On dependent generalized sensitivity indices and asymptotic distributions

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Abstract: In this paper, we propose a novel methodology for better performing uncertainty and sensitivity analysis for complex mathematical models under constraints and/or with dependent input variables, including correlated variables. Our approach allows for assessing the single, overall and interactions effects of any subset of input variables, that account for the dependencies structures inferred by the constraints. Using the variance as importance measure among others, we define the main-effect and total sensitivity indices of input(s) with the former index less than the latter. We also derive the consistent estimators and asymptotic distributions of such indices by distinguishing the case of the multivariate and/or functional outputs, including spatio-temporal models and dynamic models.

Keywords and phrases: Copulas, Dependent multivariate sensitivity analysis, Multivariate conditional quantile transform, Conditional quantile regression.

1. Introduction

Performing uncertainty and sensitivity analysis of complex mathematical models under constraints and in presence of dependent and/or correlated input variables still remains a challenge issue when one is interested in assessing the contribution of any subset of input variables and their interactions. Indeed, the dependencies inferred by the constraints on mathematical models and/or input variables, and the dependencies among inputs may have significant impact on the results of Sobol’ indices and generalized sensitivity analysis ([31, 36, 35, 9, 10, 61, 32]).

In the presence of dependent and/or correlated input variables, most existing variance-based methodologies provide the same main-effect index of one input or one block of dependent inputs ([60, 37, 27, 13, 2, 26]). Some of these approaches provide the total index of inputs, and there can be cases for which the main-effect index is greater than the total index. To be able to rank input variables, Mara et al. ([38, 58]) and Mara and Tarantola ([58]) have proposed a methodology that ensures that the main-effect index is always less than the total index for each single input. In the same sense, Lamboni and Kucherenko ([34]) have proposed in-depth approach for quantifying the effects of each single input and some subsets of inputs (but not all of them) by making use of dependency models of dependent variables. Such approach is competitive to be used regarding the computations of dependent generalized sensitivity indices for all types of dependencies among input variables. However, their approach does not allow for quantifying the effects of two inputs.
from the same block of dependent variables for instance, and it does not address the problem of constraints on a given mathematical model.

The inverse Rosenblatt transformations ([43]) and its generalization known as the multivariate conditional quantile transform ([43, 54, 1, 49]), and the conditional distribution method ([5, 40]) imply a regression representation of dependent random variables ([54, 52, 51]) or a structural equation modeling of a random vector ([45, 46]). In this paper, we propose a generic method for better assessing the impact of any subset of uncertain inputs on mathematical models under constraints and/or with dependent variables, including correlated and/or constrained input variables. Our approach consists in i) deriving the dependency functions, including empirical dependency functions, by making use of a regression representation of a dependent random vector, ii) coupling such dependency functions with the initial models for performing uncertainty quantification (UQ) and sensitivity analysis (SA) in presence of all type of dependencies of input variables.

In Section 2, firstly, we provide generic and general dependency functions of dependent variables following any distribution. A dependency model, which captures the dependency structures of a given dependent variables, expresses a subset of dependent input variables as a function of innovation variables and the remaining variables. Secondly, we introduce the dependency function transform, which avoids searching dependency functions for some distributions by making use of some well-known dependency functions ([34]). Thirdly, the empirical dependency function is investigated when the analytical distributions of input variables are not available. It could be the case of most complex mathematical models under constraints such as the outputs belong to a given domain, which introduce some dependencies among input variables. In Section 3, we formalize different (but equivalent) representations of a mathematical model under constraints that includes dependent and/or independent random variables by using the dependency functions provided in Section 2. Such equivalent representations (in distribution) of mathematical models are useful to assess the main and total effects of any subset of dependent variables. Using Such equivalent representations, we extend the dependent MSA (dMSA) ([34]) in Section 4 by providing dependent generalized sensitivity indices (dGSIs) of any subset of inputs and for the multivariate and/or functional outputs, including spatio-temporal models and dynamic models. Section 5 aims at constructing unbiased estimators of the cross-covariances of sensitivity functionals and the consistent estimators of dGSIs defined in Section 4. We also provide the asymptotic distributions of dGSIs, which can be used for deriving the asymptotic confident intervals of dGSIs. We illustrate our approach by means of analytical test cases in Section 6, and we conclude this work in Section 7.
General notation

For integer $d \in \mathbb{N}^*$, we use $\mathbf{X} := (X_1, \ldots, X_d)$ for a vector of input variables. For $v \subseteq \{1, \ldots, d\}$, we use $\mathbf{X}_v := (X_j, j \in v)$, $\mathbf{X}_{\sim v} := (X_j, j \in \{1, \ldots, d\} \setminus v)$ and $|v|$ for its cardinality (i.e., the number of elements in $v$). Thus, we have the partition $\mathbf{X} = (\mathbf{X}_v, \mathbf{X}_{\sim v})$. We also use $\mathbf{Z} \overset{d}{=} (\mathbf{X}_v, \mathbf{X}_{\sim v})$ to say that $\mathbf{Z}$ and $(\mathbf{X}_v, \mathbf{X}_{\sim v})$ have the same CDF. For $\mathbf{a} \in \mathbb{R}^n$, we use $||\mathbf{a}||_{L^2}$ for the Euclidean norm. For a matrix $\Sigma \in \mathbb{R}^{n \times n}$, we use $\text{Tr}(\Sigma)$ for the trace of $\Sigma$, and $||\Sigma||_F := \sqrt{\text{Tr}(\Sigma \Sigma^T)}$ for the Frobenius norm of $\Sigma$. We use $\mathbb{E}[:]$ for the expectation and $\mathbb{V}[:]$ for the variance-covariance. In what follows, we consider only deterministic functions.

2. Dependency function of dependent random variables

This section provides generic dependency functions of dependent variables following any distribution. A dependency function, which captures the dependency structures of a given dependent variables, aims at expressing a subset of dependent input variables as a function of independent ones consisted of the remaining variables and new variables.

It is common to say that a vector of $d$ random variables $\mathbf{X}$ has $F$ as the joint cumulative distribution function (CDF) and $C$ as copula, that is, $F(\mathbf{X}) = C(F_1(X_1), \ldots, F_d(X_d))$ with $F_j$ or $F_j^{-1}$ the marginal CDF of $X_j$, $j = 1, \ldots, d$. We use $F_j^{-1}$ for the generalized inverse of $F_j$, that is, $F_j^{-1}(z) := \inf_{x \in \mathbb{R}} \{x : F_j(x) \geq z\}$. When $X_j$ is a continuous random variable, we have $F_j^{-1} =: F_j^{-1}$. We use $F_{jk}$ for the conditional distribution of $X_j$ given $X_k$ with $j, k = 1, \ldots, d$ and $j \neq k$.

For the sequel of generality, let us consider the distribution transform of $X_j$ given by $\tau_{F_j}(x_i, \lambda_i) = \mathbb{P}(X_i < x_i) + \lambda_i \mathbb{P}(X_i = x_i)$ with $\lambda_i \in [0, 1]$ and $i = 1, \ldots, d$. Such distribution transform ensures that ([8, 49, 50, 51])

$$\tau_{F_j}(X_i, U_i) \sim \mathcal{U}(0, 1), \quad (1)$$

$$\lambda_i \overset{d}{=} \tau_{F_j}^{-1}(\tau_{F_j}(X_i, U_i)) \quad \text{a.s.} \quad (2)$$

with $U_i \sim \mathcal{U}(0, 1)$. For absolutely continuous distributions, it is to be noted that Equation (1) comes down to the Rosenblatt transform ([47]), and Equation (2) is equivalent to the inverse of the Rosenblatt transform (i.e., $X_i \overset{d}{=} F_i^{-1}(Z_i)$) ([43]). Equation (2) is part of the multivariate conditional quantile transform ([43, 1, 49]), which implies a regression representation of dependent variables ([54, 52, 51]).

Namely, we use $w := (w_1, \ldots, w_{d-1})$ for an arbitrary permutation of $\{1, \ldots, d\} \setminus \{j\}$, $\mathbf{X}_{\sim j} := (X_{w_1}, \ldots, X_{w_{d-1}})$ and $\mathbf{Z} \sim \mathcal{U}(0, 1)^{d-1}$ for $d - 1$ independent uniform variables, a regression repre-
sentation of $X$ is given by ([54, 52, 50, 51])

$$
X_{w_1} = f_{w_1}(X_j, Z_{w_1})
X_{w_{d-1}} = f_{w_{d-1}}(X_j, X_{w_1}, ..., X_{w_{d-2}}, Z_{w_{d-1}}),
$$

(3)

where $(f_{w_1}, ..., f_{w_{d-1}})$ are measurable functions and $Z$ some innovation. The regression representation of $X$ given by Equation (3) implies the existence of a dependency function $r_j : \mathbb{R}^d \to \mathbb{R}^{d-1}$ given by ([34])

$$
X_{\sim j} \overset{d}{=} r_j(X_j, Z) = \begin{bmatrix}
  r_{w_1}(X_j, Z_{w_1}) = f_{w_1}(X_j, Z_{w_1}) \\
  r_{w_2}(X_j, Z_{w_1}, Z_{w_2}) = f_{w_2}(X_j, r_{w_1}(X_j, Z_{w_1}), Z_{w_2}) \\
  \vdots \\
  r_{w_{d-1}}(X_j, Z) = f_{w_{d-1}}(X_j, r_{w_1}(X_j, Z_{w_1}), ..., r_{w_{d-2}}(\cdot), Z_{w_{d-1}})
\end{bmatrix},
$$

(4)

where $(r_{w_1}, ..., r_{w_{d-1}})$ are measurable functions, $Z$ and $X_j$ are independent. In general, for integer $p \leq d - 1$ and $u := (j, w_1, \ldots, w_p)$, there exists a measurable function $r_u : \mathbb{R}^d \to \mathbb{R}^{d-|u|}$ and independent random variables $Z_{\sim u} \sim U(0, 1)^{d-|u|}$ such that

$$
X_{\sim u} = r_u(X_u, Z_{\sim u}),
$$

(5)

where $X_u$ is independent of $Z_{\sim u}$.

It is to be noted that the dependency functions $r_u$ is not unique. For instance, one may replace the uniform distribution with any continuous distribution. If we want to keep working with the initial marginal distribution, we can replace the variable $Z_{w_i}$ with

$$
\begin{cases}
  F_{w_i}(X_{w_i}) & \text{if } F_{w_i} \text{ is continuous} \\
  \tau_{F_{w_i}}(X_{w_i}, U_{w_i}) & \text{if } F_{w_i} \text{ is discrete}
\end{cases}.
$$

**Proposition 1** Consider the generic dependency function $r_j = (r_{w_1}, ..., r_{w_{d-1}})$ given by (4) and an integer $p \leq d - 1$.

(i) If we use $u = \{j, w_1, \ldots, w_p\}$, then

$$
X_u \overset{d}{=} (X_j, r_{w_1}(X_j, Z_1), \ldots, r_{w_p}(X_j, Z_1, \ldots, Z_{w_p})) ,
$$

(6)

(ii) For all permutation of $u$ noted $v$ and $Z_{\sim u} \sim U(0, 1)^{d-|u|}$, we have

$$
X_{\sim u} \overset{d}{=} r_u(X_u, Z_{\sim u}) \overset{d}{=} r_v(X_v, Z_{\sim u}) .
$$

(7)
2.1. Distribution-based and copula-based expressions of dependency functions

The distribution-based dependency function is derived from the regression representation of $X$ ([54, 52, 50, 51], and it is given by ([34])

$$
 r^*_j (X_j, \mathbf{Z}) = \begin{bmatrix}
 F^{-1}_{u_1|j} (Z_{w_1} | X_j) \\
 \vdots \\
 F^{-1}_{w_{d-1}|j,w_1,...,w_{d-2}} (Z_{w_{d-1}} | X_j, r_{w_1}(X_j, Z_{w_1}), \ldots, r_{w_{d-2}}(X_j, Z_{w_1}, \ldots, Z_{w_{d-2}})) 
\end{bmatrix}. \tag{8}
$$

Likewise, the copula-based dependency function is of interest to master all joint distributions with the same copula, and it is derived from [50]. For independent variables $U \sim \mathcal{U}(0, 1)^d$, $\mathbf{Z}$ and $X_j$, the copula-based expression of $r^*_j$ is given by

$$
 r^*_j (X_j, \mathbf{Z}, U) = \begin{bmatrix}
 \tau^*_F (C^{-1}_{u_1|j} (Z_{w_1} | r_{F_j}(X_j, U_j))) \\
 \vdots \\
 \tau^*_F (C^{-1}_{w_{d-1}|j} (Z_{w_{d-1}} | \tau_{F_j}(X_j, U_j), \tau_{F_{u_1}} (r_{w_1}(X_j, Z_{w_1}, U_j), U_{w_1}), \ldots)) 
\end{bmatrix}, \tag{9}
$$

bearing in mind a general sampling algorithm based on copulas ([41, 40]).

