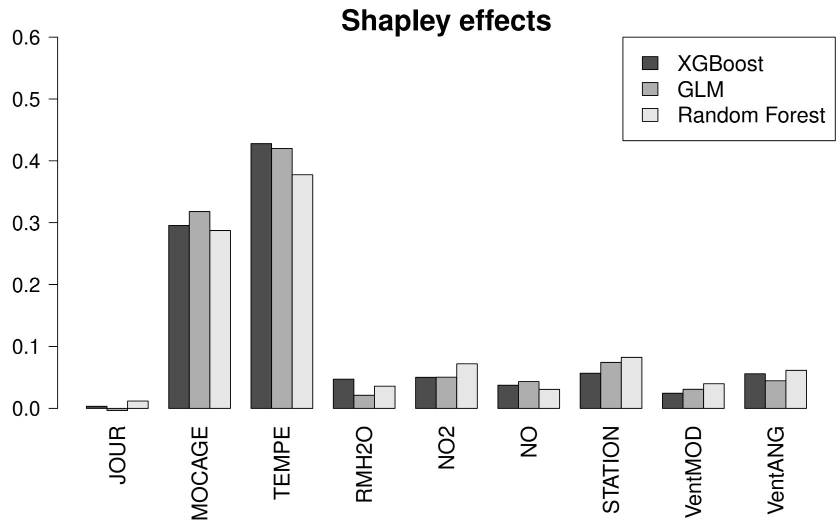


Figure 2.5: Estimation of the Shapley effects for three metamodels: XGBoost, GLM and Random Forest.

a high quality of the metamodel. Hence, one may expect that since the estimated values of $\mathrm{Var}(\mathrm{E}(\tilde{Y}|Y))/\mathrm{Var}(\mathrm{E}(\tilde{Y}|X))$ *are close to one for the three metamodels in our case (see Table 2.1), then these metamodels are of high quality.*

For each metamodel, we estimate the Shapley effects with the subset W-aggregation procedure and the double Monte-Carlo estimator $\widehat{E}_{u,MC}^{knn}$, with $N_I = 3$ and $N_{tot} = 50000$ (but the real cost is actually 40176, see Remark 18). For each metamodel, the computation time of all the Shapley effects on a personal computer is around 5 minutes. The results are presented in Figure 2.5.

We remark that the three metamodels yield similar Shapley effects. This is reassuring, since observing different behaviours of the metamodels would be a sign of inaccuracy for some of them. Only two variables have a significant impact on the ozone concentration: the predicted ozone concentration (MOCAGE) and the predicted temperature (TEMPE). This comforts the results of [BMM+07] as they use regression trees whose two most important variables are the predicted ozone concentration and the predicted temperature. All the other variables have a much smaller impact. The Shapley effect of the predicted temperature is larger than the one of the predicted ozone concentration. It could be from the better accuracy of the predicted temperature (given by the official meteorology service of France) than the predicted ozone concentration (given by a fluid mechanics model). Finally, we remark that the type of the day (holiday or not) has no impact on the ozone concentration. The corresponding Shapley effect is even estimated by a slightly negative value for the GLM, which stems from the small error estimation.

To conclude, the Shapley effect estimator given by the subset W-aggregation procedure and the double Monte-Carlo estimator $\widehat{E}_{u,MC}^{knn}$ enables us to estimate the Shapley effects on real data. The estimator only requires a data frame of the inputs-output and handles heterogeneous data, with some categorical inputs and some continuous inputs. Here, the estimator was applied to a metamodel output. This illustrates the interest of the Shapley effects (and of sensitivity analysis) to understand and interpret the predictions of complex black-box machine learning procedures [RSG16, BGLR18].

This estimator has been implemented in the R package `sensitivity` as the function "shapleySubsetMc".

G Conclusion

In this chapter, we focused on the estimation of the Shapley effects. We explained that this estimation is divided into two parts: the estimation of the conditional elements $(W_u)_{\emptyset \subsetneq u \subsetneq [1:p]}$ and the W-aggregation procedure. We suggested the new subset W-aggregation procedure and we explained how the already existing random-permutation W-aggregation procedure of [SNS16] minimizes the variance. However, the subset W-aggregation procedure is more efficient by using all the estimates of the conditional elements for each Shapley effect estimation. We highlighted this efficiency by numerical experiments. In a second part, we suggested various estimators of $(W_u)_{\emptyset \subsetneq u \subsetneq [1:p]}$ when the input distribution is unknown and when we only observe an i.i.d. sample of the input variables. We proved their consistency and gave the rates of convergence. Then, we used these new estimators to estimate the Shapley effects with consistency. We illustrated the efficiency of these estimators with numerical experiments and we tested one estimator on real heterogeneous data.

Part III

The Shapley effects using the Gaussian linear framework

Chapter 3

The Shapley effects in the Gaussian linear framework

In this chapter, we focus on the computation of the Shapley effects in the Gaussian linear framework for two reasons.

Firstly, [OP17] and [IP19] show that the Shapley effects can be explicitly computed in this framework. It is very convenient when we know the difficulties to estimate the Shapley effects in the general framework (see Chapter 2). Indeed, in Chapter 2 Section E.3, with 10 input variables, we needed around 6.5 minutes to provide quite accurate estimates of the Shapley effects using a sample of size 10000. We will see that, in the Gaussian linear framework with 10 inputs variables, the computation of the Shapley effects is instantaneous.

Secondly, the Gaussian linear framework is widely used to model physical phenomena (see for example [KHF$^+$06, HT11, Ros04]). Indeed, uncertainties are often modelled as Gaussian variables and an unknown function is commonly estimated by its linear approximation. Our collaboration with CEA/DES/ISAS/DM2S, and in particular with Pietro Mosca and Laura Clouvel, helped us to be aware about some needs in research on nuclear safety. Moreover, as explained in Section 4 of [BBCM20], sensitivity analysis is an important tool in the field of calculation codes, e.g. in nuclear safety, evaluating the impact of the input uncertainties to the uncertainty on the output of a computer code, in order to prioritize efforts for uncertainty reduction. Since the international libraries [McL05, JEF13, JEN11] on real data from the field of nuclear safety provide the average and covariance matrix of the input variables, it is natural to model them with the Gaussian distribution. Moreover, [Clo19] highlights linear relations between some physical quantities.

In Section A, we suggest an algorithm to compute the Shapley effects in the Gaussian linear framework. In Section B, we give numerical experiments with an industrial application showed in [MCL$^+$17]. Finally, in Section C, we give a conclusion with an introduction to the rest of Part III. Remark that, in this short chapter, no theoretical result is provide, and it can be seen as an introduction to Part III.

In this chapter, we assume that $X \sim \mathcal{N}(\mu, \Sigma)$, with $\Sigma \in S_p^{++}(\mathbb{R})$, and that $f : x \longmapsto \beta_0 + \beta^T x$, for a fixed $\beta_0 \in \mathbb{R}$ and a fixed vector $\beta \in \mathbb{R}^p$. We can assume without loss of generality that $\mu = 0$ and $\beta_0 = 0$, since the Shapley effects do not depend on these parameters.

A Algorithm

Recall that, in the Gaussian linear framework, the Shapley effects can be computed using

$$\eta_i := \frac{1}{p\mathrm{Var}(Y)} \sum_{u \subset -i} \begin{pmatrix} p-1 \\ |u| \end{pmatrix}^{-1} \left(E_{u \cup \{i\}} - E_u \right). \tag{3.1}$$

and that, for all subset $u \subset [1:p]$, we have

$$E_u = \mathrm{Var}(\beta_u^T X_u | X_{-u}) = \beta_u^T (\Sigma_{u,u} - \Sigma_{u,-u} \Sigma_{-u,-u}^{-1} \Sigma_{-u,u}) \beta_u, \tag{3.2}$$

One issue remains though, namely computing numerically the sum in Equation (3.1). Indeed, we have to sum over all the subsets of $[1:p]$ which do not contain i. We also have to group the subsets u and $u \cup \{i\}$. For this purpose, we suggest to use the following bijective map:

$$h : \begin{array}{ccc} \mathcal{P}([1:p]) & \longrightarrow & [0 : 2^p - 1] \\ u & \longmapsto & \sum_{i \in u} 2^{i-1}. \end{array}$$

We remark that:

$$u \subset -i \Longleftrightarrow \left\lfloor \frac{h(u)}{2^{i-1}} \right\rfloor \equiv 0 \; mod \; 2.$$

Finally, we can see that if $u \subset -i$, then $h(u \cup \{i\}) = h(u) + h(\{i\})$.

Based on this map and Equations (3.1) and (3.2), we suggest an algorithm that we call "LG-Indices" (for Linear Gaussian). This algorithm computes the Shapley effects in the linear Gaussian framework.

Algorithm 2 (LG-Indices)

Inputs: β, Σ.

1. Let $\text{Var}(Y) = \beta^T \Sigma \beta$ and let $\text{Var}(Y|X) = 0$.
2. (Compute the conditional variances) For $j = 0, \cdots, 2^p - 1$, do the following:
   (a) Compute $u = h^{-1}(j)$.
   (b) Compute $E_u := \text{Var}(Y|X_{-u})$ using Equation (3.2).
3. (Compute the Shapley effects) For $i = 1, \cdots, p$, do the following:
   (a) Initialize $\eta = (0, \cdots, 0) \in \mathbb{R}^p$.
   (b) For $k = 0, ..., 2^p - 1$, do the following:
      i. If $\left\lfloor \frac{k}{2^{i-1}} \right\rfloor \equiv 0 \; mod \; 2$, let $u = h^{-1}(k)$ and $u \cup \{i\} = h^{-1}(k + 2^{i-1})$. Then update :

$$\eta_i = \eta_i + \binom{p-1}{|u|}^{-1} \left(E_{u \cup \{i\}} - E_u \right) . \tag{3.3}$$

   (c) Let $\eta_i = \eta_i / (p\text{Var}(Y))$.

Outputs η.

This algorithm has been implemented in the URANIE platform of CEA DEN and we will see in Section C.1 that an improvement of this algorithm has been implemented in the R package `sensitivity`.

B Numerical experiments

B.1 Application on generated data

To position our work with respect to the state of art, we compare the algorithm "LG-Indices" with the existing algorithms designed to compute the Shapley effects for global sensitivity analysis suggested in [SNS16]. However, as we focus on the linear Gaussian framework, for a fair comparison, we adapt the algorithm suggested in [SNS16] to this particular framework replacing the estimations of $(\text{E}(\text{Var}(Y|X_{-u})))_{u \subset [1:p]}$ by their theoretical values given by Equation (3.2). Hence, using the terms of Chapter 2, we compare the algorithm "LG-Indices" with the random-permutation W-aggregation procedure (see Section C.2 of Chapter 2) and with the exact-permutation W-aggregation procedure (see Remark 22 in Section C.2 of Chapter 2) where the conditional elements are computed by Equation (3.2). We call these two algorithms "random-permutation Algorithm" and "exact-permutation Algorithm".

Let us consider a simulated toy example. We generate β by a $\mathcal{N}(0, I_p)$ random variable and Σ by writing $\Sigma = AA^T$, where the coefficients of A are generated independently with a standard normal distribution.

First, we compare "LG-Indices" with exact-permutations Algorithm. Both provide the exact Shapley values but with different computational times. Table 3.1 provides the computation times in seconds for different values of p, the number of input variables.

	$p=6$	$p=7$	$p=8$	$p=9$	$p=10$
exact-permutations	0.11	0.78	7.31	77.6	925
LG-Indices	0.004	0.008	0.018	0.039	0.086

Table 3.1: Computational time (in seconds) for exact-permutations Algorithm and LG-Indices for different values of p.

We remark that "LG-indices" is much faster than exact-permutations Algorithm.

We can also compare "LG-Indices" with random-permutations Algorithm. For the latter, we choose M, the number of permutations generated in random-permutations Algorithm, so that the computational time is the same as LG-Indices. Yet, while our algorithm gives the exact Shapley effects, the random-permutations Algorithm provides an estimation of them. Hence, the performance of the latter algorithm is evaluated by computing the coefficients of variation in %, for different values of p. We give in Table 3.2 the average of the p coefficients of variations. We recall that the coefficient of variation corresponds to the ratio of the standard deviation over the mean value. We see that the random-permutation Algorithm has quite large coefficients of variation when we choose M so that the computational time is the same as our algorithm. However, this variation decreases with the number of inputs p. We can explain that by saying that the computational time of LG-Indices is exponential with p. So, we can see that the precision of random-permutations Algorithm increases with M.

	$p=3$	$p=4$	$p=5$	$p=6$	$p=7$
M chosen	10	12	18	30	50
mean of coefficients of variation	31%	26%	22%	18%	13%

Table 3.2: Mean of the coefficients of variation of Shapley effects estimated by random-permutations Algorithm for the same computational time as LG-Indices.

B.2 Application on nuclear data

We present here an industrial application related to safety studies of pressurized water reactors (PWR) detailed in [Clo19] (Chapter V, Section 3.2.2). Here, the quantity of interest Y is the neutron fluence in a hot spot used to monitor the effects of irradiation on the vessel of a PWR. The quality of radiation damage prediction depends in part on the fast neutron flux. The objective is to identify the parameters which could, with a better knowledge, reduce the uncertainty of the fast neutron flux.

Here, we focus on the propagation of the uncertainty of the released power of ^{235}U from 24 different locations in the PWR (see Figure V.17 of [Clo19] for the names of the different locations). As mentioned above, the Gaussian linear framework is a favorable setting.

We present in Figure 3.1 the Shapley effects computed by Algorithm 2 on a linear model of the neutron fluence in function of the released power of ^{235}U from 24 different locations. As pointed out by [Clo19], the peripheral locations (A9, A8) that are closest to the hot spot, are those with the highest Shapley effects. Here, the Shapley effects in dimension 24 have been computed in 8 hours.

C Conclusion and preamble to the other chapters of Part III

We have seen that the Gaussian linear framework is very convenient to compute the Shapley effects. We gave an algorithm that compute the exact values of the Shapley effects. Hence, in the rest of Part III, we develop these works on the Gaussian linear framework.

Chapter 4 deals with the computation cost when the number of input variables p is larger than 30, using block-diagonal structures of the covariance matrix. The setting of Chapter 4 is wider than the Gaussian linear framework with block-diagonal covariances but concludes by giving Algorithm 3, with an improvement of Algorithm 2 in this particular setting. We give an industrial application on real data from the field of nuclear safety that can only be treated by Algorithm 3.

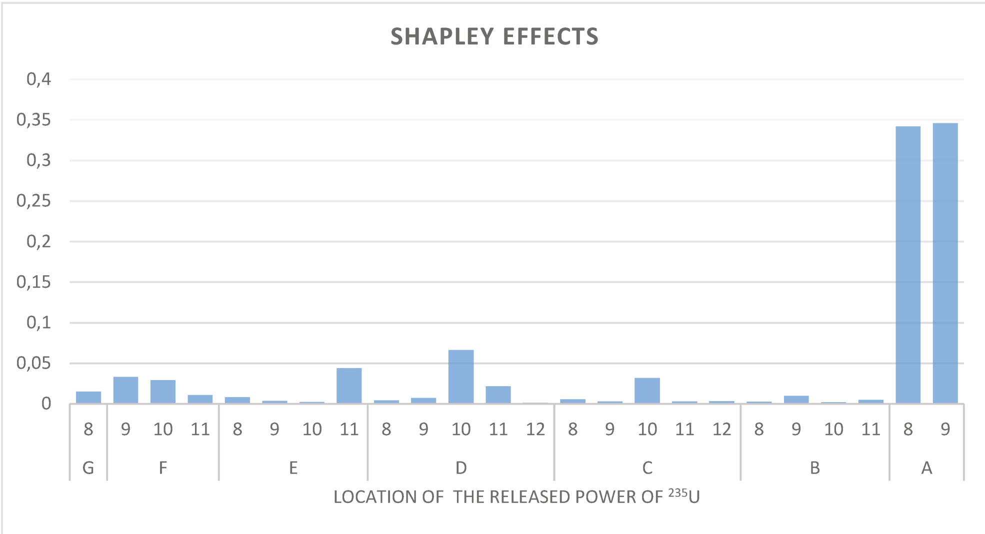


Figure 3.1: Shapley effects of the neutron fluence in the hot spot in function of the released power of ${}^{235}U$ from 24 different locations in the PWR.

Chapter 5 extends the framework of Algorithm 3 to the case where the parameters of the Gaussian distribution and of the linear model are unknown and we only observe an i.i.d. sample of the inputs-output, with a focus on the high dimension.

Finally, Chapter 6 aims to understand the impact on the Shapley effects of estimating a general setting by the Gaussian linear framework, since it is more convenient for the Shapley effects computation.

Chapter 4

Shapley effects and Sobol indices for independent groups of variables

A A high-dimensional problem

Despite the analytical formula from Equation (1.26), the computational cost of the Shapley effects in the Gaussian linear framework remains an issue when the number of input variables p is too large. Based on an implementation in the R software, Algorithm 2 provides almost instantaneous results for $p \leq 15$, but becomes impracticable for $p \geq 30$. Indeed, we have to compute and to store 2^p values, namely the $(E_u)_{u \subset [1:p]}$, and this can be a significant issue.

Fortunately, when p is large, it can frequently be the case that there are independent groups of random variables. That is, after a permutation of the variables, the covariance matrix Σ is a block-diagonal matrix. We show that, in this case, this high dimensional computational problem boils down to a collection of lower dimensional problems.

In the following, we give theoretical results in the general case, and not only for Gaussian linear models. Then, we focus on these results in the particular case of the Gaussian linear models.

B Sensitivity indices with independent groups of variables

B.1 Notations for the independent groups for general models

Let $B = \{B_1, ..., B_K\}$ be a partition of $[1 : p]$ such that the groups of random variables $(X_{B_j})_{j\in[1:K]}$ are independent. Let $A_j := X_{B_j}$. Let us write

$$Y = f(X_1, ..., X_p) = g(A_1, ..., A_K).$$

Is $w \subset [1 : K]$, we define

$$V_w^g := \mathrm{Var}(\mathrm{E}(Y|A_w)).$$

As the inputs $(A_1, ...A_K)$ are independent, the Hoeffding decomposition (see Proposition 1 of Chapter 1) of g is given by:

$$g(A) = \sum_{w\subset[1:K]} g_w(A_w). \tag{4.1}$$

Similarly to Definition 4 and Equation (1.8) in Chapter 1, the Sobol indices of g are given by

$$S_w^g := \frac{\mathrm{Var}(g_w(A_w))}{\mathrm{Var}(Y)} = \frac{1}{\mathrm{Var}(Y)} \sum_{z\subset w} (-1)^{|w|-|z|} V_z^g. \tag{4.2}$$

Remark 31. *As the inputs $(A_1, ..., A_K)$ are independent, the Sobol index S_w^g of g is the variance of g_w divided by $\mathrm{Var}(Y)$ and so is non-negative. Moreover, we can estimate it without trouble because the quantities $(V_z^g)_{z\subset w}$ are easy to estimate (using the Pick-and-Freeze estimators for example).*

We also define

$$V_u^{g,w} := \mathrm{Var}(\mathrm{E}(g_w(A_w)|X_u)).$$

Writing $B_w := \bigcup_{j\in w} B_j$, we have $V_u^{g,w} = V_{u\cap B_w}^{g,w}$. If $u \subset B_w$, let $S_u^{g,w}$ be the Sobol index of X_u on g_w:

$$S_u^{g,w} := \frac{1}{\mathrm{Var}(g_w(A_w))} \sum_{v\subset u} (-1)^{|u|-|v|} V_v^{g,w}.$$

Equivalently, if $i \in B_w$, let $\eta_i^{g,w}$ be the Shapley effect of X_i on g_w:

$$\eta_i^{g,w} = \frac{1}{|B_w|\mathrm{Var}(g_w(A_w))} \sum_{u\subset B_w\setminus\{i\}} \binom{|B_w|-1}{|u|}^{-1} (V_{u\cup i}^{g,w} - V_u^{g,w}). \tag{4.3}$$

Finally, for all $i \in [1 : p]$, let $j(i) \in [1 : K]$ be the index such that $i \in B_{j(i)}$.

B.2 Main results for general models

We will study the Sobol indices and the Shapley effects in the case of block-independent variables. First, we show a proposition about the $(V_u)_{u\subset[1:p]}$.

Proposition 16. *For all $u \subset [1:p]$, we have:*

$$V_u = \sum_{w\subset[1:K]} V^{g,w}_{u\cap B_w}. \tag{4.4}$$

Dividing by the variance of Y, we can deduce directly an identical decomposition for the closed Sobol indices defined by Equation (1.1).
We then provide a consequence of Proposition 16 on Sobol indices:

Proposition 17. *For all $u \subset [1:p]$, we have:*

$$S_u = \sum_{\substack{w\subset[1:K],\\ s.t.\ u\subset B_w}} S^g_w S^{g,w}_u. \tag{4.5}$$

Proposition 17 improves the interpretation of the Sobol indices. It states that the Sobol indices for the output Y are linear combinations of the Sobol indices when considering the outputs $g_w(A_w)$ and that the weighting coefficients are the S^g_w.

This proposition can be beneficial for the estimation of the Sobol indices. We could estimate the coefficients S^g_w by Pick-and-Freeze. If many of them are close to 0, the corresponding Sobol indices $S^{g,w}_u$ are irrelevant for the total output Y, and it is unnecessary to estimate them.

We also provide a consequence of Proposition 16 on Shapley effects:

Proposition 18. *For all $i \in [1:p]$, we have*

$$\eta_i = \sum_{\substack{w\subset[1:K],\\ s.t.\ j(i)\in w}} S^g_w \eta^{g,w}_i. \tag{4.6}$$

As for the Sobol indices, Proposition 18 provides the computation of the Shapley effects for the output Y by summing the Shapley effects when considering the outputs $g_w(A_w)$ and multiplying them by the coefficient S^g_w.

B.3 Main results for block-additive models

B.3.i) Theoretical results

In the following, we detail the consequences of Propositions 17 and 18 to the particular case of a block-additive model:

$$Y = \sum_{j=1}^{K} g_j(A_j), \tag{4.7}$$

i.e. when the functions $(g_w)_{w\subset[1:K]}$ of the Hoeffding decomposition are equal to 0 except for w equal to a singleton.

Corollary 3. *If the model is block-additive, for all u such that $u \not\subset B_j$ for all j, we have $S_u = 0$.*

This corollary states that the majority of Sobol indices for block additive models a equal to zero. It remains only $\sum_{j=1}^{K} 2^{B_j} - 1$ unknown non-zero Sobol indices instead of $2^p - 1$.

Corollary 4. *For block-additive models, we have*

$$\eta_i = S^g_{j(i)}\eta_i^{g,j(i)}. \tag{4.8}$$

For example, if we apply this corollary in the case where X_i is the only variable in its group, then we have $\eta_i = S_i$.
To compute the Shapley effect η_i in block additive models, the previous corollary reduces the sum from all the subsets of $[1:p]\setminus\{i\}$ to all the subset of $B_{j(i)}\setminus\{i\}$. Then, the computational gain is the same as in Corollary 3.

C Linear Gaussian framework with independent groups of variables

C.1 Algorithm "LG-GroupsIndices"

As we explained in Section A, the computation of the Shapley effects in the Gaussian linear framework appears impracticable when the dimension p is large. However, when there are independent groups of variables, Corollaries 3 and 4 show that this high dimensional computational problem boils down to a collection of lower dimensional problems.

In this framework, we have seen in Corollaries 3 and 4 that we only have to calculate the $\sum_{j=1}^{k} 2^{|B_j|}$ values $\{\mathrm{Var}(Y|X_u),\ u\subset B_j,\ j\in[1:K]\}$ instead of all the 2^p values $\{\mathrm{Var}(Y|X_u),\ u\subset[1:p]\}$. We detail this idea in the algorithm "LG-GroupsIndices".

Algorithm 3 (LG-GroupsIndices)

Inputs: β, Σ.

1. By Breath-First-Search (BFS), let $B_1,...,B_K$ be the independent groups of variables.

2. Let η be a vector of size p.

3. For $j = 1, ..., K$, do the following:

   (a) Let $\tilde{\eta} \in \mathbb{R}^{|B_j|}$ be the output of the algorithm LG-Indices with the inputs β_{B_j} and Σ_{B_j,B_j}.

   (b) Let

$$\eta_{B_j} = \frac{\beta_{B_j}^T \Sigma_{B_j,B_j} \beta_{B_j}}{\beta^T \Sigma \beta^T} \tilde{\eta}.$$

Ouputs: η.

This algorithm has been implemented in the R package `sensitivity` as the function "ShapleyLinearGaussian".

The complexity of the computation of the Shapley effects is $O(K2^m)$, where K denotes the number of groups and m denotes the size of the maximal group. Note that the complexity of BFS is $O(pm^2)$.
To find the independent groups of variables by BFS (see for example [Ski98], section 5.7.1), one can for example use the function "graph_from_adjacency_matrix" of the R package `igraph`[CN06].

C.2 Numerical experiments

With independent groups of inputs, to the best of our knowledge, LG-GroupsIndices is the only algorithm which can compute the exact Shapley effects for large values of p (the number of inputs). Indeed, random-permutations Algorithm can handle large values of p but always computes estimations of Shapley effects. On the other hand, LG-Indices computes exact Shapley effects but becomes too costly for $p \geq 20$ (the computation time is exponential in p).

First, we compare the computation time of LG-Indices and LG-GroupsIndices for low values of p on a toy simulated example as in Section B of Chapter 3. We generate K independent groups of m variables (with the same size). We give these results in Table 4.1.

Now, we compare LG-GroupsIndices with random-permutations Algorithm as in Section B of Chapter 3: we choose M so that the computational time is the same and we give the average c of the p coefficients of variation of random-permutations Algorithm in Table 4.2.

Here, the mean of the coefficients of variation remains quite large (around 35%) when we chose $K = m$. However, when we choose K larger (resp. lower) than m, this variation increases (resp. decreases).

	$K=3$ $m=3$	$K=4$ $m=3$	$K=4$ $m=4$	$K=5$ $m=4$
LG-Indices	0.04	0.47	8.45	168.03
LG-GroupsIndices	0.002	0.003	0.004	0.007

Table 4.1: Computation time (in seconds) for LG-Indices and LG-GroupsIndices for different values of K and m.

	$K=3$ $m=3$	$K=4$ $m=4$	$K=5$ $m=5$	$K=6$ $m=6$	$K=10$ $m=5$	$K=5$ $m=10$
M chosen	7	8	9	10	5	98
c	34%	38%	34%	36%	40%	12%

Table 4.2: Mean of the coefficients of variation c of Shapley effects estimated by random-permutations Algorithm for the same computational time as LG-GroupsIndices.

C.3 Application on nuclear data

We could apply Algorithm 3 to nuclear data thanks to our collaboration with Laura Clouvel, from CEA/DES/ISAS/DM2S/SERMA.

In this application, the output is the neutron flux Y which is a quantity of interest in safety nuclear reactor studies. For example, it can be calculated to evaluate the vessel neutron irradiation which is in fact one of the limiting factors for pressurized water reactor (PWR) lifetime (see Chapter 3 Section B.2).

As in the previous nuclear application, the cross sections are the inputs X of our model. The values of the cross sections and their uncertainties are provided by international libraries as the American Library ENDF/B-VII [McL05], the European library JEFF-3 [JEF13], and the Japan Library JENDL-4 [JEN11]. Using the standardized format, each cross section is defined for an isotope iso of the target nuclei, an energy level E of the target nuclei and a reaction number mt (see [McL05] for more information on mt numbers).

We assume that if $(iso, mt) \neq (iso', mt')$, then, $X_{(iso,mt,E)} \perp\!\!\!\perp X_{(iso',mt',E')}$ for any E, E'. Thus, the covariance Σ is block-diagonal, where each block corresponds to a value of (iso, mt). Here, we have 292 input variables divided in 50 groups of size between 2 and 18. Using reference data, [Clo19] has shown that the perturbation of the cross sections of the ^{56}Fe, ^{1}H, ^{16}O isotopes are linearly related to the

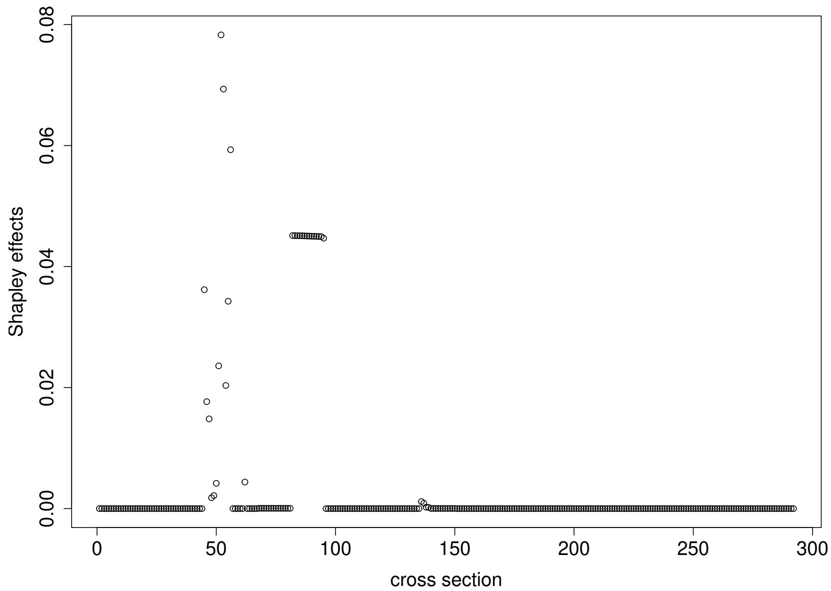


Figure 4.1: Shapley effects of all the cross sections.

perturbation of the flux:

$$Y = \sum_{j \in \{(iso,mt,E)\}} \beta_j X_j. \tag{4.9}$$

Thus, the Shapley effects are easily computable using Algorithm 3. We show the values of the Shapley effects in Figure 4.1.

We can remark that almost all the Shapley effects are close to 0. Now, we plot all the Shapley effects that are larger than 1% on Figure 4.2 with the names of the corresponding cross sections. For example, "Fe56_S4_950050" means the cross section for the isotope ^{56}Fe, the reaction scattering 4 and a level of energy larger than $950050 eV$ (and smaller than $1353400 eV$).

We remark than only 23 cross sections have a Shapley effect larger than 1%. The latter are associated with the lower energies (around 1 to 6 MeV). Moreover, they all come from three different groups of (iso, mt): (^{56}Fe, scattering 4), (^{56}Fe, scattering 2) and (^{1}H, scattering 2).

We can notice that all the Shapley effects of the cross sections from (^{1}H, scattering 2) are close, and that comes from the fact that the correlations between these different levels of energy are close to 1 in this group. We can find in [BBCM20] a physical interpretation of these Shapley effects which is insightful and consistent with the available expert knowledge.

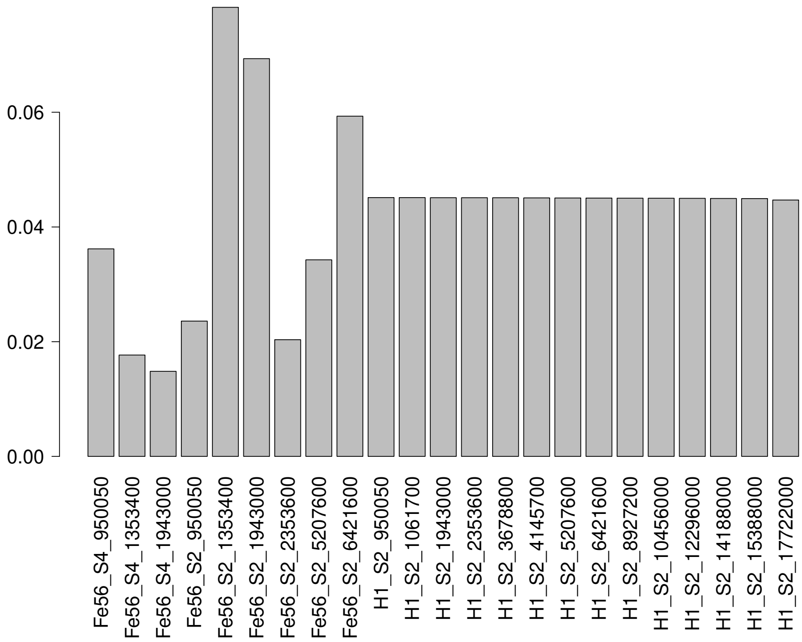


Figure 4.2: Shapley effects larger than 1%.

D Conclusion

In Chapter 4, we gave new theoretical results about the variance-based sensitivity indices for independent groups of inputs. These results drastically reduce the computational cost of these indices when the model is block-additive. Then, we applied these results to the linear Gaussian framework and we suggested an algorithm that computes efficiently the Shapley effects for a block diagonal covariance matrix. Numerical experiments on Shapley effects computations highlight this efficiency and the benefit compared to existing methods.

Chapter 5

Estimation of the Shapley effects in the Gaussian linear framework with unknown parameters

A Introduction

In Chapter 4, we have seen Algorithm 3 which computes the Shapley effects in the Gaussian linear framework for large values of p when the block-diagonal covariance matrix Σ and the linear model β are available. However, in many cases, these parameters are unknown, and we only observe a sample of the inputs-output. In this setting, the Shapley effects need to be estimated, replacing the true vector β by its estimation and the theoretical covariance matrix Σ by an estimated covariance matrix.

There exists a fair amount of work on high-dimensional covariance matrix estimation. Many researchers took an interest in the empirical covariance matrix in high dimension [MP67, Wac78, Sil85, BS10a]. For particular covariance matrices, different estimators than the empirical covariance matrix can be preferred. For some well-conditioned families of covariance matrices, [BL08] suggests a banded version of the empirical covariance matrix, and several works address the problem of estimating a sparse covariance matrix [HLPL06, LF09, EK08].

However, in general, given a high-dimensional covariance matrix, we have seen that the computation cost of the corresponding Shapley effects using Algorithm 2 or Algorithm 3 grows exponentially with the dimension. The only setting where a procedure to compute the Shapley effects with a non-exponential cost is the setting of block-diagonal matrices, using Algorithm 3. Hence, in high dimension, block-diagonal covariance matrices are a very favorable setting for the estimation of the Shapley effects. Thus, we focus on the estimation of high-dimensional block-diagonal covariance matrices. In contrast, we remark that the above methods are not relevant for the estimation of the Shapley effects, since they do not provide block-diagonal matrices.

In our framework, we assume that the true covariance matrix is block-diagonal and we want to estimate this matrix with a similar structure to compute the deduced Shapley effects. Some works address the block-diagonal estimation of covariance matrices. [PDLL18] gives a numerical procedure to estimate such covariance matrices and [HSNP15] suggests a test to verify the independence of the blocks. A block-diagonal estimator of the covariance matrix is proposed in [DG18]. The authors of [DG18] choose a more general framework, without assuming that the true covariance matrix is block-diagonal. They obtain the estimated block-diagonal structure by thresholding the empirical correlation matrix. They also give theoretical guaranties by bounding the average of the squared Hellinger distance between the estimated probability density function and the true one. This bound depends on the dimension p and the sample size n. When p/n converges to some constant $y \in]0,1[$, this bound is larger than 1 and is no longer relevant as the Hellinger distance is always smaller than 1.

Here, we focus on the high dimension setting, when p/n converges to some constant $y \in]0,1[$, and when the true covariance matrix is assumed to be block-diagonal. We give different estimators of the block-diagonal structure and we show that their complexity is small. Then, we provide new asymptotic results for these estimators. Under mild conditions, we show that the estimators of the block structure are equal to the true block structure, with probability converging to one. Furthermore, the square Frobenius distance between the estimated covariance matrices and the true one, normalized by p, converges to zero at rate $1/n$. Thus, our work complements the one of [DG18]. We also study the fixed-dimensional setting, where we show that one of our suggested estimators is asymptotically efficient.

From the estimated block-diagonal covariance matrices, we deduce estimators of the Shapley effects in the high dimensional linear Gaussian framework, with reduced computational cost. We recall that in high dimension, the computation of the Shapley effects requires that the corresponding covariance matrix be block-diagonal. We show that the relative estimation error of these estimators goes to zero at the parametric rate $1/n^{1/2}$, up to a logarithm factor, even if the linear model is estimated from noisy observations.

Our convergence results are confirmed by numerical experiments.We also apply our algorithm to semi-generated data from nuclear applications.

B Estimation of block-diagonal covariance matrices

B.1 Problem and notation

We assume that we observe $(X^{(l)})_{l\in[1:n]}$, an i.i.d. sample with distribution $\mathcal{N}(\mu,\Sigma)$, where $\mu\in\mathbb{R}^p$ and Σ are not known. We assume that $\Sigma=(\sigma_{ij})_{i,j\in[1:p]}\in S_p^{++}(\mathbb{R})$ and has a block-diagonal decomposition. To be more precise on this block-diagonal decomposition, we need to introduce some notation.

Let us write $\mathcal{P}_p$ the set of all the partitions of $[1:p]$. We endow the set $\mathcal{P}_p$ with the following partial order. If $B,B'\in\mathcal{P}_p$, we say that B is finer than B', and we write $B\leq B'$, if for all $A\in B'$, there exists $A_1,...,A_i\in B$ such that $A=\bigsqcup_{j=1}^i A_j$. We also compare the elements of a partition $B\in\mathcal{P}_p$ with their smallest element; that enables us to talk about "the k-th element" of B. If $B\in\mathcal{P}_p$ and $a_1,...,a_i\in[1:p]$, we write $(a_1,...,a_i)\in B$ if there exists $A\in B$ such that $\{a_1,...,a_i\}\subset A$ (in other words, if $a_1,...,a_i$ are in the same group of B). If $\Gamma\in S_p^{++}(\mathbb{R})$ with $\Gamma=(\gamma_{ij})_{i,j\in[1:p]}$ and if $B\in\mathcal{P}_p$, we define Γ_B by

$$(\Gamma_B)_{i,j}=\begin{cases}\gamma_{ij} & \text{if } (i,j)\in B\\ 0 & \text{otherwise.}\end{cases}$$

Let us define

$$S_p^{++}(\mathbb{R},B):=\{\Gamma\in S_p^{++}(\mathbb{R})\mid \Gamma=\Gamma_B,\ \text{and}\ \forall B'<B,\ \Gamma\neq\Gamma_{B'}\},$$

where we define $B'<B$ if $B'\leq B$ and if $B'\neq B$. Thus $S_p^{++}(\mathbb{R})=\bigsqcup_{B\in\mathcal{P}_p}S_p^{++}(\mathbb{R},B)$ and for all $\Gamma\in S_p^{++}(\mathbb{R})$, we can define an unique $B(\Gamma)\in\mathcal{P}_p$ such that $\Gamma\in S_p^{++}(\mathbb{R},B(\Gamma))$. Here, we assume that $\Sigma\in S_p^{++}(\mathbb{R},B^*)$, i.e. B^* is the finest decomposition of Σ, i.e. $B(\Sigma)=B^*$. We say that Σ has a block-diagonal decomposition B^*.

We also write

$$\overline{X}_n:=\frac{1}{n}\sum_{l=1}^n X^{(l)},$$

and

$$S_n:=\frac{1}{n}\sum_{l=1}^n(X^{(l)}-\overline{X}_n)(X^{(l)}-\overline{X}_n)^T,$$

which are the empirical estimators of μ and Σ. To simplify notation, we write $\overline{X}$ for $\overline{X}_n$ and S for S_n (the dependency on n is implicit). We know that, for all $\Gamma \in S_p^{++}(\mathbb{R})$, $\overline{X}$ maximizes the likelihood $L_{\Gamma,m}(X^{(1)},...,X^{(n)})$ over the mean parameter m, where

$$L_{\Gamma,m}(X^{(1)},...,X^{(n)}) := \frac{1}{(2\pi)^{\frac{n}{2}}|\Gamma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}\sum_{l=1}^{n}(X^{(l)}-m)^T\Gamma^{-1}(X^{(l)}-m)\right),$$

and $|\Gamma|$ is the determinant of Γ. Thus, for all $\Gamma \in S_p^{++}(\mathbb{R})$, we define

$$l_\Gamma := -\frac{2}{p}\log\left(L_{\Gamma,\overline{X}}(X^{(1)},...,X^{(n)})\right) - \frac{n}{p}\log(2\pi) = \frac{1}{p}\left(\log|\Gamma| + \mathrm{Tr}(\Gamma^{-1}S)\right).$$

As we assume that the true covariance matrix is block-diagonal, we consider a block-diagonal promoting penalization of the form

$$\mathrm{pen}(\Gamma) := \mathrm{pen}(B(\Gamma)) := \sum_{k=1}^{K} p_k^2,$$

if $B(\Gamma) = \{B_1, ..., B_K\}$ and $|B_k| = p_k$ for all $k \in [1:K]$. We consider the penalized log-likelihood criterion

$$\Phi : \begin{array}{ccc} S_p^{++}(\mathbb{R}) & \longrightarrow & \mathbb{R} \\ \Gamma & \longmapsto & l_\Gamma + \kappa\,\mathrm{pen}(\Gamma), \end{array}$$

where $\kappa \geq 0$. In this work, we suggest to estimate Σ by the minimizer of Φ, for some choice of penalisation κ. First, we show in Proposition 19 that a minimizer of Φ can only be a block-diagonal decomposition of S.

Proposition 19. *If Γ is a minimizer of Φ, then, there exists $B \in \mathcal{P}_p$ such that $\Gamma = S_B$.*

Hence, the minimization problem on $S_p^{++}(\mathbb{R})$ becomes a minimization problem on the finite set $\{S_B,\ B \in \mathcal{P}_p\}$. So, we define $\Psi(B) := \Phi(S_B)$ and we suggest to estimate B^* by

$$\widehat{B}_{tot} := \arg\min_{B\in\mathcal{P}_p} \Psi(B), \tag{5.1}$$

as the minimum structure of the penalized log-likelihood. In Section B, we study theoretically this estimator of B^*. However, it is unimplementable in high dimension since the number of partitions $B \in \mathcal{P}_p$ is too large. Hence, we will also define other estimators less costly, and study them theoretically.

B.2 Convergence in high dimension

B.2.i) Assumptions

In Section B.2, we assume that p and n go to infinity. The true covariance matrix Σ is not constant and depends on n (or p). Nevertheless, to simplify notation, we do not write the dependency on n. In all Section B.2, we choose a penalisation coefficient $\kappa = \frac{1}{pn^\delta}$ for a fixed $\delta \in]1/2, 1[$.

We also add the following assumptions on Σ along Section B.2.

Condition 1. $p/n \longrightarrow y \in]0, 1[$.

Condition 2. *There exist* $\lambda_{\inf} > 0$ *and* $\lambda_{\sup} < +\infty$ *such that, for all* n*, the eigenvalues of* Σ *are in* $[\lambda_{\inf}, \lambda_{\sup}]$.

Condition 3. *There exists* $m \in \mathbb{N}^*$ *such that for all* n*, all the blocks of* Σ *are smaller than* m*, i.e.* $\forall A \in B^*$*, we have* $|A| \leq m$.

For a $q \times q$ matrix $M = (m_{ij})_{(i,j)\in[1:q]^2}$, we let $\|M\|_{\max} = \max_{(i,j)\in[1:q]^2} |m_{ij}|$.

Condition 4. *There exists* $a > 0$ *such that for all* n *and for all* $B < B^*$*, we have* $\|\Sigma_B - \Sigma\|_{\max} \geq an^{-1/4}$.

These four mild assumptions are discussed in Section B.2.iv). However, we also focus on the case when Condition 4 does not hold. We will provide similar results, both when assuming Conditions 1 to 4, and when only Conditions 1, 2 and 3 hold.

B.2.ii) Convergence of $\widehat{B}_{tot}$ and reduction of the cost

Now that we have defined our estimator $\widehat{B}_{tot}$ of the true decomposition B^* in Equation (5.1) and we have added assumptions in Section B.2.i), we give the convergence of $\widehat{B}_{tot}$ in Proposition 20. Although $\widehat{B}_{tot}$ is not computable in practice, its convergence remains interesting to strengthen the choice of the penalized likelihood criterion and will be useful to prove the convergence of more practical estimators. In Section B.2, all the limits statements are given as $n, p \to +\infty$.

Proposition 20. *Under Conditions 1 to 4 and for a fixed* $\delta \in]1/2, 1[$*, we have*

$$\mathbb{P}\left(\widehat{B}_{tot} = B^*\right) \longrightarrow 1.$$

Hence, under Conditions 1 to 4, the estimator $\widehat{B}_{tot}$ is equal to the true decomposition B^* with probability which goes to one. When Condition 4 does not hold, we can not state such a convergence result but we get a weaker result in Proposition 21. In this case, we need to define $B(\alpha)$ as the partition given by thresholding Σ by $n^{-\alpha}$. In other words, $B(\alpha)$ is the smallest (or finest) partition B such that $\|\Sigma_B - \Sigma\|_{\max} \leq n^{-\alpha}$.

Proposition 21. *Under Conditions 1, 2 and 3, for all $\alpha_1 < \delta/2$ and $\alpha_2 > \delta/2$, we have*

$$\mathbb{P}\left(B(\alpha_1) \not> \widehat{B}_{tot} \leq B(\alpha_2)\right) \longrightarrow 1,$$

where $B(\alpha_1) \not> \widehat{B}_{tot}$ means "the partition $B(\alpha_1)$ is not strictly greater (in the sense given in Section B.1) than $\widehat{B}_{tot}$".

Thus, we defined a consistent estimator of B^* that theoretically solves our problem of the lack of knowledge of the true decomposition B^*. However, computing $\widehat{B}_{tot}$ is very costly in practice. Indeed, the number of partitions of $[1:p]$ (the Bell number) is exponential in p. As in [DG18], we suggest to restrict our estimates of B^* to the partitions given by thresholding the empirical correlation matrix $\widehat{C} := (\widehat{C}_{ij})_{i,j\in[1:p]}$ where $\widehat{C}_{ij} := s_{ij}/\sqrt{s_{ii}s_{jj}}$, with $S = (s_{ij})_{(i,j)\in[1:p]^2}$. If $\lambda \in [0,1]$, let B_λ be the finest partition of the thresholded empirical correlation matrix $\widehat{C}_\lambda := (\widehat{C}_{ij}\mathbb{1}_{|\widehat{C}_{i,j}|>\lambda})_{i,j\leq p}$. In other words, $B_\lambda := B(\widehat{C}_\lambda)$. For some value $\lambda \in [0,1]$, B_λ can be found by "Breath-First-Search" (BFS) [Lee61]. Furthermore, we do not need to compute B_λ for all $\lambda \in [0,1]$ and we suggest in the following three different choices of grids for λ.

First, we suggest the grid $A_{\widehat{C}} := \{|\widehat{C}_{ij}| \mid 1 \leq i < j \leq p\}$ and we define the estimator $\widehat{B}_{\widehat{C}} := \underset{B_\lambda \mid \lambda\in A_{\widehat{C}}}{\arg\min}\, \Psi(B)$. This grid is the finest one because that gives all the partitions $\{B_\lambda \mid \lambda \in]0,1[\}$. Almost surely, the coefficients $(\widehat{C}_{ij})_{i<j}$ are all different. Thus, when we increase the threshold to the next value of $A_{\widehat{C}}$, we only remove two symmetric coefficients from the empirical correlation matrix.

Proposition 22. *The computational complexity of $\widehat{B}_{\widehat{C}}$ is $O(p^4)$.*

Using the rate of convergence of the estimated covariances and by Condition 4, we then suggest the estimator $\widehat{B}_\lambda := B_{n^{-1/3}}$, the partition of the empirical correlation matrix thresholded by $n^{-1/3}$. With this threshold, we can not find all the partitions given by thresholded correlation matrix, but we only have to threshold by only one value.

Proposition 23. *The computational complexity of $\widehat{B}_\lambda$ is $O(p^2)$.*

One can see that reducing the grid of thresholds to one value reduces the complexity of the estimator of B^*. Finally, we suggest a third grid, in the case where the maximal size of the groups m is known.

Let $A_s := \{s/p, (s+1)/p, ..., (p-1)/p, 1\}$, where s is the smallest integer such that all the groups of $B_{s/p}$ have a cardinal smaller than m. The deduced estimator is $\widehat{B}_s := \underset{B_\lambda \mid \lambda\in A_s}{\arg\min}\, \Psi(B)$. So, this grid is the set $\{l/p \mid l \in [1:p]\}$ restricted to the thresholds that give fine enough partition (with groups of size smaller than m).

Proposition 24. *The computational complexity of* $\widehat{B}_s$ *is* $O(p^2)$*.*

One can see that the complexity of this estimator is as small as the complexity of the previous estimator $\widehat{B}_\lambda$. Furthermore, it ensures that the estimated blocks are not too large, which was not the case with the previous estimator. However, the computation of $\widehat{B}_s$ requires the knowledge of m while the other estimators do not.

Now that we have defined new estimators of B^*, we give their convergence in the following proposition.

Proposition 25. *Let* $\widehat{B}$ *be either* $\widehat{B}_{tot}$, $\widehat{B}_{\widehat{C}}$, $\widehat{B}_\lambda$ *or* $\widehat{B}_s$ *indifferently. Under Conditions 1 to 4 and for a fixed* $\delta \in]1/2, 1[$*, we have*

$$\mathbb{P}\left(\widehat{B} = B^*\right) \longrightarrow 1.$$

When Condition 4 is not satisfied, we do not study the convergence of the previous estimators. In this case, we suggest to estimate B^* by $B_{n^{-\delta/2}}$, which is the partition given by the empirical correlation matrix thresholded by $n^{-\delta/2}$. The complexity of this estimator is $O(p^2)$, as for the previous estimator $\widehat{B}_\lambda = B_{n^{-1/3}}$. We show the convergence of this estimator in Proposition 26.

Proposition 26. *Under Conditions 1, 2 and 3, if* $\alpha_1 < \delta/2$ *and* $\alpha_2 > \delta/2$*,*

$$\mathbb{P}\left(B(\alpha_1) \leq B_{n^{-\delta/2}} \leq B(\alpha_2)\right) \longrightarrow 1.$$

As Condition 4 is not satisfied, the true partition B^* is again not reached by this estimator. Nevertheless, we get stronger results for the practical estimator $B_{n^{-\delta/2}}$ than for the theoretical estimator $\widehat{B}_{tot}$ when Condition 4 is not verified. Indeed, the condition "to be larger or equal than" is stronger that "not to be smaller than".

B.2.iii) Convergence of the estimator of the covariance matrix

We have seen in Propositions 25 and 26 how to estimate the decomposition B^* by $\widehat{B}$. Now to estimate the covariance matrix Σ, it suffices to impose the block-diagonal decomposition $\widehat{B}$ to the empirical covariance matrix $S_{\widehat{B}}$. We show in Proposition 27 that the resulting block-diagonal matrix estimator $S_{\widehat{B}}$ reaches the optimal rate of convergence under Conditions 1 to 4.

Proposition 27. *Let $\|\cdot\|_F$ be the Frobenius norm defined by $\|\Gamma\|_F^2 := \sum_{i,j=1}^p \gamma_{ij}^2$. Let $\widehat{B}$ be either $\widehat{B}_{tot}$, $\widehat{B}_{\widehat{C}}, \widehat{B}_\lambda$ or $\widehat{B}_s$. Under Conditions 1 to 4 and for a fixed $\delta \in]1/2, 1[$, we have*

$$\frac{1}{p}\|S_{B^*} - \Sigma\|_F^2 = O_p(1/n)$$

and

$$\frac{1}{p}\|S_{\widehat{B}} - \Sigma\|_F^2 = O_p(1/n).$$

Moreover, it is the best rate that we can have because

$$\frac{1}{p}\|S_{B^*} - \Sigma\|_F^2 \neq o_p(1/n).$$

Thus, we see that the quantity $\frac{1}{p}\|S_{\widehat{B}} - \Sigma\|_F^2$ decreases to 0 in probability with rate $1/n$, which is the same rate as S_{B^*} if we know the true decomposition B^*. Thus, the lack of knowledge of B^* does not deteriorate the convergence of our estimator.

Now that we have given the rate of convergence of our estimator $S_{\widehat{B}}$, we compare it with that of the empirical estimator S in the next proposition.

Proposition 28. *Under Conditions 1 and 2, the rate of the empirical covariance is*

$$\frac{1}{p}\|S - \Sigma\|_F^2 = O_p(p/n).$$

and we have

$$\mathrm{E}\left(\frac{1}{p}\|S - \Sigma\|_F^2\right) \geq \frac{\lambda_{\inf}^2 p}{2n}.$$

So, we know that $\frac{1}{p}\|S - \Sigma\|_F^2$ is lower-bounded in average and is bounded in probability. Thus, the rate of convergence of our suggested estimator $S_{\widehat{B}}$ is better than the empirical covariance matrix S.

If Condition 4 does not hold, the rate of convergence is given in the following proposition.

Proposition 29. *Under Conditions 1, 2 and 3, for all $\delta \in]0, 1[$ and for all $\varepsilon > 0$, we have*

$$\frac{1}{p}\|S_{B_{n^{-\delta/2}}} - \Sigma\|_F^2 = o_p\left(\frac{1}{n^{\delta-\varepsilon}}\right).$$

We remark that, for δ close to 1, this rate of convergence almost reaches the optimal rate of S_{B^*}, whereas the partition estimator $B_{n^{-\delta/2}}$ does not reach the true decomposition B^*. That comes from the fact that the elements σ_{ij} of Σ such that the indices (i,j) are not in the estimated partition $B_{n^{-\delta/2}}$ are small (with high probability). Hence, estimating these values by 0 does not increase so much the error $\frac{1}{p}\|S_{B_{n^{-\delta/2}}} - \Sigma\|_F^2$.

Theoretical guaranties for a block-diagonal estimator of the covariance matrix are also provided in [DG18]. Their framework is more general, with a true covariance matrix which is not necessarily block-diagonal. They bound the average of the square Hellinger distance between the true normal density and the density with the block-diagonal estimated covariance matrix. However, when p/n does not go to 0, their theoretical results becom uninformative. Indeed, they give an upper-bound which is larger than one, while the square Hellinger distance remains always smaller than 1.

B.2.iv) Discussion about the assumptions

For the previous results, we needed to make four assumptions on Σ (Conditions 1 to 4, given in Section B.2.i)).

Condition 1 provides a standard setting for high-dimensional problems, in particular for estimation of covariance matrices [MP67, Sil85]. Studying an higher dimensional setting where $p/n \longrightarrow +\infty$ would be interesting in future work.

Condition 2 is needed to bound the operator norm of Σ and Σ^{-1} and the eigenvalues of the empirical covariance matrix (with high probability). It also enables to bound the diagonal terms of Σ, which allow to derive the rate of convergence of each component of the empirical covariance matrix (using in particular Bernstein's inequality, see the proofs for more details).

Condition 3 states that the blocks of the true decomposition have a maximal size. It implies that the number of non-zero terms of Σ is $O(p)$.

Condition 4 requires that a finer block decomposition Σ_B is not too close to the true Σ. This condition is needed to not confuse B^* with a finer decomposition. However, Condition 4 seems to be less mild than the others. That is why we also focus on the case when Condition 4 is not satisfied.

Nevertheless, even Condition 4 is not so restrictive. Indeed, we suggest in Proposition 30 a reasonable example where Σ is randomly generated and where a condition similar to Condition 4 holds.

Proposition 30. *Let $L \in \mathbb{N}$ and $\varepsilon > 0$. Assume that for all p, Σ is generated in the following way:*

- *Let B^* be a partition of $[1:p]$ such that all its elements have a cardinal between 10 and $m \geq 10$. Let K be the number of groups (the cardinal of B^*). For all $k \in [1:K]$, let p_k be the cardinal of the "k-th element" of B^*.*

- *For all $k \in [1:K]$, let $(U_i^{(l)})_{i\in[1:p_k],\, l\in[1:L]}$ be i.i.d. with distribution $\mathcal{U}([-1,1])$. Let $U \in \mathcal{M}_{L,p_k}(\mathbb{R})$ such that the coefficient (l,i) is $U_i^{(l)}$. Let $\Sigma_{B_k^*} = U^T U + \varepsilon I_{p_k}$, where $\Sigma_{B_k^*}$ is the sub-matrix of Σ indexed by the elements of B_k^*.*
- *Let $\sigma_{ij} = 0$ for all $(i,j) \notin B^*$.*

Then, Conditions 2 and 3 are verified and the following slightly modified version of Condition 4 is satisfied for all $a > 0$:

$$\mathbb{P}\left(\exists B < B^*,\ \|\Sigma_B - \Sigma\|_{\max} < an^{-\frac{1}{4}}\right) \longrightarrow 0.$$

Thus, if $p/n \longrightarrow y \in]0,1[$, the conclusions of Propositions 20, 25 and 27 remain true when the probabilities are defined with respect to Σ and X which distribution conditionally to Σ is $\mathcal{N}(\mu,\Sigma)$.

B.2.v) Numerical applications

We present here numerical applications of the previous results with simulated data. We generate a covariance matrix Σ as in Proposition 30 with blocks of random size distributed uniformly on $[10:15]$, with $L = 5$ and $\varepsilon = 0.2$. We assume here that we know that the maximal size of the block is $m = 15$, so we can use the estimator $\widehat{B} = \widehat{B}_s$ given in Proposition 25 to reduce the complexity to $O(p^2)$ and to prevent the blocks from being too large.

We plot in Figure 5.1 the Frobenius norm of the error of the empirical covariance matrix S and the Frobenius norm of the error of the suggested estimator $S_{\widehat{B}}$, with $n = Np$ for different values of N. We can remark that the error of S is in $\sqrt{K}$ (where K is the number of groups) whereas the error of $S_{\widehat{B}}$ stays bounded as in Proposition 27. For $K = 100$, the Frobenius error of $S_{\widehat{B}}$ on Figure 5.1 is about 10 times smaller than the one of S.

B.3 Convergence and efficiency in fixed dimension

In this section, p and Σ are fixed and n goes to $+\infty$. We choose a different penalisation $\kappa = \frac{1}{pn^{\delta}}$ with $\delta \in]0,1/2[$ (instead of $\delta \in]1/2,1[$ in the previous setting). This framework enables to study the efficiency of estimators of Σ. Contrary to the high-dimensional setting of Section B.2, we do not assume particular condition in addition to the ones given in Section B.1.

We first give the convergence of $\widehat{B}_{tot}$ defined in Equation (5.1) in the next proposition.

Proposition 31. *We have*

$$\mathbb{P}\left(\widehat{B}_{tot} = B^*\right) \longrightarrow 1.$$

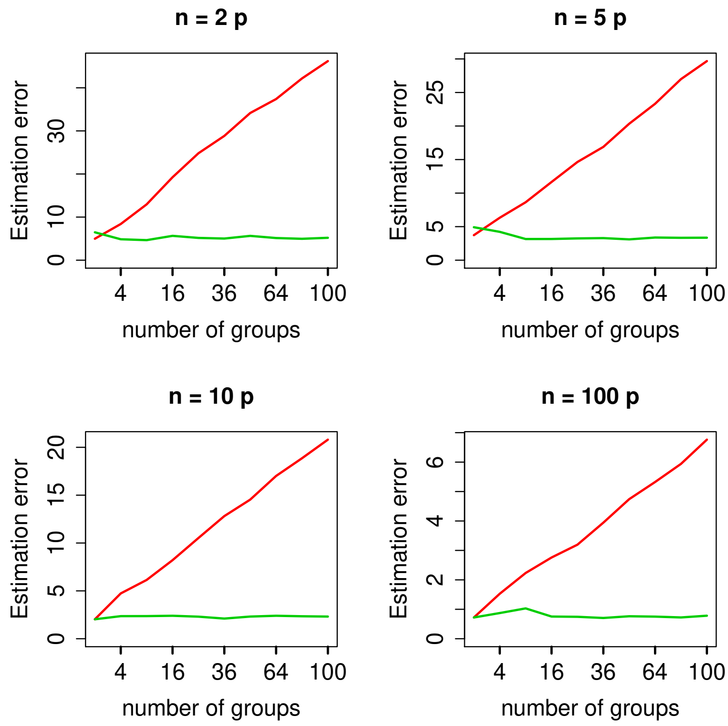


Figure 5.1: Frobenius error of the empirical covariance matrix S in red and the suggested estimator $S_{\widehat{B}}$ in green, in function of the number of groups K. The scale of the x-axis is in $\sqrt{K}$.

Corollary 5. *Let* $\widehat{B}_{\widehat{C}} := \underset{B_\lambda \mid \lambda \in A_{\widehat{C}}}{\arg\min}\, \Psi(B)$*, where* $A_{\widehat{C}} := \{|\widehat{C}_{ij}| \mid 1 \leq i < j \leq p\}$ *as in Proposition 25. Then*

$$\mathbb{P}\left(\widehat{B}_{\widehat{C}} = B^*\right) \longrightarrow 1.$$

In the rest of Section B.3, we write $\widehat{B}$ for $\widehat{B}_{tot}$ or $\widehat{B}_{\widehat{C}}$. The aim of this framework is to show that the suggested estimator $S_{\widehat{B}}$ is asymptotically efficient as if the true decomposition B^* were known.

As the parameter Σ is in the set $S_p^{++}(\mathbb{R})$ or even $S_p^{++}(\mathbb{R}, B^*)$, which are not open subsets of $\mathbb{R}^{p^2}$, the classical Cramér-Rao bound is no longer a lower-bound for the estimation error. Furthermore, as B^* is not known, the number of parameters of $S_{\widehat{B}}$ is not constant. That is why the classical Cramér-Rao bound is not relevant in our setting. We remark that applying this classical Cramér-Rao bound to a subset of the matrix estimator does not solve this problem.

A specific Cramér-Rao bound is suggested in [SN98] for parameters and estimators which satisfy continuously differentiable constraints. We shall consider linear constraints here. We let $\theta \in \mathbb{R}^d$ be the parameter, that is assumed to be restricted to a linear subspace V of dimension q in $\mathbb{R}^d$. In this case, if $U \in \mathcal{M}_{d,q}(\mathbb{R})$ is a matrix whose columns are the elements of an orthonormal basis of V and if J is the Fisher Information Matrix (FIM) of θ in the non-constraint case, [SN98] states that for unbiased estimator $\widehat{\theta} \in V$, we have

$$\mathrm{E}\left[(\widehat{\theta}-\theta)(\widehat{\theta}-\theta)^T\right] \geq U(U^T J U)^{-1} U^T, \tag{5.2}$$

where $\leq$ is the partial order on the symmetric positive semi-definite matrices.

In our setting, remark that $S_p^{++}(\mathbb{R})$ is an open subset of the linear subspace $S_p(\mathbb{R})$ of symmetric matrices and $S_p^{++}(\mathbb{R}, B^*)$ is an open subset of the linear subspace $\overline{S_p(\mathbb{R}, B^*)} := \{\Gamma \in S_p(\mathbb{R}),\ \Gamma_{B^*} = \Gamma\}$. We let $\mathrm{vec}(\Sigma)$ be the column vectorization of Σ. Hence, the parameter is $\mathrm{vec}(\Sigma)$ and there are $p(p-1)/2$ linear constraints arising from the symmetry and $p(p-1)/2 - \sum_{k=1}^K p_k(p_k-1)/2$ linear constraints arising from the block structure B^*.

So, the Cramér-Rao bound of Equation (5.2) is adapted to our framework, by considering the parameter $\mathrm{vec}(\Sigma) \in \mathbb{R}^{p^2}$, and we say that an estimator is efficient if it reaches the Cramér-Rao bound (5.2) (meaning that there is an equality in this equation), where the constraints (symmetry only or symmetry and block structure) will be stated explicitly.

Proposition 32 states that, in general, the empirical covariance matrix is efficient with this Cramér-Rao bound. This supports this choice of Cramér-Rao Bound, since in fixed dimension, one would expect that the empirical matrix is the most appropriate estimator.

If the empirical covariance matrix did not reach the Cramér-Rao Bound, we could not hope that $S_{\widehat{B}}$ would be efficient in the model where B^* was known, and this Cramér-Rao bound would not be well tuned to our problem.

Proposition 32. *If μ is known, the empirical estimator S is an efficient estimator of Σ in the model $\{\mathcal{N}(\mu, \Sigma),\ \Sigma \in S_p^{++}(\mathbb{R})\}$.*

Remark 32. *In Proposition 32, we assume that μ is known to reach the Cramér-Rao bound for fixed n (and not only asymptotically). This will be the same in Proposition 33.*

Now, we deduce the efficiency of S_{B^*} when B^* is known.

Proposition 33. *If μ and B^* are known, S_{B^*} is an efficient estimator of Σ in the model $\{\mathcal{N}(0, \Sigma),\ \Sigma \in S_p^{++}(\mathbb{R}, B^*)\}$.*

Finally, Proposition 34 states the asymptotic efficiency of our estimator $S_{\widehat{B}}$ (even for unknown μ)

Proposition 34.

$$\sqrt{n}(\mathrm{vec}(S_{\widehat{B}}) - \mathrm{vec}(\Sigma)) \underset{n\to+\infty}{\overset{\mathcal{L}}{\longrightarrow}} \mathcal{N}(0, \mathrm{CR}(\Sigma, B^*)),$$

where $\mathrm{CR}(\Sigma, B^*)$ *is the Cramér-Rao bound of* $\mathrm{vec}(\Sigma)$ *in the model* $\{\mathcal{N}(0,\Sigma),\ \Sigma \in S_p^{++}(\mathbb{R}, B^*)\}$.

The explicit expression of the $p^2 \times p^2$ matrix $\mathrm{CR}(\Sigma, B^*)$ can be found in the appendix where Propositions 32, 33 and 34 are proved.

C Application to the estimation of the Shapley effects

In this section, we apply the block-diagonal estimation of the covariance matrix Σ to estimate the Shapley effects in high dimension and for Gaussian linear models. In Section C.1, we address the problem of estimating the Shapley effects when the covariance matrix Σ and the vector β are estimated. We derive the convergence of the estimators of the Shapley effects from the results of Section B.

C.1 Estimation of the Shapley effects with noisy observations

We assume that we just observe a sample $(X^{(l)}, \tilde{Y}^{(l)})_{l\in[1:n]}$ where $\tilde{Y} = (\tilde{Y}^{(l)})_{l\in[1:n]}$ are noisy observations:

$$\tilde{Y}^{(l)} = \beta_0 + \beta^T X^{(l)} + \varepsilon^{(l)},$$

for $l \in [1:n]$ where $(\varepsilon^{(l)})_{l\in[1:n]}$ are i.i.d. with distribution $\mathcal{N}(0, \sigma_n^2)$ and where $\sigma_n \leq C_{\text{sup}}$ is unknown, where C_{sup} is a fixed finite constant.

Remark that the computation of the Shapley effects requires the parameters β and Σ (see Algorithm 3). Here, as we do not know the parameters β and Σ, we will estimate them and replace the true parameters by their estimation in Algorithm 3.

First, we estimate $(\beta_0\ \beta^T)^T$ as usual by

$$\begin{pmatrix} \widehat{\beta}_0 \\ \widehat{\beta} \end{pmatrix} := (A^T A)^{-1} A^T \tilde{Y},$$

where $A \in \mathcal{M}_{n,p+1}(\mathbb{R})$ is defined by $A_{l,i+1} := X_i^{(l)}$ and $A_{l,1} = 1$, and where $n > p$.

C.2 Estimation of the Shapley effects in high-dimension

At first glance, we could estimate Σ by the empirical covariance matrix S and replace it in Algorithm 3. However, B^* is not known and we can not find it using BFS with the empirical covariance matrix S (which usually has the simple structure $\{[1:p]\}$ with probability one). Thus, we can not use any particular block-diagonal structure and Algorithm 3 would only apply Algorithm 2. However, as we have seen, the complexity of this computation would be exponential in p and it would be no longer tractable for $p \geq 30$. Furthermore, in high dimension, the Frobenius error between S and Σ does not go to 0 (see Proposition 27). Thus, using the empirical covariance matrix could yield estimators of the Shapley effects that do not converge.

For that reason, to estimate $\eta = (\eta_i)_{i\in[1:p]}$, we suggest to estimate B^* by $\widehat{B}$ (defined in Section B.2.ii)) and Σ by $S_{\widehat{B}}$ and to replace them in Algorithm 3. We write $\widehat{\eta} = (\widehat{\eta}_i)_{i\in[1:p]}$ the estimator of the Shapley effects obtained replacing Σ by $S_{\widehat{B}}$ and β by $\widehat{\beta}$ in Algorithm 3. We use our previous results on the estimation of the covariance matrix to obtain the convergence rate of $\widehat{\eta}$.

We focus on the high dimensional case, when p and n go to $+\infty$. In this case, β and Σ are not fixed but depend on n (or p). As in Section B.2, we choose $\kappa = \frac{1}{pn^\delta}$ with $\delta \in]1/2, 1[$ to compute $\widehat{B}$. To prevent problematic cases, we also add an assumption on the vector β.

Condition 5. *There exist $\beta_{\inf} > 0$ and $\beta_{\sup} < +\infty$ such that for all n and for all $j \leq p$, we have $\beta_{\inf} \leq |\beta_j| \leq \beta_{\sup}$.*

Proposition 35. *Under Conditions 1 to 5 and if $\delta \in]1/2, 1[$, then for all $\gamma > 1/2$, we have*

$$\sum_{i=1}^{p} |\widehat{\eta}_i - \eta_i| = o_p\left(\frac{\log(n)^\gamma}{\sqrt{n}}\right).$$

Recall that $\sum_{i=1}^p \eta_i = 1$. Thus, to quantify the error estimation, the value of $\sum_{i=1}^p |\widehat{\eta}_i - \eta_i|$ is a relative error. Proposition 35 states that this relative error goes to zero at the parametric rate $1/n^{1/2}$, up to a logarithm factor.

We have seen in Section C.1 of Chapter 4 that, once we have the block-diagonal covariance matrix, the computation of the Shapley effects has the complexity $O(K2^m)$ which is equal to $O(n)$ under Condition 3. In Section B.2, we gave four different choices of $\widehat{B}$, with four different complexities, all larger than $O(n)$. Thus, the complexity of the whole estimation of the Shapley effects (including the estimation of Σ) is the same as the complexity of $\widehat{B}$ (see Section B.2.ii)).

When Condition 4 is not satisfied, we still have the convergence of the relative error, with almost the same rate.

Proposition 36. *Under Conditions 1, 2, 3 and 5, for all $\delta \in]0,1[$, choosing the partition $B_{n^{-\delta/2}}$ and for all $\varepsilon > 0$, we have*

$$\sum_{i=1}^{p} |\widehat{\eta}_i - \eta_i| = o_p\left(\frac{1}{n^{-(\delta-\varepsilon)/2}}\right).$$

Remark 33. *When the dimension p is fixed, the rate of convergence is $O_p(1/\sqrt{n})$, as if we estimated Σ by the empirical covariance matrix. Moreover, we have seen in Proposition 34 that the computation of $S_{\widehat{B}}$ enables to reach asymptotically the Cramér-Rao bound of [SN98] as if B^* were known. We then deduce the asymptotic efficiency of $\widehat{\eta}$. If β is known, we define $g : \Sigma \mapsto \eta(\beta, \Sigma)$, let $\mathrm{CR}(\eta, B^*) := Dg(\Sigma)\mathrm{CR}(\Sigma, B^*)Dg(\Sigma)$ be the Cramér-Rao bound of η in the model $\{\mathcal{N}(\mu, \Sigma),\ \Sigma \in S_p^{++}(\mathbb{R}, B^*)\}$. Thus,*

$$\sqrt{n}(\widehat{\eta} - \eta) \underset{n\to+\infty}{\overset{\mathcal{L}}{\longrightarrow}} \mathcal{N}(0, \mathrm{CR}(\eta, B^*)).$$

C.3 Numerical application

We have seen in Proposition 30 a way to generate Σ which verifies Conditions 1 to 3 and some slightly modified version of Condition 4. So, with this choice of Σ, we derive in Proposition 37 the convergence of the Shapley effects estimation.

Proposition 37. *Under Condition 5, if Σ is generated as in Proposition 30, then, for all $\gamma > 1/2$,*

$$\sum_{i=1}^{p} |\widehat{\eta}_i - \eta_i| = o_p\left(\frac{\log(n)^{\gamma}}{\sqrt{n}}\right),$$

where the probabilities are defined with respect to Σ and X, which distribution conditionally to Σ is $\mathcal{N}(\mu, \Sigma)$.

We now present a numerical application of Proposition 37. The matrix Σ is generated by Proposition 30 as in Section B.2.v), with blocks of random size distributed uniformly on $[10, 15]$, $L = 5$ and $\varepsilon = 0.2$. For all p, the vector β is generated with distribution $\mathcal{U}([1,2]^p)$, so that Condition 5 is satisfied. As in Section B.2.v), we assume that we know that the maximal size of the block is $m = 15$, so we can use the estimator $\widehat{B} = \widehat{B}_s$ given in Proposition 25. As the computation of the Shapley effects is exponential in the maximal block size, the estimator $\widehat{B}_s$ is preferred. The complexity of the estimation of the Shapley effects is then in $O(p^2)$.

We plot in Figure 5.2 the sum of the Shapley effects estimation error $\sum_{i=1}^{p} |\widehat{\eta}_i - \eta_i|$, with $n = N\,p$ for different values of N. We can remark that the sum of the errors seems to be of order $1/\sqrt{K}$, which is confirmed by Proposition 37.

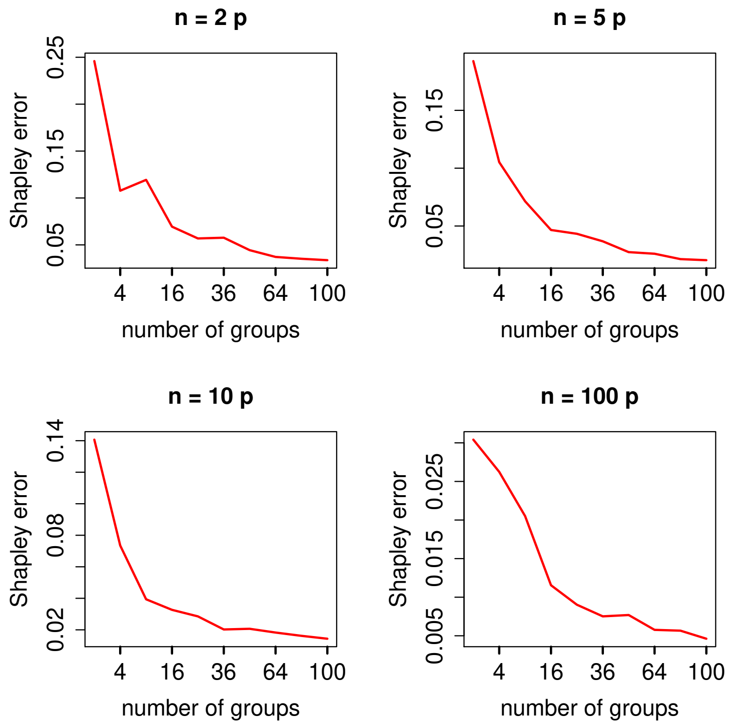


Figure 5.2: Sum of errors of the Shapley effects estimations in function of the number of groups K. The scale of the x-axis is in $\sqrt{K}$.

D Application on real data

In this section, we consider the same nuclear data as in Chapter 4 Section C.3. Recall that the output Y models the neutron flux and the inputs are the cross-sections. Here, there are 292 inputs divided into 50 groups of size between 2 and 18. The covariance matrix Σ and the vector β are available. However, in order to assess the efficiency of our suggested estimation procedures of the Shapley effects, we now assume that the true covariance matrix Σ is unknown and that we observe an i.i.d. sample $(X^{(l)})_{l\in[1:n]}$ with distribution $\mathcal{N}(\mu, \Sigma)$ (with μ unknown). We assume that the maximal group size is known to be smaller or equal to 20 and that the vector β is known. Then, we estimate the block-diagonal structure by the block-diagonal structure $\widehat{B}$ that maximizes the penalized likelihood Φ among all the block-diagonal structures obtained by thresholding the empirical correlation matrix from its largest value to the smallest value such that the maximal size of the blocks is smaller or equal to 20. Thus, our estimator $\widehat{B}$ is a mix of the estimators $\widehat{B}_{\widehat{C}}$ and $\widehat{B}_s$ detailed in Section B.2.ii).

We plot the Frobenius error of the estimated covariance matrix and the sum

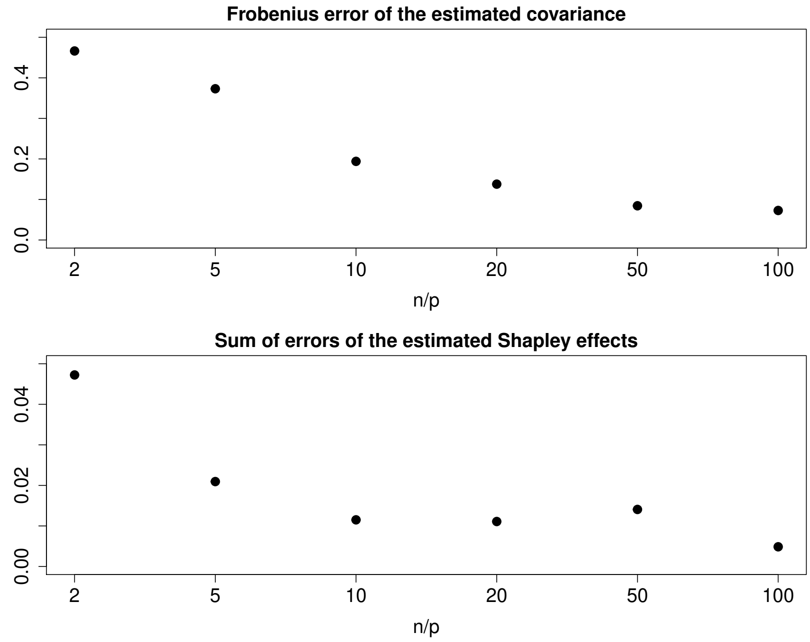


Figure 5.3: Errors of the estimated covariance matrix and the corresponding Shapley effects for different values of $\frac{n}{p}$.

of the absolute values of the errors of the estimated Shapley effects for different values of $y = p/n$ in Figure 5.3, where $p = 292$.

We can remark that the errors decrease globally when the value of $\frac{n}{p}$ increases. The larger value of the sum of the errors of the estimated Shapley effects for $n/p = 50$ is due to the randomness of the estimated Shapley effects. Note that, even when $n = 2p$, the sum of the errors of the Shapley effects is less than 0.05 (recall that, in comparison, the sum of the Shapley effects is 1). We plot in Figure 5.4 the estimated Shapley effects that are larger than 1% with $n/p = 2$. Remark that these estimated values are similar to the true ones displayed in Figure 4.2 and the physical interpretation is the same.

In conclusion, we implemented an estimator of the block-diagonal covariance matrix originating from nuclear data when we only observe an i.i.d. sample of the inputs. Then, the derived estimated Shapley effects are shown to be very close to the true Shapley effects, that quantify the impact of the uncertainties of cross sections on the uncertainty on the neutron flux. When the sample size n is equal to $2p$, the physical conclusions are the same as when the true covariance matrix is known.

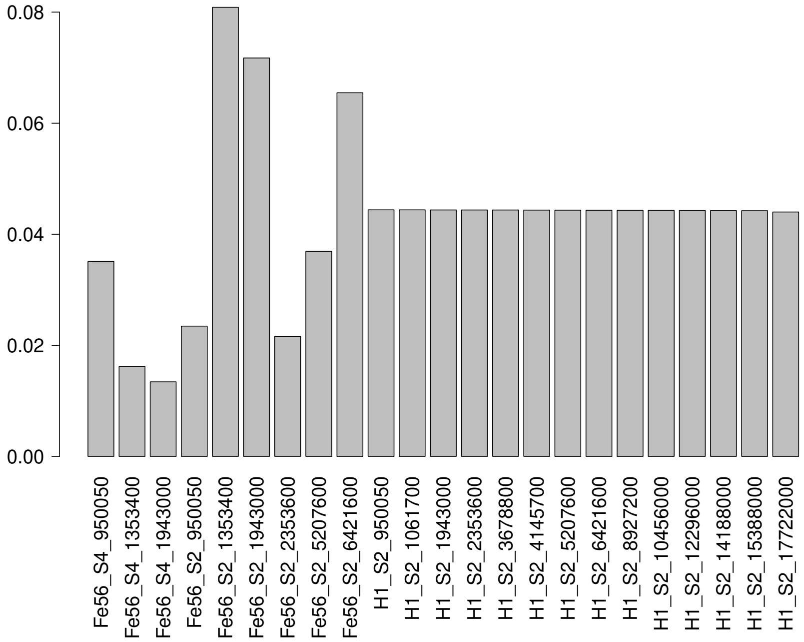


Figure 5.4: Shapley effects that are larger that 1% estimated with $n/p = 2$.