For the Gauss copula with absolutely continuous margins, the dependency function in Equation (9) has a particular form (see [34]). In order to give a dependency function that is suitable for discrete and/or continuous margins, let $C^{Gauss}(U_1, \ldots, U_d, \mathcal{R})$ be the Gauss copula having $\mathcal{R}$ as the correlation matrix, $\mathcal{L}$ be the Cholesky factor of $\mathcal{R}$, that is, $\mathcal{R} = \mathcal{L} \mathcal{L}^T$, $\Phi$ be the CDF of the standard Gaussian distribution and $\mathcal{I}$ be the identity matrix.

Lemma 1 Consider independent variables $\mathbf{Z} \sim \mathcal{N}_{d-1} (0, \mathcal{I})$ and $U_j \sim \mathcal{U}(0, 1)$.

If $X = (X_j, X_{\sim j})$ has the copula $C^{Gauss} (U_j, U_{w_1}, \ldots, U_{w_{d-1}}, \mathcal{R})$ and margins $F_i$, $i = 1, \ldots, d$, then, the dependency function $r^*_j : \mathbb{R}^{d+1} \rightarrow \mathbb{R}^{d-1}$ is given by

$$
 X_{\sim j} \overset{d}{=}_j r^*_j (X_j, \mathbf{Z}, U_j) = \begin{bmatrix}
 X_{w_1} = F^{-1}_{w_1} [\Phi (Y_{w_1})] \\
 \vdots \\
 X_{w_{d-1}} = F^{-1}_{w_{d-1}} [\Phi (Y_{w_{d-1}})] 
\end{bmatrix}, \tag{10}
$$

where

$$
 Y_{\sim j} = \mathcal{L} \begin{bmatrix}
 \Phi^{-1} (\tau_{F_j}(X_j, U_j)) \\
 \mathbf{Z}
\end{bmatrix}_{\sim 1}.
$$

The symbol $[\bullet]_{\sim 1}$ means that the first coordinate is excluded.

Proof. See Appendix A.
It is worth noting that we have to replace $\tau F_j(X_j, U_j)$ with $F_j(X_j)$ in Lemma 1 for continuous variable $X_j$.

For the Student copula, we use $t(\nu, 0, 1)$ for the standard $t$-distribution with $\nu$ degrees of freedom and $T_\nu$ for its CDF. We provide the dependency function in Lemma 2.

**Lemma 2** Consider independent variables $Z_{w_i} \sim t(\nu + i, 0, 1)$, $i = 1, \ldots, d - 1$ and $U_j \sim U(0, 1)$.

If $X = (X_j, X_{-j})$ has the Student copula $C_{St} (U_j, U_{w_1}, \ldots, U_{w_{d-1}}, \nu, R)$ and margins $F_i$, $i = 1, \ldots, d$, then, the dependency function $r_j : \mathbb{R}^{d+1} \to \mathbb{R}^{d-1}$ is given by

$$X_{-j} \overset{d}{=} r_j (X_j, Z, U_j) = \begin{bmatrix}
X_{w_1} &=& F_{w_1}^{-1} \left( T_\nu \left( Y_{w_1} \right) \right) \\
\vdots \\
X_{w_{d-1}} &=& F_{w_{d-1}}^{-1} \left( T_\nu \left( Y_{w_{d-1}} \right) \right)
\end{bmatrix},$$

where

$$Y_{-j} = \mathcal{L} \begin{bmatrix}
\sqrt{\nu + (T^{-1}_\nu (\tau F_j (X_j, U_j)))^2} Z_{w_1} \\
\vdots \\
\sqrt{\nu + (T^{-1}_\nu (\tau F_j (X_j, U_j)))^2} \prod_{k=1}^{d-2} (\nu + k)^2 Z_{w_{d-1}}
\end{bmatrix} \sim 1.$$

**Proof.** See Appendix B.

### 2.2. Transform of dependency functions

Many transformations such as monotonic transformations are widely used in probability and statistics, and it is interesting to investigate the derivation of the dependency functions of dependent variables defined through such transformations (see Proposition 2). To that end, for an invertible transformation $T$, we use $T^{-1}$ for the inverse of $T$. For a matrix $\Sigma \in \mathbb{R}^{n \times d}$ and $j \in \{1, \ldots, d\}$, we use $\Sigma_{j-\theta} \in \mathbb{R}^{1 \times d}$ for the matrix containing only the $j^{th}$ row of $\Sigma$ and $\Sigma_{-j-\theta} \in \mathbb{R}^{n-1 \times d}$ for the matrix containing all rows of $\Sigma$ except the $j^{th}$ row. We use $S$ for a sign random variable, that is, $\mathbb{P}(S = 1) = \mathbb{P}(S = -1) = 1/2$. It is also known that $S$ is Rademacher-distributed.

**Proposition 2** Consider a dependency function $r_u (X_u, Z, U)$ of $X$. Let $T_u : \mathbb{R}^{[u]} \to \mathbb{R}^{[u]}$ be an invertible transformation, $T_{-u} : \mathbb{R}^{d-[u]} \to \mathbb{R}^{n}$ be a measurable function and $S := (S_1, \ldots, S_n)$ be independent sign variables.
(i) If $Y := (Y_u, Y_w_u) \overset{d}{=} (T_u(X_u), T_w_u(X_w_u))$, then we have

$$Y_{\sim u} = T_{\sim u} \left( r_u \left( T_u^{-1}(Y_u), Z, U \right) \right). \tag{12}$$

(ii) If $|Y_u|, |Y_w_u| \overset{d}{=} (T_u(X_u), T_w_u(X_w_u))$, $Y$ is independent of $S$ and $Y_i$ has a symmetric distribution about 0 for all $i \in \{ \{1, \ldots, d\} \setminus u \}$, then we have

$$Y_{\sim u} = \text{diag}(S) T_{\sim u} \left( r_u \left( T_u^{-1}(|Y_u|), Z, U \right) \right), \tag{13}$$

with $\text{diag}(S)$ a diagonal random matrix of size $n \times n$.

**Proof.** See Appendix C. \hfill \square

**Corollary 1** Let $r_j(X_j, Z, U)$ be a dependency function of $X$, $S := (S_1, \ldots, S_d)$ be independent sign variables, $\Sigma := \begin{bmatrix} \Sigma_{j \sim \emptyset} & \Sigma_{j \sim 0} \\ \Sigma_{\sim j \sim \emptyset} & \Sigma_{\sim j \sim 0} \end{bmatrix} \in \mathbb{R}^{n \times d}$ and $\mu \in \mathbb{R}^n$.

(i) If $(Y_j, Y_{\sim j}) = \Sigma X + \mu$ with $\Sigma_{j \sim \emptyset} = [\Sigma_{jj}, 0, \ldots, 0]$ and $\Sigma_{jj} \neq 0$, then

$$Y_{\sim j} = \Sigma_{\sim j \sim \emptyset} r_j \left( \frac{Y_j - \mu_j}{\Sigma_{jj}}, Z, U \right) + \mu_{\sim j}. \tag{14}$$

(ii) If $Y_i = T_i(X_i)$ with $i = 1, \ldots, d$ and $T_j$ is invertible, then we have

$$Y_{w_i} = T_{w_i} \left( r_{w_i} \left( T_j^{-1}(Y_j), Z_{w_1}, \ldots, Z_{w_i}, U_j, U_{w_1}, \ldots, U_{w_i} \right) \right). \tag{15}$$

(iii) If $|Y_i| = T_i(X_i)$ with $i = 1, \ldots, d$, $Y$ is independent of $S$, $T_j$ is invertible and $Y_j$ has a symmetric distribution about 0 with $j \in \{1, \ldots, d\} \setminus \{j_0\}$, then we have

$$Y_{w_i} = S_{w_i} \times T_{w_i} \left( r_{w_i} \left( T_j^{-1}(|Y_j|), Z_{w_1}, \ldots, Z_{w_i}, U_j, U_{w_1}, \ldots, U_{w_i} \right) \right). \tag{16}$$

**Proof.** See Appendix D. \hfill \square

When the transformation $T_j$ is strictly increasing on the range of $X_j$ with $j = 1, \ldots, d$, Equation (15) is still valid, and it provides a dependency function of $(T_1(X_1), \ldots, T_d(X_d))$. In particular, for continuous variable $X_j$, it is known that $(T_1(X_1), \ldots, T_d(X_d))$ and $X$ have the same copula but different margins. Therefore, Corollary 1 gives a way for deriving the dependency function of $(T_1(X_1), \ldots, T_d(X_d))$ without explicitly using its margins. Proposition 2 and Corollary 1 extend the multivariate conditional method, as the dependency function can be used for sampling random values as well.
2.3. Empirical dependency functions

This section deals with the derivation of dependency functions for unknown distributions or known distributions under complex constraints such as \( c(X) \) belongs to a domain of interest \( D \) with \( c: \mathbb{R}^d \to \mathbb{R}^n \) a measurable function. For instance, \( c \) may represent a complex mathematical model that simulates a phenomenon of interest or any function of the latter, that is, \( c = h \circ f \) with \( f \) the model and \( h \) a given function.

Formally, we are interested in deriving a dependency function of a random vector defined by

\[
X^c \overset{d}{=} \{ X \sim F : c(X) \in D \}.
\]

(17)

It is clear that the constraint \( c(X) \in D \) infers dependencies on input variables \( X \). While for some distributions and constraints, we are able to derive the analytical distribution of \( X^c \) and the associated dependency function (see [34]), we have to estimate the dependency function in general.

It is common to assume that we observe or we can generate a sample of \( X^c \), that is, \( X^c_1, \ldots, X^c_m \) using Equation (17). With such sample, there is a huge literature about fitting a distribution to that observations. We distinguish mainly two ways to derive the empirical dependency functions.

2.3.1. Distribution-based empirical dependency functions

One may use either the parametric or semi parametric or non-parametric approach for estimating the distribution of \( X^c \) and its dependency functions. The following bullets summary non-exhaustive properties of the above methods.

- A parametric approach requires assuming the form of the distribution with unknown parameters. The method of moments or the maximum likelihood methods are then applied to obtain the estimations of the unknown parameters.

- A non-parametric methods such as the kernel methods ([48, 44, 7, 53]) and the empirical distribution (i.e., \( F_n \)) avoid any assumption about the form of the distribution.

- A combination of both approaches can lead to a semi-parametric methods.

Copulas remain a successful way of modeling dependence for multivariate distributions ([3, 17, 40, 50, 55, 6]). With the sample \( X^c_1, \ldots, X^c_m \), we are able to form a pseudo-sample from the copula \( C \) and use a copula approach to estimate the distribution of \( X^c \). A copula approach consists in i) fitting all the marginal distribution using one of the above methods, ii) generating a pseudo-sample from the copula, that is, \( \hat{F}_1(X^c_{i1}), \ldots, \hat{F}_d(X^c_{id}) \) for absolutely continuous variables and
\( \tau_{F_1}(X_{c1}^i, U_1), \ldots, \tau_{F_d}(X_{c1}^d, U_d) \) in general with \( i = 1, \ldots, m \), iii) adjusting a copula to the observations. Such approach is computationally attractive in high dimension when the associated copula has few parameters to be estimated. More details about different ways to fit a copula to a data or observations and their drawbacks can be found in [12, 11, 17, 16, 39, 41, 40, 18, 6].

For parametric copulas such as the Gauss and Student copulas, we can use the pairwise inversion of the extended Spearman rho given by

\[
\rho_S := \rho\left(\tau_{F_1}(X_{j1}, U_{j1}), \tau_{F_2}(X_{j2}, U_{j2})\right) = 12\mathbb{E}[C(Z_{j1}, Z_{j2})] - 3,
\]

or the Kendall tau to estimate the correlation matrix of the associated copula ([12, 16, 39]). The Kendall tau for continuous variables \( X_{j1} \) and \( X_{j2} \) is given by

\[
\rho_{\tau} := \mathbb{E}\left[\text{sign}\left((X_{j1} - X'_{j1})(X_{j2} - X'_{j2})\right)\right] = 4\mathbb{E}[C(U_1, U_2)] - 1,
\]

where \((U_1, U_2) \sim C\), \(X'_{j1}\) and \(X'_{j2}\) are independent copies of \(X_{j1}\) and \(X_{j2}\), respectively.

The Spearman rho is linked to the correlation of the Gauss copula as follows:

\[
\rho_S = \frac{6}{\pi} \arcsin \left(\frac{R_{j1,j2}}{2}\right).
\]

For elliptical copulas, including Gauss and Student copulas, we have the identify

\[
\rho_{\tau} = \frac{2}{\pi} \arcsin (R_{j1,j2}).
\]

We then derive the dependency function using Equation (9) or other equations provided in Sections 2.1-2.2.