E Conclusion

In this chapter, we suggested an estimator of a block-diagonal covariance matrix for Gaussian data. We proved that in high dimension, this estimator converges to the same block-diagonal structure with complexity in $O(p^2)$. For fixed dimension, we also proved the asymptotic efficiency of this estimator, that performs asymptotically as well as as if the true block-diagonal structure were known. Then, we deduced convergent estimators of the Shapley effects in high dimension for Gaussian linear models. These estimators are still available for thousands input variables, as long as the maximal block is not too large. Moreover, we proved the convergence of the Shapley effects estimators when the observations of the output are noisy and so the parameter β is estimated. Finally, we applied these estimator on real nuclear data.

In future works, it would be interesting to treat the higher dimension setting when p/n goes to $+\infty$.

Chapter 6

Linear Gaussian approximation for the Shapley effects

We have seen in Chapter 3 that in the linear Gaussian framework, we can easily compute the Shapley effects as long as the number of inputs is not too large using Algorithm 2. Hence, one could legitimately wonder if the values of the Shapley effects given by Algorithm 2 are relevant when we are close to the linear Gaussian framework. The aim of this chapter is to use the values of the Shapley effects in the linear Gaussian framework as estimates of the Shapley effects in more general settings.

In Section A, we show how the approximation of the true model by a linear function impacts the Shapley effects when the inputs form a Gaussian vector with a covariance matrix converging to 0. In Section B, we prove that, when the inputs are given by an empirical mean, if we want to compute the Shapley effects, we can assume asymptotically that the input vector is a Gaussian vector with a covariance matrix converging to 0. Hence using the results of Section A, the Shapley effects of the Gaussian linear framework give a good estimate of the true ones.

If Z is a random vector in $\mathbb{R}^p$ and g is a function from $\mathbb{R}^p$ to $\mathbb{R}$ such that $\mathrm{E}(g(Z)^2) < +\infty$ and $\mathrm{Var}(g(Z)) > 0$, let $\eta(Z, g) \in \mathbb{R}^p$ be the vector containing all the Shapley effects with input vector Z and model g.

A Approximation of a model by a linear model

A.1 Introduction and notation

To model uncertain physical values, it can be convenient to consider them as a Gaussian vector. For example, the international libraries [McL05, JEF13, JEN11] on real data from the field of nuclear safety provide the average and covariance matrix of the input variables, so it is natural to model them with the Gaussian distribution. Hence, to quantify the impact of the uncertainties of the physical inputs of a model on a quantity of interest, it is commonly the case to estimate the Shapley effects of Gaussian inputs. The model f is in general non-linear and the estimation procedures dedicated to non-linear models [SNS16, BBD20] are typically computationally costly, with an accuracy that can be sensitive to the specific situation. Nevertheless, when the uncertainty on the inputs become small, the input vector converges to its mean μ, and a linear approximation of the model at μ seems more and more appropriate.

To formalize this idea, let $X^{\{n\}} \sim \mathcal{N}(\mu^{\{n\}}, \Sigma^{\{n\}})$ be the input vector, with a sequence of mean vectors $(\mu^{\{n\}})$ and a sequence of covariance matrices $(\Sigma^{\{n\}})$. The index n can represent for instance the number of measures of an uncertain input, in which case the covariance matrix $\Sigma^{\{n\}}$ will decrease with n.

Assumption 9. *The covariance matrix $\Sigma^{\{n\}}$ decreases to 0 such that the eigenvalues of $a^{\{n\}}\Sigma^{\{n\}}$ are lower-bounded and upper-bounded in $\mathbb{R}_+^*$, with $a^{\{n\}} \underset{n\to+\infty}{\longrightarrow} +\infty$. Moreover, $\mu^{\{n\}} \underset{n\to+\infty}{\longrightarrow} \mu$, where μ is a fixed vector.*

In Assumption 1, the condition on the eigenvalues of $a^{\{n\}}\Sigma^{\{n\}}$ means that the correlation matrix obtained from $\Sigma^{\{n\}}$ can not get close to a singular matrix. This condition is necessary in our proofs.

If $j \in \mathbb{N}$ and if f is $\mathcal{C}^j$ at $\mu^{\{n\}}$, we will write $f_j^{\{n\}}(x) = \frac{1}{j!}D^j f(\mu^{\{n\}})(x - \mu^{\{n\}})$ (where $D^j(\mu^{\{n\}})(z)$ is the image of $(z, z, \cdots, z) \in (\mathbb{R}^p)^j$ through the multilinear function $D^j f(\mu^{\{n\}})$, which gathers all the partial derivatives of order j of f at $\mu^{\{n\}}$) and $R_j^{\{n\}}(x) = f(x) - \sum_{l=0}^j f_l^{\{n\}}(x)$ the remainder of the j-th order Taylor approximation of f at $\mu^{\{n\}}$. In particular, $f_1^{\{n\}}(x) = Df(\mu^{\{n\}})(x - \mu^{\{n\}})$, where $Df = D^1 f$. We identify the linear function $Df(\mu^{\{n\}})$ with the corresponding row gradient vector of size $1 \times p$ and the bilinear function $D^2 f(\mu^{\{n\}})$ with the corresponding Hessian matrix of size $p \times p$. We also write $f_1(x) = Df(\mu)(x - \mu)$.

Finally, we assume that the function f is subpolynomial, that is, there exist $k \in \mathbb{N}$ and $C > 0$ such that,

$$\forall x \in \mathbb{R}^p, \ |f(x)| \leq C(1 + \|x\|^k).$$

A.2 Theoretical results

A.2.i) First-order Taylor polynomial

First, we study the asymptotic difference between the Shapley effects given by the true model f and the ones given by the first-order Taylor polynomial of f at $\mu^{\{n\}}$.

Remark that adding a constant to the function does not affect the values of the Shapley effects. Thus, the Shapley effects $\eta(X^{\{n\}}, f(\mu^{\{n\}}) + f_1^{\{n\}})$ given by the first-order Taylor polynomial of f at $\mu^{\{n\}}$ are equal to $\eta(X^{\{n\}}, f_1^{\{n\}})$. In the next proposition, we show that approximating the true Shapley effects of the non-linear f by the Shapley effects of the linear approximation $f_1^{\{n\}}$ yields a vanishing error of order $1/a^{\{n\}}$ as $n \to \infty$.

Proposition 38. *Assume that $X^{\{n\}} \sim \mathcal{N}(\mu^{\{n\}}, \Sigma^{\{n\}})$, Assumption 9 holds and f is subpolynomial and $\mathcal{C}^3$ on a neighbourhood of μ and $Df(\mu) \neq 0$. Then,*

$$\|\eta(X^{\{n\}}, f) - \eta(X^{\{n\}}, f_1^{\{n\}})\| = O\left(\frac{1}{a^{\{n\}}}\right).$$

We remark that, when f is a computer model, it can be the case that the gradient vector is available. First, the computer model can already provide them, by means of the Adjoint Sensitivity Method [Cac03]. Second, automatic differentiation methods can be used on the source file of the code and yield a differentiated code [HP04].

Remark 34. *The rate $O(1/a^{\{n\}})$ is the best rate that we can reach under the assumptions of Proposition 38. Indeed, letting $X^{\{n\}} = (X_1^{\{n\}}, X_2^{\{n\}}) \sim \mathcal{N}(0, \frac{1}{a^{\{n\}}} I_2)$ and $Y^{\{n\}} = f(X^{\{n\}}) = X_1^{\{n\}} + X_2^{\{n\}2}$, we have $\eta_1(X^{\{n\}}, f_1^{\{n\}}) = 1$ and $\eta_2(X^{\{n\}}, f_1^{\{n\}}) = 0$. Moreover, $\eta_1(X^{\{n\}}, f) = \frac{a^{\{n\}}}{a^{\{n\}}+2}$ and $\eta_2(X^{\{n\}}, f) = \frac{2}{a^{\{n\}}+2}$. Thus, the rate of the difference between $\eta(X^{\{n\}}, f)$ and $\eta(X^{\{n\}}, f_1^{\{n\}})$ is exactly $1/a^{\{n\}}$.*

In Proposition 38, we bound the difference between the Shapley effects given by f and the ones given by the first-order Taylor polynomial of f. Moreover, when the matrix $a^{\{n\}}\Sigma^{\{n\}}$ converges, Proposition 39 shows that the Shapley effects given by the Taylor polynomial converge.

Proposition 39. *Assume that $X^{\{n\}} \sim \mathcal{N}(\mu^{\{n\}}, \Sigma^{\{n\}})$, Assumption 9 holds, f is $\mathcal{C}^1$ on a neighbourhood of μ, $Df(\mu) \neq 0$ and $a^{\{n\}}\Sigma^{\{n\}} \underset{n\to+\infty}{\longrightarrow} \Sigma \in S_p^{++}(\mathbb{R})$. Then, if $X^* \sim \mathcal{N}(\mu, \Sigma)$,*

$$\|\eta(X^{\{n\}}, f_1^{\{n\}}) - \eta(X^*, f_1)\| = O(\|\mu^{\{n\}} - \mu\|) + O(\|a^{\{n\}}\Sigma^{\{n\}} - \Sigma\|).$$

Proposition 38 shows that replacing f by its first-order Taylor polynomial $f_1^{\{n\}}$ does not impact significantly the Shapley effects when the input variances are small. Thus, the knowledge of $f_1^{\{n\}}$ would enable us to use the explicit expression of the Gaussian linear case, and for instance the function "ShapleyLinearGaussian" of the package `sensitivity`, to estimate the true Shapley effects $\eta(X^{\{n\}}, f)$. However, in practice, the first-order Taylor polynomial $f_1^{\{n\}}$ is not always available, except for instance in situations described above. Thus, one may be interested in replacing the true first-order Taylor polynomial $f_1^{\{n\}}$ by an approximation. We will study two such approximations given by finite difference and linear regression.

A.2.ii) Finite difference approximation

For $h=(h_1,\cdots,h_p)\in(\mathbb{R}_+^*)^p$ and writing $(e_1,\cdots,e_p)$ the canonical basis of $\mathbb{R}^p$, let

$$\widehat{D}_h f(x) := \left(\frac{f(x+e_1h_1)-f(x-e_1h_1)}{2h_1},\cdots,\frac{f(x+e_ph_p)-f(x-e_ph_p)}{2h_p}\right), \tag{6.1}$$

be the approximation of the differential of f at x with the steps $h_1,\cdots,h_p$. If $(h^{\{n\}})_n$ is a sequence of $(\mathbb{R}_+^*)^p$ converging to 0, let

$$\tilde{f}^{\{n\}}_{1,h^{\{n\}}}(x) := \tilde{f}^{\{n\}}_{1,h^{\{n\}},\mu^{\{n\}}}(x) := \widehat{D}_{h^{\{n\}}} f(\mu^{\{n\}})(x-\mu^{\{n\}})$$

be the approximation of the first-order Taylor polynomial of $f-f(\mu^{\{n\}})$ at $\mu^{\{n\}}$ with the steps $h_1,\cdots,h_p$. The next proposition ensures that the Shapley effects computed from the true Taylor polynomial and the approximated one are close, for small steps.

Proposition 40. *Under the assumptions of Proposition 38, we have*

$$\|\eta(X^{\{n\}},f_1^{\{n\}})-\eta(X^{\{n\}},\tilde{f}^{\{n\}}_{1,h^{\{n\}}})\| = O\left(\|h^{\{n\}}\|^2\right).$$

Then, the next corollary extends Propositions 38 and 39 to the approximated Taylor polynomial based on finite differences.

Corollary 6. *Under the assumptions of Proposition 38, and if $\|h^{\{n\}}\|\leq \frac{C_{\sup}}{\sqrt{a^{\{n\}}}}$ (for example, choosing $h_i^{\{n\}} := \sqrt{\mathrm{Var}(X_i^{\{n\}})}$, the standard deviation of $X_i^{\{n\}}$), we have*

$$\|\eta(X^{\{n\}},f)-\eta(X^{\{n\}},\tilde{f}^{\{n\}}_{1,h^{\{n\}}})\| = O(\frac{1}{a^{\{n\}}}).$$

Moreover, if $a^{\{n\}}\Sigma^{\{n\}} \underset{n\to+\infty}{\longrightarrow} \Sigma$, then, letting $X^*\sim\mathcal{N}(\mu,\Sigma)$,

$$\|\eta(X^{\{n\}},\tilde{f}^{\{n\}}_{1,h^{\{n\}}})-\eta(X^*,f_1)\| = O(\|\mu^{\{n\}}-\mu\|)+O(\|a^{\{n\}}\Sigma^{\{n\}}-\Sigma\|)+O\left(\frac{1}{a^{\{n\}}}\right).$$

A.2.iii) Linear regression

For $n\in\mathbb{N}$ and $N\in\mathbb{N}^*$, let $(X^{\{n\}(l)})_{l\in[1:N]}$ be an i.i.d. sample of $X^{\{n\}}$ of size N and assume that we compute the image of f at each sample point, obtaining the vector $Y^{\{n\}}$. Then, we can approximate f with a linear regression, by least squares. In this case, we estimate the coefficients of the linear regression by the vector:

$$\begin{pmatrix}\widehat{\beta}_0^{\{n\}}\\ \widehat{\beta}^{\{n\}}\end{pmatrix} = \left(A^{\{n\}T}A^{\{n\}}\right)^{-1}A^{\{n\}T}Y^{\{n\}},$$

where $A^{\{n\}} \in \mathcal{M}_{N,p+1}(\mathbb{R})$ is such that, for all $j \in [1:N]$, the j-th line of $A^{\{n\}}$ is $(1\ X^{\{n\}(j)T})$. The function f is then approximated by

$$\widehat{f}_{lin}^{\{n\}(N)} : x \longmapsto \widehat{\beta}_0^{\{n\}} + \widehat{\beta}^{\{n\}T} x.$$

Remark that the linear function $\widehat{f}_{lin}^{\{n\}(N)}$ is random and so, the deduced Shapley effects $\eta(X^{\{n\}}, \widehat{f}_{lin}^{\{n\}(N)})$ are random variables. The next proposition and corollary correspond to Proposition 40 and Corollary 6, for the linear regression approximation of f.

Proposition 41. *Under Assumption 9, if f is $\mathcal{C}^2$ on a neighbourhood of μ with $Df(\mu) \neq 0$, there exist $C_{\inf} > 0$, $C_{\sup}^{(1)} < +\infty$ and $C_{\sup}^{(2)} < +\infty$ such that, with probability at least $1 - C_{\sup}^{(1)} \exp(-C_{\inf} N)$, we have*

$$\|\eta(X^{\{n\}}, f_1^{\{n\}}) - \eta(X^{\{n\}}, \widehat{f}_{lin}^{\{n\}(N)})\| \leq C_{\sup}^{(2)} \frac{1}{\sqrt{a^{\{n\}}}}.$$

Corollary 7. *Under the assumptions of Proposition 38, there exist $C_{\inf} > 0$, $C_{\sup}^{(1)} < +\infty$ and $C_{\sup}^{(2)} < +\infty$ such that, with probability at least $1-C_{\sup}^{(1)} \exp(-C_{\inf} N)$, we have*

$$\|\eta(X^{\{n\}}, f) - \eta(X^{\{n\}}, \widehat{f}_{lin}^{\{n\}(N)})\| \leq C_{\sup}^{(2)} \frac{1}{\sqrt{a^{\{n\}}}}.$$

Moreover, if $a^{\{n\}}\Sigma^{\{n\}} \underset{n\to+\infty}{\longrightarrow} \Sigma$, then, letting $X^* \sim \mathcal{N}(\mu, \Sigma)$, there exists $C_{\sup}^{(3)} < +\infty$ such that, with probability at least $1 - C_{\sup}^{(1)} \exp(-C_{\inf} N)$,

$$\|\eta(X^{\{n\}}, \widehat{f}_{lin}^{\{n\}(N)}) - \eta(X^*, f_1)\| \leq C_{\sup}^{(3)} \left(\|\mu^{\{n\}} - \mu\| + \|a^{\{n\}}\Sigma^{\{n\}} - \Sigma\| + \frac{1}{\sqrt{a^{\{n\}}}} \right).$$

A.3 Numerical experiments

In this section, we compute the Shapley effects of the true function f and the ones obtained from the three previous linear approximations to illustrate the previous theoretical results. Let $p = 4$ and

$$f(x) = \cos(x_1)x_2 + \sin(x_2) + 2\cos(x_3)x_1 - \sin(x_4).$$

This function is 1-Lipschitz continuous and $\mathcal{C}^\infty$ on $\mathbb{R}^4$. We choose $\Sigma^{\{n\}} = \frac{1}{n^2}\Sigma$ (that is, $a^{\{n\}} = n^2$), where Σ is defined by:

$$\Sigma = A^T A, \quad A = \begin{pmatrix} -2 & -1 & 0 & 1 \\ 2 & -2 & -1 & 0 \\ 1 & 2 & -2 & -1 \\ 0 & 1 & 2 & -2 \end{pmatrix}.$$

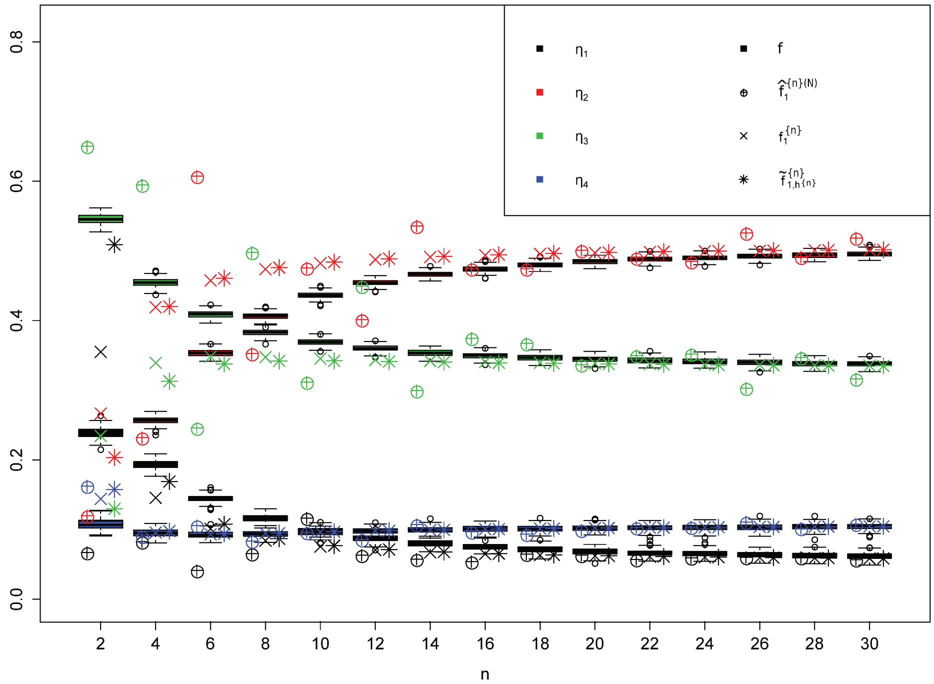


Figure 6.1: Shapley effects of the linear approximations $\widehat{f}_{lin}^{\{n\}(N)}$, $f_1^{\{n\}}$, $\tilde{f}_{1,h^{\{n\}}}^{\{n\}}$ and boxplots of estimates of the Shapley effects of the function f.

Let $\mu = (1, 0, 2, 1)$ and $\mu^{\{n\}} = \mu + \frac{1}{n}(1, 1, 1, 1)$.

On Figure 6.1, we plot, for different values of n, the vector $\eta(X^{\{n\}}, \widehat{f}_{lin}^{\{n\}(N)})$ (given by the linear regression), the vector $\eta(X^{\{n\}}, f_1^{\{n\}})$ (given by the true Taylor polynomial), the vector $\eta(X^{\{n\}}, \tilde{f}_{1,h^{\{n\}}}^{\{n\}})$ (given by the finite difference approximation of the derivatives) and the boxplots of 200 estimates of $\eta(X^{\{n\}}, f)$ computed by the R function "shapleyPermRand" from the R package `sensitivity` (see [SNS16, IP19]), which is adapted to non-linear functions, with parameters $N_V = 10^5$, $m = 10^3$ and $N_I = 3$. To compute the linear regression, we observed a sample of size $N = 40$. To compute the finite difference approximation, we took $h_i^{\{n\}} = \sqrt{\mathrm{Var}(X_i^{\{n\}})}$.

The differences between the Shapley effects given by f and the ones given by the linear approximations of f seem to converge to 0, as it is proved by Propositions 38, 40 and 41. Moreover, Figure 6.1 emphasizes that the Shapley effects obtained from the linear regression get closer slower to the true ones than the ones given by the other linear approximations.

We remark that we have here $\Sigma^{\{n\}} = \frac{1}{a^{\{n\}}}\Sigma$ and thus the assumptions of Proposition 39 hold. Hence, the values of the true Shapley effects $\eta(X^{\{n\}}, f)$ converge, as we can see on Figure 6.1.

The computation time for each estimate of the Shapley effects is around 5 seconds using "shapleyPermRand", 1.9×10^{-3} using the linear approximation $f_1^{\{n\}}$ or $\tilde{f}^{\{n\}}_{1,h^{\{n\}}}$ and 2.4×10^{-3} using the linear approximation $\widehat{f}^{\{n\}(N)}_{lin}$. Remark that this time difference can become more accentuated if the function f is a costly computer code.

B Approximation of the empirical mean by a Gaussian vector

B.1 Theoretical results

Here, we extend the results of Section A to the case where the distribution of the input (that we now write $\widehat{X}^{\{n\}}$) is close to a Gaussian distribution $X^{\{n\}}$. We focus on the setting where the input vector is an empirical mean

$$\widehat{X}^{\{n\}} = \frac{1}{n}\sum_{l=1}^{n} U^{(l)},$$

where $(U^{(l)})_{l\in[1:n]}$ is an i.i.d. sample of a random vector U in $\mathbb{R}^p$ such that $\mathrm{E}(\|U\|^2) < +\infty$ and $\mathrm{Var}(U) \neq 0$. Let $\mu := \mathrm{E}(U)$ and Σ be the covariance matrix of U. Remark that, as is Section A, the input vector $\widehat{X}^{\{n\}}$ is a random vector converging to its mean, and its covariance matrix $\Sigma^{\{n\}}$ is equal to $\frac{1}{n}\Sigma$.

Contrary to Section A, $\widehat{X}^{\{n\}}$ is not Gaussian, but, thanks to the central limit theorem, its distribution is close to $\mathcal{N}(\mu, \frac{1}{n}\Sigma)$. Hence, we would like to estimate the Shapley effects $\eta(\widehat{X}^{\{n\}}, f)$ by $\eta(X^*, Df(\mu))$, where $X^* \sim \mathcal{N}(0, \Sigma)$, since $\eta(X^*, Df(\mu))$ can be computed using the explicit expression of the Gaussian linear case, and for instance the function "ShapleyLinearGaussian" of the package `sensitivity`.

Proposition 42. *Assume that f is $\mathcal{C}^3$ on a neighbourhood of μ with $Df(\mu) \neq 0$ and that f is subpolynomial, that is there exist $k \in \mathbb{N}^*$ and $C > 0$ such that for all $x \in \mathbb{R}^p$, we have $|f(x)| \leq C(1 + \|x\|^k)$. If $\mathrm{E}(\|U\|^{4k}) < +\infty$ and if U has a bounded probability density function, then*

$$\eta(\widehat{X}^{\{n\}}, f) \underset{n\to+\infty}{\longrightarrow} \eta(X^*, Df(\mu)).$$

Proposition 42 justifies that $\eta(X^*, Df(\mu))$ is a good approximation of $\eta(\widehat{X}^{\{n\}}, f)$. Furthermore, if μ, Σ and $Df(\mu)$ are unknown, the following corollary shows that they can be replaced by approximations. Let $(U^{\{l\}\prime})_{l\in[1:n']}$ and $(U^{\{l\}\prime\prime})_{l\in[1:n'']}$ be independent of $(U^{\{l\}})_{l\in[1:n]}$, composed of i.i.d. copies of U and with $n'=n'(n)$ and $n''=n''(n)$ such that $n',n''\to\infty$ when $n\to\infty$. We can estimate μ (resp. Σ) by the empirical mean $\widehat{X}^{\{n'\}\prime}$ of $(U^{\{l\}\prime})_{l\in[1:n']}$ (resp. the empirical covariance matrix $\widehat{\Sigma}^{\{n''\}\prime\prime}$ of $(U^{\{l\}\prime\prime})_{l\in[1:n'']}$), and we can estimate Df by a finite difference approximation. The next corollary guarantees that the error stemming from these additional estimations goes to 0 as $n\to\infty$.

Corollary 8. *Assume that the assumptions of Proposition 42 hold and that $(h^{\{n\}})_{n\in\mathbb{N}}$ is a sequence of $(\mathbb{R}_+^*)^p$ converging to 0. Let X^{*n} be a random vector with distribution $\mathcal{N}(\mu,\widehat{\Sigma}^{\{n''\}\prime\prime})$ conditionally to $\widehat{\Sigma}^{\{n''\}\prime\prime}$. Then*

$$\left\|\eta(\widehat{X}^{\{n\}},f)-\eta(X^{*n},\tilde{f}^{\{n\}}_{1,h^{\{n\}},\widehat{X}^{\{n'\}\prime}})\right\|\xrightarrow[n\to+\infty]{a.s.}0,$$

where $\tilde{f}^{\{n\}}_{1,h^{\{n\}},\widehat{X}^{\{n'\}\prime}}$ is the linear approximation of f at $\widehat{X}^{\{n'\}\prime}$ obtained from Equation (6.1) by replacing $\mu^{\{n\}}$ by $\widehat{X}^{\{n'\}\prime}$.

Remark 35. *If μ, Σ or Df is known, the previous corollary holds replacing $\widehat{X}^{\{n'\}\prime}$, $\widehat{\Sigma}^{\{n''\}\prime\prime}$ or $\tilde{f}^{\{n\}}_{1,h^{\{n\}},\widehat{X}^{\{n'\}\prime}}$ by μ,Σ or $Df(\widehat{X}^{\{n'\}\prime})$ respectively.*

Remark 36. *The notation $\eta(X^{*n},\tilde{f}^{\{n\}}_{1,h^{\{n\}},\widehat{X}^{\{n'\}\prime}})$ is to be understood conditionally to $\widehat{\Sigma}^{\{n''\}\prime\prime},\widehat{X}^{\{n'\}\prime}$. That is, conditionally to $\widehat{\Sigma}^{\{n''\}\prime\prime},\widehat{X}^{\{n'\}\prime}$, the Shapley effects $\eta(X^{*n},\tilde{f}^{\{n\}}_{1,h^{\{n\}},\widehat{X}^{\{n'\}\prime}})$ are defined with the fixed linear function $\tilde{f}^{\{n\}}_{1,h^{\{n\}},\widehat{X}^{\{n'\}\prime}}$ and the Gaussian distribution for X^{*n}.*

B.2 Application to the impact of individual estimation errors

Let us show an example of application of the results of Section B.1. Let U be a continuous random vector of $\mathbb{R}^p$, with a bounded density and with an unknown mean μ. Assume that we observe an i.i.d. sample $(U^{(l)})_{l\in[1:n]}$ of U and that we focus on the estimation of a parameter $\theta=f(\mu)$, where f is $\mathcal{C}^3$. This parameter is estimated by $f(\widehat{X}^{\{n\}})$ (which is asymptotically efficient by the delta-method), where $\widehat{X}^{\{n\}}$ is the empirical mean of $(U^{(l)})_{l\in[1:n]}$. The estimation error of each variable $\widehat{X}_i^{\{n\}}$ (for $i=1,\cdots,p$) propagates through f. To quantify the part of the estimation error of $Y=f(\widehat{X}^{\{n\}})$ caused by the individual estimation errors of each $\widehat{X}_i^{\{n\}}$ (for $i=1,\cdots,p$), one can estimate the Shapley effects $\eta(\widehat{X}^{\{n\}},f)=\eta(\widehat{X}^{\{n\}}-\mu,f(\cdot+\mu)-f(\mu))$ which assess the impact of individual errors on the global error. To that end, Proposition 42 and Corollary 8 state that the Shapley effects can be estimated using a Gaussian linear approximation, with an error that vanishes as n increases.

For example, let $f = \|\cdot\|^2$ and $p = 5$. In this case, the derivative Df is known and no finite difference approximation is required. To generate U with a bounded density and with dependencies, we define $A_1 \sim \mathcal{U}([5, 10])$, $A_2 \sim \mathcal{N}(0, 4)$, A_3 with a symmetric triangular distribution $T(-1, 8)$, $A_4 \sim 5Beta(1, 2)$ and $A_5 \sim Exp(1)$. Then, we define

$$\begin{cases} U_1 & = A_1 + 2A_2 - 0.5A_3 \\ U_2 & = A_2 + 2A_1 - 0.5A_5 \\ U_3 & = A_3 + 2A_2 - 0.5A_5 \\ U_4 & = A_4 + 2A_1 - 0.5A_2 \\ U_5 & = A_5 + 2A_3 - 0.5A_4. \end{cases}$$

Since the mean μ and the covariance matrix Σ are unknown, we need to estimate them (as in Corollary 8). Using the notation of Section B.1, we choose $n = n' = n''$ and $(U^{(l)\prime})_{l\in[1:n']} = (U^{(l)\prime\prime})_{l\in[1:n']}$ (that is, we estimate the empirical mean and the empirical covariance matrix with the same sample). We estimate the Shapley effects $\eta(\widehat{X}^{\{n\}}, f)$ by $\eta(X^{*n}, Df(\widehat{X}^{\{n\}\prime}))$, where X^{*n} is a random vector with distribution $\mathcal{N}(\mu, \widehat{\Sigma}^{\{n\}\prime\prime})$ conditionally to $\widehat{\Sigma}^{\{n\}\prime\prime}$. By Corollary 8 and Remark 35, the difference between $\eta(\widehat{X}^{\{n\}}, f)$ and $\eta(X^{*n}, Df(\widehat{X}^{\{n\}\prime}))$ converges to 0 almost surely when n goes to $+\infty$.

Here, we compute 1000 estimates of μ and Σ and we compute the 1000 corresponding Shapley effects of the Gaussian linear approximation $\eta(X^{*n}, Df(\widehat{X}^{\{n\}\prime}))$. To compare with these estimates, we also compute 1000 estimates given by the function "shapleySubsetMC" suggested in [BBD20], with parameters $N_{tot} = 1000$, $N_i = 3$ and with an i.i.d. sample of $\widehat{X}^{\{n\}}$ with size 1000. We plot the results on Figure 6.2.

We observe that the estimates of the Shapley effects given by "shapleySubsetMC" and the Gaussian linear approximation are rather similar, even for $n = 100$. However, the variance of the estimates given by the Gaussian linear approximation is smaller than the one of the general estimates given by "shapleySubsetMC". Moreover, each Gaussian linear estimation requires only a sample of $(U^{(l)\prime})_{l\in[1:n]}$ (to compute $\widehat{X}^{\{n\}\prime}$ and $\widehat{\Sigma}^{\{n\}\prime\prime}$) and takes around 0.007 second on a personal computer, whereas each general estimation with "shapleySubsetMC" requires here 1000 samples of $(U^{(l)\prime})_{l\in[1:n]}$ and takes around 11 seconds. Remark that this time difference can become more accentuated if the function f is a costly computer code. Finally, the estimator of the Shapley effects given by the linear approximation converges almost surely when n goes to $+\infty$, whereas the estimator

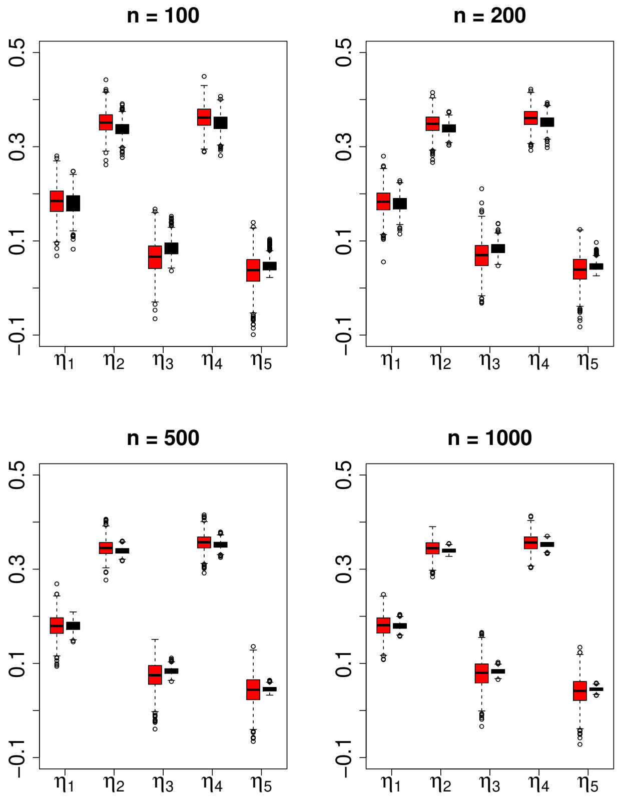


Figure 6.2: Boxplots of the estimates of the Shapley effects given by the general estimation function "shapleySubsetMC" (in red) and by the Gaussian linear approximation (in black).

of the Shapley effects given by "shapleySubsetMC" is only shown to converge in probability when the sample size and N_{tot} go to $+\infty$ (see [BBD20]).

To conclude, we have provided a framework where the theoretical results of Section B.1 can be applied. We have illustrated this framework with numerical experiments on generated data. We have showed that, in this framework, to estimate the Shapley effects, the Gaussian linear approximation provides an estimator much faster and much more accurate than the general estimator given by "shapleySubsetMC".

C Conclusion

In this chapter, we worked on the Gaussian linear framework approximation to estimate the Shapley effects, in order to take advantage of the simplicity brought by this framework. First, we focused on the case where the inputs are Gaussian variables converging to their means. This setting is motivated, in particular, by the case of uncertainties on physical quantities that are reduced by taking more and more measurements. We showed that, to estimate the Shapley effects, one can replace the true model f by three possible linear approximations: the exact Taylor polynomial approximation, a finite difference approximation and a linear regression. We gave the rate of convergence of the difference between the Shapley effects of the linear approximations and the Shapley effects of the true model. These results are illustrated by a simulated application that highlights the accuracy of the approximations. Then, we focused on the case where the inputs are given by an empirical mean. In this case, we proved that the instinctive idea to replace the empirical mean by a Gaussian vector and the true model by a linear approximation around the mean indeed gives good approximations of the Shapley effects. We highlighted the benefits of these estimators on numerical experiments.

Several questions remain open to future work. In particular, it would be valuable to obtain more insight on the choice between the general estimator of the Shapley effects for non-linear models and the estimators based on Gaussian linear approximations. Quantitative criteria for this choice, based for instance on the magnitude of the input uncertainties or on the number of input samples that are available, would be beneficial. Regarding the results on the impact of individual estimation errors in Section B.2, it would be interesting to obtain extensions to estimators of quantities of interest that are not only empirical means, for instance general M-estimators.

Chapter 7

Conclusion and perspectives

In this thesis, we developed the tools of sensitivity analysis for real data. Since the assumption of independent inputs rarely holds with industrial data, we focused on the Shapley effects, that keep interesting properties with dependent inputs.

General estimation of the Shapley effects

First, we focused on the estimation of the conditional elements. In the dependent case, [SNS16] estimated them by double Monte-Carlo, whereas in the independent case, the Pick-and-Freeze estimator was the most widespread estimator in the literature. Hence, we extended the Pick-and-Freeze estimator to the dependent case and we compared it to the double Monte-Carlo estimator in numerical experiments, to the latter's advantage.

We also improved the already existing algorithm [SNS16] to estimate the Shapley indices, suggesting to estimate once every conditional element for all the Shapley effects. We also detailed which part of the total budget should be allocated to the estimation of each conditional element in order to minimize the total variance. We proved the convergence of our suggested estimator and of the one suggested in [SNS16]. We emphasized the accuracy of our estimator with numerical experiments on simulated data.

In order to make the estimation of the Shapley effects possible in more practical cases, we extended these estimators to the case where we only observe an i.i.d. sample of the inputs, with either the computer code of f or the corresponding i.i.d. sample of the output. We proved the convergence under some mild assumptions that include heterogeneous data. We also provided rates of convergence of the estimators of the conditional elements for real continuous inputs when the probability density function of the inputs vector is upper-bounded and lower-bounded on its support. We implemented one of our suggested estimator of the Shapley effects on the R package `sensitivity`.

Numerical experiments seem to indicate that, to estimate the conditional elements (that is, more or less the Sobol indices), the double Monte-Carlo estimator is more accurate than the Pick-and-Freeze estimator. However, we could not prove such results theoretically and a particular study on the comparison of these estimators could be done is future works.

On the convergence result of the Shapley effects estimators where we only observe and i.i.d. sample of the inputs, it could be interesting to alleviate the assumption of the bound of the model f and of the density f_X. However, the assumption of the continuous density f_X seems to be indispensable to prove Lemma 5 of Chapter I in the appendix. The alleviation of the assumption of the upper-bound and the lower-bound of the density for the rate of convergence of the estimators of the conditional elements could be the subject of future works. Finally, it could be interesting to provide the optimal allocation of the total budget to the estimation of the conditional elements to minimize the total variance of the Shapley effects estimation when we only observe an i.i.d. sample of the real continuous inputs, using the rates of convergence.

Study of the linear Gaussian framework

We implemented a function to compute the Shapley effects in the linear Gaussian framework which has been integrated in the URANIE platform of CEA DES. We suggested solutions to compute the Shapley effects for large values of p (the number of inputs), when the covariance matrix is block-diagonal. That made possible applications on nuclear safety where one frequently has a large number of inputs but the physical measures enable to compute only covariances between variables of the same group, and the different groups are thus assumed to be independent.

Then, we focused on the estimation of the Shapley effects when the parameters of the block-diagonal linear Gaussian framework are unknown. When the number of inputs p is fixed, we suggested an estimator which is asymptotically efficient when the sample-size n goes to $+\infty$. To model cases with a large number of inputs, we assumed that p goes to $+\infty$ at the same rate as n. We provided different estimators of the Shapley effects which have a computational cost in $O(p^2)$. We proved that, under some conditions, the relative error goes to 0 at the parametric rate, up to a logarithm factor. We also bound the relative error under milder assumptions. We applied one of these estimators to semi-generated data. We remarked on this example that the values of the Shapley effects when the parameters are estimated with $n = 2p$ are almost the same as when the parameters are known.

Finally, we worked on estimation of the Shapley effects replacing a non linear Gaussian setting by the linear Gaussian framework. We gave the rate of convergence of the difference of the Shapley effects corresponding to the true model f and a linear approximation of f when the input vector is Gaussian with a covariance matrix converging to 0. This assumption enables to include physical applications where the uncertain inputs are modeled by a Gaussian vector with a small covariance matrix. In this case, the Shapley effects can be estimated by using the linear Gaussian framework instead of a costly approximate algorithm. We also proved the convergence of the estimation of the Shapley effects when the input vector is an empirical mean by the Shapley effects corresponding to a Gaussian linear framework.

In future works, it would be interesting to extend the works on the estimation of the Shapley effects in the "almost linear Gaussian framework". In particular, one could try to study the block-diagonal linear Gaussian approximation for general frameworks in high dimension.

Appendix I

Proofs of Chapter 2

A Proofs for the double Monte-Carlo and Pick-and-Freeze estimators: Theorems 3, 4, 5 and 6

To unify notation, let us write

$$
\begin{aligned}
\Phi_{MC}^{mix}: \quad (x^{(1)},...,x^{(N_I)}) \quad &\longmapsto \frac{1}{N_I-1}\sum_{k=1}^{N_I}\left(f(x_{-u}^{(1)},x_u^{(k)})-\frac{1}{N_I}\sum_{l=1}^{N_I}f(x_{-u}^{(1)},x_u^{(l)})\right)^2,\\
\Phi_{MC}^{knn}: \quad (x^{(1)},...,x^{(N_I)}) \quad &\longmapsto \frac{1}{N_I-1}\sum_{k=1}^{N_I}\left(f(x^{(k)})-\frac{1}{N_I}\sum_{l=1}^{N_I}f(x^{(l)})\right)^2,\\
\Phi_{PF}^{mix}: \quad (x^{(1)},x^{(2)}) \quad &\longmapsto f(x^{(1)})f(x_u^{(1)},x_{-u}^{(2)})-\mathrm{E}(Y)^2,\\
\Phi_{PF}^{knn}: \quad (x^{(1)},x^{(2)}) \quad &\longmapsto f(x^{(1)})f(x^{(2)})-\mathrm{E}(Y)^2.
\end{aligned}
$$

Remark that all these four functions are bounded as f is bounded. When we do not write the exponent mix or knn of Φ or of the estimators, it means that we refer to both of them (mix and knn). We write the proofs only for $\widehat{E}_{u,MC}$. For the estimators $\widehat{V}_{u,PF}$, it suffices to replace Φ_{MC} by Φ_{PF}, $-u$ by u (and vice-versa), E_u by V_u, $\mathrm{Var}(Y|X_{-u})$ by $\mathrm{E}(Y|X_u)^2-\mathrm{E}(Y)^2$ and N_I by 2. Hence, we shall only write the complete proofs for Theorems 3 and 4. To simplify notation, we will write $\widehat{E}_u$ for $\widehat{E}_{u,MC}$, $\widehat{E}_{u,l}$ for $\widehat{E}_{u,l,MC}$ and Φ for Φ_{MC}. N_I is a fixed integer. We also write $k_N(l,i) := k_N^{-u}(l,i)$, and the dependence on $-u$ is implicit.

A.1 Proof of consistency: Theorems 3 and 5

Recall that for all $i \in [1:p]$, $(\mathcal{X}_i, d_i)$ is a Polish space. Then, for all $v \subset [1:p]$, $\mathcal{X}_v := \prod_{i\in v} \mathcal{X}_i$ is a Polish space for the distance $d_v := \max_{i\in v} d_i$. We will write $B_v(x_v, r)$ the open ball in $\mathcal{X}_v$ of radius r and center x_v. We also let $\mu_v := \bigotimes_{i\in v} \mu_i$. Recall that the choice of the N_I-nearest neighbours could be not unique. In this case, conditionally to $(X_{-u}^{(n)})_{n\le N}$, the $(k_N(l,i))_{l\in[1:N], i\in[1:N_I]}$ are random variables that we choose in the following way. Conditionally to $(X_{-u}^{(n)})_{n\le N}$, we choose $k_N(l,i)$ uniformly over all the indices of the i-th nearest neighbours of $X_{-u}^{(l)}$, such that the $(k_N(l,i))_{i\le N_I}$ are two by two distinct and independent of all the other random variables conditionally to $(X_{-u}^{(n)})_{n\le N}$.

In particular, as we want to prove asymptotic results, we assume (without loss of generality) that we have an infinite i.i.d. sample $(X^{(n)})_{n\in\mathbb{N}^*}$, and we assume that for all $N \in \mathbb{N}^*$, conditionally to $(X_{-u}^{(n)})_{n\le N}$,

$$(k_N(l,i))_{i\le N_I} \perp\!\!\!\perp \sigma\left((X_u^{(n)})_{n\le N}, (X^{(n)})_{n>N}, (k_{N'}(l',i'))_{(N',l')\neq(N,l),\, i'\in[1:N_I]}\right).$$

Hence, for all $N \in \mathbb{N}^*$ and $l \in [1:N]$, conditionally to $(X_{-u}^{(n)})_{n\in\mathbb{N}}$, we have

$$(k_N(l,i))_{i\le N_I} \perp\!\!\!\perp \sigma\left((X_u^{(n)})_{n\in\mathbb{N}}, (k_{N'}(l',i'))_{(N',l')\neq(N,l),\, i'\in[1:N_I]}\right).$$

To simplify notation, let us write $k_N(i) := k_N(1,i)$ (the index of one i-th neighbour of $X_{-u}^{(1)}$) and $k'_N(i) := k_N(2,i)$ (the index of one i-th neighbour of $X_{-u}^{(2)}$). Remark that $X_{-u}^{(k_N(i))}$ does not depend on $k_N(i)$. Let $\mathbf{k} := (k_N(i))_{i\le N_I, N\in\mathbb{N}^*}$ and $\mathbf{k}_N := (k_N(i))_{i\le N_I}$. We will use the letter $\mathbf{h}$ for the realizations of the variable $\mathbf{k}$.

To begin with, let us recall two well-known results that we will use in the following.

Lemma 2. *Let A be a real random variable. If $\mathcal{H}$ is independent of $\sigma(\sigma(A), \mathcal{G})$, then*

$$\mathrm{E}(A|\sigma(\mathcal{G},\mathcal{H})) = \mathrm{E}(A|\mathcal{G}).$$

Lemma 3. *Let A, B be random variables. For all measurable ϕ,*

$$\mathcal{L}(\phi(A,B)|A=a) = \mathcal{L}(\phi(a,B)|A=a)$$

and if B is independent of A, then

$$\mathcal{L}(\phi(A,B)|A=a) = \mathcal{L}(\phi(a,B)).$$

Now, to prove Theorem 3, we need to prove several intermediate results.

Lemma 4. *For all $l \in \mathbb{N}^*$,*

$$X_{-u}^{(k_N(l))} \xrightarrow[N\to+\infty]{a.s.} X_{-u}^{(1)}. \tag{I.1}$$

Proof. First, let us show that for all $\varepsilon > 0$, $\mathbb{P}(d_{-u}(X_{-u}^{(1)}, X_{-u}^{(2)}) < \varepsilon) > 0$. Indeed, as $\mathcal{X}_{-u}$ is a Polish space, its support has measure 1. Thus

$$\begin{aligned}
\mathbb{P}(d_{-u}(X_{-u}^{(1)}, X_{-u}^{(2)}) < \varepsilon) &= \int_{\mathcal{X}_{-u}^2} \mathbb{1}_{d_{-u}(x_{-u},x'_{-u})<\varepsilon} d\mathbb{P}_{X_{-u}} \otimes \mathbb{P}_{X_{-u}}(x_{-u}, x'_{-u}) \\
&= \int_{\mathcal{X}_{-u}} \mathbb{P}_{X_{-u}}(B_{-u}(x_{-u}, \varepsilon)) d\mathbb{P}_{X_{-u}}(x_{-u}) \\
&= \int_{supp(\mathcal{X}_{-u})} \mathbb{P}_{X_{-u}}(B_{-u}(x_{-u}, \varepsilon)) d\mathbb{P}_{X_{-u}}(x_{-u}) \\
&> 0,
\end{aligned}$$

because if $x_{-u} \in supp(\mathcal{X}_{-u})$, then $B_{-u}(x_{-u}, \varepsilon) \not\subset supp(\mathcal{X}_{-u})^c$ and $\mathbb{P}_{X_{-u}}(B_{-u}(x_{-u}, \varepsilon)) > 0$.

Next, remark that

$$X_{-u}^{(k_N(l))} \xrightarrow[N\to+\infty]{a.s.} X_{-u}^{(1)} \iff X_{-u}^{(k_N(2))} \xrightarrow[N\to+\infty]{a.s.} X_{-u}^{(1)},$$

and,

$$\begin{aligned}
\mathbb{P}\left(\left\{X_{-u}^{(k_N(2))} \xrightarrow[N\to+\infty]{} X_{-u}^{(1)}\right\}^c\right) &= \mathbb{P}\left(\bigcup_{k\geq 1}\bigcap_{n\geq 2} d_{-u}(X_{-u}^{(n)}, X_{-u}^{(1)}) \geq \frac{1}{k}\right) \\
&\leq \sum_{k\geq 1} \mathbb{P}\left(\bigcap_{n\geq 2} d_{-u}(X_{-u}^{(n)}, X_{-u}^{(1)}) \geq \frac{1}{k}\right) \\
&= \sum_{k\geq 1} \lim_{N\to+\infty} \mathbb{P}\left(d_{-u}(X_{-u}^{(2)}, X_{-u}^{(1)}) \geq \frac{1}{k}\right)^N \\
&= \sum_{k\geq 1} \lim_{N\to+\infty} \left[1 - \mathbb{P}\left(d_{-u}(X_{-u}^{(2)}, X_{-u}^{(1)}) < \frac{1}{k}\right)\right]^N \\
&= \sum_{k\geq 1} 0 \\
&= 0.
\end{aligned}$$

□

Lemma 5. *There exists a version of*

$$\mathcal{L}(X_u|X_{-u} = \cdot) : (\mathcal{X}_{-u}, d_{-u}) \longrightarrow (\mathcal{M}_1(\mathcal{X}_u), \mathcal{T}(weak))$$

which is continuous $\mathbb{P}_{X_{-u}}$-a.e., where $\mathcal{M}_1(\mathcal{X}_u)$ is the set of probability measures on $\mathcal{X}_u$ and $\mathcal{T}(weak)$ is the topology of weak convergence.

Proof. We assumed that there exists a version of f_X which is bounded and $\mathbb{P}_X$-a.e. continuous. Let

$$f_{X_{-u}}(x_{-u}) := \int_{\mathcal{X}_u} f_X(x_u, x_{-u}) d\mu_u(x_u),$$

which is bounded by $\mu_u(\mathcal{X}_u)\|f_X\|_\infty$ and is a $\mathbb{P}_{X_{-u}}$-a.e. continuous (thanks to the dominated converging Theorem) version of the density of X_{-u} with respect to μ_{-u}. Let $x_{-u} \in \mathcal{X}_{-u}$ such that $f_{X_{-u}}(x_{-u}) \leq \|f_{X_{-u}}\|_\infty$, $f_{X_{-u}}(x_{-u}) > 0$ and such that $f_{X_{-u}}$ is continuous at x_{-u}. We have that

$$f_{X_u|X_{-u}=x_{-u}}(x_u) := \frac{f_X(x_u, x_{-u})}{f_{X_{-u}}(x_{-u})}$$

is a version of the density of X_u conditionally to $X_{-u} = x_{-u}$ (defined for almost all x_{-u}). Let $(x_{-u}^{(n)})$ be a sequence converging to x_{-u}. There exists n_0 such that for all $n \geq n_0$, $f_{X_{-u}}(x_{-u}^{(n)}) > 0$. Thus, by continuity of f which respect to x_{-u} and of $f_{X_{-u}}$, we have $f_{X_u|X_{-u}=x_{-u}}(x_u) = \lim_{n\to+\infty} f_{X_u|X_{-u}=x_{-u}^{(n)}}(x_u)$ for almost all x_u. Then, using the dominated converging Theorem,

$$\mathcal{L}(X_u|X_{-u} = x_{-u}^{(n)}) \underset{N\to+\infty}{\overset{weakly}{\longrightarrow}} \mathcal{L}(X_u|X_{-u} = x_{-u}).$$

$\square$

Remark 37. *The assumption "$X = (X_u, X_{-u})$ has a bounded density f_X with respect to a finite measure $\mu = \bigotimes_{i=1}^p \mu_i$, which is continuous $\mathbb{P}_X$-a.e." is only used in the proof of Lemma 5. It would be interesting in future work to prove 5 with a weaker assumption.*

Remark 38. *There exists a different proof of Lemma 5 if we assume that μ is regular. Theorem 8.1 of [Tju74] ensures that the conditional distribution in the sense of Tjur is defined for all x_{-u} such that $f_{X_{-u}} > 0$ (and not only for almost all x_{-u}) and the continuity of $f_{X_u|X_{-u}=x_{-u}}(x_u)$ with respect to x_{-u} comes from Theorem 22.1 of [Tju74].*

Remark 39. *To avoid confusion, we can now define $\mathcal{L}(X_u|X_{-u} = x_{-u})$ as the probability measure of density $\frac{f(\cdot,x_{-u})}{f_{X_{-u}}(x_{-u})}$, which is defined for all (and not "almost all") x_{-u} in $\{f_{X_{-u}} > 0\}$.*

Proposition 43. *If*

$$\mathcal{L}(X_u|X_{-u} = .) : (\mathcal{X}_{-u}, d_{-u}) \longrightarrow (\mathcal{M}_1(\mathcal{X}_u), \mathcal{T}(weak))$$

is continuous (where $\mathcal{T}(weak)$ is the topology of weak convergence) almost everywhere, then, for almost all $\left((x_{-u}^{(n)})_n, \mathbf{h}\right)$, we have

$$\mathrm{E}\left(\widehat{E}_{u,1}\left|(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k} = \mathbf{h}\right.\right) \underset{N\to+\infty}{\longrightarrow} \mathrm{Var}(Y|X_{-u} = x_{-u}^{(1)}) \tag{I.2}$$

and,

$$\mathrm{E}(\widehat{E}_{u,1}) \underset{N\to+\infty}{\longrightarrow} E_u. \tag{I.3}$$

Proof. Let $\mathbf{Z} = (\mathbf{Z}_1, ..., \mathbf{Z}_{N_I}) : (\Omega, \mathcal{A}) \to (\mathcal{X}^{N_I}, \mathcal{E}^{\otimes N_I})$ measurable, where $\mathcal{E}$ is the σ-algebra on $\mathcal{X}$, such that for almost all $\left((x_{-u}^{(n)})_n, \mathbf{h}\right)$, we have

$$\mathcal{L}\left(\mathbf{Z}|(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k} = \mathbf{h}\right) = \bigotimes_{i=1}^{N_I} \mathcal{L}(X^{(1)}|X_{-u}^{(1)} = x_{-u}^{(1)}).$$

It suffices to show that, for almost all $\left((x_{-u}^{(n)})_n, \mathbf{h}\right)$,

$$(X^{(k_N(i))})_{i\leq N_I} \underset{N\to+\infty}{\overset{\mathcal{L}_{|(X_{-u}^{(n)})_n=(x_{-u}^{(n)})_n,\mathbf{k}=\mathbf{h}}}{\longrightarrow}} \mathbf{Z}. \tag{I.4}$$

Indeed, if Equation (I.4) is true, then, using that Φ is bounded,

$$\begin{aligned}
& \mathrm{E}\left(\widehat{E}_{u,1}\left|(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k} = \mathbf{h}\right.\right) \\
= \quad & \mathrm{E}\left[\Phi\left((X^{(k_N(i))})_{i\leq N_I}\right)\left|(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k} = \mathbf{h}\right.\right] \\
\underset{N\to+\infty}{\longrightarrow} \quad & \mathrm{E}(\Phi(\mathbf{Z})\left|(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k} = \mathbf{h}\right.) \\
= \quad & \mathrm{Var}(Y|X_{-u} = x_{-u}^{(1)}),
\end{aligned}$$

by definition of $\mathbf{Z}$ and of Φ. Thus, we have Equation I.2. Furthermore, using dominated convergence theorem, integrating on $\left((x_{-u}^{(n)})_n, \mathbf{h}\right)$, we obtain Equation I.3.

Thus, it remains to show that conditionally to $(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k} = \mathbf{h}$, the random vector $(X^{(k_N(i))})_{i\leq N_I}$ converges in distribution to $\mathbf{Z}$. We prove this convergence step by step.

Lemma 6. *For almost all $(x_{-u}^{(n)})_n$,*

$$\mathcal{L}((X_u^{(n)})_n|(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n) = \bigotimes_{n\geq 1} \mathcal{L}(X_u|X_{-u} = x_{-u}^{(n)}).$$

Proof. Let $(\tilde{X}_{-u}^{(n)})_n : \Omega \to \mathcal{X}_{-u}^{\mathbb{N}}$ be an i.i.d. sequence of distribution $\mathcal{L}(X_{-u})$. Then, we let $(\tilde{X}_u^{(n)})_n : \Omega \to \mathcal{X}_u^{\mathbb{N}}$ be a sequence with conditional distribution

$$\mathcal{L}((\tilde{X}_u^{(n)})_n | (\tilde{X}_{-u}^{(n)})_n = (x_{-u}^{(n)})_n) = \bigotimes_{n \geq 1} \mathcal{L}(X_u | X_{-u} = x_{-u}^{(n)}).$$

We just have to prove that $(\tilde{X}^{(n)})_n$ is an i.i.d. sample of distribution $\mathcal{L}(X)$.

Each $\tilde{X}^{(n)}$ has a distribution $\mathcal{L}(X)$ because for all bounded measurable ϕ,

$$\begin{aligned}
\mathrm{E}(\phi(\tilde{X}^{(n)})) &= \int_\Omega \phi(\tilde{X}^{(n)}(\omega)) d\mathbb{P}(\omega) \\
&= \int_{\mathcal{X}_u \times \mathcal{X}_{-u}} \phi(x_u, x_{-u}) d\mathbb{P}_{(\tilde{X}_u, \tilde{X}_{-u})}(x_u, x_{-u}) \\
&= \int_{\mathcal{X}_{-u}} \left(\int_{\mathcal{X}_u} \phi(x_u, x_{-u}) d\mathbb{P}_{X_u | X_{-u} = x_{-u}}(x_u) \right) d\mathbb{P}_{X_{-u}}(x_{-u}) \\
&= \int_{\mathcal{X}} \phi(x) d\mathbb{P}_X(x).
\end{aligned}$$

Moreover, $(\tilde{X}^{(n)})_n$ are independent because if $n \neq m$, then, for all bounded Borel functions ϕ_1 and ϕ_2, we have:

$$\begin{aligned}
& \mathrm{E}(\phi_1(\tilde{X}^{(n)})\phi_2(\tilde{X}^{(m)})) \\
= & \int_{\mathcal{X}_u^2 \times \mathcal{X}_{-u}^2} \phi_1(x_u^{(n)}, x_{-u}^{(n)}) \phi_2(x_u^{(m)}, x_{-u}^{(m)}) d\mathbb{P}_{(\tilde{X}_u^{(n)}, \tilde{X}_u^{(m)}, \tilde{X}_{-u}^{(n)}, \tilde{X}_{-u}^{(m)})}(x_u^{(n)}, x_u^{(m)}, x_{-u}^{(n)}, x_{-u}^{(m)}) \\
= & \int_{\mathcal{X}_{-u}^2} \left(\int_{\mathcal{X}_u^2} \phi_1(x_u^{(n)}, x_{-u}^{(n)}) \phi_2(x_u^{(m)}, x_{-u}^{(m)}) \right. \\
& \left. d\mathbb{P}_{(\tilde{X}_u^{(n)}, \tilde{X}_u^{(m)}) | (\tilde{X}_{-u}^{(n)}, \tilde{X}_{-u}^{(m)}) = (x_{-u}^{(n)}, x_{-u}^{(m)})}(x_u^{(n)}, x_u^{(m)}) \right) d\mathbb{P}_{(\tilde{X}_{-u}^{(n)}, \tilde{X}_{-u}^{(m)})}(x_{-u}^{(n)}, x_{-u}^{(m)}) \\
= & \int_{\mathcal{X}_{-u}^2} \left(\int_{\mathcal{X}_u^2} \phi_1(x_u^{(n)}, x_{-u}^{(n)}) \phi_2(x_u^{(m)}, x_{-u}^{(m)}) \right. \\
& \left. d\mathbb{P}_{X_u | X_{-u} = x_{-u}^{(n)}} \otimes \mathbb{P}_{X_u | X_{-u} = x_{-u}^{(m)}}(x_u^{(n)}, x_u^{(m)}) \right) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(n)}, x_{-u}^{(m)}) \\
= & \int_{\mathcal{X}_{-u}^2} \left(\int_{\mathcal{X}_u} \phi_1(x_u^{(n)}, x_{-u}^{(n)}) d\mathbb{P}_{X_u | X_{-u} = x_{-u}^{(n)}}(x_u^{(n)}) \right) \\
& \left(\int_{\mathcal{X}_u} \phi_2(x_u^{(m)}, x_{-u}^{(m)}) d\mathbb{P}_{X_u | X_{-u} = x_{-u}^{(m)}}(x_u^{(m)}) \right) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(n)}, x_{-u}^{(m)}) \\
= & \int_{\mathcal{X}_{-u}} \left(\int_{\mathcal{X}_u} \phi_1(x_u^{(n)}, x_{-u}^{(n)}) d\mathbb{P}_{\tilde{X}_u | \tilde{X}_{-u} = x_{-u}^{(n)}}(x_u^{(n)}) \right) d\mathbb{P}_{\tilde{X}_{-u}}(x_{-u}^{(n)})
\end{aligned}$$

$$
\begin{aligned}
& \left(\int_{\mathcal{X}_u} \phi_2(x_u^{(m)}, x_{-u}^{(m)}) d\mathbb{P}_{\tilde{X}_u|\tilde{X}_{-u}=x_{-u}^{(m)}}(x_u^{(m)})\right) d\mathbb{P}_{\tilde{X}_{-u}}(x_{-u}^{(m)}) \\
= \quad & \mathrm{E}(\phi_1(\tilde{X}^{(n)}))\mathrm{E}(\phi_2(\tilde{X}^{(m)})).
\end{aligned}
$$

The above calculation can be extended to finite products of more than two terms. That concludes the proof of Lemma 6. □

Lemma 7. *For almost all* $\left((x_{-u}^{(n)})_n, \mathbf{h}\right)$, *we have:*

$$
\mathcal{L}\left((X_u^{(k_N(i))})_{i\leq N_I}|(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k}=\mathbf{h}\right) = \bigotimes_{i=1}^{N_I} \mathcal{L}\left(X_u|X_{-u} = x_{-u}^{(h_N(i))}\right).
$$

Proof. For all bounded Borel function ϕ,

$$
\begin{aligned}
& \mathrm{E}\left(\phi((X_u^{(k_N(i))})_{i\leq N_I})|(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k}=\mathbf{h}\right) \\
= \quad & \mathrm{E}\left(\phi\left((X_u^{(k_N(i))})_{i\leq N_I})\right)\Big|\,(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, (k_{N'}(i))_{i\leq N_I, N'\in\mathbb{N}^*} = (h_{N'}(i))_{i\leq N_I, N'\in\mathbb{N}^*}\right) \\
= \quad & \mathrm{E}\left(\phi\left((X_u^{(k_N(i))})_{i\leq N_I}\right)\Big|\,(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, (k_N(i))_{i\leq N_I} = (h_N(i))_{i\leq N_I}\right) \\
= \quad & \mathrm{E}\left(\phi\left((X_u^{(h_N(i))})_{i\leq N_I}\right)|(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n\right),
\end{aligned}
$$

using Lemmas 2 and 3 conditionally to $(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n$. Then,

$$
\begin{aligned}
& \mathrm{E}\left(\phi\left((X_u^{(h_N(i))})_{i\leq N_I}\right)|(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n\right) \\
= \quad & \int_{\mathcal{X}_u^{N_I}} \phi(x_u^{(1)}, ..., x_u^{(N_I)}) d\mathbb{P}_{(X_u^{(h_N(i))})_{i\leq N_I}|(X_{-u}^{(n)})_n=(x_{-u}^{(n)})_n}(x_u^{(1)}, ..., x_u^{(N_I)}) \\
= \quad & \int_{\mathcal{X}_u^{N_I}} \phi(x_u^{(1)}, ..., x_u^{(N_I)}) d\bigotimes_{i=1}^{N_I} \mathbb{P}_{X_u|X_{-u}=x_{-u}^{(h_N(i))}}(x_u^{(1)}, ..., x_u^{(N_I)}).
\end{aligned}
$$

That concludes the proof of Lemma 7. □

Recall that $X_{-u}^{(k_N(i)))} \underset{N\to+\infty}{\longrightarrow} X_{-u}^{(1)}$ $\mathbb{P}$-a.e., thus, for almost all $\left((x_{-u}^{(n)})_n, \mathbf{h}\right)$,

$$
x_{-u}^{(h_N(i))} \underset{N\to+\infty}{\longrightarrow} x_{-u}^{(1)}.
$$

Thus, using the continuity of the conditional distribution given by Lemma 5, for almost all $\left((x_{-u}^{(n)})_n, \mathbf{h}\right)$, we have,

$$
\mathcal{L}(X_u|X_{-u} = x_{-u}^{(h_N(i))}) \underset{N\to+\infty}{\overset{weakly}{\longrightarrow}} \mathcal{L}(X_u|X_{-u} = x_{-u}^{(1)}).
$$

Thus, for almost all $\left((x_{-u}^{(n)})_n, \mathbf{h}\right)$,

$$\bigotimes_{i=1}^{N_I} \mathcal{L}(X_u|X_{-u} = x_{-u}^{(h_N(i))}) \underset{N\to+\infty}{\overset{weakly}{\longrightarrow}} \bigotimes_{i=1}^{N_I} \mathcal{L}(X_u|X_{-u} = x_{-u}^{(1)}) = \mathcal{L}(\mathbf{Z}_u|X_{-u}^{(1)} = x_{-u}^{(1)}).$$

So, using Lemma 7, for almost all $\left((x_{-u}^{(n)})_n, \mathbf{h}\right)$,

$$\mathcal{L}\left((X_u^{(k_N(i))})_{i\leq N_I}|(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k} = \mathbf{h}\right) \underset{N\to+\infty}{\overset{weakly}{\longrightarrow}} \mathcal{L}(\mathbf{Z}_u|X_{-u}^{(1)} = x_{-u}^{(1)}).$$

So, for almost all $\left((x_{-u}^{(n)})_n, \mathbf{h}\right)$,

$$\mathcal{L}\left((X_u^{(k_N(i))})_{i\leq N_I}|(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k} = \mathbf{h}\right) \underset{N\to+\infty}{\overset{weakly}{\longrightarrow}} \mathcal{L}\left(\mathbf{Z}_u|(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k} = \mathbf{h}\right).$$

Using Slutsky lemma, for almost all $\left((x_{-u}^{(n)})_n, \mathbf{h}\right)$,

$$\mathcal{L}\left((X^{(k_N(i))})_{i\leq N_I}|(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k} = \mathbf{h}\right) \underset{N\to+\infty}{\overset{weakly}{\longrightarrow}} \mathcal{L}\left(\mathbf{Z}|(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k} = \mathbf{h}\right),$$

that concludes the proof of Proposition 43. □

Lemma 8. *The value of* $\mathrm{Var}(\widehat{E}_{u,1,MC})$ *is bounded by* $128\|f\|_\infty^4$.

Proof. As f is bounded, Φ is bounded by $\frac{1}{N_I-1}\sum_{k=1}^{N_I}(2\|f\|_\infty)^2 = \frac{N_I}{N_I-1}4\|f\|_\infty^2 \leq 8\|f\|_\infty^2$ so $\mathrm{Var}(\widehat{E}_{u,1})$ is bounded by $2\|\Phi\|_\infty^2 \leq 128\|f\|_\infty^4$. □

Proposition 44. *We have*

$$\mathrm{cov}(\widehat{E}_{u,1}, \widehat{E}_{u,2}) \underset{N\to+\infty}{\longrightarrow} 0.$$

Proof. We use the law of total covariance

$$\mathrm{cov}(\widehat{E}_{u,1}, \widehat{E}_{u,2}) = \mathrm{E}\left(\mathrm{cov}\left(\widehat{E}_{u,1}, \widehat{E}_{u,2}|X_{-u}^{(1)}, X_{-u}^{(2)}\right)\right) + \mathrm{cov}\left(\mathrm{E}(\widehat{E}_{u,1}|X_{-u}^{(1)}, X_{-u}^{(2)}), \mathrm{E}(\widehat{E}_{u,2}|X_{-u}^{(1)}, X_{-u}^{(2)})\right). \tag{I.5}$$

We will show that both terms go to 0 as N goes to $+\infty$. Let us compute the second term. Using Proposition 43,

$$\begin{aligned} & \mathrm{cov}\left(\mathrm{E}(\widehat{E}_{u,1}|X_{-u}^{(1)}, X_{-u}^{(2)}), \mathrm{E}(\widehat{E}_{u,2}|X_{-u}^{(1)}, X_{-u}^{(2)})\right) \\ = \; & \mathrm{E}\left(\mathrm{E}(\widehat{E}_{u,1}|X_{-u}^{(1)}, X_{-u}^{(2)})\mathrm{E}(\widehat{E}_{u,2}|X_{-u}^{(1)}, X_{-u}^{(2)})\right) - \mathrm{E}(\widehat{E}_{u,1})\mathrm{E}(\widehat{E}_{u,2}) \end{aligned}$$

$$
\begin{aligned}
\underset{N\to+\infty}{\longrightarrow} & \quad \mathrm{E}\left(\mathrm{Var}(Y|X_{-u}=X_{-u}^{(1)})\mathrm{Var}(Y|X_{-u}=X_{-u}^{(2)})\right)-E_u^2 \\
= & \quad 0.
\end{aligned}
$$

It remains to prove that $\mathrm{E}\left(\mathrm{cov}\left(\widehat{E}_{u,1},\widehat{E}_{u,2}|X_{-u}^{(1)},X_{-u}^{(2)}\right)\right)$ goes to 0. By dominated convergence theorem, it suffices to show that for almost all $(x_{-u}^{(1)},x_{-u}^{(2)})$,

$$
\mathrm{cov}\left(\widehat{E}_{u,1},\widehat{E}_{u,2}|X_{-u}^{(1)}=x_{-u}^{(1)},X_{-u}^{(2)}=x_{-u}^{(2)}\right)\underset{N\to+\infty}{\longrightarrow}0. \tag{I.6}
$$

From now on, we aim to proving Equation (I.6).

First, we want to prove Equation (I.6) for $x_{-u}^{(1)}\neq x_{-u}^{(2)}$. Using dominated convergence theorem and Proposition 43, it will suffice to show that (conditionally to $X_{-u}^{(1)}=x_{-u}^{(1)},\ X_{-u}^{(2)}=x_{-u}^{(2)}$), for almost all $((x_{-u}^{(n)})_{n\geq 3},\mathbf{h},\mathbf{h}')$,

$$
\mathrm{E}\left(\widehat{E}_{u,1},\widehat{E}_{u,2}|(X_{-u}^{(n)})_n=(x_{-u}^{(n)})_n,\mathbf{k}=\mathbf{h},\mathbf{k}'=\mathbf{h}'\right)\underset{N\to+\infty}{\longrightarrow}\mathrm{Var}\left(Y|X_{-u}=x_{-u}^{(1)}\right)\mathrm{Var}\left(Y|X_{-u}=x_{-u}^{(2)}\right).
$$

Let

$$
A:=\left\{\left((x_{-u}^{(n)})_n,\mathbf{h},\mathbf{h}'\right)\mid x_{-u}^{h_N(N_1)}\underset{N\to+\infty}{\longrightarrow}x_{-u}^{(1)},\ x_{-u}^{h'_N(N_1)}\underset{N\to+\infty}{\longrightarrow}x_{-u}^{(2)}\right\}.
$$

The set A has probability 1 thanks to Lemma 4. Let $\left((x_{-u}^{(n)})_n,\mathbf{h},\mathbf{h}'\right)\in A$ be such that $x_{-u}^{(1)}\neq x_{-u}^{(2)}$ and let $\delta:=d_{-u}(x_{-u}^{(1)},x_{-u}^{(2)})/2$. There exists N_1 such that for all $N\geq N_1$,

$$
d_{-u}\left(x_{-u}^{(1)},x_{-u}^{(h_N(N_I))}\right)<\frac{\delta}{2},\quad d_{-u}\left(x_{-u}^{(2)},x_{-u}^{(h'_N(N_I))}\right)<\frac{\delta}{2}.
$$

Thus, for all $N\geq N_1$,

$$
\begin{aligned}
& E(\widehat{E}_{u,1}\widehat{E}_{u,2}|(X_{-u}^{(n)})_n=(x_{-u}^{(n)})_n,\mathbf{k}=\mathbf{h},\mathbf{k}'=\mathbf{h}') \\
= & \quad \mathrm{E}\left[\Phi\left((X^{k_N(i)})_{i\leq N_I}\right)\Phi\left((X^{k'_N(i)})_{i\leq N_I}\right)\Big|\,(X_{-u}^{(n)})_n=(x_{-u}^{(n)})_n,\mathbf{k}=\mathbf{h},\mathbf{k}'=\mathbf{h}'\right] \\
= & \quad \mathrm{E}\left[\Phi\left((X^{k_N(i)})_{i\leq N_I}\right)\Phi\left((X^{k'_N(i)})_{i\leq N_I}\right)\Big|\,(X_{-u}^{(n)})_n=(x_{-u}^{(n)})_n,\mathbf{k}_N=\mathbf{h}_N,\mathbf{k}'_N=\mathbf{h}'_N\right] \\
= & \quad \mathrm{E}\left[\Phi\left((X^{h_N(i)})_{i\leq N_I}\right)\Phi\left((X^{k'_N(i)})_{i\leq N_I}\right)\Big|\,(X_{-u}^{(n)})_n=(x_{-u}^{(n)})_n,\mathbf{k}'_N=\mathbf{h}'_N\right] \\
= & \quad \mathrm{E}\left[\Phi\left((X^{h_N(i)})_{i\leq N_I}\right)\Phi\left((X^{h'_N(i)})_{i\leq N_I}\right)\Big|\,(X_{-u}^{(n)})_n=(x_{-u}^{(n)})_n\right] \\
= & \quad \mathrm{E}\left[\Phi\left((x_{-u}^{h_N(i)})_{i\leq N_I},(X_u^{h_N(i)})_{i\leq N_I}\right)\Phi\left((x_{-u}^{h'_N(i)})_{i\leq N_I},(X_u^{h'_N(i)})_{i\leq N_I}\right)\Big|\,(X_{-u}^{(n)})_n=(x_{-u}^{(n)})_n\right] \\
= & \quad \mathrm{E}\left[\Phi\left((x_{-u}^{h_N(i)})_{i\leq N_I},(X_u^{h_N(i)})_{i\leq N_I}\right)\Big|\,(X_{-u}^{(n)})_n=(x_{-u}^{(n)})_n\right] \\
& \quad \mathrm{E}\left[\Phi\left((x_{-u}^{h'_N(i)})_{i\leq N_I},(X_u^{h'_N(i)})_{i\leq N_I}\right)\Big|\,(X_{-u}^{(n)})_n=(x_{-u}^{(n)})_n\right]
\end{aligned}
$$

$$\begin{aligned} &= \quad \mathrm{E}\left[\widehat{E}_{u,1}\middle|\,(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k}=\mathbf{h}\right] \mathrm{E}\left[\widehat{E}_{u,2}\middle|\,(X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k}'=\mathbf{h}'\right] \\ &\underset{N\to+\infty}{\longrightarrow} \quad \mathrm{Var}\left[Y|\,X_{-u}=x_{-u}^{(1)}\right] \mathrm{Var}\left[Y|\,X_{-u}=x_{-u}^{(2)}\right], \end{aligned}$$

thanks to Proposition 43.

Assume now that $X_{-u}^{(1)} = X_{-u}^{(2)} = x_{-u}$. We can assume without lost of generality that $\mathbb{P}(X_{-u}=x_{-u})>0$ because if we write $H := \{x_{-u}|\ \mathbb{P}(X_{-u}=x_{-u})=0\}$, we have $\mathbb{P}(X_{-u}^{(1)} = X_{-u}^{(2)} \in H)=0$. We have to show that

$$\mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1)} = X_{-u}^{(2)} = x_{-u}\right) - \mathrm{Var}(Y|X_{-u}=x_{-u})^2 \underset{N\to+\infty}{\longrightarrow} 0.$$

Let $\varepsilon>0$.

Let M_N the number of observations which are equal to x_{-u},

$$M_N := \#\{n\leq N\ :\ X_{-u}^{(n)} = x_{-u}\},$$

and let H_N be the number of nearest neighbours (up to N_I-nearest) shared by $X_{-u}^{(1)}$ and $X_{-u}^{(2)}$,

$$H_N := \#\left[\{k_N(i)\ :\ i\leq N_I\}\cap\{k'_N(i)\ :\ i\leq N_I\}\right].$$

If $M_n = m \geq 2N_I$, $X_{-u}^{(1)} = x_{-u} = X_{-u}^{(2)}$, then the N_I-nearest neighbours $\mathbf{k}_N$ of $X_{-u}^{(1)}$ and $\mathbf{k}'_N$ of $X_{-u}^{(2)}$ are independent and are samples of uniformly distributed variables on the same set of cardinal m, without replacement. Thus,

$$\begin{aligned} & \mathbb{P}(H_N=0|M_N=m, X_{-u}^{(1)} = X_{-u}^{(2)} = x_{-u}) \\ = \quad & \frac{\begin{pmatrix} m-N_I \\ N_I\end{pmatrix}}{\begin{pmatrix} m \\ N_I\end{pmatrix}} \\ = \quad & \frac{(m-2N_I+1)(m-2N_I+2)...(m-N_I)}{(m-N_I+1)(m-N_I+2)...m} \\ \underset{m\to+\infty}{\longrightarrow} \quad & 1. \end{aligned}$$

Thus, there exists m_1 such that

$$\alpha_{m_1} := \mathbb{P}(H_N=0|M_N\geq m_1, X_{-u}^{(1)} = X_{-u}^{(2)} = x_{-u}) > 1 - \frac{\varepsilon}{5\|\Phi\|_\infty^2}. \tag{I.7}$$

So,

$$\begin{aligned}
& \mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u}\right) \\
= & \mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u},M_N<m_1\right)\mathbb{P}(M_N<m_1|X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u}) \\
& +\mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u},M_N\geq m_1\right)\mathbb{P}(M_N\geq m_1|X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u}).
\end{aligned}$$

Let

$$\beta_N := \mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u},M_N<m_1\right)\mathbb{P}(M_N<m_1|X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u}).$$

Conditionally to $X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u}$, we know that $M_N-2\sim\mathcal{B}\left(N-2,\mathbb{P}(X_{-u}=x_{-u})\right)$, the binomial distribution. Thus, there exists N_1 such that for all $N\geq N_1$,

$$\mathbb{P}\left(M_N<m_1|X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u}\right)<\frac{\varepsilon}{5\max(1,\|\Phi\|_\infty^2)}, \tag{I.8}$$

and so, for all $N\geq N_1$, $\beta_N<\varepsilon/5$. Furthermore

$$\begin{aligned}
& \mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u},M_N\geq m_1\right) \\
= & \mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u},M_N\geq m_1,H_N=0\right) \\
& \times\mathbb{P}(H_N=0|X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u},M_N\geq m_1) \\
& +\mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u},M_N\geq m_1,H_N\geq 1\right) \\
& \times\mathbb{P}(H_N\geq 1|X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u},M_N\geq m_1).
\end{aligned}$$

Let

$$\gamma_N := \mathbb{P}\left(M_N\geq m_1|X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u}\right).$$

Moreover, conditionally to $X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u},M_N\geq m_1$, $H_N=0$ implies that $\widehat{E}_{u,1}\perp\!\!\!\perp\widehat{E}_{u,2}$ thanks to Lemma 9.

Lemma 9. *Conditionally to $X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u},M_N\geq m_1$, $H_N=0$, the vector $\left((X^{(k_N(i))})_{i\leq N_I},(X^{(k'_N(i))})_{i\leq N_I}\right)$ is composed of $2N_I$ i.i.d. random variables of distribution X conditionally to $X_{-u}=x_{-u}$.*

Proof. We know that, conditionally to $X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u},M_N\geq m_1$, $H_N=0$, the vector $\left((X_{-u}^{(k_N(i))})_{i\leq N_I},(X_{-u}^{(k'_N(i))})_{i\leq N_I}\right)$ is constant equal to $(x_{-u})_{i\leq 2N_I}$. It suffices to show that, conditionally to $X_{-u}^{(1)}=X_{-u}^{(2)}=x_{-u},M_N\geq m_1$, $H_N=0$, the vector $\left((X_{u}^{(k_N(i))})_{i\leq N_I},(X_{u}^{(k'_N(i))})_{i\leq N_I}\right)$ is composed of $2N_I$ i.i.d. random variables of distribution X conditionally to $X_{-u} = x_{-u}$. Let $((x_{-u}^{(n)})_n, \mathbf{h}_N, \mathbf{h}'_N)$ such that $X_{-u}^{(1)} = X_{-u}^{(2)} = x_{-u}, M_N \geq m_1$ and $H_N = 0$. As $M_N \geq m_1 \geq N_I$, for all $i \leq N_I$, we have $x_{-u}^{(k_N(i))} = x_{-u} = x_{-u}^{(k'_N(i))}$. As $H_N = 0$, then, for all i and j smaller than N_I, $h_N(i) \neq h'_N(j)$. Thus, we have for any bounded Borel function ϕ,

$$\begin{aligned}
& \mathrm{E}\left(\phi\left[(X_u^{(k_N(i))})_{i\leq N_I}, (X_u^{(k'_N(i))})_{i\leq N_I}\right]\Big|\, (X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k}_N = \mathbf{h}_N, \mathbf{k}'_N = \mathbf{h}'_N\right) \\
= \ & \mathrm{E}\left(\phi\left[(X_u^{(h_N(i))})_{i\leq N_I}, (X_u^{(k'_N(i))})_{i\leq N_I}\right]\Big|\, (X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \mathbf{k}'_N = \mathbf{h}'_N\right) \\
= \ & \mathrm{E}\left(\phi\left[(X_u^{(h_N(i))})_{i\leq N_I}, (X_u^{(h'_N(i))})_{i\leq N_I}\right]\Big|\, (X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n, \right) \\
= \ & \mathrm{E}\Bigg(\phi\left[(X_u^{(h_N(i))})_{i\leq N_I}, (X_u^{(h'_N(i))})_{i\leq N_I}\right]\Bigg|(X_{-u}^{(h_N(i))})_{i\leq N_I} = (x_{-u})_{i\leq N_I}, \\
& (X_{-u}^{(h'_N(i))})_{i\leq N_I} = (x_{-u})_{i\leq N_I}\Bigg) \\
= \ & \mathrm{E}\left(\phi\left[(X_u^{(i)})_{i\leq N_I}, (X_u^{(i+N_I)})_{i\leq N_I}\right]\big|\, (X_{-u}^{(i)})_{i\leq 2N_I} = (x_{-u})_{i\leq 2N_I}\right).
\end{aligned}$$

Thus,

$$\begin{aligned}
& \mathrm{E}\left(\phi\left[(X_u^{(k_N(i))})_{i\leq N_I}, (X_u^{(k'_N(i))})_{i\leq N_I}\right]\Big|\, X_{-u}^{(1)} = X_{-u}^{(2)} = x_{-u}, M_N \geq m_1, H_N = 0\right) \\
= \ & \mathrm{E}\Bigg\{\mathrm{E}\Bigg(\phi\left[(X_u^{(k_N(i))})_{i\leq N_I}, (X_u^{(k'_N(i))})_{i\leq N_I}\right]\Bigg|X_{-u}^{(1)} = X_{-u}^{(2)} = x_{-u}, \\
& M_N \geq m_1, H_N = 0, (X_{-u}^{(n)})_n, \mathbf{k}, \mathbf{k}'\Bigg)\Bigg\} \\
= \ & \mathrm{E}\left\{\mathrm{E}\left(\phi\left[(X_u^{(i)})_{i\leq N_I}, (X_u^{(i+N_I)})_{i\leq N_I}\right]\big|\, (X_{-u}^{(i)})_{i\leq 2N_I} = (x_{-u})_{i\leq 2N_I}\right)\right\} \\
= \ & \mathrm{E}\left(\phi\left[(X_u^{(i)})_{i\leq N_I}, (X_u^{(i+N_I)})_{i\leq N_I}\right]\big|\, (X_{-u}^{(i)})_{i\leq 2N_I} = (x_{-u})_{i\leq 2N_I}\right),
\end{aligned}$$

that concludes the proof of Lemma 9. □

Thus

$$\begin{aligned}
& \mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1)} = X_{-u}^{(2)} = x_{-u}, M_N \geq m_1,\ H_N = 0\right) \\
= \ & \mathrm{E}\left(\widehat{E}_{u,1}|X_{-u}^{(1)} = X_{-u}^{(2)} = x_{-u}, M_N \geq m_1,\ H_N = 0\right)^2
\end{aligned}$$

and so, using Proposition 43, there exists N_2 such that for all $N \geq N_2$,

$$\left|\mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1)} = X_{-u}^{(2)} = x_{-u}, M_N \geq m_1,\ H_N = 0\right) - \mathrm{Var}(Y|X_{-u} = x_{-u})^2\right| < \frac{\varepsilon}{5}. \tag{I.9}$$

Thus, for all $N \geq \max(N_1, N_2)$,

$$\begin{aligned}
& \left| \mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1)} = X_{-u}^{(2)} = x_{-u}\right) - \mathrm{Var}(Y|X_{-u} = x_{-u})^2 \right| \\
\leq \quad & |\beta_N| + \left|\gamma_N \mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1)} = X_{-u}^{(2)} = x_{-u}, M_N \geq m_1,\ H_N \geq 1\right)(1-\alpha_{m_1})\right| \\
& + \left|\gamma_N \alpha_{m_1} \mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1)} = X_{-u}^{(2)} = x_{-u}, M_N \geq m_1,\ H_N = 0\right) - \mathrm{Var}(Y|X_{-u} = x_{-u})^2\right|.
\end{aligned}$$

The upper-bound is a sum of three terms. The first one is bounded by $\varepsilon/5$ using Equation I.8 and the second one is bounded by $\varepsilon/5$ using Equation I.7. For the last one, we use that, for all $C \in \mathbb{R}$,

$$\gamma_N \alpha_{m_1} C = (\gamma_N \alpha_{m_1} - 1)C + C.$$

Thus,

$$\begin{aligned}
& \left| \mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1)} = X_{-u}^{(2)} = x_{-u}\right) - \mathrm{Var}(Y|X_{-u} = x_{-u})^2 \right| \\
\leq \quad & \frac{\varepsilon}{5} + \frac{\varepsilon}{5} + |\gamma_N \alpha_{m_1} - 1| \, \|\Phi\|_\infty^2 \\
& + \left| \mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1)} = X_{-u}^{(2)} = x_{-u}, M_N \geq m_1,\ H_N = 0\right) - \mathrm{Var}(Y|X_{-u} = x_{-u})^2 \right| \\
\leq \quad & \frac{3\varepsilon}{5} + \left(|\gamma_N - 1|\alpha_N + |\alpha_N - 1|\right) \|\Phi\|_\infty^2 \quad \text{using Equation I.9} \\
\leq \quad & \varepsilon,
\end{aligned}$$

using Equation I.8 and Equation I.7. Finally, we proved that

$$\mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1)} = X_{-u}^{(2)} = x_{-u}\right) - \mathrm{Var}(Y|X_{-u} = x_{-u})^2 \underset{N \to +\infty}{\longrightarrow} 0.$$

Hence, Equation (I.6) is proved and the proof of Proposition 44 is concluded. ☐

Proposition 45. *We have*

$$\widehat{E}_u - \mathrm{E}\left(\widehat{E}_{u,1}\right) \underset{\substack{N \to +\infty, \\ N_u \to +\infty}}{\overset{\mathbb{P}}{\longrightarrow}} 0. \tag{I.10}$$

Proof. Let $\varepsilon > 0$. By Chebyshev's inequality,

$$\mathbb{P}\left(\left|\widehat{E}_u - \mathrm{E}\left(\widehat{E}_u\right)\right| > \varepsilon\right) \leq \frac{\mathrm{Var}(\widehat{E}_u)}{\varepsilon^2}. \tag{I.11}$$

If $(s(l))_{l \leq N_u}$ is a sample of uniformly distributed variables on $[1:N]$ with replacement, we remark that for all $i \neq j$,

$$\mathrm{cov}\left(\widehat{E}_{u,s(i)}, \widehat{E}_{u,s(j)}\right)$$

$$\begin{aligned}
&= \mathrm{E}(\widehat{E}_{u,s(i)}\widehat{E}_{u,s(j)}) - \mathrm{E}(\widehat{E}_{u,s(i)})\mathrm{E}(\widehat{E}_{u,s(j)}) \\
&= \mathrm{E}(\widehat{E}_{u,s(i)}\widehat{E}_{u,s(j)}|s(i) \neq s(j))\mathbb{P}(s(i) \neq s(j)) \\
&\quad +\mathrm{E}(\widehat{E}_{u,s(i)}\widehat{E}_{u,s(j)}|s(i) = s(j))\mathbb{P}(s(i) = s(j)) - \mathrm{E}(\widehat{E}_{u,s(i)})\mathrm{E}(\widehat{E}_{u,s(j)}) \\
&= \left[\mathrm{E}(\widehat{E}_{u,s(i)}\widehat{E}_{u,s(j)}|s(i) \neq s(j)) - \mathrm{E}(\widehat{E}_{u,1})\mathrm{E}(\widehat{E}_{u,2})\right]\mathbb{P}(s(i) \neq s(j)) \\
&\quad + \left[\mathrm{E}(\widehat{E}_{u,s(i)}\widehat{E}_{u,s(i)}|s(i) = s(j)) - \mathrm{E}(\widehat{E}_{u,1})^2\right]\mathbb{P}(s(i) = s(j)) \\
&= \left[\mathrm{E}(\widehat{E}_{u,1}\widehat{E}_{u,2}|s(i) = 1, s(j) = 2) - \mathrm{E}(\widehat{E}_{u,1})\mathrm{E}(\widehat{E}_{u,2})\right]\mathbb{P}(s(i) \neq s(j)) \\
&\quad + \left[\mathrm{E}(\widehat{E}_{u,1}\widehat{E}_{u,1}|s(i) = s(j) = 1) - \mathrm{E}(\widehat{E}_{u,1})^2\right]\mathbb{P}(s(i) = s(j)) \\
&= \mathrm{cov}\left(\widehat{E}_{u,1}, \widehat{E}_{u,2}\right)\mathbb{P}(s(i) \neq s(j)) + \mathrm{Var}\left(\widehat{E}_{u,1}\right)\mathbb{P}(s(i) = s(j)),
\end{aligned}$$

thus

$$\begin{aligned}
\mathrm{Var}(\widehat{E}_u) &= \frac{1}{N_u^2}\sum_{i,j=1}^{N_u}\mathrm{cov}\left(\widehat{E}_{u,s(i)}, \widehat{E}_{u,s(j)}\right) \\
&= \frac{1}{N_u^2}\sum_{i\neq j=1}^{N_u}\mathrm{cov}\left(\widehat{E}_{u,1}, \widehat{E}_{u,2}\right)\mathbb{P}(s(i) \neq s(j)) \\
&\quad +\frac{1}{N_u^2}\sum_{i\neq j=1}^{N_u}\mathrm{Var}\left(\widehat{E}_{u,1}\right)\mathbb{P}(s(i) = s(j)) + \frac{1}{N_u^2}\sum_{i=1}^{N_u}\mathrm{Var}\left(\widehat{E}_{u,s(i)}\right) \\
&\leq \frac{1}{N_u^2}\sum_{i\neq j=1}^{N_u}\left|\mathrm{cov}\left(\widehat{E}_{u,1}, \widehat{E}_{u,2}\right)\right| \\
&\quad +\frac{1}{N_u^2}\sum_{i\neq j=1}^{N_u}\mathrm{Var}\left(\widehat{E}_{u,1}\right)\frac{1}{N} + \frac{1}{N_u^2}\sum_{i=1}^{N_u}\mathrm{Var}\left(\widehat{E}_{u,1}\right) \\
&\leq \left|\mathrm{cov}\left(\widehat{E}_{u,1}, \widehat{E}_{u,2}\right)\right| + \mathrm{Var}\left(\widehat{E}_{u,1}\right)\left(\frac{1}{N} + \frac{1}{N_u}\right).
\end{aligned}$$

If $(s(l))_{l\leq N_u}$ is a sample of uniformly distributed variables on $[1:N]$ without replacement, we have

$$\begin{aligned}
\mathrm{Var}(\widehat{E}_u) &= \frac{1}{N_u^2}\sum_{i,j=1}^{N_u}\mathrm{cov}\left(\widehat{E}_{u,s(i)}, \widehat{E}_{u,s(j)}\right) \\
&= \frac{1}{N_u^2}\sum_{i\neq j=1}^{N_u}\mathrm{cov}\left(\widehat{E}_{u,s(i)}, \widehat{E}_{u,s(j)}\right) + \frac{1}{N_u^2}\sum_{i=1}^{N_u}\mathrm{Var}\left(\widehat{E}_{u,s(i)}\right)
\end{aligned}$$

$$= \frac{N_u - 1}{N_u} \mathrm{cov}\left(\widehat{E}_{u,1}, \widehat{E}_{u,2}\right) + \frac{1}{N_u} \mathrm{Var}\left(\widehat{E}_{u,1}\right).$$

In both cases (with or without replacement), thanks to Proposition 44, we have

$$\mathbb{P}\left(\left|\widehat{E}_u - \mathrm{E}\left(\widehat{E}_u\right)\right| > \varepsilon\right) \underset{\substack{N \to +\infty,\\ N_u \to +\infty}}{\longrightarrow} 0.$$

□

Now, to prove Theorem 3, we only have to use Proposition 43 (which can be applied thanks to Lemma 5) and Proposition 45.

A.2 Proof for rate of convergence: Theorems 4 and 6

We want to prove Theorems 4 and 6 about the rate of convergence of the double Monte-Carlo and Pick-and-Freeze estimators. We have to add some notation. We will write $C_{\sup}$ for a generic non-negative finite constant (depending only on u, f and the distribution of X). The actual value of $C_{\sup}$ is of no interest and can change in the same sequence of equations. Similarly, we will write $C_{\inf}$ a generic strictly positive constant. We will write $C_{\sup}(\varepsilon)$ for a generic non-negative finite constant depending only on ε, u, f and the distribution of X.

Recall that for all i, $\mathcal{X}_i$ is a compact subset of $\mathbb{R}$ and that f is $\mathcal{C}^1$. Moreover recall that X has a probability density f_X with respect to λ_p (the Lebesgue measure on $\mathbb{R}^p$) such that λ_p-a.e., we have $0 < C_{\inf} \leq f_X \leq C_{\sup}$, and such that f_X is Lipschitz continuous.

Note that with these assumptions, Φ is $\mathcal{C}^1$ on the compact set $\mathcal{X}$ and so Lipschitz continuous. For all n, we will write d for the euclidean distance on $\mathbb{R}^n$ (for any value of n) and $B(x, r)$ for the open ball of radius r and center x in $\mathbb{R}^n$. We also let $\mathcal{S}(x, r)$ be the sphere of center x and radius r.

Remark that

$$\begin{aligned}
& \mathbb{P}\left(d(X_{-u}^{(1)}, X_{-u}^{(2)}) = d(X_{-u}^{(1)}, X_{-u}^{(3)})\right) \\
= & \int_{\mathcal{X}_{-u}^2} \mathbb{P}\left(d(x_{-u}^{(1)}, x_{-u}^{(2)}) = d(x_{-u}^{(1)}, X_{-u}^{(3)})\right) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)}, x_{-u}^{(2)}) \\
\leq & \; C_{\sup} \int_{\mathcal{X}_{-u}^2} \lambda_{|-u|}\left(\mathcal{S}(x_{-u}^{(1)}, d(x_{-u}^{(1)}, x_{-u}^{(2)}))\right) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)}, x_{-u}^{(2)}) \\
= & \; 0,
\end{aligned}$$

because the Lebesgue measure of the sphere $\mathcal{S}(x_{-u}^{(1)}, d(x_{-u}^{(1)}, x_{-u}^{(2)}))$ is zero. Thus, almost everywhere, for all l and all $i \neq j$,

$$d\left(X_{-u}^{(l)}, X_{-u}^{(i)}\right) \neq d\left(X_{-u}^{(l)}, X_{-u}^{(j)}\right).$$

Thus, the indices of the nearest neighbours $(k_N(l,i))_{l,i}$ are constant random variables conditionally to $(X_{-u}^{(n)})_n$ or to $(X_{-u}^{(n)})_{n\leq N}$. In particular, for all N and l, $k_N(l,1) = l$. Thanks to Doob-Dynkin lemma, we can write, abusing notation, $k_N(l,i)(\omega) = k_N(l,i)[(X_{-u}^{(n)}(\omega))_n] = k_N(l,i)[(X_{-u}^{(n)}(\omega))_{n\leq N}]$. To simplify notation, let us write $k_N(i) := k_N(1,i)$ (the index of one i-th neighbour of $X_{-u}^{(1)}$) and $k'_N(i) := k_N(2,i)$ (the index of one i-th neighbour of $X_{-u}^{(2)}$).

Remark 40. *We can prove the rate of convergence in a more general framework than the Euclidean space with the Lebesgue measure. It suffices to have a compact set $\mathcal{X}$ with a dominating finite measure $\mu = \bigotimes \mu_i$ such that for μ_i-almost all $x_i \in \mathcal{X}_i$ and for all $\delta > 0$,*

$$C_{\inf}\delta \leq \mu_i(B(x_i,\delta)) = \mu_i(\overline{B}(x_i,\delta)) \leq C_{\sup}\delta.$$

We prove Theorems 4 and 6 step by step.

Lemma 10. *Assume that $(a_i)_i$ and $(b_i)_i$ are sequences such that for all i, $|a_i| \leq M$, $|b_i| \leq M$ and $|a_i - b_i| \leq \varepsilon$. Then, for all $N \in \mathbb{N}^*$*

$$\left|\prod_{i=1}^N a_i - \prod_{i=1}^N b_i\right| \leq NM^{N-1}\varepsilon.$$

Proof. By induction. □

Lemma 11. *If for all $i \leq N$, $d(x_{-u}^{(i)}, \mathbf{y}_{-u}^{(i)}) < \varepsilon$, then, for all $(\mathbf{a}_{-u}^{(i)})_{i\leq N_I} \in \mathcal{X}_{-u}^{N_I}$,*

$$\begin{aligned} &\left| \mathrm{E}\left[\Phi\left((\mathbf{a}_{-u}^{(i)})_{i\leq N_I}, (X_u^{(i)})_{i\leq N_I}\right) \middle| (X_{-u}^{(i)})_{i\leq N_I} = (x_{-u}^{(i)})_{i\leq N_I}\right]\right. \\ - \;& \left.\mathrm{E}\left[\Phi\left((\mathbf{a}_{-u}^{(i)})_{i\leq N_I}, (X_u^{(i)})_{i\leq N_I}\right) \middle| (X_{-u}^{(i)})_{i\leq N_I} = (\mathbf{y}_{-u}^{(i)})_{i\leq N_I}\right]\right| \;\leq C_{\sup}\varepsilon. \end{aligned}$$

Proof.

$$\begin{aligned} & \left| \mathrm{E}\left[\Phi\left((\mathbf{a}_{-u}^{(i)})_{i\leq N_I}, (X_u^{(i)})_{i\leq N_I}\right) \middle| (X_{-u}^{(i)})_{i\leq N_I} = (x_{-u}^{(i)})_{i\leq N_I}\right]\right. \\ & \left. - \mathrm{E}\left[\Phi\left((\mathbf{a}_{-u}^{(i)})_{i\leq N_I}, (X_u^{(i)})_{i\leq N_I}\right) \middle| (X_{-u}^{(i)})_{i\leq N_I} = (\mathbf{y}_{-u}^{(i)})_{i\leq N_I}\right]\right| \\ = \;& \left| \int_{\mathcal{X}_u^{N_I}} \Phi((\mathbf{a}_{-u}^{(i)})_{i\leq N_I}, (x_u^{(i)})_{i\leq N_I}) \left(f_{(X_u^{(i)})_{i\leq N_I}|(X_{-u}^{(i)})_{i\leq N_I}=(x_{-u}^{(i)})_{i\leq N_I}}((x_u^{(i)})_{i\leq N_I})\right.\right. \\ & \left.\left. - f_{(X_u^{(i)})_{i\leq N_I}|(X_{-u}^{(i)})_{i\leq N_I}=(\mathbf{y}_{-u}^{(i)})_{i\leq N_I}}((x_u^{(i)})_{i\leq k})\right) d((x_u^{(i)})_{i\leq N_I})\right| \\ \leq \;& C_{\sup} \int_{\mathcal{X}_u^{N_I}} \left| \prod_{i=1}^{N_I} f_{X_u|X_{-u}=x_{-u}^{(i)}}(x_u^{(i)}) - \prod_{i=1}^{N_I} f_{X_u|X_{-u}=\mathbf{y}_{-u}^{(i)}}(x_u^{(i)})\right| d((x_u^{(i)})_{i\leq N_I}). \end{aligned}$$

We know that,

$$\begin{aligned}
& \left|f_{X_u|X_{-u}=x_{-u}}(x_u) - f_{X_u|X_{-u}=\mathbf{y}_{-u}}(x_u)\right| \\
\leq & \left|\frac{f_X(x_u,x_{-u})}{\int_{\mathcal{X}_u} f_X(x'_u,x_{-u})d(x'_u)} - \frac{f_X(x_u,\mathbf{y}_{-u})}{\int_{\mathcal{X}_u} f_X(x'_u,\mathbf{y}_{-u})d(x'_u)}\right| \\
\leq & \frac{1}{\int_{\mathcal{X}_u} f_X(x'_u,x_{-u})d(x'_u)} \left|f_X(x_u,x_{-u}) - f_X(x_u,\mathbf{y}_{-u})\right| \\
& + f_X(x_u,\mathbf{y}_{-u}) \left|\frac{1}{\int_{\mathcal{X}_u} f_X(x'_u,x_{-u})d(x'_u)} - \frac{1}{\int_{\mathcal{X}_u} f_X(x'_u,\mathbf{y}_{-u})d(x'_u)}\right| \\
\leq & C_{\sup}\left|f_X(x_u,x_{-u}) - f_X(x_u,\mathbf{y}_{-u})\right| + C_{\sup}\left|f_X(x_u,x_{-u}) - f_X(x_u,\mathbf{y}_{-u})\right| \\
\leq & C_{\sup} d(x_{-u},\mathbf{y}_{-u}).
\end{aligned}$$

Thus, for all $i \in [1:N_i]$ and for all $x_u^{(i)}$,

$$\left|f_{X_u|X_{-u}=x_{-u}^{(i)}}(x_u^{(i)}) - f_{X_u|X_{-u}=\mathbf{y}_{-u}^{(i)}}(x_u^{(i)})\right| \leq C_{\sup}\varepsilon.$$

Thus, using Lemma 10,

$$\begin{aligned}
& \left|\mathrm{E}\left[\Phi\left((\mathbf{a}_{-u}^{(i)})_{i\leq N_I},(X_u^{(i)})_{i\leq N_I}\right)\middle|(X_{-u}^{(i)})_{i\leq N_I} = (x_{-u}^{(i)})_{i\leq N_I}\right]\right. \\
& \left.-\,\mathrm{E}\left[\Phi\left((\mathbf{a}_{-u}^{(i)})_{i\leq N_I},(X_u^{(i)})_{i\leq N_I}\right)\middle|(X_{-u}^{(i)})_{i\leq N_I} = (\mathbf{y}_{-u}^{(i)})_{i\leq N_I}\right]\right| \leq C_{\sup}\varepsilon.
\end{aligned}$$

□

Lemma 12. *If for all i, $d(x_{-u}^{(i)},\mathbf{y}_{-u}^{(i)}) < \varepsilon$, then*

$$\begin{aligned}
& \left|\mathrm{E}\left[\Phi\left((x_{-u}^{(i)})_{i\leq N_I},(X_u^{(i)})_{i\leq N_I}\right)\middle|(X_{-u}^{(i)})_{i\leq N_I} = (x_{-u}^{(i)})_{i\leq N_I}\right]\right. \\
- & \left.\mathrm{E}\left[\Phi\left((\mathbf{y}_{-u}^{(i)})_{i\leq N_I},(X_u^{(i)})_{i\leq N_I}\right)\middle|(X_{-u}^{(i)})_{i\leq N_I} = (\mathbf{y}_{-u}^{(i)})_{i\leq N_I}\right]\right| \quad \leq C_{\sup}\varepsilon.
\end{aligned}$$

Proof.

$$\begin{aligned}
& \left|\mathrm{E}\left[\Phi\left((x_{-u}^{(i)})_{i\leq N_I},(X_u^{(i)})_{i\leq N_I}\right)\middle|(X_{-u}^{(i)})_{i\leq N_I} = (x_{-u}^{(i)})_{i\leq N_I}\right]\right. \\
& \left.-\,\mathrm{E}\left[\Phi\left((\mathbf{y}_{-u}^{(i)})_{i\leq N_I},(X_u^{(i)})_{i\leq N_I}\right)\middle|(X_{-u}^{(i)})_{i\leq N_I} = (\mathbf{y}_{-u}^{(i)})_{i\leq N_I}\right]\right| \\
\leq & \left|\mathrm{E}\left[\Phi\left((x_{-u}^{(i)})_{i\leq N_I},(X_u^{(i)})_{i\leq N_I}\right)\middle|(X_{-u}^{(i)})_{i\leq N_I} = (x_{-u}^{(i)})_{i\leq N_I}\right]\right. \\
& \left.-\,\mathrm{E}\left[\Phi\left((x_{-u}^{(i)})_{i\leq N_I},(X_u^{(i)})_{i\leq N_I}\right)\middle|(X_{-u}^{(i)})_{i\leq N_I} = (\mathbf{y}_{-u}^{(i)})_{i\leq N_I}\right]\right| \\
& +\left|\mathrm{E}\left[\Phi\left((x_{-u}^{(i)})_{i\leq N_I},(X_u^{(i)})_{i\leq N_I}\right) - \Phi\left((\mathbf{y}_{-u}^{(i)})_{i\leq N_I},(X_u^{(i)})_{i\leq N_I}\right)|(X_{-u}^{(i)})_{i\leq N_I} = (\mathbf{y}_{-u}^{(i)})_{i\leq N_I}\right]\right| \\
\leq & C_{\sup}\varepsilon + C_{\sup}\varepsilon,
\end{aligned}$$

using Lemma 11 and using that Φ is Lipschitz continuous on $\mathcal{X}$. □

Lemma 13. *There exists $C_{\sup} < +\infty$ such that for all $a > 0$,*

$$\mathbb{P}\left(d\left(X_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}\right) \geq a \middle| X_{-u}^{(1)}\right) \leq C_{\sup} N^{N_I} (1 - C_{\inf} a^{|-u|})^{N-N_I}. \tag{I.12}$$

Proof. Let $K(a) := \#\{n \in [2:N],\ d(X_{-u}^{(1)}, X_{-u}^{(n)}) < a\}$. Conditionally to $X_{-u}^{(1)}$, $K(a) \sim \mathcal{B}(N-1, p(a, X_{-u}^{(1)}))$, writing $p(a, X_{-u}^{(1)}) := \mathbb{P}(d(X_{-u}^{(1)}, X_{-u}^{(2)}) < a | X_{-u}^{(1)})$. Thus,

$$\begin{aligned}
& \mathbb{P}\left(d\left(X_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}\right) \geq a \middle| X_{-u}^{(1)}\right) \\
= \ & \mathbb{P}\left(K(a) \leq N_I - 1 | X_{-u}^{(1)}\right) \\
= \ & \sum_{k=0}^{N_I-1} \binom{N-1}{k} p(a, X_{-u}^{(1)})^k (1 - p(a, X_{-u}^{(1)}))^{N-1-k} \\
\leq \ & N_I \binom{N-1}{N_I-1} (1 - p(a, X_{-u}^{(1)}))^{N-N_I} \\
\leq \ & C_{\sup} N^{N_I} (1 - p(a, X_{-u}^{(1)}))^{N-N_I}.
\end{aligned}$$

We know that

$$\begin{aligned}
p(a, X_{-u}^{(1)}) &= \int_{B(X_{-u}^{(1)}, a)} f_{X_{-u}}(x_{-u}) dx_{-u} \\
&\geq C_{\inf} \lambda_{|-u|}\left(B(X_{-u}^{(1)}, a)\right) \\
&\geq C_{\inf} a^{|-u|}.
\end{aligned}$$

Thus

$$\mathbb{P}\left(d\left(X_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}\right) \geq a \middle| X_{-u}^{(1)}\right) \leq C_{\sup} N^{N_I} (1 - C_{\inf} a^{|-u|})^{N-N_I}. \tag{I.13}$$

□

Remark 41. *For the estimators $\widehat{V}_{u,PF}$, we choose only one nearest neighbour different from $X_u^{(1)}$ in $\widehat{V}_{u,1,PF}$, which is $X_u^{(k_N(2))}$. Thus, in the previous computation, we do not have the N^{N_I}. Remark that this is also true for $\widehat{E}_{u,MC}$ taking $N_I = 2$.*

Lemma 14. *For all $\varepsilon > 0$, there exists $C_{\sup}(\varepsilon)$ such that*

$$\mathrm{E}\left(d\left(X_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}\right)\right) \leq \frac{C_{\sup}(\varepsilon)}{N^{\frac{1}{p-|u|}-\varepsilon}}, \tag{I.14}$$

and for all $x_{-u}^{(1)}$,

$$\mathrm{E}\left(d\left(X_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}\right) \middle| X_{-u}^{(1)} = x_{-u}^{(1)}\right) \leq \frac{C_{\sup}(\varepsilon)}{N^{\frac{1}{p-|u|}-\varepsilon}}. \tag{I.15}$$

Proof. Using Lemma 13, we have

$$\begin{aligned}
& \mathrm{E}\left((N-N_I)^{\frac{1}{|-u|}-\varepsilon} d\left(X_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}\right) \middle| X_{-u}^{(1)}\right) \\
= & \int_0^{+\infty} \mathbb{P}\left((N-N_I)^{\frac{1}{|-u|}-\varepsilon} d\left(X_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}\right) > t \middle| X_{-u}^{(1)}\right) dt \\
\leq & 1 + \int_1^{+\infty} \mathbb{P}\left(d\left(X_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}\right) > t (N-N_I)^{-\frac{1}{|-u|}+\varepsilon} \middle| X_{-u}^{(1)}\right) dt \\
= & 1 + \frac{1}{|-u|} \int_1^{+\infty} s^{\frac{1}{|-u|}-1} \mathbb{P}\left(d\left(X_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}\right) > s^{\frac{1}{|-u|}} (N-N_I)^{-\frac{1}{|-u|}+\varepsilon} \middle| X_{-u}^{(1)}\right) ds \\
\leq & 1 + \frac{1}{|-u|} \int_1^{+\infty} C_{\sup} N^{N_I} (1 - C_{\inf} s (N-N_I)^{|-u|\varepsilon - 1})^{N-N_I} ds,
\end{aligned}$$

and

$$\begin{aligned}
(1 - C_{\inf} s (N-N_I)^{|-u|\varepsilon-1})^{N-N_I} & = \exp\left[(N-N_I) \ln\left(1 - C_{\inf} s (N-N_I)^{|-u|\varepsilon-1}\right)\right] \\
& \leq \exp\left[(N-N_I)\left(-C_{\inf} s (N-N_I)^{|-u|\varepsilon-1}\right)\right] \\
& = \exp(-C_{\inf} s (N-N_I)^{|-u|\varepsilon}).
\end{aligned}$$

Thus,

$$\begin{aligned}
& \mathrm{E}\left((N-N_I)^{\frac{1}{|-u|}-\varepsilon} d\left(X_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}\right) \middle| X_{-u}^{(1)}\right) \\
\leq & 1 + C_{\sup} \int_1^{+\infty} N^{N_I} \exp(-C_{\inf} s (N-N_I)^{|-u|\varepsilon}) ds \\
\leq & 1 + C_{\sup} \left[N^{N_I} \exp(-C_{\inf} \frac{1}{2} (N-N_I)^{|-u|\varepsilon}) \right] \int_1^{+\infty} \exp(-C_{\inf} \frac{s}{2} (N-N_I)^{|-u|\varepsilon}) ds \\
\leq & 1 + C_{\sup}(\varepsilon).
\end{aligned}$$

Indeed, the values $N^{N_I} \exp(-C_{\inf} \frac{1}{2} (N-N_I)^{|-u|\varepsilon}$ and $\int_1^{+\infty} \exp(-C_{\inf} \frac{s}{2} (N-N_I)^{|-u|\varepsilon}) ds$ go to 0 when N do $+\infty$. Thus

$$\mathrm{E}\left(d\left(X_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}\right) \middle| X_{-u}^{(1)}\right) \leq \frac{1 + C_{\sup}(\varepsilon)}{(N-N_I)^{\frac{1}{p-|u|}-\varepsilon}} \leq \frac{C_{\sup}(\varepsilon)}{N^{\frac{1}{p-|u|}-\varepsilon}}.$$

That concludes the proof of Lemma 14. ◻

Remark 42. *For the estimators $\widehat{V}_{u,PF}$, we do not have the N^{N_I}. Thus, we can choose $\varepsilon = 0$ up to Proposition 46.*

Proposition 46. *For all $\varepsilon > 0$, there exists $C_{\sup}(\varepsilon)$ such that*

$$\left| \mathrm{E}\left(\widehat{E}_u\right) - E_u \right| \leq \frac{C_{\sup}(\varepsilon)}{N^{\frac{1}{p-|u|}-\varepsilon}} \tag{I.16}$$

and for almost all $x_{-u}^{(1)}$*,*

$$\left| \mathrm{E}\left(\widehat{E}_{u,1} | X_{-u}^{(1)} = x_{-u}^{(1)} \right) - \mathrm{Var}(Y|X_{-u} = x_{-u}^{(1)}) \right| \leq \frac{C_{\sup}(\varepsilon)}{N^{\frac{1}{p-|u|}-\varepsilon}}. \tag{I.17}$$

Proof. For almost all $(x_{-u}^{(n)})_n$, using the definition of the random variable $\mathbf{Z}$ (in the proof of Proposition 43) and using Lemma 7,

$$\begin{aligned}
& \left| \mathrm{E}\left(\Phi\left((X_{-u}^{(k_N(i)[(X_{-u}^{(n)})_n])})_{i\leq N_I}, (X_u^{(k_N(i)[(X_{-u}^{(n)})_n])})_{i\leq N_I} \right) \middle| (X_{-u}^{(n)})_n = (x_{-u}^{(n)})_n \right) \right. \\
& \left. -\mathrm{E}\left(\Phi\left(\mathbf{Z}\right) \middle| X_{-u}^{(1)} = x_{-u}^{(1)} \right) \right| \\
= & \left| \mathrm{E}\left(\Phi\left((x_{-u}^{(k_N(i)[(x_{-u}^{(n)})_n])})_{i\leq N_I}, (X_u^{(i)})_{i\leq N_I} \right) \middle| (X_{-u}^{(i)})_{i\leq N_I} = (x_{-u}^{(k_N(i)[(x_{-u}^{(n)})_n])})_{i\leq N_I} \right) \right. \\
& \left. -\mathrm{E}\left(\Phi\left((x_{-u}^{(1)})_{i\leq N_I}, (X_u^{(i)})_{i\leq N_I} \right) \middle| (X_{-u}^{(i)})_{i\leq N_I} = (x_{-u}^{(1)})_{i\leq N_I} \right) \right| \\
\leq & \; C_{\sup} d\left(x_{-u}^{(k_N(N_I)[(x_{-u}^{(n)})_n])}, x_{-u}^{(1)} \right),
\end{aligned}$$

thanks to Lemma 12. Thus, using Lemma 14, for all $\varepsilon > 0$,

$$\begin{aligned}
\left| \mathrm{E}\left(\widehat{E}_{u,1} | X_{-u}^{(1)} = x_{-u}^{(1)} \right) - \mathrm{Var}(Y|X_{-u} = x_{-u}^{(1)}) \right| & \leq C_{\sup} \mathrm{E}\left(d\left(X_{-u}^{(1)}, X_{-u}^{(k_N(N_I))} \right) \middle| X_{-u}^{(1)} = x_{-u}^{(1)} \right) \\
& \leq C_{\sup} \frac{C_{\sup}(\varepsilon)}{N^{\frac{1}{p-|u|}-\varepsilon}}.
\end{aligned}$$

□

In the following, to simplify notation, we may write "$X_{-u}^{(1,2)} = x_{-u}^{(1,2)}$" for "$X_{-u}^{(1)} = x_{-u}^{(1)}$ and $X_{-u}^{(2)} = x_{-u}^{(2)}$".

Lemma 15. *For almost all* $(x_{-u}^{(1)}, x_{-u}^{(2)})$ *and for all* $a \geq 0$*, we have*

$$\mathbb{P}\left(d(x_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}) \geq a \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)} \right) \leq \mathbb{P}\left(d(x_{-u}^{(1)}, X_{-u}^{(k_{N-1}(N_I))}) \geq a \middle| X_{-u}^{(1)} = x_{-u}^{(1)} \right),$$

and thus, integrating a *on* $\mathbb{R}_+$*,*

$$\mathrm{E}\left(d\left(X_{-u}^{(k_N(N_I))}, X_{-u}^{(1)} \right) \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)} \right) \leq \mathrm{E}\left(d\left(X_{-u}^{(k_{N-1}(N_I))}, X_{-u}^{(1)} \right) \middle| X_{-u}^{(1)} = x_{-u}^{(1)} \right).$$

Proof. Let $g_N(i)$ be the index of the i-th nearest neighbour of $X_{-u}^{(1)}$ in $(X_{-u}^{(n)})_{n\in[1:N]\setminus\{2\}}$. For almost all $(x_{-u}^{(1)}, x_{-u}^{(2)})$, we have

$$\mathbb{P}\left(d(x_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}) \geq a \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)} \right)$$

$$\begin{aligned}
= \quad & \mathbb{P}\left(d(x_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}) \geq a \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)}, d(x_{-u}^{(1)}, x_{-u}^{(2)}) > d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \right) \\
& \mathbb{P}\left(d(x_{-u}^{(1)}, x_{-u}^{(2)}) > d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)} \right) \\
& + \mathbb{P}\left(d(x_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}) \geq a \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)}, d(x_{-u}^{(1)}, x_{-u}^{(2)}) \leq d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \right) \\
& \mathbb{P}\left(d(x_{-u}^{(1)}, x_{-u}^{(2)}) \leq d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)} \right).
\end{aligned}$$

Moreover, conditionally to $X_{-u}^{(1,2)} = x_{-u}^{(1,2)}$, if $d(x_{-u}^{(1)}, x_{-u}^{(2)}) > d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))})$, then the N_I-nearest neighbours of $X_{-u}^{(1)}$ do not change if we do not take into account $X_{-u}^{(2)}$. Thus

$$\begin{aligned}
& \mathbb{P}\left(d(x_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}) \geq a \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)}, d(x_{-u}^{(1)}, x_{-u}^{(2)}) > d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \right) \\
= \quad & \mathbb{P}\left(d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \geq a \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)}, d(x_{-u}^{(1)}, x_{-u}^{(2)}) > d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \right) \\
= \quad & \mathbb{P}\left(d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \geq a \middle| X_{-u}^{(1)} = x_{-u}^{(1)}, d(x_{-u}^{(1)}, x_{-u}^{(2)}) > d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \right).
\end{aligned}$$

Similarly, conditionally to $X_{-u}^{(1,2)} = x_{-u}^{(1,2)}$, if $d(x_{-u}^{(1)}, x_{-u}^{(2)}) \leq d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}$, then $x_{-u}^{(2)}$ is one of the N_I-nearest neighbours of $X_{-u}^{(1)}$. Thus

$$\begin{aligned}
& \mathbb{P}\left(d(x_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}) \geq a \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)}, d(x_{-u}^{(1)}, x_{-u}^{(2)}) \leq d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \right) \\
\leq \quad & \mathbb{P}\left(d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \geq a \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)}, d(x_{-u}^{(1)}, x_{-u}^{(2)}) \leq d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \right) \\
= \quad & \mathbb{P}\left(d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \geq a \middle| X_{-u}^{(1)} = x_{-u}^{(1)}, d(x_{-u}^{(1)}, x_{-u}^{(2)}) \leq d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \right).
\end{aligned}$$

Finally,

$$\begin{aligned}
& \mathbb{P}\left(d(x_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}) \geq a \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)} \right) \\
\leq \quad & \mathbb{P}\left(d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \geq a \middle| X_{-u}^{(1)} = x_{-u}^{(1)}, d(x_{-u}^{(1)}, x_{-u}^{(2)}) > d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \right) \\
& \mathbb{P}\left(d(x_{-u}^{(1)}, x_{-u}^{(2)}) > d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \middle| X_{-u}^{(1)} = x_{-u}^{(1)} \right) \\
& + \mathbb{P}\left(d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \geq a \middle| X_{-u}^{(1)} = x_{-u}^{(1)}, d(x_{-u}^{(1)}, x_{-u}^{(2)}) \leq d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \right) \\
& \mathbb{P}\left(d(x_{-u}^{(1)}, x_{-u}^{(2)}) \leq d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \middle| X_{-u}^{(1)} = x_{-u}^{(1)} \right) \\
= \quad & \mathbb{P}\left(d(x_{-u}^{(1)}, X_{-u}^{(g_N(N_I))}) \geq a \middle| X_{-u}^{(1)} = x_{-u}^{(1)} \right) \\
= \quad & \mathbb{P}\left(d(x_{-u}^{(1)}, X_{-u}^{(k_{N-1}(N_I))}) \geq a \middle| X_{-u}^{(1)} = x_{-u}^{(1)} \right),
\end{aligned}$$

and we proved Lemma 15. □

Proposition 47. *For all $\varepsilon > 0$, there exists $C_{\sup}(\varepsilon)$ such that*

$$\left|\mathrm{cov}(\widehat{E}_{u,1}, \widehat{E}_{u,2})\right| \leq \frac{C_{\sup}(\varepsilon)}{N^{\frac{1}{p-|u|}-\varepsilon}}. \tag{I.18}$$

Proof. We use the law of total covariance,

$$\mathrm{cov}(\widehat{E}_1, \widehat{E}_2) = \mathrm{E}\left[\mathrm{cov}\left(\widehat{E}_1, \widehat{E}_2 \middle| X_{-u}^{(1)}, X_{-u}^{(2)}\right)\right] + \mathrm{cov}\left[\mathrm{E}\left(\widehat{E}_{u,1}|X_{-u}^{(1)}, X_{-u}^{(2)}\right), \mathrm{E}\left(\widehat{E}_{u,2}|X_{-u}^{(1)}, X_{-u}^{(2)}\right)\right]. \tag{I.19}$$

Part 1: First, we will bound the second term of Equation I.19. Thanks to Lemma 12, we have

$$\begin{aligned}
&\left|\mathrm{E}\left(\widehat{E}_{u,1}|X_{-u}^{(1)} = x_{-u}^{(1)}, X_{-u}^{(2)} = x_{-u}^{(2)}\right) - \mathrm{Var}\left(Y|X_{-u} = x_{-u}^{(1)})\right)\right| \\
\leq\ & \mathrm{E}\left\{\left|\mathrm{E}\left[\Phi\left((X^{(k_N(i))})_{i\leq N_I}\right) \middle| X_{-u}^{(1)} = x_{-u}^{(1)}, X_{-u}^{(2)} = x_{-u}^{(2)}, (X_{-u}^{(n)})_{n\geq 3}\right] - \mathrm{Var}\left(Y|X_{-u} = x_{-u}^{(1)})\right)\right|\right\} \\
\leq\ & C_{\sup}\mathrm{E}\left(d\left(X_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}\right)\middle| X_{-u}^{(1)} = x_{-u}^{(1)}, X_{-u}^{(2)} = x_{-u}^{(2)}\right) \qquad \text{using Lemma 12,} \\
\leq\ & C_{\sup}\mathrm{E}\left(d\left(X_{-u}^{(1)}, X_{-u}^{(k_{N-1}(N_I))}\right)\middle| X_{-u}^{(1)} = x_{-u}^{(1)}\right) \qquad \text{using Lemma 15,} \\
\leq\ & \frac{C_{\sup}(\varepsilon)}{(N-1)^{\frac{1}{p-|u|}-\varepsilon}} \qquad \text{using Lemma 14,} \\
\leq\ & \frac{C_{\sup}(\varepsilon)}{N^{\frac{1}{p-|u|}-\varepsilon}}.
\end{aligned}$$

Similarly,

$$\left|\mathrm{E}\left(\widehat{E}_{u,2}|X_{-u}^{(1)} = x_{-u}^{(1)}, X_{-u}^{(2)} = x_{-u}^{(2)}\right) - \mathrm{Var}\left(Y|X_{-u} = x_{-u}^{(2)})\right)\right| \leq \frac{C_{\sup}(\varepsilon)}{N^{\frac{1}{p-|u|}-\varepsilon}}.$$

Thus, using that Φ is bounded,

$$\begin{aligned}
&\Big|\mathrm{E}\left(\widehat{E}_{u,1}|X_{-u}^{(1)} = x_{-u}^{(1)}, X_{-u}^{(2)} = x_{-u}^{(2)}\right)\mathrm{E}\left(\widehat{E}_{u,2}|X_{-u}^{(1)} = x_{-u}^{(1)}, X_{-u}^{(2)} = x_{-u}^{(2)}\right) \\
&\quad -\mathrm{Var}\left(Y|X_{-u} = x_{-u}^{(1)})\right)\mathrm{Var}\left(Y|X_{-u} = x_{-u}^{(2)})\right)\Big| \leq \tfrac{C_{\sup}(\varepsilon)}{N^{\frac{1}{p-|u|}-\varepsilon}}.
\end{aligned}$$

Moreover, using Proposition 46, we have

$$\begin{aligned}
&\Big|\mathrm{E}\left(\widehat{E}_{u,1}|X_{-u}^{(1)} = x_{-u}^{(1)}\right)\mathrm{E}\left(\widehat{E}_{u,2}|X_{-u}^{(2)} = x_{-u}^{(2)}\right) \\
&-\mathrm{Var}\left(Y|X_{-u} = x_{-u}^{(1)})\right)\mathrm{Var}\left(Y|X_{-u} = x_{-u}^{(2)})\right)\Big| \leq \tfrac{C_{\sup}(\varepsilon)}{N^{\frac{1}{p-|u|}-\varepsilon}}.
\end{aligned}$$

Thus,

$$\left|\mathrm{E}\left(\widehat{E}_{u,1}|X_{-u}^{(1)}=x_{-u}^{(1)},X_{-u}^{(2)}=x_{-u}^{(2)}\right)\mathrm{E}\left(\widehat{E}_{u,2}|X_{-u}^{(1)}=x_{-u}^{(1)},X_{-u}^{(2)}=x_{-u}^{(2)}\right)\right.$$
$$\left.-\mathrm{E}\left(\widehat{E}_{u,1}|X_{-u}^{(1)}=x_{-u}^{(1)}\right)\mathrm{E}\left(\widehat{E}_{u,2}|X_{-u}^{(2)}=x_{-u}^{(2)}\right)\right| \leq \frac{C_{\sup}(\varepsilon)}{N^{\frac{1}{p-|u|}-\varepsilon}}.$$

Finally,

$$\begin{aligned}
& \left|\operatorname{cov}\left[\mathrm{E}\left(\widehat{E}_{u,1}|X_{-u}^{(1)},X_{-u}^{(2)}\right),\mathrm{E}\left(\widehat{E}_{u,2}|X_{-u}^{(1)},X_{-u}^{(2)}\right)\right]\right| \\
= & \left|\mathrm{E}\left[\mathrm{E}\left(\widehat{E}_{u,1}|X_{-u}^{(1)},X_{-u}^{(2)}\right)\mathrm{E}\left(\widehat{E}_{u,2}|X_{-u}^{(1)},X_{-u}^{(2)}\right)\right]-\mathrm{E}\left[\mathrm{E}\left(\widehat{E}_{u,1}|X_{-u}^{(1)}\right)\mathrm{E}\left(\widehat{E}_{u,2}|X_{-u}^{(2)}\right)\right]\right| \\
\leq & \ \mathrm{E}\left[\left|\mathrm{E}\left(\widehat{E}_{u,1}|X_{-u}^{(1)},X_{-u}^{(2)}\right)\mathrm{E}\left(\widehat{E}_{u,2}|X_{-u}^{(1)},X_{-u}^{(2)}\right)-\mathrm{E}\left(\widehat{E}_{u,1}|X_{-u}^{(1)}\right)\mathrm{E}\left(\widehat{E}_{u,2}|X_{-u}^{(2)}\right)\right|\right] \\
\leq & \ \frac{C_{\sup}(\varepsilon)}{N^{\frac{1}{p-|u|}-\varepsilon}}.
\end{aligned}$$

Remark 43. *In this Part 1, we can choose $\varepsilon=0$ for the estimators $\widehat{V}_{u,PF}$ or for $\widehat{E}_{u,MC}$ if we take $N_I=2$.*

Part 2: Let $\varepsilon>0$. We will bound the first term of Equation (I.19):

$$\mathrm{E}\left[\operatorname{cov}\left(\widehat{E}_1,\widehat{E}_2\middle|X_{-u}^{(1)},X_{-u}^{(2)}\right)\right].$$

We want to prove that

$$\left|\int_{\mathcal{X}_{-u}^2}\mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1,2)}=x_{-u}^{(1,2)}\right)-\mathrm{E}(\widehat{E}_{u,1}|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})\mathrm{E}(\widehat{E}_{u,2}|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})\right.$$
$$\left.d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)},x_{-u}^{(2)})\right|\leq\frac{C_{\sup}(\varepsilon)}{N^{1-\varepsilon}}.$$

Let us write

$$l(x_{-u}^{(1)},x_{-u}^{(2)}):=\min\left(d(x_{-u}^{(1)},x_{-u}^{(2)})/2,\ \frac{1}{N^{\frac{1}{|-u|}-\delta}}\right)$$

where $\delta=\varepsilon/(4|-u|)$, and

$$G(x_{-u}^{(1)},x_{-u}^{(2)}):=\left\{(x_{-u}^{(n)})_{n\in[3:N]}\middle|\quad d(x_{-u}^{(1)},x_{-u}^{(k_N(N_I)[(x_{-u}^{(n)})_{n\leq N}])})<l(x_{-u}^{(1)},x_{-u}^{(2)}),\right.$$
$$\left.d(x_{-u}^{(2)},x_{-u}^{(k'_N(N_I)[(x_{-u}^{(n)})_{n\leq N}])})<l(x_{-u}^{(1)},x_{-u}^{(2)})\right\}.$$

Part 2.A: We prove the following lemmas.

Lemma 16. *For all $\varepsilon > 0$, there exists $C_{\sup}(\varepsilon)$ such that,*

$$\int_{\mathcal{X}_{-u}^2} \mathbb{P}\left(d(X_{-u}^{(1)}, X_{-u}^{(k_{N-1}(N_I))}) \geq d(x_{-u}^{(1)}, x_{-u}^{(2)})/2 \middle| X_{-u}^{(1)} = x_{-u}^{(1)} \right) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)}, x_{-u}^{(2)}) \leq \frac{C_{\sup}(\varepsilon)}{N^{1-\varepsilon}}. \tag{I.20}$$

Proof. We divide $\mathcal{X}_{-u}^2$ in $F_1 := \{(x_{-u}^{(1)}, x_{-u}^{(2)}) \in \mathcal{X}_{-u}^2,\ d(x_{-u}^{(1)}, x_{-u}^{(2)}) < (N - N_I - 1)^{\frac{-1+\varepsilon}{|-u|}}\}$ and $F_2 := \{(x_{-u}^{(1)}, x_{-u}^{(2)}) \in \mathcal{X}_{-u}^2,\ d(x_{-u}^{(1)}, x_{-u}^{(2)}) \geq (N - N_I - 1)^{\frac{-1+\varepsilon}{|-u|}}\}$.

$$\begin{aligned}
& \int_{F_1} \mathbb{P}\left(d(X_{-u}^{(1)}, X_{-u}^{(k_{N-1}(N_I))}) \geq d(x_{-u}^{(1)}, x_{-u}^{(2)})/2 \middle| X_{-u}^{(1)} = x_{-u}^{(1)} \right) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)}, x_{-u}^{(2)}) \\
\leq\ & C_{\sup} \lambda_{|-u|}^{\otimes 2}(F_1) \\
\leq\ & C_{\sup} \int_{\mathcal{X}_{-u}} \lambda_{|-u|} \left(B\left[x_{-u}, (N - N_I - 1)^{\frac{-1+\varepsilon}{|-u|}} \right] \right) dx_{-u} \\
\leq\ & C_{\sup} \int_{\mathcal{X}_{-u}} (N - N_I - 1)^{\frac{-1+\varepsilon}{|-u|}|-u|} dx_{-u} \\
\leq\ & C_{\sup}(N - N_I - 1)^{-1+\varepsilon} \\
\leq\ & \frac{C_{\sup}}{N^{1-\varepsilon}}.
\end{aligned}$$

Furthermore, using Lemma 13, we have

$$\begin{aligned}
& \int_{F_2} \mathbb{P}\left(d(X_{-u}^{(1)}, X_{-u}^{(k_{N-1}(N_I))}) \geq d(x_{-u}^{(1)}, x_{-u}^{(2)})/2 \middle| X_{-u}^{(1)} = x_{-u}^{(1)} \right) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)}, x_{-u}^{(2)}) \\
\leq & \int_{F_2} C_{\sup}(N-1)^{N_I} (1 - C_{\inf} d(x_{-u}^{(1)}, x_{-u}^{(2)})^{|-u|})^{N-1-N_I} d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)}, x_{-u}^{(2)}) \\
\leq & \lambda_{|-u|}(\mathcal{X}_{-u})^2 C_{\sup}(N-1)^{N_I} (1 - C_{\inf}(N - N_I - 1)^{\frac{-1+\varepsilon}{|-u|}|-u|})^{N-1-N_I} \\
\leq & C_{\sup}(N-1)^{N_I}(1 - C_{\inf}(N - N_I - 1)^{-1+\varepsilon})^{N-1-N_I} \\
\leq & C_{\sup}(N-1)^{N_I} \exp\left[(N - 1 - N_I) \ln\left(1 - C_{\inf}(N - N_I - 1)^{-1+\varepsilon}\right) \right] \\
\leq & C_{\sup}(N-1)^{N_I} \exp\left[-C_{\inf}(N - N_I - 1)^{\varepsilon} + o((N - N_I - 1)^{\varepsilon}) \right] \\
\leq & \frac{C_{\sup}(\varepsilon)}{N^{1-\varepsilon}}.
\end{aligned}$$

□

Remark 44. *In Lemma 16, we need $\varepsilon > 0$ even for the Pick-and-Freeze estimators. That explains the rate of convergence when $|u| = 1$ for the Pick-and-Freeze estimators.*

Lemma 17. *For all $\varepsilon > 0$, there exists $C_{\sup}(\varepsilon)$ such that,*

$$\int_{\mathcal{X}_{-u}^2} \mathbb{P}_{X_{-u}}^{\otimes(N-2)}(G(x_{-u}^{(1)}, x_{-u}^{(2)})^c) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)}, x_{-u}^{(2)}) \leq \frac{C_{\sup}(\varepsilon)}{N^{1-\varepsilon}}. \tag{I.21}$$

Proof. Using Lemma 13, we have

$$\mathbb{P}\left(d(X_{-u}^{(k_{N-1}(N_I))}, x_{-u}^{(1)}) \geq N^{-\frac{1}{|-u|}+\delta} | X_{-u}^{(1)}\right) \leq C_{\sup}(N-1)^{N_I}(1-C_{\inf}N^{-1+\delta|-u|})^{N-1-N_I},$$

so

$$\mathbb{P}\left(d(X_{-u}^{(k_{N-1}(N_I))}, x_{-u}^{(1)}) \geq N^{-\frac{1}{|-u|}+\delta} | X_{-u}^{(1)}\right) \leq \frac{C_{\sup}(\varepsilon)}{N}. \tag{I.22}$$

Thus, we have

$$\begin{aligned}
& \int_{\mathcal{X}_{-u}^2} \mathbb{P}_{X_{-u}}^{\otimes(N-2)}(G(x_{-u}^{(1)}, x_{-u}^{(2)})^c) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)}, x_{-u}^{(2)}) \\
\leq \; & \int_{\mathcal{X}_{-u}^2} \mathbb{P}\left(d(X_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}) \geq d(x_{-u}^{(1)}, x_{-u}^{(2)})/2 \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)}\right) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)}, x_{-u}^{(2)}) \\
& + \int_{\mathcal{X}_{-u}^2} \mathbb{P}\left(d(X_{-u}^{(2)}, X_{-u}^{(k'_N(N_I))}) \geq d(x_{-u}^{(1)}, x_{-u}^{(2)})/2 \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)}\right) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)}, x_{-u}^{(2)}) \\
& + \int_{\mathcal{X}_{-u}^2} \mathbb{P}\left(d(X_{-u}^{(1)}, X_{-u}^{(k_N(N_I))}) \geq N^{-\frac{1}{|-u|}+\delta} \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)}\right) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)}, x_{-u}^{(2)}) \\
& + \int_{\mathcal{X}_{-u}^2} \mathbb{P}\left(d(X_{-u}^{(2)}, X_{-u}^{(k'_N(N_I))}) \geq N^{-\frac{1}{|-u|}+\delta} \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)}\right) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)}, x_{-u}^{(2)}) \\
\leq \; & \int_{\mathcal{X}_{-u}^2} \mathbb{P}\left(d(X_{-u}^{(1)}, X_{-u}^{(k_{N-1}(N_I))}) \geq d(x_{-u}^{(1)}, x_{-u}^{(2)})/2 \middle| X_{-u}^{(1)} = x_{-u}^{(1)}\right) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)}, x_{-u}^{(2)}) \\
& + \int_{\mathcal{X}_{-u}^2} \mathbb{P}\left(d(X_{-u}^{(2)}, X_{-u}^{(k'_{N-1}(N_I))}) \geq d(x_{-u}^{(1)}, x_{-u}^{(2)})/2 \middle| X_{-u}^{(2)} = x_{-u}^{(2)}\right) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)}, x_{-u}^{(2)}) \\
& + \int_{\mathcal{X}_{-u}^2} \mathbb{P}\left(d(X_{-u}^{(1)}, X_{-u}^{(k_{N-1}(N_I))}) \geq N^{-\frac{1}{|-u|}+\delta} \middle| X_{-u}^{(1)} = x_{-u}^{(1)}\right) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)}, x_{-u}^{(2)}) \\
& + \int_{\mathcal{X}_{-u}^2} \mathbb{P}\left(d(X_{-u}^{(2)}, X_{-u}^{(k'_{N-1}(N_I))}) \geq N^{-\frac{1}{|-u|}+\delta} \middle| X_{-u}^{(2)} = x_{-u}^{(2)}\right) d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)}, x_{-u}^{(2)}),
\end{aligned}$$

and we conclude the proof of Lemma 17 using Lemma 16 and Equation I.22. □

For $i = 1, 2$, let B_i be the ball of center $x_{-u}^{(i)}$ and of radius $l(x_{-u}^{(1)}, x_{-u}^{(2)})$, let p_i be the probability of B_i and N_i be the number of observations $(X_{-u}^{(n)})_{n\in[3:N]}$ in the ball B_i. Remark that

$$p_i \leq \frac{C_{\sup}}{N^{1-\delta|-u|}}.$$

We have the two following lemmas.

Lemma 18. *Conditionally to $X_{-u}^{(1,2)} = x_{-u}^{(1,2)}$, the random variable N_i is binomial $\mathcal{B}(N-2, p_i)$.*
Conditionally to $X_{-u}^{(1,2)} = x_{-u}^{(1,2)}, N_j = n_j$, the random variable N_i is binomial $\mathcal{B}(N-2-n_j, p_i(1-p_j)^{-1})$.

Proof. For the first assertion, we use that the $(X_{-u}^{(n)})_n$ are i.i.d. For the second assertion, we compute $\mathbb{P}(N_i = n_i | X_{-u}^{(1,2)} = x_{-u}^{(1,2)}, N_j = n_j)$ with Bayes' theorem. □

Lemma 19. *If $N_i = n_i$, let $X_{-u}^{(\mathbf{M}_i)}$ be the random vector composed of the n_i observations in B_i of $(X_{-u}^{(n)})_{n\in[3:N]}$ and $\mathbf{M}_i \in [3:N]^{n_i}$ the vector containing the corresponding indices. We have:*

$$
\begin{aligned}
& \mathcal{L}\left(X^{(\mathbf{M}_1)}, X^{(\mathbf{M}_2)} | X_{-u}^{(1,2)} = x_{-u}^{(1,2)}, N_1 = n_1, N_2 = n_2\right) \\
= \;& \mathcal{L}\left(X^{(\mathbf{M}_1)} | X_{-u}^{(1,2)} = x_{-u}^{(1,2)}, N_1 = n_1\right) \otimes \mathcal{L}\left(X^{(\mathbf{M}_2)} | X_{-u}^{(1,2)} = x_{-u}^{(1,2)}, N_2 = n_2\right).
\end{aligned}
$$

Proof. For any bounded Borel functions ϕ_1, ϕ_2, we have

$$
\begin{aligned}
& \mathrm{E}\left(\phi_1(X^{(\mathbf{M}_1)})\phi_2(X^{(\mathbf{M}_2)}) | X_{-u}^{(1,2)} = x_{-u}^{(1,2)}, N_1 = n_1, N_2 = n_2\right) \\
= \;& \frac{\mathrm{E}\left(\phi_1(X^{(\mathbf{M}_1)})\phi_2(X^{(\mathbf{M}_2)}) \mathbb{1}_{N_1=n_1} \mathbb{1}_{N_2=n_2} | X_{-u}^{(1,2)} = x_{-u}^{(1,2)}\right)}{\mathbb{P}(N_1 = n_1, N_2 = n_2 | X_{-u}^{(1,2)} = x_{-u}^{(1,2)})}.
\end{aligned}
$$

Let

$$
\mathcal{P}([3:N], n_1) := \{(k_1, \cdots, k_{n_1}) \in [3:N]^{n_1} \;:\; k_i < k_j \text{ for } i,j \in [1:n_1],\ i<j\}
$$

be the set of all possible two-by-two distinct elements in $[3:N]$. To simplify notation, we also consider an element of $\mathcal{P}([3:N], n_1)$ with the subset of $[3:N]$ that contains its indices. We have

$$
\begin{aligned}
& \mathrm{E}\left(\phi_1(X^{(\mathbf{M}_1)})\phi_2(X^{(\mathbf{M}_2)}) \mathbb{1}_{N_1=n_1} \mathbb{1}_{N_2=n_2} \middle| X_{-u}^{(1,2)} = x_{-u}^{(1,2)}\right) \\
= \;& \sum_{\mathbf{m}_1 \in \mathcal{P}([3:N], n_1)} \sum_{\mathbf{m}_2 \in \mathcal{P}([3:N]\setminus \mathbf{m}_1, n_2)} \mathrm{E}\Big(\phi_1(X^{(\mathbf{m}_1)})\phi_2(X^{(\mathbf{m}_2)}) \mathbb{1}_{X_{-u}^{(\mathbf{m}_1)} \in B_1^{n_1}} \mathbb{1}_{X_{-u}^{(\mathbf{m}_2)} \in B_2^{n_2}} \\
& \times \prod_{i \in [3:N]\setminus(\mathbf{m}_1 \cup \mathbf{m}_2)} \mathbb{1}_{X_{-u}^{(i)} \notin B_1 \cup B_2} \Big| X_{-u}^{(1,2)} = x_{-u}^{(1,2)}\Big)
\end{aligned}
$$

Now, using the independence of $(X^{(n)})_n$ and summing over $\mathbf{m}_1$ and $\mathbf{m}_2$, we have, for any value of $\mathbf{m}_1 \in \mathcal{P}([3:N], n_1)$ and $\mathbf{m}_2 \in \mathcal{P}([3:N], n_2)$,

$$
\mathrm{E}\left(\phi_1(X^{(\mathbf{M}_1)})\phi_2(X^{(\mathbf{M}_2)}) | X_{-u}^{(1,2)} = x_{-u}^{(1,2)}, N_1 = n_1, N_2 = n_2\right)
$$

$$= \binom{N-2}{n_1}\binom{N-2-n_1}{n_2}(1-p_1-p_2)^{N-2-n_1-n_2}$$
$$\frac{\mathrm{E}\left(\phi_1(X^{(\mathbf{m}_1)})\mathbb{1}_{X_{-u}^{(\mathbf{m}_1)}\in B_1^{n_1}}\middle|X_{-u}^{(1,2)}=x_{-u}^{(1,2)}\right)\mathrm{E}\left(\phi_2(X^{(\mathbf{m}_2)})\mathbb{1}_{X_{-u}^{(\mathbf{m}_2)}\in B_2^{n_2}}\middle|X_{-u}^{(1,2)}=x_{-u}^{(1,2)}\right)}{\binom{N-2}{n_1}\binom{N-2-n_1}{n_2}p_1^{n_1}p_2^{n_2}(1-p_1-p_2)^{N-2-n_1-n_2}}$$
$$= \frac{\mathrm{E}\left(\phi_1(X^{(\mathbf{m}_1)})\mathbb{1}_{X_{-u}^{(\mathbf{m}_1)}\in B_1^{n_1}}\middle|X_{-u}^{(1,2)}=x_{-u}^{(1,2)}\right)}{p_1^{n_1}}\frac{\mathrm{E}\left(\phi_2(X^{(\mathbf{m}_2)})\mathbb{1}_{X_{-u}^{(\mathbf{m}_2)}\in B_2^{n_2}}\middle|X_{-u}^{(1,2)}=x_{-u}^{(1,2)}\right)}{p_2^{n_2}}$$
$$= \frac{\mathrm{E}\left(\phi_1(X^{(\mathbf{m}_1)})\mathbb{1}_{X_{-u}^{(\mathbf{m}_1)}\in B_1^{n_1}}\prod_{i\in[3:N]\setminus\mathbf{m}_1}\mathbb{1}_{X_{-u}^{(i)}\notin B_1}\middle|X_{-u}^{(1,2)}=x_{-u}^{(1,2)}\right)}{p_1^{n_1}(1-p_1)^{n_1}}$$
$$\frac{\mathrm{E}\left(\phi_2(X^{(\mathbf{m}_2)})\mathbb{1}_{X_{-u}^{(\mathbf{m}_2)}\in B_2^{n_2}}\prod_{i\in[3:N]\setminus\mathbf{m}_2}\mathbb{1}_{X_{-u}^{(i)}\notin B_2}\middle|X_{-u}^{(1,2)}=x_{-u}^{(1,2)}\right)}{p_2^{n_2}(1-p_2)^{n_2}}$$
$$= \mathrm{E}\left(\phi_1(X^{(\mathbf{M}_1)})\middle|X_{-u}^{(1,2)}=x_{-u}^{(1,2)},N_1=n_1\right)\mathrm{E}\left(\phi_2(X^{(\mathbf{M}_2)})\middle|X_{-u}^{(1,2)}=x_{-u}^{(1,2)},N_2=n_2\right).$$

That concludes the proof of Lemma 19. □

Part 2.B: We aim to proving that

$$\left|\int_{\mathcal{X}_{-u}^2}\mathrm{E}\left(\widehat{E}_{u,1}\widehat{E}_{u,2}|X_{-u}^{(1,2)}=x_{-u}^{(1,2)}\right)-\mathrm{E}(\widehat{E}_{u,1}|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})\mathrm{E}(\widehat{E}_{u,2}|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})\right.$$
$$\left.d\mathbb{P}_{X_{-u}}^{\otimes 2}(x_{-u}^{(1)},x_{-u}^{(2)})\right|\leq\frac{C_{\sup}(\varepsilon)}{N^{1-\varepsilon}}.$$

To simplify notation, let $X^{(\mathbf{k}_N)}:=(X^{(k_N(i))})_{i\leq N_I}$ and $X^{(\mathbf{k}'_N)}:=(X^{(k'_N(i))})_{i\leq N_I}$. We have

$$\mathrm{E}\left(\Phi(X^{(\mathbf{k}_N)})\Phi(X^{(\mathbf{k}'_N)})|X_{-u}^{(1,2)}=x_{-u}^{(1,2)}\right)$$
$$= \sum_{n_1,n_2=0}^{N-2}\mathrm{E}\left(\Phi(X^{(\mathbf{k}_N)})|N_1=n_1,X_{-u}^{(1,2)}=x_{-u}^{(1,2)}\right)\mathrm{E}\left(\Phi(X^{(\mathbf{k}'_N)})|N_2=n_2,X_{-u}^{(1,2)}=x_{-u}^{(1,2)}\right)$$
$$\times\mathbb{P}(N_1=n_1,N_2=n_2|X_{-u}^{(1,2)}=x_{-u}^{(1,2)}).$$

On the other hand, we have

$$\mathrm{E}\left(\Phi(X^{(\mathbf{k}_N)})|X_{-u}^{(1,2)}=x_{-u}^{(1,2)}\right)\mathrm{E}\left(\Phi(X^{(\mathbf{k}'_N)})|X_{-u}^{(1,2)}=x_{-u}^{(1,2)}\right)$$

$$= \sum_{n_1,n_2=0}^{N-2} \mathrm{E}\left(\Phi(X^{(\mathbf{k}_N)})|N_1=n_1, X_{-u}^{(1,2)}=x_{-u}^{(1,2)}\right) \mathrm{E}\left(\Phi(X^{(\mathbf{k}'_N)})|N_2=n_2, X_{-u}^{(1,2)}=x_{-u}^{(1,2)}\right)$$
$$\times \mathbb{P}(N_1=n_1|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})\mathbb{P}(N_2=n_2|X_{-u}^{(1,2)}=x_{-u}^{(1,2)}).$$

Thus, using that Φ is bounded and using Lemma 17, it suffices to show that

$$\sum_{n_1,n_2=N_I-1}^{N-2} \big|\mathbb{P}(N_1=n_1,N_2=n_2|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})$$
$$-\mathbb{P}(N_1=n_1|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})\mathbb{P}(N_2=n_2|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})\big| \leq \frac{C_{\sup}(\varepsilon)}{N^{1-\varepsilon}}.$$

Let $K_N := \lfloor N^\alpha \rfloor$, where $\alpha = \varepsilon/3$. We divide the previous sum into two sums:

$$A(x_{-u}^{(1)}, x_{-u}^{(2)}) := \sum_{n_1,n_2=N_I-2}^{K_N} \big|\mathbb{P}(N_1=n_1,N_2=n_2|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})$$
$$-\mathbb{P}(N_1=n_1|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})\mathbb{P}(N_2=n_2|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})\big|,$$
$$B(x_{-u}^{(1)}, x_{-u}^{(2)}) := \sum_{\substack{n_1,n_2=N_I-1,\\ s.t.\ n_1>K_N \text{ or } n_2>K_N}}^{N-2} \big|\mathbb{P}(N_1=n_1,N_2=n_2|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})$$
$$-\mathbb{P}(N_1=n_1|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})\mathbb{P}(N_2=n_2|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})\big|.$$

Let us bound these two terms.

First, we have

$$A(x_{-u}^{(1)}, x_{-u}^{(2)}) = \sum_{n_1,n_2=N_I-1}^{K_N} \mathbb{P}(N_1=n_1|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})\mathbb{P}(N_2=n_2|N_1=n_1,X_{-u}^{(1,2)}=x_{-u}^{(1,2)})$$
$$\times\left|1-\frac{\mathbb{P}(N_2=n_2|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})}{\mathbb{P}(N_2=n_2|N_1=n_1,X_{-u}^{(1,2)}=x_{-u}^{(1,2)})}\right|.$$

Thus, it suffices to bound

$$\left|1-\frac{\mathbb{P}(N_2=n_2|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})}{\mathbb{P}(N_2=n_2|N_1=n_1,X_{-u}^{(1,2)}=x_{-u}^{(1,2)})}\right| \leq \frac{C_{\sup}(\varepsilon)}{N^{1-\varepsilon}}.$$

Thus, it suffices to show

$$\left|\log\left(\frac{\mathbb{P}(N_2=n_2|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})}{\mathbb{P}(N_2=n_2|N_1=n_1,X_{-u}^{(1,2)}=x_{-u}^{(1,2)})}\right)\right| \leq \frac{C_{\sup}(\varepsilon)}{N^{1-\varepsilon}}.$$

To simplify notation, let $T = N-2$. Thanks to Lemma 18, we have,

$$\log\left(\frac{\mathbb{P}(N_2=n_2|X_{-u}^{(1,2)}=x_{-u}^{(1,2)})}{\mathbb{P}(N_2=n_2|N_1=n_1,X_{-u}^{(1,2)}=x_{-u}^{(1,2)})}\right)$$

$$\begin{aligned}
&= \log\left(\frac{T(T-1)...(T-n_1+1)}{(T-n_2)(T-n_2-1)...(T-n_2-n_1+1)}\frac{(1-p_1)^{T-n_1}(1-p_2)^{T-n_2}}{(1-p_1-p_2)^{T-n_1-n_2}}\right)\\
&= \log\left(1(1-\frac{1}{T})...(1-\frac{n_1-1}{T})\right) - \log\left((1-\frac{n_2}{T})(1-\frac{n_2+1}{T})...(1-\frac{n_2+n_1-1}{T})\right)\\
&\quad (T-n_1)\log(1-p_1) + (T-n_2)\log(1-p_2) - (T-n_1-n_2)\log(1-p_1-p_2)\\
&= -\frac{n_1(n_1-1)}{2T} + n_1 O(\frac{n_1^2}{T^2}) + \frac{n_1(n_1+2n_2-1)}{2T} + n_1 O(\frac{(n_1+n_2)^2}{T^2})\\
&\quad -(T-n_2)p_2 + (T-n_2)O(p_2^2) - (T-n_1)p_1 + (T-n_1)O(p_1^2)\\
&\quad +(T-n_1-n_2)(p_1+p_2) + (T-n_1-n_2)O((p_1+p_2)^2)\\
&= \frac{n_1 n_2}{T} + O(\frac{n_1^3}{T}) + O(\frac{n_1(n_1+n_2)^2}{T^2}) - n_2 p_1 - n_1 p_2\\
&\quad +(T-n_2)O(p_1^2) + (T-n_1)O(p_2^2) + (T-n_1-n_2)O((p_1+p_2)^2).
\end{aligned}$$

We know that

$$K_N p_i \leq \frac{C_{\text{sup}}}{N^{1-\delta|-u|-\alpha}} \leq \frac{C_{\text{sup}}}{N^{1-\varepsilon}}.$$

So, for all $n_1 \leq K_N$ and all $n_2 \leq K_N$,

$$\left|\log\left(\frac{\mathbb{P}(N_2 = n_2 | X_{-u}^{(1,2)} = x_{-u}^{(1,2)})}{\mathbb{P}(N_2 = n_2 | N_1 = n_1, X_{-u}^{(1,2)} = x_{-u}^{(1,2)})}\right)\right| \leq \frac{C_{\text{sup}}(\varepsilon)}{N^{1-\varepsilon}}.$$

Thus, we have shown that we have

$$A(x_{-u}^{(1)}, x_{-u}^{(2)}) \leq \frac{C_{\text{sup}}}{N^{1-\varepsilon}}.$$

Now, let us bound $B(x_{-u}^{(1)}, x_{-u}^{(2)})$. Remark that $\{(n_1, n_2) \in [N_I - 1 : N-2] |\ n_1 > K_N \text{ or } n_2 > K_N\}$ is a subset of

$$([K_N + 1 : N-2] \times [N_I - 1 : N-2]) \cup ([N_I - 1 : N-2] \times [K_N + 1 : N-2]).$$

Thus, it suffices to bound

$$\begin{aligned}
\textstyle\sum_{n_1=K_N+1}^{N-2}\sum_{n_2=N_I-1}^{N-2} \quad & \big|\mathbb{P}(N_1 = n_1, N_2 = n_2 | X_{-u}^{(1,2)} = x_{-u}^{(1,2)})\\
& -\mathbb{P}(N_1 = n_1 | X_{-u}^{(1,2)} = x_{-u}^{(1,2)})\mathbb{P}(N_2 = n_2 | X_{-u}^{(1,2)} = x_{-u}^{(1,2)})\big|\\
= \quad & \sum_{n_1=K_N+1}^{N-2} \mathbb{P}(N_1 = n_1 | X_{-u}^{(1,2)} = x_{-u}^{(1,2)})\\
& \sum_{n_2=N_I-1}^{N-2} \left|\mathbb{P}(N_2 = n_2 | N_1 = n_1, X_{-u}^{(1,2)} = x_{-u}^{(1,2)}) - \mathbb{P}(N_2 = n_2 | X_{-u}^{(1,2)} = x_{-u}^{(1,2)})\right|.
\end{aligned}$$

Thus, it suffices to bound

$$\sum_{n_1=K_N+1}^{N-2} \mathbb{P}(N_1 = n_1 | X_{-u}^{(1,2)} = x_{-u}^{(1,2)}).$$

Let $T := N-2$. We know that N_1 has a binomial distribution with parameters T and p_1. Thus,

$$\mathrm{E}(N_1) = p_1 T \leq C_{\sup} N^{\delta|-u|} \leq C_{\sup} N^{\frac{\varepsilon}{4}}.$$

Thus, there exists N_ε such that for $N \geq N_\varepsilon$, we have that, $\mathrm{E}(N_1) \leq K_T + 1$. Thus, for N large enough and for all $n_1 > K_T$ and, we have

$$\mathbb{P}(N_1 = n_1 | X_{-u}^{(1,2)} = x_{-u}^{(1,2)}) \leq \mathbb{P}(N_1 = K_T + 1 | X_{-u}^{(1,2)} = x_{-u}^{(1,2)}).$$

Thus, for $N \geq N_\varepsilon$,

$$\begin{aligned}
&\sum_{n_1=K_N+1}^{N-2} \mathbb{P}(N_1 = n_1 | X_{-u}^{(1,2)} = x_{-u}^{(1,2)}) \\
\leq \;& (T-K_T)\mathbb{P}(N_1 = K_T+1 | X_{-u}^{(1,2)} = x_{-u}^{(1,2)}) \\
= \;& (T-K_T)\frac{T!}{(T-K_T-1)!(K_T+1)!} p_1^{K_T+1}(1-p_1)^{T-K_T+1} \\
\leq \;& (T-K_T)\frac{T!}{(T-K_T-1)!(K_T+1)!} p_1^{K_T+1} \\
\leq \;& C_{\sup} \frac{(T-K_T)\sqrt{2\pi T}\left(\frac{T}{e}\right)^T \left(\frac{C_{\sup}}{T^{1-\delta|-u|}}\right)^{K_T+1}}{\sqrt{2\pi(K_T+1)}\left(\frac{K_T+1}{e}\right)^{(K_T+1)}\sqrt{2\pi(T-K_T-1)}\left(\frac{T-K_T-1}{e}\right)^{(T-K_T-1)}} \\
\leq \;& C_{\sup} \frac{(T-K_T)\sqrt{T}T^T C_{\sup}^{K_T+1}}{\sqrt{(K_T+1)(T-K_T-1)}(K_T+1)^{K_T+1}(T-K_T-1)^{T-K_T-1}T^{(1-\delta|-u|)(K_T+1)}} \\
\leq \;& C_{\sup}(T-K_T)^{K_T+\frac{3}{2}-T}(K_T+1)^{-K_T-\frac{3}{2}}T^{T-\frac{1}{2}+\delta|-u|(K_T+1)-K_T}C_{\sup}^{K_T+1}.
\end{aligned}$$

Using the Taylor expansion of $x \mapsto \log(1-x)$ at 0, we can see that

$$(T-K_T)^{-T}T^T \leq C_{\sup}\exp(K_T) \leq C_{\sup}^{K_T}.$$

Moreover, we have

$$(K_T+1)T^{1-\delta|-u|} \geq T^{\frac{\varepsilon}{3}}T^{1-\frac{\varepsilon}{4}} = T^{1+\frac{\varepsilon}{12}},$$

and so

$$(T-K_T)^{K_T}(K_T+1)^{-K_T}T^{-K_T(1-\delta|-u|)}C_{\sup}^{K_T} \;\leq\; \exp\left(K_T \log\left[C_{\sup}\frac{T-K_T}{T^{1+\frac{\varepsilon}{12}}}\right]\right)$$

$$\leq \quad C_{\sup}(\varepsilon)e^{-K_T}.$$

Thus, we have

$$\begin{aligned}
&\sum_{n_1=K_N+1}^{N-2} \mathbb{P}(N_1 = n_1 | X_{-u}^{(1,2)} = x_{-u}^{(1,2)}) \\
\leq\ & C_{\sup}(\varepsilon)e^{-K_T}(T-K_T)^{\frac{3}{2}}(K_T+1)^{-\frac{3}{2}}T^{-\frac{1}{2}+\delta|-u|} \\
\leq\ & \frac{C_{\sup}(\varepsilon)}{T} \\
\leq\ & \frac{C_{\sup}(\varepsilon)}{N}.
\end{aligned}$$

Finally, we have

$$A(x_{-u}^{(1)}, x_{-u}^{(2)}) \leq \frac{C_{\sup}}{N^{1-\varepsilon}}, \quad \text{and} \quad B(x_{-u}^{(1)}, x_{-u}^{(2)}) \leq \frac{C_{\sup}(\varepsilon)}{N}.$$

Thus

$$\begin{aligned}
\textstyle\sum_{n_1,n_2=N_I}^{N} \quad & \big|\mathbb{P}(N_1 = n_1, N_2 = n_2 | X_{-u}^{(1,2)} = x_{-u}^{(1,2)}) \\
& -\mathbb{P}(N_1 = n_1 | X_{-u}^{(1,2)} = x_{-u}^{(1,2)})\mathbb{P}(N_2 = n_2 | X_{-u}^{(1,2)} = x_{-u}^{(1,2)})\big| \leq \frac{C_{\sup}(\varepsilon)}{N^{1-\varepsilon}}.
\end{aligned}$$

So, we have proved Proposition 47. □

We conclude by the proof of Theorem 4.