2.3.2. Empirical conditional quantile estimator as dependency functions

This section aims at using a non-parametric estimation of conditional quantile function ([22, 59, 15, 24, 23, 19, 21, 57]) to derive a dependency function. Considering the loss function of Koenker and Bassett ([22]), that is, \( L(x, u) = x \left( u - \mathbb{I}_{\{x < 0\}} \right) \) with \( u \in [0, 1] \), we can express a dependency function as follows:

\[
r_j(X_{j1}^c, Z_{w1}) := \arg\min_{f \in \mathcal{F}} \mathbb{E}\left[ L(X_{w1}^c, f(X_{j1}^c), Z_{w1}) \mid X_{j1}^c, Z_{w1} \right],
\]

where \( \mathcal{F} \) is a class of smooth functions, and \( Z_{w1} \sim \mathcal{U}(0, 1) \) is independent of \((X_{j1}^c, X_{w1}^c)\). While a value of \( Z_{w1} \) controls the quantile of interest, all the values of \( Z_{w1} \) are important for a dependency function.
Since the distribution of \((X^c_j, X^c_{w1})\) is unknown, and we have only a sample of \((X^c_j, X^c_{w1})\), the M-estimator of a dependency function with penalty is given by ([57], Lemma 3)

$$\hat{r}_j(X^c_j, Z_{w1}) := \arg \min \limits_{f \in H} \sum_{i=1}^{m} L(X^c_{i,w1} - f(X^c_{i,j}), Z_{w1}) + \frac{\lambda}{2} \|f(X^c_j) - b\|_H^2,$$

where \(\lambda \in \mathbb{R}^+\) is a bandwidth, \(\|\cdot\|_H\) is a norm defined on RKHS \(H\), and \(b \in \mathbb{R}\).

We can extend Equation (18) to obtain a dependency function of the form

$$r_u(X^c_{u1}, Z_{w1}) := \arg \min \limits_{f \in F} E \left[ L(X^c_{w1} - f(X^c_u), Z_{w1}) \mid X^c_{u1}, Z_{w1} \right].$$

2.3.3. Extension

When the constrained function \(c\) involves a complex mathematical model, which is time demanding to get one model run, we should replace such model with its emulator. The Gaussian process ([4, 14, 20, 42]) is an interesting candidate, as it handles dependent variables as well.

As a conclusion of this section, we assume in what follows that the dependency functions for any distribution is known and ready to be used.

3. Representation of functions with dependent variables

This section formalizes different representations of a function that includes dependent and/or independent random variables. Formally, for \(\Theta \subseteq \mathbb{R}\) and \(d, n \in \mathbb{N}^*\), we consider a function \(f : \mathbb{R}^d \times \Theta \to \mathbb{R}^n\), which may represent any multivariate and functional outputs such as spatio-temporal models or dynamic models. When \(\Theta = \{\theta_0\}\), it is clear that we obtain a class of functions with multivariate outputs or the multivariate response models. For \(\theta \in \Theta\), the function \(f(\cdot, \theta)\) may includes independent and/or dependent variables. In what follows, we assume that

(A1): the random vector \(X := (X_j, j \in \{1, \ldots, d\})\) is consisted of \(K\) independent random vector(s), that is, \(X = (X_k, k = 1, \ldots, K)\) where \(X_{k_1}\) is independent of \(X_{k_2}\) for \(k_1, k_2 \in \{1, \ldots, K\}\) and \(k_1 \neq k_2\). Without loss of generality, we suppose \(X_{1}\) is a random vector of \(d_1 \geq 0\) independent variable(s); \(X_k\) with \(k \geq 2\) is a random vector of \(d_k \geq 2\) dependent variables.

Assumption (A1) is always hold, and under (A1), we have \(d = \sum_{k=1}^{K} d_k\). When \(K = 1\) we have only independent input variables, and when \(d_1 = 0\) we have only \(K - 1\) independent random vector(s) of dependent variables. When \(d_1 \geq 1\), we use \(\mathbf{o} := \{1, \ldots, d_1\}\) and \(X_\mathbf{o}\) represents \(X_{1}\), the original independent variables. For all \(j_k \in \{1, \ldots, d_k\}\), we use \(X_{j_k}\) for an element of \(X_k\) with \(k = 2, \ldots, K\). We also use \(\mathbf{s} := \{j_k, k = 2, \ldots, K\}\), \(X_\mathbf{s} := (X_j, j \in \mathbf{s})\) for a vector of \(K - 1\)
selected variables from \((X_k, k = 2, \ldots, K)\) and \(X_{\sim \mathbf{s}} := (X_{\sim j_k}, k = 2, \ldots, K)\). Thus, we have the following partitions of input variables

\[
(X_k, k = 2, \ldots, K) = (X_s, X_{\sim \mathbf{s}}), \quad X = (X_o, X_s, X_{\sim \mathbf{s}}).
\]  

(20)

Bearing in mind the dependency function (see Section 2), we can represent \(X_k\) with \(k = 2, \ldots, K\) as follows:

\[
\begin{aligned}
X_{\sim j_2} &\overset{d}{=} r_{j_2} (X_{j_2}, Z_2) \\
& \vdots \\
X_{\sim j_K} &\overset{d}{=} r_{j_K} (X_{j_K}, Z_K)
\end{aligned}
\]

(21)

where \(Z_k := (Z_{w_1, k}, \ldots, Z_{w_{d_k-1}, k})\) is a random vector of \(d_k - 1\) independent variables, \(X_{j_k}\) is independent of \(Z_k\) with \(k = 2, \ldots, K\). When we use \(Z := (Z_k, k = 2, \ldots, K)\) and assumption (A1) holds, then \((X_o, X_s, Z)\) is a random vector of independent variables. By compiling all the dependency functions given by (21) in one function, we obtain the function \(r_s : \mathbb{R}^{d-d_1} \to \mathbb{R}^{d-d_1-K+1}\) given by

\[
r_s(X_s, Z) = (r_{j_2} (X_{j_2}, Z_2), \ldots, r_{j_K} (X_{j_K}, Z_K)) .
\]

(22)

Thus, Equation (21) becomes

\[
X_{\sim \mathbf{s}} \overset{d}{=} r_s(X_s, Z),
\]

(23)

and we have the following partition

\[
X \overset{d}{=} (X_o, X_s, r_s(X_s, Z)) .
\]

(24)

**Remark 1** It worth noting that when some inputs are discrete, we have sometime to include additional and independent uniformly distributed variables \(U\) in the dependency function (see Equation (1)). Indeed, we have \(U_{w_i} = \tau_{F_{w_i}} (X_i, U_{w_i})\) and the copula-based dependency function becomes

\[
X_{\sim \mathbf{s}} \overset{d}{=} r_s(X_s, Z_o, U), \quad X \overset{d}{=} (X_o, X_s, r_s(X_s, Z_c, U)) ,
\]

where \((Z_c, U)\) is a vector of independent variables with \(U\) a vector of size the number of discrete variables. We can see that \(Z_o\) and \(X_{\sim \mathbf{s}}\) have the same dimension. For concise notation, we use \(Z = (Z_c, U)\).

Now, let us take a function that includes \(X\) as inputs, that is, \(f(X, \theta)\) and consider a function \(g : \mathbb{R}^{|\mathbf{x}|} \times \Theta \to \mathbb{R}^n\) given by

\[
g(X_o, X_s, Z, \theta) = f(X_o, X_s, r_s(X_s, Z), \theta) .
\]

(25)

The function \(g\) is a composition of \(f(\cdot, \theta)\) by the dependency function (24), and it includes only independent variables \((X_o, X_s, Z)\). Lemma 3 provides useful properties of \(g(X_o, X_s, Z, \theta)\) linked
to \( f(X, \theta) \). Namely, we use \((w_{1,k}, \ldots, w_{d_k-1,k})\) for an arbitrary permutation of \(\{1, \ldots, d_k\} \setminus \{j_k\}\), \(v_k := (w_{1,k}, \ldots, w_{p_k,k})\) where \(0 \leq p_k \leq d_k - 1\) and \(u_k := (j_k, v_k)\) with \(k = 2, \ldots, K\). When \(p_k = 0\) we have \(v_k = \emptyset\) and \(u_k = \{j_k\}\) by definition.

**Lemma 3** Consider \(u_0 \subseteq \emptyset\) and \(\{k_1, \ldots, k_m\} \subseteq \{2, \ldots, K\}\). Under assumption (A1), we have the following equalities in distribution.

\[
\begin{align*}
f(X, \theta) | X_{u_0}, X_{j_{k_1}}, \ldots, X_{j_{k_m}} & \stackrel{d}{=} g(X_{u_0}, X_{s}, Z, \theta) | X_{u_0}, X_{j_{k_1}}, \ldots, X_{j_{k_m}}, \quad (26) \\
\text{for all } \{j_{k_1}, \ldots, j_{k_m}\} & \subseteq s, \\
f(X, \theta) | X_{u_0}, X_{u_{k_1}}, \ldots, X_{u_{k_m}} & \stackrel{d}{=} g(X_{u_0}, X_{s}, Z, \theta) | X_{u_0}, X_{j_{k_1}}, X_{v_{k_1}}, \ldots, X_{j_{k_m}}, Z_{v_{k_m}}, \quad (27)
\end{align*}
\]

**Proof.** See Appendix E.

It comes out from Lemma 3 that the distribution of \(f(X, \theta)\) given the inputs \((X_{u_0}, X_{u_{k_1}}, \ldots, X_{u_{k_m}})\) is equivalent (in distribution) to the conditional distribution of \(g(X_{o}, X_{s}, Z, \theta)\) given \((X_{u_0}, X_{j_{k_1}}, Z_{v_{k_1}}, \ldots, X_{j_{k_m}}, Z_{v_{k_m}})\). Thus, Lemma 3 gives us the ability to assess the effect of the inputs \((X_{u_0}, X_{u_{k_1}}, \ldots, X_{u_{k_m}})\) on \(f(X, \theta)\) by making use of the function \(g(X_{o}, X_{s}, Z, \theta)\) and some of its inputs, that is,

\((X_{u_0}, X_{j_{k_1}}, Z_{v_{k_1}}, \ldots, X_{j_{k_m}}, Z_{v_{k_m}})\).

**Definition 1** Let \(u \subseteq \{1, \ldots, d\}\) and \(g(X_{o}, X_{s}, Z, \theta)\) be a function that includes independent inputs.

A function \(g(\cdot)\) is said to be an equivalent representation of \(f(X, \theta)\) regarding the input \(X_u\) if we can determine the distribution \(f(X, \theta)|X_u\) using \(g(\cdot)\) and some of its inputs.

Thus, according to Lemma 3, \(g(X_{o}, X_{s}, Z, \theta)\) is an equivalent representation of \(f\) regarding \((X_{u_0}, X_{u_{k_1}}, \ldots, X_{u_{k_m}})\). Such representation, which is associated with the selected inputs \(X_s\), can be used to assess the effects of all inputs given by \((X_{u_0}, X_{u_{k_2}}, \ldots, X_{u_{k_m}})\) with \(u_0 \subseteq \emptyset\), \(\{k_1, \ldots, k_m\} \subseteq \{2, \ldots, K\}\). Another representations of \(f(X, \theta)\) are necessary for assessing the effects of the variables that belong to \(X_{\sim j_k}\) with \(k = 2, \ldots, K\). A permutation of the elements of the vector \(X_k\) with \(k = 2, \ldots, K\) will allow for assessing more inputs’ effects. Of course, we have \(R_{j_k} := (d_k - 1)! \left( \prod_{k=2}^{K} d_k! \right)^{-1} \) equivalent representations of \(f\) (out of \(\prod_{k=2}^{K} d_k!\)) that allow for assessing the effects of \(X_{j_{k_1}}\). However, such representations are not sufficient for quantifying all the effects of inputs (or group of inputs).
Definition 2 For \( v \subseteq \{1, \ldots, d\} \), let \( X_v \) be the variables of interest, and consider two equivalent representations of \( f \) such as \( g_1, g_2 \) with \( g_1 \neq g_2 \).

The functions \( g_1, g_2 \) are said replicated representations of \( f \) regarding \( X_v \) if both representations allow for determining the conditional distribution \( f(X, \theta)|X_v \).

Obviously, such replicated representations should be avoided when we are only interested in the conditional distribution of \( f \) given \( X_v \). However, remark that replicated representations are sometime necessary to determine other conditional distributions. Therefore, replicated representations regarding an input or group of inputs should be avoided as much as possible. Since a replicated representation of \( f \) can be obtained by just permuting some elements of \( \{1, \ldots, d\} \), it is interesting to be able to recover all the subsets of \( \{1, \ldots, d\} \) by using few and necessary permutations of \( \{1, \ldots, d\} \). Namely, let \( \pi_{\ell_k}(\{1, \ldots, d\}) \) be the \( \ell_k \)th permutation of \( \{1, \ldots, d\} \) with \( \ell_k = 1, \ldots, d! \) for all \( k \in \{2, \ldots, K\} \). We use Algorithm 1 to select such necessary permutations (see Lemma 4). Formally, let us consider integers given by

\[
j_{0,k} = \begin{cases} \frac{d_k}{2} & \text{if } d_k \text{ is even} \\ \frac{d_k+1}{2} & \text{otherwise} \end{cases}, \quad k = 2, \ldots, K, \tag{28}
\]

and the sets \( A_{j_{0,k}} \) given by

\[
A_{j_{0,k}} = \{ u \subseteq \{1, \ldots, d\} : |u| = j_{0,k} \}, \quad k = 2, \ldots, K.
\]

The set \( A_{j_{0,k}} \) is consisted of all the subsets of \( \{1, \ldots, d\} \) that contain exactly \( j_{0,k} \) elements, and we can see that the cardinal of \( A_{j_{0,k}} \) is given by \( |A_{j_{0,k}}| = \binom{d_k}{j_{0,k}} \). For a given permutation \( w_k := \pi_{\ell_k}(\{1, \ldots, d\}) \), we use the vector \( w_k = (w_{1,k}, \ldots, w_{d_k,k}) \) to report (in order) the elements of that permutation. For instance, \( w_{1,k} \) is the first element of that permutation, and \( w_{d_k,k} \) is the...
Algorithm 1: Construction of the sets $B_k$ and $P_k$, $k = 2, \ldots, K$.

**Initialization:**

$B_k \leftarrow P_k \leftarrow \mathcal{E} \leftarrow \emptyset$; $i \leftarrow e_0 \leftarrow 1$;

$A_{j_0,k} \leftarrow \{u \subseteq \{1, \ldots, d_k\} : |u| = j_0,k\}$;

while $|A_{j_0,k}| > 0$ do

Find a permutation $w_k \leftarrow \pi_{e_k}(1, \ldots, d_k)$ such that:

- $\{w_{1,k}, \ldots, w_{j_0,k}\} \notin B_k$, $\forall j = e_0, \ldots, j_0,k$ and
- $\{w_{d_k-j_0,k+1}, \ldots, w_{d_k,k}\} \notin \mathcal{E}$, $\forall j = e_0, \ldots, j_0,k$ and $\{w_{1,k}, \ldots, w_{j_0,k,k}\} \in A_{j_0,k}$;

$A_{j_0,k} \leftarrow A_{j_0,k} \setminus \{w_{1,k}, \ldots, w_{j_0,k,k}\}$;

$B_k \leftarrow B_k \cup \{w_{1,k}, \ldots, w_{j_0,k}\}$,

$\forall j = e_0, \ldots, d_k - e_0 + 1$;

$\mathcal{E} \leftarrow \mathcal{E} \cup \{w_{j,k}, \ldots, w_{d_k,k} : j = j_0,k + 1, \ldots, d_k - e_0 + 1\}$;

$P_k \leftarrow P_k \cup w_k$;

$i \leftarrow i + 1$;

if $(d_k)_{e_0} < i \leq (d_k)_{e_0+1}$ then

$e_0 \leftarrow e_0 + 1$;

end

end

The set $P_k$ from Algorithm 1 contains $(d_k)_{j_0,k}$ permutations $(w_k)$ selected out of $d_k!$ permutations.

The set $B_k$ is built using the set $P_k$, and it is consisted of sets containing the first $j$ elements of $w_k$ with $j = 1, \ldots, d_k$ and for all $w_k \in P_k$. Lemma 4 provides interesting properties of the sets $P_k$ and $B_k$.

**Lemma 4** Consider an integer $j_0,k$ given by (28) and the sets $B_k, P_k$ given by Algorithm 1. Then, we have

$$B_k = \{u \subseteq \{1, \ldots, d_k\} : |u| > 0\}.$$  \hspace{1cm} (29)

$$B_k = \{\{w_{1,k}, \ldots, w_{j,k}\}, j = 1, \ldots, d_k : \forall w_k \in P_k\}.$$  \hspace{1cm} (30)

**Proof.** See Appendix F.

Using Lemma 4, we are able to quantify the necessary and sufficient number of equivalent representation(s) of $f$ given $X_u$ for all $u \subseteq \{1, \ldots, d\}$ (see Theorem 1). For $w_k \in P_k$, recall that $w_{\sim,1,k} := (w_{2,k}, \ldots, w_{d_k,k})$ and the cardinal $|P_k| = (d_k)_{j_0,k}$ with $k = 2, \ldots, K$. 

Theorem 1 Let $X$ be $d$ dependent variables, $p_2, \ldots, p_K$ be integers, and assume that (A1) holds. Then,

(i) the minimal number of equivalent representations of $f$ given $X_v$ for all $v \subseteq \{1, \ldots, d\}$ (i.e., $g$) is given by

$$R_{\text{min}} := \prod_{k=2}^{K} \binom{d_k}{j_0,k}.$$ \hspace{1cm} (31)

Such representations are given by

$$f(X, \theta) \overset{d}{=} g_{\ell}(X_o, X_{w_1,2}, \ldots, X_{w_{-1,K}}, Z_{w_{-1,1,K}}, \theta),$$ \hspace{1cm} (32)

where $\ell := (w_{2}, \ldots, w_{K})$ for all $w_k \in \mathcal{P}_k$ and $k = 2, \ldots, K$.

(ii) The minimal number of representations of $f$ given $X_v$ for all

$$v \in \{\{u_0, u_2, \ldots, u_K\} : u_0 \subseteq \mathcal{O}, u_k \subseteq \{1, \ldots, d_k\}, |u_k| \leq p_k \leq j_0,k, k = 2, \ldots, K\}$$

is given by

$$R_{p_2,\ldots,p_K} := \max_{2 \leq k \leq K} \binom{d_k}{p_k}.$$ \hspace{1cm} (33)

Proof. See Appendix G.

\[\square\]

Equation (32) from Theorem 1 provides generic representations of $f$. It is worth noting that any representation of $f$ shares the same distribution with $f$ (see Lemma 3), and two different representations of $f$ must be independent to avoid misleading dependencies. When the function includes only independent variables, it is obvious that the number of representation $R_{\text{min}} = 1$. Reducing $R_{\text{min}}$ will depend on the analysis of interest. For instance, one representation of $f$ is sufficient to determine the conditional distribution of $f$ given $X_v$ for all

$$v \in \{\{u_0, w_{1,k}, \ldots, w_{j,k}\} : u_0 \subseteq \mathcal{O}, j = 0, \ldots, d_k, k = 2, \ldots, K\}.$$ \hspace{1cm} (34)

In the same sense, $R_1 = \max(d_2, \ldots, d_K)$ equivalent representations of $f$ can be used for assessing the effects of $X_j$ for all $j \in \{1, \ldots, d\}$. It is worth noting that the above number of representations can lead to assess the effects of other inputs or groups of inputs.

4. Dependent multivariate sensitivity analysis

In this section, we define and study the properties of dependent generalized sensitivity indices (dGSIs) for any model $f$ that includes dependent and/or independent variables by making use of its equivalent representations. For the sequel of generality, let us consider a function that includes $d$ input variables $X$ and provides $n$ functional outputs given by $f(X, \theta) \in \mathbb{R}^n$ with $\theta \in \Theta$ and
\( \Theta \subseteq \mathbb{R} \). Under assumption (A1), let us recall an equivalent representation of \( f \) (see Equation (32)), that is,

\[
\begin{align*}
    f (X, \theta) & \overset{d}{=} g_\ell (X_\alpha, X_{w,2}, Z_{w,-1,2}, \ldots, X_{w,1,K}, Z_{w,1,K}, \theta),
\end{align*}
\]

where \( \ell = (w_2, \ldots, w_K) \), \( w_k \in \mathcal{P}_k \) and \( k = 2, \ldots, K \).

It is to be noted that the function \( g_\ell (X_\alpha, X_{w,2}, Z_{w,-1,2}, \ldots, X_{w,1,K}, Z_{w,1,K}, \theta) \) includes only independent variables, and we are going to define the dGSIs by using the classical multivariate sensitivity analysis ([36, 9, 31, 30]) associated with \( g_\ell \). To ensure that the proposed dGSIs in this section are well defined, we assume that

\[
(A2): 0 < \int_{\Theta} \mathbb{E} \left[ ||f (X, \theta)||^2_{L_2} \right] d\theta < +\infty.
\]

The definitions of GSIs and dGSIs are based on sensitivity functionals (SFs), which contain all information about the single and overall contributions of input variables over the whole model outputs ([28, 29, 30, 31, 32, 33, 34]).

Namely, for integer \( p_k \) with \( 0 \leq p_k \leq d_k \), we use \( v_k := \{w_{2,k}, \ldots, w_{p_k,k}\} \) and \( u_k = \{w_{1,k}, v_k\} \) with \( k = 2, \ldots, K \). For instance, when \( p_{k_0} = 0 \) with \( k_0 \in \{2, \ldots, K\} \) we have \( u_{k_0} = v_{k_0} = \emptyset \) by definition. When \( p_{k_0} = 1 \), we have \( u_{k_0} = \{w_{1,k_0}\}, v_{k_0} = \emptyset \).

According to Lemma 4 and Lemma 3, for all \( u \subseteq \{1, \ldots, d\} \), there exists \( u_0 \subseteq \alpha \), a vector \( w_k \in \mathcal{P}_k \) and integer \( p_k \) with \( k = 2, \ldots, K \), such that

\[
X_u = (X_{u_0}, X_{u_2}, \ldots, X_{u_K}),
\]

and

\[
f(X, \theta)|X_u \overset{d}{=} g_\ell (X_\alpha, X_{w,2}, Z_{w,-1,2}, \ldots, X_{w,1,K}, Z_{w,1,K}, \theta) \mid X_{u_0}, Y_{u_2}, \ldots, Y_{u_K}, \tag{34}
\]

where \( Y_{u_k} := (X_{w,1,k}, Z_{u_k}), k = 2, \ldots, K \).

Therefore, the effect of inputs \( X_u \) is equal to the effect of \( X_{u_0}, Y_{u_2}, \ldots, Y_{u_K} \) or \( X_{u_0}, (X_{w,1,2}, Z_{u_2}), \ldots, (X_{w,1,K}, Z_{u_K}) \) using \( g_\ell \). The value of \( p_k \) allows for choosing particular subsets of \( X \). For instance, \( u = u_0 \) if \( p_k = 0 \) for all \( k \in \{2, \ldots, K\} \), and when \( p_{k_0} = 1 \), we have \( Y_{u_{k_0}} = X_{w,1,k_0} \). When \( 0 \leq p_k \leq 1 \), we are interested in assessing the effects of \( X_u \) with \( u \subseteq \{\alpha, w_{1,2}, \ldots, w_{1,K}\} \), which have been addressed in [34]. In what follows, we allow \( 0 \leq p_k \leq d_k \) in order to assess the effect of any subset of inputs.
X. It is worth noting that with the equivalent representation \( g_t \) given by (34), we can assess the effect of inputs of the form

\[
(X_{u_0}, X_{u_2}, \ldots, X_{u_K}), \quad \forall u_0 \subseteq \{0, \ldots, d_k\}, \quad k = 2, \ldots K. \tag{35}
\]

The first-order SF of \( X_u \) with \( u = \{u_0, u_2, \ldots, u_K\} \) is given by

\[
f_u^{fo}(X_{u_0}, Y_{u_2}, \ldots, Y_{u_K}, \theta) := \mathbb{E} \left[ g_t(X_0, X_s, Z_{w_{-1,2}}, \ldots, Z_{w_{-1,K}}, \theta) \right] \big| X_{u_0}, Y_{u_2}, \ldots, Y_{u_K} \right]
\]

\[
-\mathbb{E} \left[ g_t(X_0, X_s, Z_{w_{-1,2}}, \ldots, Z_{w_{-1,K}}, \theta) \right], \tag{36}
\]

where \( s = \{w_1, \ldots, w_{1,K}\} \), and \( \theta \in \Theta \). While the first-order SF is used to assess the single contribution of \( X_u \), the total SF contains the overall information about the effect of \( X_u \), and it is given by

\[
f_u^{tot}(X_0, X_s, Z_{w_{-1,2}}, \ldots, Z_{w_{-1,K}}, \theta) := g_t(X_0, X_s, Z_{w_{-1,2}}, \ldots, Z_{w_{-1,K}}, \theta)
\]

\[
-\mathbb{E}_{X_0, Y_{u_2}, \ldots, Y_{u_K}} \left[ g_t(X_0, X_s, Z_{w_{-1,2}}, \ldots, Z_{w_{-1,K}}, \theta) \right], \tag{37}
\]

where \( \mathbb{E}_Y \) means that the expectation is taken w.r.t. \( Y \).