Proof.

$$\begin{aligned}
& \mathbb{P}\left(\left|\widehat{E}_u - E_u\right| > \varepsilon\right) \\
\leq\ & \mathbb{P}\left(\left|\widehat{E}_u - \mathrm{E}(\widehat{E}_u)\right| > \frac{\varepsilon}{2}\right) + \mathbb{P}\left(\left|\mathrm{E}(\widehat{E}_u) - E_u\right| > \frac{\varepsilon}{2}\right).
\end{aligned}$$

Then, we use the proof of Proposition 45. If $(s(l))_{l\leq N_u}$ is a sample of uniformly distributed variables on $[1:N]$ with replacement, then for all $\varepsilon > 0$,

$$\begin{aligned}
\mathbb{P}\left(\left|\widehat{E}_u - \mathrm{E}(\widehat{E}_u)\right| > \frac{\varepsilon}{2}\right) \quad & \leq \quad \frac{4}{\varepsilon^2}\left(\left|\mathrm{cov}\left(\widehat{E}_{u,1}, \widehat{E}_{u,2}\right)\right| + \mathrm{Var}\left(\widehat{E}_{u,1}\right)\left(\frac{1}{N} + \frac{1}{N_u}\right)\right) \\
& \leq \quad \frac{1}{\varepsilon^2}\left(\frac{C_{\sup}(\varepsilon')}{N^{\frac{1}{p-|u|}-\varepsilon'}} + \frac{C_{\sup}}{N_u}\right),
\end{aligned}$$

for all $\varepsilon' > 0$, thanks to Proposition 47. If $(s(l))_{l\leq N_u}$ is a sample of uniformly distributed variables on $[1:N]$ without replacement, then for all $\varepsilon > 0$,

$$\mathbb{P}\left(\left|\widehat{E}_u - \mathrm{E}(\widehat{E}_u)\right| > \frac{\varepsilon}{2}\right) \quad \leq \quad \frac{4}{\varepsilon^2}\left(\frac{N_u - 1}{N_u}\mathrm{cov}\left(\widehat{E}_{u,1}, \widehat{E}_{u,2}\right) + \frac{1}{N_u}\mathrm{Var}\left(\widehat{E}_{u,1}\right)\right)$$

$$\leq \frac{1}{\varepsilon^2}\left(\frac{C_{\sup}(\varepsilon')}{N^{\frac{1}{p-|u|}-\varepsilon'}} + \frac{C_{\sup}}{N_u}\right),$$

for all $\varepsilon' > 0$, thanks to Proposition 47. Moreover, for all $\varepsilon > 0$,

$$\begin{aligned}\mathbb{P}\left(\left|\widehat{E}_u - E_u\right| > \frac{\varepsilon}{2}\right) &\leq \frac{2}{\varepsilon}\left|\mathrm{E}(\widehat{E}_u) - E_u\right| \\ &\leq \frac{C_{\sup}(\varepsilon')}{\varepsilon N^{\frac{1}{p-|u|}-\varepsilon'}},\end{aligned}$$

for all $\varepsilon' > 0$, thanks to Proposition 46. Finally, for all $\varepsilon > 0$, $\varepsilon' > 0$, we have

$$\mathbb{P}\left(\left|\widehat{E}_u - E_u\right| > \varepsilon\right) \leq \frac{1}{\varepsilon^2}\left(\frac{C_{\sup}(\varepsilon')}{N^{\frac{1}{p-|u|}-\varepsilon'}} + \frac{C_{\sup}}{N_u}\right).$$

That concludes the proof. □

B Other proofs

Proof of Proposition 9

Proof.

$$\begin{aligned}& \mathrm{E}(f(X)f(X^u)) \\ =\ & \mathrm{E}(\mathrm{E}(f(X)f(X^u)|X_u)) \\ =\ & \mathrm{E}\left(\int_{\mathcal{X}_{-u}^2} f(X_u, x_{-u}) f(X_u, x'_{-u}) d\mathbb{P}_{X_{-u}|X_u} \otimes \mathbb{P}_{X_{-u}|X_u}(x_{-u}, x'_{-u})\right) \\ =\ & \mathrm{E}\left(\int_{\mathcal{X}_{-u}} f(X_u, x_{-u}) d\mathbb{P}_{X_{-u}|X_u}(x_{-u}) \int_{\mathcal{X}_{-u}} f(X_u, x'_{-u}) d\mathbb{P}_{X_{-u}|X_u}(x'_{-u})\right) \\ =\ & \mathrm{E}\left(\mathrm{E}(f(X)|X_u)^2\right).\end{aligned}$$

That concludes the proof of Proposition 9. □

Proof of Proposition 10

Proof. Let

$$A_{i,u} := \begin{cases} -\frac{1}{p}\binom{p-1}{|u|}^{-1} & \text{if } i \notin u \\ \frac{1}{p}\binom{p-1}{|u|-1}^{-1} & \text{if } i \in u. \end{cases}$$

Under Assumption 2, we have

$$\begin{aligned}
\mathrm{Var}(Y)^2\sum_{i=1}^p \mathrm{Var}(\widehat{\eta}_i) &= \sum_{i=1}^p \sum_{\emptyset\subsetneq u\subsetneq[1:p]} A_{i,u}^2 \mathrm{Var}(\widehat{W}_u)\\
&= \sum_{\emptyset\subsetneq u\subsetneq[1:p]} \mathrm{Var}(\widehat{W}_u)\sum_{i=1}^p A_{i,u}^2\\
&= \sum_{\emptyset\subsetneq u\subsetneq[1:p]} \frac{\mathrm{Var}(\widehat{W}_u^{(1)})}{N_u}\sum_{i=1}^p A_{i,u}^2.
\end{aligned}$$

Moreover,

$$\begin{aligned}
\sum_{i=1}^p A_{i,u}^2 &= \sum_{i\in -u}\frac{1}{p^2}\binom{p-1}{|u|}^{-2}+\sum_{i\in u}\frac{1}{p^2}\binom{p-1}{|u|-1}^{-2}\\
&= \frac{1}{p!^2}\left((p-|u|)|u|!^2(p-|u|-1)!^2+|u|(|u|-1)!^2(p-|u|)!^2\right)\\
&= \frac{(p-|u|)!|u|!}{p!^2}(p-|u|-1)!(|u|-1)!(|u|+p-|u|)\\
&= \frac{(p-|u|)!|u|!}{p!}\frac{(p-|u|-1)!(|u|-1)!}{(p-1)!}\\
&=: C(|u|,p).
\end{aligned}$$

Thus, we want to minimize

$$\sum_{\emptyset\subsetneq u\subsetneq[1:p]} \frac{\mathrm{Var}(\widehat{W}_u^{(1)})}{N_u}C(|u|,p)$$

subject to

$$\sum_{\emptyset\subsetneq u\subsetneq[1:p]} N_u=\frac{N_{tot}}{\kappa}.$$

Let $U=(\mathbb{R}_+^*)^{2^p-2}$. If $x\in U$, we index the components of x by the subsets $\emptyset\subsetneq u\subsetneq[1:p]$ and we write $x=(x_u)_{\emptyset\subsetneq u\subsetneq[1:p]}$. Let h be the C^1 function on U defined by $h(x)=\sum_{\emptyset\subsetneq u\subsetneq[1:p]}\frac{C(|u|,p)\mathrm{Var}(\widehat{W}_u^{(1)})}{x_u}$, let g be the C^1 function on U defined by $g(x)=\left(\sum_{\emptyset\subsetneq u\subsetneq[1:p]}x_u\right)-N_{tot}/\kappa$ and let $A=g^{-1}(\{0\})$. Using the method of Lagrange multipliers, if $h_{|A}$ has a local minimum in $\mathbf{a}$, there exists c such that $Dh(\mathbf{a})=cDg(\mathbf{a})$, i.e. $\nabla h(\mathbf{a})=\nabla g(\mathbf{a})$ i.e.

$$\mathbf{a}=\frac{N_{tot}}{\kappa\sum_{\emptyset\subsetneq v\subsetneq[1:p]}\sqrt{C(|v|,p)\mathrm{Var}(\widehat{W}_v^{(1)})}}\left(\sqrt{C(|u|,p)\mathrm{Var}(\widehat{W}_u^{(1)})}\right)_{\emptyset\subsetneq u\subsetneq[1:p]}.$$

Moreover, note that h is strictly convex and the set A is convex, thus $h_{|A}$ is strictly convex. Thus $\mathbf{a}$ is the strict global minimum point of $h_{|A}$. □

Proof of Proposition 12

Proof. Let us write $V := \mathrm{Var}(\widehat{W}_u^{(1)})$ that does not depend on u by assumption. To simplify notation, let $N_0 = N_p = +\infty$. In this way, we have, for all $u \subset [1:p]$, $\mathrm{Var}(\widehat{W}_u(m)) = V/N_{|u|}$.

We have

$$\begin{aligned}
\mathrm{Var}\left(\widehat{\eta}_i | (\sigma_m)_{m\leq M}\right) &= \frac{1}{p^2\mathrm{Var}(Y)^2}\sum_{u\subset -i}\frac{1}{M^2}\sum_{m=1}^M\left[\mathrm{Var}\left(\widehat{W}_{u\cup\{i\}}(m)\right)+\mathrm{Var}\left(\widehat{W}_u(m)\right)\right]\mathbb{1}_{P_i(\sigma_m)=u}\\
&= \frac{V}{p^2\mathrm{Var}(Y)^2}\sum_{u\subset -i}\frac{1}{M^2}\sum_{m=1}^M\left[\frac{1}{N_{|u\cup\{i\}|}}+\frac{1}{N_u}\right]\mathbb{1}_{P_i(\sigma_m)=u}.
\end{aligned}$$

Thus,

$$\begin{aligned}
\mathrm{E}\left[\mathrm{Var}\left(\widehat{\eta}_i | (\sigma_m)_{m\leq M}\right)\right] &= \frac{V}{p^2\mathrm{Var}(Y)^2}\sum_{u\subset -i}\frac{1}{M^2}\sum_{m=1}^M\left[\frac{1}{N_{|u\cup\{i\}|}}+\frac{1}{N_u}\right]\mathbb{P}(P_i(\sigma_m)=u)\\
&= \frac{V}{p^2\mathrm{Var}(Y)^2}\sum_{u\subset -i}\frac{1}{M^2}\sum_{m=1}^M\frac{1}{p}\begin{pmatrix}p-1\\|u|\end{pmatrix}^{-1}\left[\frac{1}{N_{|u\cup\{i\}|}}+\frac{1}{N_{|u|}}\right]\\
&= \frac{V}{p^2\mathrm{Var}(Y)^2}\sum_{u\subset[1:p]}a_{i,u}\frac{1}{N_{|u|}},
\end{aligned}$$

where

$$a_{i,u} := \begin{cases}\frac{1}{p}\begin{pmatrix}p-1\\|u|\end{pmatrix}^{-1} & \text{if } i\notin u\\ \begin{pmatrix}p-1\\|u|-1\end{pmatrix}^{-1} & \text{if } i\in u.\end{cases}$$

Remark that $\sum_{i=1}^p a_{i,u} = 2\begin{pmatrix}p\\|u|\end{pmatrix}^{-1}$. Then,

$$\begin{aligned}
\mathrm{E}\left[\sum_{i=1}^p\mathrm{Var}\left(\widehat{\eta}_i | (\sigma_m)_{m\leq M}\right)\right] &= \sum_{i=1}^p\frac{V}{p^2\mathrm{Var}(Y)^2}\sum_{u\subset[1:p]}a_{i,u}\frac{1}{N_{|u|}}\\
&= \frac{V}{p^2\mathrm{Var}(Y)^2}\sum_{u\subset[1:p]}\frac{1}{N_{|u|}}\sum_{i=1}^p a_{i,u}
\end{aligned}$$

$$
\begin{aligned}
&= \frac{2V}{p^2\mathrm{Var}(Y)^2} \sum_{u \subset [1:p]} \frac{1}{N_{|u|}} \binom{p}{|u|}^{-1} \\
&= \frac{2V}{p^2\mathrm{Var}(Y)^2} \sum_{k=1}^{p-1} \frac{1}{N_k}
\end{aligned}
$$

We get the relaxed problem

$$
\min_{(N_k)_{k\in[1:p-1]}} \frac{2V}{p^2\mathrm{Var}(Y)^2} \sum_{k=1}^{p-1} \frac{1}{N_k}
$$

subject to $M\sum_{k=1}^{p-1} N_k = MN_O(p-1)$. Let $U = (\mathbb{R}_+^*)^{p-1}$. Let h be the C^1 function on U defined by $h(x) = \frac{2V}{p^2\mathrm{Var}(Y)^2}\sum_{k=1}^{p-1}\frac{1}{x_k}$, g be the C^1 function on U defined by $g(x) = M\sum_{k=1}^{p-1} x_k - MN_O(p-1)$. Finally, let $A = g^{-1}(\{0\})$. Using the method of Lagrange multipliers, if $h_{|A}$ has a local minimum in $\mathbf{a}$, there exists c such that $Dh(\mathbf{a}) = cDg(\mathbf{a})$, i.e. $\nabla h(\mathbf{a}) = \nabla g(\mathbf{a})$ i.e. $\forall u$, $-\frac{1}{a_u^2} = c'$ i.e. $a_u = c''$. To sum up, if $h_{|A}$ has a local minimum, it is in $\mathbf{a}$ defined by

$$
a_u = N_O M p_u.
$$

Moreover, note that h is strictly convex and the set A is convex, thus $h_{|A}$ is strictly convex. Thus $\mathbf{a}$ is the strict global minimum point of $h_{|A}$. Thus, $\mathbf{a}$ is the global minimum on the constraint problem (where the inputs are integers). □

Proof of Proposition 13 This proof totally arises from the appendix of [SNS16]. The computations are the same.

Proof. Under Assumption 4, we have

$$
\begin{aligned}
\mathrm{Var}(\widehat{\eta}_i) &= \frac{1}{M\mathrm{Var}(Y)^2}\left(\mathrm{Var}\left(\widehat{W}_{P_i(\sigma_1)\cup\{i\}}\right) + \mathrm{Var}\left(\widehat{W}_{P_i(\sigma_1)}\right)\right) \\
&= \frac{1}{M\mathrm{Var}(Y)^2}\Big(\mathrm{Var}(\mathrm{E}(\widehat{W}_{P_i(\sigma_1)\cup\{i\}}|\sigma_1)) + \mathrm{E}(\mathrm{Var}(\widehat{W}_{P_i(\sigma_1)\cup\{i\}}|\sigma_1)) \\
&\quad + \mathrm{Var}(\mathrm{E}(\widehat{W}_{P_i(\sigma_1)}|\sigma_1)) + \mathrm{E}(\mathrm{Var}(\widehat{W}_{P_i(\sigma_1)}|\sigma_1))\Big) \\
&= \frac{1}{C\mathrm{Var}(Y)^2}\Big(N_O\mathrm{Var}(W_{P_i(\sigma_1)\cup\{i\}}) + N_O\mathrm{Var}(W_{P_i(\sigma_1)}) \\
&\quad + \mathrm{E}(\mathrm{Var}(\widehat{W}^{(1)}_{P_i(\sigma_1)\cup\{i\}}|\sigma_1)) + \mathrm{E}(\mathrm{Var}(\widehat{W}^{(1)}_{P_i(\sigma_1)}|\sigma_1))\Big).
\end{aligned}
$$

Thus, the minimum is with $N_O = 1$. □

Proof of Proposition 14

Proof. We only prove the second item. The first one is easier and uses the same idea. Let $i \in [1:p]$. Remark that

$$\begin{aligned}\widehat{\eta}_i &= \frac{1}{M\mathrm{Var}(Y)} \sum_{m=1}^{M} \left(\widehat{W}_{P_i(\sigma_m)\cup\{i\}}(m) - \widehat{W}_{P_i(\sigma_m)}(m) \right) \\ &= \frac{1}{p\mathrm{Var}(Y)} \sum_{u \subset -i} \binom{p-1}{|u|}^{-1} \left(\tilde{W}_{u\cup\{i\},i} - \tilde{W}_{u,i} \right)\end{aligned}$$

with

$$\tilde{W}_{u,i} := \binom{p-1}{|u|} \frac{p}{M} \sum_{m|\ P_i(\sigma_m)=u} \widehat{W}_u(m) \quad \text{and} \quad \tilde{W}_{u\cup\{i\},i} := \binom{p-1}{|u|} \frac{p}{M} \sum_{m|\ P_i(\sigma_m)=u} \widehat{W}_{u\cup\{i\}}(m),$$

where we sum over all the integers $m \in [1:M]$ such that $P_i(\sigma_m) = u$. Thus, for all u,

$$\tilde{W}_{u,i} \sim \binom{p-1}{|u \setminus \{i\}|} \frac{p}{M} \tilde{N}_{u,i,M} \widehat{W}_u^{\tilde{N}_{u,i,M}},$$

where

$$\widehat{W}_u^{\tilde{N}_{u,i,M}} := \frac{1}{\tilde{N}_{u,i,M}} \sum_{k=1}^{\tilde{N}_{u,i,M}} \widehat{W}_u(k),$$

and $\tilde{N}_{u,i,M} = \tilde{N}_{u\cup\{i\},i,M} \sim \mathcal{B}(M, \frac{|u|!(p-1-|u|)!}{p!})$ (the binomial distribution). Now, remark that M goes to $+\infty$ when N_{tot} goes to $+\infty$ (recall that $N_{tot} = \kappa M(p-1)$). Hence,

$$\binom{p-1}{|u \setminus \{i\}|} \frac{p}{M} \tilde{N}_{u,i,M} \underset{N_{tot}\to+\infty}{\overset{\mathbb{P}}{\longrightarrow}} 1.$$

It suffices to show that for all $u \subset [1:p]$, the estimator $\omega \mapsto \widehat{W}_u^{\tilde{N}_{u,i,M}(\omega)}(\omega)$ converges to W_u in probability when N and N_{tot} go to $+\infty$ and we could conclude by

$$\begin{aligned}\widehat{\eta}_i &= \frac{1}{p\mathrm{Var}(Y)} \sum_{u \subset -i} \binom{p-1}{|u|}^{-1} \left(\tilde{W}_{u\cup\{i\},i} - \tilde{W}_{u,i} \right) \\ &\underset{\substack{N_{tot}\to+\infty \\ N\to+\infty}}{\overset{\mathbb{P}}{\longrightarrow}} \frac{1}{p\mathrm{Var}(Y)} \sum_{u \subset -i} \binom{p-1}{|u|}^{-1} \left(W_{u\cup\{i\}} - W_u \right) \\ &= \eta_i.\end{aligned}$$

Let $\varepsilon > 0$ and $\delta > 0$. Using the assumptions and Chebyshev's inequality, we have that $(\widehat{W}_u^{N_O})_{N_O,N}$ is consistent, thus there exists N_{O1} and N_1 such that for all $N_O \geq N_{O1}$ and all $N \geq N_1$,

$$\mathbb{P}\left(\left|\widehat{W}_u^{N_O} - W_u\right| > \delta\right) < \frac{\varepsilon}{2}.$$

Moreover,

$$\mathbb{P}(\tilde{N}_{u,M} \leq N_{O1}) \underset{M\to+\infty}{\longrightarrow} 0.$$

Thus, there exists M_1 such that for all $M \geq M_1$,

$$\mathbb{P}(\tilde{N}_{u,M} \leq N_{O1}) < \frac{\varepsilon}{2}.$$

Thus, there exists N_{tot1} such that for all $N_{tot} \geq N_{tot1}$,

$$\mathbb{P}(\tilde{N}_{u,M} \leq N_{O1}) < \frac{\varepsilon}{2}.$$

Finally, for all $N_{tot} \geq N_{tot1}$ and $N \geq N_1$, we have

$$\begin{aligned}\mathbb{P}\left(\left|\widehat{W}_u^{\tilde{N}_{u,M}} - W_u\right| > \delta\right) &\leq \mathbb{P}\left(\left|\widehat{W}_u^{\tilde{N}_{u,M}} - W_u\right| > \delta,\ \ \tilde{N}_{u,M} \geq N_{O1}\right) + \mathbb{P}(\tilde{N}_{u,M} \leq N_{O1}) \\ &< \varepsilon.\end{aligned}$$

That proves that the estimator $\omega \mapsto \widehat{W}_u^{\tilde{N}_{u,i,M}(\omega)}(\omega)$ converges to W_u in probability when N and N_{tot} go to $+\infty$. □

Proof of Corollary 1 and Corollary 2

We do the proof for Corollary 1. The proof of Corollary 2 uses the same idea.

Proof. Let $\delta > 0$. Thanks to Theorem 4, with $\varepsilon' = \delta$, we have

$$\mathbb{P}\left(N^{\frac{1}{2(p-|u|)}-\delta}\left|\widehat{E}_{u,MC} - E_u\right| > \varepsilon\right) \leq \frac{C_{\sup}(\delta)N^{\frac{1}{p-|u|}-2\delta}}{\varepsilon^2 N^{\frac{1}{p-|u|}-\delta}} \underset{N\to+\infty}{\longrightarrow} 0.$$

That concludes the proof of Corollary 1. □

Proof of Proposition 15

Proof. If we use the subset W-aggregation procedure, we just have to use the consistency of $\widehat{W}_u$ from Theorems 3 and 5 and to use Proposition 11.

If we use the subset W-aggregation procedure, the consistency of the estimators of the Shapley effects comes from the second part of Proposition 14. We just have to verify Assumption 5. Let $\widehat{W}_u(m)$ of Proposition 14 be $\widehat{E}_{u,s(m),MC}$ or $\widehat{V}_{u,s(m),PF}$

defined in Section E.1, where $(s(m))_m$ are independent and uniformly distributed on $[1:N]$. Then, following the end of the proof of Theorems 3 and 5, we obtain

$$\frac{1}{M^2}\sum_{m,m'=1}^{M}\operatorname{cov}\left(\widehat{W}_u(m),\widehat{W}_u(m')\right)\underset{N,M\to+\infty}{\longrightarrow}0,$$

and, by Proposition 43, we have

$$\mathrm{E}\left(\widehat{W}_u(1)\right)=\mathrm{E}\left(\widehat{W}_u^{(1)}\right)\underset{N\to+\infty}{\longrightarrow}W_u.$$

Thus, Assumption 5 holds. $\square$

Appendix II

Proofs of Chapter 4

Proof of Proposition 16:
We use the Hoeffding decomposition of g:

$$
\begin{aligned}
V_u &= \mathrm{Var}(\mathrm{E}(Y|X_u)) \\
&= \mathrm{Var}\left[\sum_{w\subset[1:K]} \mathrm{E}(g_w(A_w)|X_{u\cap B_w})\right] \\
&= \sum_{w\subset[1:K]} \mathrm{Var}\left[\mathrm{E}(g_w(A_w)|X_{u\cap B_w})\right] \\
&= \sum_{w\subset[1:K]} V^{g,w}_{u\cap B_w}.
\end{aligned}
$$

$\square$

Proof of Proposition 17:
We have

$$
\begin{aligned}
S_u &= \frac{1}{\mathrm{Var}(Y)} \sum_{v\subset u} (-1)^{|u|-|v|} V_v \\
&= \frac{1}{\mathrm{Var}(Y)} \sum_{v\subset u} (-1)^{|u|-|v|} \sum_{w\subset[1:K]} V^{g,w}_{v\cap B_w} \\
&= \frac{1}{\mathrm{Var}(Y)} \sum_{w\subset[1:K]} \sum_{v\subset u} (-1)^{|u|-|v|} V^{g,w}_{v\cap B_w} \\
&= \frac{1}{\mathrm{Var}(Y)} \sum_{w\subset[1:K]} \sum_{v_1\subset u\cap B_w} V^{g,w}_{v_1} \sum_{\substack{v_2\subset -B_w,\\ \text{s.t.} v_1\cup v_2\subset u}} (-1)^{|u|-|v_1|-|v_2|}.
\end{aligned}
$$

One can remark that, if $u \setminus B_w \neq \emptyset$,

$$\sum_{\substack{v_2 \subset -B_w, \\ \text{s.t.} v_1 \cup v_2 \subset u}} (-1)^{|u|-|v_1|-|v_2|} = (-1)^{|u|-|v_1|} \sum_{n=0}^{|u \setminus B_w|} \binom{|u \setminus B_w|}{n} (-1)^n = 0.$$

Thus,

$$\begin{aligned} S_u &= \frac{1}{\mathrm{Var}(Y)} \sum_{\substack{w \subset [1:K], \\ s.t.\ u \subset B_w}} \sum_{v_1 \subset u} (-1)^{|u|-|v_1|} V_{v_1}^{g,w} \\ &= \sum_{\substack{w \subset [1:K], \\ s.t.\ u \subset B_w}} \frac{\mathrm{Var}(g_w(A_w))}{\mathrm{Var}(Y)} S_u^{g,w}. \end{aligned}$$

$\square$

Proof of Proposition 18:

$$\begin{aligned} \eta_i &= \frac{1}{p\mathrm{Var}(Y)} \sum_{u \subset -i} \binom{p-1}{|u|}^{-1} (V_{u \cup \{i\}} - V_u) \\ &= \frac{1}{p\mathrm{Var}(Y)} \sum_{u \subset -i} \binom{p-1}{|u|}^{-1} \sum_{w \subset [1:K]} (V^{g,w}_{(u \cup i) \cap B_w} - V^{g,w}_{u \cap B_w}) \\ &= \frac{1}{p\mathrm{Var}(Y)} \sum_{\substack{w \subset [1:K], \\ \text{s.t. } j(i) \in w}} \sum_{u \subset -i} \binom{p-1}{|u|}^{-1} (V^{g,w}_{(u \cup i) \cap B_w} - V^{g,w}_{u \cap B_w}) \\ &= \frac{1}{p\mathrm{Var}(Y)} \sum_{\substack{w \subset [1:K], \\ \text{s.t. } j(i) \in w}} \sum_{u \subset B_w \setminus \{i\}} \left[\sum_{v \subset -B_w} \binom{p-1}{|u \cup v|}^{-1} \right] (V^{g,w}_{u \cup i} - V^{g,w}_u) \\ &= \frac{1}{p\mathrm{Var}(Y)} \sum_{\substack{w \subset [1:K], \\ \text{s.t. } j(i) \in w}} \sum_{u \subset B_w \setminus \{i\}} \left[\sum_{j=0}^{p-|B_w|} \binom{p-|B_w|}{j} \binom{p-1}{|u|+j}^{-1} \right] (V^{g,w}_{u \cup i} - V^{g,w}_u). \end{aligned}$$

It remains to prove the following equation:

$$\frac{1}{p} \sum_{j=0}^{p-|B_w|} \binom{p-|B_w|}{j} \binom{p-1}{|u|+j}^{-1} = \frac{1}{|B_w|} \binom{|B_w|-1}{|u|}^{-1}. \tag{II.1}$$

In the interest of simplifying notation, until the end of the proof, we will write u (resp. c) instead of $|u|$ (resp. $|B_w|$). We can verify that Equation (II.1) is equivalent to the following equations:

$$\begin{aligned} & \frac{1}{p}\sum_{j=0}^{p-c}\frac{(p-c)!}{j!(p-c-j)!}\frac{(u+j)!(p-1-u-j)!}{(p-1)!} = \frac{1}{c}\frac{u!(c-1-u)!}{(c-1)!} \\ \iff & \sum_{j=0}^{p-c}\binom{u+j}{u}\binom{p-1-u-j}{c-u-1} = \binom{p}{c}. \end{aligned} \tag{II.2}$$

We will show Equation (II.2). Now, we can remark that we have:

$$\frac{x^c}{(1-x)^{c+1}} = x\frac{x^u}{(1-x)^{u+1}}\frac{x^{c-u-1}}{(1-x)^{c-u}}. \tag{II.3}$$

Giving their power series, we have:

$$x\left(\sum_{k\geq 0}\binom{k}{u}x^k\right)\left(\sum_{k'\geq 0}\binom{k'}{c-u-1}x^{k'}\right) = \sum_{k''\geq 0}\binom{k''}{c}x^{k''}. \tag{II.4}$$

We have the equality of the coefficient of x^p. Then:

$$\begin{aligned} \binom{p}{c} &= \sum_{k+k'=p-1}\binom{k}{u}\binom{k'}{c-u-1} = \sum_{k=u}^{p-1}\binom{k}{u}\binom{p-1-k}{c-u-1} = \sum_{j=0}^{p-1-u}\binom{u+j}{u}\binom{p-1-u-j}{c-u-1} \\ &= \sum_{j=0}^{p-c}\binom{u+j}{u}\binom{p-1-u-j}{c-u-1}. \end{aligned}$$

For the last equality, we remark that if $j > p-c$, then $p-1-u-j < c-u-1$ so the last terms of the sum are equal to zero. We have proven Equation (II.2). To conclude, we have

$$\begin{aligned} \eta_i &= \frac{1}{p\mathrm{Var}(Y)}\sum_{\substack{w\subset[1:K],\\ \text{s.t. } j(i)\in w}}\sum_{u\subset B_w\setminus\{i\}}\left[\sum_{j=0}^{p-|B_w|}\binom{p-|B_w|}{j}\binom{p-1}{|u|+j}^{-1}\right](V_{u\cup\{i\}}-V_u) \\ &= \sum_{\substack{w\subset[1:K],\\ \text{s.t. } j(i)\in w}} S_w^g\frac{1}{|B_w|\mathrm{Var}(g_w(A_w))}\sum_{u\subset B_w\setminus\{i\}}\binom{|B_w|-1}{|u|}^{-1}(V_{u\cup i}^{g,w}-V_u^{g,w}) \\ &= \sum_{\substack{w\subset[1:K],\\ \text{s.t. } j(i)\in w}} S_w^g\eta_i^{g,w}. \end{aligned}$$

□

Appendix III

Proofs of Chapter 5

Notation

We will write $C_{\sup}$ for a generic non-negative finite constant (depending only on $\lambda_{\inf}$, $\lambda_{\sup}$ and m in Conditions 2 and 3). The actual value of $C_{\sup}$ is of no interest and can change in the same sequence of equations. Similarly, we will write $C_{\inf}$ for a generic strictly positive constant.

If $B, B' \in \mathcal{P}_p$, and $(i,j) \in [1:p]^2$, we will write $(i,j) \in B \setminus B'$ if $(i,j) \in B$ and $(i,j) \notin B'$, that is, if i and j are in the same group with the partition B and are in different groups with the partition B'.

If $B, B' \in \mathcal{P}_p$, we define $B \cap B'$ as the maximal partition B'' such that $B'' \leq B$ and $B'' \leq B'$.

If $\Gamma \in \mathcal{M}_p(\mathbb{R})$ (the set of the matrices of dimension $p \times p$), and if $u, v \subset [1:p]$, we define $\Gamma_{u,v} := (\Gamma_{i,j})_{i \in u, j \in v}$ and $\Gamma_u := \Gamma_{u,u}$.

Recall that $\mathrm{vec} : \mathcal{M}_p(\mathbb{R}) \to \mathbb{R}^{p^2}$ is defined by $(\mathrm{vec}(M))_{p(j-1)+i} := M_{i,j}$.

If $\Gamma \in S_p(\mathbb{R})$ (the set of the symmetric positive definite matrices) and $i \in [1:p]$, let $\phi_i(M)$ be the i-th largest eigenvalue of M. We also write $\lambda_{\max}(M)$ (resp. $\lambda_{\min}(M)$) for the largest (resp. smallest) eigenvalue of M.

We define $\widehat{\Sigma} := \frac{1}{n-1}\sum_{l=1}^{l}(X^{(l)} - \overline{X})(X^{(l)} - \overline{X})^T = \frac{n}{n-1}S$, the unbiased empirical estimator of Σ. Let $(\widehat{\sigma}_{ij})_{i,j \leq p}$ be the coefficients of $\widehat{\Sigma}$ and $(s_{ij})_{i,j \leq p}$ be the coefficients of S.

Recall that when Condition 4 does not hold, we need to define $B(\alpha)$ as the partition given by thresholding Σ by $n^{-\alpha}$. We also define $K(\alpha) := |B(\alpha)|$ and write $B(\alpha) = \{B_1(\alpha), B_2(\alpha), ...B_{K(\alpha)}(\alpha)\}$.

Proof of Proposition 19

Proof. Let us write

$$\overline{S_p^{++}(\mathbb{R}, B)} := \bigsqcup_{B' \leq B} S_p^{++}(\mathbb{R}, B') = \{\Gamma \in S_p^{++},\ \Gamma = \Gamma_B\},$$

which is the closure of $S_p^{++}(\mathbb{R}, B)$ in $S_p^{++}(\mathbb{R})$.

First, let us show that, for all B, S_B is the minimum of $\Gamma \mapsto l_\Gamma$ on $\overline{S_p^{++}(\mathbb{R}, B)}$. If $\Gamma_B \in \overline{S_p^{++}(\mathbb{R}, B)}$, we have

$$\begin{aligned} p\left(l_{\Gamma_B} - l_{S_B}\right) &= -\log(|\Gamma_B^{-1}|) + \mathrm{Tr}(\Gamma_B^{-1}S) + \log(|S_B^{-1}|) - \mathrm{Tr}(S_B^{-1}S) \\ &= -\log\left(\left|\Gamma_B^{-1}S_B\right|\right) + \mathrm{Tr}\left(\Gamma_B^{-1}S_B\right) - p \\ &= \sum_{i=1}^{p}\left\{-\log\left(\phi_i\left[\Gamma_B^{-1/2}S_B\Gamma_B^{-1/2}\right]\right) + \phi_i\left(\Gamma_B^{-1/2}S_B\Gamma_B^{-1/2}\right) - 1\right\}. \end{aligned}$$

The function $f : \mathbb{R}_+^* \to \mathbb{R}$ defined by $f(t) := -\log(t)+t-1$ has an unique minimum at 1. Thus, the function $g : S_p^{++} \to \mathbb{R}$ defined by $g(M) := \sum_{i=1}^p -\log\left(\phi_i\left[M\right]\right) + \phi_i\left(M\right) - 1$ has an unique minimum at I_p. Thus $\Gamma_B \in \overline{S_p^{++}(\mathbb{R}, B)} \mapsto l_{\Gamma_B} - l_{S_B}$ has an unique minimum at $\Gamma_B = S_B$.

Now, the penalisation term is constant on each $S_p^{++}(\mathbb{R}, B)$. Thus Φ has a global minimum (not necessary unique) at S_B, for some $B \in \mathcal{P}_p$. □

Notation for Section B.2

Here and in all the proofs of Section B.2, we assume Conditions 1 to 3 of Section B.2.i).

In the following, we introduce some notation.

We know that

$$\sum_{k=1}^{n}(X^{(k)} - \overline{X})(X^{(k)} - \overline{X})^T \sim \mathcal{W}(n-1, \Sigma),$$

where $\mathcal{W}(n-1, \Sigma)$ is the Wishart distribution with parameter $n-1$ and Σ [GN99]. Thus, if we write $(M^{(k)})_k$ i.i.d. with distribution $\mathcal{N}(0, \Sigma)$, we have

$$\widehat{\Sigma} := \frac{1}{n-1}\sum_{k=1}^{n}(X^{(k)} - \overline{X})(X^{(k)} - \overline{X})^T \sim \frac{1}{n-1}\sum_{k=1}^{n-1} M^{(k)}M^{(k)T}.$$

Lemma 20. *For all $C_{\inf} > 0$,*

$$\mathbb{P}\left(\lambda_{\max}(S) > \lambda_{\sup}(1+\sqrt{y})^2 + C_{\inf}\right) \longrightarrow 0,$$
$$\mathbb{P}\left(\lambda_{\max}(S) < \lambda_{\inf}(1+\sqrt{y})^2 - C_{\inf}\right) \longrightarrow 0,$$
$$\mathbb{P}\left(\lambda_{\min}(S) < \lambda_{\inf}(1-\sqrt{y})^2 - C_{\inf}\right) \longrightarrow 0,$$

and

$$\mathbb{P}\left(\lambda_{\min}(S) > \lambda_{\sup}(1-\sqrt{y})^2 + C_{\inf}\right) \longrightarrow 0.$$

Moreover, that holds also for $\widehat{\Sigma}$ instead of S.

Proof. Let $(A^{(k)})_k$ i.i.d. with distribution $\mathcal{N}(0, I_p)$. Using the result in [Sil85] which states that

$$\lambda_{\max}\left(\frac{1}{n-1}\sum_{k=1}^{n-1} A^{(k)}A^{(k)T}\right) \xrightarrow[n\to+\infty]{a.s.} (1+\sqrt{y})^2,$$

we have,

$$\begin{aligned}
\lambda_{\max}(S) &= \frac{n}{n-1}\lambda_{\max}\left(\frac{1}{n-1}\sum_{k=1}^{n-1} M^{(k)}M^{(k)T}\right) \\
&\leq \frac{n}{n-1}\lambda_{\sup}\lambda_{\max}\left(\frac{1}{n-1}\sum_{k=1}^{n-1} A^{(k)}A^{(k)T}\right) \\
&= \lambda_{\sup}(1+\sqrt{y})^2 + o_p(1),
\end{aligned}$$

and

$$\lambda_{\max}(S) \geq \frac{n}{n-1}\lambda_{\inf}\lambda_{\max}\left(\frac{1}{n-1}\sum_{k=1}^{n-1} A^{(k)}A^{(k)T}\right) = \lambda_{\inf}(1+\sqrt{y})^2 + o_p(1).$$

Thus,

$$\lambda_{\inf}(1+\sqrt{y})^2 + o_p(1) \leq \lambda_{\max}(S) \leq \lambda_{\sup}(1+\sqrt{y})^2 + o_p(1).$$

The proof is the same for $\lambda_{\min}$. □

We also verify the assumptions of Bernstein's inequality (see for example Theorem 2.8.1 in [Ver18]). For all i, j, k, let

$$Z_{ij}^{(k)} := M_i^{(k)}M_j^{(k)} - \sigma_{ij}. \tag{III.1}$$

The random-variables $(Z_{ij}^{(k)})_k$ are independent, mean zero, sub-exponential and we have $\|Z_{ik}^{(k)}\|_{\psi_1} \leq \|M_i\|_{\psi_2}\|M_j\|_{\psi_2} \leq C_{\sup}\sqrt{\sigma_{ii}\sigma_{jj}} \leq C_{\sup}$, where $\|.\|_{\psi_1}$ is the sub-exponential norm (for example, see Definition 2.7.5 in [Ver18]). So, we can use Bernstein's inequality with $(Z_{ij}^{(k)})_k$: there exists $C_{\inf}$ such that, for all $\varepsilon > 0$ and $n \in \mathbb{N}$,

$$\max_{i,j\in[1:p]} \mathbb{P}\left(\left|\sum_{k=1}^{n} Z_{ij}^{(k)}\right| \geq n\varepsilon\right) \leq 2\exp\left(-C_{\inf} n \min(\varepsilon, \varepsilon^2)\right).$$

Proof of Proposition 20

In this proof, we assume that Conditions 1 to 4 are satisfied. We first show several Lemmas.

Lemma 21. *For all symmetric positive definite* Γ *and for all* $B \in \mathcal{P}_p$*, if we write* $\Delta = \Gamma - \Gamma_B$*, we have:*

- $v \mapsto \lambda_{\min}(\Gamma_B + v\Delta)$ *decreases and so* $\min_{v\in[0,1]} \lambda_{\min}(\Gamma_B + v\Delta) = \lambda_{\min}(\Gamma)$.
- $v \mapsto \lambda_{\max}(\Gamma_B + v\Delta)$ *increases and so* $\max_{v\in[0,1]} \lambda_{\max}(\Gamma_B + v\Delta) = \lambda_{\max}(\Gamma)$.

Proof. Let us show that $v \mapsto \lambda_{\max}(\Gamma_B + v\Delta)$ increases (the proof if the same for $\lambda_{\min}$).

For all $v \in [0, 1]$, let $\Gamma_v = \Gamma_B + v\Delta$, $\lambda_v = \lambda_{\max}(\Gamma_v)$ and e_v an unit eigenvector of Γ_v associated to λ_v. Let $v, v' \in [0, 1]$, $v < v'$. Thus

$$\lambda_{v'} = \max_{u,\ \|u\|=1} u^T(\Gamma_B + v'\Delta)u \geq e_v^T(\Gamma_B + v'\Delta)e_v = \lambda_v + (v - v')e_v^T\Delta e_v.$$

If we show that $e_v^T\Delta e_v \geq 0$, we proved that $v \mapsto \lambda_v$ increases. First, assume that $v = 0$. If we write B_k the group of the largest eigenvalue of Γ_B, then $(e_0)_i$ is equal to zero for all $i \notin B_k$, so $(e_0^T\Delta)_j$ is equal to zero for all $j \in B_k$, and so $e_0^T\Delta e_0$ is equal to zero.

Assume now that $v > 0$ and let us show that $e_v^T\Delta e_v \geq 0$ by contradiction. Assume that $e_v^T\Delta e_v < 0$. Then

$$e_v^T(\Gamma_B + v\Delta)e_v < e_v^T\Gamma_B e_v \leq e_0^T\Gamma_B e_0.$$

Furthermore, we have seen that $e_0^T\Delta e_0 = 0$. Thus, we have

$$e_v^T(\Gamma_B + v\Delta)e_v < e_0^T(\Gamma_B + v\Delta)e_0,$$

that is in contradiction with $e_v \in \arg\max_{u,\ \|u\|=1} u^T(\Gamma_B + v\Delta)u$. □

In the following, let $\Delta_{B,B'} := S_B - S_{B'}$ for all $B, B' \in \mathcal{P}_p$.

Lemma 22. *For all* $B \in \mathcal{P}_p$*, we have*

$$l_{S_{B\cap B^*}} - l_{S_B} \leq \frac{1}{2\lambda_{\min}(S)}\frac{1}{p}\|\Delta_{B,B\cap B^*}\|_F^2. \tag{III.2}$$

Moreover, for all $B < B^*$*, we have*

$$l_{S_B} - l_{S_{B^*}} \geq \frac{1}{2\lambda_{\max}(S_{B^*})}\frac{1}{p}\|\Delta_{B^*,B}\|_F^2. \tag{III.3}$$

Proof. First, we prove Equation (III.2). Doing the Taylor expansion of

$$t \mapsto \log\circ\det\left(S_{B\cap B^*} + t\Delta_{B,B\cap B^*}\right)$$

and using the integral form of the remainder (as Equation (9) of [RBLZ08] or in [LF09]), we have

$$
\begin{aligned}
& p\left(l_{S_{B\cap B^*}} - l_{S_B}\right) \\
= \; & \log(|S_{B\cap B^*}|) - \log(|S_B|) \\
= \; & -\operatorname{Tr}(S_{B\cap B^*}\Delta_{B,B\cap B^*}) + \operatorname{vec}(\Delta_{B,B\cap B^*})^T \left[\int_0^1 (S_{B\cap B^*} + v\Delta_{B,B\cap B^*})^{-1} \right. \\
& \left. \otimes (S_{B\cap B^*} + v\Delta_{B,B\cap B^*})^{-1}(1-v)dv \right] \operatorname{vec}(\Delta_{B,B\cap B^*}),
\end{aligned}
$$

where $\otimes$ is the Kronecker product. The trace is equal to zero. Now,

$$
\begin{aligned}
p\left(l_{S_{B\cap B^*}} - l_{S_B}\right) & \leq 1/2 \max_{0\leq v\leq 1} \lambda^2_{\max}[(S_{B\cap B^*} + v\Delta_{B,B\cap B^*})^{-1}] \| \operatorname{vec}(\Delta_{B,B\cap B^*})\|^2 \\
& = 1/2 \max_{0\leq v\leq 1} \lambda^{-2}_{\min}(S_{B\cap B^*} + v\Delta_{B,B\cap B^*}) \| \operatorname{vec}(\Delta_{B,B\cap B^*})\|^2 \\
& = \frac{1}{2\min_v(\lambda_{\min}(S_{B\cap B^*} + v\Delta_{B,B\cap B^*}))^2} \| \operatorname{vec}(\Delta_{B,B\cap B^*})\|^2 \\
& = \frac{1}{2\lambda_{\min}(S_B)^2} \| \operatorname{vec}(\Delta_{B,B\cap B^*})\|^2 \\
& \leq \frac{1}{2\lambda_{\min}(S)^2} \| \operatorname{vec}(\Delta_{B,B\cap B^*})\|^2,
\end{aligned}
$$

using Lemma 21 for the two last steps.

Now, we prove Equation (III.3) similarly. We have, using Lemma 21,

$$
\begin{aligned}
p\left(l_{S_B} - l_{S_{B^*}}\right) & = -\operatorname{Tr}(S_B\Delta_{B^*,B}) + \operatorname{vec}(\Delta_{B^*,B})^T \left[\int_0^1 (S_B + v\Delta_{B^*,B})^{-1} \right. \\
& \quad \left. \otimes (S_B + v\Delta_{B^*,B})^{-1}(1-v)dv \right] \operatorname{vec}(\Delta_{B^*,B}) \\
& \geq 1/2 \min_{0\leq v\leq 1} \lambda^2_{\min}[(S_B + v\Delta_{B^*,B})^{-1}] \| \operatorname{vec}(\Delta_{B^*,B})\|^2 \\
& = 1/2 \min_{0\leq v\leq 1} \lambda^{-2}_{\max}(S_B + v\Delta_{B^*,B}) \| \operatorname{vec}(\Delta_{B^*,B})\|^2 \\
& = \frac{1}{2\max_v(\lambda_{\max}(S_B + v\Delta_{B^*,B}))^2} \| \operatorname{vec}(\Delta_{B^*,B})\|^2 \\
& = \frac{1}{2\lambda_{\max}(S_B)^2} \| \operatorname{vec}(\Delta_{B^*,B})\|^2 \\
& \geq \frac{1}{2\lambda_{\max}(S)^2} \| \operatorname{vec}(\Delta_{B^*,B})\|^2.
\end{aligned}
$$

□

Lemma 23.

$$\mathbb{P}\left(\max_{B \nsubseteq B^*} \Phi(B \cap B^*) - \Phi(B) \geq 0\right) \longrightarrow 0.$$

Proof. Using Lemma 22, we have

$$\begin{aligned}
& \mathbb{P}\left(\max_{B \nsubseteq B^*} \Phi(B \cap B^*) - \Phi(B) \geq 0\right) \\
\leq \; & \mathbb{P}\left(\max_{B \nsubseteq B^*} \left[l_{S_{B\cap B^*}} - l_{S_B} - \frac{1}{pn^\delta}\left(\mathrm{pen}(B) - \mathrm{pen}(B \cap B^*)\right)\right] \geq 0\right) \\
\leq \; & \mathbb{P}\left(\max_{B \nsubseteq B^*} \left[\frac{1}{2\lambda_{\min}(S)^2}\|\Delta_{B,B\cap B^*}\|_F^2 - \frac{1}{n^\delta}\left(\mathrm{pen}(B) - \mathrm{pen}(B \cap B^*)\right)\right] \geq 0\right) \\
\leq \; & \mathbb{P}\left(\lambda_{\min}(S) \leq \frac{1}{2}\lambda_{\inf}(1-\sqrt{y})^2\right) \\
& + \mathbb{P}\left(\max_{B \nsubseteq B^*} \left[\frac{1}{(1-\sqrt{y})^4\lambda_{\inf}^2}\|\Delta_{B,B\cap B^*}\|_F^2 - \frac{1}{n^\delta}\left(\mathrm{pen}(B) - \mathrm{pen}(B \cap B^*)\right)\right] \geq 0\right).
\end{aligned}$$

We show that the two terms go to 0. The first term goes to 0 with Lemma 20. For the second term, we have

$$\begin{aligned}
& \mathbb{P}\left(\max_{B \nsubseteq B^*} \left[\frac{1}{(1-\sqrt{y})^4\lambda_{\inf}^2}\|\Delta_{B,B\cap B^*}\|_F^2 - \frac{1}{n^\delta}\left(\mathrm{pen}(B) - \mathrm{pen}(B \cap B^*)\right)\right] \geq 0\right) \\
= \; & \mathbb{P}\left(\max_{B \nsubseteq B^*} \left[\sum_{(i,j)\in B\setminus B^*} \left\{\frac{1}{(1-\sqrt{y})^4\lambda_{\inf}^2} s_{ij}^2 - \frac{1}{n^\delta}\right\}\right] \geq 0\right) \\
\leq \; & \mathbb{P}\left(\exists (i,j) \notin B^*, \; \frac{1}{(1-\sqrt{y})^4\lambda_{\inf}^2} s_{ij}^2 - \frac{1}{n^\delta} \geq 0\right) \\
\leq \; & \mathbb{P}\left(\exists (i,j) \notin B^*, \; \frac{2}{(1-\sqrt{y})^4\lambda_{\inf}^2} \widehat{\sigma}_{ij}^2 - \frac{1}{n^\delta} \geq 0\right) \\
\leq \; & p^2 \max_{(i,j)\notin B^*} \mathbb{P}\left(\frac{2}{(1-\sqrt{y})^4\lambda_{\inf}^2} \widehat{\sigma}_{ij}^2 - \frac{1}{n^\delta} \geq 0\right) \\
\leq \; & p^2 \max_{(i,j)\notin B^*} \mathbb{P}\left(\frac{\sqrt{2}}{(1-\sqrt{y})^2\lambda_{\inf}} |\widehat{\sigma}_{ij}| \geq \frac{1}{n^{\delta/2}}\right) \\
\leq \; & p^2 \max_{(i,j)\notin B^*} \mathbb{P}\left(\left|\sum_{k=1}^{n-1} Z_{ij}^{(k)}\right| \geq \frac{(1-\sqrt{y})^2}{\sqrt{2}}\lambda_{\inf} n^{1-\delta/2}\right) \\
\leq \; & 2p^2 \exp\left(-C_{\inf} n^{1-\delta}\right) \longrightarrow 0,
\end{aligned}$$

using Bernstein's inequality, where $Z_{ij}^{(k)}$ is defined in Equation (III.1). That concludes the proof. □

Lemma 24.

$$\mathbb{P}\left(\max_{B<B^*} \Phi(B^*) - \Phi(B) \geq 0\right) \longrightarrow 0.$$

Proof. Using Lemma 22, we have

$$\begin{aligned}
& \mathbb{P}\left(\max_{B<B^*} \Phi(B^*) - \Phi(B) \geq 0\right) \\
\leq\ & \mathbb{P}\left(\min_{B<B^*} \left[l_{S_B} - l_{S_{B^*}} - \frac{1}{pn^\delta}\left(\mathrm{pen}(B^*) - \mathrm{pen}(B)\right)\right] \leq 0\right) \\
\leq\ & \mathbb{P}\left(\min_{B<B^*} \left[\frac{1}{2\lambda_{\max}(S_{B^*})^2}\|\Delta_{B^*,B}\|_F^2 - \frac{1}{n^\delta}\left(\mathrm{pen}(B^*) - \mathrm{pen}(B)\right)\right] \leq 0\right) \\
\leq\ & \mathbb{P}\left(\lambda_{\max}(S_B) \leq \frac{\lambda_{\inf}(1+\sqrt{y})^2}{2}\right) \\
& + \mathbb{P}\left(\min_{B<B^*} \left[\frac{1}{(1+\sqrt{y})^4\lambda_{\inf}^2}\|\Delta_{B^*,B}\|_F^2 - \frac{1}{n^\delta}\left(\mathrm{pen}(B^*) - \mathrm{pen}(B)\right)\right] \leq 0\right).
\end{aligned}$$

The first term goes to 0 with Lemma 20. The second term is

$$\begin{aligned}
& \mathbb{P}\left(\exists B < B^*,\ \sum_{(i,j)\in B^*\setminus B} \left[\frac{1}{(1+\sqrt{y})^4\lambda_{\inf}^2} s_{i,j}^2 - n^{-\delta}\right] \leq 0\right) \\
\leq\ & \mathbb{P}\left(\exists B < B^*,\ \sum_{(i,j)\in B^*\setminus B} \left[\frac{1}{\lambda_{\inf}^2} s_{i,j}^2 - n^{-\delta}\right] \leq 0\right) \\
\leq\ & \mathbb{P}\left(\exists k \in [1:K],\ \emptyset \subsetneq B_1 \subsetneq B_k^*,\ \sum_{i\in B_1,\, j\in B_k^*\setminus B_1} \left[\frac{1}{\lambda_{\inf}^2} s_{ij}^2 - n^{-\delta}\right] \leq 0\right) \\
\leq\ & p2^m \max_{\substack{k\in[1:K],\\ \emptyset\subsetneq B_1\subsetneq B_k^*}} \mathbb{P}\left(\sum_{i\in B_1,\, j\in B_k^*\setminus B_1} \left[\frac{1}{\lambda_{\inf}^2} s_{ij}^2 - n^{-\delta}\right] \leq 0\right) \\
\leq\ & p2^m \max_{\substack{k\in[1:K],\\ \emptyset\subsetneq B_1\subsetneq B_k^*}} \mathbb{P}\left(\sum_{i\in B_1,\, j\in B_k^*\setminus B_1} \left[\frac{1}{2\lambda_{\inf}^2} \widehat{\sigma}_{ij}^2 - n^{-\delta}\right] \leq 0\right).
\end{aligned}$$

Now, for all $k \in [1;K]$ and for all $\emptyset \subsetneq B_1 \subsetneq B_k^*$, let $(i^*, j^*) \in \arg\max_{i\in B_1, j\in B_k^*\setminus B_1} |\sigma_{ij}|$ (with an implicit dependence on k and B_1). Remark that

$$\frac{1}{2\lambda_{\inf}^2}\widehat{\sigma}_{i^*j^*}^2 \geq m^2 n^{-\delta} \Longrightarrow \sum_{i\in B_1,\, j\in B_k^*\setminus B_1} \left(\frac{1}{2\lambda_{\inf}^2}\widehat{\sigma}_{ij}^2 - n^{-\delta}\right) \geq 0.$$

Thus,

$$
\begin{aligned}
&\mathbb{P}\left(\exists B < B^*, \sum_{(i,j)\in B^*\setminus B}\left[\frac{1}{\lambda_{\inf}^2}s_{i,j}^2 - n^{-\delta}\right] \leq 0\right) \\
\leq\ & p2^m \max_{\substack{k\in[1:K],\\ \emptyset\subsetneq B_1\subsetneq B_k^*}} \mathbb{P}\left(\frac{1}{2\lambda_{\inf}^2}\widehat{\sigma}_{i^*j^*}^2 \leq m^2 n^{-\delta}\right) \\
=\ & p2^m \max_{\substack{k\in[1:K],\\ \emptyset\subsetneq B_1\subsetneq B_k^*}} \mathbb{P}\left(|\widehat{\sigma}_{i^*j^*}| \leq \sqrt{2}\lambda_{\inf} m n^{-\delta/2}\right) \\
\leq\ & p2^m \max_{\substack{k\in[1:K],\\ \emptyset\subsetneq B_1\subsetneq B_k^*}} \mathbb{P}\left(|\widehat{\sigma}_{i^*j^*} - \sigma_{i^*j^*}| \geq |\sigma_{i^*j^*}| - \sqrt{2}\lambda_{\inf} m n^{-\delta/2}\right) \\
=\ & p2^m \max_{\substack{k\in[1:K],\\ \emptyset\subsetneq B_1\subsetneq B_k^*}} \mathbb{P}\left(\left|\sum_{k=1}^{n-1} Z_{i^*j^*}^{(k)}\right| \geq n\left[|\sigma_{i^*j^*}| - \sqrt{2}\lambda_{\inf} m n^{-\delta/2}\right]\right) \\
=\ & p2^m \mathbb{P}\left(\left|\sum_{k=1}^{n-1} Z_{i^*j^*}^{(k)}\right| \geq n \min_{\substack{k\in[1:K],\\ \emptyset\subsetneq B_1\subsetneq B_k^*}}\left[|\sigma_{i^*j^*}| - \sqrt{2}\lambda_{\inf} m n^{-\delta/2}\right]\right).
\end{aligned}
$$

Now, by Condition 4, we know that $\min_{\substack{k\in[1:K],\\ \emptyset\subsetneq B_1\subsetneq B_k^*}} |\sigma_{i^*j^*}| \geq a n^{-1/4}$, so, for n large enough,

$$
\min_{\substack{k\in[1:K],\\ \emptyset\subsetneq B_1\subsetneq B_k^*}}\left[|\sigma_{i^*j^*}| - \sqrt{2}\lambda_{\inf} m n^{-\delta/2}\right] \geq C_{\inf}(n^{-1/4} - n^{-\delta/2}) \geq C_{\inf}(\delta) n^{-1/4}.
$$

Thus, by Bernstein's inequality, for n large enough,

$$
\begin{aligned}
&\mathbb{P}\left(\exists B < B^*, \sum_{(i,j)\in B^*\setminus B}\left[\frac{1}{(1-\sqrt{y})^2\lambda_{\inf}^2}s_{i,j}^2 - n^{-\delta}\right] \leq 0\right) \\
&\leq p2^{m+1}\exp\left(-C_{\inf}(\delta) n^{1/2}\right) \longrightarrow 0.
\end{aligned}
$$

□

Now, we can prove Proposition 20.

Proof. We have

$$
\mathbb{P}\left(\max_{B\neq B^*} \Phi(B^*) - \Phi(B) \geq 0\right) \ \leq\ \mathbb{P}\left(\max_{B< B^*} \Phi(B^*) - \Phi(B) \geq 0\right)
$$

$$+\mathbb{P}\left(\max_{B>B^*}\Phi(B^*)-\Phi(B)\geq 0\right)$$
$$+\mathbb{P}\left(\max_{B\nleq B^*,\,B\ngeq B^*}\Phi(B^*)-\Phi(B)\geq 0\right).$$

The two first terms go to 0 tanks to Lemmas 23 and 24. For the last term, we have

$$\begin{aligned}
&\mathbb{P}\left(\max_{B\nleq B^*,\,B\ngeq B^*}\Phi(B^*)-\Phi(B)\geq 0\right)\\
=\;&\mathbb{P}\left(\max_{B\nleq B^*,\,B\ngeq B^*}\Phi(B^*)-\Phi(B\cap B^*)+\Phi(B\cap B^*)-\Phi(B)\geq 0\right)\\
\leq\;&\mathbb{P}\left(\max_{B\nleq B^*,\,B\ngeq B^*}\Phi(B^*)-\Phi(B\cap B^*)\geq 0\right)\\
&+\mathbb{P}\left(\max_{B\nleq B^*,\,B\ngeq B^*}\Phi(B\cap B^*)-\Phi(B)\geq 0\right)\\
\leq\;&\mathbb{P}\left(\max_{B'<B^*}\Phi(B^*)-\Phi(B')\geq 0\right)\\
&+\mathbb{P}\left(\max_{B\nleq B^*}\Phi(B\cap B^*)-\Phi(B)\geq 0\right).
\end{aligned}$$

These two last terms go to 0 thanks to Lemmas 23 and 24.

□

Proofs of Proposition 21

In this proof, we assume that Conditions 1 to 3 hold.

Lemma 25. *For all $B\in\mathcal{P}_p$, we have*

$$l_{S_{B\cap B(\alpha_2)}}-l_{S_B}\leq\frac{1}{2\lambda_{\min}(S)}\frac{1}{p}\|\Delta_{B,B\cap B(\alpha_2)}\|_F^2. \tag{III.4}$$

Moreover, for all $B<B(\alpha_2)$, we have

$$l_{S_B}-l_{S_{B(\alpha_2)}}\geq\frac{1}{2\lambda_{\max}(S_{B(\alpha_2)})}\frac{1}{p}\|\Delta_{B(\alpha_2),B}\|_F^2. \tag{III.5}$$

Proof. Same proof as Lemma 22 replacing B^* by $B(\alpha_2)$. □

Lemma 26. *If $\alpha_2>\delta/2$, then,*

$$\mathbb{P}\left(\max_{B\nleq B(\alpha_2)}\Phi(B\cap B(\alpha_2))-\Phi(B)\geq 0\right)\longrightarrow 0.$$

Proof. Following the proof of Lemma 23 (and using Lemma 25), it is enough to prove that the following term goes to 0:

$$
\begin{aligned}
& \mathbb{P}\left(\max_{B \nsubseteq B(\alpha_2)} \left[\frac{1}{(1-\sqrt{y})^4 \lambda_{\inf}^2} \|\Delta_{B, B\cap B(\alpha_2)}\|_F^2 - \frac{1}{n^\delta}\left(\mathrm{pen}(B) - \mathrm{pen}(B \cap B(\alpha_2))\right)\right] \geq 0\right) \\
= \; & \mathbb{P}\left(\max_{B \nsubseteq B(\alpha_2)} \left[\sum_{(i,j)\in B\setminus B(\alpha_2)} \left\{\frac{1}{(1-\sqrt{y})^4 \lambda_{\inf}^2} s_{ij}^2 - \frac{1}{n^\delta}\right\}\right] \geq 0\right) \\
\leq \; & \mathbb{P}\left(\exists (i,j) \notin B(\alpha_2),\; \frac{1}{(1-\sqrt{y})^4 \lambda_{\inf}^2} s_{ij}^2 - \frac{1}{n^\delta} \geq 0\right) \\
\leq \; & \mathbb{P}\left(\exists (i,j) \notin B(\alpha_2),\; \frac{2}{(1-\sqrt{y})^4 \lambda_{\inf}^2} \widehat{\sigma}_{ij}^2 - \frac{1}{n^\delta} \geq 0\right) \\
\leq \; & p^2 \max_{(i,j)\notin B(\alpha_2)} \mathbb{P}\left(\frac{2}{(1-\sqrt{y})^4 \lambda_{\inf}^2} \widehat{\sigma}_{ij}^2 - \frac{1}{n^\delta} \geq 0\right) \\
\leq \; & p^2 \max_{(i,j)\notin B(\alpha_2)} \mathbb{P}\left(\frac{\sqrt{2}}{(1-\sqrt{y})^2 \lambda_{\inf}} |\widehat{\sigma}_{ij}| \geq \frac{1}{n^{\delta/2}}\right) \\
\leq \; & p^2 \max_{(i,j)\notin B(\alpha_2)} \mathbb{P}\left(\frac{\sqrt{2}}{(1-\sqrt{y})^2 \lambda_{\inf}} |\widehat{\sigma}_{ij} - \sigma_{ij}| \geq \frac{1}{n^{\delta/2}} - \frac{\sqrt{2}}{(1-\sqrt{y})^2 \lambda_{\inf}} n^{-\alpha_2}\right) \\
\leq \; & 2p^2 \exp\left(-C_{\inf} n^{1-\delta}\right) \longrightarrow 0,
\end{aligned}
$$

using again Bernstein's inequality. That concludes the proof. □

Lemma 27. *If $\alpha_1 < \delta/2$, then,*

$$\mathbb{P}\left(\max_{B < B(\alpha_1)} \Phi(B(\alpha_1)) - \Phi(B) \geq 0\right) \longrightarrow 0.$$

Proof. Following the proof of Lemma 24, it suffices to prove that

$$p 2^m \mathbb{P}\left(\left|\sum_{k=1}^{n-1} Z_{i^*j^*}^{(k)}\right| \geq n \min_{\substack{k\in[1:K(\alpha_1)],\\ \emptyset \subsetneq B_1 \subsetneq B_k(\alpha_1)}} \left[|\sigma_{i^*j^*}| - \sqrt{2}\lambda_{\inf} m n^{-\delta/2}\right]\right) \longrightarrow 0.$$

Now, by definition of $B(\alpha_1)$, we know that $\min_{\substack{k\in[1:K(\alpha_1)],\\ \emptyset \subsetneq B_1 \subsetneq B_k(\alpha_1)}} |\sigma_{i^*j^*}| \geq n^{-\alpha_1}$, so, for n large enough,

$$\min_{\substack{k\in[1:K(\alpha_1)],\\ \emptyset \subsetneq B_1 \subsetneq B_k(\alpha_1)}} \left[|\sigma_{i^*j^*}| - \sqrt{2}\lambda_{\inf} m n^{-\delta/2}\right] \geq C_{\inf}(n^{-\alpha_1} - n^{-\delta/2}) \geq C_{\inf}(\alpha_1, \delta) n^{-\alpha_1}.$$

Thus, by Bernstein's inequality, for n large enough,

$$\begin{aligned}
&\mathbb{P}\left(\exists B < B(\alpha_1), \sum_{(i,j)\in B(\alpha_1)\setminus B}\left[\frac{1}{(1-\sqrt{y})^2\lambda_{\text{inf}}^2}s_{i,j}^2 - n^{-\delta}\right] \leq 0\right) \\
&\leq p2^{m+1}\exp\left(-C_{\text{inf}}(\alpha_1,\delta)n^{1-2\alpha_1}\right) \longrightarrow 0.
\end{aligned}$$

□

We can now prove Proposition 21.

Proof. We have

$$\begin{aligned}
& \mathbb{P}\left(\left\{B(\alpha_1) \not> \widehat{B}_{tot} \leq B(\alpha_2)\right\}^c\right) \\
= \ & \mathbb{P}\left(\min_{B<B(\alpha_1) \text{ or } B\nleq B(\alpha_2)} \Phi(B) \leq \min_{B\not<B(\alpha_1) \text{ and } B\leq B(\alpha_2)} \Phi(B)\right) \\
\leq \ & \mathbb{P}\left(\min_{B<B(\alpha_1)} \Phi(B) \leq \min_{B\not<B(\alpha_1) \text{ and } B\leq B(\alpha_2)} \Phi(B)\right) \\
& + \mathbb{P}\left(\min_{B\nleq B(\alpha_2) \text{ s.t. } B\cap B(\alpha_2)\not<B(\alpha_1)} \Phi(B) \leq \min_{B\not<B(\alpha_1) \text{ and } B\leq B(\alpha_2)} \Phi(B)\right) \\
& + \mathbb{P}\left(\min_{B\nleq B(\alpha_2) \text{ s.t. } B\cap B(\alpha_2)<B(\alpha_1)} \Phi(B) \leq \min_{B\not<B(\alpha_1) \text{ and } B\leq B(\alpha_2)} \Phi(B)\right).
\end{aligned}$$

First,

$$\begin{aligned}
& \mathbb{P}\left(\min_{B<B(\alpha_1)} \Phi(B) \leq \min_{B\not<B(\alpha_1) \text{ and } B\leq B(\alpha_2)} \Phi(B)\right) \\
\leq \ & \mathbb{P}\left(\min_{B<B(\alpha_1)} \Phi(B) - \Phi(B(\alpha_1)) \leq 0\right) \longrightarrow 0,
\end{aligned}$$

from Lemma 27. Secondly,

$$\begin{aligned}
& \mathbb{P}\left(\min_{B\nleq B(\alpha_2) \text{ s.t. } B\cap B(\alpha_2)\not<B(\alpha_1)} \Phi(B) \leq \min_{B\not<B(\alpha_1) \text{ and } B\leq B(\alpha_2)} \Phi(B)\right) \\
\leq \ & \mathbb{P}\left(\min_{B\nleq B(\alpha_2) \text{ s.t. } B\cap B(\alpha_2)\not<B(\alpha_1)} \Phi(B) - \Phi(B\cap B(\alpha_2)) \leq 0\right) \longrightarrow 0,
\end{aligned}$$

from Lemma 26. Finally,

$$\mathbb{P}\left(\min_{B\nleq B(\alpha_2) \text{ s.t. } B\cap B(\alpha_2)<B(\alpha_1)} \Phi(B) \leq \min_{B\not<B(\alpha_1) \text{ and } B\leq B(\alpha_2)} \Phi(B)\right)$$

$$
\begin{aligned}
&\leq \mathbb{P}\left(\min_{B\nleq B(\alpha_2) \text{ s.t. } B\cap B(\alpha_2)<B(\alpha_1)} \Phi(B)\leq \Phi(B(\alpha_1))\right)\\
&\leq \mathbb{P}\Bigg(\min_{B\nleq B(\alpha_2) \text{ s.t. } B\cap B(\alpha_2)<B(\alpha_1)} \Phi(B)-\Phi(B\cap B(\alpha_2))\\
&\quad +\Phi(B\cap B(\alpha_2))-\Phi(B(\alpha_1)\leq 0\Bigg)\\
&\leq \mathbb{P}\left(\min_{B\nleq B(\alpha_2) \text{ s.t. } B\cap B(\alpha_2)<B(\alpha_1)} \Phi(B)-\Phi(B\cap B(\alpha_2))\leq 0\right)\\
&\quad +\mathbb{P}\left(\min_{B\nleq B(\alpha_2) \text{ s.t. } B\cap B(\alpha_2)<B(\alpha_1)} \Phi(B\cap B(\alpha_2))-\Phi(B(\alpha_1)\leq 0\right)\\
&\leq \mathbb{P}\left(\min_{B\nleq B(\alpha_2)} \Phi(B)-\Phi(B\cap B(\alpha_2))\leq 0\right)\\
&\quad +\mathbb{P}\left(\min_{B<B(\alpha_1)} \Phi(B)-\Phi(B(\alpha_1)\leq 0\right)\\
&\longrightarrow 0,
\end{aligned}
$$

from Lemmas 26 and 27. □

Proofs of Propositions 22, 23 and 24

Proof. In the three cases, the computation of $\widehat{B}$ requires carrying out the BFS algorithm for B_λ and the computation of a determinant for $\Psi(B_\lambda)$. Recall that if $G=(V,E)$ is a graph (where V is the set of vertices and E the set of edges), the complexity of the BFS algorithm is $O(|V|+|E|)$. Recall that, if M is a squared matrix of size p, the complexity of $\det(M)$ is $O(p^3)$ using the LU decomposition.

Now, we compute the complexity of the three estimators $\widehat{B}_{\widehat{C}}$, $\widehat{B}_A$ and $\widehat{B}_s$.

- For all $\lambda\in A_{\widehat{C}}$, the complexity of B_λ is $O(p^2)$, and the cardinal of $A_{\widehat{C}}$ is $O(p^2)$. Thus, the complexity of the computation of $\{B_\lambda \mid \lambda\in A_{\widehat{C}}\}$ is $O(p^4)$.

  Now, for all $\lambda\in A_{\widehat{C}}$, the complexity of $\Psi(B_\lambda)$ is $O(p^3)$ and the cardinal of $\{B_\lambda \mid \lambda\in A_{\widehat{C}}\}$ is $O(p)$ (because the function $\lambda\mapsto B_\lambda$ decreases). Thus, the complexity of the evaluations $\{\Psi(B),\ B\in\{B_\lambda \mid \lambda\in A_{\widehat{C}}\}\}$ is $O(p^4)$

  So the complexity of $\widehat{B}_{\widehat{C}}$ is $O(p^4)$.

- For the threshold $n^{-1/3}$, the complexity of $B_{n^{-1/3}}$ is $O(p^2)$.

  So the complexity of $\widehat{B}_\lambda$ is $O(p^2)$.

- One can divide the computation of $\widehat{B}_s$ into two steps.

For the first step, as we do not know the value of s, we have to compute $B_{l/p}$ from $l = p$ to $l = s-1$, verifying each time if the maximal size of group is smaller than m or not. First, for each value of l from p decreasing to s, the complexity of the BFS algorithm to $B_{l/p}$ is $O(p \times m^2) = O(p)$, thus, the complexity of all these partitions is $O(p^2)$. Then, for $l = s-1$, the complexity of $B_{(s-1)/p}$ is $O(p^2)$. So, the complexity of this first step is $O(p^2)$. In the second step, we have to evaluate $\Psi(B_{l/p})$ for all $l \in [s : p]$. The complexity of each evaluation is $O(pm^3) = O(p)$, and the the number of evaluations is $O(p)$. Thus, the complexity of this second step is $O(p^2)$.

□

Proof of Proposition 25

To prove the convergence of $\widehat{B}$ in the three cases, we need the three following Lemmas.

Lemma 28. *For all sequence $(\lambda_n)_n$ such that for all n, $\lambda_n \in [n^{-1/3}, an^{-1/4}/3\lambda_{\sup}(1+\sqrt{y})^2]$ (we assume that n is large enough and that subset is not empty), we have*

$$\mathbb{P}(B_\lambda = B^*) \longrightarrow 1.$$

Proof. Step 1: $B_\lambda \leq B^*$ with probability which goes to 1.

$$\begin{aligned}
& \mathbb{P}\left(B_\lambda \not\leq B^*\right) \\
= \ & \mathbb{P}\left(\exists (i,j) \notin B^*,\ |\widehat{C}_{ij}| \geq \lambda\right) \\
\leq \ & \mathbb{P}\left(\exists (i,j) \notin B^*,\ |\widehat{\sigma}_{ij}| \geq \lambda \frac{\lambda_{\inf}(1-\sqrt{y})^2}{2}\right) + \mathbb{P}\left(\exists i \leq p,\ \widehat{\sigma}_{ii} < \lambda_{\inf}\frac{(1-\sqrt{y})^2}{2}\right) \\
\leq \ & p^2 \max_{(i,j)\notin B^*} \mathbb{P}\left(|\widehat{\sigma}_{ij}| \geq \lambda \frac{\lambda_{\inf}(1-\sqrt{y})^2}{2}\right) + \mathbb{P}\left(\lambda_{\min}(\widehat{\Sigma}) < \lambda_{\inf}\frac{(1-\sqrt{y})^2}{2}\right) \\
\leq \ & p^2 \max_{(i,j)\notin B^*} \mathbb{P}\left(|\widehat{\sigma}_{ij}| \geq \frac{\lambda_{\inf}(1-\sqrt{y})^2}{2} n^{-1/3}\right) + o(1) \\
\leq \ & 2p^2 \exp\left(-C_{\inf} n^{1/3}\right) + o(1) \longrightarrow 0,
\end{aligned}$$

using Lemma 20 and Bernstein's inequality.

Step 2: $B_\lambda \geq B^*$ with probability which goes to 1.

For all $k \in [1 : K]$, and all $\emptyset \subsetneq B_1 \subsetneq B_k^*$, let $B_2 := B_k^* \setminus B_1$ and $(i^*, j^*) := \arg\max_{(i,j)\in B_1 \times B_2} |\sigma_{ij}|$, where the dependency on k and B_1 is implicit. Thanks to Condition 4, we have $|\sigma_{i^*j^*}| \geq an^{-1/4}$. Then, using Lemma 20,

$$\mathbb{P}\left(B_\lambda \not\geq B^*\right)$$

$$\begin{aligned}
&= \mathbb{P}\left(\exists k \in [1:K],\ \exists\, \emptyset \subsetneq B_1 \subsetneq B_k^*,\ \max_{(i,j)\in B_1\times B_2} |\widehat{C}_{ij}| < \lambda\right) \\
&\le \mathbb{P}\left(\exists k \in [1:K],\ \exists\, \emptyset \subsetneq B_1 \subsetneq B_k^*,\ \max_{(i,j)\in B_1\times B_2} |\widehat{\sigma}_{ij}| < 2\lambda\lambda_{\sup}(1+\sqrt{y})^2\right) \\
&\quad + \mathbb{P}\left(\exists i \le p,\ \widehat{\sigma}_{ii} \ge 2\lambda_{\sup}(1+\sqrt{y})^2\right) \\
&\le \mathbb{P}\left(\exists k \in [1:K],\ \exists\, \emptyset \subsetneq B_1 \subsetneq B_k^*,\ |\widehat{\sigma}_{i^*j^*}| < \frac{2}{3}an^{-1/4}\right) \\
&\quad + \mathbb{P}\left(\lambda_{\max}(\widehat{\Sigma}) \ge 2\lambda_{\sup}(1+\sqrt{y})^2\right) \\
&\le \mathbb{P}\left(\exists k \in [1:K],\ \exists\, \emptyset \subsetneq B_1 \subsetneq B_k^*,\ |\widehat{\sigma}_{i^*j^*} - \sigma_{i^*j^*}| > \frac{1}{3}an^{-1/4}\right) + o(1) \\
&\le \mathbb{P}\left(\exists (i,j) \in [1:p]^2,\ |\widehat{\sigma}_{ij} - \sigma_{ij}| > \frac{1}{3}an^{-1/4}\right) + o(1) \\
&\le p^2 \max_{(i,j)} \mathbb{P}\left(|\widehat{\sigma}_{ij} - \sigma_{ij}| > \frac{1}{3}an^{-1/4}\right) + o(1) \\
&\le 2p^2 \exp\left(-C_{\inf} n^{1/2}\right) + o(1) \longrightarrow 0,
\end{aligned}$$

by Bernstein's inequality. □

Lemma 29. *Let $c > 0$. Let $\tilde{A} := \{a_0,\ a_1, ...,\ a_L\}$ such that $a_0 = 0,\ a_L = 1,\ 0 < a_{l+1} - a_l < c/\sqrt{p}$ for all $l \in [0 : L-1]$. Then,*

$$\mathbb{P}\left(B^* \in \left\{B_\lambda,\ \lambda \in \tilde{A}\right\}\right) \longrightarrow 1.$$

Proof. Thanks to Lemma 28, it suffices to show that, for n large enough, there exists $l \in [0 : L]$ such that $a_l \in [n^{-1/3}, an^{-1/4}/3\lambda_{\sup}(1+\sqrt{y})^2]$. By contradiction, let us assume that there does not exist such l. Let $j \in [0 : L]$ such that $a_j < n^{-1/3}$ and $a_{j+1} > an^{-1/4}/3\lambda_{\sup}$. Thus, we have

$$\begin{aligned}
\sqrt{p}\,(a_{j+1} - a_j) &> \sqrt{p}\left(\frac{an^{-1/4}}{3\lambda_{\sup}(1+\sqrt{y})^2} - n^{-1/3}\right) \\
&\ge C_{\inf} n^{1/4} \longrightarrow +\infty,
\end{aligned}$$

which is in contradiction with the definition of $\tilde{A}$.

□

Lemma 30. *We have,*

$$\mathbb{P}\left(B^* \in \{B_\lambda,\ \lambda \in A_s\}\right) \longrightarrow 1.$$

Proof. Let $\mathcal{P}_p(m)$ be the set of the partitions of $[1:p]$ such that all their elements have cardinal smaller than m. By assumption (Condition 3), $B^* \in \mathcal{P}_p(m)$. Let $G := \{l/p | \; l \in [0,p]\}$. Thus G verifies the assumption of $\tilde{A}$ in Lemma 29, so

$$\mathbb{P}\left(B^* \in \{B_\lambda, \; \lambda \in G\}\right) \longrightarrow 1.$$

Thus

$$\mathbb{P}\left(B^* \in \{B_\lambda, \; \lambda \in G\} \cap \mathcal{P}_p(m)\right) \longrightarrow 1.$$

To conclude, it suffices to prove that $\{B_\lambda, \; \lambda \in G_s\} \cap \mathcal{P}_p(m) = \{B_\lambda, \; \lambda \in A_s\}$.