Likewise, if we use \( \omega := (\omega_0, \omega_2, \ldots, \omega_K) \) with \( \omega_0 \subseteq u_0 \) and \( \omega_k \subseteq u_k \) for all \( k \in \{2, \ldots, K\} \), the total-interaction SF of \( X_u \) is given by ([32])

\[
f_u^{sup}(X_0, X_s, Z_{w_{-1,2}}, \ldots, Z_{w_{-1,K}}, \theta) := \sum_{\omega \subset u} (-1)^{|\omega|+|\omega|+1} f_u^{tot}(X_0, X_s, Z_{w_{-1,2}}, \ldots, Z_{w_{-1,K}}, \theta). \tag{38}
\]

The SFs given by (36)-(38) are random vectors for a given \( \theta \), and their components may be correlated and/or dependent. Using SFs and the variance or covariance as importance measure, a definition of the sensitivity indices for the multivariate and/or functional outputs with dependent variables should be based on the following cross-covariances of SFs.

The cross-covariance of \( f_u^{fo} \) is given by

\[
\Sigma_u(\theta_1, \theta_2) := \mathbb{E} \left[ f_u^{fo}(X_{u_0}, Y_{u_2}, \ldots, Y_{u_K}, \theta_1) f_u^{fo}(X_{u_0}, Y_{u_2}, \ldots, Y_{u_K}, \theta_2)^T \right], \tag{39}
\]

with \( \theta_1, \theta_2 \in \Theta \).

Further, the cross-covariances of \( f_u^{tot} \) and \( f_u^{sup} \) are given in Equations (40)-(42), respectively.

\[
\Sigma_u^{tot}(\theta_1, \theta_2) := \mathbb{E} \left[ f_u^{tot}(X_0, X_s, Z_{w_{-1,2}}, \ldots, Z_{w_{-1,K}}, \theta_1) \right] \times f_u^{tot}(X_0, X_s, Z_{w_{-1,2}}, \ldots, Z_{w_{-1,K}}, \theta_2)^T, \tag{40}
\]

\[
\Sigma_u^{sup}(\theta_1, \theta_2) := \mathbb{E} \left[ f_u^{sup}(X_0, X_s, Z_{w_{-1,2}}, \ldots, Z_{w_{-1,K}}, \theta_1) \right] \times f_u^{sup}(X_0, X_s, Z_{w_{-1,2}}, \ldots, Z_{w_{-1,K}}, \theta_2)^T. \tag{41}
\]
The cross-covariance of \( f(X, \theta) \) is given by
\[
\Sigma(\theta_1, \theta_2) := \mathbb{E} \left[ f(X, \theta_1) f(X, \theta_2)^T \right] - \mathbb{E} \left[ f(X, \theta_1) \right] \mathbb{E} \left[ f(X, \theta_2)^T \right] \quad (42)
\]
\[
= \mathbb{E} \left[ g_{\ell}(X_0, X_s, Z_{w_{1,2}}, \ldots, Z_{w_{1,K}}, \theta_1) g_{\ell}(X_0, X_s, Z_{w_{1,2}}, \ldots, Z_{w_{1,K}}, \theta_2)^T \right] - \mathbb{E} \left[ g_{\ell}(X_0, X_s, Z_{w_{1,2}}, \ldots, Z_{w_{1,K}}, \theta_1) \right] \mathbb{E} \left[ g_{\ell}(X_0, X_s, Z_{w_{1,2}}, \ldots, Z_{w_{1,K}}, \theta_2)^T \right].
\]

Using the above cross-covariances, Definition 3 provides the dGSIs of \( X_u \) given by \((35)\) for the multivariate and functional outputs, including dynamic models.

**Definition 3** Consider the cross-covariances of SFs, and assume that (A1) and (A2) hold.

(i) The first-type dGSIs are defined below.

The first-order dGSI of \( X_u \) is given by
\[
dGSI_{1u}^1 := \frac{\int_{\Theta} \text{Tr}(\Sigma_u(\theta, \theta)) \, d\theta}{\int_{\Theta} \text{Tr}(\Sigma(\theta, \theta)) \, d\theta}.
\]

Further, the total dGSI of \( X_u \) is given by
\[
dGSI_{1u}^{\text{tot}} := \frac{\int_{\Theta} \text{Tr}(\Sigma_{u}^{\text{tot}}(\theta, \theta)) \, d\theta}{\int_{\Theta} \text{Tr}(\Sigma(\theta, \theta)) \, d\theta},
\]

and the total-interaction dGSI of \( X_u \) is given by
\[
dGSI_{1u}^{\text{sup}} := \frac{\int_{\Theta} \text{Tr}(\Sigma_{u}^{\text{sup}}(\theta, \theta)) \, d\theta}{\int_{\Theta} \text{Tr}(\Sigma(\theta, \theta)) \, d\theta}.
\]

(ii) The prime second-type dGSIs are defined as follows:
\[
dGSI_{2u}^{\ell} := \left( \frac{\int_{\Theta} \| \Sigma_u(\theta, \theta) \|_F^2 \, d\theta}{\int_{\Theta} \| \Sigma(\theta, \theta) \|_F^2 \, d\theta} \right)^{1/2};
\]
\[
dGSI_{2u}^{\text{tot}} := \left( \frac{\int_{\Theta} \| \Sigma_{u}^{\text{tot}}(\theta, \theta) \|_F^2 \, d\theta}{\int_{\Theta} \| \Sigma(\theta, \theta) \|_F^2 \, d\theta} \right)^{1/2};
\]
\[
dGSI_{2u}^{\text{sup}} := \left( \frac{\int_{\Theta} \| \Sigma_{u}^{\text{sup}}(\theta, \theta) \|_F^2 \, d\theta}{\int_{\Theta} \| \Sigma(\theta, \theta) \|_F^2 \, d\theta} \right)^{1/2}.
\]

(iii) The second-type dGSIs are given as follows:
\[
dGSI_{1u}^{\ell} := \left( \frac{\int_{\Theta_1} \| \Sigma_{u}(\theta_1, \theta_2) \|_F^2 \, d\theta_1 \, d\theta_2}{\int_{\Theta_1} \| \Sigma(\theta_1, \theta_2) \|_F^2 \, d\theta_1 \, d\theta_2} \right)^{1/2};
\]
\[
dGSI_{1u}^{\text{tot}} := \left( \frac{\int_{\Theta_1} \| \Sigma_{u}^{\text{tot}}(\theta_1, \theta_2) \|_F^2 \, d\theta_1 \, d\theta_2}{\int_{\Theta_1} \| \Sigma(\theta_1, \theta_2) \|_F^2 \, d\theta_1 \, d\theta_2} \right)^{1/2};
\]
\[
dGSI_{1u}^{\text{sup}} := \left( \frac{\int_{\Theta_1} \| \Sigma_{u}^{\text{sup}}(\theta_1, \theta_2) \|_F^2 \, d\theta_1 \, d\theta_2}{\int_{\Theta_1} \| \Sigma(\theta_1, \theta_2) \|_F^2 \, d\theta_1 \, d\theta_2} \right)^{1/2}.
\]
The first-type and the prime second-type dGSIs treat independently the outputs \( f(X, \theta_1) \) and \( f(X, \theta_2) \) with \( \theta_1 \neq \theta_2 \), but the prime second-type dGSIs account for the correlations among the components of SFs from the same output \( f(X, \theta) \). Furthermore, the second-type dGSIs account for the correlations among the components of SFs from the same output and the correlations among the cross-components of SFs. Of course, the prime second-type dGSIs and the second-type dGSIs are equal when the outputs \( f(X, \theta_1) \) and \( f(X, \theta_2) \) are not correlated with \( \theta_1, \theta_2 \in \Theta \) and \( \theta_1 \neq \theta_2 \).

4.1. Properties of dependent generalized sensitivity indices

The two types of dGSIs share the same properties as those proposed in [34] with \( 0 \leq p_k \leq 1 \), only. Proposition 3 summaries such properties.

**Proposition 3** Consider the dGSIs given in Definition 3 under assumptions (A1)-(A2).

(i) We have the following relationships between dGSIs

\[
0 \leq \text{dGSI}_1 u \leq \text{dGSI}_1 T_u \leq 1,
\]

(52)

\[
0 \leq \text{dGSI}'_2 u \leq \text{dGSI}'_2 T_u \leq 1.
\]

(53)

(ii) If the cross-covariances are positive semi-definite, we have

\[
0 \leq \text{dGSI}_2 u \leq \text{dGSI}_2 T_u \leq 1.
\]

(54)

(iii) For all orthogonal matrix \( V \in \mathbb{R}^{n \times n} \) (i.e., \( VV^T = V^TV = I \)), we have

\[
\text{dGSI}_i u (Vf) = \text{dGSI}_i u, \quad (55)
\]

\[
\text{dGSI}_i T_u (Vf) = \text{dGSI}_i T_u, \quad (56)
\]

\[
\text{dGSI}'_i T_u (Vf) = \text{dGSI}'_i T_u, \quad (57)
\]

where \( i = 1, 2', 2 \) is associated with the first-type, the prime second-type and second-type dGSIs, respectively.

**Proof.** See Appendix H.

To give some strategies for fixing non-influential inputs using our dGSIs, recall that we are able to assess the total effects of all subsets of \( X \) (i.e., total dGSIs) using \( R_{\min} \) equivalent representations of \( f \). Thus, when the total dGSI of the subset \( X_u \) is zero or almost zero, we have to fix \( X_u = (X_{u_0}, X_{u_1}, \ldots, X_{u_K}) \) using the dependency functions associated with each \( X_k, k = 2, \ldots, K \).
Indeed, for the following dependency function $X_u^k = r_u^k (X_{u^k}, Z_{u^k})$, fixing $X_u^k$ comes down to fix $Z_{u^k}$ to its nominal values. Instead of fixing $Z_{u^k}$, one may also take an average over $Z_{u^k}$. Since we can compute the total $dGSI$ of each block of dependent variables $X_k$ using any equivalent representations of $f$, it becomes possible to quickly identify the non-influential block of dependent variables, and then put our computational efforts on the other groups of dependent variables (i.e., reduce $R_{\min}$).

Regarding the ranking of input variables, Proposition 4 provides conditions that ensure the equivalence between using either $dGSI_1^T$ or $dGSI_2^T$. To that end, we use $A_1 \preceq A_2$ to say that $A_2 - A_1$ is positive semi-definite, known as the Loewner partial ordering between matrices.

**Proposition 4** Let $X_u$ and $X_\omega$ be two subsets of $X$ having the following total-effect cross-covariances $\Sigma_u^{tot}(\theta, \theta)$, $\Sigma_\omega^{tot}(\theta, \theta)$, respectively.

If $\Sigma_u^{tot}(\theta, \theta) \preceq \Sigma_\omega^{tot}(\theta, \theta)$, then we have

$$dGSI_1^T \leq dGSI_1^T, \quad dGSI_2^T \leq dGSI_2^T$$

(58)

When assumption $\Sigma_u^{tot}(\theta, \theta) \preceq \Sigma_\omega^{tot}(\theta, \theta)$ is not satisfied, we may have different ranking of inputs using both types of dGSIs (see Section 6.3 in [34]).

**Remark 2** Case of the multivariate dynamic function

Consider a model that includes $d$ input variables $X$ and provides $n$ dynamic(s) such as a spatio-temporal model. Formally, for $T \in \mathbb{R}_+$, we can see that the multivariate dynamic model given by $f : \mathbb{R}^d \times [0, T] \rightarrow \mathbb{R}^n$, $f(X, t) \in \mathbb{R}^n$ with $t \in [0, T] = \Theta$ is a particular case of the multivariate and functional outputs. Therefore, the dGSIs provided in Definition 3 can be used for quantifying the effects of input variables.

4.2. Case of the multivariate response models

When $\Theta = \{\theta_0\}$, the multivariate and functional outputs $f(X, \theta)$ come down to $f(X, \theta_0) =: h(X)$, which is a multivariate response function, that is, $h : \mathbb{R}^d \rightarrow \mathbb{R}^n$. Therefore, the dGSIs provided in Definition 3 can be used for quantifying the effect of inputs. It is worth noting that the second-type dGSIs are equal to the prime second-type dGSIs, and both types of dGSIs boil down to the second-type dGSIs proposed in Definition 4. Moreover, the cross-covariances become the covariances, and we use $\Sigma_u := \Sigma_u(\theta_0, \theta_0)$, $\Sigma_u^{tot} := \Sigma_u^{tot}(\theta_0, \theta_0)$ and $\Sigma := \Sigma(\theta_0, \theta_0)$.