We have immediately $\{B_\lambda, \; \lambda \in A_s\} \subset \{B_\lambda, \; \lambda \in G\} \cap \mathcal{P}_p(m)$. We have to prove the other inclusion. Assume that $B \in \{B_\lambda, \; \lambda \in G\} \cap \mathcal{P}_p(m)$. We know that there exists $\lambda = l/p \in G$ such that $B = B_\lambda$. As $B_{l/p} \in \mathcal{P}_p(m)$, we know by definition of s that $l \geq s$ and thus $\lambda \in A$. □

Now, we prove Proposition 25.

Proof.
- Using Lemma 28, Proposition 20, and the fact that $\{B_\lambda \mid \lambda \in A_{\widehat{C}}\} = \{B_\lambda \mid \lambda \in [0,1[\}$, we have $\mathbb{P}\left(\widehat{B}_{\widehat{C}} = B^*\right) \longrightarrow 1$.
- Using Lemma 28 and Proposition 20, we have $\mathbb{P}\left(\widehat{B}_\lambda = B^*\right) \longrightarrow 1$.
- Using Lemma 30 and Proposition 20, we have $\mathbb{P}\left(\widehat{B}_s = B^*\right) \longrightarrow 1$.

□

Proof of Proposition 26

Proof. We follow the proof of Lemma 28.

Step 1: $B_{n^{-\delta/2}} \leq B(\alpha_2)$ with probability which goes to 1.

$$\begin{aligned}
& \mathbb{P}\left(B_{n^{-\delta/2}} \not\leq B(\alpha_2)\right) \\
= \; & \mathbb{P}\left(\exists (i,j) \notin B(\alpha_2), \; |\widehat{C}_{ij}| \geq n^{-\delta/2}\right) \\
\leq \; & \mathbb{P}\left(\exists (i,j) \notin B(\alpha_2), \; |\widehat{\sigma}_{ij}| \geq n^{-\delta} \frac{\lambda_{\inf}(1-\sqrt{y})^2}{2}\right) + \mathbb{P}\left(\exists i \leq p, \; \widehat{\sigma}_{ii} < \lambda_{\inf} \frac{(1-\sqrt{y})^2}{2}\right) \\
\leq \; & p^2 \max_{(i,j)\notin B(\alpha_2)} \mathbb{P}\left(|\widehat{\sigma}_{ij}| \geq n^{-\delta/2} \frac{\lambda_{\inf}(1-\sqrt{y})^2}{2}\right) + \mathbb{P}\left(\lambda_{\min}(\widehat{\Sigma}) < \lambda_{\inf} \frac{(1-\sqrt{y})^2}{2}\right) \\
\leq \; & p^2 \max_{(i,j)\notin B(\alpha_2)} \mathbb{P}\left(|\widehat{\sigma}_{ij} - \sigma_{ij}| \geq n^{-\delta/2} \frac{\lambda_{\inf}(1-\sqrt{y})^2}{2} - n^{-\alpha_2}\right) + o(1)
\end{aligned}$$

$$\leq \quad 2p^2 \exp\left(-C_{\inf}(\delta,\alpha_2)n^{1-\delta}\right) + o(1) \longrightarrow 0,$$

using Lemma 20 and Bernstein's inequality.

Step 2: $B_{n^{-\delta/2}} \geq \mathcal{B}(\alpha_1)$ with probability which goes to 1.

For all $k \in [1 : K(\alpha_1)]$, and all $\emptyset \subsetneq B_1 \subsetneq B_k(\alpha_1)$, let $B_2 := B_k(\alpha_1) \setminus B_1$ and $(i^*, j^*) := \arg\max_{(i,j)\in B_1\times B_2} |\sigma_{ij}|$, where the dependency on k and B_1 is implicit. Then, using Lemma 20,

$$\begin{aligned}
& \mathbb{P}\left(B_{n^{-\delta/2}} \not\geq \mathcal{B}(\alpha_1)\right) \\
= \quad & \mathbb{P}\left(\exists k \in [1 : K(\alpha_1)],\ \exists\, \emptyset \subsetneq B_1 \subsetneq B_k(\alpha_1),\ \max_{(i,j)\in B_1\times B_2} |\widehat{C}_{ij}| < n^{-\alpha_1}\right) \\
\leq \quad & \mathbb{P}\left(\exists k \in [1 : K(\alpha_1)],\ \exists\, \emptyset \subsetneq B_1 \subsetneq B_k(\alpha_1),\ |\widehat{\sigma}_{i^*j^*}| < 2\lambda_{\sup}(1+\sqrt{y})^2 n^{-\alpha_1}\right) \\
& + \mathbb{P}\left(\exists i \leq p,\ \widehat{\sigma}_{ii} \geq 2\lambda_{\sup}(1+\sqrt{y})^2\right) \\
\leq \quad & \mathbb{P}\left(\exists k \in [1 : K(\alpha_1)],\ \exists\, \emptyset \subsetneq B_1 \subsetneq B_k(\alpha_1),\ |\widehat{\sigma}_{i^*j^*}| < 2\lambda_{\sup}(1+\sqrt{y})^2 n^{-\alpha_1}\right) \\
& + \mathbb{P}\left(\lambda_{\max}(\widehat{\Sigma}) \geq 2\lambda_{\sup}(1+\sqrt{y})^2\right) \\
\leq \quad & \mathbb{P}\left(\exists k \in [1 : K],\ \exists\, \emptyset \subsetneq B_1 \subsetneq B_k^*,\ |\widehat{\sigma}_{i^*j^*} - \sigma_{i^*j^*}| > n^{-\alpha_1} - 2\lambda_{\sup}(1+\sqrt{y})^2 n^{-\delta/2}\right) + o(1) \\
\leq \quad & \mathbb{P}\left(\exists (i,j) \in [1 : p]^2,\ |\widehat{\sigma}_{ij} - \sigma_{ij}| > n^{-\alpha_1} - 2\lambda_{\sup}(1+\sqrt{y})^2 n^{-\delta/2}\right) + o(1) \\
\leq \quad & p^2 \max_{(i,j)} \mathbb{P}\left(|\widehat{\sigma}_{ij} - \sigma_{ij}| > n^{-\alpha_1} - 2\lambda_{\sup}(1+\sqrt{y})^2 n^{-\delta/2}\right) + o(1) \\
\leq \quad & 2p^2 \exp\left(-C_{\inf}(\delta,\alpha_1)n^{1-2\alpha_1}\right) + o(1) \longrightarrow 0,
\end{aligned}$$

by Bernstein's inequality.

□

Proof of Proposition 27

Proof. First, we prove the results for $\widehat{\Sigma}_{B^*}$. We have, using again the notation $M \sim \mathcal{N}(0, \Sigma)$,

$$\begin{aligned}
\mathrm{E}\left(\frac{n}{p}\|\widehat{\Sigma}_{B^*} - \Sigma\|_F^2\right) \quad & \leq \quad n\, m^2 \max_{(i,j)\in B^*} \mathrm{E}\left[(\widehat{\sigma}_{ij} - \sigma_{ij})^2\right] \\
& = \quad n\, m^2 \max_{(i,j)\in B^*} \mathrm{Var}\left(\widehat{\sigma}_{ij}\right) \\
& \leq \quad m^2 \frac{n}{n-1} \max_{(i,j)\in B^*} \mathrm{Var}\left(M_i M_j\right) \\
& \leq \quad 2m^2 \max_{(i,j)\in B^*} \left(\sigma_{ii}\sigma_{jj} + 2\sigma_{ij}^2\right)
\end{aligned}$$

$$\leq \quad 6m^2\lambda_{\sup}^2.$$

By Markov's inequality, that proves

$$\frac{1}{p}\|\widehat{\Sigma}_{B^*} - \Sigma\|_F^2 = O_p(1/n).$$

Now, we want to prove that

$$\frac{1}{p}\|\widehat{\Sigma}_{B^*} - \Sigma\|_F^2 \neq o_p(1/n).$$

First, we have

$$\begin{aligned}
\mathrm{E}\left(\frac{n}{p}\|\widehat{\Sigma}_{B^*} - \Sigma\|_F^2\right) &\geq n \min_{i\in[1:p]} \mathrm{E}\left[(\widehat{\sigma}_{ii} - \sigma_{ii})^2\right] \\
&= n \min_{i\in[1:p]} \mathrm{Var}\left(\widehat{\sigma}_{ii}\right) \\
&\geq \frac{n}{n-1}\mathrm{Var}(M_{ii}^2) \\
&\geq \min_{i\in[1:p]} 2\sigma_{ii}^2 \\
&\geq 2\lambda_{\inf}^2.
\end{aligned}$$

Now, the variance is

$$\mathrm{Var}\left(\frac{1}{p}\|\widehat{\Sigma}_{B^*} - \Sigma\|_F^2\right) = \sum_{k=1}^{K} \mathrm{Var}\left(\frac{1}{p}\|\widehat{\Sigma}_{B_k^*} - \Sigma_{B_k^*}\|_F^2\right) \leq p \max_{k\in[1:K]} \mathrm{Var}\left(\frac{1}{p}\|\widehat{\Sigma}_{B_k^*} - \Sigma_{B_k^*}\|_F^2\right).$$

Now,

$$\mathrm{Var}\left(\frac{1}{p}\|\widehat{\Sigma}_{B_k^*} - \Sigma_{B_k^*}\|_F^2\right) = \frac{1}{p^2}\mathrm{Var}\left(\sum_{i,j\in B_k^*} (\widehat{\sigma}_{ij} - \sigma_{ij})^2\right).$$

Remark that if $A_1, ..., A_d$ are random variables, we have

$$\begin{aligned}
\mathrm{Var}\left(\sum_{i=1}^{d} A_i\right) &= \sum_{i,j=1}^{d} \mathrm{cov}(A_i, A_j) \\
&\leq \sum_{i,j=1}^{d} \sqrt{\mathrm{Var}(A_i)}\sqrt{\mathrm{Var}(A_j)} \\
&= \left(\sum_{i=1}^{d} \sqrt{\mathrm{Var}(A_i)}\right)^2
\end{aligned}$$

$$\leq \ d \sum_{i=1}^{d} \mathrm{Var}(A_i).$$

Thus

$$\mathrm{Var}\left(\frac{1}{p}\|\widehat{\Sigma}_{B_k^*} - \Sigma_{B_k^*}\|_F^2\right) \ \leq \ \frac{m^4}{p^2} \max_{i,j \in B_k^*} \mathrm{Var}\left((\widehat{\sigma}_{ij} - \sigma_{ij})^2\right).$$

Let $i, j \in B_k^*$ for some k. We want to upper-bound $\mathrm{Var}\left((\widehat{\sigma}_{ij} - \sigma_{ij})^2\right)$. Let us define $a_k := X_i^{(k)} X_j^{(k)} - \sigma_{ij}$. We know that

$$(\widehat{\sigma}_{ij} - \sigma_{ij})^2 = \left(\frac{1}{n}\sum_{k=1}^{n} a_k\right)^2 = \frac{1}{n^2}\sum_{k=1}^{n} a_k^2 + \frac{1}{n^2}\sum_{k \neq k'} a_k a_{k'}.$$

So, using the independence of $a_1, ..., a_n$, we obtain

$$\begin{aligned}
\mathrm{Var}\left((\widehat{\sigma}_{ij} - \sigma_{ij})^2\right) \ &= \ \frac{1}{n^4} \sum_{k_1,k_2=1}^{n} \mathrm{cov}\left(a_{k_1}^2, a_{k_2}^2\right) + 2\frac{1}{n^4} \sum_{\substack{k_1,k_2,k_2'=1, \\ k_2 \neq k_2'}}^{n} \mathrm{cov}\left(a_{k_1}^2, a_{k_2} a_{k_2'}\right) \\
&\quad + \frac{1}{n^4} \sum_{\substack{k_1,k_1',k_2,k_2'=1, \\ k_1 \neq k_1',\ k_2 \neq k_2'}}^{n} \mathrm{cov}\left(a_{k_1} a_{k_1'}, a_{k_2} a_{k_2'}\right) \\
&= \ \frac{1}{n^3}\mathrm{cov}\left(a_1^2, a_1^2\right) + 4\frac{n-1}{n^3}\mathrm{cov}\left(a_1^2, a_1 a_2\right) \\
&\quad + 2\frac{n-1}{n^3}\mathrm{cov}\left(a_1 a_2, a_1 a_2\right),
\end{aligned}$$

where we observed that $\mathrm{cov}(a_1 a_2, a_1, a_3) = 0$. Now, by Isserlis' theorem and using the fact that σ_{ij} is upper-bounded by λ_{sup}, we have $\mathrm{cov}\left(a_1^2, a_1^2\right) \leq C_{\mathrm{sup}}$, $\mathrm{cov}\left(a_1^2, a_1 a_2\right) \leq C_{\mathrm{sup}}$ and $\mathrm{cov}\left(a_1 a_2, a_1 a_2\right) \leq C_{\mathrm{sup}}$ (and these bounds do not depend on k, i, j). So

$$\mathrm{Var}\left(\widehat{\sigma}_{ij}^2\right) \leq \frac{C_{\mathrm{sup}}}{n^2}.$$

Thus,

$$\mathrm{Var}\left(\frac{1}{p}\|\widehat{\Sigma}_{B_k^*} - \Sigma_{B_k^*}\|_F^2\right) \leq \frac{C_{\mathrm{sup}}}{p^2 n^2},$$

and

$$\mathrm{Var}\left(\frac{1}{p}\|\widehat{\Sigma}_{B^*} - \Sigma\|_F^2\right) \leq \frac{C_{\mathrm{sup}}}{p\, n^2}.$$

Thus, by Chebyshev's inequality

$$\begin{aligned}
& \mathbb{P}\left(\frac{1}{p}\|\widehat{\Sigma}_{B^*}-\Sigma\|_F^2 < \frac{\lambda_{\inf}^2}{n}\right) \\
\leq\ & \mathbb{P}\left(\left|\frac{1}{p}\|\widehat{\Sigma}_{B^*}-\Sigma\|_F^2 - \mathrm{E}\left[\frac{1}{p}\|\widehat{\Sigma}_{B^*}-\Sigma\|_F^2\right]\right| > \frac{\lambda_{\inf}^2}{n}\right) \\
\leq\ & \frac{\mathrm{Var}\left(\frac{1}{p}\|\widehat{\Sigma}_{B^*}-\Sigma\|_F^2\right) n^2}{\lambda_{\inf}^4} \\
\leq\ & \frac{C_{\sup}}{p} \longrightarrow 0.
\end{aligned}$$

So, we proved that $\frac{1}{p}\|\widehat{\Sigma}_{B^*}-\Sigma\|_F^2$ is not an $o_p(1/n)$.

Now, we show that the same results hold for S_{B^*} proving that $\frac{1}{p}\|S_{B^*}-\Sigma\|_F^2 - \frac{1}{p}\|\widehat{\Sigma}_{B^*}-\Sigma\|_F^2 = o_p(1/n)$. We have

$$\begin{aligned}
& \left|\frac{1}{p}\|S_{B^*}-\Sigma\|_F^2 - \frac{1}{p}\|\widehat{\Sigma}_{B^*}-\Sigma\|_F^2\right| \\
=\ & \left|\frac{1}{p}\sum_{(i,j)\in B^*} 2\sigma_{ij}\widehat{\sigma}_{ij}\frac{1}{n} - \widehat{\sigma}_{ij}^2\frac{2n-1}{n^2}\right| \\
\leq\ & \frac{m^2}{n}\max_{(i,j)\in B^*}\left|2\sigma_{ij}\widehat{\sigma}_{ij} - \frac{2n-1}{n}\widehat{\sigma}_{ij}^2\right| \\
\leq\ & \frac{m^2}{n}\max_{(i,j)\in B^*}\left(2|\widehat{\sigma}_{ij}||\widehat{\sigma}_{ij}-\sigma_{ij}| + |\widehat{\sigma}_{ij}^2|/n\right).
\end{aligned}$$

Yet, by Bernstein's inequality,

$$\max_{(i,j)\in B^*}|\widehat{\sigma}_{ij}| = O_p(1),$$

$$\max_{(i,j)\in B^*}|\widehat{\sigma}_{ij}-\sigma_{ij}| = o_p(1),$$

and

$$\max_{(i,j)\in B^*}\widehat{\sigma}_{ij}^2 = O_p(1).$$

That proves

$$\frac{1}{p}\|S_{B^*}-\Sigma\|_F^2 - \frac{1}{p}\|\widehat{\Sigma}_{B^*}-\Sigma\|_F^2 = o_p(1/n).$$

Now, on the one hand, we have

$$\frac{1}{p}\|S_{B^*}-\Sigma\|_F^2 = O_p(1/n),$$

and by Proposition 25,

$$\frac{1}{p}\|S_{\widehat{B}} - \Sigma\|_F^2 = O_p(1/n).$$

On the other hand,

$$\frac{1}{p}\|S_{B^*} - \Sigma\|_F^2 \neq o_p(1/n).$$

□

Proof of Proposition 28

Proof. It suffices to prove that

$$\frac{\lambda_{\inf}^2}{2} \leq \mathrm{E}\left(\frac{n}{p^2}\|S - \Sigma\|_F^2\right) \leq C_{\sup}. \tag{III.6}$$

First,

$$\begin{aligned}
\mathrm{E}\left(\frac{n}{p^2}\|S - \Sigma\|_F^2\right) &\leq n \max_{(i,j)\in[1:p]^2} \mathrm{E}\left[(s_{ij} - \sigma_{ij})^2\right] \\
&= n \max_{(i,j)\in[1:p]^2} \mathrm{Var}\left(s_{ij}\right) + \frac{\sigma_{ij}^2}{n} \\
&= \frac{n-1}{n} \max_{(i,j)\in[1:p]^2} \mathrm{Var}\left(M_i M_j\right) + \frac{\sigma_{ij}^2}{n} \\
&\leq \max_{(i,j)\in[1:p]^2} \left(\sigma_{ii}\sigma_{jj} + \sigma_{ij}^2 + \frac{\sigma_{ij}^2}{n}\right) \\
&\leq 3\lambda_{\sup}^2.
\end{aligned}$$

Secondly,

$$\begin{aligned}
\mathrm{E}\left(\frac{n}{p^2}\|S - \Sigma\|_F^2\right) &\geq n \min_{(i,j)\in[1:p]^2} \mathrm{E}\left[(s_{ij} - \sigma_{ij})^2\right] \\
&\geq n \min_{(i,j)\in[1:p]^2} \mathrm{Var}\left(s_{ij}\right) \\
&= \frac{n-1}{n} \min_{(i,j)\in[1:p]^2} \left(\sigma_{ii}\sigma_{jj} + \sigma_{ij}^2\right) \\
&\geq \frac{1}{2}\lambda_{\inf}^2.
\end{aligned}$$

□

Proof of Proposition 29

Proof. We follow the proof of Proposition 27. Let $\delta \in]1/2, 1[$, $\varepsilon > 0$, and $\alpha_1 := \delta/2 - \varepsilon/4$.

We have

$$\begin{aligned}
& \max_{B(\alpha_1) \le B \le B^*} \mathrm{E}\left(\frac{n^{\delta-\varepsilon}}{p} \|\widehat{\Sigma}_B - \Sigma\|_F^2\right) \\
= & \max_{B(\alpha_1) \le B \le B^*} \frac{n^{\delta-\varepsilon}}{p} \sum_{k=1}^{K} \left[\sum_{\substack{i,j \in B_k^*, \\ (i,j) \in B}} \mathrm{E}\left((\widehat{\sigma}_{ij} - \sigma_{ij})^2\right) + \sum_{\substack{i,j \in B_k^*, \\ (i,j) \in B}} \sigma_{ij}^2 \right] \\
\le & \; n^{\delta-\varepsilon} m^2 \left(\max_{(i,j) \in B^*} \mathrm{E}\left(\widehat{\sigma}_{ij} - \sigma_{ij}\right)^2\right) + \max_{B(\alpha_1) \le B \le B^*} \max_{(i,j) \in B^* \setminus B} \sigma_{ij}^2 \right) \\
\le & \; n^{\delta-\varepsilon} m^2 \left(O\left(\frac{1}{n}\right) + n^{-2\alpha_1} \right) \longrightarrow 0.
\end{aligned}$$

Thus,

$$\max_{B(\alpha_1) \le B \le B^*} \frac{1}{p} \|\widehat{\Sigma}_B - \Sigma\|_F^2 = o_p\left(\frac{1}{n^{\delta-\varepsilon}}\right),$$

and thus

$$\max_{B(\alpha_1) \le B \le B^*} \frac{1}{p} \|S_B - \Sigma\|_F^2 = o_p\left(\frac{1}{n^{\delta-\varepsilon}}\right).$$

We conclude using Proposition 26 and using that $B(\alpha_2) \le B^*$. $\square$

Proof of Proposition 30

Proof. The eigenvalues of Σ are lower-bounded by ε and upper-bounded by mL, so Σ verifies Condition 2. Condition 3 is verified by construction. It remains to prove the slightly modified Condition 4 given in Proposition 30. Let $a > 0$.

$$\begin{aligned}
& \mathbb{P}\left(\exists B < B^*, \; \|\Sigma_B - \Sigma\|_{\max} < an^{-1/4}\right) \\
= & \; \mathbb{P}\left(\exists k, \max_{i,j \in B_k^*, \, i \ne j} |\sigma_{ij}| < an^{-1/4}\right) \\
\le & \; p\mathbb{P}\left(\max_{i,j \in [1:10], \, i \ne j} |\sum_{l=1}^{L} U_i^{(l)} U_j^{(l)}| \le an^{-1/4}\right),
\end{aligned}$$

using an union bound and the fact that all the blocks have a size larger that 10. Then, by independence of $\left(\sum_{l=1}^{L} U_{2k-1}^{(l)} U_{2k}^{(l)}\right)_{k \le 5}$, we have

$$\mathbb{P}\left(\exists B < B^*, \; \|\Sigma_B - \Sigma\|_{\max} < an^{-1/4}\right) \le p\mathbb{P}\left(|\sum_{l=1}^{L} U_1^{(l)} U_2^{(l)}| \le an^{-1/4}\right)^5$$

Let $U_i := (U_i^{(l)})_{l\leq L} \in \mathbb{R}^L$ for $i = 1, 2$. Then, U_1 and U_2 are independent and uniformly distributed on $[-1, 1]^L$. Thus

$$\mathbb{P}\left(|\sum_{l=1}^{L} U_1^{(l)} U_2^{(l)}| \leq an^{-1/4}\right) = \mathrm{E}\left[\mathbb{P}\left(|\langle U_1, U_2\rangle| \leq an^{-1/4}\middle| U_2\right)\right]$$

Let $u_2 \in [-1, 1]^L \setminus \{0\}$. The set $\{u_1 \in [-1, 1]^L |\ |\langle u_1, u_2\rangle| \leq an^{-1/4}\}$ is a subset of $\{\sum_{l=1}^{L} x_i e_i |\ -an^{-1/4}\|u_2\| \leq x_1 \leq an^{-1/4}\|u_2\|,\ |x_l| \leq \sqrt{L}\ \forall l\}$ where $e_1 = u_2/\|u_2\|$ and $(e_1, ..., e_L)$ is an orthonormal basis of $\mathbb{R}^L$. The Lebesgue measure of this subset is $(2\sqrt{L})^{L-1} 2an^{-1/4}\|u_2\|$. Furthermore, (conditionally to $U_2 = u_2$) the probability density function of U_1 on this set is either 0 or 2^{-L}. So, for all $u_2 \in [-1, 1]^L \setminus \{0\}$,

$$\mathbb{P}\left(|\langle U_1, U_2\rangle| \leq an^{-1/4}\middle| U_2 = u_2\right) \leq (2\sqrt{L})^{L-1} 2an^{-1/4}\|u_2\| 2^{-L} \leq \sqrt{L}^{L-1} an^{-1/4}.$$

Thus

$$\mathbb{P}\left(|\sum_{l=1}^{L} U_1^{(l)} U_2^{(l)}| \leq an^{-1/4}\right) \leq \sqrt{L}^{L-1} an^{-1/4}.$$

Then

$$\mathbb{P}\left(\exists B < B^*,\ \|\Sigma_B - \Sigma\|_{\max} < an^{-1/4}\right) \leq p(\sqrt{L}^{L-1} an^{-1/4})^5 \longrightarrow 0.$$

Hence, it remains to prove that the conclusion of Proposition 20 holds. That will imply the same for Propositions 25 and 27. Let $a > 0$ and $E := \{\Gamma \in S_p^{++}(\mathbb{R}, B^*)|\ \forall B < B^*,\ \|\Sigma_B - \Sigma\|_{\max} \geq an^{-1/4}\}$, where the generation of B^* is defined in Proposition 30. We have

$$\begin{aligned} \mathbb{P}\left(\widehat{B}_{tot} \neq B^*\right) &\leq \mathbb{P}\left(\Sigma \notin E\right) + \mathbb{P}\left(\widehat{B}_{tot} \neq B^* \middle| \Sigma \in E\right) \\ &\leq o(1) + \int_E \mathbb{P}\left(\widehat{B}_{tot} \neq B^* \middle| \Sigma = \Gamma\right) d\mathbb{P}_\Sigma(\Gamma). \end{aligned}$$

Yet, for all $\Sigma \in E$, $\mathbb{P}\left(\widehat{B}_{tot} \neq B^* \middle| \Sigma = \Gamma\right) \longrightarrow 0$ thanks to Proposition 20 (even in Condition 4 is not verified, the proof is still valid since the covariance matrix is in E). We conclude by dominated convergence theorem. □

Notation for the proofs of Section B.3

For all $i, j \in [1 : p]$, let $e_i \in \mathbb{R}^p$ be such that all coefficients are zero except the i-th one which is equal to 1, and let $e_{ij} \in \mathcal{M}_p(\mathbb{R})$ be such that all coefficients are zero except the (i, j)-th one which is equal to 1. Let γ_{ij} be the (i, j)-th coefficient of Σ^{-1}. Finally, as we use matrices M of size $p^2 \times p^2$, and vectors v of size p^2, we define $v_{ij} := v_{(j-1)p+i}$ and $M_{ij,kl} := M_{(j-1)p+i,(l-1)p+k}$.

Proof of Proposition 31

We see that, for all $B \in \mathcal{P}_p$, $l_{S_B} = \log(|S_B|)/p + \frac{n-1}{n}$ converges almost surely to $\log(|\Sigma_B|)/p + 1$. The following Lemma gives a central limit theorem for this convergence.

Lemma 31. *For all $B \in \mathcal{P}_p$, we have*

$$\sqrt{n}(\log|S_B| - \log|\Sigma_B|) \xrightarrow[n\to+\infty]{\mathcal{L}} \mathcal{N}(0, 2\,\mathrm{Tr}(\Sigma_B^{-1}\Sigma\Sigma_B^{-1}\Sigma)/p), \tag{III.7}$$

with $2\,\mathrm{Tr}(\Sigma_B^{-1}\Sigma\Sigma_B^{-1}\Sigma)/p \leq 2p$. In particular

$$\sqrt{n}(\log|S| - \log|\Sigma|) \xrightarrow[n\to+\infty]{\mathcal{L}} \mathcal{N}(0, 2).$$

Proof. Let $Z^{(k)} = M^{(k)}M^{(k)T}$, where $M^{(k)} = (M_i^{(k)})_{i\leq p} \in R^p$. We know that $\mathrm{E}(Z) = \Sigma$ and $\mathrm{cov}(Z_{i,j}, Z_{k,l}) = \mathrm{E}(X_iX_jX_kX_l) - \sigma_{ij}\sigma_{kl} = \sigma_{ij}\sigma_{kl} + \sigma_{ik}\sigma_{jl} + \sigma_{il}\sigma_{jk} - \sigma_{ij}\sigma_{kl} = \sigma_{ik}\sigma_{jl} + \sigma_{il}\sigma_{jk}$. Let $\Gamma \in \mathcal{M}_{p^2,p^2}$, be such that $\Gamma_{ij,kl} := \sigma_{ik}\sigma_{jl} + \sigma_{il}\sigma_{jk} = \mathrm{cov}(Z_{i,j}, Z_{k,l})$. Using the central limit Theorem,

$$\sqrt{n-1}\left(\mathrm{vec}(\widehat{\Sigma}_B) - \mathrm{vec}(\Sigma_B)\right)) \xrightarrow[n\to+\infty]{\mathcal{L}} \mathcal{N}(0, \Gamma_B),$$

and by Slutsky Lemma,

$$\sqrt{n}\,(\mathrm{vec}(S_B) - \mathrm{vec}(\Sigma_B)) \xrightarrow[n\to+\infty]{\mathcal{L}} \mathcal{N}(0, \Gamma_B), \tag{III.8}$$

where $(\Gamma_B)_{ij,kl} = \Gamma_{ij,kl}$ if $(i,j) \in B$ and $(k,l) \in B$ and $(\Gamma_B)_{ij,kl} = 0$ otherwise.

Let us apply the Delta-method to (III.8) with the function $\log \circ \det \circ \mathrm{mat}$, where $\mathrm{mat} = \mathbb{R}^{p^2} \to \mathcal{M}_p(\mathbb{R})$ is the inverse function of vec. If we write L the Jacobian matrix of $\log \circ \det \circ \mathrm{mat}$, we have:

$$\sqrt{n}(\log|S_B| - \log|\Sigma_B|) \xrightarrow[n\to+\infty]{\mathcal{L}} \mathcal{N}(0, L(\mathrm{vec}(\Sigma_B))\Gamma_B L(\mathrm{vec}(\Sigma_B))^T).$$

Let us compute the linear map $L(\mathrm{vec}(\Sigma_B)) : \mathbb{R}^{p^2} \to \mathbb{R}$, that we identify with its matrix. Let us recall that, for the dot product $\langle A, B\rangle := Tr(A^TB)$, the gradient of $\log \circ \det$ on A is A^{-1}. Thus, if $v \in \mathbb{R}^{p^2}$, we have

$$\begin{aligned}
L(\mathrm{vec}(\Sigma_B))(v) &= D(\log\circ\det)(\mathrm{mat}(\mathrm{vec}(\Sigma_B)) \circ D\,\mathrm{mat}(\mathrm{vec}(\Sigma_B))(v) \\
&= \langle \nabla(\log\circ\det)(\Sigma_B), D\,\mathrm{mat}(\mathrm{vec}(\Sigma))(v)\rangle, \\
&= \langle \Sigma_B^{-1}, \Sigma\rangle \\
&= \mathrm{Tr}(\Sigma_B^{-1}\,\mathrm{mat}(v)) \\
&= \mathrm{vec}(\Sigma_B^{-1})^T v.
\end{aligned}$$

So $L(\mathrm{vec}(\Sigma_B)) = \mathrm{vec}(\Sigma_B^{-1})^T$, then

$$\sqrt{n}(\log|S_B| - \log|\Sigma_B|) \underset{n\to+\infty}{\xrightarrow{\mathcal{L}}} \mathcal{N}(0, \mathrm{vec}(\Sigma_B^{-1})^T \Gamma_B \,\mathrm{vec}(\Sigma_B^{-1})).$$

Now,

$$\begin{aligned}
& \mathrm{vec}(\Sigma_B^{-1})^T \Gamma_B \,\mathrm{vec}(\Sigma_B^{-1}) \\
= & \sum_{i,j,k,l} (\Sigma_B)^{-1}_{i,j} (\sigma_{ik}\sigma_{jl} + \sigma_{il}\sigma_{jk})(\Sigma_B)^{-1}_{k,l} \\
= & \sum_{i,j,k,l} (\Sigma_B)^{-1}_{i,j} \sigma_{ik}\sigma_{jl}(\Sigma_B)^{-1}_{k,l} + \sum_{i,j,k,l} (\Sigma_B)^{-1}_{i,j} \sigma_{il}\sigma_{jk}(\Sigma_B)^{-1}_{k,l} \\
= & \; 2\,\mathrm{Tr}(\Sigma_B^{-1}\Sigma\Sigma_B^{-1}\Sigma) \\
= & \; 2\,\mathrm{Tr}\left[\left(\Sigma_B^{-\frac{1}{2}}\Sigma\Sigma_B^{-\frac{1}{2}}\right)\left(\Sigma_B^{-\frac{1}{2}}\Sigma\Sigma_B^{-\frac{1}{2}}\right)\right] \\
\leq & \; 2\,\mathrm{Tr}\left(\Sigma_B^{-\frac{1}{2}}\Sigma\Sigma_B^{-\frac{1}{2}}\right)^2 \\
= & \; 2\,\mathrm{Tr}(\Sigma_B^{-1}\Sigma)^2 \\
= & \; 2p^2.
\end{aligned}$$

Indeed, as $A := \Sigma_B^{-\frac{1}{2}}\Sigma\Sigma_B^{-\frac{1}{2}}$ is symmetric positive definite, we have $\mathrm{Tr}(AA) \leq \mathrm{Tr}(A)^2$. □

Lemma 32. *For all $\Gamma \in S_p^{++}(\mathbb{R})$ and for all $B \in \mathcal{P}_p$ such that $\Gamma \neq \Gamma_B$, we have* $\det(\Gamma_B) > \det(\Gamma)$.

Proof. First, let us prove it for $|B| = K = 2$. We have $B = \{I, J\}$.

$$\det(\Gamma) = \det(\Gamma_{I,I}) \det(\Gamma_{J,J} - \Gamma_{J,I}\Gamma_{I,I}^{-1}\Gamma_{I,J}).$$

Now, $\det(\Gamma_B) = \det(\Gamma_{I,I})\det(\Gamma_{J,J})$. Thus, it suffices to show that $\det(\Gamma_{J,J}) > \det(\Gamma_{J,J} - \Gamma_{J,I}\Gamma_{I,I}^{-1}\Gamma_{I,J})$. We then write $A_1 := \Gamma_{J,J} - \Gamma_{J,I}\Gamma_{I,I}^{-1}\Gamma_{I,J}$ which is symmetric positive definite (Schur's complement), and $A_2 = \Gamma_{J,I}\Gamma_{I,I}^{-1}\Gamma_{I,J}$ which is also symmetric positive definite. Then, we have

$$\det(A_1 + A_2) = \det(A_1)\det(I_p + A_1^{-\frac{1}{2}}A_2A_1^{-\frac{1}{2}}) > \det(A_1),$$

because $\det(I_p + A_1^{-\frac{1}{2}}A_2A_1^{-\frac{1}{2}}) = \prod_{i=1}^p (1 + \phi_i(A_1^{-\frac{1}{2}}A_2A_1^{-\frac{1}{2}}))$.

Now, we prove the lemma for any value of $|B| = K$. Let $\Gamma \in S_p^{++}(\mathbb{R})$ and $B \in \mathcal{P}_p$ such that $\Gamma \neq \Gamma_B$. Let $B^{(j)} := \{\bigcup_{i=1}^j B_i, \bigcup_{i=j+1}^K B_i\}$ for all $j \in [1 : K-1]$. We now define $(\Gamma^{(j)})_{j\in[1,K]}$ with the recurrence relation $\Gamma_{(j+1)} = \Gamma^{(j)}_{B^{(j)}}$ and with $\Gamma^{(1)} = \Gamma$, we then have $\Gamma_B = \Gamma^K$. Thus

$$\det(\Gamma_B) = \det(\Gamma^{(K)}) \geq \det(\Gamma^{(K-1)}) \geq ... \geq \det(\Gamma^{(1)}) = \det(\Gamma).$$

Furthermore, as $\Gamma \neq \Gamma_B$, there exists j such that $\Gamma^{(j)}_{B^{(j)}} \neq \Gamma^{(j)}$. Thus, at least one of the previous inequality is strict, and so $\det(\Gamma_B) > \det(\Gamma)$. □

Using Lemmas 31 and 32, we can prove Proposition 31.

Proof. It suffices to show that, for all $B \neq B^*$,

$$\mathbb{P}(\widehat{B}_{tot} = B) \underset{n\to+\infty}{\longrightarrow} 0.$$

We split the proof into two steps: for $B \ngeq B^*$ and for $B > B^*$.

Step 1: $B \ngeq B^*$.
Let $h := \min\{\log(|\Sigma_B|) - \log(|\Sigma|) |\ B \ngeq B^*\} = \min\{\log(|\Sigma_B|) - \log(|\Sigma|),\ B < B^*\}$, since $\Sigma_B = \Sigma_{B\cap B^*}$. Thanks to Lemma 32, we know that $h > 0$.

Let $B \ngeq B^*$. Using the convergence in probability of $l_{S'_B}$, we know that $\mathbb{P}(l_{S_B} < \log|\Sigma_B|/p + 1 - h/3) \underset{n\to+\infty}{\longrightarrow} 0$ and $\mathbb{P}(l_{S_{B^*}} > \log|\Sigma|/p + 1 + h/3) \underset{n\to+\infty}{\longrightarrow} 0$.

Now, we know that for $n > (3p/h)^{1/\delta}$, the term of penalisation satisfies $\kappa\,\mathrm{pen}(B^*) < h/3$. Thus,

$$\mathbb{P}(\widehat{B}_{tot} = B) \underset{n\to+\infty}{\longrightarrow} 0.$$

Step 2: $B > B^*$.
Let $B > B^*$. We know that

$$\begin{aligned} & \sqrt{n}\,(\Psi(B) - \Psi(B^*)) \\ = \ & \sqrt{n}\,(l_{S_B} + \kappa\,\mathrm{pen}(B) - l_{S_{B^*}} - \kappa\,\mathrm{pen}(B^*)) \\ = \ & \sqrt{n}\kappa(\mathrm{pen}(B) - \mathrm{pen}(B^*)) + \sqrt{n}(l_{S_B} - l_{\Sigma_B}) - \sqrt{n}(l_{S_{B^*}} - l_{\Sigma_{B^*}}), \end{aligned}$$

since $\Sigma_B = \Sigma_{B^*}$ for $B > B^*$. Let a_n be equal to $\sqrt{n}\kappa(\mathrm{pen}(B) - \mathrm{pen}(B^*))$ (which converges to $+\infty$), b_n to be equal to $\sqrt{n}(l_{S_B} - l_{\Sigma_B})$ (which converges to a zero mean normal distribution) and c_n to be equal to $\sqrt{n}(l_{S_{B^*}} - l_{\Sigma_{B^*}})$ (which converges to a zero mean normal distribution). We have

$$\begin{aligned} \mathbb{P}\left[\sqrt{n}\,(\Psi(B) - \Psi(B^*)) > 0\right] &= \mathbb{P}(b_n - c_n < -a_n) \\ &\leq \mathbb{P}(b_n \leq -a_n/2 \text{ or } c_n \geq a_n/2) \\ &\leq \mathbb{P}(b_n \leq -a_n/2) + \mathbb{P}(c_n \geq a_n/2) \underset{n\to+\infty}{\longrightarrow} 0. \end{aligned}$$

Thus, $\mathbb{P}(\widehat{B}_{tot} = B) \underset{n\to+\infty}{\longrightarrow} 0$. □

Proof of Proposition 32

Proof. We follow the notation of [SN98].

An othonormal basis of $S_p(\mathbb{R})$ is $\{\frac{1}{\sqrt{2}}(e_{ij}+e_{ji})|\ i<j\} \cup \{e_{ii}|\ i \le p\}$ with the following total order on $\{(i,j) \in [1:p]^2|\ i \le j\}$: we write $(i,j) \le (i',j')$ if $j<j'$ or if $j=j$ and $i \le i'$. We define $U \in \mathcal{M}_{p^2,p(p+1)/2}(\mathbb{R})$ as the matrix which columns are the vectorizations of the components of this basis of $\mathrm{vec}(S_p(\mathbb{R}))$. Thus $U_{ij,kl} = \frac{1}{\sqrt{2}}(\mathbb{1}_{(i,j)=(k,l)} + \mathbb{1}_{(i,j)=(l,k)})$, for all $k<l$ and $U_{ij,kk} = \mathbb{1}_{(i,j)=(k,k)}$.

Thus, $U(U^TJU)^{-1}U^T$ is the Cramér-Rao bound, where J is the standard Fisher information matrix in the model $\{\mathcal{N}(\mu,\Sigma),\ \Sigma \in \mathcal{M}_p(\mathbb{R})\}$. As the sample is i.i.d, it suffices to prove if with $n=1$. In the rest of the proof, we compute the Cramér-Rao bound, and we show that this bound is equal to $\mathrm{E}\left((S-\Sigma)(S-\Sigma)^T\right)$. We split the proof into several Lemmas.

Lemma 33. *Recall that* $\Sigma^{-1} = (\gamma_{ij})_{i,j\le p}$. *Let* $A = (A_{mn,m'n'})_{m\le n, m'\le n'} \in \mathcal{M}_{p(p+1)/2}(\mathbb{R})$ *defined by*

$$A_{mn,m'n'} = \begin{cases} \frac{1}{2}(\gamma_{mm'}\gamma_{nn'} + \gamma_{mn'}\gamma_{nm'}) & \text{if } m<n \text{ and } m'<n' \\ \frac{1}{\sqrt{2}}\gamma_{mm'}\gamma_{nn'} & \text{if either } m=n \text{ or } m'=n' \\ \frac{1}{2}\gamma_{mm'}^2 & \text{if } m=n \text{ and } m'=n', \end{cases}$$

Then, $A = U^TJU$.

Proof. Deriving twice the log-likelihood with respect to σ_{ij} and σ_{kl} (for $i,j,k,l \in [1:p]$) and taking the expectation, we get

$$\begin{aligned} J_{ij,kl} &= \frac{1}{2}\mathrm{Tr}\left(\Sigma^{-1}e_ie_j^T\Sigma^{-1}e_ke_l^T\right) \\ &= \frac{1}{2}\gamma_{li}\gamma_{jk}. \end{aligned}$$

Thus, for all $m<n,\ m'<n'$, we have

$$\begin{aligned} (U^TJU)_{mn,m'n'} &= \sum_{i,j,k,l=1}^{p} U_{ij,mn}J_{ij,kl}U_{kl,m'n'} \\ &= \sum_{i,j,k,l=1}^{p} \frac{1}{\sqrt{2}}(\mathbb{1}_{(i,j)=(m,n)} + \mathbb{1}_{(i,j)=(n,m)})J_{ij,kl}\frac{1}{\sqrt{2}}(\mathbb{1}_{(k,l)=(m',n')} + \mathbb{1}_{(k,l)=(n',m')}) \\ &= \frac{1}{2}(J_{mn,m'n'} + J_{mn,n'm'} + J_{nm,m'n'} + J_{nm,n'm'}) \\ &= \frac{1}{2}(\gamma_{mm'}\gamma_{nn'} + \gamma_{mn'}\gamma_{nm'}). \end{aligned}$$

Now, if $m'<n'$, we have

$$(U^TJU)_{mm,m'n'} = \sum_{i,j,k,l=1}^{p} U_{ij,mm}J_{ij,kl}U_{kl,m'n'}$$

$$
\begin{aligned}
&= \sum_{i,j,k,l=1}^{p} \mathbb{1}_{(i,j)=(m,m)} J_{ij,kl} \frac{1}{\sqrt{2}} (\mathbb{1}_{(k,l)=(m',n')} + \mathbb{1}_{(k,l)=(n',m')}) \\
&= \frac{1}{\sqrt{2}} (J_{mm,m'n'} + J_{mm,n'm'}) \\
&= \frac{1}{\sqrt{2}} \gamma_{mm'} \gamma_{mn'}.
\end{aligned}
$$

If $m < n$, we have

$$
\begin{aligned}
(U^T JU)_{mn,m'm'} &= \sum_{i,j,k,l=1}^{p} U_{ij,mn} J_{ij,kl} U_{kl,m'm'} \\
&= \sum_{i,j,k,l=1}^{p} \frac{1}{\sqrt{2}} (\mathbb{1}_{(i,j)=(m,n)} + \mathbb{1}_{(i,j)=(n,m)}) J_{ij,kl} \mathbb{1}_{(k,l)=(m',m')} \\
&= \frac{1}{\sqrt{2}} (J_{mn,m'm'} + J_{nm,m'm'}) \\
&= \frac{1}{\sqrt{2}} \gamma_{mm'} \gamma_{nm'}.
\end{aligned}
$$

Finally,

$$
\begin{aligned}
(U^T JU)_{mm,m'm'} &= \sum_{i,j,k,l=1}^{p} U_{ij,mm} J_{ij,kl} U_{kl,m'm'} \\
&= \sum_{i,j,k,l=1}^{p} \mathbb{1}_{(i,j)=(m,m)} J_{ij,kl} \mathbb{1}_{(k,l)=(m',m')} \\
&= J_{mm,m'm'} \\
&= \frac{1}{2} \gamma_{mm'}^2.
\end{aligned}
$$

$\square$

Lemma 34. *Let $B = (B_{mn,m'n'})_{m \le n, m' \le n'} \in \mathcal{M}_{p(p+1)/2}(\mathbb{R})$ defined by*

$$
B_{mn,m'n'} = \begin{cases} 2(\sigma_{mm'}\sigma_{nn'} + \sigma_{mn'}\sigma_{nm'}) & \text{if } m < n \text{ and } m' < n' \\ 2\sqrt{2}\sigma_{mm'}\sigma_{nn'} & \text{if either } m = n \text{ or } m' = n' \\ 2\sigma_{mm'}^2 & \text{if } m = n \text{ and } m' = n', \end{cases}
$$

then, $B = A^{-1}$. Moreover $(UBU^T)_{ij,i'j'} = \sigma_{ii'}\sigma_{jj'} + \sigma_{ij'}\sigma_{ji'}$ for all $i, j, i', j' \in [1 : p]$.

Proof. We compute the product $A\ B$. First of all, let $m < n$ and $m' < n'$. We have

$$\begin{aligned}
(A\ B)_{mn,m'n'} &= \sum_{i\le j} A_{mn,ij} B_{ij,m'n'} \\
&= \sum_{i<j} A_{mn,ij} B_{ij,m'n'} + \sum_{i=j} A_{mn,ij} B_{ij,m'n'} \\
&= \sum_{i<j} \left(\gamma_{mi}\gamma_{nj} + \gamma_{mj}\gamma_{ni}\right)\left(\sigma_{im'}\sigma_{jn'} + \sigma_{in'}\sigma_{jm'}\right) \\
&\quad +2\sum_{i=j} \gamma_{mi}\gamma_{nj}\sigma_{im'}\sigma_{jn'} \\
&= I_1 + I_2,
\end{aligned}$$

with

$$I_1 = \sum_{i<j} \gamma_{mi}\gamma_{nj}\sigma_{im'}\sigma_{jn'} + \sum_{i<j} \gamma_{mj}\gamma_{ni}\sigma_{in'}\sigma_{jm'} + \sum_{i=j} \gamma_{mi}\gamma_{nj}\sigma_{im'}\sigma_{jn'},$$

and

$$I_2 = \sum_{i<j} \gamma_{mj}\gamma_{ni}\sigma_{im'}\sigma_{jn'} + \sum_{i<j} \gamma_{mi}\gamma_{nj}\sigma_{in'}\sigma_{jm'} + \sum_{i=j} \gamma_{mj}\gamma_{ni}\sigma_{im'}\sigma_{jn'}.$$

We then have

$$\begin{aligned}
I_1 &= \sum_{i<j} \gamma_{mi}\gamma_{nj}\sigma_{im'}\sigma_{jn'} + \sum_{j<i} \gamma_{mi}\gamma_{nj}\sigma_{jn'}\sigma_{im'} + \sum_{i=j} \gamma_{im}\gamma_{jn}\sigma_{im'}\sigma_{jn'} \\
&= \sum_{i,j} \gamma_{mi}\gamma_{nj}\sigma_{im'}\sigma_{jn'} \\
&= \sum_{i} \gamma_{mi}\sigma_{im'} \sum_{j} \gamma_{nj}\sigma_{jn'} \\
&= \mathbb{1}_{(m,n)=(m',n')}.
\end{aligned}$$

Similarly,

$$\begin{aligned}
I_2 &= \sum_{i<j} \gamma_{mj}\gamma_{ni}\sigma_{im'}\sigma_{jn'} + \sum_{j<i} \gamma_{mj}\gamma_{ni}\sigma_{jn'}\sigma_{im'} + \sum_{i=j} \gamma_{mj}\gamma_{ni}\sigma_{im'}\sigma_{jn'} \\
&= \sum_{i,j} \gamma_{mj}\gamma_{ni}\sigma_{im'}\sigma_{jn'} \\
&= \sum_{i} \gamma_{ni}\sigma_{im'} \sum_{j} \gamma_{mj}\sigma_{jn'} \\
&= \mathbb{1}_{(n,m)=(m',n')}
\end{aligned}$$

$$= \quad 0.$$

Now, if $m' < n'$

$$\begin{aligned}
(A\ B)_{mm,m'n'} &= \sum_{i\leq j} A_{mm,ij} B_{ij,m'n'} \\
&= \sum_{i<j} A_{mm,ij} B_{ij,m'n'} + \sum_{i=j} A_{mm,ij} B_{ij,m'n'} \\
&= \sqrt{2} \sum_{i<j} \gamma_{mi}\gamma_{mj} \left(\sigma_{im'}\sigma_{jn'} + \sigma_{in'}\sigma_{jm'}\right) \\
&\quad + \sqrt{2} \sum_{i=j} \gamma_{mi}\gamma_{mj}\sigma_{im'}\sigma_{jn'} \\
&= \sqrt{2} \sum_{i,j} \gamma_{mi}\gamma_{mj}\sigma_{im'}\sigma_{jn'} \\
&= \sqrt{2} \sum_{i} \gamma_{mi}\sigma_{im'} \sum_{j} \gamma_{mj}\sigma_{jn'} \\
&= \sqrt{2}\mathbb{1}_{(m,m)=(m',n')} \\
&= 0.
\end{aligned}$$

If $m < n$, then

$$\begin{aligned}
(A\ B)_{mn,m'm'} &= \sum_{i\leq j} A_{mn,ij} B_{ij,m'm'} \\
&= \sum_{i<j} A_{mn,ij} B_{ij,m'm'} + \sum_{i=j} A_{mn,ij} B_{ij,m'm'} \\
&= \sqrt{2} \sum_{i<j} \left(\gamma_{mi}\gamma_{nj} + \gamma_{mj}\gamma_{ni}\right) \sigma_{im'}\sigma_{jm'} \\
&\quad + \sqrt{2} \sum_{i=j} \gamma_{mi}\gamma_{nj}\sigma_{im'}\sigma_{jm'} \\
&= \sqrt{2} \sum_{i,j} \gamma_{mi}\gamma_{nj}\sigma_{im'}\sigma_{jm'} \\
&= \sqrt{2} \sum_{i} \gamma_{mi}\sigma_{im'} \sum_{j} \gamma_{nj}\sigma_{jn'} \\
&= \sqrt{2}\mathbb{1}_{(m,n)=(m',m')} \\
&= 0.
\end{aligned}$$

Finally,

$$(A\ B)_{mm,m'm'} = \sum_{i\leq j} A_{mm,ij} B_{ij,m'm'}$$

$$
\begin{aligned}
&= \sum_{i<j} A_{mm,ij} B_{ij,m'm'} + \sum_{i=j} A_{mm,ij} B_{ij,m'm'} \\
&= 2 \sum_{i<j} \gamma_{mi}\gamma_{mj}\sigma_{im'}\sigma_{jm'} \\
&\quad + \sum_{i=j} \gamma_{mi}\gamma_{mj}\sigma_{im'}\sigma_{jm'} \\
&= \sum_{i,j} \gamma_{mi}\gamma_{mj}\sigma_{im'}\sigma_{jm'} \\
&= \mathbb{1}_{m=m'}.
\end{aligned}
$$

We proved that $B = A^{-1}$. Let us show that $(U^T BU)_{ij,i'j'} = \sigma_{ii'}\sigma_{jj'} + \sigma_{ij'}\sigma_{ji'}$ for all i, j, i', j'. First of all, assume $i \neq j$ and $i' \neq j'$. Assume for example $i < j$ and $i' < j'$. Then we have

$$
\begin{aligned}
& (UBU^T)_{ij,i'j'} \\
= & \sum_{m\leq n, m'\leq n'} U_{ij,mn} B_{mn,m'n'} U_{i'j',m'n'} \\
= & \sum_{m\leq n, m'\leq n'} \frac{1}{\sqrt{2}} (\mathbb{1}_{(m,n)=(i,j)} + \mathbb{1}_{(m,n)=(j,i)}) B_{mn,m'n'} \frac{1}{\sqrt{2}} (\mathbb{1}_{(m',n')=(i',j')} + \mathbb{1}_{(m',n')=(j',i')}) \\
= & \frac{1}{2} B_{ij,i'j'} \\
= & \sigma_{ii'}\sigma_{jj'} + \sigma_{ij'}\sigma_{ji'}.
\end{aligned}
$$

We apply the same method for $i < j$ and $i' > j'$, for $i > j$ and $i' < j'$, and for $i > j$ and $i' > j'$. Then, let $i = j$ and $i' \neq j'$, for example $i' < j'$. We have

$$
\begin{aligned}
& (UBU^T)_{ii,i'j'} \\
= & \sum_{m\leq n, m'\leq n'} U_{ii,mn} B_{mn,m'n'} U_{i'j',m'n'} \\
= & \sum_{m\leq n, m'\leq n'} \mathbb{1}_{(m,n)=(i,i)} B_{mn,m'n'} \frac{1}{\sqrt{2}} (\mathbb{1}_{(m',n')=(i',j')} + \mathbb{1}_{(m',n')=(j',i')}) \\
= & \frac{1}{\sqrt{2}} B_{ii,i'j'} \\
= & \sigma_{ii'}\sigma_{ij'} + \sigma_{ij'}\sigma_{ii'}.
\end{aligned}
$$

The other cases are similar. □

We thus have the component of the Cramér-Rao bound:

$$
\left[U(U^T JU)^{-1} U^T\right]_{ij,i'j'} = \sigma_{ii'}\sigma_{jj'} + \sigma_{ij'}\sigma_{ji'}.
$$

This matrix is equal to $\mathrm{E}\left((\mathrm{vec}(S)-\mathrm{vec}(\Sigma))(\mathrm{vec}(S)-\mathrm{vec}(\Sigma))^T\right)$ for $n=1$ and when the mean μ is known. $\square$

Proof of Proposition 33

Proof. An orthonormal basis of $S_p(\mathbb{R}, B^*)$ is $\{\frac{1}{\sqrt{2}}(e_{ij}+e_{ji})|\ i<j,\ (i,j)\in B^*\}\cup\{e_{ii}|\ i\leq p\}$ with the following total order on $\{(i,j)\in[1:p]^2|\ i\leq j,\ (i,j)\in B^*\}$: we write $(i,j)\leq(i',j')$ if $j<j'$ or if $j=j$ and $i\leq i'$. Thus, we define U as the matrix which the columns are the vectorizations of the components of this basis of $S_p(\mathbb{R}, B^*)$. We have $U_{ij,kl}=\frac{1}{\sqrt{2}}(\mathbb{1}_{(i,j)=(k,l)}+\mathbb{1}_{(i,j)=(l,k)})$, for all $k<l$ with $(k,l)\in B^*$ and $U_{ij,kk}=\mathbb{1}_{(i,j)=(kk)}$.

Thus, $U(U^TJU)^{-1}U^T$ is the Cramér-Rao bound. As the sample is i.i.d, it suffices to prove the proposition with $n=1$.

Lemma 35. *Let $A=(A_{mn,m'n'})_{(m,n),\ (m',n')\in B^*,\ m\leq n,\ m'\leq n'}$ defined by*

$$A_{mn,m'n'}=\begin{cases}\frac{1}{2}(\gamma_{mm'}\gamma_{nn'}+\gamma_{mn'}\gamma_{nm'}) & \text{if } m<n \text{ and } m'<n'\\ \frac{1}{\sqrt{2}}\gamma_{mm'}\gamma_{nn'} & \text{if either } m=n \text{ or } m'=n'\\ \frac{1}{2}\gamma_{mm'}^2 & \text{if } m=n \text{ and } m'=n',\end{cases}$$

Then, $A=U^TJU$.

Proof. The proof is similar to the proof of Lemma 33, except that the values of m,n,m' and n' are more constraint. First of all

$$\begin{aligned}J_{ij,kl} &= \frac{1}{2}\mathrm{Tr}\left(\Sigma^{-1}e_ie_j^T\Sigma^{-1}e_ke_l^T\right)\\ &= \frac{1}{2}\gamma_{il}\gamma_{jk}.\end{aligned}$$

Now, if $(m,n)\in B^*,\ (m',n')\in B^*,\ m<n,\ m'<n'$,

$$\begin{aligned}(U^TJU)_{mn,m'n'} &= \sum_{i,j,k,l=1}^{p}U_{ij,mn}J_{ij,kl}U_{kl,m'n'}\\ &= \sum_{i,j,k,l=1}^{p}\frac{1}{\sqrt{2}}(\mathbb{1}_{(i,j)=(m,n)}+\mathbb{1}_{(i,j)=(n,m)})J_{ij,kl}\frac{1}{\sqrt{2}}(\mathbb{1}_{(k,l)=(m',n')}+\mathbb{1}_{(k,l)=(n',m')})\\ &= \frac{1}{2}\left(J_{mn,m'n'}+J_{mn,n'm'}+J_{nm,m'n'}+J_{nm,n'm'}\right)\\ &= \frac{1}{2}(\gamma_{mm'}\gamma_{nn'}+\gamma_{mn'}\gamma_{nm'}).\end{aligned}$$

If $m' < n'$ and $(m', n') \in B^*$,

$$\begin{aligned}
(U^T JU)_{mm,m'n'} &= \sum_{i,j,k,l=1}^{p} U_{ij,mm} J_{ij,kl} U_{kl,m'n'} \\
&= \sum_{i,j,k,l=1}^{p} \mathbb{1}_{(i,j)=(m,m)} J_{ij,kl} \frac{1}{\sqrt{2}} \big(\mathbb{1}_{(k,l)=(m',n')} + \mathbb{1}_{(k,l)=(n',m')} \big) \\
&= \frac{1}{\sqrt{2}} (J_{mm,m'n'} + J_{mm,n'm'}) \\
&= \frac{1}{\sqrt{2}} \gamma_{mm'} \gamma_{mn'}.
\end{aligned}$$

If $m < n$ and $(m, n) \in B^*$, we have

$$\begin{aligned}
(U^T JU)_{mn,m'm'} &= \sum_{i,j,k,l=1}^{p} U_{ij,mn} J_{ij,kl} U_{kl,m'm'} \\
&= \sum_{i,j,k,l=1}^{p} \frac{1}{\sqrt{2}} \big(\mathbb{1}_{(i,j)=(m,n)} + \mathbb{1}_{(i,j)=(n,m)} \big) J_{ij,kl} \mathbb{1}_{(k,l)=(m',m')} \\
&= \frac{1}{\sqrt{2}} (J_{mn,m'm'} + J_{nm,m'm'}) \\
&= \frac{1}{\sqrt{2}} \gamma_{mm'} \gamma_{nm'}.
\end{aligned}$$

Finally,

$$\begin{aligned}
(U^T JU)_{mm,m'm'} &= \sum_{i,j,k,l=1}^{p} U_{ij,mm} J_{ij,kl} U_{kl,m'm'} \\
&= \sum_{i,j,k,l=1}^{p} \mathbb{1}_{(i,j)=(m,m)} J_{ij,kl} \mathbb{1}_{(k,l)=(m',m')} \\
&= J_{mm,m'm'} \\
&= \frac{1}{2} \gamma_{mm'}^2.
\end{aligned}$$

□

Lemma 36. *Let* $B = (B_{mn,m'n'})_{m \le n, m' \le n',\ (m,n) \in B^*, (m',n') \in B^*}$ *defined by*

$$B_{mn,m'n'} = \begin{cases} 2(\sigma_{mm'}\sigma_{nn'} + \sigma_{mn'}\sigma_{nm'}) & \text{if } m < n \text{ and } m' < n' \\ 2\sqrt{2}\sigma_{mm'}\sigma_{nn'} & \text{if either } m = n \text{ or } m' = n' \\ 2\sigma_{mm'}^2 & \text{if } m = n \text{ and } m' = n', \end{cases}$$

then, $B = A^{-1}$. Moreover $(UBU^T)_{ij,i'j'} = \sigma_{ii'}\sigma_{jj'} + \sigma_{ij'}\sigma_{ji'}$ for all $(i,j,i',j') \in B^*$ and $(UBU^T)_{ij,i'j'} = 0$ for all $(i,j,i',j') \notin B^*$. Recall that we write $(i,j,i',j') \in B^*$ if there exists $A \in B^*$ such that $\{i,j,i',j'\} \subset A$.

Proof. We introduce the following notation: if $l \in B_k^*$, let $[l]_k$ to be the index of l in B_k^*.

Step 1: Let us prove that $B = A^{-1}$.

We compute the product AB. Assume that $m, n \in B_k^*$ with $m \leq n$ and $m', n' \in B_{k'}^*$ with $m' \leq n'$ and $k \neq k'$. We then have

$$\begin{aligned}
(A\ B)_{mn,m'n'} &= \sum_{(a,b)\in B^*,\ a\leq b} A_{mn,ab}B_{ab,m'n'} \\
&= \sum_{a,b\in B_k^*,\ a\leq b} A_{mn,ab}B_{ab,m'n'} + \sum_{a,b\in B_{k'}^*,\ a\leq b} A_{mn,ab}B_{ab,m'n'} \\
&= \sum_{a,b\in B_k^*,\ a\leq b} A_{mn,ab}0 + \sum_{a,b\in B_{k'}^*,\ a\leq b} 0B_{ab,m'n'} \\
&= 0,
\end{aligned}$$

using that $B_{ab,m'n'} = 0$ if $a, b \in B_k^*$ and $m', n' \in B_{k'}^*$ because Σ is block-diagonal, and using that $A_{mn,a,b} = 0$ if $m, n \in B_k^*$ and $a, b \in B_{k'}^*$ because Σ^{-1} is block-diagonal. Assume that $m, n, m', n' \in B_k^*$ with $m \leq n$ and $m' \leq n'$. We have,

$$\begin{aligned}
(A\ B)_{mn,m'n'} &= \sum_{(a,b)\in B^*,\ a\leq b} A_{mn,ab}B_{ab,m'n'} \\
&= \left(A_{B_k^*}B_{B_k^*}\right)_{[m]_k[n]_k,[m']_k[n']_k} \\
&= \mathbb{1}_{([m]_k,[n]_k)=([m']_k,[n']_k)} \\
&= \mathbb{1}_{(m,n)=(m',n')},
\end{aligned}$$

thanks to Lemma 34 applied to the matrix $\Sigma_{B_k^*}$. We proved that $B = A^{-1}$.

Step 2.A : We show that $(UBU^T)_{ij,i'j'} = \sigma_{ii'}\sigma_{jj'} + \sigma_{ij'}\sigma_{ji'}$ for all $(i,j,i',j') \in B^*$.

Assume that $(i,j,i',j') \in B^*$. First, assume that $i \neq j$ and $i' \neq j'$. Assume for example that $i < j$ and $i' < j'$ (the other cases are similar). We then have

$$\begin{aligned}
&(UBU^T)_{ij,i'j'} \\
= &\sum_{\substack{(m,n)\in B^*, m\leq n,\\ (m',n')\in B^*, m'\leq n'}} U_{ij,mn}B_{mn,m'n'}U_{i'j',m'n'}
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{\substack{(m,n)\in B^*, m\le n,\\ (m',n')\in B^*, m'\le n'}} \frac{1}{\sqrt{2}}(\mathbb{1}_{(m,n)=(i,j)} + \mathbb{1}_{(m,n)=(j,i)})B_{mn,m'n'}\frac{1}{\sqrt{2}}(\mathbb{1}_{(m',n')=(i',j')} + \mathbb{1}_{(m',n')=(j',i')})\\
&= \frac{1}{2}B_{ij,i'j'}\\
&= \sigma_{ii'}\sigma_{jj'} + \sigma_{ij'}\sigma_{ji'}.
\end{aligned}
$$

Let us take the case where $(i,j,i',j') \in B^*$ with either $i = j$, or $i' = j'$. For example $i = j$ and $i' < j'$. We then have

$$
\begin{aligned}
&(U^T BU)_{ii,i'j'}\\
&= \sum_{\substack{(m,n)\in B^*, m\le n,\\ (m',n')\in B^*, m'\le n'}} U_{mn,ii}B_{mn,m'n'}U_{m'n',i'j'}\\
&= \sum_{\substack{(m,n)\in B^*, m\le n,\\ (m',n')\in B^*, m'\le n'}} \mathbb{1}_{(m,n)=(i,i)}B_{mn,m'n'}\frac{1}{\sqrt{2}}(\mathbb{1}_{(m',n')=(i',j')} + \mathbb{1}_{(m',n')=(j',i')})\\
&= \frac{1}{\sqrt{2}}B_{ii,i'j'}\\
&= \sigma_{ii'}\sigma_{ij'} + \sigma_{ij'}\sigma_{ii'}.
\end{aligned}
$$

It is the same for $i = j$ and $i' > j'$, then for $i \neq j$ and $i' = j'$. We also can prove the equality similarly when $i = i'$ and $j = j'$.

Step 2.B: Let us prove that $(UBU^T)_{ij,i'j'} = 0$ for all $(i,j,i',j') \notin B^*$.

Assume that $(i,j,i',j') \notin B^*$. If $(i,j) \notin B^*$, or if $(i',j') \notin B^*$, we have

$$
\begin{aligned}
&(UBU^T)_{ij,i'j'}\\
&= \sum_{\substack{(m,n)\in B^*, m\le n,\\ (m',n')\in B^*, m'\le n'}} U_{ij,mn}B_{mn,m'n'}U_{i'j',m'n'}\\
&= \sum_{\substack{(m,n)\in B^*, m\le n,\\ (m',n')\in B^*, m'\le n'}} \frac{1}{\sqrt{2}}(\mathbb{1}_{(m,n)=(i,j)} + \mathbb{1}_{(m,n)=(j,i)})B_{mn,m'n'}\frac{1}{\sqrt{2}}(\mathbb{1}_{(m',n')=(i',j')} + \mathbb{1}_{(m',n')=(j',i')})\\
&= 0,
\end{aligned}
$$

because if $(i,j) \notin B^*$, the term $(\mathbb{1}_{(m,n)=(i,j)} + \mathbb{1}_{(m,n)=(j,i)})$ is equal to 0. Similarly, if $(i',j') \notin B^*$, the term $(\mathbb{1}_{(m',n')=(i',j')} + \mathbb{1}_{(m',n')=(j',i')})$ is equal to 0.

It remains the case where $i,j \in B_k^*$ and $i',j' \in B_{k'}^*$ with $k \neq k'$. Then, $(U^T BU)_{ij,i'j'} = \sigma_{ii'}\sigma_{jj'} + \sigma_{ij'}\sigma_{ji'} = 0$. $\square$

To conlude the proof, we remark that, if $(i,j,i',j') \in B^*$, then

$$\operatorname{cov}((S_{B^*})_{ij}, (S_{B^*})_{i'j'}) = \operatorname{cov}(X_i X_j, X_{i'} X_{j'}) = \sigma_{ii'}\sigma_{jj'} + \sigma_{ij'}\sigma_{ji'}.$$

Now, assume that $(i,j,i',j') \notin B^*$. If $(i,j) \notin B^*$ or if $(i',j') \notin B^*$, then $\operatorname{cov}((S_{B^*})_{ij}, (S_{B^*})_{i'j'}) = 0$ because one of the two terms is zero. Assume that $i,j \in B^*_k$ and $i',j' \in B^*_{k'}$ with $k \neq k'$. Then

$$\operatorname{cov}((S_{B^*})_{ij}, (S_{B^*})_{i'j'}) = \operatorname{cov}(X_i X_j, X_{i'} X_{j'}) = \sigma_{ii'}\sigma_{jj'} + \sigma_{ij'}\sigma_{ji'} = 0.$$

Thus, the covariance matrix of $\operatorname{vec}(S_{B^*})$ is equal to the Cramér-Rao bound. $\square$

Proof of Proposition 34

Proof. Using the central limit Theorem and Proposion 33, we have

$$\sqrt{n-1}(\operatorname{vec}(\widehat{\Sigma}_{B^*}) - \operatorname{vec}(\Sigma)) \xrightarrow[n\to+\infty]{\mathcal{L}} \mathcal{N}(0, CR).$$

Then, by Proposition 31, we have

$$\sqrt{n-1}(\operatorname{vec}(\widehat{\Sigma}_{\widehat{B}}) - \operatorname{vec}(\Sigma)) \xrightarrow[n\to+\infty]{\mathcal{L}} \mathcal{N}(0, CR),$$

and by Slutsky,

$$\sqrt{n}(\operatorname{vec}(S_{\widehat{B}}) - \operatorname{vec}(\Sigma)) \xrightarrow[n\to+\infty]{\mathcal{L}} \mathcal{N}(0, CR).$$

$\square$

Proof of Proposition 35

Lemma 37. *Under Conditions 1 to 4, for all $\gamma > 1/2$*

$$\|S_{B^*} - \Sigma\|_2 = o_p\left(\frac{\log(n)^\gamma}{\sqrt{n}}\right),$$

where $\|.\|_2$ is the operator norm, and it is equal to $\lambda_{max}(.)$ on the set of the symmetric positive semi-definite matrices.

Proof.

$$
\begin{aligned}
& \mathbb{P}\left(\|S_{B^*}-\Sigma\|_2 > \frac{\varepsilon\log(n)^\gamma}{\sqrt{n}}\right) \\
= \; & \mathbb{P}\left(\exists k\in[1:K],\ \|S_{B_k^*}-\Sigma_{B_k^*}\|_2 > \frac{\varepsilon\log(n)^\gamma}{\sqrt{n}}\right) \\
\leq \; & K\max_{k\in[1:K]}\mathbb{P}\left(\|S_{B_k^*}-\Sigma_{B_k^*}\|_2 > \frac{\varepsilon\log(n)^\gamma}{\sqrt{n}}\right) \\
\leq \; & K\max_{k\in[1:K]}\mathbb{P}\left(m\max_{i,j\in B_k^*}|s_{ij}-\sigma_{ij}| > \frac{\varepsilon\log(n)^\gamma}{\sqrt{n}}\right) \\
\leq \; & K\max_{k\in[1:K]}\mathbb{P}\left(\max_{i,j\in B_k^*}|s_{ij}-\widehat{\sigma}_{ij}|+|\widehat{\sigma}_{ij}-\sigma_{ij}| > \frac{\varepsilon\log(n)^\gamma}{m\sqrt{n}}\right) \\
\leq \; & Km^2\max_{k\in[1:K]}\max_{i,j\in B_k^*}\mathbb{P}\left(|s_{ij}-\widehat{\sigma}_{ij}|+|\widehat{\sigma}_{ij}-\sigma_{ij}| > \frac{\varepsilon\log(n)^\gamma}{m\sqrt{n}}\right).
\end{aligned}
$$

Now, on the one hand,

$$
\begin{aligned}
& Km^2\max_{k\in[1:K]}\max_{i,j\in B_k^*}\mathbb{P}\left(|\widehat{\sigma}_{ij}-\sigma_{ij}| > \frac{\varepsilon\log(n)^\gamma}{2m\sqrt{n}}\right) \\
\leq \; & 2Km^2\exp\left(-C_{\inf}n\frac{\varepsilon^2\log(n)^{2\gamma}}{4m^2n}\right)\longrightarrow 0,
\end{aligned}
$$

by Bernstein's inequality. On the other hand,

$$
\begin{aligned}
& Km^2\max_{k\in[1:K]}\max_{i,j\in B_k^*}\mathbb{P}\left(|s_{ij}-\widehat{\sigma}_{ij}| > \frac{\varepsilon\log(n)^\gamma}{2m\sqrt{n}}\right) \\
= \; & Km^2\max_{k\in[1:K]}\max_{i,j\in B_k^*}\mathbb{P}\left(|\widehat{\sigma}_{ij}| > n\frac{\varepsilon\log(n)^\gamma}{2m\sqrt{n}}\right)\longrightarrow 0,
\end{aligned}
$$

by Bernstein's inequality. □

Lemma 38. *Under Conditions 1 to 5, for all $\gamma > \frac{1}{2}$,*

$$
\max_{i\in[1:p]}|\widehat{\beta}_i-\beta_i| = o_p\left(\frac{\log(n)^\gamma}{\sqrt{n}}\right).
$$

Proof. We know that $\widehat{\beta}-\beta\sim\mathcal{N}\left(0,\sigma_n^2[(A^TA)^{-1}]_{-1,-1}\right)$. To simplify notation, let $Q := \frac{1}{n}A^TA$. Remark that $Q_{1,1}=1$, $Q_{-1,1}=\frac{1}{n}\sum_{k=1}^n X^{(k)}$ and $Q_{-1,-1}=\frac{1}{n}\sum_{k=1}^n X^{(k)}X^{(k)T}$. Now, we know that

$$
[Q^{-1}]_{-1,-1} \; = \; \left(Q_{-1,-1}-Q_{-1,1}Q_{1,1}^{-1}Q_{1,-1}\right)^{-1}
$$

$$
\begin{aligned}
&= \left(\frac{1}{n}\sum_{k=1}^{n} X^{(k)}X^{(k)T} - \left[\frac{1}{n}\sum_{k=1}^{n} X^{(k)}\right]\left[\frac{1}{n}\sum_{k=1}^{n} X^{(k)}\right]^T \right)^{-1} \\
&= S^{-1}.
\end{aligned}
$$

Thus, $\widehat{\beta} - \beta \sim \mathcal{N}\left(0, \frac{\sigma^2}{n} S^{-1}\right)$.

Now, by Lemma 20,

$$
\mathbb{P}\left(\lambda_{\max}(S^{-1}) \geq \frac{2}{(1-\sqrt{y})^2\lambda_{\inf}}\right) = o(1).
$$

Let $\varepsilon > 0$ and $\gamma > \frac{1}{2}$. We have,

$$
\begin{aligned}
& \mathbb{P}\left(\max_{i\in[1:p]} |\widehat{\beta}_i - \beta_i| > \frac{\varepsilon \log(n)^\gamma}{n^{\frac{1}{2}}}\right) \\
\leq\ & \mathbb{P}\left(\max_{i\in[1:p]} |\widehat{\beta}_i - \beta_i| > \frac{\varepsilon \log(n)^\gamma}{n^{\frac{1}{2}}},\ \lambda_{\max}(S^{-1}) < \frac{2}{(1-\sqrt{y})^2\lambda_{\inf}}\right) + o(1) \\
\leq\ & o(1) + p\max_{i\in[1:p]} \mathbb{P}\left(|\widehat{\beta}_i - \beta_i| > \frac{\varepsilon \log(n)^\gamma}{n^{\frac{1}{2}}},\ \lambda_{\max}(S^{-1}) < \frac{2}{(1-\sqrt{y})^2\lambda_{\inf}}\right) \\
\leq\ & o(1) + p\max_{i\in[1:p]} \mathbb{P}\left(\frac{n^{\frac{1}{2}}|\widehat{\beta}_i - \beta_i|}{\sigma_n\sqrt{(S^{-1})_{i,i}}} > \frac{\varepsilon \log(n)^\gamma}{\sigma_n\sqrt{(S^{-1})_{i,i}}},\ \lambda_{\max}(S^{-1}) < \frac{2}{(1-\sqrt{y})^2\lambda_{\inf}}\right) \\
\leq\ & o(1) + p\max_{i\in[1:p]} \mathbb{P}\left(\frac{n^{\frac{1}{2}}|\widehat{\beta}_i - \beta_i|}{\sigma_n\sqrt{(S^{-1})_{i,i}}} > \frac{(1-\sqrt{y})\sqrt{\lambda_{\inf}}\varepsilon \log(n)^\gamma}{\sigma_n\sqrt{2}}\right) \\
\leq\ & o(1) + p\exp\left(-C_{\inf}\log(n)^{2\gamma}\right) \underset{n\to+\infty}{\longrightarrow} 0.
\end{aligned}
$$

□

Lemma 39. *Under Conditions 1 to 5, for all $\gamma > 1/2$,*

$$
\left|\frac{p}{\widehat{\beta}^T S_{B^*}\widehat{\beta}} - \frac{p}{\beta^T\Sigma\beta}\right| = o_p\left(\frac{\log(n)^\gamma}{\sqrt{n}}\right).
$$

Proof. We have

$$
\begin{aligned}
& \frac{1}{p}\left|\widehat{\beta}^T S_{B^*}\widehat{\beta} - \beta^T\Sigma\beta\right| \\
\leq\ & \frac{1}{p}\left|\widehat{\beta}^T S_{B^*}\widehat{\beta} - \beta^T S_{B^*}\beta\right| + \frac{1}{p}\left|\beta^T(S_{B^*} - \Sigma)\beta\right| \\
\leq\ & \frac{\|\widehat{\beta}\|_2 + \|\beta\|_2}{\sqrt{p}}\|S_{B^*}\|_2 \frac{\|\widehat{\beta} - \beta\|_2}{\sqrt{p}} + \frac{\|\beta\|_2^2}{p}\|S_{B^*} - \Sigma\|_2
\end{aligned}
$$

$$= \quad o_p\left(\frac{\log(n)^\gamma}{\sqrt{n}}\right),$$

by Lemmas 38 and 37. Now, with probability which goes to one 1, by Lemmas 20 and 38, we have $\widehat{\beta}^T S_{B^*}\widehat{\beta}/p \geq \lambda_{\inf}(1-\sqrt{y})^2\beta_{\inf}^2/2$. Moreover, $\beta^T\Sigma\beta/p \geq \lambda_{\inf}\beta_{\inf}^2 \geq \lambda_{\inf}(1-\sqrt{y})^2\beta_{\inf}^2/2$. Thus, with probability which goes to one 1, we have

$$\left|\frac{p}{\beta^T S_{B^*}\beta} - \frac{p}{\beta^T\Sigma\beta}\right| \leq \frac{4}{\lambda_{\inf}^2(1-\sqrt{y})^4\beta_{\inf}^4}\left|\frac{\beta^T S_{B^*}\beta}{p} - \frac{\beta^T\Sigma\beta}{p}\right| = o_p\left(\frac{\log(n)^\gamma}{\sqrt{n}}\right).$$

□

We can now prove Proposition 35

Proof. Let $\tilde{\eta}_i$ be the estimator of η_i obtained replacing Σ by S_{B^*} and β by $\widehat{\beta}$ in Algorithm 3. For all $\varepsilon > 0$ and $\gamma > 1/2$, we have

$$\begin{aligned}
&\mathbb{P}\left(\sum_{i=1}^p |\widehat{\eta}_i - \eta_i| > \frac{\varepsilon\log(n)^\gamma}{\sqrt{n}}\right)\\
\leq\ &\mathbb{P}\left(\sum_{i=1}^p |\tilde{\eta}_i - \eta_i| > \frac{\varepsilon\log(n)^\gamma}{\sqrt{n}}\right) + \mathbb{P}(\widehat{B} \neq B^*)\\
\leq\ &\mathbb{P}\left(p\max_{i\in[1:p]} |\tilde{\eta}_i - \eta_i| > \frac{\varepsilon\log(n)^\gamma}{\sqrt{n}}\right) + \mathbb{P}(\widehat{B} \neq B^*).
\end{aligned}$$

The term $\mathbb{P}(\widehat{B} = B^*)$ goes to 0 from Proposition 20. It remains to prove that

$$\mathbb{P}\left(p\max_{i\in[1:p]} |\tilde{\eta}_i - \eta_i| > \frac{\varepsilon\log(n)^\gamma}{\sqrt{n}}\right) \longrightarrow 0. \tag{III.9}$$

For all $k \in [1:K]$ and all $u \subset B_k^*$, let us write

$$\begin{aligned}
V_u^k &:= \beta_{B_k^*-u}^T\left(\Sigma_{B_k^*-u,B_k^*-u} - \Sigma_{B_k^*-u,u}\Sigma_{u,u}^{-1}\Sigma_{u,B_k^*-u}\right)\beta_{B_k^*-u}\\
\tilde{V}_u^k &:= \widehat{\beta}_{B_k^*-u}^T\left(S_{B_k^*-u,B_k^*-u} - S_{B_k^*-u,u}S_{u,u}^{-1}S_{u,B_k^*-u}\right)\widehat{\beta}_{B_k^*-u}\\
V &:= \beta^T\Sigma\beta\\
\tilde{V} &:= \widehat{\beta}^T S_{B^*}\widehat{\beta}\\
\alpha_u &:= \frac{V_u^k}{V}\\
\tilde{\alpha}_u &:= \frac{\tilde{V}_u^k}{\tilde{V}}.
\end{aligned}$$

Let, for all $C \subset [1:p]$, $C \neq \emptyset$,

$$L\left((a_u)_{u\in C}; C\right) := \left(\frac{1}{|C|} \sum_{u \subset C-i} \binom{|C|-1}{|u|}^{-1} [a_{u+i} - a_u] \right)_{i\in C}.$$

We then have $(\eta_i)_{i\in B_k^*} = L\left((\alpha_u)_{u\in B_k^*}; B_k^*\right)$ et $(\tilde{\eta}_i)_{i\in B_k^*} = L\left((\tilde{\alpha}_u)_{u\in B_k^*}; B_k^*\right)$.