**Definition 4** Consider the covariances of SFs and assume that (A1)-(A2) hold.
(i) The first-type dGSIs for a given multivariate response function are
\[
dGSI^{1,M}_u := \frac{\text{Tr}(\Sigma_u)}{\text{Tr}(\Sigma)},
\]
(59)
\[
dGSI^{1,M}_T_u := \frac{\text{Tr}(\Sigma^\text{tot}_u)}{\text{Tr}(\Sigma)}.
\]
(60)

(ii) The second-type dGSIs are defined as follows:
\[
dGSI^{2,M}_u := \frac{||\Sigma_u||_F}{||\Sigma||_F};
\]
(61)
\[
dGSI^{2,M}_T_u := \frac{||\Sigma^\text{tot}_u||_F}{||\Sigma||_F},
\]
(62)
with \(||\Sigma||_F = \text{Tr}(\Sigma\Sigma^T)\).

Obviously, the dGSIs from Definition 4 satisfy the properties listed in Proposition 3, and when \(n = 1\), both types of dGSIs are equal and boil down to the dependent sensitivity indices (dSIs) for the single response models (see Definition 5).

**Definition 5** Consider a function \(f : \mathbb{R}^d \rightarrow \mathbb{R}\) and assume that (A1)-(A2) hold. The first-order and total dSIs of \(X_u\) are given by
\[
dS_u := \frac{\Sigma_u}{\Sigma},
\]
(63)
\[
dS^T_u := \frac{\Sigma^\text{tot}_u}{\Sigma}.
\]
(64)

5. Estimators of dependent generalized sensitivity indices

In this section, we provide unbiased estimators of the cross-covariances of SFs, consistent estimators of dGSIs and their asymptotic distributions. First, we derive new expressions of the cross-covariances of SFs so as to construct the estimators of dGSIs from Definition 3 and study their statistical performances. Second, we deduce the estimators of dGSIs from Definition 4 and Definition 5. We provide such estimators by i) using the distributions of independent variables \(X_{\{o,s\}}\) and the innovation \(Z\), ii) assuming that the dependency function \(r_u\) is invertible.

5.1. Case 1: making use of the distribution of the innovation

The cross-covariances of SFs (Equations (40)-(39)) are directly based on the definition of such SFs. In Proposition 5, we derive new expressions of such cross-covariances by making use of an equivalent representation of \(f(X, \theta)\) given by Equation (34). Recall that for all \(u \subseteq \{1, \ldots, d\}\), we can write (see Equation (35))
\[
X_u = (X_{u_0}, X_{u_2}, \ldots, X_{u_K}),
\]
and that subset of inputs of \( f \) is associated with the following inputs (see Lemma 3)

\[
(X_{u_{l_0}}, Y_{u_2}, \ldots, Y_{u_K}) = (X_{u_{l_0}}, (X_{w_{1,2}}, Z_{v_2}), \ldots, (X_{w_{1,K}}, Z_{v_K})),
\]

of

\[
g_t(X_{(o,s)}, Z_{w_{-1,2}}, \ldots, Z_{w_{-1,K}}, \theta) = f(X_{(o,s)}, r_s(X_s, Z_{w_{-1,2}}, \ldots, Z_{w_{-1,K}}), \theta)
\]

\[
= f(X_{(o,s)}, r_{w_{1,2}}(X_{w_{1,2}}, Z_{w_{-1,2}}), \ldots, r_{w_{1,K}}(X_{w_{1,K}}, Z_{w_{-1,K}}), \theta),
\]

with \( s = \{w_{1,2}, \ldots, w_{1,K}\} \). For concise notation, we use \( w_{-1} := \{w_{1,2}, \ldots, w_{1,K}\}, v := \{v_2, \ldots, v_K\}, w_{-1} \cap v := \{w_{1,2} \cap v_2, \ldots, w_{1,K} \cap v_K\} \) and \( w_{-1} \setminus v := \{w_{1,2} \setminus v_2, \ldots, w_{1,K} \setminus v_K\} \) in what follows. For instance, we have

\[
Z_{w_{-1}} := (Z_{w_{-1,2}}, \ldots, Z_{w_{-1,K}}), \quad Z_v := (Z_{v_2}, \ldots, Z_{v_K}).
\]

**Proposition 5** Let \( (X^{(1)}_{(o,s)}, Z^{(1)}_{w_{-1}}) \) and \( (X^{(2)}_{(o,s)}, Z^{(2)}_{w_{-1}}) \) be two independent copies of \( (X_{(o,s)}, Z_{w_{-1}}) \) and \( X^{(1)} := (X^{(1)}_{(o,s)}, r_s(X^{(1)}_s, Z^{(1)}_{w_{-1}})) \). Assume that assumptions (A1, A2) hold.

(i) The first-order cross-covariance is given by

\[
\Sigma_u(\theta_1, \theta_2) = -E \left[ f(X^{(1)}, \theta_1) \right] E \left[ f(X^{(1)}, \theta_2) \right]^T - E \left[ f(X^{(1)}, \theta_1) f(X^{(1)}, \theta_2)^T \right] + E \left[ f(X^{(1)}, \theta_1) f(X^{(1)}_{(o,s)} \cap u, X^{(2)}_{(o,s)} \setminus u, r_s(X^{(1)}_{u \cap w}, X^{(1)}_{w \setminus u}, Z^{(1)}_{w_{-1} \cap v}, Z^{(2)}_{w_{-1} \setminus v}), \theta_2)^T \right].
\]

(ii) The total-effect cross-covariance is given by

\[
\Sigma^t_u(\theta_1, \theta_2) = E \left[ f(X^{(1)}, \theta_1) f(X^{(1)}, \theta_2)^T \right] - E \left[ f(X^{(1)}, \theta_1) f(X^{(2)}_{(o,s)} \cap u, X^{(1)}_{(o,s)} \setminus u, r_s(X^{(2)}_{u \cap w}, X^{(1)}_{w \setminus u}, Z^{(2)}_{w_{-1} \cap v}, Z^{(1)}_{w_{-1} \setminus v}), \theta_2)^T \right].
\]

**Proof.** See Appendix 1.

While Proposition 5 can be used to obtain the analytical values of dGSIs, Theorem 2 provides the estimators of the cross-covariances that are useful for estimating the dGSIs for complex models.

**Theorem 2** Let \( (X^{(1)}_{i,(o,s)}, Z^{(1)}_{i,w_{-1}}) \) and \( (X^{(2)}_{i,(o,s)}, Z^{(2)}_{i,w_{-1}}) \) with \( i = 1, \ldots, m \) be two independent samples of size \( m \) from \( (X_{(o,s)}, Z_{w_{-1}}) \). Consider two random vectors \( X^{(1)} := (X^{(1)}_{i,(o,s)}, r_s(X^{(1)}_{i,s}, Z^{(1)}_{i,w_{-1}})) \) and \( X^{(2)} := (X^{(2)}_{i,(o,s)}, r_s(X^{(2)}_{i,s}, Z^{(2)}_{i,w_{-1}})) \) with \( i = 1, \ldots, m \), and assume that (A1)-(A2) hold.
(i) An unbiased estimator of $\Sigma_u(\theta_1, \theta_2)$ is given by
\[
\bar{\Sigma}_u(\theta_1, \theta_2) := \frac{1}{4m} \sum_{i=1}^{m} \left( \left[ f \left( X_i^{(1)}(1) \right) - f \left( X_i^{(2)} \cap u \right) \sum_{u} X_i^{(1)} \sum_{u} Z_i^{(2)} \sum_{u} Z_i^{(1)} ; \theta_1 \right] \right) \times \left[ f \left( X_i^{(1)}(2) \cap u \right) \sum_{u} X_i^{(1)}(2) \sum_{u} Z_i^{(2)} \sum_{u} Z_i^{(1)} ; \theta_2 \right) - f \left( X_i^{(2)}(2) \cap u \right) \sum_{u} X_i^{(2)}(2) \sum_{u} Z_i^{(2)} \sum_{u} Z_i^{(1)} ; \theta_2 \right) \right) \bigg) T \right] ,
\]
and
\[E \left( \bar{\Sigma}_u(\theta_1, \theta_2) \right) = \Sigma_u(\theta_1, \theta_2) ;
\]

The estimator $\bar{\Sigma}_u(\theta_1, \theta_2)$ is consistent, that is, when $m \to +\infty$
\[\bar{\Sigma}_u(\theta_1, \theta_2) \xrightarrow{T} \Sigma_u(\theta_1, \theta_2) ,
\]
with $T \to$ the convergence in probability.

(ii) An unbiased estimator of $\Sigma_u^{tot}(\theta_1, \theta_2)$ is given by
\[
\bar{\Sigma}_u^{tot}(\theta_1, \theta_2) := \frac{1}{4m} \sum_{i=1}^{m} \left( \left[ f \left( X_i^{(1)}(1) \right) - f \left( X_i^{(2)} \cap u \right) \sum_{u} X_i^{(1)} \sum_{u} Z_i^{(2)} \sum_{u} Z_i^{(1)} ; \theta_1 \right] \right) \times \left[ f \left( X_i^{(1)}(2) \cap u \right) \sum_{u} X_i^{(1)}(2) \sum_{u} Z_i^{(2)} \sum_{u} Z_i^{(1)} ; \theta_2 \right) - f \left( X_i^{(2)}(2) \cap u \right) \sum_{u} X_i^{(2)}(2) \sum_{u} Z_i^{(2)} \sum_{u} Z_i^{(1)} ; \theta_2 \right) \right) \bigg) T \right] ,
\]
and
\[E \left( \bar{\Sigma}_u^{tot}(\theta_1, \theta_2) \right) = \Sigma_u^{tot}(\theta_1, \theta_2) ;
\]

If $m \to +\infty$, then we have
\[\bar{\Sigma}_u^{tot}(\theta_1, \theta_2) \xrightarrow{T} \Sigma_u^{tot}(\theta_1, \theta_2) ,
\]

(iii) An unbiased estimator of $\Sigma(\theta_1, \theta_2)$ is given by
\[
\bar{\Sigma}(\theta_1, \theta_2) := \frac{1}{2m} \sum_{i=1}^{m} \left[ f \left( X_i^{(1)}(1) \right) - f \left( X_i^{(2)}(1) \right) \right] \bigg) \left[ f \left( X_i^{(1)}(2) \right) - f \left( X_i^{(2)}(2) \right) \right] T \right] ,
\]
and
\[E \left( \bar{\Sigma}(\theta_1, \theta_2) \right) = \Sigma(\theta_1, \theta_2) ;
\]
\[\bar{\Sigma}(\theta_1, \theta_2) \xrightarrow{T} \Sigma(\theta_1, \theta_2) ,
\]
when $m \to +\infty$. 

Proof. See Appendix J. □

It is to be noted that when \( \theta_1 = \theta_2 = \theta \) the estimators from Theorem 2 have minimum variances.

Using Theorem 2, we can deduce the estimators of the variances or covariances of SFs for the multivariate response models, including the single response models. Corollary 2 provides such results.

**Corollary 2** Assume that \( f \) has finite fourth moments (A3) and (A1)-(A2) hold.

(i) The minimum variance unbiased (MVU) estimator of \( \Sigma_u \) is given by

\[
\hat{\Sigma}_u := \frac{1}{4m} \sum_{i=1}^{m} \left( \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2)} \right) \right] \right) \left( \begin{array}{c} X_i^{(1)} \setminus \{ o \} \setminus \{ u \} \setminus \{ v \} \setminus \{ w \} \\ \end{array} \right) \cdot \left( \begin{array}{c} X_i^{(1)} \setminus \{ o \} \setminus \{ u \} \setminus \{ v \} \setminus \{ w \} \\ \end{array} \right) ^T
\]

where

\[
\hat{\Sigma}_u := \frac{1}{4m} \sum_{i=1}^{m} \left( \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2)} \right) \right] \right) \left( \begin{array}{c} X_i^{(1)} \setminus \{ o \} \setminus \{ u \} \setminus \{ v \} \setminus \{ w \} \\ \end{array} \right) \cdot \left( \begin{array}{c} X_i^{(1)} \setminus \{ o \} \setminus \{ u \} \setminus \{ v \} \setminus \{ w \} \\ \end{array} \right) ^T
\]

and we have

\[
\hat{\Sigma}_u \overset{p}{\to} \Sigma_u.
\]

(ii) The MVU estimator of \( \Sigma_{tot} \) is given by

\[
\hat{\Sigma}_{tot} := \frac{1}{4m} \sum_{i=1}^{m} \left( \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2)} \right) \right] \right) \left( \begin{array}{c} X_i^{(1)} \setminus \{ o \} \setminus \{ u \} \setminus \{ v \} \setminus \{ w \} \\ \end{array} \right) \cdot \left( \begin{array}{c} X_i^{(1)} \setminus \{ o \} \setminus \{ u \} \setminus \{ v \} \setminus \{ w \} \\ \end{array} \right) ^T
\]

where

\[
\hat{\Sigma} := \frac{1}{2m} \sum_{i=1}^{m} \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2)} \right) \right] \left( \begin{array}{c} X_i^{(1)} \setminus \{ o \} \setminus \{ u \} \setminus \{ v \} \setminus \{ w \} \\ \end{array} \right) \cdot \left( \begin{array}{c} X_i^{(1)} \setminus \{ o \} \setminus \{ u \} \setminus \{ v \} \setminus \{ w \} \\ \end{array} \right) ^T
\]

We also have

\[
\hat{\Sigma} \overset{p}{\to} \Sigma.
\]
Proof. See Appendix K.