As $L(.;C)$ is linear, it is Lipschitz continuous from $(R^{2^{|C|}}, \|.\|_\infty)$ to $(R^{|C|}, \|.\|_\infty)$, with constant $l_{|C|}$ (we can show that $l_{|C|} = 2$). Let $l := \max_{j\in[1:m]} l_j < +\infty$ (we have in fact $l = 2$). We then have,

$$p \max_{i\in[1:p]} |\tilde{\eta}_i - \eta_i| \leq p\, l \max_{k\in[1:K]} \max_{u\subset B_k^*} |\tilde{\alpha}_u - \alpha_u|.$$

It suffices to show that

$$p \max_{k\in[1:K]} \max_{u\subset B_k^*} |\tilde{\alpha}_u - \alpha_u| = o_p\left(\frac{\log(n)^\gamma}{\sqrt{n}}\right).$$

Now,

$$\begin{aligned} p\,|\tilde{\alpha}_u - \alpha_u| &\leq \left| \frac{p\tilde{V}_u^k}{\tilde{V}} - \frac{pV_u^k}{\tilde{V}} \right| + \left| \frac{pV_u^k}{\tilde{V}} - \frac{pV_u^k}{V} \right| \\ &\leq \frac{p}{\tilde{V}} \left| \tilde{V}_u^k - V_u^k \right| + V_u^k \left| \frac{p}{\tilde{V}} - \frac{p}{V} \right|. \end{aligned}$$

The term $\max_{k\in[1:K]} \max_{u\subset B_k^*} V_u^k$ is bounded from Conditions 2 and 5 and $\left|\frac{p}{\tilde{V}} - \frac{p}{V}\right| = o_p(\log(n)^\gamma/\sqrt{n})$ thanks to Lemma 39. The term $\frac{p}{\tilde{V}}$ is bounded in probability using Lemma 39, Conditions 2 and 5. Thus, it suffices to show that $\max_{k\in[1:K]} \max_{u\subset B_k^*} \left|\tilde{V}_u^k - V_u^k\right| = o_p(\log(n)^\gamma/\sqrt{n})$. We will use that the operator norm of a sub-matrix is smaller than the operator norm of the whole matrix.

For all $k \in [1:K]$ and $u \subset B_k^*$, we have

$$\begin{aligned} &\left|\tilde{V}_u^k - V_u^k\right| \\ \leq\ & \Big|\widehat{\beta}_{B_k^*-u}^T \left(S_{B_k^*-u,B_k^*-u} - S_{B_k^*-u,u} S_{u,u}^{-1} S_{u,B_k^*-u}\right) \widehat{\beta}_{B_k^*-u} \\ & -\beta_{B_k^*-u}^T \left(S_{B_k^*-u,B_k^*-u} - S_{B_k^*-u,u} S_{u,u}^{-1} S_{u,B_k^*-u}\right) \beta_{B_k^*-u}\Big| \\ & +\Big|\beta_{B_k^*-u}^T \left(S_{B_k^*-u,B_k^*-u} - S_{B_k^*-u,u} S_{u,u}^{-1} S_{u,B_k^*-u}\right) \beta_{B_k^*-u} \\ & -\beta_{B_k^*-u}^T \left(\Sigma_{B_k^*-u,B_k^*-u} - \Sigma_{B_k^*-u,u} \Sigma_{u,u}^{-1} \Sigma_{u,B_k^*-u}\right) \beta_{B_k^*-u}\Big| \end{aligned}$$

$$\leq \|\widehat{\beta}_{B_k^*-u} - \beta^T_{B_k^*-u}\|_2 \|S_{B_k^*-u,B_k^*-u} - S_{B_k^*-u,u}S_{u,u}^{-1}S_{u,B_k^*-u}\|_2 \left(\|\widehat{\beta}_{B_k^*-u}\|_2 + \|\beta_{B_k^*-u}\|_2\right)$$
$$+m\beta_{\text{sup}}^2 \|S_{B_k^*-u} - \Sigma_{B_k^*-u}\|_2 + m\beta_{\text{sup}}^2 \|S_{B_k^*-u,u}S_{u,u}^{-1}S_{u,B_k^*-u} - \Sigma_{B_k^*-u,u}\Sigma_{u,u}^{-1}\Sigma_{u,B_k^*-u}\|_2.$$

Thus, we obtain a sum a three terms, and we have to prove that each term is $o_p(\log(n)^\gamma/\sqrt{n})$. The first term is $o_p(\log(n)^\gamma/\sqrt{n})$ thanks to Lemmas 20 and 38.

For the second term, $\|S_{B_k^*-u} - \Sigma_{B_k^*-u}\|_2 \leq \|S_{B_k^*} - \Sigma_{B_k^*}\|_2$ so is $o_p(\log(n)^\gamma/\sqrt{n})$ from Lemma 37.

Finally, for the third term,

$$\begin{aligned}
& \|S_{B_k^*-u,u}S_{u,u}^{-1}S_{u,B_k^*-u} - \Sigma_{B_k^*-u,u}\Sigma_{u,u}^{-1}\Sigma_{u,B_k^*-u}\|_2 \\
\leq\ & \|S_{B_k^*-u,u}S_{u,u}^{-1}\left(S_{u,B_k^*-u} - \Sigma_{u,B_k^*-u}\right)\|_2 \\
& + \|S_{B_k^*-u,u}\left(S_{u,u}^{-1} - \Sigma_{u,u}^{-1}\right)\Sigma_{u,B_k^*-u}\|_2 \\
& + \|\left(S_{B_k^*-u,u} - \Sigma_{B_k^*-u,u}\right)\Sigma_{u,u}^{-1}\Sigma_{u,B_k^*-u}\|_2 \\
\leq\ & \|S_{B_k^*}\|_2\|S_{B_k^*}^{-1}\|_2\|S_{B_k^*} - \Sigma_{B_k^*}\|_2 + \|S_{B_k^*}\|_2\|S_{B_k^*}^{-1} - \Sigma_{B_k^*}^{-1}\|_2\|\Sigma_{B_k^*}\|_2 + \|S_{B_k^*} - \Sigma_{B_k^*}\|_2\|\Sigma_{B_k^*}^{-1}\|_2\|\Sigma_{B_k^*}\|_2 \\
\leq\ & \|S\|_2\|S^{-1}\|_2\|S-\Sigma\|_2 + \|S\|_2\|S^{-1}-\Sigma^{-1}\|_2\|\Sigma\|_2 + \|S-\Sigma\|_2\|\Sigma^{-1}\|_2\|\Sigma\|_2,
\end{aligned}$$

which do not depend on k and u. Finally, remark that $\|\Sigma\|_2$ and $\|\Sigma^{-1}\|_2$ are bounded from Condition 2, that $\|S\|_2$ are $\|S^{-1}\|_2$ bounded in probability from Lemma 20, that $\|S-\Sigma\|_2 = o_p(\log(n)^\gamma/\sqrt{n})$ from Lemma 37 and Proposition 20 and that

$$\|S^{-1} - \Sigma^{-1}\|_2 \leq \|\Sigma^{-1}\|_2\|S^{-1}\|_2\|S-\Sigma\|_2 = o_p(\log(n)^\gamma/\sqrt{n}).$$

Thus, we proved that

$$p \max_{k\in[1:K]} \max_{u\subset B_k^*} |\tilde{\alpha}_u - \alpha_u| = o_p(\log(n)^\gamma/\sqrt{n}).$$

□

Proof of Proposition 36

Lemma 40. *Under Conditions 1, 2 and 3, for all penalization coefficient $\delta \in]0,1[$ and for all $\varepsilon > 0$,*

$$\max_{B(\alpha_1)\leq B\leq B^*} \|S_B - \Sigma\|_2 = o_p\left(\frac{1}{n^{(\delta-\varepsilon)/2}}\right),$$

where $\|.\|_2$ is the operator norm, and it is equal to $\lambda_{max}(.)$ on the set of the symmetric positive semi-definite matrices.

Proof. Let $\alpha_1 := \delta/2 - \varepsilon/4$.

$$
\begin{aligned}
& \mathbb{P}\left(\max_{B(\alpha_1)\leq B\leq B^*} \|S_B - \Sigma\|_2 > \frac{\epsilon}{n^{(\delta-\varepsilon)/2}}\right) \\
= \;& \mathbb{P}\left(\exists k \in [1:K], \max_{B(\alpha_1)\leq B\leq B^*} \|(S_B)_{B_k^*} - \Sigma_{B_k^*}\|_2 > \frac{\epsilon}{n^{(\delta-\varepsilon)/2}}\right) \\
\leq \;& K \max_{k\in[1:K]} \mathbb{P}\left(\max_{B(\alpha_1)\leq B\leq B^*} \|(S_B)_{B_k^*} - \Sigma_{B_k^*}\|_2 > \frac{\epsilon}{n^{(\delta-\varepsilon)/2}}\right) \\
\leq \;& K \max_{k\in[1:K]} \mathbb{P}\left(m \max_{B(\alpha_1)\leq B\leq B^*} \max_{i,j\in B_k^*} |(S_B)_{i,j} - \sigma_{ij}| > \frac{\epsilon}{n^{(\delta-\varepsilon)/2}}\right) \\
\leq \;& K \max_{k\in[1:K]} \mathbb{P}\left(m \max_{i,j\in B_k^*} |s_{ij} - \sigma_{ij}| + mn^{-\alpha_1} > \frac{\epsilon}{n^{(\delta-\varepsilon)/2}}\right) \\
\leq \;& K \max_{k\in[1:K]} \mathbb{P}\left(m \max_{i,j\in B_k^*} |s_{ij} - \sigma_{ij}| > C_{\inf}(\varepsilon,\delta,\epsilon) n^{-(\delta-\varepsilon)/2}\right),
\end{aligned}
$$

that goes to 0 following the proof of 37. □

Lemma 41. *Under Conditions 1, 2, 3 and 5, for all penalization coefficient* $\delta \in]0,1[$ *and for all* $\varepsilon > 0$,

$$
\left|\frac{p}{\widehat{\beta}^T S_{B^*}\widehat{\beta}} - \frac{p}{\beta^T\Sigma\beta}\right| = o_p\left(\frac{1}{n^{(\delta-\varepsilon)/2}}\right).
$$

Proof. The proof is similar to the proof of Lemma 39. □

We now can prove Proposition 36.

Proof. For all $B \in \mathcal{P}_p$, we define $\tilde{\eta}(B)_i$ as the estimator of η_i obtained replacing B^* by B, Σ by S_B and β by $\widehat{\beta}$ in Algorithm 3. We also define $\widehat{\eta}_i := \tilde{\eta}(B_{n^{-\delta/2}})_i$.

$$
\begin{aligned}
& \mathbb{P}\left(\sum_{i=1}^p |\widehat{\eta}_i - \eta_i| > \frac{\epsilon}{n^{-(\delta-\varepsilon)/2}}\right) \\
\leq \;& \mathbb{P}\left(\max_{B(\alpha_1)\leq B\leq B^*} \sum_{i=1}^p |\tilde{\eta}(B)_i - \eta_i| > \frac{\epsilon}{n^{-(\delta-\varepsilon)/2}}\right) + \mathbb{P}(\{B(\alpha_1) \leq B_{n^{-\delta/2}} \leq B^*\}^c) \\
\leq \;& \mathbb{P}\left(p \max_{B(\alpha_1)\leq B\leq B^*} \max_{i\in[1:p]} |\tilde{\eta}(B)_i - \eta_i| > \frac{\epsilon}{n^{-(\delta-\varepsilon)/2}}\right) + \mathbb{P}(\{B(\alpha_1) \leq B_{n^{-\delta/2}} \leq B^*\}^c).
\end{aligned}
$$

By Proposition 26, $\mathbb{P}(\{B(\alpha_1) \leq B_{n^{-\delta/2}} \leq B^*\}^c) \longrightarrow 0$.

Finally, we prove that

$$\mathbb{P}\left(p \max_{B(\alpha_1)\leq B\leq B^*} \max_{i\in[1:p]} |\tilde{\eta}(B)_i - \eta_i| > \frac{\epsilon}{n^{-(\delta-\varepsilon)/2}}\right) \longrightarrow 0,$$

following the proof of Proposition 35. $\square$

Proof of Proposition 37

Proof. Remark that Σ verifies Conditions 1 to 3. Let $a > 0$. Let $\check{\Sigma} := \Sigma$ if $\forall B < B^*$, $\|\Sigma_B - \Sigma\|_{\max} \geq an^{-1/4}$ and $\check{\Sigma} = I_p$ otherwise. Let $\check{\eta}$ and $\check{\hat{\eta}}$ be defined as η and $\widehat{\eta}$ in Proposition 35 but replacing Σ by $\check{\Sigma}$. As $\check{\Sigma}$ verify the Conditions 1 to 3 and the slightly modified Condition 4 given in Proposition 30, conditionally to $\check{\Sigma}$

$$\sum_{i=1}^{p} \left|\check{\hat{\eta}}_i - \check{\eta}_i\right| = o_p\left(\frac{\log(n)^\gamma}{\sqrt{n}}\right).$$

Thus, for all $\varepsilon > 0$,

$$\mathbb{P}\left(\sum_{i=1}^{p} \left|\check{\hat{\eta}}_i - \check{\eta}_i\right| > \frac{\varepsilon \log(n)^\gamma}{\sqrt{n}} \middle| \check{\Sigma}\right) \longrightarrow 0,$$

so, by dominated convergence theorem,

$$\sum_{i=1}^{p} \left|\check{\hat{\eta}}_i - \check{\eta}_i\right| = o_p\left(\frac{\log(n)^\gamma}{\sqrt{n}}\right),$$

unconditionally to $\check{\Sigma}$.

We conclude saying that $\check{\Sigma} = \Sigma$ with probability which converges to 1 from Proposition 30, so $\check{\hat{\eta}} = \widehat{\eta}$ and $\check{\eta} = \eta$ with probability which converges to 1. $\square$

Appendix IV

Proofs of Chapter 6

In the chapter, we will write $C_{\sup}$ for a generic non-negative finite constant. The actual value of $C_{\sup}$ is of no interest and can change in the same sequence of equations. Similarly, we will write $C_{\inf}$ for a generic strictly positive constant. Moreover, for all $u \subset [1:p]$, if Z is a random vector in $\mathbb{R}^p$ and g is a function from $\mathbb{R}^p$ to $\mathbb{R}$ such that $\mathrm{E}(g(Z)^2) < +\infty$ and $\mathrm{Var}(g(Z)) > 0$, let $S_u^{cl}(Z, g)$ be the closed Sobol index for the input vector Z and the model g, defined by:

$$S_u^{cl}(Z, g) = \frac{\mathrm{Var}(\mathrm{E}(g(Z)|Z_u))}{\mathrm{Var}(g(Z))}.$$

A Proofs of Section A

Proof of Proposition 38

We divide the proof into several lemmas. We assume that the assumptions of Proposition 38 hold throughout this proof.

Let $\varepsilon \in]0,1[$ be such that f is $\mathcal{C}^3$ on $\overline{B}(\mu, \varepsilon)$ and such that, for all $x \in \overline{B}(\mu, \varepsilon)$, we have $Df(x) \neq 0$. Since $\mu^{\{n\}}$ converges to μ, there exists $N \in \mathbb{N}$ such that, for all $n \geq N$, $\mu^{\{n\}} \in B(\mu, \varepsilon/2)$. In the following, we assume that n is larger than N.

Lemma 42. *For all $x \in B(\mu^{\{n\}}, \varepsilon/2)$, we have*

$$|R_1^{\{n\}}(x)| \leq C_1 \|x - \mu^{\{n\}}\|^2, \quad |R_2^{\{n\}}(x)| \leq C_1' \|x - \mu^{\{n\}}\|^3$$

and for all $x \notin B(\mu^{\{n\}}, \varepsilon/2)$,

$$|R_1^{\{n\}}(x)| \leq C_2 \|x - \mu^{\{n\}}\|^k, \quad |R_2^{\{n\}}(x)| \leq C_2' \|x - \mu^{\{n\}}\|^k,$$

where C_1, C_1', C_2 and C_2' are positive constants that do not depend on n.

Proof. Using Taylor's theorem, for all $x \in B(\mu^{\{n\}}, \frac{\varepsilon}{2})$, there exist $\theta_2(n,x), \theta_3(n,x) \in]0,1[$ such that

$$\begin{aligned} f(x) &= f_0^{\{n\}} + f_1^{\{n\}}(x) + \frac{1}{2}D^2 f(\mu^{\{n\}} + \theta_2(n,x)(x-\mu^{\{n\}}))(x-\mu^{\{n\}}) \\ &= f_0^{\{n\}} + f_1^{\{n\}}(x) + f_2^{\{n\}}(x) \\ &\quad + \frac{1}{6}D^3 f(\mu^{\{n\}} + \theta_3(n,x)(x-\mu^{\{n\}}))(x-\mu^{\{n\}}). \end{aligned}$$

Let $C_1 = \frac{1}{2}\max_{x\in\overline{B}(\mu,\varepsilon)} \|D^2 f(x)\|$ and $C_1' = \frac{1}{6}\max_{x\in\overline{B}(\mu,\varepsilon)} \|D^3 f(x)\|$, where $\|\cdot\|$ also means the operator norm of a multilinear form. Thus, for all $x \in B(\mu, \frac{\varepsilon}{2})$,

$$|R_1^{\{n\}}(x)| \leq C_1 \|x-\mu^{\{n\}}\|^2, \quad |R_2^{\{n\}}(x)| \leq C_1' \|x-\mu^{\{n\}}\|^3.$$

Moreover, f is subpolynomial, so $\exists k \geq 3$, and $C < +\infty$ such that, $\forall x \in \mathbb{R}^p$,

$$|f(x)| \leq C(1 + \|x\|^k).$$

Hence, taking $C' = C(2\|\mu\| + 2)^k$, we have

$$|f(x)| \leq C(1 + 2^k\|x-\mu^{\{n\}}\|^k + 2^k\|\mu^{\{n\}}\|^k) \leq C'(1 + \|x-\mu^{\{n\}}\|^k).$$

Hence, taking $C'' := C' + \max_{y\in\overline{B}(\mu,\varepsilon)} \|Df(y)\|$, we have

$$|R_1^{\{n\}}(x)| \leq |f(x)| + \max_{y\in\overline{B}(\mu,\varepsilon)} \|Df(y)\| \|x-\mu^{\{n\}}\| \leq C''(1 + \|x-\mu^{\{n\}}\|^k).$$

Now, taking $C_2 := C''\left(1 + (\frac{2}{\varepsilon})^k\right)$, we have, for all $x \notin B(\mu^{\{n\}}, \varepsilon/2)$,

$$|R_1^{\{n\}}(x)| \leq C'' + C''\|x-\mu^{\{n\}}\|^k \leq C_2\|x-\mu^{\{n\}}\|^k.$$

Similarly, there exists $C_2' < +\infty$ such that

$$|R_2^{\{n\}}(x)| \leq C_2'\|x-\mu^{\{n\}}\|^k.$$

□

Lemma 43. *We have*

$$\mathrm{cov}(\mathrm{E}(f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}), f_2^{\{n\}}(X^{\{n\}})|X_u^{\{n\}})) = 0.$$

Proof. Let $n \in \mathbb{N}$. To simplify notation, let $A = X^{\{n\}} - \mu^{\{n\}}$, $\beta \in \mathbb{R}^p$ be the vector of the linear application $Df(\mu^{\{n\}})$ and $\Gamma \in \mathcal{M}_p(\mathbb{R})$ be symmetric the matrix of the quadratic form $\frac{1}{2}D^2 f(\mu^{\{n\}})$. Then,

$$\mathrm{cov}(\mathrm{E}(f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}), \mathrm{E}(f_2^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}))$$

$$
\begin{aligned}
&= \operatorname{cov}(\mathrm{E}(\beta^T A)|A_u), \mathrm{E}(A^T \Gamma A|A_u)) \\
&= \mathrm{E}\left(\left[\beta_u^T A_u + \beta_{-u}^T \mathrm{E}(A_{-u}|A_u)\right]\left[A_u^T \Gamma_{u,u} A_u + 2A_u^T \Gamma_{u,-u} \mathrm{E}(A_{-u}|A_u) + \mathrm{E}(A_{-u}^T \Gamma_{-u,-u} A_{-u}|A_u)\right]\right) \\
&= \mathrm{E}\left(\left[\beta_u^T A_u + \beta_{-u}^T \mathrm{E}(A_{-u}|A_u)\right] \mathrm{E}(A_{-u}^T \Gamma_{-u,-u} A_{-u}|A_u)\right)
\end{aligned}
$$

since all the other terms are linear combinations of expectations of products of three zero-mean Gaussian variables. Indeed, the coefficients of $\mathrm{E}(A_{-u}|A_u)$ are linear combinations of the coefficients of A_u. Now,

$$
\begin{aligned}
\mathrm{E}\left(\beta_u^T A_u \times \mathrm{E}(A_{-u}^T \Gamma_{-u,-u} A_{-u}|A_u)\right) &= \mathrm{E}\left(\mathrm{E}(\beta_u^T A_u \times A_{-u}^T \Gamma_{-u,-u} A_{-u}|A_u)\right) \\
&= \mathrm{E}(\beta_u^T A_u \times A_{-u}^T \Gamma_{-u,-u} A_{-u}) \\
&= 0.
\end{aligned}
$$

Similarly, the term $\mathrm{E}\left(\beta_{-u}\mathrm{E}(A_{-u}|A_u)\mathrm{E}(A_{-u}^T \Gamma_{-u,-u} A_{-u}|A_u)\right)$ is equal to 0. □

Lemma 44. *There exists $C_{\sup} < +\infty$ such that, for all $u \subset [1:p]$,*

$$
\operatorname{Var}(\mathrm{E}(\sqrt{a^{\{n\}}} R_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}})) \leq \frac{C_{\sup}}{a^{\{n\}}},
$$

and

$$
\left|\operatorname{cov}(\mathrm{E}(\sqrt{a^{\{n\}}} f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}), \mathrm{E}(\sqrt{a^{\{n\}}} R_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}))\right| \leq \frac{C_{\sup}}{a^{\{n\}}}.
$$

Proof. Using Lemma 42, we have,

$$
\begin{aligned}
\mathrm{E}(|\sqrt{a^{\{n\}}} R_1^{\{n\}}(X^{\{n\}})|^2) &= \mathrm{E}(|\sqrt{a^{\{n\}}} R_1^{\{n\}}(X^{\{n\}})|^2 \mathbb{1}_{\|X_n\| < \frac{\varepsilon}{2}}) + \mathrm{E}(|\sqrt{a^{\{n\}}} R_1^{\{n\}}(X^{\{n\}})|^2 \mathbb{1}_{\|X_n\| \geq \frac{\varepsilon}{2}}) \\
&\leq \frac{C_1^2}{a^{\{n\}}} \mathrm{E}(\|\sqrt{a^{\{n\}}}(X^{\{n\}} - \mu^{\{n\}})\|^4) \\
&\quad + \frac{C_2^2}{a^{\{n\}(k-1)}} \mathrm{E}(\|\sqrt{a^{\{n\}}}(X^{\{n\}} - \mu^{\{n\}})\|^{2k}) \\
&\leq \frac{C_{\sup}}{a^{\{n\}}},
\end{aligned}
$$

since $a^{\{n\}}\Sigma^{\{n\}}$ is bounded. Hence,

$$
\operatorname{Var}(\sqrt{a^{\{n\}}} R_1^{\{n\}}(X^{\{n\}})) \leq \frac{C_{\sup}}{a^{\{n\}}}.
$$

Moreover, for all $u \subset [1:p]$,

$$
0 \leq \operatorname{Var}(\mathrm{E}(a^{\{n\}} R_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}})) \leq \operatorname{Var}(a^{\{n\}} R_1^{\{n\}}(X^{\{n\}})) \leq \frac{C_{\sup}}{a^{\{n\}}}.
$$

For all $u \subset [1:p]$,

$$\begin{aligned}
& \mathrm{cov}(\mathrm{E}(\sqrt{a^{\{n\}}} f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}), \mathrm{E}(\sqrt{a^{\{n\}}} R_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}})) \\
= & \mathrm{cov}(\mathrm{E}(\sqrt{a^{\{n\}}} f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}), \mathrm{E}(\sqrt{a^{\{n\}}} f_2^{\{n\}}(X^{\{n\}})|X_u^{\{n\}})) \\
& + \mathrm{cov}(\mathrm{E}(\sqrt{a^{\{n\}}} f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}), \mathrm{E}(\sqrt{a^{\{n\}}} R_2^{\{n\}}(X^{\{n\}})|X_u^{\{n\}})) \\
= & \mathrm{cov}(\mathrm{E}(\sqrt{a^{\{n\}}} f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}), \mathrm{E}(\sqrt{a^{\{n\}}} R_2^{\{n\}}(X^{\{n\}})|X_u^{\{n\}})),
\end{aligned}$$

using Lemma 43. Now, by Cauchy-Schwarz inequality,

$$\begin{aligned}
& \left|\mathrm{cov}(\mathrm{E}(\sqrt{a^{\{n\}}} f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}), \mathrm{E}(\sqrt{a^{\{n\}}} R_2^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}))\right| \\
\leq & \sqrt{\mathrm{Var}(\sqrt{a^{\{n\}}} f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}})} \sqrt{\mathrm{Var}(\sqrt{a^{\{n\}}} R_2^{\{n\}}(X^{\{n\}})|X_u^{\{n\}})} \\
\leq & \sqrt{\mathrm{Var}(\sqrt{a^{\{n\}}} f_1^{\{n\}}(X^{\{n\}}))} \sqrt{\mathrm{Var}(\sqrt{a^{\{n\}}} R_2^{\{n\}}(X^{\{n\}}))}.
\end{aligned}$$

Now, by Lemma 42, we have,

$$\begin{aligned}
& \mathrm{E}(|\sqrt{a^{\{n\}}} R_2^{\{n\}}(X^{\{n\}})|^2) \\
= & \mathrm{E}(|\sqrt{a^{\{n\}}} R_2^{\{n\}}(X^{\{n\}})|^2 \mathbb{1}_{\|X_n\| \leq \frac{\varepsilon}{2}}) + \mathrm{E}(|\sqrt{a^{\{n\}}} R_2^{\{n\}}(X^{\{n\}})|^2 \mathbb{1}_{\|X_n\| \geq \frac{\varepsilon}{2}}) \\
\leq & \frac{C_1^2}{a^{\{n\}2}} \mathrm{E}(\|\sqrt{a^{\{n\}}}(X^{\{n\}} - \mu^{\{n\}})\|^6) \\
& + \frac{C_2^2}{a^{\{n\}(k-1)}} \mathrm{E}(\|\sqrt{a^{\{n\}}}(X^{\{n\}} - \mu^{\{n\}})\|^{k \times 2}) \\
\leq & \frac{C_{\sup}}{a^{\{n\}2}}.
\end{aligned}$$

Furthermore,

$$\begin{aligned}
\mathrm{Var}(\sqrt{a^{\{n\}}} f_1^{\{n\}}(X^{\{n\}})) & \leq \max_{x \in \overline{B}(\mu^{\{n\}}, \varepsilon/2)} \|Df(x)\| \mathrm{E}\left(\|\sqrt{a^{\{n\}}}(X^{\{n\}} - \mu^{\{n\}})\|\right) \\
& \leq C_{\sup}.
\end{aligned}$$

Finally,

$$\left|\mathrm{cov}(\mathrm{E}(\sqrt{a^{\{n\}}} f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}), \mathrm{E}(\sqrt{a^{\{n\}}} R_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}))\right| \leq \frac{C_{\sup}}{a^{\{n\}}},$$

that concludes the proof of Lemma 44. □

Lemma 45. *For all $u \subset [1:p]$,*

$$S_u^{cl}(X^{\{n\}}, f) = S_u^{cl}(X^{\{n\}}, f_1^{\{n\}}) + O\left(\frac{1}{a^{\{n\}}}\right).$$

Proof. We have

$$f(X^{\{n\}}) = f(\mu^{\{n\}}) + f_1^{\{n\}}(X^{\{n\}}) + R_1^{\{n\}}(X^{\{n\}}).$$

For all $u \subset [1:p]$, we have

$$\mathrm{E}(f(X^{\{n\}})|X_u^{\{n\}}) = f(\mu^{\{n\}}) + \mathrm{E}(f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}) + \mathrm{E}(R_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}),$$

so,

$$\begin{aligned}
& a^{\{n\}}\mathrm{Var}(\mathrm{E}(f(X^{\{n\}})|X_u^{\{n\}})) \\
= \;& \mathrm{Var}(\mathrm{E}(\sqrt{a^{\{n\}}}f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}})) + \mathrm{Var}(\mathrm{E}(\sqrt{a^{\{n\}}}R_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}})) \\
& +2\mathrm{cov}(\mathrm{E}(\sqrt{a^{\{n\}}}f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}), \mathrm{E}(\sqrt{a^{\{n\}}}R_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}})) \\
= \;& \mathrm{Var}(\mathrm{E}(\sqrt{a^{\{n\}}}f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}})) + O(\frac{1}{a^{\{n\}}}),
\end{aligned}$$

by Lemma 44. Hence, for $u = [1:p]$, we have

$$a^{\{n\}}\mathrm{Var}(f(X^{\{n\}})) = \mathrm{Var}(\sqrt{a^{\{n\}}}f_1^{\{n\}}(X^{\{n\}})) + O(\frac{1}{a^{\{n\}}}).$$

Thus, for all $u \subset [1:p]$,

$$\begin{aligned}
S_u^{cl}(X^{\{n\}}, f) &= \frac{\mathrm{Var}(\mathrm{E}(f(X^{\{n\}})|X_u^{\{n\}}))}{\mathrm{Var}(f(X^{\{n\}}))} \\
&= \frac{a^{\{n\}}\mathrm{Var}(\mathrm{E}(f(X^{\{n\}})|X_u^{\{n\}}))}{a^{\{n\}}\mathrm{Var}(f(X^{\{n\}}))} \\
&= \frac{\mathrm{Var}(\mathrm{E}(\sqrt{a^{\{n\}}}f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}})) + O(\frac{1}{a^{\{n\}}})}{\mathrm{Var}(\sqrt{a^{\{n\}}}f_1^{\{n\}}(X^{\{n\}})) + O(\frac{1}{a^{\{n\}}})} \\
&= \frac{\mathrm{Var}(\sqrt{a^{\{n\}}}f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}})}{\mathrm{Var}(\sqrt{a^{\{n\}}}f_1^{\{n\}}(X^{\{n\}}))} + O(\frac{1}{a^{\{n\}}}) \\
&= S_u^{cl}(X^{\{n\}}, f_1^{\{n\}}) + O\left(\frac{1}{a^{\{n\}}}\right),
\end{aligned}$$

where we used that,

$$\begin{aligned}
\mathrm{Var}(\sqrt{a^{\{n\}}}f_1^{\{n\}}(X^{\{n\}})) &= Df(\mu^{\{n\}})(a^{\{n\}}\Sigma^{\{n\}})Df(\mu^{\{n\}})^T \\
&\geq \lambda_{\min}(a^{\{n\}}\Sigma^{\{n\}}) \inf_{x\in\overline{B}(\mu,\varepsilon/2)} \|Df(x)\|^2 \\
&\geq C_{inf}.
\end{aligned}$$

$\square$

Now we have proved the convergence of the closed Sobol indices, we can prove Proposition 38 easily.

Proof. By Lemma 45 and applying the linearity of the Shapley effects with respect to the Sobol indices, we have

$$\eta(X^{\{n\}}, f) = \eta(X^{\{n\}}, f_1^{\{n\}}) + O(\frac{1}{a^{\{n\}}}).$$

□

Proof of Remark 34

Proof. Let $X^{\{n\}} = (X_1^{\{n\}}, X_2^{\{n\}}) \sim \mathcal{N}(0, \frac{1}{a^{\{n\}}} I_2)$ and $Y^{\{n\}} = f(X^{\{n\}}) = X_1^{\{n\}} + X_2^{\{n\}2}$, we have $f_1^{\{n\}}(X^{\{n\}}) = X_1^{\{n\}}$ and $R_1^{\{n\}}(X^{\{n\}}) = X_2^{\{n\}2}$. Thus, $\eta_1(X^{\{n\}}, f_1^{\{n\}}) = 1$ and $\eta_2(X^{\{n\}}, f_1^{\{n\}}) = 0$. Now, let us compute the Shapley effects $\eta(X^{\{n\}}, f)$. We have

$$\begin{aligned}
\mathrm{Var}(f(X^{\{n\}})) &= \mathrm{Var}(X_1^{\{n\}}) + \mathrm{Var}(X_2^{\{n\}2}) \\
&= \mathrm{Var}(X_1^{\{n\}}) + \mathrm{E}(X_2^{\{n\}4}) - \mathrm{E}(X_2^{\{n\}2})^2 \\
&= \frac{1}{a^{\{n\}}} + \frac{3}{a^{\{n\}2}} - \frac{1}{a^{\{n\}2}} \\
&= \frac{a^{\{n\}} + 2}{a^{\{n\}2}}.
\end{aligned}$$

Moreover,

$$\mathrm{Var}(\mathrm{E}(f(X^{\{n\}})|X_1^{\{n\}})) = \mathrm{Var}(X_1^{\{n\}} + \frac{1}{a^{\{n\}}}) = \mathrm{Var}(X_1^{\{n\}}) = \frac{1}{a^{\{n\}}}$$

and

$$\mathrm{Var}(\mathrm{E}(f(X^{\{n\}})|X_2^{\{n\}})) = \mathrm{Var}(X_2^{\{n\}2}) = \mathrm{E}(X_2^{\{n\}4}) - \mathrm{E}(X_2^{\{n\}2})^2 = \frac{3-1}{a^{\{n\}2}} = \frac{2}{a^{\{n\}2}}.$$

Hence,

$$\eta_1(X^{\{n\}}, f) = \frac{a^{\{n\}2}}{(a^{\{n\}} + 2)2} \left(\frac{1}{a^{\{n\}}} + \frac{a^{\{n\}} + 2}{a^{\{n\}2}} - \frac{2}{a^{\{n\}2}} \right) = \frac{a^{\{n\}}}{a^{\{n\}} + 2},$$

and

$$\eta_2(X^{\{n\}}, f) = \frac{2}{a^{\{n\}} + 2}.$$

□

Proof of Proposition 39

As in the proof of Proposition 38, we first prove the convergence for the closed Sobol indices. To simplify notation, let $\Gamma^{\{n\}} := a^{\{n\}}\Sigma^{\{n\}}$.

Lemma 46. *Under the assumptions of Proposition 39, for all $u \subset [1:p]$, we have*

$$S_u^{cl}(f_1^{\{n\}}(X^{\{n\}})) = S_u^{cl}(f_1(X^*)) + O(\|\mu^{\{n\}} - \mu\|) + O(\|\Gamma^{\{n\}} - \Sigma\|).$$

Proof. We have

$$\begin{aligned}
& \mathrm{Var}(\sqrt{a^{\{n\}}} f_1^{\{n\}}(X^{\{n\}})) - \mathrm{Var}(f_1(X^*)) \\
= \; & Df(\mu^{\{n\}})\Gamma^{\{n\}} Df(\mu^{\{n\}})^T - Df(\mu)\Sigma Df(\mu)^T \\
= \; & Df(\mu^{\{n\}})\Gamma^{\{n\}} \left[Df(\mu^{\{n\}})^T - Df(\mu)^T\right] + Df(\mu^{\{n\}}) \left[\Gamma^{\{n\}} - \Sigma\right] Df(\mu)^T \\
& \left[Df(\mu^{\{n\}}) - Df(\mu)\right] \Sigma Df(\mu)^T \\
= \; & O(\|Df(\mu^{\{n\}}) - Df(\mu)\|) + O(\|\Gamma^{\{n\}} - \Sigma\|) \\
= \; & O(\|\mu^{\{n\}} - \mu\|) + O(\|\Gamma^{\{n\}} - \Sigma\|),
\end{aligned}$$

using that Df is Lipschitz continuous on a neighbourhood of μ (thanks to the continuity of $D^2 f$).

Moreover, for all $\emptyset \subsetneq u \subsetneq [1:p]$, we have

$$\begin{aligned}
& \mathrm{Var}(\mathrm{E}(\sqrt{a^{\{n\}}} f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}})) - \mathrm{Var}(\mathrm{E}(f_1(X^*)|X_u^*)) \\
= \; & \mathrm{Var}(\sqrt{a^{\{n\}}} f_1^{\{n\}}(X^{\{n\}})) - \mathrm{E}(\mathrm{Var}(\sqrt{a^{\{n\}}} f_1(X^{\{n\}})|X_{-u}^{\{n\}})) - \mathrm{Var}(f_1(X^*)) + \mathrm{E}(\mathrm{Var}(f_1(X^*)|X_u^*)) \\
= \; & Df(\mu^{\{n\}})\Gamma^{\{n\}} Df(\mu^{\{n\}})^T - Df(\mu^{\{n\}})_u(\Gamma_{u,u}^{\{n\}} - \Gamma_{u,-u}^{\{n\}}\Gamma_{-u,-u}^{\{n\}-1}\Gamma_{-u,u}^{\{n\}}) Df(\mu^{\{n\}})_u^T \\
& - Df(\mu)\Sigma Df(\mu)^T - Df(\mu)_u(\Sigma_{u,u} - \Sigma_{u,-u}\Sigma_{-u,-u}^{-1}\Sigma_{-u,u}) Df(\mu)_u^T \\
= \; & O(\|\mu^{\{n\}} - \mu\|) + O(\|\Gamma^{\{n\}} - \Sigma\|),
\end{aligned}$$

proceeding as previously and using the fact that the operator norm of a submatrix is smaller than the operator norm of the whole matrix.

Hence,

$$S_u^{cl}(X^{\{n\}}, f_1^{\{n\}}) = S_u^{cl}(X^*, f_1) + O(\|\mu^{\{n\}} - \mu\|) + O(\|\Gamma^{\{n\}} - \Sigma\|).$$

□

Now, we can easily prove Proposition 39.

Proof. By Lemma 46 and applying the linearity of the Shapley effects with respect to the Sobol indices, we have

$$\eta(f_1^{\{n\}}(X^{\{n\}})) = \eta(f_1(X^*)) + O(\|\mu^{\{n\}} - \mu\|) + O(\|\Gamma^{\{n\}} - \Sigma\|).$$

□

Proof of Proposition 40

Under the assumption of Proposition 40, let $\varepsilon > 0$ be such that f is $\mathcal{C}^3$ on $\overline{B}(\mu,\varepsilon)$ and such that, for all $x \in \overline{B}(\mu,\varepsilon)$, we have $Df(x) \neq 0$. Since $\mu^{\{n\}}$ converges to μ, there exists $N \in \mathbb{N}$ such that, for all $n \geq N$, $\mu^{\{n\}} \in B(\mu,\varepsilon/2)$. In the following, we assume that n is larger than N.

Lemma 47. *For all $x \in \overline{B}(\mu,\frac{\varepsilon}{2})$ and $h \in (\mathbb{R}_+^*)^p$ such that $\|h\| \leq \frac{\varepsilon}{2}$, we have*

$$\|\widehat{D}_h f(x) - Df(x)\| \leq \frac{1}{6} \max_{i\in[1:p]} \max_{y \in \overline{B}(\mu,\varepsilon)} |\partial_i^3 f(y)| \|h\|^2$$

Proof. Let $x \in \overline{B}(\mu,\frac{\varepsilon}{2})$ and $h \in (\mathbb{R}_+^*)^p$ such that $\|h\| \leq \frac{\varepsilon}{2}$. For all $i \in [1:p]$, using Taylor's theorem, there exist $\theta^+_{x,h,i}, \theta^-_{x,h,i} \in]0,1[$ such that

$$\frac{f(x+e_ih_i) - f(x-e_ih_i)}{2h_i} = \partial_i f(x) + \frac{h_i^2}{12}\left(\partial_i^3 f(x+\theta^+_{x,h,i}h) + \partial_i^3 f(x-\theta^-_{x,h,i}h)\right).$$

Hence,

$$\begin{aligned}
\|\widehat{D}_h f(x) - Df(x)\| &\leq \sum_{i=1}^p \left|\left[\widehat{D}_h f(x) - Df(x)\right]_i\right| \\
&\leq \frac{1}{6} \max_{i\in[1:p]} \max_{y \in \overline{B}(\mu,\varepsilon)} |\partial_i^3 f(y)| \sum_{i=1}^p h_i^2 \\
&= \frac{1}{6} \max_{i\in[1:p]} \max_{y \in \overline{B}(\mu,\varepsilon)} |\partial_i^3 f(y)| \|h\|^2.
\end{aligned}$$

□

Lemma 48. *For all linear functions l_1 and l_2 from $\mathbb{R}^p$ to $\mathbb{R}$, we have*

$$\left|\mathrm{Var}(\mathrm{E}(l_1(X^{\{n\}})|X_u^{\{n\}}) - \mathrm{Var}(\mathrm{E}(l_2(X^{\{n\}})|X_u^{\{n\}})\right| \leq \frac{C_{\sup}}{a^{\{n\}}}\|l_1 - l_2\|.$$

Proof. For all $u \subset [1:p]$, let $\phi_u^{\{n\}} : \mathbb{R}^{|u|} \longrightarrow \mathbb{R}^p$ be defined by

$$\phi_u^{\{n\}}(x_u) = \begin{pmatrix} x_u \\ \mu_{-u}^{\{n\}} + \Gamma_{-u,u}^{\{n\}} \Gamma_{u,u}^{\{n\}-1}(x_u - \mu_u^{\{n\}}) \end{pmatrix}$$

and $\phi_{[1:p]}^{\{n\}} = id_{\mathbb{R}^p}$.

Let $u \subset [1:p]$. Then

$$\mathrm{E}(X^{\{n\}}|X_u^{\{n\}}) = \phi_u^{\{n\}}(X_u^{\{n\}}).$$

Now, for all linear function $l : \mathbb{R}^p \longrightarrow \mathbb{R}$, we have

$$\mathrm{E}(l(X^{\{n\}})|X_u^{\{n\}}) = l\left(\mathrm{E}(X^{\{n\}}|X_u^{\{n\}})\right) = l(\phi_u^{\{n\}}(X_u^{\{n\}})),$$

so, identifying a linear function from $\mathbb{R}^p$ to $\mathbb{R}$ with its matrix of size $1 \times p$, we have

$$\mathrm{Var}\left(\mathrm{E}(l(X^{\{n\}})|X_u^{\{n\}})\right) = l\phi_u^{\{n\}} \frac{\Gamma_{u,u}^{\{n\}}}{a^{\{n\}}} \phi_u^{\{n\}T} l^T.$$

Hence, for $l = l_1$ and $l = l_2$, one can show that,

$$\left|\mathrm{Var}(\mathrm{E}(l_1(X^{\{n\}})|X_u^{\{n\}})) - \mathrm{Var}(\mathrm{E}(l_2(X^{\{n\}})|X_u^{\{n\}}))\right| \leq \frac{C_{\sup}}{a^{\{n\}}}\|l_1 - l_2\|.$$

□

Now, we can prove Proposition 40.

Proof. By Lemmas 47 and 48, we have, for all $u \subset [1:p]$,

$$\mathrm{Var}(\mathrm{E}(\sqrt{a^{\{n\}}} f_1^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}) - \mathrm{Var}(\mathrm{E}(\sqrt{a^{\{n\}}} \tilde{f}_{1,h^{\{n\}}}^{\{n\}}(X^{\{n\}})|X_u^{\{n\}}) = O\left(\|h^{\{n\}}\|^2\right).$$

Thus,

$$S_u^{cl}(X^{\{n\}}, f_1^{\{n\}}) - S_u^{cl}(X^{\{n\}}, \tilde{f}_{1,h^{\{n\}}}^{\{n\}}) = O\left(\|h^{\{n\}}\|^2\right),$$

so

$$\eta(X^{\{n\}}, f_1^{\{n\}}) - \eta(X^{\{n\}}, \tilde{f}_{1,h^{\{n\}}}^{\{n\}}) = O\left(\|h^{\{n\}}\|^2\right).$$

□

Proof of Proposition 41

Under the assumption of Proposition 40, let $\varepsilon > 0$ be such that f is $\mathcal{C}^3$ on $\overline{B}(\mu, \varepsilon)$ and such that, for all $x \in \overline{B}(\mu, \varepsilon)$, we have $Df(x) \neq 0$. Since $\mu^{\{n\}}$ converges to μ, there exists $N \in \mathbb{N}$ such that, for all $n \geq N$, $\mu^{\{n\}} \in B(\mu, \varepsilon/2)$. In the following, we assume that n is larger than N.

Lemma 49. *There exists $C_{\sup}$ such that, with probability at least $1 - 2p^2 \exp(-C_{\inf} N) - 4p \exp(-C_{\inf} N^2)$,*

$$\left\|\left(A^{\{n\}T}A^{\{n\}}\right)^{-1} A^{\{n\}T}\right\| \leq C_{\sup} \frac{\sqrt{a^{\{n\}}}}{\sqrt{N}}.$$

Proof.

$$\begin{aligned}
\left\|\left(A^{\{n\}T}A^{\{n\}}\right)^{-1} A^{\{n\}T}\right\|^2 &= \lambda_{\max}\left[\left(A^{\{n\}T}A^{\{n\}}\right)^{-1}\right] \\
&= \frac{a^{\{n\}}}{N} \lambda_{\max}\left[\left(\frac{a^{\{n\}}}{N} A^{\{n\}T}A^{\{n\}}\right)^{-1}\right].
\end{aligned}$$

Now, by the strong law of large numbers, we have almost surely

$$\frac{a^{\{n\}}}{N}A^{\{n\}T}A^{\{n\}}-(a^{\{n\}}-1)\begin{pmatrix}1\\ \mu^{\{n\}}\end{pmatrix}\begin{pmatrix}1\\ \mu^{\{n\}}\end{pmatrix}^T \underset{N\to+\infty}{\longrightarrow} M_1^{\{n\}} := \begin{pmatrix}1 & \mu^{\{n\}T}\\ \mu^{\{n\}} & \Gamma^{\{n\}}+\mu^{\{n\}}\mu^{\{n\}T}\end{pmatrix}.$$

Let $M_2^{\{n\}} := \begin{pmatrix}1 & \mu^{\{n\}T}\\ \mu^{\{n\}} & \lambda_{\inf}I_p+\mu^{\{n\}}\mu^{\{n\}T}\end{pmatrix}$ and $M_2 := \begin{pmatrix}1 & \mu^T\\ \mu & \lambda_{\inf}I_p+\mu\mu^T\end{pmatrix}$, where $\lambda_{\inf}>0$ is a lower-bound of the eigenvalues of $(\Gamma^{\{n\}})_n$. We can see that

$$M_1^{\{n\}} \geq M_2^{\{n\}} \underset{n\to+\infty}{\longrightarrow} M_2.$$

Now,

$$\det(M_2)=\det(1)\det\left([\lambda_{\inf}I_p+\mu\mu^T]-\mu 1^{-1}\mu^T\right)=\lambda_{\inf}^p>0.$$

Hence, writing $\lambda'_{\inf}>0$ the smallest eigenvalue of M_2, we have that the eigenvalues of $M_1^{\{n\}}$ are lower-bounded by $\lambda'_{\inf}/2$ for n large enough.

Similarly, let $M_3^{\{n\}} := \begin{pmatrix}1 & \mu^{\{n\}T}\\ \mu^{\{n\}} & \lambda_{\sup}I_p+\mu^{\{n\}}\mu^{\{n\}T}\end{pmatrix}$ and $M_3 := \begin{pmatrix}1 & \mu^T\\ \mu & \lambda_{\sup}I_p+\mu\mu^T\end{pmatrix}$, where $\lambda_{\sup}>0$ is an upper-bound of the eigenvalues of $(\Gamma^{\{n\}})_n$. Writing $\lambda'_{\sup}<+\infty$ the largest eigenvalue of M_3, we have that the eigenvalues of $M_1^{\{n\}}$ are upper-bounded by $2\lambda'_{\sup}$ for n large enough.

Now, since the eigenvalues of $(M_1^{\{n\}})_n$ are lower-bounded and upper-bounded, there exists $\alpha>0$ such that, for all $n\in\mathbb{N}$ (large enough), $\forall M\in S_p(\mathbb{R})$,

$$\|M-M_1^{\{n\}}\|\leq\alpha \Longrightarrow |\lambda_{\min}(M)-\lambda_{\min}(M_1^{\{n\}})|\leq\frac{\lambda'_{\inf}}{4}.$$

Now, by Bernstein inequality,

$$\begin{aligned}&\mathbb{P}\left(\left\|\frac{a^{\{n\}}}{N}A^{\{n\}T}A^{\{n\}}-(a^{\{n\}}-1)\begin{pmatrix}1\\ \mu^{\{n\}}\end{pmatrix}\begin{pmatrix}1\\ \mu^{\{n\}}\end{pmatrix}^T-M_1^{\{n\}}\right\|\leq\alpha\right)\\ \geq\ & 1-2p^2\exp(-C_{\inf}N)-2\times 2p\exp(-C_{\inf}N^2)\\ \geq\ & 1-C_{\sup}\exp(-C_{\inf}N),\end{aligned}$$

where the term $2p^2\exp(-C_{\inf}N)$ bounds the difference of the submatrices of index $[2:p+1]\times[2:p+1]$ and the term $2\times 2p\exp(-C_{\inf}N^2)$ bounds the differences of the submatrices of index $\{1\}\times[2:p+1]$ and $[2:p+1]\times\{1\}$.

Hence, with probability at least $1-C_{\sup}\exp(-C_{\inf}N)$, we have

$$\lambda_{\min}\left(\frac{a^{\{n\}}}{N}A^{\{n\}T}A^{\{n\}}-(a^{\{n\}}-1)\begin{pmatrix}1\\ \mu^{\{n\}}\end{pmatrix}\begin{pmatrix}1\\ \mu^{\{n\}}\end{pmatrix}^T\right)\geq\frac{\lambda'_{\inf}}{4},$$

and so

$$\lambda_{\min}\left(\frac{a^{\{n\}}}{N}A^{\{n\}T}A^{\{n\}}\right) \geq \frac{\lambda'_{\inf}}{4}.$$

□

Lemma 50. *With probability at least* $1 - C_{\sup}\exp(-C_{\inf}N)$*, we have*

$$\left\|\widehat{\beta}^{\{n\}} - \nabla f(\mu^{\{n\}})\right\| \leq C_{\sup}\frac{1}{\sqrt{a^{\{n\}}}}.$$

Proof. Let $Z^{\{n\}} \sim \mathcal{N}(0, \Gamma^{\{n\}})$. Then $\|X^{\{n\}} - \mu^{\{n\}}\| \leq \frac{\varepsilon}{2}$ with probability $\mathbb{P}(\|Z^{\{n\}}\| \leq \frac{a^{\{n\}}\varepsilon}{2}) \underset{n\to+\infty}{\longrightarrow} 1$. Let $\Omega_N^{\{n\}} := \{\omega \in \Omega \mid \forall j \in [1:N], \|X^{\{n\}(j)}(\omega) - \mu^{\{n\}}\| \leq \frac{\varepsilon}{2}\}$. Hence,

$$\mathbb{P}(\Omega_N^{\{n\}}) \geq 1 - 2N\exp\left(-C_{\inf}a^{\{n\}}\right) \underset{n\to+\infty}{\longrightarrow} 1.$$

On $\overline{B}(\mu^{\{n\}}, \frac{\varepsilon}{2})$, we have $f = f(\mu^{\{n\}}) + f_1^{\{n\}} + R_1^{\{n\}}$. Hence, on $\Omega_N^{\{n\}}$, for all $j \in [1:N]$,

$$f(X^{\{n\}(j)}) = f(\mu^{\{n\}}) + f_1^{\{n\}}(X^{\{n\}(j)}) + R_1^{\{n\}}(X^{\{n\}(j)}).$$

Thus,

$$\widehat{\beta}^{\{n\}} = \left(A^{\{n\}T}A^{\{n\}}\right)^{-1}A^{\{n\}T}\left(f(\mu^{\{n\}}) + f_1^{\{n\}}(X^{\{n\}(j)}) + R_1^{\{n\}}(X^{\{n\}(j)})\right)_{j\in[1:N]}.$$

Since $f(\mu^{\{n\}}) + f_1^{\{n\}}$ is a linear function with gradient vector $\nabla f(\mu^{\{n\}})$ and with value at zero $f(\mu^{\{n\}}) - Df(\mu^{\{n\}})\mu^{\{n\}}$, we have,

$$\left(A^{\{n\}T}A^{\{n\}}\right)^{-1}A^{\{n\}T}(f(\mu^{\{n\}}) + f_1^{\{n\}}(X^{\{n\}(j)}))_{j\in[1:N]} = \begin{pmatrix} f(\mu^{\{n\}}) - Df(\mu^{\{n\}})\mu^{\{n\}} \\ \nabla f(\mu^{\{n\}}) \end{pmatrix}.$$

Hence, it remains to see if

$$\left(A^{\{n\}T}A^{\{n\}}\right)^{-1}A^{\{n\}T}(R_1^{\{n\}}(X^{\{n\}(j)}))_{j\in[1:N]}$$

is small enough. By Lemma 42, we have on $\Omega_N^{\{n\}}$,

$$\begin{aligned}\|(R_1^{\{n\}}(X^{\{n\}(j)}))_{j\in[1:N]}\|^2 &= \sum_{j=1}^{N} R_1^{\{n\}}(X^{\{n\}(j)})^2 \\ &\leq C_{\sup}\sum_{j=1}^{N}\|X^{\{n\}(j)} - \mu^{\{n\}}\|^4\end{aligned}$$

$$\leq \frac{C_{\sup}}{a^{\{n\}2}} \sum_{j=1}^{N} \|\sqrt{a^{\{n\}}}(X^{\{n\}(j)} - \mu^{\{n\}})\|^4.$$

Hence, on $\Omega_N^{\{n\}}$,

$$\|(R_1^{\{n\}}(X^{\{n\}(j)}))_{j\in[1:N]}\| \leq C_{\sup}\frac{\sqrt{N}}{a^{\{n\}}}.$$

Thus,

$$\begin{aligned} & \left\|\left(A^{\{n\}T}A^{\{n\}}\right)^{-1} A^{\{n\}T}(R_1^{\{n\}}(X^{\{n\}(j)}))_{j\in[1:N]}\right\| \\ \leq & \left\|\left(A^{\{n\}T}A^{\{n\}}\right)^{-1} A^{\{n\}T}\right\| \left\|(R_1^{\{n\}}(X^{\{n\}(j)}))_{j\in[1:N]}\right\| \\ \leq & C_{\sup}\frac{1}{\sqrt{a^{\{n\}}}}, \end{aligned}$$

with probability at least $1 - C_{\sup}\exp(-C_{\inf}N)$. □

Now, it is easy to prove Proposition 41.

Proof. By Lemma 48 for $l_1 = \widehat{\beta}^{\{n\}T}$ and $l_2 = Df(\mu^{\{n\}})$, and by Lemma 50 we have, with probability at least $1 - C_{\sup}\exp(-C_{\inf}N)$,

$$\begin{aligned} & \left|\mathrm{Var}(\mathrm{E}(\sqrt{a^{\{n\}}}Df(\mu^{\{n\}})X^{\{n\}}|X_u^{\{n\}})) - \mathrm{Var}(\mathrm{E}(\sqrt{a^{\{n\}}}\widehat{\beta}^{\{n\}T}X^{\{n\}}|X_u^{\{n\}}))\right| \\ \leq & C_{\sup}\|Df(\mu^{\{n\}}) - \widehat{\beta}^{\{n\}T}\| \\ \leq & C_{\sup}\frac{1}{\sqrt{a^{\{n\}}}}, \end{aligned}$$

where the conditional expectations and the variances are conditional to $(X^{\{n\}(j)})_{j\in[1:N]}$. Thus, with probability at least $1 - C_{\sup}\exp(-C_{\inf}N)$, there exists $C_{\inf} > 0$ such that, for n large enough $\|\widehat{\beta}^{\{n\}T}\| \geq C_{\inf}$, thus $\mathrm{Var}(\sqrt{a^{\{n\}}}\widehat{\beta}^{\{n\}^T}X^{\{n\}})$ is lower-bounded. Hence, with probability at least $1 - C_{\sup}\exp(-C_{\inf}N)$,

$$\left|S_u^{cl}(X^{\{n\}}, f_1^{\{n\}}) - S_u^{cl}(X^{\{n\}}, \widehat{\beta}^{\{n\}T})\right| \leq C_{\sup}\frac{1}{\sqrt{a^{\{n\}}}},$$

and so

$$\left\|\eta(X^{\{n\}}, f_1^{\{n\}}) - \eta(X^{\{n\}}, \widehat{\beta}^{\{n\}T})\right\| \leq C_{\sup}\frac{1}{\sqrt{a^{\{n\}}}}.$$

□

B Proof of Proposition 42

In this section, we prove Proposition 42 in Subsections B.1 to B.6 and we prove Corollary 8 in Subsection B.7.

B.1 Introduction to the proof of Proposition 42

Recall that $(U^{(l)})_{l\in[1:n]}$ is an i.i.d. sample of U with $\mathrm{E}(U)=\mu$ and $\mathrm{Var}(U)=\Sigma$ and

$$\widehat{X}^{\{n\}}=\frac{1}{n}\sum_{l=1}^{n}U^{(l)}.$$

Let $X^{\{n\}}\sim\mathcal{N}(\mu,\frac{1}{n}\Sigma)$. By Proposition 38, we have

$$\eta\left(X^{\{n\}},f\right)=\eta\left(X^{\{n\}},Df(\mu)\right)+O\left(\frac{1}{a^{\{n\}}}\right)=\eta\left(X^{*},Df(\mu)\right)+O\left(\frac{1}{a^{\{n\}}}\right).$$

Hence, it remains to prove that

$$\left\|\eta\left(\widehat{X}^{\{n\}},f\right)-\eta\left(X^{\{n\}},f\right)\right\|\underset{n\to+\infty}{\longrightarrow}0,$$

that is, writing $f_n:=\sqrt{n}\left(f\left(\frac{\cdot}{\sqrt{n}}+\mu\right)-f(\mu)\right)$ and $\tilde{X}^{\{n\}}:=\sqrt{n}(\widehat{X}^{\{n\}}-\mu)$, that

$$\left\|\eta\left(\tilde{X}^{\{n\}},f_n\right)-\eta\left(X^{*},f_n\right)\right\|\underset{n\to+\infty}{\longrightarrow}0.$$

In Section B.2, we give some lemmas of f_n. Then, defining

$$E_{u,n,K}(Z):=\mathrm{E}\left(\mathrm{E}\left[f_n(Z)^2\mathbb{1}_{\|Z\|_\infty\leq K}\middle|Z_u\right]^2\right),$$

$$E_{u,n}(Z):=\mathrm{E}\left(\mathrm{E}\left[f_n(Z)^2\middle|Z_u\right]^2\right),$$

we prove in Section B.3 that $\sup_n|E_{u,n,K}(\tilde{X}^{\{n\}})-E_{u,n}(\tilde{X}^{\{n\}})|$ converges to 0 when $K\to+\infty$. In particular, for $U\sim\mathcal{N}(\mu,\Sigma)$, the result holds for $\tilde{X}^{\{n\}}=X^*$.

Hence, for any $\varepsilon>0$, choosing K such that $|E_{u,n,K}(\tilde{X}^{\{n\}})-E_{u,n}(\tilde{X}^{\{n\}})|<\varepsilon/3$ and $|E_{u,n,K}(X^*)-E_{u,n}(X^*)|<\varepsilon/3$, we show in Section B.4 that

$$|E_{u,n,K}(X^*)-E_{u,n,K}(\tilde{X}^{\{n\}})|\underset{n\to+\infty}{\longrightarrow}0.$$

In Section B.5, we conclude the proof that

$$\left|\mathrm{Var}(\mathrm{E}(f_n(\tilde{X}^{\{n\}})|\tilde{X}_u^{\{n\}}))-\mathrm{Var}(\mathrm{E}(f_n(X^*)|X_u^*))\right|\underset{n\to+\infty}{\longrightarrow}0.$$

In Section B.6, we conclude the proof that

$$\left\|\eta\left(\tilde{X}^{\{n\}},f_n\right)-\eta\left(X^{*},f_n\right)\right\|\underset{n\to+\infty}{\longrightarrow}0.$$

The key of the proof is that the probability density function of $\tilde{X}^{\{n\}}$ converges uniformly to the one of X^* by local limit theorem (see [She71] or Theorem 19.1 of [BR86]).

B.2 Part 1

Lemma 51. *There exists $C_{\sup} < +\infty$ such that, for all $x \in \mathbb{R}^p$,*

$$|f_n(x)| \leq C_{\sup}\left(\|x\|\mathbb{1}_{\|x\|\leq\sqrt{n}} + \frac{\|x\|^k}{\sqrt{n}^{k-1}}\mathbb{1}_{\|x\|>\sqrt{n}})\right),$$

where we recall that $k \in \mathbb{N}^*$ is such that for all $x \in \mathbb{R}^p$, we have $|f(x)| \leq C(1 + \|x\|^k)$.

Proof. For all $x \in \mathbb{R}^p$, we have

$$\begin{aligned}
\left|f\left(\frac{x}{\sqrt{n}}+\mu\right)-f\left(\mu\right)\right| &\leq \left|f\left(\frac{x}{\sqrt{n}}+\mu\right)\right| + |f\left(\mu\right)| \\
&\leq C_{\sup}\left(1+\left\|\frac{x}{\sqrt{n}}+\mu\right\|^k\right) + |f\left(\mu\right)| \\
&\leq C_{\sup}\left(1+\left\|\frac{x}{\sqrt{n}}\right\|^k\right).
\end{aligned}$$

Thus, for all $\|x\| \geq \sqrt{n}$, we have

$$|f_n(x)| \leq C_{\sup}\frac{\|x\|^k}{\sqrt{n}^{k-1}}.$$

If $\|x\| \leq \sqrt{n}$, we have

$$\begin{aligned}
\left|f\left(\frac{x}{\sqrt{n}}+\mu\right)-f\left(\mu\right)\right| &\leq \max_{\|y\|\leq 1+\|\mu\|}\|Df(y)\|\left\|\frac{x}{\sqrt{n}}+\mu-\mu\right\| \\
&\leq C_{\sup}\left\|\frac{x}{\sqrt{n}}\right\|,
\end{aligned}$$

and thus,

$$|f_n(x)| \leq C_{\sup}\|x\|.$$

$\square$

In particular,

$$|f_n(x)| \leq C_{\sup}(\|x\| + \|x\|^k), \quad f_n(x)^2 \leq C_{\sup}(\|x\|^2 + \|x\|^{2k})$$

Lemma 52. *For $i = 1, 2$, we have*

$$\mathrm{E}(f_n(\tilde{X}^{\{n\}})^{2i}) \leq C_{\sup}.$$

Proof. We have

$$\begin{aligned} \mathrm{E}(f_n(\tilde{X}^{\{n\}})^{2i}) &\leq C_{\sup}\left(\mathrm{E}(\|\tilde{X}^{\{n\}}\|^{2ik}) + \mathrm{E}(\|\tilde{X}^{\{n\}}\|^{2i})\right) \\ &\leq C_{\sup}\left(\mathrm{E}(\|\tilde{X}^{\{n\}}\|_{2ik}^{2ik}) + \mathrm{E}(\|\tilde{X}^{\{n\}}\|_{2i}^{2i})\right). \end{aligned}$$

Now, by Rosenthal inequality [Ros70], we have

$$\begin{aligned} \mathrm{E}(|\tilde{X}_j|^{2ik}) &= \frac{1}{n^{ik}}\mathrm{E}\left[\left(\sum_{l=1}^{n} U_j^{(l)} - \mu_j\right)^{2ik}\right] \\ &\leq \frac{C_{\sup}}{n^{ik}} \max\left(n\mathrm{E}([U_j^{(1)} - \mu_j]^{2ik}), \left[n\mathrm{E}([U_j^{(1)} - \mu_j]^2)\right]^{ik}\right) \\ &\leq C_{\sup}. \end{aligned}$$

$\square$

Lemma 53. *For all $v \subset [1:p]$, $v \neq \emptyset$ and for $i = 1, 2$, we have*

$$\sup_n \mathrm{E}\left(f_n(\tilde{X}^{\{n\}})^i \mathbb{1}_{\tilde{X}_v^{\{n\}} \notin [-K,K]^{|v|}}\right) \underset{K\to+\infty}{\longrightarrow} 0.$$

Proof. We have

$$\begin{aligned} &\mathrm{E}\left(f_n(\tilde{X}^{\{n\}})^i \mathbb{1}_{\tilde{X}_v^{\{n\}} \notin [-K,K]^{|v|}}\right) \\ \leq\ & \sqrt{\mathrm{E}\left(f_n(\tilde{X}^{\{n\}})^{2i}\right)}\sqrt{\mathbb{P}(\tilde{X}_v^{\{n\}} \notin [-K,K]^{|v|})}. \end{aligned}$$

By Lemma 52, $\sup_n \sqrt{\mathrm{E}\left(f_n(\tilde{X}^{\{n\}})^{2i}\right)}$ is bounded.

Now, since $(\tilde{X}_v^{\{n\}})_n$ converges in distribution, it is a tight sequence, hence

$$\sup_n \mathbb{P}\left(\tilde{X}_v^{\{n\}} \notin [-K,K]^{|v|}\right) \leq \sup_n \mathbb{P}(\|\tilde{X}_v^{\{n\}}\| \geq K) \underset{K\to+\infty}{\longrightarrow} 0.$$

$\square$

Lemma 54. *The sequence $(f_n)_n$ converges pointwise to $Df(\mu)$.*

Proof. For all $x \in \mathbb{R}$,

$$f\left(\frac{x}{\sqrt{n}} + \mu\right) - f(\mu) = Df(\mu)\frac{x}{\sqrt{n}} + O\left(\left\|\frac{x}{\sqrt{n}}\right\|^2\right),$$

so,

$$f_n(x) = Df(\mu)\,x + O\left(\frac{\|x\|^2}{\sqrt{n}}\right).$$

$\square$

B.3 Part 2

We want to prove that, for all $u \subset [1:p]$, $u \neq \emptyset$, we have

$$\sup_n |E_{u,n,K}(\tilde{X}^{\{n\}}) - E_{u,n}(\tilde{X}^{\{n\}})| \underset{K \to +\infty}{\longrightarrow} 0.$$

We will prove this result for $\emptyset \subsetneq u \subsetneq [1:p]$, since it is easier for $u = [1:p]$ (see Remark 45).

We have

$$\begin{aligned}
& \left| \int_{\mathbb{R}^{|u|}} \left(\int_{\mathbb{R}^{|-u|}} f_n(x) d\mathbb{P}_{\tilde{X}_{-u}^{\{n\}} | \tilde{X}_u^{\{n\}} = x_u}(x_{-u}) \right)^2 d\mathbb{P}_{\tilde{X}_u^{\{n\}}}(x_u) \right. \\
& \left. - \int_{[-K,K]^{|u|}} \left(\int_{[-K,K]^{|-u|}} f_n(x) d\mathbb{P}_{\tilde{X}_{-u}^{\{n\}} | \tilde{X}_u^{\{n\}} = x_u}(x_{-u}) \right)^2 d\mathbb{P}_{\tilde{X}_u^{\{n\}}}(x_u) \right| \\
\leq & \int_{([-K,K]^{|u|})^c} \left(\int_{\mathbb{R}^{|-u|}} f_n(x) d\mathbb{P}_{\tilde{X}_{-u}^{\{n\}} | \tilde{X}_u^{\{n\}} = x_u}(x_{-u}) \right)^2 d\mathbb{P}_{\tilde{X}_u^{\{n\}}}(x_u) \\
& + \int_{[-K,K]^{|u|}} \left| \left(\int_{\mathbb{R}^{|-u|}} f_n(x) d\mathbb{P}_{\tilde{X}_{-u}^{\{n\}} | \tilde{X}_u^{\{n\}} = x_u}(x_{-u}) \right)^2 \right. \\
& \left. - \left(\int_{[-K,K]^{|-u|}} f_n(x) d\mathbb{P}_{\tilde{X}_{-u}^{\{n\}} | \tilde{X}_u^{\{n\}} = x_u}(x_{-u}) \right)^2 \right| d\mathbb{P}_{\tilde{X}_u^{\{n\}}}(x_u).
\end{aligned}$$

We have to bound the two summands of the previous upper-bound.

The first term converges to 0 by Lemma 53. Let us bound the second term. By mean-value inequality with the square function, we have

$$\begin{aligned}
& \int_{[-K,K]^{|u|}} \left| \left(\int_{\mathbb{R}^{|-u|}} f_n(x) d\mathbb{P}_{\tilde{X}_{-u}^{\{n\}} | \tilde{X}_u^{\{n\}} = x_u}(x_{-u}) \right)^2 \right. \\
& \left. - \left(\int_{[-K,K]^{|-u|}} f_n(x) d\mathbb{P}_{\tilde{X}_{-u}^{\{n\}} | \tilde{X}_u^{\{n\}} = x_u}(x_{-u}) \right)^2 \right| d\mathbb{P}_{\tilde{X}_u^{\{n\}}}(x_u) \\
\leq & \; 2 \int_{[-K,K]^{|u|}} \left(\int_{\mathbb{R}^{|-u|}} |f_n(x)| d\mathbb{P}_{\tilde{X}_{-u}^{\{n\}} | \tilde{X}_u^{\{n\}} = x_u}(x_{-u}) \right) \\
& \left| \int_{\mathbb{R}^{|-u|}} \mathbb{1}_{x_{-u} \notin [-K,K]^{|-u|}} f_n(x) d\mathbb{P}_{\tilde{X}_{-u}^{\{n\}} | \tilde{X}_u^{\{n\}} = x_u}(x_{-u}) \right| d\mathbb{P}_{\tilde{X}_u^{\{n\}}}(x_u) \\
\leq & \; 2 \int_{[-K,K]^{|u|}} \left(\int_{\mathbb{R}^{|-u|}} |f_n(x)| d\mathbb{P}_{\tilde{X}_{-u}^{\{n\}} | \tilde{X}_u^{\{n\}} = x_u}(x_{-u}) \right) \\
& \times \left(\int_{\mathbb{R}^{|-u|}} \mathbb{1}_{x_{-u} \notin [-K,K]^{|-u|}} |f_n(x)| d\mathbb{P}_{\tilde{X}_{-u}^{\{n\}} | \tilde{X}_u^{\{n\}} = x_u}(x_{-u}) \right) d\mathbb{P}_{\tilde{X}_u^{\{n\}}}(x_u)
\end{aligned}$$

$$\leq 2\sqrt{\mathrm{E}(\mathrm{E}(|f_n(\tilde{X}^{\{n\}})|\ |\tilde{X}_u^{\{n\}})^2)}$$
$$\times\sqrt{\int_{\mathbb{R}^{|u|}}\left(\int_{\mathbb{R}^{|-u|}}\mathbb{1}_{x_{-u}\notin[-K,K]^{|-u|}}|f_n(x)|d\mathbb{P}_{\tilde{X}_{-u}^{\{n\}}|\tilde{X}_u^{\{n\}}=x_u}(x_{-u})\right)^2 d\mathbb{P}_{\tilde{X}_u^{\{n\}}}(x_u)}.$$

Now, $\mathrm{E}(\mathrm{E}(|f_n(\tilde{X}^{\{n\}})|\ |\tilde{X}_u^{\{n\}})^2) \leq \mathrm{E}(f_n(\tilde{X}^{\{n\}})^2)$ which is bounded by Lemma 52 and the other term converges to 0 uniformly on n by Lemma 53.

Remark 45. *In the case where $u = [1:p]$, it is much simpler, since*

$$\mathrm{E}(f_n(\tilde{X}^{\{n\}})^2) - \mathrm{E}(f_n(\tilde{X}^{\{n\}})^2\mathbb{1}_{\tilde{X}^{\{n\}}\in[-K,K]^p}) = \mathrm{E}(f_n(\tilde{X}^{\{n\}})^2\mathbb{1}_{\tilde{X}^{\{n\}}\notin[-K,K]^p}),$$

which converges to 0 uniformly on n when $K \to +\infty$ by Lemma 53.

B.4 Part 3

Let $K \in \mathbb{R}_+^*$ and $u \subset [1:p]$ such that $u \neq \emptyset$. We want to prove that

$$|E_{u,n,K}(X^*) - E_{u,n,K}(\tilde{X}^{\{n\}})| \underset{n\to+\infty}{\longrightarrow} 0.$$

The case $u = [1:p]$ is much easier (see Remark 46), hence, assume that $\emptyset \subsetneq u \subsetneq [1:p]$. Since K is fixed, the probability density function f_{X^*} of X^* is lower-bounded by $a > 0$ on $[-K,K]^p$. Let $\varepsilon_n := \max_{\emptyset\subsetneq u\subset[1:p]}\sup_{x\in\mathbb{R}^p}|f_{X^*}(x) - f_{\tilde{X}^{\{n\}}}(x)|$. Using local limit theorem (see Theorem 19.1 of [BR86] or [She71]), $\varepsilon_n \underset{n\to+\infty}{\longrightarrow} 0$. We assume that n is large enough such that $\varepsilon_n \leq \frac{a}{2}$. Let $b < +\infty$ be the maximum of f_{X^*}.

We have

$$\begin{aligned}
&|E_{u,n,K}(X^*) - E_{u,n,K}(\tilde{X}^{\{n\}})| \\
\leq\ & \int_{[-K,K]^{|u|}}\Bigg|\left(\int_{[-K,K]^{|-u|}} f_n(x)\frac{f_{X^*}(x)}{f_{X_u^*}(x_u)}dx_{-u}\right)^2 \\
&-\left(\int_{[-K,K]^{|-u|}} f_n(x)\frac{f_{\tilde{X}^{\{n\}}}(x)}{f_{\tilde{X}_u^{\{n\}}}(x_u)}dx_{-u}\right)^2\Bigg| f_{X_u^*}(x_u)dx_u \\
&+\int_{[-K,K]^{|u|}}\left(\int_{[-K,K]^{|-u|}} f_n(x)\frac{f_{\tilde{X}^{\{n\}}}(x)}{f_{\tilde{X}_u^{\{n\}}}(x_u)}dx_{-u}\right)^2 |f_{X_u^*}(x_u) - f_{\tilde{X}_u^{\{n\}}}(x_u)|dx_u.
\end{aligned}$$

Hence, we have to prove the convergence of the two summands in the previous upper-bound. For the second term, it suffices to remark that

$$|f_{X_u^*}(x_u) - f_{\tilde{X}_u^{\{n\}}}(x_u)| \leq \varepsilon_n \leq \frac{2\varepsilon_n}{a}f_{\tilde{X}_u^{\{n\}}}(x_u).$$

Hence, the second term is smaller than $\frac{2\varepsilon_n}{a}\mathrm{E}(f_n(\tilde{X}^{\{n\}})^2)$ that converges to 0. It remains to prove that the first term converges to 0. By mean-value inequality, we have

$$\begin{aligned}
& \int_{[-K,K]^{|u|}} \Bigg| \left(\int_{[-K,K]^{|-u|}} f_n(x) \frac{f_{X^*}(x)}{f_{X_u^*}(x_u)} dx_{-u} \right)^2 \\
& - \left(\int_{[-K,K]^{|-u|}} f_n(x) \frac{f_{\tilde{X}^{\{n\}}}(x)}{f_{\tilde{X}_u^{\{n\}}}(x_u)} dx_{-u} \right)^2 \Bigg| f_{X_u^*}(x_u) dx_u \\
\leq \; & 2 \int_{[-K,K]^{|u|}} \left(\int_{[-K,K]^{|-u|}} |f_n(x)| \max\left(\frac{f_{X^*}(x)}{f_{X_u^*}(x_u)}, \frac{f_{\tilde{X}^{\{n\}}}(x)}{f_{\tilde{X}_u^{\{n\}}}(x_u)} \right) dx_{-u} \right) \\
& \times \left(\int_{[-K,K]^{|-u|}} |f_n(x)| \left| \frac{f_{X^*}(x)}{f_{X_u^*}(x_u)} - \frac{f_{\tilde{X}^{\{n\}}}(x)}{f_{\tilde{X}_u^{\{n\}}}(x_u)} \right| dx_{-u} \right) f_{X_u^*}(x_u) dx_u.
\end{aligned}$$

Now,

$$\begin{aligned}
\left| \frac{f_{X^*}(x)}{f_{X_u^*}(x_u)} - \frac{f_{\tilde{X}^{\{n\}}}(x)}{f_{\tilde{X}_u^{\{n\}}}(x_u)} \right| & \leq \frac{|f_{X^*}(x) - f_{\tilde{X}^{\{n\}}}(x)|}{f_{X_u^*}(x_u)} + f_{\tilde{X}^{\{n\}}}(x) \left| \frac{1}{f_{X_u^*}(x_u)} - \frac{1}{f_{\tilde{X}_u^{\{n\}}}(x_u)} \right| \\
& \leq \frac{|f_{X^*}(x) - f_{\tilde{X}^{\{n\}}}(x)|}{f_{X_u^*}(x_u)} + f_{\tilde{X}^{\{n\}}}(x) \frac{4}{a^2} \left| f_{X_u^*}(x_u) - f_{\tilde{X}_u^{\{n\}}}(x_u) \right| \\
& \leq \frac{\varepsilon_n}{f_{X_u^*}(x_u)} + f_{\tilde{X}^{\{n\}}}(x) \frac{4}{a^2} \varepsilon_n \\
& \leq \frac{\varepsilon_n}{f_{X_u^*}(x_u)} + f_{X^*}(x) \frac{8}{a^2} \varepsilon_n \\
& \leq \frac{\varepsilon_n}{a} \frac{f_{X^*}(x)}{f_{X_u^*}(x_u)} + \frac{8b}{a^2} \varepsilon_n \frac{f_{X^*}(x)}{f_{X_u^*}(x_u)} \\
& \leq C_{\sup} \varepsilon_n \frac{f_{X^*}(x)}{f_{X_u^*}(x_u)}.
\end{aligned}$$

Hence, for n large enough such that $C_{\sup}\varepsilon_n \leq 1$, we have

$$\begin{aligned}
& \int_{[-K,K]^{|u|}} \Bigg| \left(\int_{[-K,K]^{|-u|}} f_n(x) \frac{f_{X^*}(x)}{f_{X_u^*}(x_u)} dx_{-u} \right)^2 \\
& - \left(\int_{[-K,K]^{|-u|}} f_n(x) \frac{f_{\tilde{X}^{\{n\}}}(x)}{f_{\tilde{X}_u^{\{n\}}}(x_u)} dx_{-u} \right)^2 \Bigg| f_{X_u^*}(x_u) dx_u \\
\leq \; & 2 \int_{[-K,K]^{|u|}} \left(\int_{[-K,K]^{|-u|}} |f_n(x)| 2 \frac{f_{X^*}(x)}{f_{X_u^*}(x_u)} dx_{-u} \right)
\end{aligned}$$

$$\times \left(\int_{[-K,K]^{|-u|}} |f_n(x)| C_{\sup} \varepsilon_n \frac{f_{X^*}(x)}{f_{X_u^*}(x_u)} dx_{-u} \right) f_{X_u^*}(x_u) dx_u$$

$$\leq \; C_{\sup}\varepsilon_n \mathrm{E}(f_n(X^*)^2),$$

that converges to 0.

Remark 46. *If $u = [1:p]$, it suffices to remark that*

$$|f_{X^*}(x) - f_{\tilde{X}^{\{n\}}}(x)| \leq \varepsilon_n \leq \frac{\varepsilon_n}{a} f_{X^*}(x).$$

Thus,

$$\begin{aligned} & |E_{u,n,K}(X^*) - E_{u,n,K}(\tilde{X}^{\{n\}})| \\ \leq & \int_{[-K,K]^p} f_n(x)^2 |f_{X^*}(x) - f_{\tilde{X}^{\{n\}}}(x)| dx \\ \leq & \frac{\varepsilon_n}{a} \mathrm{E}(f_n(X^*)^2) \\ \leq & C_{\sup}\varepsilon_n. \end{aligned}$$

B.5 Part 4

Let us prove that

$$\mathrm{E}(f_n(\tilde{X}^{\{n\}})) - \mathrm{E}(f_n(X^*)) \longrightarrow 0$$

By lemma 53, we have

$$\sup_n \left| \mathrm{E}(f_n(\tilde{X}^{\{n\}}) - \mathrm{E}(f_n(\tilde{X}^{\{n\}}) \mathbb{1}_{\tilde{X}^{\{n\}} \in [-K,K]^p}) \right| \underset{K \to \infty}{\longrightarrow} 0$$

Let $\varepsilon > 0$ and let K such that

$$\sup_n \left| \mathrm{E}(f_n(\tilde{X}^{\{n\}}) - \mathrm{E}(f_n(\tilde{X}^{\{n\}}) \mathbb{1}_{\tilde{X}^{\{n\}} \in [-K,K]^p}) \right| < \frac{\varepsilon}{3}$$

and

$$\sup_n \left| \mathrm{E}(f_n(X^*) - \mathrm{E}(f_n(X^*) \mathbb{1}_{X^* \in [-K,K]^p}) \right| < \frac{\varepsilon}{3}.$$

By local limit theorem, we have

$$\left| \mathrm{E}(f_n(\tilde{X}^{\{n\}}) \mathbb{1}_{\tilde{X}^{\{n\}} \in [-K,K]^p}) - \mathrm{E}(f_n(X^*) \mathbb{1}_{X^* \in [-K,K]^p}) \right| \underset{n \to +\infty}{\longrightarrow} 0.$$

Thus, for all $u \subset [1:p]$, we have

$$\mathrm{Var}(\mathrm{E}(f_n(\tilde{X}^{\{n\}}) | \tilde{X}_u^{\{n\}})) - \mathrm{Var}(\mathrm{E}(f_n(X^*) | X_u^*)) \underset{n \to +\infty}{\longrightarrow} 0.$$

B.6 Conclusion

To prove the convergence of the Shapley effects, it suffices to prove the $\mathrm{Var}(f_n(X^*))$ is lower-bounded. Hence, we show that $\mathrm{Var}(f_n(X^*))$ converges to $\mathrm{Var}(Df(\mu)X^*)$. Let $i = 1, 2$ and let $\varepsilon > 0$. By Lemma 53, let K such that

$$\sup_n \mathrm{E}(f_n(X^*)^i \mathbb{1}_{X^* \notin [-K,K]^p}) \leq \frac{\varepsilon}{3}, \quad \mathrm{E}([Df(\mu)X^*]^i \mathbb{1}_{X^* \notin [-K,K]^p}) \leq \frac{\varepsilon}{3}.$$

By Lemmas 51 and 54 and by dominated convergence theorem, we have :

$$\mathrm{E}(f_n(X^*)^i \mathbb{1}_{X^* \in [-K,K]^p}) \underset{n\to+\infty}{\longrightarrow} \mathrm{E}([Df(\mu)X^*]^i \mathbb{1}_{X^* \in [-K,K]^p}).$$

Hence, $\mathrm{Var}(f_n(X^*))$ converges to $\mathrm{Var}(Df(\mu)X^*)$. Thus, for all $u \subset [1:p]$

$$S_u^{cl}(\tilde{X}^{\{n\}}, f_n) - S_u(X^*, f_n) \underset{n\to+\infty}{\longrightarrow} 0.$$

Hence,

$$\left\| \eta(\tilde{X}^{\{n\}}, f_n) - \eta(X, f_n) \right\| \underset{n\to+\infty}{\longrightarrow} 0.$$

B.7 Proof of Corollary 8

Since $\widehat{X}^{\{n'\}\prime} \underset{n\to+\infty}{\overset{a.s}{\longrightarrow}} \mu$ and $\widehat{\Sigma}^{\{n''\}\prime} \underset{n\to+\infty}{\overset{a.s}{\longrightarrow}} \Sigma$, it suffices to prove that, if $(x^{\{n\}})_n$ converges to μ, and $(\Sigma^{\{n\}})_n$ converges to Σ, we have

$$\left\| \eta(\widehat{X}^{\{n\}}, f) - \eta(X^{*n}, \tilde{f}^{\{n\}}_{1,h^{\{n\}},x^{\{n\}}}) \right\| \underset{n\to+\infty}{\longrightarrow} 0,$$

where X^{*n} is a random vector with distribution $\mathcal{N}(\mu, \Sigma^{\{n\}})$. Let $(x^{\{n\}})_n$ and $(\Sigma^{\{n\}})_n$ be such sequences. Recall that

$$\left\| \eta(\tilde{X}^{\{n\}}, f_n) - \eta(X^*, f_n) \right\| \underset{n\to+\infty}{\longrightarrow} 0,$$

where $X^* \sim \mathcal{N}(0, \Sigma)$, that is

$$\left\| \eta\left(\widehat{X}^{\{n\}}, f\right) - \eta\left(X^{\{n\}}, f\right) \right\| \underset{n\to+\infty}{\longrightarrow} 0,$$

where $X^{\{n\}} \sim \mathcal{N}(\mu, \frac{1}{n}\Sigma)$. Hence, we have to prove that

$$\left\| \eta(X^{\{n\}}, f) - \eta(X^{*n}, \tilde{f}^{\{n\}}_{1,h^{\{n\}},x^{\{n\}}}) \right\| \underset{n\to+\infty}{\longrightarrow} 0.$$

By Propositions 38 and Proposition 39, remark that $\eta(X^{\{n\}}, f)$ converges to $\eta(X^*, f_1)$. Moreover,

$$\eta(X^{*n}, \tilde{f}^{\{n\}}_{1,h^{\{n\}},x^{\{n\}}}) = \eta(X^{*n} + x^{\{n\}} - \mu^{\{n\}}, \tilde{f}^{\{n\}}_{1,h^{\{n\}},x^{\{n\}}}) \underset{n\to+\infty}{\longrightarrow} \eta(X^*, f_1),$$

by Corollary 6, that concludes the proof.

Appendix V

Gaussian field on the symmetric group: prediction and learning

In the framework of the supervised learning of a real function defined on an abstract space $\mathcal{X}$, the so called Kriging method stands on a real Gaussian field defined on $\mathcal{X}$. The Euclidean case is well known and has been widely studied. In this work, we explore the less classical case where $\mathcal{X}$ is the non commutative finite group of permutations. In this framework, we propose and study an harmonic analysis of the covariance operators that allows us to put into action the full machinery of Gaussian processes learning. We also consider our framework in the case of partial rankings.

A Introduction

The problem of ranking a set of items is a fundamental task in today's data driven world. Analysing observations which are not quantitative variables but rankings has been often studied in social sciences. It has also become a popular problem in statistical learning thanks to the generalization of the use of automatic recommendation systems. Rankings are labels that model an order over a finite set $E_N := \{1, \dots, N\}$. Hence, an observation is a set of preferences between these N points. It is thus a one to one relation σ acting from E_N onto E_N. In other words, σ lies in the finite symmetric group S_N of all permutations of E_N. More precisely, assume that we have a finite set $X = \{x_1, \cdots, x_N\}$ and we have to order the elements of X. A ranking on X is a statement of the form

$$x_{i_1} \succ x_{i_2} \succ \cdots \succ x_{i_N}, \tag{V.1}$$

where all the $i_j, j = 1 \cdots, N$ are different. We can associate to this ranking the permutation σ defined by $\sigma(i_k) = k$. Reversely, to a permutation σ, we can associate the following ranking

$$x_{\sigma^{-1}(1)} \succ x_{\sigma^{-1}(2)} \succ \cdots \succ x_{\sigma^{-1}(N)}. \tag{V.2}$$

We refer to the works of Douglas E. Critchlow (see for example [CFV91, Cri92, CF93]) for an introduction to rankings, together with various results.

Our aim is to predict outputs corresponding to permutations inputs. For instance, the permutation input can correspond to an ordering of tasks, in applications. In a workflow management system, there may be a large number of tasks that may be done in different orders but are all necessary to achieve the goal. Workflow prediction or optimization problems currently occur in fields such as grid computing [YBT05], and logistics [Chr16].

Another example of application is given by the maintenance of machines in a supply line. Machines in a supply line need to be tuned or monitored in order to optimize the production of a good. The machines can be tuned in different orders, each corresponding to a permutation and these choices have an impact on the quality of the production of the goods, measured by a quantitative variable Y, for instance the amount of defects in the produced goods. Hence, the objective of the model will thus be to forecast the outcome of a specific order for the maintenance of the machines in order to optimize the production.

Another interesting case of output corresponding to a permutation input is of the form $\max_{x\in X} f(\sigma, x)$, where f is a function both acting on the permutation σ and on some external variable x. This output corresponds to a worst case for the performance or the cost given by the permutation σ. Classical examples of this kind of output are the max distance criterion for Latin Hypercube Designs [MBC79, SWNW03] and the robust deviation for a tour in the robust traveling salesman problem [MBMG07]. In Section C.4, we discuss and address the example of the max distance criterion.

In this work, we will be in the framework of Gaussian processes indexed by S_N. Actually, Gaussian process models rely on the definition of a covariance function that characterizes the correlations between values of the process at different observation points. As the notion of similarity between data points is crucial, *i.e.* close location inputs are likely to have similar target values, covariance functions (symmetric positive definite kernels) are the key ingredient in using Gaussian processes for prediction. Indeed, the covariance operator contains nearness or similarity informations. In order to obtain a satisfying model one needs to choose a covariance function (*i.e.* a symmetric positive definite kernel) that respects the structure of the index space of the dataset.

A large number of applications gave rise to recent researches on ranking including *ranking aggregation* [KCS17], clustering rankings (see [CGJ11]) or kernels on rankings for supervised learning. Constructing kernels over the set of permutations has been studied following several different ways. In [Kon08], Kondor provides results about kernels in non-commutative finite groups and constructs *diffusion kernels* (which are positive definite) on S_N. These diffusion kernels are based on a discrete notion of neighbourhood. Notice that the kernels considered therein are quite different from those considered in this work. Furthermore, the diffusion kernels are not in general covariance functions because of their tricky dependency on permutations. The recent reference [JV17] proves that the Kendall and Mallow's kernels are positive definite. Further, [MRW$^+$16] extends this study characterizing both the feature spaces and the spectral properties associated with these two kernels. A real data set [Bru12] on rankings is studied in [MRW$^+$16]. The authors used a kernel regression to predict the age of a participant with his/her order of preference of six sources of news regarding scientific developments: TV, radio, newspapers and magazines, scientific magazines, the internet, school/university.

There are applications where not all of the items in (V.1) are ranked. Rather, a partial ranking is given (see for example the "sushi" dataset available at `http://www.kamishima.net` or movie datasets). The books [Cri12] and [Mar14] provide metrics on partial rankings and the papers [KB10] and [JV17] provide kernels on partial rankings and deal with the complexity reduction of their computation.

The goal in this work is threefold: first we define Gaussian processes indexed by S_N by providing a wide class of covariance kernels. We generalize previous results on the Mallow's kernel (see [JV17]). Second, we consider the Kriging models (see for instance [Ste99]) that consist in inferring the values of a Gaussian random field given observations at a finite set of observation points. Here, the observations points are permutations. We study the asymptotic properties of the maximum likelihood estimator of the parameters of the covariance function. We also prove the asymptotic accuracy of the Kriging prediction under the estimated covariance parameters. Further, we provide simulations that illustrate the very good performances of the proposed kernels. Finally, we provide an application to Gaussian process based optimization of Latin Hypercube Designs. Last, we show that the Gaussian process framework may be adapted to the cases of learning with partially observed rankings. We define a class of covariance kernels on partial rankings, for which we show how to reduce the computation complexity. In simulations, we show that our suggested kernels yield more efficient Gaussian process predictions than the kernels given in [JV17].

The work falls into the following parts. In Section B, we recall some facts on S_N and provide some covariance kernels on this set. Asymptotic results on the estimation of the covariance function are presented in Section C. Section C also contains an application to the optimization of Latin Hypercube Designs. Section D provides new covariance kernels for partial rankings with a comparison with the ones given in [JV17] in a numerical experiment. Section E concludes this chapter. The proofs are all postponed to Section F.

B Covariance model for rankings

Recall that we define S_N as the set of all permutations on $E_N := \{1, \dots, N\}$. An element σ of S_N is a bijection from E_N to E_N. We aim at constructing kernels, or covariance functions, on S_N. We will base these kernels on the three following distances on S_N (see [Dia88]). For any permutations π and σ of S_N,

- The Kendall's tau distance is defined by

$$d_\tau(\pi, \sigma) := \sum_{\substack{i,j=1,\dots,N \\ i<j}} \left(\mathbb{1}_{\sigma(i)>\sigma(j),\, \pi(i)<\pi(j)} + \mathbb{1}_{\sigma(i)<\sigma(j),\, \pi(i)>\pi(j)} \right). \tag{V.3}$$

  This distance counts the number of pairs on which the permutations disagree in ranking.

- The Hamming distance is defined by

$$d_H(\pi, \sigma) := \sum_{i=1}^{N} \mathbb{1}_{\pi(i) \neq \sigma(i)}. \tag{V.4}$$

- The Spearman's footrule distance is defined by

$$d_S(\pi, \sigma) := \sum_{i=1}^{N} |\pi(i) - \sigma(i)|. \tag{V.5}$$

These three distances are right-invariant. That is, for all π, σ, $\tau \in S_N$, $d(\pi, \sigma) = d(\pi\tau, \sigma\tau)$. Other right-invariant distances are discussed in [Dia88].

We aim at defining a Gaussian process indexed by permutations. Notice that, generally speaking, using the abstract Kolmogorov construction (see for example [DCD12] Chapter 0), the law of a Gaussian random process $(Y_x)_{x \in E}$ indexed by an abstract set E is entirely characterized by its mean and covariance functions

$$M : x \mapsto \mathrm{E}(Y_x)$$

and

$$K : (x, y) \mapsto \mathrm{Cov}(Y_x, Y_y).$$

Of course, here the framework is much simpler as S_N is finite ($|S_N| = N!$), and the Gaussian distribution is obviously completely determined by its mean and covariance matrix. Hence, if we assume that the process is centered, we only have to build a covariance function on S_N. First, we recall the definition of a positive definite kernel on an abstract space E. A symmetric map $K : E \times E \to \mathbb{R}$ is called a *positive definite kernel* if for all $n \in \mathbb{N}$ and for all $(x_1, \cdots, x_n) \in E^n$, the matrix $(K(x_i, x_j))_{i,j}$ is positive semi-definite. In this work, we say that K is a *strictly positive definite kernel* if K is symmetric and, for all $n \in \mathbb{N}$ and for all $(x_1, \cdots, x_n) \in E^n$ such that $x_i \neq x_j$ if $i \neq j$, the matrix $(K(x_i, x_j))_{i,j}$ is positive definite.

These notions are particularly interesting for S_N (and any finite set). Indeed, if K is a strictly positive definite kernel, then for any function $f : S_N \to \mathbb{R}$, there exists $(a_\sigma)_{\sigma \in S_N}$ such that

$$f = \sum_{\sigma \in S_N} a_\sigma K(., \sigma), \tag{V.6}$$

and K is of course an *universal kernel* (see [MXZ06]).

Remark 47. *Since S_N is a finite discrete space, remark that the Reproducible Kernel Hilbert Space (RKHS) of a kernel K is defined by the set of the functions of the form (V.6), and the universality of the kernel K is equivalent to the equality of its RKHS with the set of the functions from S_N to $\mathbb{R}$. This is, in turn, equivalent to the fact that K is strictly positive definite.*

We now provide two different parametric families of covariance kernels. The members of these families have the general form

$$K_{\theta_1,\theta_2}(\sigma, \sigma') := \theta_2 \exp\left(-\theta_1 d(\sigma, \sigma')\right), \quad (\theta_1, \theta_2 > 0), \tag{V.7}$$

and

$$K_{\theta_1,\theta_2,\theta_3}(\sigma, \sigma') := \theta_2 \exp\left(-\theta_1 d(\sigma, \sigma')^{\theta_3}\right), \quad (\theta_1,\ \theta_2 > 0,\ \theta_3 \in [0, 1]). \tag{V.8}$$

Here, d is one of the three distances defined in (V.3), (V.4) and (V.5). More precisely, for the Kendall's (resp. Hamming's and Spearman's footrule) distance let $K^\tau_{\theta_1,\theta_2(,\theta_3)}$ (resp. $K^H_{\theta_1,\theta_2(,\theta_3)}$, $K^S_{\theta_1,\theta_2(,\theta_3)}$) be the corresponding covariance function. For concision, sometimes we will write $K_{\theta_1,\theta_2(,\theta_3)}$ (resp. d) for one of these three kernels (resp. distances).

We show in the next proposition that K_{θ_1,θ_2} is strictly positive definite.

Proposition 48. *For all $\theta_1 > 0$ and $\theta_2 > 0$, $K^\tau_{\theta_1,\theta_2}$, $K^H_{\theta_1,\theta_2}$, $K^S_{\theta_1,\theta_2}$ are strictly positive definite kernels on S_N.*

Remark 48. *In [MRW+16], the strict positive definiteness of the Mallow's kernel, corresponding to* $K^{\tau}_{\theta_1,\theta_2}$*, is also shown. Our proof of Proposition 48 seems more direct than the one given in [MRW+16].*

We also have a similar result for $K_{\theta_1,\theta_2,\theta_3}$.

Proposition 49. *For all* $\theta_1 > 0$, $\theta_2 \geq 0$ *and* $\theta_3 \in [0, 1]$*, the maps* $K^{\tau}_{\theta_1,\theta_2,\theta_3}$, $K^{H}_{\theta_1,\theta_2,\theta_3}$, $K^{S}_{\theta_1,\theta_2,\theta_3}$ *are positive definite kernels on* S_N*.*

Propositions 48 and 49 enable to define Gaussian processes indexed by permutations.

Remark 49. *The authors of [AMR17] define strictly positive definite kernels on graphs with Euclidean edges with two different metrics: the geodesic metric and the "resistance metric". The kernels are obtained by applying completely monotonous functions to these metrics (distances). They provide different classes of such functions: the power exponential functions (which are considered in our work, see* (V.8)*), the Matérn functions (with a smoothness parameter* $0 < \nu \leq 1/2$*), the generalized Cauchy functions and the Dagum functions. One can show that Proposition 49 remains valid for all these kernels, by remarking as in [AMR17] that these kernels are based on completely monotonous functions. Some of the proofs of [AMR17] are based on techniques similar to the proof of Proposition 49, using Schoenberg's theorems.*

We remark that the finite set of permutations S_N *is a graph, when two permutations* σ_1 *and* σ_2 *are connected if there exists a transposition* π *such that* $\sigma_1 = \sigma_2\pi$*. Hence, it is natural to ask if the results of [AMR17] can imply or extend some of the results in this work. The answer however appears to be negative. Indeed, the distances considered in [AMR17] are the geodesic or the "resistance" distances, hence the distances in* (V.3), (V.4) *and* (V.5) *do not fall into this category.*

One could also consider the set of the permutations as a fully connected weighted graph, where the weight of the edge between σ_1 *and* σ_2 *is* $d(\sigma_1, \sigma_2)$ *and where* d *is* d_τ *or* d_H *or* d_S*. Nevertheless, also with this graph, the results of [AMR17] do not apply, since the graphs addressed by this reference have a particular structure (finite sequential 1-sum of Euclidean cycles and trees).*

We finally remark that [AMR17] constructs covariance functions not only on finite graphs, but between connected vertices. In contrast, the covariance functions constructed here are defined only on the finite set S_N*.*

C Gaussian fields on the symmetric group

C.1 Maximum likelihood

Let us consider a Gaussian process Y indexed by $\sigma \in S_N$, with zero mean and covariance function K_*. In a parametric setting, a classical assumption is that the covariance function K_* belongs to some parametric set of the form

$$\{K_\theta \ ; \ \theta \in \Theta\}, \tag{V.9}$$

where $\Theta \subset \mathbb{R}^p$ is given and for all $\theta \in \Theta$, K_θ is a covariance function. The parameter θ is generally called the covariance parameter. In this framework, $K_* = K_{\theta^*}$ for some parameter $\theta^* \in \Theta$.

The parameter θ^* is estimated from noisy observations of the values of the Gaussian process at several inputs. Namely, to the observation point σ_i, we associate the observation $Y(\sigma_i) + \varepsilon_i$, for $i = 1, \ldots, n$, where $(\varepsilon_i)_i$ is an independent Gaussian white noise. Let us consider a sample of random permutations $\Sigma = (\sigma_1, \sigma_2, \cdots, \sigma_n) \in S_N$. Assume that we observe Σ and a random vector $y = (y_1, y_2, \cdots, y_n)^T$ defined by, for $i \leq N$,

$$y_i = Y(\sigma_i) + \varepsilon_i. \tag{V.10}$$

Here, Y is a Gaussian process indexed by S_N and independent of Σ. We assume that Y is centered with covariance function $K_{\theta_1^*, \theta_2^*}$ (see (V.7) in Section B) and that $(\varepsilon_i)_{i \leq n} \sim \mathcal{N}(0, \theta_3^* I_n)$. Y is the unknown process to predict and ε is an additive white noise. Notice that θ_3 denotes here the variance of the nugget effect while it is a power in Section B (see (V.8)). We keep the same name in order to use the compact notation θ for the parameter of the model. The Gaussian process Y is stationary in the sense that for all $\sigma_1, \cdots, \sigma_n \in S_N$ and for all $\tau \in S_N$, the finite-dimensional distribution of Y at $\sigma_1, \cdots, \sigma_n$ is the same as the finite-dimensional distribution at $\sigma_1 \tau, \cdots, \sigma_n \tau$.

Several techniques have been proposed for constructing an estimator $\widehat{\theta} = \widehat{\theta}(\sigma_1, y_1, \cdots, \sigma_n, y_n)$ of $\theta^* := (\theta_1^*, \theta_2^*, \theta_3^*)$: maximum likelihood estimation [Whi82], restricted maximum likelihood [CL93], leave-one-out estimation [Cre92, Bac13], leave-one-out log probability [SK01]... Here, we shall focus on the maximum likelihood method. It is widely used in practice and has received a lot of theoretical attention. Assume that $\Theta \subset \prod_{i=1}^3 [\theta_{i,min}, \theta_{i,max}]$ for some given $0 < \theta_{i,min} \leq \theta_{i,max} < \infty$ $(i = 1, 2, 3)$. The maximum likelihood estimator is defined as

$$\widehat{\theta}_{ML} = \widehat{\theta}_n \in \arg\min_{\theta \in \Theta} L_\theta \tag{V.11}$$

with

$$L_\theta := \frac{1}{n} \ln(\det R_\theta) + \frac{1}{n} y^T R_\theta^{-1} y, \tag{V.12}$$

where $R_\theta = [K_{\theta_1,\theta_2}(\sigma_i,\sigma_j) + \theta_3 \mathbb{1}_{i=j}]_{1\leq i,j\leq n}$ is invertible for $\theta \in \Theta$ since $\theta_3 > 0$.

C.2 Asymptotic results

When considering the asymptotic behaviour of the maximum likelihood estimator, two different frameworks can be studied: fixed domain and increasing domain asymptotics [Ste99]. Under increasing-domain asymptotics, as $n \to \infty$, the observation points $\sigma_1, \cdots, \sigma_n$ are such that $\min_{i\neq j} d(\sigma_i,\sigma_j)$ is lower bounded and $d(\sigma_i,\sigma_j)$ becomes large with $|i-j|$, (thus we can not keep N fixed as $n \to +\infty$). Under fixed-domain asymptotics, the sequence (or triangular array) of observation points $(\sigma_1, \cdots, \sigma_n, \cdots)$ is dense in a fixed bounded subset. For a Gaussian field on $\mathbb{R}^d$, under increasing-domain asymptotics, the true covariance parameter θ^* can be estimated consistently by maximum likelihood. Furthermore, the maximum likelihood estimator is asymptotically normal [MM84, CL93, CL96, Bac14]. Moreover, prediction performed using the estimated covariance parameter $\widehat{\theta}_n$ is asymptotically as good as the one computed with θ^* as pointed out in [Bac14]. Finally, note that in the symmetric group, the fixed-domain framework can not be considered (contrary to the input space $\mathbb{R}^d$) since S_N is a finite space.

We will consider hereafter the increasing-domain framework. We thus consider a number of observations n that goes to infinity. Hence, the size N of the permutations can not be fixed, as pointed out above. We thus let the size of the permutations be a function of n, that we write N_n, with $N_n \to \infty$ as $n \to \infty$. To summarize, we consider a sequence of Gaussian processes Y_n on S_{N_n}, with $N_n \underset{n\to+\infty}{\longrightarrow} +\infty$ and where we consider a triangular array $(\sigma_i^{(n)})_{i\leq n} \subset S_{N_n}$ of observation points. However, for the sake of simplicity, we only write Y and $(\sigma_i)_{i\leq n}$ and the dependency on n is implicit. We observe values of the Gaussian process on the permutations $\Sigma = (\sigma_1, \cdots, \sigma_n)$, that are assumed to fulfill the following assumptions:

Condition 1: For $d = d_\tau$ or $d = d_H$ or $d = d_S$, there exists $\beta > 0$ such that $\forall i, j,\ d(\sigma_i,\sigma_j) \geq |i-j|^\beta$.

Condition 2: For $d = d_\tau$ or $d = d_H$ or $d = d_S$, there exists $c > 0$ such that $\forall i,\ d(\sigma_i,\sigma_{i+1}) \leq c$.

Here, we recall that d_τ, d_H and d_S are defined in Section B. Notice that β and c are assumed to be independent on n.

These conditions are natural under increasing-domain asymptotics. Indeed, Condition 1 provides asymptotic independence for pairs of observations with asymptotically distant indices. It allows to show that the variance of L_θ and of its gradient converges to 0. Condition 2 ensures the asymptotic discrimination of the covariance parameters (see Lemma 58 in Section F). These conditions can be ensured with particular choices of sampling schemes for $(\sigma_1, \cdots, \sigma_n)$ (using the distances previously discussed).

As an example consider the following setting. We fix $k \in \mathbb{N}$. For $n \in \mathbb{N}, i \in [1 : n]$, we choose $\sigma_i^{(n)} = \sigma_i = \tau_i c_i \in S_{k+n}$ (we have $N_n = k + n$) with $\tau_i \in S_k \times id_{[k+1:n+k]} := \{\sigma \in S_{n+k} | \ \sigma_{|[k+1:n+k]} = id\}$ a random permutation such that $(\tau_i)_i$ are independent (we do not make further assumptions on the law of τ_i). Let $c_i = (i+k \quad i+k-1 \quad \cdots \quad 1)$ the cycle defined by $c_i(1) = i+k$, $c_i(j) = j-1$ if $1 < j \leq i+k$ and $c_i(j) = j$ if $j > i+k$. Then, σ_i is a permutation such that $\sigma_i(1) = i+k$, $\sigma_i(j)$ is a random variable in $[2 : k]$ if $1 < j \leq k+1$, $\sigma_i(j) = j-1$ if $k+1 < j \leq i+k$ and $\sigma_i(j) = j$ if $j > i+k$. A straightforward computation shows that the Conditions 1 and 2 are satisfied with $\beta = 1$ and $c = 1 + k(k-1)/2$ for the Kendall's tau distance, $c = 2+k$ for the Hamming distance, $c = 2+k^2$ for the Spearman's footrule distance. Indeed, the three distances in S_k are upper-bounded by $k(k-1)/2$, k and k^2 respectively.

The following theorems give both the consistency and the asymptotic normality of the estimator when the number of observations increases.

Theorem 7. *Let $\widehat{\theta}_{ML}$ be defined as in (V.11), where the distance d used to define the set $\{K_\theta \ ; \ \theta \in \Theta\}$ is d_τ, d_H or d_S. Assume that Conditions 1 and 2 hold with the same choice of the distance d. Then,*

$$\widehat{\theta}_{ML} \xrightarrow[n \to +\infty]{\mathbb{P}} \theta^*. \tag{V.13}$$

Theorem 8. *Under the assumptions of Theorem 7, let M_{ML} be the 3×3 matrix defined by*

$$(M_{ML})_{i,j} = \frac{1}{2n} \operatorname{Tr}\left(R_{\theta^*}^{-1} \frac{\partial R_{\theta^*}}{\partial \theta_i} R_{\theta^*}^{-1} \frac{\partial R_{\theta^*}}{\partial \theta_j} \right). \tag{V.14}$$

Then

$$\sqrt{n} M_{ML}^{\frac{1}{2}} \left(\widehat{\theta}_{ML} - \theta^* \right) \xrightarrow[n \to +\infty]{\mathcal{L}} \mathcal{N}(0, I_3). \tag{V.15}$$

Furthermore,

$$0 < \liminf_{n \to \infty} \lambda_{\min}(M_{ML}) \leq \limsup_{n \to \infty} \lambda_{\max}(M_{ML}) < +\infty, \tag{V.16}$$

where $\lambda_{\min}(M_{ML})$ (resp. $\lambda_{\max}(M_{ML})$) is the smallest (resp. largest) eigenvalue of M_{ML}.

Given the maximum likelihood estimator $\widehat{\theta}_{ML}$, the value $Y(\overline{\sigma}_n)$, for any input $\overline{\sigma}_n \in S_{N_n}$, can be forecasted by plugging the estimated parameter in the conditional expectation expression for Gaussian processes. Hence $Y(\overline{\sigma}_n)$ is predicted by

$$\widehat{Y}_{\widehat{\theta}_{ML}}(\overline{\sigma}_n) = r_{\widehat{\theta}_{ML}}^T(\overline{\sigma}_n) R_{\widehat{\theta}_{ML}}^{-1} y \tag{V.17}$$

with

$$r_{\widehat{\theta}_{ML}}(\overline{\sigma}_n) = \begin{bmatrix} K_{\widehat{\theta}_{ML}}(\overline{\sigma}_n, \sigma_1) \\ \vdots \\ K_{\widehat{\theta}_{ML}}(\overline{\sigma}_n, \sigma_n) \end{bmatrix}.$$

We point out that $\widehat{Y}_{\widehat{\theta}_{ML}}(\overline{\sigma}_n)$ is the conditional expectation of $Y(\overline{\sigma}_n)$ given $y_1, \cdots, y_n$, when assuming that Y is a centered Gaussian process with covariance function $K_{\widehat{\theta}_{ML}}$.

The following theorem shows that the forecast with the estimated parameter behaves asymptotically as if the true covariance parameter were known.

Theorem 9. *Under the assumptions of Theorem 7, for any fixed sequence $(\overline{\sigma}_n)_{n\in\mathbb{N}}$, with $\overline{\sigma}_n \in S_{N_n}$ for $n \in \mathbb{N}$, we have*

$$\left|\widehat{Y}_{\widehat{\theta}_{ML}}(\overline{\sigma}_n) - \widehat{Y}_{\theta^*}(\overline{\sigma}_n)\right| \xrightarrow[n\to+\infty]{\mathbb{P}} 0. \tag{V.18}$$

Remark 50. *Theorem 9 does not imply that*

$$\max_{\sigma\in S_{N_n}} \left|\widehat{Y}_{\widehat{\theta}_{ML}}(\sigma) - \widehat{Y}_{\theta^*}(\sigma)\right| \xrightarrow[n\to+\infty]{\mathbb{P}} 0. \tag{V.19}$$

Indeed, letting $\overline{\sigma}_n \in \operatorname*{argmax}_{\sigma\in S_{N_n}} \left|\widehat{Y}_{\widehat{\theta}_{ML}}(\sigma) - \widehat{Y}_{\theta^*}(\sigma)\right|$, (V.19) is equivalent to

$$\left|\widehat{Y}_{\widehat{\theta}_{ML}}(\overline{\sigma}_n) - \widehat{Y}_{\theta^*}(\overline{\sigma}_n)\right| \xrightarrow[n\to+\infty]{\mathbb{P}} 0,$$

but where $\overline{\sigma}_n$ is random. Here, Theorem 9 does not imply (V.19) as it holds for deterministic sequences $(\overline{\sigma}_n)_{n\in\mathbb{N}}$. It would be interesting, in future work, to extend Theorem 9 to show (V.19).

The proofs of Theorems 7, 8 and 9 are given in Section F (Sections F.2.ii), F.2.iii) and F.2.iv) respectively). They are based on lemmas stated and proved in Section F.2.i). In [Bac14] and [BGLV17], similar results for maximum likelihood are given for Gaussian fields indexed on $\mathbb{R}^d$ and on the set of all probability measures on $\mathbb{R}$ (see also [BSG+19]). At the beginning of Section F.2, we also discuss the similarities and differences between the proofs of Theorems 7, 8 and 9 and these given in [Bac14] and [BGLV17].

C.3 Numerical experiments

As an illustration of Theorem 7, we provide a numerical illustration showing that the maximum likelihood is consistent. We generated the observations as discussed

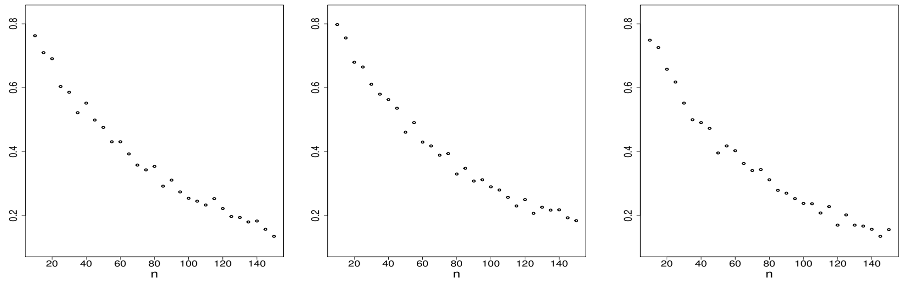


Figure V.1: Monte Carlo estimates of $\mathbb{P}(\|\widehat{\theta}_n - \theta^*\| > 0.5)$ for different values of n, the number of observations, with $\theta^* = (0.1, 0.8, 0.3)$ and Kendall's tau distance, the Hamming distance and the Spearman's footrule distance from left to right.

in Section C with $k = 3$. We recall that $N_n = k+n$ and $\sigma_i = \tau_i(i+k\ i+k-1\ \cdots 1) \in S_{k+n}$ where $\tau_i \in S_k \times id_{[k+1:k+n]}$ is a random permutation.

For each value of n, we estimate the probability $\mathbb{P}(\|\widehat{\theta}_n - \theta^*\| > \varepsilon)$ using a Monte-Carlo method and a sample of 1000 values of $\mathbb{1}_{\|\widehat{\theta}_n - \theta^*\| > \varepsilon}$. Figure V.1 depicts these estimates for $\varepsilon = 0.5$, $\theta^* = (0.1, 0.8, 0.3)$ and $\Theta = [0.02, 2] \times [0.3, 2] \times [0.1, 1]$.

In Figure V.2, we display the density of the coordinates of the maximum likelihood estimator for different values of n ranging from 20, 60 to 150. These densities have been estimated with a sample of 1000 values of the maximum likelihood estimator. We observe that the densities can be far from the true parameter for $n = 20$ or $n = 60$ but are quite close to it for $n = 150$. Further, we see that for $n = 150$, the Kendall's tau distance seems to give better estimates for θ_3^*. However, the computation time of the distance matrix is much longer with the Kendall's tau distance than with the other distances.

In Figure V.3, for a given $\overline{\sigma}_n$, we display estimates of the probability that the deviation between the prediction of $Y(\overline{\sigma}_n)$ given in (V.17) with the parameter $\widehat{\theta}_n$ and the prediction of $Y(\overline{\sigma}_n)$ with the parameter θ^* exceeds 0.3. Indeed, Theorem 9 ensures us that this probability converges to 0 as $n \to +\infty$.

C.4 Application to the optimization of Latin Hypercube Designs

We consider here an application of Proposition 49 to find an optimal Latin Hypercube Design (LHD). A LHD is a design of experiments $(X_j)_{j \le N} \in [0,1]^d$ where, for each component $i \in [1:d]$, the projections of $X_1, ..., X_N$ on the component i are equispaced in $[0,1]$ (see [MBC79]). We will thus consider that each component

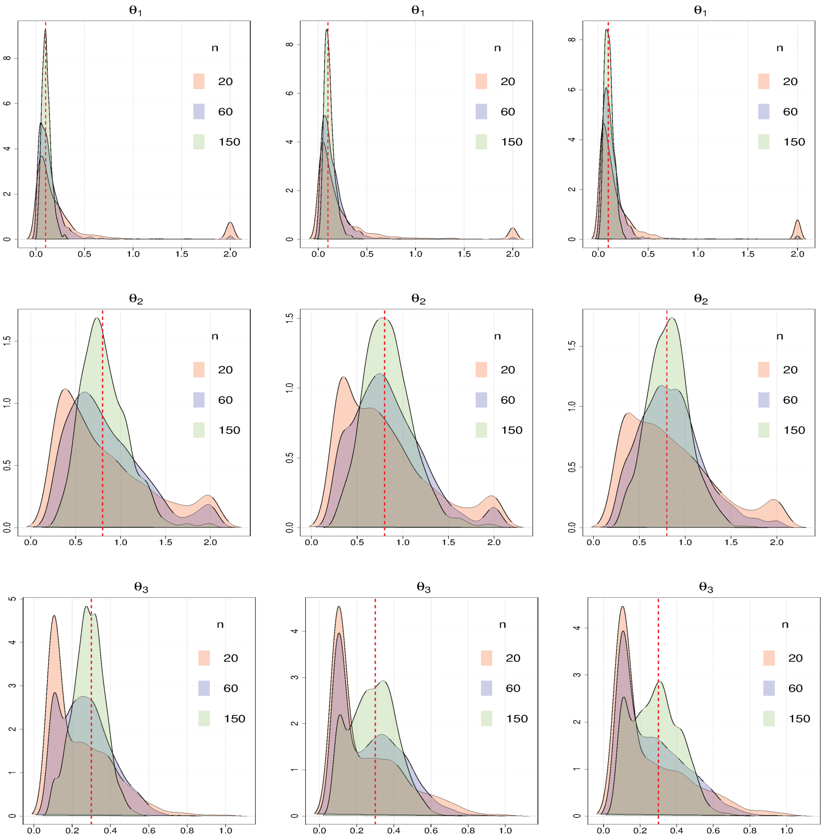


Figure V.2: Density of the coordinates of $\widehat{\theta}_{ML}$ for the number of observations $n = 20$ (in red), $n = 60$ (in blue), $n = 150$ (in green) with $\theta^* = (0.1, 0.8, 0.3)$ (represented by the red vertical line). We used the Kendall's tau distance, the Hamming distance and the Spearman's footrule distance from left to right.

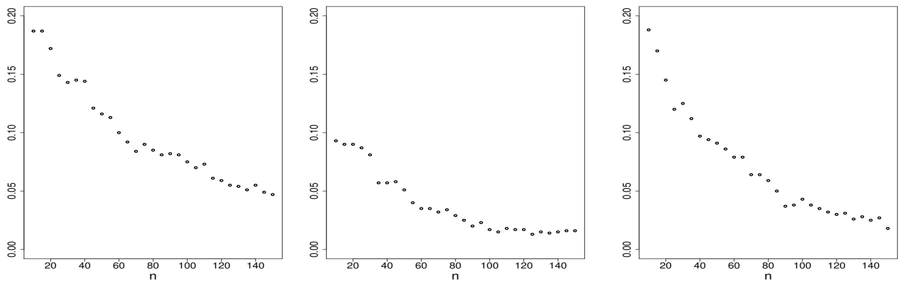


Figure V.3: Monte Carlo estimates of $\mathbb{P}\left(\left|\widehat{Y}_{\widehat{\theta}_n}(\overline{\sigma}_n) - \widehat{Y}_{\theta^*}(\overline{\sigma}_n)\right| > 0.3\right)$ for different values of n, the number of observations, with $\theta^* = (0.1, 0.8, 0.3)$, $\overline{\sigma}_n = (1\ 4\ 6) \in S_{n+3}$, and the Kendall's tau distance, the Hamming distance and the Spearman's footrule distance from left to right.

of one X_j is equal to $k/(N-1)$ for some $k \in [0 : N-1]$. We also remark that we can always permute the variables so that the first component of X_j is equal to $(j-1)/(N-1)$. So, for each LHD $(X_j)_{j \le N}$, there exist $\sigma_2, ..., \sigma_d \in S_N$ such that for all $j \in [1 : N]$, we have

$$X_j = \left(\frac{j-1}{N-1}, \frac{\sigma_2(j)-1}{N-1}, \cdots, \frac{\sigma_d(j)-1}{N-1} \right).$$

Hence, there is a bijection between the set of LHD with N points and the set S_N^{d-1}.

Now, if $(X_j)_{j \le N}$ is a LHD, we can define its measure of space filling quality as

$$f((X_j)_{j \le N}) = \sup_{x \in [0,1]^d} \min_{j \in [1:N]} \|x - X_j\|,$$

that is the largest distance of a point of $[0,1]^d$ to $(X_j)_{j \le N}$. We remark that LHDs minimizing f are called minimax [SWNW03]. Our aim is to find a minimax LHD $(X_j^*)_{j \le N}$. However, given a LHD $(X_j)_{j \le N}$, its quality $f((X_j)_{j \le N})$ is not an obvious quantity and its computation is expensive.

To estimate this quantity, we suggest to generate N_{tot} random points $(x_l)_{l \le N_{tot}}$ uniformly on $[0,1]^d$, to compute their distance to the LHD and to take the maximum value. This estimation is costly (because of the large number N_{tot}) and noisy (because of the randomness of the points $(x_l)_{l \le N_{tot}}$). Thus, we suggest to use a Gaussian process model on f and to apply the Expected Improvement (EI) strategy [JSW98]. Nevertheless, remark that f is a positive function, whereas a Gaussian process realization can take negative values. In this case, different options are possible: firstly, we can ignore the information of the inequality constraint; secondly, we can use Gaussian process under inequality constraints (see

[BLLLo19]); thirdly, we can use a transformation of the function to remove the inequality constraint. We choose here the third strategy and we model $\log(f)$ by a Gaussian process realization. We remark that $\log(f)$ can take positive and negative values.

We thus assume that the unknown function $\log(f)$ to minimize is a realization of a Gaussian process. We have to find a positive definite kernel on S_N^{d-1}. Thanks to Proposition 49, we have three positive definite kernels on S_N, thus on S_N^{d-1} (taking the tensor product of these kernels). Thus, we apply the EI strategy with these three kernels to find the best LHD with $N_{\max}$ calls to the function f. The $N_{\max}/2$ first LHDs are generated uniformly on S_N^{d-1} and the other ones are generated sequentially by following the EI strategy.

More precisely, for $i \in [N_{\max}/2 : N_{\max} - 1]$, let us explain how to choose the $i+1$-th observation, when we have observed the vectors $(\sigma_j^{(k)})_{j\in[2:d],k\in[1:i]}$ and the associated observations $\left[\log\left(f\left((\sigma_j^{(k)})_{j\in[2:d]}\right)\right)\right]_{k\in[1:i]}$ (we remark that f can be defined equivalently as a function $f(\sigma_2,\dots,\sigma_d)$ of $d-2$ permutations or as a function $f((X_j)_{j\leq N})$ of a LHD). We model $\log(f)$ by a realization of a Gaussian process Z, with a conditional mean written $\widehat{Z}_i(\sigma_2,\cdots,\sigma_d)$ and a conditional variance written $\widehat{s}_i^2(\sigma_2,\cdots,\sigma_d)$, given

$$\{Z((\sigma_j^{(k)})_{j=2,\dots,d}) = \log(f((\sigma_j^{(k)})_{j=2,\dots,d}))\}_{k=1,\dots,i}. \tag{V.20}$$

Then, we let

$$(\sigma_2^{(i+1)},\cdots,\sigma_d^{(i+1)}) \in \underset{\sigma_2,\cdots,\sigma_d\in S_N}{\operatorname{argmax}}\ EI(\sigma_2,\cdots,\sigma_d),$$

where

$$EI(\sigma_2,\cdots,\sigma_d) = \mathrm{E}_i\left(\max\left(M_i - Z(\sigma_2,\cdots,\sigma_d),0\right)\right),$$

where $M_i = \min_{k\in[1:i]} \log(f(\sigma_2^{(k)},\cdots,\sigma_d^{(k)}))$, and E_i is the expectation conditionally to the observations (V.20). We have an explicit expression of EI,

$$EI = (M_i - \widehat{Z}_i)\Phi\left(\frac{M_i-\widehat{Z}_i}{\widehat{s}_i}\right) + \widehat{s}_i\phi\left(\frac{M_i-\widehat{Z}_i}{\widehat{s}_i}\right),$$

where ϕ and Φ are the standard normal density and distribution functions. To choose $(\sigma_2^{(i+1)},\cdots,\sigma_d^{(i+1)})$, we thus solve an optimization problem for EI, which has a very small cost compared to evaluating f, since the computation of EI is instantaneous. We thus choose the set of permutations that maximizes EI over 2000 sets of uniformly distributed permutations.

We refer to [JSW98] for more details on EI. The parameters of the covariance functions are estimated by maximum likelihood at each step.

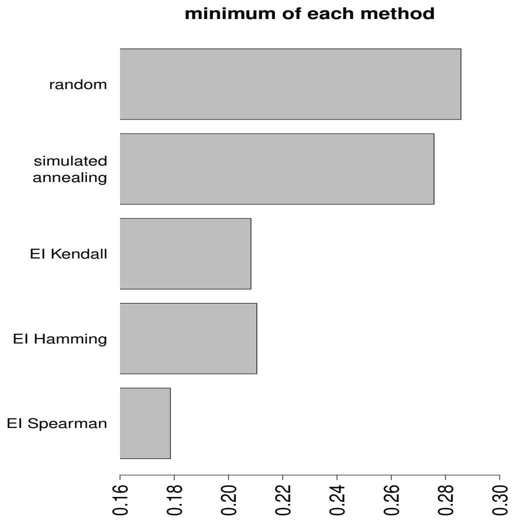


Figure V.4: Minimal quality of LHD found by the five methods.

We run an experiment where we compare the performances of the 5 following methods:

- Random sampling, to generate $N_{\max}$ LHDs of the form $\{(X_j^{(i)})_{j\leq N};\ i \leq N_{\max}\}$ by generating $\sigma_2, ..., \sigma_d$ uniformly and independently;
- Simulated annealing, choosing that two LHDs $(\sigma_j)_{2\leq j\leq d}$ and $(\sigma'_j)_{2\leq j\leq d}$ are neighbours if there exist transpositions $\tau_2, ..., \tau_d$ such that for all $j \in [2 : d]$, we have $\sigma'_j = \sigma_j \tau_j$;
- EI with Kendall distance;
- EI with Hamming distance;
- EI with Spearman distance.

For each method, the performance indicator is $\min_{i=1,...,N_{\max}} f((X_j^{(i)})_{j\leq N})$. Here, we take $d = 3$, $N = 15$, $N_{\max} = 200$ and $N_{tot} = 27 \times 10^6$.

We can see in Figure V.4 that the best LHDs are found by EI, particularly with the Spearman distance. The simulated annealing is slightly better than random sampling.

We display in Figure V.5 the distributions of the qualities $\{f((X_j^{(i)})_{j\leq N}); i \leq N_{\max}\}$ for the five methods. We can notice that the simulated annealing does not explore the set of all the LHDs and does not find the best minimum. EI performs minimisation and exploration to find better minima. We can then provide the best

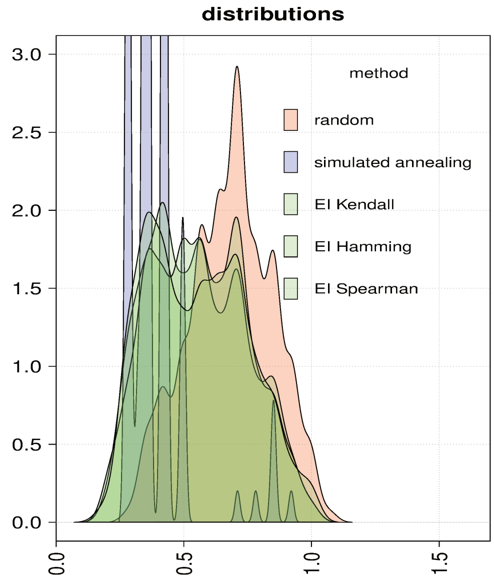


Figure V.5: Distributions of the quality of LHDs for the five methods.

LHD of EI with the Spearman distance. This LHD is given by the permutations

$$\begin{aligned}\sigma_2 &= (5, 2, 1, 7, 6, 3, 4, 8, 11, 13, 12, 9, 10, 14, 15),\\ \sigma_3 &= (3, 6, 1, 8, 4, 9, 15, 7, 12, 5, 13, 10, 2, 11, 14).\end{aligned}$$

To conclude, the kernels on permutations provided in Section B enable us to use EI that gives much better results than simulated annealing or random sampling to find the best LHD.

D Covariance model for partial ranking

D.1 A new kernel on partial rankings

In application, it can happen that partial rankings rather than complete rankings are observed. A partial ranking aims at giving an order of preference between different elements of X without comparing all the pairs in X. Hence, a partial ranking R is a statement of the form

$$X_1 \succ X_2 \succ \cdots \succ X_m, \tag{V.21}$$

where $m < N$, and $X_1, \cdots, X_m$ are disjoint sets of $X = \{x_1, x_2, \cdots, x_N\}$. The partial ranking means that any element of X_j is preferred to any element of X_{j+1}

but the elements of X_j cannot be ordered. Given a partial ranking R, we consider the following subset of S_N

$$E_R := \{\sigma \in S_N : \sigma(i_1) < \sigma(i_2) < \cdots < \sigma(i_m) \\ \text{for any choice of } (x_{i_1}, \cdots, x_{i_m}) \in X_1 \times \cdots \times X_m \}. \quad (V.22)$$

In the statistical literature, there is a natural way to extend a positive definite kernel K on S_N to the set of partial rankings (see [KB10], [JV17]). To do so, one considers for R and R' two partial rankings the following averaged kernel

$$\mathcal{K}(R, R') := \frac{1}{|E_R||E_{R'}|} \sum_{\sigma \in E_R} \sum_{\sigma' \in E_{R'}} K(\sigma, \sigma'). \quad (V.23)$$

Here, $|E_R|$ denotes the cardinal of the set E_R. Notice that, if K is a positive definite kernel on permutations, then $\mathcal{K}$ is also a positive definite kernel [Hau99]. Indeed, if $R_1, \cdots, R_n$ are partial rankings and if $(a_1, \cdots, a_n) \neq 0$, then

$$\sum_{i,j=1}^{n} a_i a_j \mathcal{K}(R_i, R_j) = \sum_{\sigma, \sigma' \in S_N} b_\sigma b_{\sigma'} K(\sigma, \sigma'), \quad (V.24)$$

where we set

$$b_\sigma := \sum_{i,\ \sigma \in R_i} \frac{a_i}{|E_{R_i}|}. \quad (V.25)$$

Observe that the computation of $\mathcal{K}$ is very costly. Indeed, we have to sum over $|E_R||E_{R'}|$ permutations. Several works aim to reduce the computation cost of this kernel (see [KB10, LM08, LRGG19]). However, its efficient computation remains an issue.

In the following, we provide another way to extend the kernels $K_{\theta_1,\theta_2,\theta_3}$ to partial rankings. We will provide computational simplifications for this extension. First, define the measure of dissimilarity d_{avg} on partial rankings as the mean of distances $d(\sigma, \sigma')$ ($\sigma \in E_R, \sigma' \in E_{R'}$). That is

$$d_{\text{avg}}(R, R') := \frac{1}{|E_R||E_{R'}|} \sum_{\sigma \in E_R} \sum_{\sigma \in E_{R'}} d(\sigma, \sigma'). \quad (V.26)$$

Since $d_{\text{avg}}(R, R) \neq 0$ in general, we need to define d_{partial} as follows

$$d_{\text{partial}}(R, R') := d_{\text{avg}}(R, R') - \frac{1}{2} d_{\text{avg}}(R, R) - \frac{1}{2} d_{\text{avg}}(R', R'). \quad (V.27)$$

Proposition 50. *$d_{\text{partial}}^{\frac{1}{2}}$ is a pseudometric on partial rankings (i.e. it satisfies the positivity, the symmetry, the triangular inequality and is equal to 0 on the diagonal $\{(R, R),\ R \text{ is a partial ranking}\}$).*

We remark that other metrics on partial rankings are defined in [Cri12], in particular the Hausdorff metrics and the fixed vector metrics (based on the group representation of S_N). These two metrics are different from the one defined in (V.27). Our suggested metric d_{partial} will enable us to define positive definite kernels in Proposition 51. In future work, it would be interesting to study the construction of positive definite kernels based on the Hausdorff and fixed vector metrics.

We further define

$$\mathcal{K}_{\theta_1,\theta_2,\theta_3}(R,R') := \theta_2 \exp(-\theta_1 d_{\text{partial}}(R,R')^{\theta_3}). \tag{V.28}$$

The next proposition warrants that this last function is in fact a covariance kernel, which will later enable to define Gaussian processes on partial rankings.

Proposition 51. *$\mathcal{K}_{\theta_1,\theta_2,\theta_3}$ is a positive definite kernel for the Kendall's tau distance, the Hamming distance and the Spearman's footrule distance.*

D.2 Kernel computation in partial ranking

At a first glance, the computation of the kernel $\mathcal{K}_{\theta_1,\theta_2,\theta_3}(R,R')$ on partial rankings may still appear very costly due to the evaluation of d_{partial}. Indeed, we have to sum $|E_R||E_{R'}|$ elements for $d_{\text{avg}}(R,R')$, $|E_R|^2$ elements for $d_{\text{avg}}(R,R)$ and $|E_{R'}|^2$ elements for $d_{\text{avg}}(R',R')$. However, this computation problem can be quite simplified. As we will show in this subsection, the mean of the distances is much easier to compute than the mean of exponential of distances. We write $d_{\tau,\text{avg}}$ (resp. $d_{H,\text{avg}}$ and $d_{S,\text{avg}}$) for the average distance in (V.26) when the distance on the permutations is d_τ (resp. d_H and d_S).
To begin with, let us consider the case of top-k partial rankings. A top-k partial ranking (or a top-k list) is a partial ranking of the form

$$x_{i_1} \succ x_{i_2} \succ \cdots \succ x_{i_k} \succ X_{rest}, \tag{V.29}$$

where $X_{rest} := X \setminus \{x_{i_1}, \cdots, x_{i_k}\}$. It can be seen as the "highest rankings". In order to alleviate the notations, let just write $I = (i_1, \cdots, i_k)$ for this top-k partial ranking. The following proposition shows that the computation cost to evaluate d_{avg} (and so the kernel values) might be reduced when the partial rankings are in fact top-k partial rankings. Before stating this proposition let us define some more mathematical objects. Let $I := (i_1, \cdots, i_k)$ and $I' := (i'_1, \cdots, i'_k)$ be two top-k partial rankings. Let

$$\{j_1, \cdots, j_p\} := \{i_1, \cdots, i_k\} \cap \{i'_1, \cdots, i'_k\}$$

where $j_1 < j_2 < \cdots < j_p$ and p is an integer no larger than k. Let, for $l = 1, \cdots p$, c_{j_l} (resp. c'_{j_l}) denotes the rank of j_l in I (resp. in I'). Further, let $r := k - p$ and define $\tilde{I}$ (resp. $\tilde{I}'$) as the complementary set of $\{j_1, \cdots, j_p\}$ in $\{i_1, \cdots, i_k\}$ (resp. in $\{i'_1, \cdots, i'_k\}$). Writing these two sets in ascending order, we may finally define for $j = 1, \cdots, r$, u_j (resp. u'_j) as the rank in I (resp I') of the j-th element of $\tilde{I}$ (resp. $\tilde{I}'$).

Example 6. *Assume that $n = 7$, $I = (3, 2, 1, 4, 5)$ and $I' = (3, 5, 1, 6, 2)$. We have $(j_1, j_2, j_3, j_4) = (1, 2, 3, 5)$ (the items ranked by I and I', in increasing order). Thus, $c_{j_1} = 3$, $c_{j_2} = 2$, $c_{j_3} = 1$, $c_{j_4} = 5$ and $c'_{j_1} = 3$, $c'_{j_2} = 5$, $c'_{j_3} = 1$, $c'_{j_4} = 2$. Further, $u_1 = 4$ and $u'_1 = 4$.*

Proposition 52. *Let I and I' be two top k-partial rankings. Set $N' := N - k - 1$ and $m := N - |I \cup I'|$. Then,*

$$\begin{aligned}
d_{\tau,avg}(I, I') &= \sum_{1 \le l < l' \le p} \mathbb{1}_{(c_{j_l} < c_{j_{l'}}, c'_{j_l} > c'_{j_{l'}}) \ or \ (c_{j_l} > c_{j_{l'}}, c'_{j_l} < c'_{j_{l'}})} + r(2k + 1 - r) \\
&\quad - \sum_{j=1}^{r} (u_j + u'_j) + r^2 + \binom{N-k}{2} - \frac{1}{2}\binom{m}{2}, \\
d_{H,avg}(I, I') &= \sum_{l=1}^{p} \mathbb{1}_{c_{j_l} \neq c'_{j_l}} + m\frac{N-k-1}{N-k} + 2r, \\
d_{S,avg}(I, I') &= \sum_{l=1}^{p} |c_{j_l} - c'_{j_l}| + r(N + k + 1) - \sum_{j=1}^{r} (u_j + u'_j) \\
&\quad + mN' - \frac{mN'(2N'+1)}{3(N'+1)}.
\end{aligned}$$

Notice that the sequences (c_{j_l}), (c'_{j_l}) and (u_j), (u'_j) are easily computable and so $d_{\text{avg}}(I, I')$ too. Let us discuss an easy example to handle the computation of the previous sequences.

Example 7. *Assume that $n = 7$, $I = (3, 2, 1, 4, 5)$ and $I' = (3, 5, 1, 6, 2)$. Proposition 52 leads to*

$$d_{\tau,avg}(I, I') = 6, \quad d_{S,avg}(I, I') = 4.5, \quad d_{S,avg}(I, I') = 11.5.$$

To compute the pseudometric d_{partial} defined in (V.27), we also need to compute $d_{\tau,\text{avg}}$ on the diagonal $\{(I, I) |\ I \text{ is a top-}k \text{ partial ranking}\}$. The following corollary gives these computations.

Corollary 9. *Let I be a top-k partial ranking. Then,*

$$\begin{aligned} d_{\tau,avg}(I,I) &= \frac{1}{2}\binom{N-k}{2}, \\ d_{H,avg}(I,I) &= N-k-1, \\ d_{S,avg}(I,I) &= (N-k)(N-k-1)+\frac{(N-k-1)(2N-2k-1)}{3}. \end{aligned}$$

Remark 51. *Similar results as Proposition 52 are stated in Sections III.B and III.C of [Cri12] for the Hausdorff metrics and the fixed vector metrics respectively.*

In the case of the Hamming distance, we may step ahead and provide a simpler computational formula for the average distance between two partial rankings whenever their associated partitions share the same number of members (see Proposition 53 below). More precisely let R_1 and R_2 be two partial rankings such that

$$R_i = X_1^i \succ \cdots \succ X_k^i,\ i=1,2, \tag{V.30}$$

assume also that for $j=1,\cdots,k$, $|X_j^1| = |X_j^2|$ and denote by γ_j this integer. Obviously, $N=\sum_{j=1}^k \gamma_j$ so that $\gamma := (\gamma_j)_j$ is an integer partition of n. Further, when $1=\gamma_1=\gamma_2=\cdots=\gamma_{k-1}$ and $\gamma_k = N-k+1$ one is in the top-$(k-1)$ partial ranking case. For $j=1,\cdots,k$, let Γ_j be the set of all integers lying in $\left[\sum_{l=1}^{j-1}\gamma_l+1, \sum_{l=1}^{j}\gamma_l\right]$. Set further,

$$S_\gamma := S_{\Gamma_1}\times S_{\Gamma_2}\times\cdots\times S_{\Gamma_k},$$

where S_{Γ_i} is the set of permutations on Γ_i. Notice that S_γ is nothing more than the subgroup of S_n letting invariant the sets Γ_j ($j=1,\cdots,k$). So that, for $i=1,2$, we can write E_{R_i} as a right coset $R_i = S_\gamma \pi_i$ for some $\pi_i \in E_{R_i}$. With these extra notations and definitions, we are now able to compute $d_{H,\text{avg}}(R_1,R_2)$.

Proposition 53. *In the previous setting, we have*

$$d_{H,avg}(R_1,R_2) = |\{i,\ \Gamma(\pi_1(i)) \neq \Gamma(\pi_2(i))\}| + \sum_{j=1}^{k}\frac{\gamma_j}{N}(\gamma_j-1), \tag{V.31}$$

where, for $1\le l\le N$, $\Gamma(l)$ is the integer j such that $l\in\Gamma_j$.

Note that in (V.31), the term $|\{i,\ \Gamma(\pi_1(i)) \neq \Gamma(\pi_2(i))\}|$ counts the number of item $i\in[1:N]$ that are ranked differently in R_1 and R_2.

kernel	$\mathcal{K}^{\tau}_{\theta_1,\theta_2,\theta_3}$	$\mathcal{K}^{H}_{\theta_1,\theta_2,\theta_3}$	$\mathcal{K}^{S}_{\theta_1,\theta_2,\theta_3}$	$\mathcal{K}_{\theta_1}$
rate	0.902	0.904	0.912	0.928
R^2	0.887	0.996	0.996	0.070

Table V.1: Rate of test points that are in the 90% confidence interval and coefficient of determination for the four kernels.

D.3 Numerical experiments

We have proposed in Section D.1 a new kernel $\mathcal{K}_{\theta_1,\theta_2,\theta_3}$ defined by (V.28) on partial rankings. We show in Section D.2 that in several cases (for example with top-k partial rankings), we can reduce drastically the computation of this kernel. Another direction is given in [JV17] by considering the averaged Kendall kernel and reducing the computation of this kernel on top-k partial rankings. This kernel is available on the R package `kernrank`. We write $\mathcal{K}$ the averaged Kendall kernel, and we define $\mathcal{K}_{\theta_1} := \theta_1 \mathcal{K}$.

In this section, we compare our new kernel $\mathcal{K}_{\theta_1,\theta_2,\theta_3}$ with the averaged Kendall kernel $\mathcal{K}_{\theta_1}$ in a numerical experiment where an objective function indexed by top-k partial rankings is predicted, by Kriging. We take $N = 10$ and for simplicity, we take the same value $k = 4$ for all the top-k partial rankings. For a top-k partial ranking $I = (i_1, i_2, i_3, i_4)$, the objective function to predict is $f(I) := 2i_1 + i_2 - i_3 - 2i_4$. We make 500 noisy observations $(y_i)_{i \leq 500}$ with $y_i = f(I_i) + \varepsilon_i$, where $(I_i)_{i \leq 500}$ are i.i.d. uniformly distributed top-k partial rankings and $(\varepsilon_i)_{i \leq 500}$ are i.i.d. $\mathcal{N}(0, \lambda^2)$, with $\lambda = \frac{1}{2}$. As in Section C, we estimate (θ, λ) by maximum likelihood. Then, we compute the predictions $(\widehat{y'_i})_{i \leq 500}$ of $y' = (y'_i)_{i \leq 500}$, with y' the observations corresponding to 500 other test points $(I'_i)_{i \leq 500}$, that are i.i.d. uniform top-k partial rankings.

For the four kernels (our kernel $\mathcal{K}_{\theta_1,\theta_2,\theta_3}$ with the 3 distances and the averaged Kendall kernel $\mathcal{K}_{\theta_1}$), we provide the rate of test points that are in the 90% confidence interval together with the coefficient of determination R^2 of the predictions of the test points. Recall that

$$R^2 := 1 - \frac{\frac{1}{500} \sum_{i=1}^{500} (y'_i - \widehat{y'_i})^2}{\frac{1}{500} \sum_{i=1}^{500} \left(y'_i - \overline{y'}\right)^2},$$

where $\overline{y'}$ is the average of y'. The results are provided in Table V.1.

The rate of test points that are in the 90% confidence interval is close to 90% for the four kernels. We can deduce that the parameters (θ, λ) are well estimated by maximum likelihood, even for the averaged Kendall kernel $\mathcal{K}_{\theta_1}$.

However, we can see that the coefficient of determination of the averaged Kendall kernel $\mathcal{K}_{\theta_1}$ is close to 0. The predictions given by the averaged Kendall kernel $\mathcal{K}_{\theta_1}$ are nearly as bad as predicting with the empirical mean. In the opposite way the coefficient of determination of our kernels is larger than 0.9 for the Kendall distance, and larger than 0.99 for the Hamming distance and the Spearman distance. That means that the prediction given by our kernels are much better than the empirical mean.

To conclude, we provide a class of positive definite kernels $\mathcal{K}_{\theta_1,\theta_2,\theta_3}$ which seems to be significantly more efficient than the averaged Kendall kernel $\mathcal{K}_{\theta_1}$, in the case of Gaussian process models on partial rankings.

E Conclusion

In this work, we provide a Gaussian process model for permutations. Following the recent works of [JV17] and [MRW+16], we propose kernels to model the covariance of such processes and show the relevance of such choices. Based on the three distances on the set of permutations, Kendall's tau, Hamming distance and Spearman's footrule distance, we obtain parametric families of relevant covariance models. To show the practical efficiency of these parametric families, we apply them to the optimization of Latin Hypercube Designs. In this framework, we prove under some assumptions on the set of observations, that the parameters of the model can be estimated and the process can be forecasted using linear combinations of the observations, with asymptotic efficiency. Such results enable to extend the well-known properties of Kriging methods to the case where the process is indexed by ranks and tackle a large variety of problems. We remark that our asymptotic setting corresponds to the increasing domain asymptotic framework for Gaussian processes on the Euclidean space. It would be interesting to extend our results to more general sets of permutations under designs that do not necessarily satisfy Conditions 1 and 2.

We also show that the Gaussian process framework can be extended to the case of partially observed ranks. This corresponds to many practical cases. We provide new kernels on partial rankings, together with results that significantly simplify their computation. We show the efficiency of these kernels in simulations. We leave a specific asymptotic study of Gaussian processes indexed by partial rankings open for further research.

As highlighted in [Mar14], data consisting of rankings arise from many different fields. Our suggested kernels on total rankings and partial rankings could lead to different applications to real ranking data. We treated the case of regression in Sections C.3 and D.3. In Section C.4, we used these kernels for an optimization problem. One could also use our suggested kernels in classification, as it is done in [JV17], in [MRW+16] or in [KB10], and also using Gaussian process based classification [RW06] with ranking inputs.

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F Proofs

F.1 Proofs for Sections B and D

Proof of Proposition 48

Proof. We show that K_{θ_1,θ_2} is a strictly positive definite kernel on S_n. It suffices to prove that, if $\nu > 0$, the map K defined by

$$K(\sigma,\sigma') := e^{-\nu d(\sigma,\sigma')} \tag{V.32}$$

is a strictly positive definite kernel.

Case of the Kendall's tau distance. It has been shown in Theorem 5 of [MRW+16] that K is a strictly positive definite kernel on S_N for the Kendall's tau distance. Nevertheless, we provide here an other shorter and easier proof. The idea is to write $K(\sigma_1,\sigma_2)$ as $M(\Phi(\sigma_1),\Phi(\sigma_2))$, for an application Φ defined below, for a function M defined below and for $\sigma_1,\sigma_2 \in S_N$. We will then show that M is strictly positive definite and which will imply that K also is.

Let

$$\Phi : \begin{array}{ccc} S_N & \longrightarrow & \{0,1\}^{\frac{N(N-1)}{2}} \\ \sigma & \longmapsto & (\mathbb{1}_{\sigma(i)<\sigma(j)})_{1\leq i<j\leq N}. \end{array}$$

Further, define

$$M : \begin{array}{ccc} \{0,1\}^{\frac{N(N-1)}{2}} \times \{0,1\}^{\frac{N(N-1)}{2}} & \longrightarrow & \mathbb{R} \\ ((a_{i,j})_{i,j},(b_{i,j})_{i,j}) & \longmapsto & \exp\left(-\nu \sum_{i<j} |a_{i,j}-b_{i,j}|\right). \end{array}$$

Remark that for all σ,σ', we have

$$K(\sigma,\sigma') = M(\Phi(\sigma),\Phi(\sigma')).$$

Now, assume that M is a strictly positive definite kernel. Let $n \in \mathbb{N}$ and let $\sigma_1,\cdots,\sigma_n \in S_N$ such that $\sigma_i \neq \sigma_j$ if $i \neq j$. As Φ is injective, we have $\Phi(\sigma_i) \neq \Phi(\sigma_j)$ if $i \neq j$, and so $(K(\sigma_i,\sigma_j))_{1\leq i,j\leq n} = (M(\Phi(\sigma_i),\Phi(\sigma_j)))_{1\leq i,j\leq n}$ is a symmetric positive definite matrix. Thus, K is a strictly positive definite kernel.

It remains to prove that M is a strictly positive kernel. For all $k \in \mathbb{N}^*$, we index the elements of $\{0,1\}^k$ using the following bijective map

$$N_k : \begin{array}{ccc} \{0,1\}^k & \longrightarrow & [1:2^k] \\ (a_i)_{i\leq k} & \longmapsto & 1+\sum_{i=1}^k a_i 2^{i-1}. \end{array}$$

With this indexation, we let $\tilde{M}$ be the square matrix of size $2^{\frac{N(N-1)}{2}}$ defined by

$$\tilde{M}_{i,j} := M(N^{-1}_{\frac{N(N-1)}{2}}(i), N^{-1}_{\frac{N(N-1)}{2}}(j)).$$

By induction on k, we show that the $2^k \times 2^k$ matrix $M^{(k)}$ defined by

$$M_{i,j}^{(k)} := \exp\left(-\nu \sum_{l=1}^{k} |N_k^{-1}(i)_l - N_k^{(-1)}(j)_l|\right), \quad (i,j \in [1:2^k]),$$

is the Kronecker product of k matrices A_ν defined by

$$A_\nu := \begin{pmatrix} 1 & e^{-\nu} \\ e^{-\nu} & 1 \end{pmatrix}, \quad (\nu > 0).$$

This is obvious for $k = 1$. Assume that this is true for some k. Thus, for all $i \leq 2^k$ and $j \leq 2^k$, we have

$$\begin{aligned}
(A_\nu \otimes M^{(k)})_{i,j} &= 1M_{i,j}^{(k)} \\
&= \exp\left(-\nu \sum_{l=1}^{k} |N_k^{-1}(i)_l - N_k^{(-1)}(j)_l|\right) \\
&= \exp\left(-\nu \sum_{l=1}^{k+1} |N_{k+1}^{-1}(i)_l - N_{k+1}^{(-1)}(j)_l|\right) \\
&= M_{i,j}^{(k+1)}.
\end{aligned}$$

With the same computation, we have

$$(A_\nu \otimes M^{(k)})_{i+2^k,j+2^k} = M_{i+2^k,j+2^k}^{(k+1)}.$$

We also have

$$\begin{aligned}
(A_\nu \otimes M^{(k)})_{i+2^k,j} &= e^{-\nu} M_{i,j}^{(k)} \\
&= \exp\left(-\nu \left[1 + \sum_{l=1}^{k} |N_k^{-1}(i)_l - N_k^{(-1)}(j)_l|\right]\right) \\
&= \exp\left(-\nu \sum_{l=1}^{k+1} |N_{k+1}^{-1}(i)_l - N_{k+1}^{(-1)}(j)_l|\right) \\
&= M_{i+2^k,j}^{(k+1)},
\end{aligned}$$

and with the same computation,

$$(A_\nu \otimes M^{(k)})_{i,j+2^k} = M_{i,j+2^k}^{(k+1)}.$$

So we conclude the induction. Using this result with $k = \frac{N(N-1)}{2}$, we have that the matrix $\tilde{M}$ is the Kronecker product of positive definite matrices, thus it is positive definite and so, M is a strictly positive definite kernel.

Remark 52. *We could have showed that M is a positive definite kernel using Example 21.5.1 and Property 21.5.8 of [RKSF13] (it is a straightforward consequence of these example and property). However, these example an property do not prove the strict positive definiteness of M.*

<u>**Case of the other distances.**</u> For the Hamming distance and the Spearman's footrule distance, we show that the kernel K is strictly positive definite on the set F of the functions from $[1:N]$ to $[1:N]$. Indeed, if "for all $n \in \mathbb{N}$ and all $f_1, \cdots, f_n \in F$ such that $f_i \neq f_j$ if $i \neq j$, $(K(f_i, f_j))_{1 \leq i,j \leq n}$ is a symmetric positive definite matrix", then "for all $n \in \mathbb{N}$ and all $\sigma_1, \cdots, \sigma_n \in S_N \subset F$ such that $\sigma_i \neq \sigma_j$ if $i \neq j$, $(K(\sigma_i, \sigma_j))_{1 \leq i,j \leq n}$ is a symmetric positive definite matrix". Now, to prove the strict positive definiteness of K on F, it suffices to index the elements of F by $f_1, \cdots, f_{N^N}$ and to prove that the matrix $\tilde{M} := (K(f_i, f_j))_{1 \leq i,j \leq N^N}$ is symmetric positive definite. We index the elements of F using the following bijective map

$$J_N : \begin{array}{ccc} F & \longrightarrow & [1:N^N] \\ f & \longmapsto & 1 + \sum_{i=1}^N N^i (f(i) - 1). \end{array}$$

Thus, it suffices to show that the $N^N \times N^N$ matrices $\tilde{M}$ defined by

$$\tilde{M}_{i,j} := K\left(J_N^{-1}(i), J_N^{-1}(j)\right),$$

are positive definite matrices for these three distances. Straightforward computations show that

- For the Hamming distance, $\tilde{M}$ is the Kronecker product of N matrices, all equal to $(\exp(-\nu \mathbb{1}_{i \neq j}))_{i,j \in [1:N]}$.
- For the Spearman Footrule distance, $\tilde{M}$ is the Kronecker product of N matrices, all equal to $(\exp(-\nu|i-j|))_{i,j \in [1:N]}$.

In all cases, $\tilde{M}$ is a Kronecker product of positive definite matrices thus is also a positive definite matrix.

$\square$

Lemma 55. *For all the three distances, there exist constants $d_N \in \mathbb{N}^*$, $C_N \in \mathbb{R}$ and a function $\Phi : S_N \to \mathbb{R}^{d_N}$ such that $d(\sigma, \sigma') = C_N - \langle \Phi(\sigma), \Phi(\sigma') \rangle$. Here $\langle \cdot, \cdot \rangle$ denotes the standard scalar product on $\mathbb{R}^{d_N}$.*

Proof.

- $\frac{N(N-1)}{4} - d_\tau(\sigma, \sigma') = \frac{1}{2} \sum_{i<j} \mathbb{1}_{\sigma(i)<\sigma(j),\, \sigma'(i)<\sigma'(j)} + \mathbb{1}_{\sigma(i)>\sigma(j),\, \sigma'(i)>\sigma'(j)} - \frac{1}{2} \sum_{i<j} \mathbb{1}_{\sigma(i)<\sigma(j),\, \sigma'(i)>\sigma'(j)} + \mathbb{1}_{\sigma(i)>\sigma(j),\, \sigma'(i)<\sigma'(j)} = \langle \Phi(\sigma), \Phi(\sigma') \rangle$ where $\Phi(\sigma) \in \mathbb{R}^{\frac{N(N-1)}{2}}$ is defined by $\Phi(\sigma)_{i,j} := \frac{1}{\sqrt{2}} (\mathbb{1}_{\sigma(i)>\sigma(j)} - \mathbb{1}_{\sigma(i)<\sigma(j)})$, for all $1 \leq i < j \leq N$.