□

When $n = 1$ the MVU estimators of the covariances of SFs in Corollary 2 have simple expressions given below.

**Corollary 3** Assume that $n = 1$ and assumptions (A1), (A2) and (A3) hold.

(i) The MVU estimator $\tilde{\Sigma}_u$ becomes

$$
\tilde{\sigma}_u := \frac{1}{2m} \sum_{i=1}^{m} \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2), i, \{o,s\} \cap u}, X_i^{(1), i, \{o,s\} \setminus u} : r_s \left( X_i^{(2), i, \{o,s\} \cap u}, X_i^{(1), i, \{o,s\} \setminus u} : Z_{i, \{w_{-1,1}\} \cap u}, Z_{i, \{w_{-1,1}\} \setminus u} \right) \right] \times \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2), i, \{o,s\} \cap u}, X_i^{(1), i, \{o,s\} \setminus u} : r_s \left( X_i^{(2), i, \{o,s\} \cap u}, X_i^{(1), i, \{o,s\} \setminus u} : Z_{i, \{w_{-1,1}\} \cap u}, Z_{i, \{w_{-1,1}\} \setminus u} \right) \right] - f \left( X_i^{(2)} \right) \right] .
$$

(ii) The MVU estimator $\tilde{\Sigma}^{tot}_u$ becomes

$$
\tilde{\sigma}^{tot}_u := \frac{1}{4m} \sum_{i=1}^{m} \left( \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2), i, \{o,s\} \cap u}, X_i^{(1), i, \{o,s\} \setminus u} : r_s \left( X_i^{(2), i, \{o,s\} \cap u}, X_i^{(1), i, \{o,s\} \setminus u} : Z_{i, \{w_{-1,1}\} \cap u}, Z_{i, \{w_{-1,1}\} \setminus u} \right) \right] \right)^2 + \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2), i, \{o,s\} \cap u}, X_i^{(1), i, \{o,s\} \setminus u} : r_s \left( X_i^{(2), i, \{o,s\} \cap u}, X_i^{(1), i, \{o,s\} \setminus u} : Z_{i, \{w_{-1,1}\} \cap u}, Z_{i, \{w_{-1,1}\} \setminus u} \right) \right] - f \left( X_i^{(2)} \right) \right)^2 .
$$

(iii) The MVU estimator $\tilde{\Sigma}$ becomes

$$
\tilde{\sigma} := \frac{1}{2m} \sum_{i=1}^{m} \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2)} \right) \right]^2 .
$$

Proof. The proof is obvious using Corollary 2.

□

If we are only interested in the total-effects, we should use the expressions of $\tilde{\Sigma}^{tot}_u$ and $\tilde{\sigma}^{tot}_u$ given by

$$
\frac{1}{2m} \sum_{i=1}^{m} \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2), i, \{o,s\} \cap u}, X_i^{(1), i, \{o,s\} \setminus u} : r_s \left( X_i^{(2), i, \{o,s\} \cap u}, X_i^{(1), i, \{o,s\} \setminus u} : Z_{i, \{w_{-1,1}\} \cap u}, Z_{i, \{w_{-1,1}\} \setminus u} \right) \right] \right] \times \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2), i, \{o,s\} \cap u}, X_i^{(1), i, \{o,s\} \setminus u} : r_s \left( X_i^{(2), i, \{o,s\} \cap u}, X_i^{(1), i, \{o,s\} \setminus u} : Z_{i, \{w_{-1,1}\} \cap u}, Z_{i, \{w_{-1,1}\} \setminus u} \right) \right] - f \left( X_i^{(2)} \right) \right] = 0 ,
$$

and

$$
\frac{1}{2m} \sum_{i=1}^{m} \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2), i, \{o,s\} \cap u}, X_i^{(1), i, \{o,s\} \setminus u} : r_s \left( X_i^{(2), i, \{o,s\} \cap u}, X_i^{(1), i, \{o,s\} \setminus u} : Z_{i, \{w_{-1,1}\} \cap u}, Z_{i, \{w_{-1,1}\} \setminus u} \right) \right] \right]^T = 0 ,
$$

respectively.

Using the results from Theorem 2, Corollary 2 and Corollary 3, we derive the estimators of dGSIs and dSIs in Theorem 3, Theorem 4 and Corollary 4 for the multivariate and functional outputs, the multivariate response models and the single response models, respectively.
Theorem 3 Consider the estimators of the cross-covariances from Theorem 2. Assume that (A1)-(A3) hold.

If we observe the model outputs at $\theta_\ell \in \Theta$ with $\ell = 1, \ldots, L$, then

(i) the estimators of the first-type dGSIs are given as follows:

$$d\overline{GSI}_u^1 := \frac{\sum_{\ell=1}^L \text{Tr} \left( \Sigma_u(\theta_\ell, \theta_\ell) \right)}{\sum_{\ell=1}^L \text{Tr} \left( \Sigma(\theta_\ell, \theta_\ell) \right)},$$

and if $L \to \infty$, $m \to \infty$ we have

$$\overline{dGSI}_u^1 \overset{P}{\to} d\overline{GSI}_u^1.$$  

(ii) The estimators of the prime second-type dGSIs are given as follows:

$$d\overline{GSI}_u^2' := \left( \frac{\sum_{\ell=1}^L \left\| \Sigma_u(\theta_\ell, \theta_\ell) \right\|_F^2}{\sum_{\ell=1}^L \left\| \Sigma(\theta_\ell, \theta_\ell) \right\|_F^2} \right)^{1/2} \overset{P}{\to} d\overline{GSI}_u^2',$$

(iii) The estimators of the second-type dGSIs are given as follows:

$$d\overline{GSI}_u^2 := \left( \frac{\sum_{\ell_1=1}^L \sum_{\ell_2=1}^L \left\| \Sigma_u(\theta_{\ell_1}, \theta_{\ell_2}) \right\|_F^2}{\sum_{\ell_1=1}^L \sum_{\ell_2=1}^L \left\| \Sigma(\theta_{\ell_1}, \theta_{\ell_2}) \right\|_F^2} \right)^{1/2},$$

with $\ell_1, \ell_2 \in \{1, \ldots, L\}$. If $L \to \infty$, $m \to \infty$, then we have

$$\overline{dGSI}_u^2 \overset{P}{\to} d\overline{GSI}_u^2.$$

$$d\overline{GSI}_u^2 := \left( \frac{\sum_{\ell_1=1}^L \sum_{\ell_2=1}^L \left\| \Sigma_u(\theta_{\ell_1}, \theta_{\ell_2}) \right\|_F^2}{\sum_{\ell_1=1}^L \sum_{\ell_2=1}^L \left\| \Sigma(\theta_{\ell_1}, \theta_{\ell_2}) \right\|_F^2} \right)^{1/2} \overset{P}{\to} d\overline{GSI}_u^2.$$  

Proof. See Appendix L.

Remark 3 It is worth noting that the consistency of the above estimators are still valid for finite value of $L$, which corresponds to the case when $\Theta \subseteq \mathbb{N}$ with finite number of elements (i.e., $L < \infty$). In this case, the consistency is taken w.r.t. to $m \to \infty$. 

□
Thus, it comes out from Corollary 2 that Equations (71)-(72) become
\[
\begin{align*}
\text{Theorem 4} \\
\text{Assume that (A1)-(A3) hold, and we use } d \times (d + 1) \text{ model runs for computing the model variance or covariances ([31, 34]). Such model runs can be used for computing the model variance or covariances. In what follows, we suppose that } M \text{ model runs are used for computing the model variance or covariance.}
\end{align*}
\]
Namely, let us consider the following kernels
\[
K(X_i) := 
\left[ f \left( X^{(1)}_i \right) - f \left( X^{(2)}_i \right) \right] 
\times 
\left[ f \left( X^{(1)}_i \right) - f \left( X^{(2)}_i \right) \right]^T
\]
\[
K_{\text{tot}}(X_i) := 
\left[ f \left( X^{(1)}_i \right) - f \left( X^{(2)}_i \right) \right] 
\times 
\left[ f \left( X^{(1)}_i \right) - f \left( X^{(2)}_i \right) \right]^T
\]
Thus, it comes out from Corollary 2 that Equations (71)-(72) become
\[
\hat{\Sigma}_u = \frac{1}{4m} \sum_{i=1}^{m} K(X_i), \\
\hat{\Sigma}_{\text{tot}} = \frac{1}{4m} \sum_{i=1}^{m} K_{\text{tot}}(X_i),
\]
and
\[
\hat{\Sigma} := \frac{1}{2M} \sum_{i=1}^{M} \left[ f \left( X^{(1)}_i \right) - f \left( X^{(2)}_i \right) \right] \left[ f \left( X^{(1)}_i \right) - f \left( X^{(2)}_i \right) \right]^T.
\]
We use the operator Vec(·) to transform a matrix \( \Sigma \in \mathbb{R}^{n \times n} \) into a vector, that is, Vec(\( \Sigma \)) \( \in \mathbb{R}^{n^2} \), and we use \( O \in \mathbb{R}^{n \times n} \) for the null matrix.

\textbf{Theorem 4} Assume that (A1)-(A3) hold, \( m \to +\infty, \ M \to +\infty \) and \( m/M \to 0 \).

(i) The estimators of the first-type dGSIs are given below.

The estimator of the first-order dGSI of \( X_u \) is consistent, that is,
\[
d\text{GSI}^{1,M}_u := \frac{\text{Tr} \left( \hat{\Sigma}_u \right)}{\text{Tr} \left( \hat{\Sigma} \right)} \xrightarrow{p} d\text{GSI}^{1,M}_u, \tag{85}
\]
and we have the asymptotic normality, that is,

\[ \sqrt{m} \left( \hat{dGSI}_M^{1,M} - dGSI_M^{1,M} \right) \xrightarrow{D} N \left( 0, \frac{\mathbb{V} \left[ \text{Tr}(K(X_1)) \right]}{\left( \text{Tr}(\Sigma) \right)^2} \right) . \]

Further, the estimator of the total dGSI of \( X_u \) is consistent, that is,

\[ \hat{dGSI}_T^{1,M} := \text{Tr} \left( \hat{\Sigma} \right) \xrightarrow{P} dGSI_T^{1,M} , \quad (86) \]

and we have

\[ \sqrt{m} \left( \hat{dGSI}_T^{1,M} - dGSI_T^{1,M} \right) \xrightarrow{D} N \left( 0, \mathbb{V} \left[ \text{Tr}(K(X_1)) \right] \right) \cdot \]

(ii) For the second-type dGSIs, we can write

\[ \hat{dGSI}_u^{2,M} := \left| \left| \hat{\Sigma}_u \right| \right|_F \xrightarrow{P} dGSI_u^{2,M} , \quad (87) \]

and if \( \Sigma_u \neq O \), we have

\[ \sqrt{m} \left( \hat{dGSI}_u^{2,M} - dGSI_u^{2,M} \right) \xrightarrow{D} N \left( 0, \frac{\text{Vec}(\Sigma_u)^T \mathbb{V} \left[ \text{Vec}(K(X_1)) \right] \text{Vec}(\Sigma_u)}{\left( \left| \Sigma \right| \right)_F^2} \right) . \]

We also have

\[ \hat{dGSI}_T^{2,M} := \left| \left| \hat{\Sigma}_u \right| \right|_F \xrightarrow{P} dGSI_T^{2,M} , \quad (88) \]

\[ \sqrt{m} \left( \hat{dGSI}_T^{2,M} - dGSI_T^{2,M} \right) \xrightarrow{D} N \left( 0, \frac{\text{Vec}(\Sigma_u)^T \mathbb{V} \left[ \text{Vec}(K(X_1)) \right] \text{Vec}(\Sigma_u)}{\left( \left| \Sigma \right| \right)_F^2} \right) , \]

provided that \( \Sigma_u \neq O \).

**Proof.** See Appendix M.

Using Theorem 4, we derive the estimators of dSIs provided in Definition 5 in Corollary 4.