- $N - d_H(\sigma,\sigma') = \sum_{i=1}^N \mathbb{1}_{\sigma(i)=\sigma(j)} = \langle \Phi(\sigma), \Phi(\sigma')\rangle$ where $\Phi(\sigma) \in \mathcal{M}_N(\mathbb{R})$ is defined by $\Phi(\sigma) := (\mathbb{1}_{\sigma(i)=j})_{i,j}$,
- $N^2 - d_S(\sigma,\sigma') = \sum_{i=1}^N \min(\sigma(i),\sigma'(i)) + N - \max(\sigma(i),\sigma'(i)) = \langle \Phi(\sigma), \Phi(\sigma')\rangle$ where $\Phi(\sigma) \in \mathcal{M}_N(\mathbb{R})^2$ is defined by

$$\Phi(\sigma)_{i,j,1} := \begin{cases} 1 & \text{if } j \leq \sigma(i) \\ 0 & \text{otherwise,} \end{cases} \qquad \Phi(\sigma)_{i,j,2} := \begin{cases} 0 & \text{if } j < \sigma(i) \\ 1 & \text{otherwise.} \end{cases}$$

□

Proof of Proposition 49

Proof. Let us prove that d is a definite negative kernel, that is, for all $c_1, ..., c_k \in \mathbb{R}$ such that $\sum_{i=1}^k c_i = 0$, we have $\sum_{i,j=1}^k c_i c_j d(\sigma_i, \sigma_j) \leq 0$. Let $c_1, ..., c_k \in \mathbb{R}$ such that $\sum_{i=1}^k c_i = 0$ and let $\sigma_1, ..., \sigma_k \in S_N$. We have

$$\sum_{i,j=1}^k c_i c_j d(\sigma_i, \sigma_j) \quad = \quad C_N \sum_{i,j=1}^k c_i c_j - \sum_{i,j=1}^k c_i c_j \langle \Phi(\sigma_i), \Phi(\sigma_j)\rangle \leq 0,$$

as $C_N \sum_{i,j=1}^k c_i c_j = C_N \left(\sum_{i=1}^N c_i\right)^2$ is equal to 0. So, d is a negative definite kernel. Hence d^{θ_3} is a definite negative kernel for all $\theta_3 \in [0,1]$ (see for example Property 21.5.9 in [RKSF13]). The function $F : t \mapsto \theta_2 \exp(-\theta_1 t)$ is completely monotone, thus, using Schoenberg's theorem (see [BCR84] for the definitions of these notions and Schoenberg's theorem), $K_{\theta_1,\theta_2,\theta_3}$ is a positive definite kernel. □

Proof of Proposition 50

Proof. Let us write, with the notation of Lemma 55,

$$\Phi_{\text{avg}} : R \longmapsto \frac{1}{|E_R|} \sum_{\sigma \in E_R} \Phi(\sigma). \tag{V.33}$$

Then,

$$\begin{aligned} C_N - d_{\text{avg}}(R,R') &= C_N - \frac{1}{|E||E'|} \sum_{\sigma \in E_R} \sum_{\sigma \in E_{R'}} d(\sigma,\sigma') \\ &= \frac{1}{|E_R||E_{R'}|} \sum_{\sigma \in E_R} \sum_{\sigma \in E_{R'}} C_N - d(\sigma,\sigma') \\ &= \frac{1}{|E_R||E_{R'}|} \sum_{\sigma \in E_R} \sum_{\sigma \in E_{R'}} \langle \Phi(\sigma), \Phi(\sigma')\rangle \end{aligned}$$

$$= \langle \Phi_{\text{avg}}(R), \Phi_{\text{avg}}(R') \rangle.$$

Thus,

$$\begin{aligned}
d_{\text{partial}}(R, R') &= d_{\text{avg}}(R, R') - \frac{1}{2} d_{\text{avg}}(R, R) - \frac{1}{2} d_{\text{avg}}(R', R') \\
&= \frac{1}{2} \left[\left(C_N - d_{\text{avg}}(R, R) \right) + \left(C_N - d_{\text{avg}}(R', R') \right) - 2 \left(C_N - d_{\text{avg}}(R, R') \right) \right] \\
&= \frac{1}{2} \left(\|\Phi_{\text{avg}}(R)\|^2 + \|\Phi_{\text{avg}}(R')\|^2 - 2 \langle \Phi_{\text{avg}}(R), \Phi_{\text{avg}}(R') \rangle \right) \\
&= \|\Phi_{\text{avg}}(R) - \Phi_{\text{avg}}(R')\|^2.
\end{aligned}$$

□

Proof of Proposition 51

Proof. Let us prove that d_{partial} is a definite negative kernel. We define

$$D_{\text{avg}}(R, R') := \Phi_{\text{avg}}(R)^T \Phi_{\text{avg}}(R'). \tag{V.34}$$

Let $(c_1, ..., c_k) \in \mathbb{R}^k$ such that $\sum_{i=1}^k c_i = 0$. We have

$$\begin{aligned}
\sum_{i,j=1}^k c_i c_j d_{\text{partial}}(R_i, R_j) &= \sum_{i,j=1}^k c_i c_j \left[d_{\text{avg}}(R_i, R_j) - \frac{1}{2} d_{\text{avg}}(R_i, R_i) - \frac{1}{2} d_{\text{avg}}(R_j, R_j) \right] \\
&= \sum_{i,j=1}^k c_i c_j d_{\text{avg}}(R_i, R_j) - \frac{1}{2} \sum_{i=1}^k c_i d_{\text{avg}}(R_i, R_i) \sum_{j=1}^k c_j \\
&\quad - \frac{1}{2} \sum_{j=1}^k c_j d_{\text{avg}}(R_j, R_j) \sum_{i=1}^k c_i \\
&= \sum_{i,j=1}^k c_i c_j d_{\text{avg}}(R_i, R_j) \\
&= \sum_{i,j=1}^k c_i c_j \left[C_N - D_{\text{avg}}(R_i, R_j) \right] \\
&= - \sum_{i,j=1}^k c_i c_j D_{\text{avg}}(R_i, R_j) \\
&\leq 0.
\end{aligned}$$

So, d_{partial} is a definite negative kernel, and we may conclude as in the proof of Proposition 49.

□

Proof of Proposition 52

Proof. Assume that σ (resp. σ') is a uniform random variable of E_I (resp. $E_{I'}$). We have to compute $\mathrm{E}(d(\sigma,\sigma')) = d_{\text{avg}}(I,I')$ for the three distances: Kendall's tau, Hamming and Spearman's footrule.

First, we compute $\mathrm{E}(d_\tau(\sigma,\sigma'))$. Following the proof of Lemma 3.1 of [FKS03], we have

$$\mathrm{E}(d_\tau(\sigma,\sigma')) = \sum_{a<b} \mathrm{E}(K_{a,b}(\sigma,\sigma')),$$

with

$$K_{a,b}(\sigma,\sigma') = \mathbb{1}_{(\sigma(a)<\sigma(b),\sigma'(a)>\sigma'(b)) \text{ or } (\sigma(a)>\sigma(b),\sigma'(a)<\sigma'(b))}.$$

We now compute $\mathrm{E}(K_{a,b}(\sigma,\sigma'))$ for (a,b) in different cases. Let us write $J := \{j_1,\cdots,j_p\}$ and we keep the notation I (resp. I') for the set $\{i_1,...,i_k\}$ (resp. $\{i'_1,...,i'_k\}$). In this way, we have $I = J \sqcup \tilde{I}$ and $I' = J \sqcup \tilde{I}'$.

1. Consider the case where a and b are in J. There exists l and $l' \in [1:p]$ such that $a = j_l$ and $b = j_{l'}$. Then

$$K_{a,b}(\sigma,\sigma') = \mathbb{1}_{(c_{j_l}<c_{j_{l'}},c'_{j_l}>c'_{j_{l'}}) \text{ or } (c_{j_l}>c_{j_{l'}},c'_{j_l}<c'_{j_{l'}})}.$$

Thus, the total contribution of the pairs in this case is

$$\sum_{1\leq l<l'\leq p} \mathbb{1}_{(c_{j_l}<c_{j_{l'}},c'_{j_l}>c'_{j_{l'}}) \text{ or } (c_{j_l}>c_{j_{l'}},c'_{j_l}<c'_{j_{l'}})}.$$

2. Consider the case where a and b both appear in one top-k partial ranking (say I) and exactly one of i or j, say i appear in the other top-k partial ranking. Let us call P_2 the set of (a,b) such that $a<b$ and (a,b) is in this case. We have

$$\sum_{(a,b)\in P_2} K_{a,b}(\sigma,\sigma') = \sum_{\substack{a\in J,\\ b\in\tilde{I}}} K_{a,b}(\sigma,\sigma') + \sum_{\substack{a\in J,\\ b\in\tilde{I}'}} K_{a,b}(\sigma,\sigma')$$

Let us compute the first sum. Recall that $\tilde{I} = \{i_{u_1},...,i_{u_r}\}$.

$$\begin{aligned}
\sum_{\substack{a\in J,\\ b\in\tilde{I}}} K_{a,b}(\sigma,\sigma') &= \sum_{b\in\tilde{I}}\sum_{a\in J} K_{a,b}(\sigma,\sigma') \\
&= \sum_{b\in\tilde{I}} \#\{a\in J,\ \sigma(a)>\sigma(b)\} \\
&= \sum_{l=1}^{r} \#\{a\in J,\ \sigma(a)>\sigma(i_{u_l})\}
\end{aligned}$$

We order $u_1, \cdots, u_r$ such that $u_1 < \cdots < u_r$. Let $l \in [1 : r]$. Remark that $\sigma(i_{u_l}) = u_l$. We have $\#\{a \in I,\ \sigma(a) > u_l\} = k - u_l$ and $\#\{a \in \tilde{I},\ \sigma(a) > u_l\} = r - l$, thus $\#\{a \in J,\ \sigma(a) > u_l\} = k - u_l - r + l$. Then,

$$\sum_{\substack{a \in J, \\ b \in \tilde{I}}} K_{a,b}(\sigma, \sigma') = r\left(k + \frac{1-r}{2}\right) - \sum_{l=1}^{r} u_l.$$

Likewise, we have

$$\sum_{\substack{a \in J, \\ b \in \tilde{I}'}} K_{a,b}(\sigma, \sigma') = r\left(k + \frac{1-r}{2}\right) - \sum_{l=1}^{r} u'_l. \tag{V.35}$$

Finally, the total contribution of the pairs in this case is

$$r(2k + 1 - r) - \sum_{j=1}^{r} (u_j + u'_j).$$

3. Consider the case where a, but not b, appears in one top-k partial ranking (say I), and b, but not a, appears in the other top-k partial ranking (I'). Then $K_{a,b}(\sigma, \sigma') = 1$ and the total contribution of these pairs is r^2.

4. Consider the case where a and b do not appear in the same top-k partial ranking (say I). It is the only case where $K_{a,b}(\sigma, \sigma')$ is a non constant random variable. First, we show that in this case, $\mathrm{E}(K_{a,b}(\sigma, \sigma')) = 1/2$. Assume for example that I does not contain a and b. Let $(a\ b)$ be the transposition which exchanges a and b and does not change the other elements. We have

   $$\{\pi \in E_I, \pi(a) < \pi(b)\} = (a\ b)\{\pi \in E_I, \pi(a) > \pi(b)\}.$$

   Thus, there are as many $\pi \in E_I$ such that $\pi(a) < \pi(b)$ as there are $\pi \in E_I$ such that $\pi(a) > \pi(b)$. That proves that $\mathrm{E}(K_{a,b}(\sigma, \sigma')) = 1/2$.

   Then, the total distribution of the pairs in this case is

   $$\frac{1}{2}\left[\binom{|I^c|}{2} + \binom{|I'^c|}{2} - \binom{|I^c \cap I'^c|}{2}\right] = \binom{N-k}{2} - \frac{1}{2}\binom{m}{2}.$$

That concludes the computation for the Kendall's tau distance.

To compute $\mathrm{E}(d_H(\sigma,\sigma'))$, it suffices to see that

$$\begin{aligned}
\mathrm{E}(d_H(\sigma,\sigma')) &= \mathrm{E}\left(\sum_{i=1}^{n} \mathbb{1}_{\sigma(i)\neq\sigma'(i)}\right) \\
&= \sum_{l=1}^{p} \mathbb{1}_{c_{j_l}\neq c'_{j_l}} + \mathrm{E}\left(\sum_{i\neq I\cup I'} \mathbb{1}_{\sigma(i)\neq\sigma'(i)}\right) \\
&\quad + \mathrm{E}\left(\sum_{j=1}^{r} \mathbb{1}_{u_j\neq\sigma'(i_{u_j})}\right) + \mathrm{E}\left(\sum_{j=1}^{r} \mathbb{1}_{\sigma(i_{u'_j})\neq u'_j}\right) \\
&= \sum_{l=1}^{p} \mathbb{1}_{c_{j_l}\neq c'_{j_l}} + m\frac{N-k-1}{N-k} + 2r.
\end{aligned}$$

Finally, let compute $\mathrm{E}(d_S(\sigma,\sigma'))$. First, we define

- $A_c := \sum_{j=1}^{p} |c_j - c'_j|$
- $A_u(\sigma') := \sum_{j=1}^{r} |u_j - \sigma'(i_{u_j})|$
- $A_{u'}(\sigma) := \sum_{j=1}^{r} |\sigma(i'_{u'_j}) - u'_j|$
- $R(\sigma,\sigma') := \sum_{i\neq I\cup I'} |\sigma(i) - \sigma'(i)|$.

We have

$$\mathrm{E}(d_S(\sigma,\sigma')) = \mathrm{E}(A_c) + \mathrm{E}(A_u(\sigma')) + \mathrm{E}(A_{u'}(\sigma)) + \mathrm{E}(R(\sigma,\sigma')).$$

It remains to compute all the expectations appearing here.

1. $\mathrm{E}(A_c) = A_c$.

2. $\mathrm{E}(A_u(\sigma')) = \sum_{j=1}^{r} \mathrm{E}(|u_j - \sigma'(i_{u_j})|)$. If σ' is uniform on $E_{I'}$, then $\sigma'(i_{u_j})$ is uniform on $[k+1:N]$ so:

$$\mathrm{E}(|u_j - \sigma'(i_{u_j})|) = \mathrm{E}(\sigma'(i_{u_j}) - u_j) = \frac{N+k+1}{2} - u_j.$$

   Finally,

$$\mathrm{E}(A_u(\sigma')) = r\frac{N+k+1}{2} - \sum_{j=1}^{r} u_j. \tag{V.36}$$

3. $\mathrm{E}(A_{u'}(\sigma)) = r\frac{N+k+1}{2} - \sum_{j=1}^{r} u'_j$.

4. $\mathrm{E}(R(\sigma,\sigma')) = \sum_{i\neq I\cup I'} \mathrm{E}(|\sigma(i)-\sigma'(i)|)$. $\sigma(i)$ and $\sigma'(i)$ are independent uniform random variables on $[k+1:N]$.

$$\begin{aligned}\mathrm{E}(|\sigma(i)-\sigma'(i)|) &= \sum_{j=1}^{N-k-1} j\mathbb{P}(|\sigma(i)-\sigma'(i)|=j)\\ &= \sum_{j=1}^{N-k-1} j2\frac{N-k-j}{(N-k)^2}.\end{aligned}$$

Then

$$\begin{aligned}\mathrm{E}(R(\sigma,\sigma')) &= \frac{2m}{(N'+1)^2}\sum_{j=1}^{N'} j(N'+1-j)\\ &= \frac{2m}{(N'+1)^2}\left(\frac{N'(N'+1)^2}{2}-\frac{N'(N'+1)(2N'+1)}{6}\right)\\ &= mN' - \frac{mN'(2N'+1)}{3(N'+1)}.\end{aligned}$$

That concludes the proof of Proposition 52. □

Proof of Proposition 53

Proof. We define

$$\begin{aligned}a_j^{\gamma}(\sigma,\sigma') &:= |\{i\in[1:N],\ \sigma(i)\in\Gamma_j,\sigma'(i)\in\Gamma_j,\ \sigma(i)\neq\sigma'(i)\}|,\\ b_{j,l}^{\gamma}(\sigma,\sigma') &:= |\{i\in[1:N],\ \sigma(i)\in\Gamma_j,\sigma'(i)\in\Gamma_l,\ j\neq l\}|.\end{aligned}$$

Now, assume that $\sigma,\sigma'\sim\mathcal{U}(S_\gamma)$ and $\sigma_j,\sigma_j'\sim\mathcal{U}(S_{\gamma_j})$. We have

$$\begin{aligned}\mathrm{E}\left(d_H(\sigma,\sigma')\right) &= \mathrm{E}\left(\sum_{j,l=1}^{k} b_{j,l}^{\gamma}(\sigma\pi_1,\sigma'\pi_2)+\sum_{j=1}^{k} a_j^{\gamma}(\sigma\pi_1,\sigma'\pi_2)\right)\\ &= \sum_{j,l=1}^{k} b_{j,l}^{\gamma}(\pi_1,\pi_2)+\sum_{j=1}^{k}|\{i,\ \pi_1(i),\pi_2(i)\in\Gamma_j\}|\frac{\gamma_j-1}{\gamma_j}\\ &= |\{i,\ \Gamma(\pi_1(i))\neq\Gamma(\pi_2(i))\}|+\sum_{j=1}^{k}\frac{\gamma_j}{n}(\gamma_j-1).\end{aligned}$$

□

F.2 Proofs for Section C

In the following, let us write $\|.\|$ for the operator norm (for a linear mapping of $\mathbb{R}^n$ with the Euclidean norm) of a squared matrix of size n, $\|.\|_F$ for its Frobenius norm defined by $\|M\|_F^2 := \sum_{i,j=1}^n m_{ij}^2$ for $M = (m_{ij})_{1\leq i,j\leq n} \in \mathcal{M}_n(\mathbb{R})$, and let us define the norm $|\cdot|$ by $|M|^2 := \frac{1}{n}\|M\|_F^2$. We remark that, when M is a symmetric positive definite matrix, $\|M\|$ is its largest eigenvalue. In this case, we may also write $\|M\| = \lambda_{\max}(M)$, where $\lambda_{\max}(M)$ has been defined in Section C.2 and is the largest value of M. For a vector u of $\mathbb{R}^d$, for $d \in \mathbb{R}$, recall that $\|u\|$ is the Euclidean norm of u.

The proofs of Theorems 7, 8 and 9 are given in Section F.2.ii), F.2.iii) and F.2.iv) respectively. These proofs are based on Lemmas 56 to 59, that are stated and proved in Section F.2.i). The proofs of these lemmas are new. Then, having at hand the lemmas, the proof of the theorems follows [BGLV17]. We write all the proofs to be self-contained.

F.2.i) Lemmas

The following Lemmas are useful for the proofs of Theorems 7, 8 and 9.

Lemma 56. *The eigenvalues of R_θ are lower-bounded by $\theta_{3,\min} > 0$ uniformly in n, θ and Σ.*

Proof. R_θ is the sum of a symmetric positive matrix and $\theta_3 I_n$. Thus, the eigenvalues are lower-bounded by $\theta_{3,\min}$. □

Lemma 57. *For all $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{N}^3$, with $|\alpha| = \alpha_1 + \alpha_2 + \alpha_3$ and with $\partial\theta^\alpha = \partial\theta_1^{\alpha_1}\partial\theta_2^{\alpha_2}\partial\theta_3^{\alpha_3}$, the eigenvalues of $\frac{\partial^{|\alpha|}R_\theta}{\partial\theta^\alpha}$ are upper-bounded uniformly in n, θ and Σ.*

Proof. It is easy to prove when $\alpha_1 = \alpha_2 = 0$. Indeed:

1. If $\alpha_3 = 0$, then $\lambda_{\max}(R_\theta) \leq \lambda_{\max}\left((K_{\theta_1,\theta_2}(\sigma_i,\sigma_j))_{i,j}\right) + \theta_{3,\max}$ and we show that $\lambda_{\max}\left(K_{\theta_1,\theta_2}(\sigma_i,\sigma_j)_{i,j}\right)$ is uniformly bounded using Gershgorin circle theorem ([Ger31]).

2. If $\alpha_3 = 1$, then $\frac{\partial^{|\alpha|}R_\theta}{\partial\theta^\alpha} = I_n$.

3. If $\alpha_3 > 1$, then $\frac{\partial^{|\alpha|}R_\theta}{\partial\theta^\alpha} = 0$.

Then, we suppose that $(\alpha_1, \alpha_2) \neq (0,0)$. Thus,

$$\frac{\partial^{|\alpha|}R_\theta}{\partial\theta^\alpha} = \frac{\partial^{|\alpha|}\left(K_{\theta_1,\theta_2}(\sigma_i,\sigma_j)_{i,j}\right)}{\partial\theta^\alpha}.$$

It does not depend on α_3 so we can assume that $\alpha \in \mathbb{N}^2$. We have

$$\left| \frac{\partial^{|\alpha|} K_{\theta_1,\theta_2}(\sigma,\sigma')}{\partial \theta^\alpha} \right| \leq \max(1,\theta_{2,\max}) d(\sigma,\sigma')^{\alpha_1} e^{-\theta_{1,\min} d(\sigma,\sigma')}. \tag{V.37}$$

We conclude using Gershgorin circle theorem [Ger31]. □

Lemma 58. *Uniformly in* Σ,

$$\forall \alpha > 0, \ \liminf_{n\to+\infty} \inf_{\|\theta-\theta^*\|\geq\alpha} \frac{1}{n} \sum_{i,j=1}^n (R_{\theta,i,j} - R_{\theta^*,i,j})^2 > 0. \tag{V.38}$$

Proof. Let N be the norm on $\mathbb{R}^3$ defined by

$$N(x) := \max(4c\theta_{2,\max}|x_1|, 2|x_2|, |x_3|), \tag{V.39}$$

with c as in Condition 2. Let $\alpha > 0$. We want to find a positive lower-bound over $\theta \in \Theta \setminus B_N(\theta^*,\alpha)$, where $B_N(\theta^*,\alpha)$ is the ball with the norm N of center θ^* and radius α, of

$$\frac{1}{n} \sum_{i,j=1}^n (R_{\theta,i,j} - R_{\theta^*,i,j})^2. \tag{V.40}$$

Let $\theta \in \Theta \setminus B_N(\theta^*,\alpha)$.

1. Consider the case where $|\theta_1 - \theta_1^*| \geq \alpha/(4c\theta_{2,\max})$. Let $k_\alpha \in \mathbb{N}$ be the first integer such that

$$k_\alpha^\beta \geq 4c\theta_{2,\max} \frac{2 + \ln(\theta_{2,\max}) - \ln(\theta_{2,\min})}{\alpha}. \tag{V.41}$$

Then, for all $i \in \mathbb{N}^*$,

$$\left| \frac{(\theta_1^* - \theta_1) d(\sigma_i,\sigma_{i+k_\alpha}) + \ln(\theta_2) - \ln(\theta_2^*)}{2} \right| \geq 1.$$

For all $n \geq k_\alpha$,

$$\begin{aligned} & \frac{1}{n} \sum_{i,j=1}^n (R_{\theta,i,j} - R_{\theta^*,i,j})^2 \\ \geq\ & \frac{1}{n} \sum_{i=1}^{n-k_\alpha} (R_{\theta,i,i+k_\alpha} - R_{\theta^*,i,i+k_\alpha})^2 \\ \geq\ & \frac{1}{n} \sum_{i=1}^{n-k_\alpha} e^{-2\theta_{1,\max} c k_\alpha + 2\ln(\theta_{2,\min})} 4\sinh^2\left(\frac{(\theta_1^* - \theta_1) d(\sigma_i,\sigma_{i+k_\alpha}) + \ln(\theta_2) - \ln(\theta_2^*)}{2} \right) \\ \geq\ & C_{1,\alpha} \frac{n-k_\alpha}{n}, \end{aligned}$$

where we write $C_{1,\alpha} = e^{-2\theta_{1,\max} c k_\alpha + 2\ln(\theta_{2,\min})} 4\sinh^2(1)$.

2. Consider the case where $|\theta_1 - \theta_1^*| \leq \alpha/(4c\theta_{2,\max})$.

   (a) If $|\theta_2 - \theta_2^*| \geq \alpha/2$, we have

$$\begin{aligned} \frac{|\theta_1 - \theta_1^*|}{2} d(\sigma_i, \sigma_{i+1}) &< \frac{\alpha}{8\theta_{2,\max}} \\ &= \frac{\alpha}{4\theta_{2,\max}} - \frac{\alpha}{8\theta_{2,\max}} \\ &\leq \frac{|\ln(\theta_2^*) - \ln(\theta_2)|}{2} - \frac{\alpha}{8\theta_{2,\max}}. \end{aligned}$$

   Thus,

$$\left| \frac{(\theta_1^* - \theta_1) d(\sigma_i, \sigma_{i+1}) + \ln(\theta_2) - \ln(\theta_2^*)}{2} \right| \geq \frac{\alpha}{8\theta_{2,\max}}, \tag{V.42}$$

   and we have

$$\begin{aligned} & \frac{1}{n} \sum_{i,j=1}^{n} (R_{\theta,i,j} - R_{\theta^*,i,j})^2 \\ \geq\ & \frac{1}{n} \sum_{i=1}^{n-1} (R_{\theta,i,i+1} - R_{\theta^*,i,i+1})^2 \\ \geq\ & \frac{1}{n} \sum_{i=1}^{n-1} e^{-2\theta_{1,\max} c + 2\ln(\theta_{2,\min})} 4 \sinh^2 \left(\frac{\alpha}{8\theta_{2,\max}} \right) \\ =\ & C_{2,\alpha} \frac{n-1}{n}, \end{aligned}$$

   where we write $C_{2,\alpha} := e^{-2\theta_{1,\max} c + 2\ln(\theta_{2,\min})} 4 \sinh^2 \left(\frac{\alpha}{8\theta_{2,\max}} \right)$.

   (b) If $|\theta_2 - \theta_2^*| < \alpha/2$, we have $|\theta_3 - \theta_3^*| \geq \alpha$. Thus,

$$\begin{aligned} & \frac{1}{n} \sum_{i,j=1}^{n} (R_{\theta,i,j} - R_{\theta^*,i,j})^2 \\ \geq\ & \frac{1}{n} \sum_{i=1}^{n} (R_{\theta,i,i} - R_{\theta^*,i,i})^2 \\ =\ & \frac{1}{n} \sum_{i=1}^{n} (\theta_2 + \theta_3 - \theta_2^* - \theta_3^*)^2 \\ \geq\ & \frac{\alpha^2}{4}. \end{aligned}$$

Finally, if we write

$$C_\alpha := \min\left(C_{1,\alpha}, C_{2,\alpha}, \frac{\alpha^2}{2}\right), \tag{V.43}$$

we have

$$\inf_{N(\theta-\theta^*)\geq\alpha} \frac{1}{n}\sum_{i,j=1}^{n}(R_{\theta,i,j}-R_{\theta^*,i,j})^2 \geq \frac{n-k_\alpha}{n}C_\alpha. \tag{V.44}$$

To conclude, by equivalence of norms in $\mathbb{R}^3$, there exists $h>0$ such that $\|.\|_2 \leq hN(.)$, thus

$$\liminf_{n\to+\infty} \inf_{\|\theta-\theta^*\|\geq\alpha} \frac{1}{n}\sum_{i,j=1}^{n}(R_{\theta,i,j}-R_{\theta^*,i,j})^2 \geq C_{\alpha/h} > 0. \tag{V.45}$$

□

Lemma 59. $\forall(\lambda_1,\lambda_2,\lambda_3)\neq(0,0,0)$, *uniformly in* σ,

$$\liminf_{n\to+\infty}\frac{1}{n}\sum_{i,j=1}^{n}\left(\sum_{k=1}^{3}\lambda_i\frac{\partial}{\partial\theta_k}R_{\theta^*,i,j}\right)^2 > 0. \tag{V.46}$$

Proof. We have

$$\begin{aligned}
\frac{\partial}{\partial\theta_1}R_{\theta^*,i,j} &= -\theta_2^* d(\sigma_i,\sigma_j)e^{-\theta_1^* d(\sigma_i,\sigma_j)},\\
\frac{\partial}{\partial\theta_2}R_{\theta^*,i,j} &= e^{-\theta_1^* d(\sigma_i,\sigma_j)},\\
\frac{\partial}{\partial\theta_3}R_{\theta^*,i,j} &= \mathbb{1}_{i=j}.
\end{aligned}$$

Let $(\lambda_1,\lambda_2,\lambda_3)\neq(0,0,0)$. We have

$$\begin{aligned}
&\frac{1}{n}\sum_{i,j=1}^{n}\left(\sum_{k=1}^{3}\lambda_k\frac{\partial}{\partial\theta_k}R_{\theta^*,i,j}\right)^2\\
=\ &\frac{1}{n}\sum_{i\neq j=1}^{n}\left(\sum_{k=1}^{2}\lambda_k\frac{\partial}{\partial\theta_k}R_{\theta^*,i,j}\right)^2 + (\lambda_2+\lambda_3)^2\\
=\ &\frac{1}{n}\sum_{i\neq j=1}^{n} e^{-2\theta_1^* d(\sigma_i,\sigma_j)}\left(\lambda_2-\lambda_1\theta_2^* d(\sigma_i,\sigma_j)\right)^2 + (\lambda_2+\lambda_3)^2.
\end{aligned}$$

If $\lambda_1\neq 0$, then for conditions 1 and 2, we can find $\epsilon>0, \tau>0, k\in\mathbb{Z}$ so that for $|i-j|=k$, we have $(\lambda_2-\lambda_1 d(\sigma_i,\sigma_j))^2\geq\epsilon$ and $e^{-2\theta_1^* d(\sigma_i,\sigma_j)}\geq\tau$. This concludes the proof in the case $\lambda_1 \neq 0$. The proof in the case $\lambda_1 = 0$ can then be obtained by considering the pairs $(j, j+1)$ in the above display.

$\square$

With these lemmas we are ready to prove the main asymptotic results.

F.2.ii) Proof of Theorem 7

Proof. Step 1: It suffices to prove that, uniformly in Σ where we recall that $\Sigma = (\sigma_1, \cdots, \sigma_n) \in S_{N_n}$,

$$\mathbb{P}\left(\sup_{\theta\in\Theta} |(L_\theta - L_{\theta^*}) - (\mathrm{E}(L_\theta|\Sigma) - \mathrm{E}(L_{\theta^*}|\Sigma))| \geq \epsilon \middle| \Sigma\right) \to_{n\to\infty} 0, \tag{V.47}$$

and that there exists $a > 0$ such that

$$\mathrm{E}(L_\theta|\Sigma) - \mathrm{E}(L_{\theta^*}|\Sigma) \geq a\frac{1}{n}\sum_{i,j=1}^{n}(K_\theta(\sigma_i,\sigma_j) - K_{\theta^*}(\sigma_i,\sigma_j))^2. \tag{V.48}$$

Indeed, by contradiction, assume that we have (V.47), (V.48) but not the consistency of the maximum likelihood estimator. We will use a subsequence argument and thus we explicit here the dependence on n of the likelihood function (resp. the estimated parameter) writing it $L_{n,\theta}$ (resp. $\widehat{\theta}_{ML}$). Then,

$$\exists\epsilon > 0,\ \exists\alpha > 0,\ \forall n \in \mathbb{N},\ \exists m_n \geq n,\ \mathbb{P}(\|\widehat{\theta}_{m_n} - \theta^*\| \geq \epsilon) \geq \alpha. \tag{V.49}$$

Thus, with probability at least α, we have, for all n:
$\|\widehat{\theta}_{m_n} - \theta^*\| \geq \epsilon$ thus $\inf_{\|\theta-\theta^*\|\geq\epsilon} L_{m_n,\theta} \leq L_{m_n,\widehat{\theta}_{m_n}}$.
However, by definition of $\widehat{\theta}_{m_n}$, we have $L_{m_n,\widehat{\theta}_{m_n}} \leq L_{m_n,\theta^*}$.
Thus: $\inf_{\|\theta-\theta^*\|\geq\epsilon} L_{m_n,\theta} \leq L_{m_n,\theta^*}$.
Finally, with probability at least α:

$$\begin{aligned}
0 &\geq \inf_{\|\theta-\theta^*\|\geq\epsilon}(L_{m_n,\theta} - L_{m_n,\theta^*}) \\
&\geq \inf_{\|\theta-\theta^*\|\geq\epsilon} \mathrm{E}\left(L_{m_n,\theta} - L_{m_n,\theta^*}|\Sigma\right) \\
&\quad - \sup_{\|\theta-\theta^*\|\geq\epsilon} |(L_{m_n,\theta} - L_{m_n,\theta^*}) - (\mathrm{E}(L_{m_n,\theta} - L_{m_n,\theta^*}|\Sigma)| \\
&\geq \inf_{\|\theta-\theta^*\|\geq\epsilon} a|R_\theta - R_{\theta^*}|^2 - \sup_{\|\theta-\theta^*\|\geq\epsilon} |(L_{m_n,\theta} - L_{m_n,\theta^*}) - (\mathrm{E}(L_{m_n,\theta} - L_{m_n,\theta^*}|\Sigma)|,
\end{aligned}$$

using (V.48), which is contradicted using (V.47) and recalling Lemma 58. In the above display, we recall that the norm $|\cdot|$ for matrices is defined at the beginning of Section F.2. It remains to prove (V.47) and (V.48).

Step 2: We prove (V.47).
For all $\sigma \in (S_{N_n})^n$ satisfying Conditions 1 and 2, recalling that $\|\cdot\|_F^2$ and $\|\cdot\|$ are defined at the beginning of Section F.2,

$$\begin{aligned}
\mathrm{Var}(L_\theta|\Sigma=\sigma) &= \mathrm{Var}\left(\frac{1}{n}\det(R_\theta) + \frac{1}{n} y^T R_\theta^{-1} y | \Sigma = \sigma\right) \\
&= \frac{2}{n^2}\mathrm{Tr}(R_{\theta^*}R_\theta^{-1}R_{\theta^*}R_\theta^{-1}) \\
&= \frac{2}{n^2}\left\| R_{\theta^*}^{\frac{1}{2}} R_{\theta^*}^{-1} R_{\theta^*}^{\frac{1}{2}}\right\|_F^2 .
\end{aligned}$$

The previous display holds true because, with $R_{\theta^*}^{\frac{1}{2}}$, the unique matrix square root of R_{θ^*}, we have

$$\mathrm{Tr}(R_{\theta^*}R_\theta^{-1}R_{\theta^*}R_\theta^{-1}) = \mathrm{Tr}\left[\left(R_{\theta^*}^{\frac{1}{2}} R_{\theta^*}^{-1} R_{\theta^*}^{\frac{1}{2}}\right)^T \left(R_{\theta^*}^{\frac{1}{2}} R_{\theta^*}^{-1} R_{\theta^*}^{\frac{1}{2}}\right)\right] = \left\| R_{\theta^*}^{\frac{1}{2}} R_{\theta^*}^{-1} R_{\theta^*}^{\frac{1}{2}}\right\|_F^2 .$$

Then, we have the relation $\|AB\|_F^2 \leq \|A\|^2\|B\|_F^2$. Thus, we have

$$\begin{aligned}
\mathrm{Var}(L_\theta|\Sigma=\sigma) &\leq \frac{2}{n^2}\left\| R_{\theta^*}^{\frac{1}{2}} R_{\theta^*}^{-1} R_{\theta^*}^{\frac{1}{2}}\right\|_F^2 \\
&\leq \frac{2}{n^2}\left\| R_{\theta^*}^{\frac{1}{2}}\right\|^2 \|R_{\theta^*}^{-1}\|_F^2 \left\| R_{\theta^*}^{\frac{1}{2}}\right\|^2 \\
&\leq \frac{2}{n^2}\|R_{\theta^*}^{\frac{1}{2}}\|^4 n \|R_\theta^{-1}\|^2 \\
&\leq \frac{2}{n}\|R_{\theta^*}\|^2\|R_\theta^{-1}\|^2 .
\end{aligned}$$

Hence, we have

$$\mathrm{Var}(L_\theta|\Sigma=\sigma) \leq \frac{C}{n},$$

where $C>0$ is some constant independent on n, θ and Σ, using Lemmas 56 and 57 (Lemmas 56 to 59 are stated and proved in Section F.2.i)). Thus, for all σ,

$$\mathrm{Var}(L_\theta|\Sigma=\sigma) = \mathrm{E}\left((L_\theta - \mathrm{E}(L_\theta|\Sigma=\sigma))^2|\Sigma=\sigma\right) \leq \frac{C}{n},$$

so

$$\mathrm{E}\left((L_\theta - \mathrm{E}(L_\theta|\Sigma=\sigma))^2\right) \leq \frac{C}{n},$$

thus $L_\theta - \mathrm{E}(L_\theta|\Sigma) = o_{\mathbb{P}}(1)$. Let us write $z := R_\theta^{-\frac{1}{2}} y$. For $i \in \{1,2,3\}$,

$$\sup_{\theta\in\Theta}\left|\frac{\partial L_\theta}{\partial \theta_i}\right| = \sup_{\theta\in\Theta}\frac{1}{n}\left(\mathrm{Tr}\left(R_\theta^{-1}\frac{\partial R_\theta}{\partial\theta_i}\right) + z^T R_{\theta^*}^{\frac{1}{2}} R_\theta^{-1}\frac{\partial R_\theta}{\partial\theta_i}R_\theta^{-1}R_{\theta^*}^{\frac{1}{2}} z\right)$$

$$\leq \sup_{\theta\in\Theta}\left(\max\left(\|R_\theta^{-1}\|\left\|\frac{\partial R_\theta}{\partial \theta_i}\right\|, \|R_{\theta^*}\|\|R_\theta^{-2}\|\left\|\frac{\partial R_\theta}{\partial \theta_i}\right\|\right)\right)\left(1+\frac{1}{n}\|z\|^2\right).$$

Here, we have used $z^T A z \leq \|z\|^2\|A\|$ for a symmetric positive definite matrix A , the fact that $\|AB\| \leq \|A\|\|B\|$ for matrices A and B, and the fact that, by Cauchy-Schwarz,

$$\mathrm{Tr}(AB) \leq \|A\|_F\|B\|_F \leq n\|A\|\|B\|.$$

Hence, $\sup_{\theta\in\Theta}\left|\frac{\partial L_\theta}{\partial \theta_i}\right|$ is bounded in probability conditionally to $\Sigma = \sigma$, uniformly in σ. Indeed $z \sim \mathcal{N}(0, I_n)$ thus $1/n\ \|z\|^2$ is bounded in probability, conditionally to Σ and uniformly in Σ.

Then $\sup_{i\in[1:3],\theta\in\Theta}\left|\frac{\partial L_\theta}{\partial \theta_i}\right|$ is bounded in probability.

Thanks to the pointwise convergence and the boundedness of the derivatives, we have

$$\sup_{\theta\in\Theta}|L_\theta - \mathrm{E}(L_\theta)| =: r_1, \tag{V.50}$$

where r_1 depends on Σ and, for all $\varepsilon > 0$, $\mathbb{P}(|r_1| > \varepsilon) \underset{n\to+\infty}{\longrightarrow} 0$ uniformly in Σ. Hence,

$$\sup_{\theta\in\Theta}|L_\theta - \mathrm{E}(L_\theta|\Sigma)| + |L_{\theta^*} - \mathrm{E}(L_{\theta^*}|\Sigma)| =: r_2,$$

where r_2 depends on Σ and, for all $\varepsilon > 0$, $\mathbb{P}(|r_2| > \varepsilon) \underset{n\to+\infty}{\longrightarrow} 0$ uniformly in Σ. Now, let us write $D_{\theta,\theta^*} := \mathrm{E}(L_\theta|\Sigma) - \mathrm{E}(L_{\theta^*}|\Sigma)$. Thanks to (V.50),

$$\sup_{\theta\in\Theta}|L_\theta - L_{\theta^*} - D_{\theta,\theta^*}| \leq \sup_{\theta}|L_\theta - \mathrm{E}(L_\theta|\Sigma)| + |L_{\theta^*} - \mathrm{E}(L_{\theta^*}|\Sigma)|. \tag{V.51}$$

Thus

$$\sup_{\theta\in\Theta}|L_\theta - L_{\theta^*} - D_{\theta,\theta^*}| =: r_3,$$

where r_3 depends on Σ and, for all $\varepsilon > 0$, $\mathbb{P}(|r_3| > \varepsilon) \underset{n\to+\infty}{\longrightarrow} 0$ uniformly in Σ.

Step 3: We prove (V.48).
We have

$$\mathrm{E}(y^T R_\theta y|\Sigma) = \mathrm{E}(\mathrm{Tr}(y^T R_\theta y)|\Sigma) = \mathrm{E}(\mathrm{Tr}(R_\theta y y^T)|\Sigma)) = \mathrm{Tr}(R_\theta \mathrm{E}(y^T y)).$$

Thus

$$\mathrm{E}(L_\theta|\Sigma) = \frac{1}{n}\ln(\det(R_\theta)) + \frac{1}{n}\mathrm{Tr}(R_\theta^{-1}R_{\theta^*}), \tag{V.52}$$

Let us write $\phi_1(M), \cdots, \phi_n(M)$ the eigenvalues of a symmetric $n\times n$ matrix M. We have

$$D_{\theta,\theta^*} = \frac{1}{n}\ln(\det(R_\theta)) + \frac{1}{n}\mathrm{Tr}(R_\theta^{-1}R_{\theta^*}) - \frac{1}{n}\ln(\det(R_{\theta^*})) - 1$$

$$
\begin{aligned}
&= \frac{1}{n}\left(-\ln\left((\det(R_\theta^{-1})\det(R_{\theta^*})\right) + \mathrm{Tr}(R_\theta^{-1}R_{\theta^*}) - 1\right) \\
&= \frac{1}{n}\left(-\ln\left((\det(R_{\theta^*}^{\frac{1}{2}}R_\theta^{-1}R_{\theta^*}^{\frac{1}{2}})\right) + \mathrm{Tr}(R_{\theta^*}^{\frac{1}{2}}R_\theta^{-1}R_{\theta^*}^{\frac{1}{2}}) - 1\right) \\
&= \frac{1}{n}\sum_{i=1}^{n}\left(-\ln\left[\phi_i\left(R_{\theta^*}^{\frac{1}{2}}R_\theta^{-1}R_{\theta^*}^{\frac{1}{2}}\right)\right] + \phi_i\left(R_{\theta^*}^{\frac{1}{2}}R_\theta^{-1}R_{\theta^*}^{\frac{1}{2}}\right) - 1\right).
\end{aligned}
$$

Thanks to Lemmas 57 and 58, the eigenvalues of R_θ and R_θ^{-1} are uniformly bounded in θ and Σ. Thus, there exist $a > 0$ and $b > 0$ such that for all σ, n and θ, we have

$$\forall i,\ a < \phi_i\left(R_{\theta^*}^{\frac{1}{2}}R_\theta R_{\theta^*}^{\frac{1}{2}}\right) < b.$$

Let us define $f(t) := -\ln(t) + t - 1$. The function f is minimal in 1 and $f'(1) = 0$ and $f''(1) = 1$. So there exists $A > 0$ such that for all $t \in [a, b]$, $f(t) \geq A(t-1)^2$. Finally:

$$
\begin{aligned}
D_{\theta,\theta^*} &\geq \frac{A}{n}\sum_{i=1}^{n}\left(1 - \phi_i(R_{\theta^*}^{\frac{1}{2}}R_\theta^{-1}R_{\theta^*}^{\frac{1}{2}})\right)^2 \\
&= \frac{A}{n}\mathrm{Tr}\left[\left(I_n - R_{\theta^*}^{\frac{1}{2}}R_\theta^{-1}R_{\theta^*}^{\frac{1}{2}}\right)^2\right] \\
&= \frac{A}{n}\mathrm{Tr}\left[\left(R_\theta^{-\frac{1}{2}}(R_\theta - R_{\theta^*})R_\theta^{-\frac{1}{2}}\right)^2\right] \\
&= \frac{A}{n}\left\|R_\theta^{-\frac{1}{2}}(R_\theta - R_{\theta^*})R_\theta^{-\frac{1}{2}}\right\|_F^2,
\end{aligned}
$$

where we have used $\mathrm{Tr}(AA^T) = \|A\|_F^2$ for a square matrix A. Furthermore, with $\lambda_{\min}(A)$ the smallest eigenvalue of a symmetric matrix A, for any squared matrix B, we have $\|AB\|_F^2 \geq \lambda_{\min}^2(A)\|B\|^2$. This yields

$$
\begin{aligned}
D_{\theta,\theta^*} &\geq \frac{A}{n}\|R_\theta - R_{\theta^*}\|_F^2\,\lambda_{\min}^2\left(R_\theta^{-\frac{1}{2}}\right)\lambda_{\min}^2\left(R_\theta^{-\frac{1}{2}}\right) \\
&\geq a|R_\theta - R_{\theta^*}|^2,
\end{aligned}
$$

by Lemma 56, writing $a = A\theta_{3,\max}^{-2}$, and recalling that $|A|^2 = \frac{1}{n}\|A\|_F^2$ for a matrix A. $\square$

F.2.iii) Proof of Theorem 8

Proof. First, we prove (V.16). For all $(\lambda_1, \lambda_2, \lambda_3) \in \mathbb{R}^3$ such that $\|(\lambda_1, \lambda_2, \lambda_3)\| = 1$, we have

$$\sum_{i,j=1}^{3}\lambda_i\lambda_j(M_{ML})_{i,j} = \frac{1}{2n}\mathrm{Tr}\left(R_{\theta^*}^{-1}\left(\sum_{i=1}^{3}\lambda_i\frac{\partial R_{\theta^*}}{\partial\theta_i}\right)R_{\theta^*}^{-1}\left(\sum_{j=1}^{3}\lambda_j\frac{\partial R_{\theta^*}}{\partial\theta_j}\right)\right)$$

$$
\begin{aligned}
&= \frac{1}{2n}\mathrm{Tr}\left(R_{\theta^*}^{-\frac{1}{2}}\left(\sum_{i=1}^{3}\lambda_i\frac{\partial R_{\theta^*}}{\partial\theta_i}\right)R_{\theta^*}^{-\frac{1}{2}}R_{\theta^*}^{-\frac{1}{2}}\left(\sum_{j=1}^{3}\lambda_j\frac{\partial R_{\theta^*}}{\partial\theta_j}\right)R_{\theta^*}^{-\frac{1}{2}}\right)\\
&= \frac{1}{2n}\left\|R_{\theta^*}^{-\frac{1}{2}}\left(\sum_{i=1}^{3}\lambda_i\frac{\partial R_{\theta^*}}{\partial\theta_i}\right)R_{\theta^*}^{-\frac{1}{2}}\right\|_F^2,
\end{aligned}
$$

where we have used $\mathrm{Tr}(AA^T)=\|A\|_F^2$ for a square matrix A. Furthermore, using $\|AB\|_F^2\geq\lambda_{\min}^2(A)\|B\|^2$ when A is symmetric, we obtain

$$
\begin{aligned}
\sum_{i,j=1}^{3}\lambda_i\lambda_j(M_{ML})_{i,j} &\geq \frac{1}{2n}\lambda_{\min}^2\left(R_{\theta^*}^{-\frac{1}{2}}\right)\left\|\left(\sum_{i=1}^{3}\lambda_i\frac{\partial R_{\theta^*}}{\partial\theta_i}\right)\right\|_F^2\lambda_{\min}^2\left(R_{\theta^*}^{-\frac{1}{2}}\right)\\
&= \frac{1}{2\theta_{3,\max}^2}\left|\left(\sum_{i=1}^{3}\lambda_i\frac{\partial R_{\theta^*}}{\partial\theta_i}\right)\right|^2,
\end{aligned}
$$

using Lemma 56 and where we recall that $\frac{1}{n}\|\cdot\|_F^2=|\cdot|$, see the beginning of Section F.2. Hence, from Lemma 59, there exists $C_{\min}>0$ such that

$$
\liminf_{n\to\infty}\lambda_{\min}(M_{ML})\geq C_{\min}. \tag{V.53}
$$

Moreover, we have, using similar manipulations of norms on matrices above, and using $|\mathrm{Tr}(AB)|\leq\|A\|_F\|B\|_F$ from Cauchy-Schwarz,

$$
\begin{aligned}
|(M_{ML})_{i,j}| &= \left|\frac{1}{2n}\mathrm{Tr}\left(R_{\theta^*}^{-1}\frac{\partial R_{\theta^*}}{\partial\theta_i}R_{\theta^*}^{-1}\frac{\partial R_{\theta^*}}{\partial\theta_j}\right)\right|\\
&\leq \frac{1}{2n}\left\|R_{\theta^*}^{-1}\frac{\partial R_{\theta^*}}{\partial\theta_i}\right\|_F\left\|R_{\theta^*}^{-1}\frac{\partial R_{\theta^*}}{\partial\theta_j}\right\|_F\\
&\leq \frac{1}{2}\left\|R_{\theta^*}^{-1}\frac{\partial R_{\theta^*}}{\partial\theta_i}\right\|\left\|R_{\theta^*}^{-1}\frac{\partial R_{\theta^*}}{\partial\theta_j}\right\|\\
&\leq \frac{1}{2}\|R_{\theta^*}^{-1}\|^2\left\|\frac{\partial R_{\theta^*}}{\partial\theta_i}\right\|\left\|\frac{\partial R_{\theta^*}}{\partial\theta_j}\right\|\\
&\leq C_{\max},
\end{aligned}
$$

for some $C_{\max}<\infty$, from Lemmas 56 and 57. Using Gershgorin circle theorem [Ger31], we obtain

$$
\limsup_{n\to\infty}\lambda_{\max}(M_{ML})<+\infty, \tag{V.54}
$$

that concludes the proof of (V.16).

By contradiction, let us now assume that

$$
\sqrt{n}M_{ML}^{\frac{1}{2}}\left(\widehat{\theta}_{ML}-\theta^*\right)\ \underset{n\to+\infty}{\overset{\mathcal{L}}{\not\longrightarrow}}\ \mathcal{N}(0,I_3). \tag{V.55}
$$

Then, there exists a bounded measurable function $g : \mathbb{R}^3 \to \mathbb{R}$, $\xi > 0$ such that, up to extracting a subsequence, we have:

$$\left| \mathrm{E}\left[g\left(\sqrt{n} M_{ML}^{\frac{1}{2}} (\widehat{\theta}_{ML} - \theta^*) \right) \right] - \mathrm{E}(g(U)) \right| \geq \xi, \tag{V.56}$$

with $U \sim \mathcal{N}(0, I_3)$. The rest of the proof consists in contradicting (V.56).

As $0 < C_{\min} \leq \lambda_{\min}(M_{ML}) \leq \lambda_{\max}(M_{ML}) \leq C_{\max}$, up to extracting another subsequence, we can assume that:

$$M_{ML} \underset{n\to\infty}{\longrightarrow} M_\infty, \tag{V.57}$$

with $\lambda_{\min}(M_\infty) > 0$.

We have:

$$\frac{\partial}{\partial \theta_i} L_\theta = \frac{1}{n}\left(\mathrm{Tr}\left(R_\theta^{-1} \frac{\partial R_\theta}{\partial \theta_i} \right) - y^T R_\theta^{-1} \frac{\partial R_\theta}{\partial \theta_i} R_\theta^{-1} y \right). \tag{V.58}$$

Let $\lambda = (\lambda_1\ \lambda_2\ \lambda_3)^T \in \mathbb{R}^3$. For a fixed σ, denoting $\sum_{k=1}^3 \lambda_k R_{\theta^*}^{-\frac{1}{2}} \frac{\partial R_{\theta^*}}{\partial \theta_k} R_{\theta^*}^{-\frac{1}{2}} = P^T D P$ with $P^T P = I_n$ and D diagonal, $z_\sigma = P R_{\theta^*}^{-\frac{1}{2}} y$ (which is a vector of i.i.d. standard Gaussian variables, conditionally to $\Sigma = \sigma$), we have, letting $\phi_1(A), \cdots, \phi_n(A)$ be the eigenvalues of a $n \times n$ symmetric matrix A,

$$\begin{aligned}
\sum_{k=1}^3 \lambda_k \sqrt{n} \frac{\partial}{\partial \theta_k} L_{\theta^*} &= \frac{1}{\sqrt{n}} \left[\mathrm{Tr}\left(\sum_{k=1}^3 \lambda_k R_{\theta^*}^{-1} \frac{\partial R_{\theta^*}}{\partial \theta_k} \right) - \sum_{i=1}^n \phi_i \left(\sum_{k=1}^3 \lambda_k R_{\theta^*}^{-\frac{1}{2}} \frac{\partial R_{\theta^*}}{\partial \theta_k} R_{\theta^*}^{-\frac{1}{2}} \right) z_{\sigma,i}^2 \right] \\
&= \frac{1}{\sqrt{n}} \left[\sum_{i=1}^n \phi_i \left(\sum_{k=1}^3 \lambda_k R_{\theta^*}^{-\frac{1}{2}} \frac{\partial R_{\theta^*}}{\partial \theta_k} R_{\theta^*}^{-\frac{1}{2}} \right) (1 - z_{\sigma,i}^2) \right].
\end{aligned}$$

Hence, we have

$$\begin{aligned}
\mathrm{Var}\left(\sum_{k=1}^3 \lambda_k \sqrt{n} \frac{\partial}{\partial \theta_k} L_{\theta^*} \middle| \Sigma \right) &= \frac{2}{n} \sum_{i=1}^n \phi_i^2 \left(\sum_{k=1}^3 \lambda_k R_{\theta^*}^{-\frac{1}{2}} \frac{\partial R_{\theta^*}}{\partial \theta_k} R_{\theta^*}^{-\frac{1}{2}} \right) \\
&= \frac{2}{n} \sum_{k,l=1}^3 \lambda_k \lambda_l \mathrm{Tr}\left(\frac{\partial R_{\theta^*}}{\partial \theta_k} R_{\theta^*}^{-1} \frac{\partial R_{\theta^*}}{\partial \theta_l} R_{\theta^*}^{-1} \right) \\
&= \lambda^T (4 M_{ML}) \lambda \underset{n\to\infty}{\longrightarrow} \lambda^T (4 M_\infty) \lambda.
\end{aligned}$$

Hence, for almost every σ, we can apply the Lindeberg-Feller criterion to the variables $\frac{1}{\sqrt{n}} \phi_i \left(\sum_{k=1}^3 \lambda_k R_{\theta^*}^{-\frac{1}{2}} \frac{\partial R_{\theta^*}}{\partial \theta_k} R_{\theta^*}^{-\frac{1}{2}} \right) (1 - z_{\sigma,i}^2)$ to show that, conditionally to $\Sigma = \sigma$,

$\sqrt{n}\frac{\partial}{\partial\theta}L_{\theta^*}$ converges in distribution to $\mathcal{N}(0, 4M_\infty)$.

Then, using the dominated convergence theorem on Σ, we show that:

$$\mathrm{E}\left(\exp\left(i\sum_{k=1}^{3}\lambda_k\sqrt{n}\frac{\partial}{\partial\theta_k}L_{\theta^*}\right)\right)\underset{n\to\infty}{\longrightarrow}\exp\left(-\frac{1}{2}\lambda^T(4M_\infty)\lambda\right). \tag{V.59}$$

Finally,

$$\sqrt{n}\frac{\partial}{\partial\theta}L_{\theta^*}\xrightarrow[n\to\infty]{\mathcal{L}}\mathcal{N}(0,4M_\infty). \tag{V.60}$$

Let us now compute

$$\begin{aligned}\frac{\partial^2}{\partial\theta_i\partial\theta_j}L_{\theta^*} &= \frac{1}{n}\mathrm{Tr}\left(-R_{\theta^*}^{-1}\frac{\partial R_{\theta^*}}{\partial\theta_i}R_{\theta^*}^{-1}\frac{\partial R_{\theta^*}}{\partial\theta_j}+R_{\theta^*}^{-1}\frac{\partial^2 R_{\theta^*}}{\partial\theta_i\partial\theta_j}\right)\\ &\quad+\frac{1}{n}y^T\left(2R_{\theta^*}^{-1}\frac{\partial R_{\theta^*}}{\partial\theta_i}R_{\theta^*}^{-1}\frac{\partial R_{\theta^*}}{\partial\theta_j}R_{\theta^*}^{-1}-R_{\theta^*}^{-1}\frac{\partial^2 R_{\theta^*}}{\partial\theta_i\partial\theta_j}R_{\theta^*}^{-1}\right)y.\end{aligned}$$

Thus, we have,

$$\mathrm{E}\left(\frac{\partial^2}{\partial\theta_i\partial\theta_j}L_{\theta^*}\right)\underset{n\to+\infty}{\longrightarrow}(2M_\infty)_{i,j}, \tag{V.61}$$

and, using Lemmas 56 and 57, and proceeding similarly as in the proof of Theorem 7,

$$\mathrm{Var}\left(\frac{\partial^2}{\partial\theta_i\partial\theta_j}L_{\theta^*}\middle|\Sigma\right)\underset{n\to+\infty}{\longrightarrow}0. \tag{V.62}$$

Hence, a.s.

$$\frac{\partial^2}{\partial\theta_i\partial\theta_j}L_{\theta^*}\xrightarrow[n\to+\infty]{\mathbb{P}_{|\Sigma}}2(M_\infty)_{i,j}. \tag{V.63}$$

Moreover, $\frac{\partial^3}{\partial\theta_i\partial\theta_j\partial\theta_k}L_\theta$ can be written as

$$\frac{1}{n}\mathrm{Tr}(A_\theta)+\frac{1}{n}y^TB_\theta y, \tag{V.64}$$

where A_θ and B_θ are sums and products of the matrices R_θ^{-1} or $\frac{\partial^{|\beta|}}{\partial\theta^\beta}$ with $\beta\in[0:3]^3$. Hence, from Lemmas 56 and 57, we have

$$\sup_{\theta\in\Theta}\left\|\frac{\partial^3}{\partial\theta_i\partial\theta_j\partial\theta_k}L_\theta\right\|=O_{\mathbb{P}_{|\Sigma}}(1). \tag{V.65}$$

We know that, for $k\in\{1,2,3\}$, from a Taylor expansion,

$$0=\frac{\partial}{\partial\theta_k}L_{\widehat{\theta}_{ML}}=\frac{\partial}{\partial\theta_k}L_{\theta^*}+\left(\frac{\partial}{\partial\theta}\frac{\partial}{\partial\theta_k}L_{\theta^*}\right)^T(\widehat{\theta}_{ML}-\theta^*)+r_k$$

with some random r_k, such that

$$|r_k| \leq C \sup_{\theta\in\Theta,i,j} \left| \frac{\partial^3 L_\theta}{\partial\theta_i\partial\theta_j\partial\theta_k} \right| \|\widehat{\theta}_{ML} - \theta^*\|^2,$$

where C is a finite constant that come from the equivalence of norms for 3×3 matrices. Hence, from (V.65), $r_k = o_{\mathbb{P}_{|\Sigma}}(|\widehat{\theta}_{ML} - \theta^*|)$. We then have, with $\frac{\partial^2}{\partial\theta^2}L_{\theta^*}$ the 3×3 Hessian matrix of L_θ at θ^*,

$$-\frac{\partial}{\partial\theta}L_{\theta^*} = \left[\left(\frac{\partial^2}{\partial\theta^2}L_{\theta^*}\right)^T + o_{\mathbb{P}_{|\Sigma}}(1)\right]\left(\widehat{\theta}_{ML} - \theta^*\right),$$

an so

$$\left(\widehat{\theta}_{ML} - \theta^*\right) = -\left[\left(\frac{\partial}{\partial\theta}\frac{\partial}{\partial\theta}L_{\theta^*}\right)^T + o_{\mathbb{P}_{|\Sigma}}(1)\right]^{-1}\frac{\partial}{\partial\theta_k}L_{\theta^*}. \tag{V.66}$$

Hence, using Slutsky lemma, (V.63) and (V.60), a.s.

$$\sqrt{n}\left(\widehat{\theta}_{ML} - \theta^*\right) \xrightarrow[n\to+\infty]{\mathcal{L}_{|\Sigma}} \mathcal{N}\left(0,(2M_\infty)^{-1}(4M_\infty)(2M_\infty)^{-1}\right) = \mathcal{N}\left(0, M_\infty^{-1}\right). \tag{V.67}$$

Moreover, using (V.57), we have

$$\sqrt{n}M_{ML}^{\frac{1}{2}}\left(\widehat{\theta}_{ML} - \theta^*\right) \xrightarrow[n\to+\infty]{\mathcal{L}_{|\Sigma}} \mathcal{N}(0, I_3). \tag{V.68}$$

Hence, using dominated convergence theorem on Σ, we have

$$\sqrt{n}M_{ML}^{\frac{1}{2}}\left(\widehat{\theta}_{ML} - \theta^*\right) \xrightarrow[n\to+\infty]{\mathcal{L}} \mathcal{N}(0, I_3). \tag{V.69}$$

To conclude, we have found a subsequence such that, after extracting,

$$\left|\mathrm{E}\left[g\left(\sqrt{n}M_{ML}^{\frac{1}{2}}(\widehat{\theta}_{ML} - \theta^*\right)\right] - \mathrm{E}(g(U))\right| \xrightarrow[n\to+\infty]{} 0, \tag{V.70}$$

which is in contradiction with (V.56). □

F.2.iv) Proof of Theorem 9

Proof. Let $\overline{\sigma}_n \in S_{N_n}$. We have:

$$\left|\widehat{Y}_{\widehat{\theta}_{ML}}(\overline{\sigma}_n) - \widehat{Y}_{\theta^*}(\overline{\sigma}_n)\right| \leq \sup_{\theta\in\Theta}\left\|\frac{\partial}{\partial\theta}\widehat{Y}_\theta(\overline{\sigma}_n)\right\| \left\|\widehat{\theta}_{ML} - \theta^*\right\|. \tag{V.71}$$

From Theorem 7, it is enough to show that, for $i \in \{1, 2, 3\}$

$$\left| \sup_{\theta \in \Theta} \frac{\partial}{\partial \theta_i} \widehat{Y}_\theta(\overline{\sigma}_n) \right| = O_{\mathbb{P}}(1). \tag{V.72}$$

From a version of Sobolev embedding theorem ($W^{1,4}(\Theta) \hookrightarrow L^\infty(\Theta)$, see Theorem 4.12, part I, case A in [AF03]), there exists a finite constant A_Θ depending only on Θ such that

$$\sup_{\theta \in \Theta} \left| \frac{\partial}{\partial \theta_i} \widehat{Y}_\theta(\overline{\sigma}_n) \right| \leq A_\Theta \int_\Theta \left| \frac{\partial}{\partial \theta_i} \widehat{Y}_\theta(\overline{\sigma}_n) \right|^4 d\theta + A_\Theta \sum_{j=1}^{3} \int_\Theta \left| \frac{\partial^2}{\partial \theta_j \partial \theta_i} \widehat{Y}_\theta(\overline{\sigma}_n) \right|^4 d\theta.$$

The rest of the proof consists in showing that these integrals are bounded in probability. We have to compute the derivatives of

$$\widehat{Y}_\theta(\overline{\sigma}_n) = r_\theta^T(\overline{\sigma}_n) R_\theta^{-1} y$$

with respect to θ. Thus, we can write these first and second derivatives as weighted sums of $w_\theta^T(\overline{\sigma}_n) W_\theta y$, where $w_\theta(\overline{\sigma}_n)$ is of the form $r_\theta(\overline{\sigma}_n)$ or $\frac{\partial}{\partial \theta_i} r_\theta(\overline{\sigma}_n)$ of $\frac{\partial^2}{\partial \theta_j \theta_i} r_\theta(\overline{\sigma}_n)$ and W_θ is product of the matrices R_θ^{-1}, $\frac{\partial}{\partial \theta_i} R_\theta$ and $\frac{\partial^2}{\partial \theta_j \theta_i} R_\theta$. It is sufficient to show that

$$\int_\Theta \left| w_\theta^T(\overline{\sigma}_n) W_\theta y \right|^4 d_\theta = O_{\mathbb{P}}(1). \tag{V.73}$$

From Fubini-Tonelli Theorem (see [Bil13]), we have

$$\mathrm{E}\left(\int_\Theta \left| w_\theta^T(\overline{\sigma}_n) W_\theta y \right|^4 d_\theta \middle| \Sigma \right) = \int_\Theta \mathrm{E}\left(\left| w_\theta^T(\overline{\sigma}_n) W_\theta y \right|^4 \middle| \Sigma \right) d_\theta.$$

There exists a constant c so that for X a centred Gaussian random variable

$$\mathrm{E}\left(|X|^4\right) = c \mathrm{Var}(X)^2,$$

hence

$$\begin{aligned} \mathrm{E}\left(\int_\Theta \left| w_\theta^T(\overline{\sigma}_n) W_\theta y \right|^4 d_\theta | \Sigma \right) &= c \int_\Theta \mathrm{Var}\left(w_\theta^T(\overline{\sigma}_n) W_\theta y | \Sigma \right)^2 d_\theta \\ &= c \int_\Theta \left(w_\theta^T(\overline{\sigma}_n) W_\theta R_\theta^* W_\theta(\overline{\sigma}_n) w_\theta(\overline{\sigma}_n) \right)^2 d_\theta. \end{aligned}$$

From Lemma 57, there exists $B < \infty$ such that, a.s.

$$\sup_{\theta \in \Theta} \| W_\theta R_{\theta^*} W_\theta \| < B.$$

Thus

$$\mathrm{E}\left(\int_{\Theta}\left|w_\theta^T(\overline{\sigma}_n)W_\theta y\right|^4 d_\theta \middle| \Sigma\right) \leq B^2 c\int_{\Theta}\|w_\theta^T(\overline{\sigma}_n)\|^2 d_\theta. \tag{V.74}$$

Finally, for some $\alpha \in [0:2]^3$ such that $|\alpha| \leq 2$, we have

$$\sup_{\theta\in\Theta}\|w_\theta^T(\overline{\sigma}_n)\|^2 \quad = \quad \sup_\theta \sum_{i=1}^n \left(\frac{\partial^{|\alpha|}}{\partial\theta^\alpha}K_\theta(\overline{\sigma}_n,\sigma_i)\right)^2.$$

Thus, it suffices to bound this term. Using the proof of Lemma 57, there exists $A < +\infty, a > 0$ such that

$$\sup_\theta \left(\frac{\partial^{|\alpha|}}{\partial\theta^\alpha}K_\theta(\overline{\sigma}_n,\sigma_i)\right)^2 \leq A\exp\left(-ad(\overline{\sigma}_n,\sigma_i)\right).$$

Yet, choosing $i^* \in [1:n]$ such that $d(\overline{\sigma}_n,\sigma_{i^*}) \leq d(\overline{\sigma}_n,\sigma_i)$ for all $i \in [1:n]$, we have

$$d(\overline{\sigma}_n,\sigma_i) \geq \frac{1}{2}d(\sigma_i,\sigma_{i^*}).$$

Thus, we have

$$\begin{aligned}
\sup_\theta \sum_{i=1}^n \left(\frac{\partial^{|\alpha|}}{\partial\theta^\alpha}K_\theta(\overline{\sigma}_n,\sigma_i)\right)^2 \quad &\leq \quad A\sum_{i=1}^n \exp\left(-\frac{a}{2}d(\sigma_i,\sigma_{i^*})\right)\\
&\leq \quad A\sum_{i=1}^n \exp\left(-\frac{a}{2}|i-i^*|^\beta\right)\\
&\leq \quad 2A\sum_{i=0}^{+\infty} \exp\left(-\frac{a}{2}i^\beta\right)\\
&\leq \quad C.
\end{aligned}$$

That concludes the proof. □

Appendix VI

List of Symbols

List of Symbols from Part I

X	random vector modeling the inputs 9
$\mathbb{P}_X$	Distribution of the random variable X 9
$\subset$	Include or equal 9
$[1:p]$	Set of integers from 1 to p 9
x_u	$(x_i)_{i\in u}$ 9
$\lvert u\rvert$	Cardinality of u 9
L^2	Set of squared integrable functions from $(\mathcal{X}, \mathcal{E}, \mathbb{P}_X)$ to $\mathbb{R}$ 9
Y	random variable modeling the output 9
f	function in L^2 of the mapping between the inputs and the output 9
$\sigma(X_u)$	σ-algebra generated by X_u 10
H_u	Linear subspace of functions $h_u \in L^2$ such that $h_u(X)$ is $\sigma(X_u)$-measurable 10
S_u^{cl}	Closed Sobol index of the group of variable X_u 10
H_u^0	Linear subspace of L^2 of the (generalized) Hoeffding decomposition 11
f_u	Component of the (generalized) Hoeffding decomposition of f 11
S_u	Sobol index of the group of variables X_u 12
ST_i	Total Sobol index of the variable X_i 13

$(x_u^{(1)}, x_{-u}^{(2)})$	Vector of $\mathcal{X}$ such that the i-th component is $x_i^{(1)}$ if $i \in u$ and $x_i^{(2)}$ otherwise 14
S_u^{gen}	Generalized Sobol index of the group of variables X_u 20
δ_u	δ-index of the group of variables X_u 24
S_i^{full}	Full Sobol index of the variable X_i 25
ST_i^{full}	Full total Sobol index of the variable X_i 25
S_i^{ind}	Independent Sobol index of the variable X_i 25
ST_i^{ind}	Independent total Sobol index of the variable X_i 25
ϕ_i	Shapley value of player i 26
$\mathcal{S}_p$	Set of permutations of $[1:p]$ 26
$T_i(\sigma)$	Set of players preceding σ in order σ 26
η_i	Shapley effect of the variable X_i 27
V_u	$\mathrm{Var}(\mathrm{E}(Y\|X_u))$ 28
E_u	$\mathrm{E}(\mathrm{Var}(Y\|X_{-u}))$ 28
$(W_u)_{u\subset[1:p]}$	Either $(V_u)_{u\subset[1:p]}$ or $(E_u)_{u\subset[1:p]}$ 28
$S_p^{++}(\mathbb{R})$	Set of symmetric positive definite matrices of size $p \times p$ with real coefficients 29
$\Sigma_{u,v}$	Sub-matrix $(\Sigma_{i,j})_{i\in u, j\in v}$ of Σ 29
$P_i(\sigma)$	$T_i(\sigma^{-1})$ 30

List of Symbols from Part II

$\widehat{E}_{u,MC}^{known}$	Double Monte-Carlo estimator of E_u when the input distribution is known 39
$\widehat{V}_{u,PF}^{known}$	Pick-and-Freeze estimator of V_u when the input distribution is known 40
$(X^{(n)})_{nin[1:N]}$	Observed i.i.d. sample of the input vector 50
f_X	Probability density function of X with respect to a finite measure μ 51
$k_N^v(l,n)$	Index such that $X_v^{(k_N^v(l,n))}$ is the (or one of the) n-th closest element to $X_v^{(l)}$ in $(X_v^{(i)})_{i\in[1:N]}$, and such that $(k_N^v(l,n))_{n\in[1:N_I]}$ are two by two distinct 52

$\widehat{E}^{mix}_{u,MC}$	”Mix” version of the double Monte-Carlo estimator of E_u when the input distribution is unknown 53
$\widehat{E}^{knn}_{u,MC}$	”Knn” version of the double Monte-Carlo estimator of E_u when the input distribution is unknown 53
$\widehat{E}_{u,MC}$	Double Monte-Carlo estimator of E_u when the input distribution is unknown (”mix” or ”knn” version) 54
$\widehat{V}^{mix}_{u,PF}$	”Mix” version of the Pick-and-Freeze estimator of V_u when the input distribution is unknown 55
$\widehat{V}^{knn}_{u,PF}$	”Knn” version of the Pick-and-Freeze estimator of V_u when the input distribution is unknown 55
$\widehat{V}_{u,PF}$	Pick-and-Freeze estimator of E_u when the input distribution is unknown (”mix” or ”knn” version) 55

List of Symbols from Part III

μ	Mean of the Gaussian input vector X 68
Σ	Covariance matrix of the Gaussian input vector X 68
β	Vector containing the coefficients of the linear function f 68
K	Number of independent groups of input variables 73
V^g_w	$\mathrm{Var}(\mathrm{E}(Y\|A_w))$ 74
g_w	Component of the Hoeffding decomposition of g corresponding to the variable A_w 74
S^g_w	Sobol index of the groups of variables A_w 74
$V^{g,w}_u$	$\mathrm{Var}(\mathrm{E}(g_w(A_w)\|X_u))$ 74
$S^{g,w}_u$	Shapley effect of the variable X_u for the function g_w 74
$\eta^{g,w}_i$	Shapley effect of the variable X_i for the function g_w 74
$j(i)$	Index of the group of i, that is $i \in B_{j(i)}$ 74
m	Maximal size of group of input variables 77

y	Limit of p/n in $]0,1[$ 82
$(X^{(l)})_{l\in[1:n]}$	Observed i.i.d. sample of the input vector 82
$\mathcal{P}_p$	Set of partitions of $[1:p]$ 83
Γ_B	block-diagonal matrix with the same coefficients as Γ in the block-diagonal structure B and with zero coefficients out of the block-diagonal structure B 83
$S_p^{++}(\mathbb{R}, B)$	Set of the symmetric positive definite matrices whose block-diagonal structure is B 83
$B(\Gamma)$	Block-diagonal structure of Γ 83
B^*	Block-diagonal structure of Σ 83
$\overline{X}$	Empirical estimator of μ 83
S	Empirical estimator of Σ 83
l_Γ	Log-likelihood in Γ and $\overline{X}$ 84
pen	Block-diagonal promoting penalization function 84
Φ	Penalized log-likelihood function from $S_p^{++}(\mathbb{R})$ 84
κ	Penalization coefficient 84
Ψ	Penalized log-likelihood function from $\mathcal{P}_p$ 84
$\widehat{B}_{tot}$	Estimator of B^* that reaches the minimum of Ψ 84
$\|M\|_{\max}$	Norm max of M 85
$B(\alpha)$	Partition given by thresholding Σ by $n^{-\alpha}$ 85
$\widehat{C}_{ij}$	Coefficient of the empirical correlation matrix 86
B_λ	Partition given by thresholding the empirical correlation matrix by λ 86
$\widehat{B}_{\widehat{C}}$	Argument of the minimum of Ψ over all the partitions given by thresholding the empirical correlation matrix 86
$\widehat{B}_\lambda$	Partition given by thresholding the empirical correlation matrix by $n^{-1/3}$ 86
$\widehat{B}_s$	Argument of the minimum of Ψ over the partitions given by thresholding the empirical correlation by $(k/p)_{k\in[1:p]}$ with a maximal size of group smaller or equal than m 86
$\|\cdot\|_F$	Frobenius norm 87

$\tilde{Y}$	Vector of noisy observations 93
$\eta(Z, g)$	vector containing all the Shapley effects with input vector Z and model g 99
$X^{\{n\}}$	Gaussian vector with parameter $\mu^{\{n\}}$ and $\Sigma^{\{n\}}$ 100
$f_1^{\{n\}}(x)$	Image of $x - \mu^{\{n\}}$ through the differential of f at $\mu^{\{n\}}$ 100
$\tilde{f}_{1,h^{\{n\}}}^{\{n\}}(x)$	Image of $x - \mu^{\{n\}}$ through a finite difference approximation of the differential of f at $\mu^{\{n\}}$ 102
$\widehat{f}_{lin}^{\{n\}(N)}$	Linear regression of f with a sample of $X^{\{n\}}$ of size N 102
$\widehat{X}^{\{n\}}$	Empirical mean of an i.i.d. sample $(U^{(l)})_{l\in[1:n]}$ 105

List of Symbols of the article on permutations

E_N	Set of integers from 1 to N 219
S_N	Set of permutations of E_N 219
d_τ	Kendall's tau distance 222
d_H	Hamming distance 222
d_S	Spearman's footrule distance 222
K_{θ_1,θ_2}	Family of strictly positive definite kernels on S_N 223
$K_{\theta_1,\theta_2,\theta_3}$	Family of positive definite kernels on S_N 223
Y	Gaussian process on S_N 224
$\widehat{\theta}_{ML}$	Maximum likelihood estimator of θ^* 225
L_θ	Log-likelihood 225
R_θ	Covariance matrix of the observations 225
$\widehat{Y}_{\widehat{\theta}_{ML}}$	Prediction of Y by plugging the estimated parameter in the conditional expectation expression for Gaussian processes 227
E_R	Subset of S_N corresponding to the partial ranking R 234
d_{avg}	Measure of dissimilarity between partial rankings 235
d_{partial}	Pseudometric on partial rankings 235
$\mathcal{K}_{\theta_1,\theta_2,\theta_3}$	Positive definite kernel on partial rankings 236

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Appendix VII

Résumé en français

L'analyse de sensibilité est un outil important qui permet d'analyser des modèles mathématiques et des codes de calculs. Elle révèle les variables d'entrées les plus influentes sur la variable de sortie, en leur affectant une valeur appelée "indice de sensibilité". Dans ce cadre, les effets de Shapley, récemment définis par Owen, permettent de gérer des variables d'entrées dépendantes. Cependant, l'estimation de ces indices n'est proposée dans l'état de l'art que dans deux cadres très particuliers : lorsque la loi du vecteur d'entrée est connue ou lorsque les entrées sont gaussiennes et le modèle est linéaire. Cette thèse se divise en deux parties, correspondantes à ces deux cadres d'estimation.

Dans la première partie, nous nous intéressons à l'estimation des effets de Shapley lorsque la loi du vecteur d'entrée est connue. L'estimateur proposé dans l'état de l'art demande de pouvoir générer des échantillons selon les lois conditionnelles de la distribution du vecteur d'entrée. Nous proposons une nouvelle méthode d'estimation plus efficace et les paramètres optimaux sont calculés dans un cadre théorique. Ensuite, nous élargissons le cadre d'application de ces estimateurs lorsque nous ne pouvons pas générer selon les lois conditionnelles mais lorsqu'un échantillon du vecteur d'entrée est disponible. Nous proposons une méthode d'estimation basée sur une méthode de plus proches voisins permettant de remplacer la connaissance des lois conditionnelles. Nous montrons la convergence de ces nouveaux estimateurs et des applications numériques sont réalisées sur des données simulées et des données réelles. Un des estimateurs, qui prend en compte des variables catégorielles et réelles (continues ou non), a été implémenté dans le package `sensitivity` sous la fonction "shapleySubsetMC".

La deuxième partie porte sur les effets de Shapley dans le cadre linéaire. A l'aide de l'état de l'art, nous proposons un algorithme permettant de calculer les valeurs théoriques des effets de Shapley dans ce cadre lorsque les paramètres sont connus. Cependant, nous soulignons les problèmes de calculs liés à la grande dimension. Nous proposons alors des solutions lorsque la matrice de covariance du vecteur d'entrée est diagonale par blocs et en déduisons un algorithme implémenté dans le package `sensitivity` sous la fonction "shapleyLinearGaussian". Cet algorithme est ensuite testé sur des données réelles provenant de la sûreté nucléaire.

Nous poursuivons les travaux sur le cadre linéaire gaussien, avec une matrice de covariance diagonale par blocs lorsque les paramètres sont inconnus. Nous traitons le cas où la dimension du vecteur d'entrée est fixé ainsi que celui où la dimension du vecteur d'entrée converge vers l'infini, à la même vitesse que le nombre d'observations. Nous proposons des estimateurs diagonaux par blocs de la matrice de covariance et nous en déduisons des estimateurs des effets de Shapley dont l'erreur totale converge vers 0 et fournissons des vitesses de convergence. Un de ces estimateurs a été implémenté dans le package `sensitivity` sous la fonction "shapleyBlockEstimation". Nous appliquons cet estimateur des effets de Shapley à des données semi-réelles.

Enfin nous nous intéressons aux cadres proches du cadre linéaire gaussien. Dans un premier temps nous traitons le cas où le vecteur d'entrée est gaussien avec une matrice de covariance convergeant vers 0 et le modèle n'est pas linéaire. Nous prouvons que la différence entre les effets de Shapley correspondant au modèle non linéaire et les effets de Shapley correspondant à une approximation linéaire du modèle converge vers 0. Nous fournissons, pour chaque approximation linéaire une vitesse de convergence. Dans un deuxième temps, nous supposons que le vecteur d'entrée est une moyenne empirique (pas nécessairement gaussienne). Nous montrons que, lorsque la taille de l'échantillon permettant de calculer la moyenne empirique tend vers l'infini, les effets de Shapley convergent vers des effets de Shapley provevant du cadre linéaire gaussien. Nous proposons enfin un cadre pratique où le vecteur d'entrée est une moyenne empirique et où les effets de Shapley fournissent des informations importantes.

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Titre: Analyse de sensibilité en présence de variables aléatoires dépendantes : Estimation des effets de Shapley pour une distribution d'entrée inconnue et pour des modèles linéaires gaussiens

Mots clés: Analyse de sensibilité, Indices de Sobol, Effets de Shapley, Estimation de matrices de covariance diagonales par blocs.

Résumé: L'analyse de sensibilité est un outil puissant qui permet d'analyser des modèles mathématiques et des codes de calculs. Elle révèle les variables d'entrées les plus influentes sur la variable de sortie, en leur affectant une valeur appelée "indice de sensibilité". Dans ce cadre, les effets de Shapley, récemment définis par Owen, permettent de gérer des variables d'entrées dépendantes. Cependant, l'estimation de ces indices ne peut se faire que dans deux cadres très particuliers : lorsque la loi du vecteur d'entrée est connue ou lorsque les entrées sont gaussiennes et le modèle est linéaire. Cette thèse se divise en deux parties. Dans la première partie, l'objectif est d'étendre les estimateurs des effets de Shapley lorsque seul un échantillon des entrées est disponible et leur loi est inconnue. La deuxième partie porte sur le cas linéaire gaussien. Le problème de la grande dimension est abordé et des solutions sont proposées lorsque les variables forment des groupes indépendants. Enfin, l'étude montre comment les effets de Shapley du cadre linéaire gaussien peuvent estimer ceux d'un cadre plus général.

Title: Sensitivity analysis with dependent random variables: Estimation of the Shapley effects for unknown input distribution and linear Gaussian models

Keywords: Sensitivity analysis, Sobol indices, Shapley effects, Estimation of block-diagonal covariance matrices.

Abstract: Sensitivity analysis is a powerful tool to study mathematical models and computer codes. It reveals the most impacting input variables on the output variable, by assigning values to the the inputs, that we call "sensitivity indices". In this setting, the Shapley effects, recently defined by Owen, enable to handle dependent input variables. However, one can only estimate these indices in two particular cases: when the distribution of the input vector is known or when the inputs are Gaussian and when the model is linear. This thesis can be divided into two parts. First, the aim is to extend the estimation of the Shapley effects when only a sample of the inputs is available and their distribution is unknown. The second part focuses on the linear Gaussian framework. The high-dimensional framework is addressed and solutions are suggested when there are independent groups of variables. Finally, it is shown how the values of the Shapley effects in the linear Gaussian framework can estimate the Shapley effects in more general settings.

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