**Corollary 4** Consider the estimators of the variances of SFs from Corollary 3. Assume that \( n = 1 \), (A1)-(A3) hold, \( m \to +\infty \), \( M \to +\infty \) and \( m/M \to 0 \). Then, we have

\[ \hat{dS}_u := \frac{\hat{\sigma}_u}{\sigma} \xrightarrow{P} dS_u ; \quad \sqrt{m} \left( \hat{dS}_u - dS_u \right) \xrightarrow{P} N \left( 0, \frac{\mathbb{V} \left[ K(X_1) \right]}{\sigma^4} \right) . \quad (89) \]

and

\[ \hat{dS}_T := \frac{\hat{\sigma}_T}{\sigma} \xrightarrow{P} dS_T ; \quad \sqrt{m} \left( \hat{dS}_T - dS_T \right) \xrightarrow{P} N \left( 0, \frac{\mathbb{V} \left[ K(X_1) \right]}{\sigma^4} \right) . \quad (90) \]

**Proof.** It is just a particular case of Theorem 4 \((n = 1)\).
The computation of the dGSIs or dSIs of \( \mathbf{X}_u \) with \( u \subseteq \{1, \ldots, d\} \) using the above estimators will require \( R_{\text{min}} \) equivalent representations of \( f \). When we are only interested in \( u \subseteq \{1, \ldots, d\} \) with \(|u| = 1\), \( R_1 = \max(d_2, \ldots, d_K) \) equivalent representations of \( f \) are sufficient, and we need \( 2 \times m(d + 1) \) model evaluations to estimate the first-order and total dGSIs or dSIs of \( \mathbf{X}_u \) for all \( u \in \{1, \ldots, d\} \).

5.2. Case 2: when the dependency function is invertible

In this section, we provide the estimators of dGSIs and dSIs by making use of independent copies of \( \mathbf{X} \) (rather than \( \mathbf{Z} \)) and the inverse of the dependency function. We first derive new expressions of the cross-covariances of SFs and then construct i) the estimators of such cross-covariances, ii) the estimators of dGSIs and dSIs. In this section, we assume that

(A4) a dependency function is invertible.

Recall that under assumption (A1), we are interested in quantifying the effect of \( \mathbf{X}_u \) where \( u = \{u_0, u_2, \ldots, u_K\} \subseteq \{1, \ldots, d\} \) with \( u_0 \subseteq \emptyset \), \( u_k = \{w_{1,k}, \ldots, w_{p_k,k}\} \) and \( w_k = \{w_{1,k}, \ldots, w_{d_k,k}\} \) for all \( k \in \{2, \ldots, K\} \). The dependency function \( \mathbf{r}_s : \mathbb{R}^{d-d_1} \rightarrow \mathbb{R}^{d-d_1-K+1} \) is given by \( \mathbf{r}_s(\mathbf{X}_s, \mathbf{Z}_{w_{-1}}) \) with \( s = \{w_{1,2}, \ldots, w_{1,K}\} \) and \( \mathbf{Z}_{w_{-1}} = (\mathbf{Z}_{w_{-1,2}}, \ldots, \mathbf{Z}_{w_{-1,K}}) \) a vector of \( d-d_1-K+1 \) independent variables (see Equations (23)-(65)). Using Equation (7), the above dependency function implies the following dependency functions

\[
\mathbf{X}_{w_k \setminus u_k} \stackrel{d}{=} \mathbf{r}_{u_k}(\mathbf{X}_{u_k}, \mathbf{Z}_{w_k \setminus u_k}), \quad k = 2, \ldots, K,
\]

which can be written in a concise way as follows:

\[
\mathbf{X}_{w \setminus u} \stackrel{d}{=} \left( \mathbf{r}_{u_k}(\mathbf{X}_{u_k}, \mathbf{Z}_{w_k \setminus u_k}) \right), \quad k = 2, \ldots, K =: \mathbf{r}_{u \setminus u_0}(\mathbf{X}_{u \setminus u_0}, \mathbf{Z}_{w \setminus u}).
\]

It is to be noted that when \( p_{k_0} = 0 \), \( u_{k_0} = \emptyset \) and \( \mathbf{X}_{w_{k_0} \setminus u_{k_0}} \) contains all the elements of \( \mathbf{X}_{k_0} \). We give the precision about the inversion of \( \mathbf{r}_{u \setminus u_0} \) in Definition 6.

**Definition 6** Consider the dependency function \( \mathbf{r}_{u \setminus u_0}(\mathbf{X}_{u \setminus u_0}, \mathbf{Z}_{w \setminus u}) \).

The function \( \mathbf{r}_{u \setminus u_0} \) is said invertible given \( \mathbf{X}_{u \setminus u_0} \) if the function \( h : \mathbb{R}^{d-d_1-K+1} \rightarrow \mathbb{R}^{d-d_1-K+1} \) given by \( h(\mathbf{Z}_{w \setminus u}) = \mathbf{r}_{u \setminus u_0}(\mathbf{X}_{u \setminus u_0}, \mathbf{Z}_{w \setminus u}) \) is invertible.

If we use \( \mathbf{r}_{u \setminus u_0}^{-1} \) for the inverse of \( \mathbf{r}_{u \setminus u_0} \), then we have

\[
\mathbf{X}_{w \setminus u} = \mathbf{r}_{u \setminus u_0}(\mathbf{X}_{u \setminus u_0}, \mathbf{Z}_{w \setminus u}) \iff \mathbf{Z}_{w \setminus u} = \mathbf{r}_{u \setminus u_0}^{-1}(\mathbf{X}_{w \setminus u} | \mathbf{X}_{u \setminus u_0}).
\]

(91)
Thus, the inversion of \( r_{u|u_0} \) is done given \( X_{u|u_0} \). It is obvious that \( r_{u|u_0} \) is invertible if and only if \( r_{u_k} \) is invertible for all \( k \in \{2, \ldots, K\} \).

**Remark 4** When the dependency function includes \( U \) (see Remark 1), the inversion concerns \( X_{w|u} \) and \( Z_c \).

Now, we are going to derive new expressions of the cross-covariances of SFs under assumption (A4).

**Proposition 6** Let \( X^{(1)}, X^{(2)}, X^{(3)}, X^{(4)} \) be independent copies of \( X \) and
\[
Y := \left( X^{(1)}_{o,u}, r_{u|u_0} \left( X^{(1)}_{u|u_0}, r_{u|u_0}^{-1} \left( X^{(3)}_{w|u}, X^{(3)}_{w|u_0} \right) \right) \right). 
\]
Assume that (A1)-(A2) and (A4) hold and \( \theta_1, \theta_2 \in \Theta \).

(i) The first-order cross-covariance is given by
\[
\Sigma_u(\theta_1, \theta_2) = -E[f(Y, \theta_1)] E[f(Y, \theta_2)]^T \tag{92}
\]
\[
+ E \left[ f(Y, \theta_1) f \left( X^{(1)}_u, X^{(2)}_{o,u|u_0}, r_{u|u_0} \left( X^{(1)}_{u|u_0}, r_{u|u_0}^{-1} \left( X^{(3)}_{w|u}, X^{(3)}_{w|u_0} \right) \right), \theta_2 \right)^T \right].
\]

(ii) The total-effect cross-covariance is given by
\[
\Sigma_{u}^{\text{tot}}(\theta_1, \theta_2) = E \left[ f(Y, \theta_1) f(Y, \theta_2)^T \right] \tag{93}
\]
\[
- E \left[ f(Y, \theta_1) f \left( X^{(1)}_u, X^{(2)}_{o,u|u_0}, r_{u|u_0} \left( X^{(1)}_{u|u_0}, r_{u|u_0}^{-1} \left( X^{(3)}_{w|u}, X^{(3)}_{w|u_0} \right) \right), \theta_2 \right)^T \right].
\]

**Proof.** See Appendix N.

Proposition 6 provides new expressions of the cross-covariances of SFs by respecting the fact that \( Z_{w,1} \) is independent of \( X_o \) and \( X_u \). In Proposition 7, we derive new versions of the cross-covariances of SFs using only two independent copies of \( X \).

**Proposition 7** Let \( X^{(1)}, X^{(2)} \) be two independent copies of \( X \). Assume that (A1)-(A2) and (A4) hold and \( \theta_1, \theta_2 \in \Theta \). Then, we have
\[
\Sigma_u(\theta_1, \theta_2) = -E[f(X^{(1)}, \theta_1)] E[f(X^{(1)}, \theta_2)]^T \tag{94}
\]
\[
+ E \left[ f \left( X^{(1)}_u, \theta_1 \right) f \left( X^{(1)}_u, X^{(2)}_{o,u|u_0}, r_{u|u_0} \left( X^{(1)}_{u|u_0}, r_{u|u_0}^{-1} \left( X^{(2)}_{w|u}, X^{(2)}_{w|u_0} \right) \right), \theta_2 \right)^T \right],
\]
and
\[
\Sigma_{u}^{\text{tot}}(\theta_1, \theta_2) = E \left[ f(X^{(1)}, \theta_1) f(X^{(1)}, \theta_2)^T \right]
\]
(95)
\[
- E \left[ f \left( X^{(1)}, \theta_1 \right) f \left( X^{(2)}, X^{(1)}_{o \setminus u_0}, r_{u \setminus u_0} \left( X^{(2)}_{u \setminus u_0}, X^{(1)}_{u \setminus u_0} \right), \theta_2 \right)^T \right].
\]

**Proof.** Using Proposition 6, the proofs are straightforward, as \( r_{u \setminus u_0}^{-1} \left( X^{(1)}_{w \setminus u} | X^{(1)}_{u \setminus u_0} \right) \) (resp. \( r_{u \setminus u_0}^{-1} \left( X^{(1)}_{w \setminus u} | X^{(1)}_{u \setminus u_0} \right) \)) is independent of \((X^{(1)}_u, X^{(2)}_o)\) (resp. \((X^{(2)}_u, X^{(1)}_o)\)).

Using the expressions of the cross-covariances of SFs from Proposition 7, Corollary 5 provides the estimators of the cross-covariances of SFs.

**Corollary 5** Let \( X^{(1)}_i, X^{(2)}_i \) with \( i = 1, 2, \ldots, m \) be two independent samples of size \( m \) from \( X \). Assume that \((A1)-(A2)\) and \((A4)\) hold and \( \theta_1, \theta_2 \in \Theta \).

(i) An unbiased estimator of \( \Sigma_u(\theta_1, \theta_2) \) is given by
\[
\Sigma_u'(\theta_1, \theta_2) := \frac{1}{4m} \sum_{i=1}^{m} \left( \left[ f \left( X^{(1)}_i, \theta_1 \right) - f \left( X^{(2)}_{i,u}, X^{(1)}_{i,o \setminus u_0}, r_{u \setminus u_0} \left( X^{(2)}_{i,w \setminus u} | X^{(1)}_{i,u \setminus u_0} \right), \theta_1 \right] \right) \times f \left( X^{(1)}_i, X^{(2)}_{i,o \setminus u_0}, r_{u \setminus u_0} \left( X^{(1)}_{i,w \setminus u} | X^{(1)}_{i,u \setminus u_0} \right), \theta_2 \right) - f \left( X^{(2)}_i, \theta_2 \right)^T \right)
+ \left( f \left( X^{(1)}_i, X^{(2)}_{i,o \setminus u_0}, r_{u \setminus u_0} \left( X^{(1)}_{i,w \setminus u} | X^{(1)}_{i,u \setminus u_0} \right), \theta_1 \right) - f \left( X^{(2)}_i, \theta_1 \right)^T \right) \times f \left( X^{(1)}_i, X^{(2)}_{i,u}, r_{u \setminus u_0} \left( X^{(1)}_{i,w \setminus u} | X^{(1)}_{i,u \setminus u_0} \right), \theta_2 \right) - f \left( X^{(2)}_i, \theta_2 \right)^T \right),
\]
and
\[
E \left( \Sigma_u'(\theta_1, \theta_2) \right) = \Sigma_u(\theta_1, \theta_2).
\]
If \( m \to +\infty \), then we have
\[
\Sigma_u'(\theta_1, \theta_2) \xrightarrow{P} \Sigma_u(\theta_1, \theta_2).
\]

(ii) An unbiased estimator of \( \Sigma_u^{\text{tot}}(\theta_1, \theta_2) \) is given by
\[
\Sigma_u^{\text{tot}}(\theta_1, \theta_2) := \frac{1}{4m} \sum_{i=1}^{m} \left( \left[ f \left( X^{(1)}_i, \theta_1 \right) - f \left( X^{(2)}_{i,u}, X^{(1)}_{i,o \setminus u_0}, r_{u \setminus u_0} \left( X^{(2)}_{i,w \setminus u} | X^{(1)}_{i,u \setminus u_0} \right), \theta_1 \right] \right) \times f \left( X^{(1)}_i, X^{(2)}_{i,o \setminus u_0}, r_{u \setminus u_0} \left( X^{(1)}_{i,w \setminus u} | X^{(1)}_{i,u \setminus u_0} \right), \theta_2 \right) - f \left( X^{(2)}_i, \theta_2 \right)^T \right)
+ \left( f \left( X^{(1)}_i, X^{(2)}_{i,o \setminus u_0}, r_{u \setminus u_0} \left( X^{(1)}_{i,w \setminus u} | X^{(1)}_{i,u \setminus u_0} \right), \theta_1 \right) - f \left( X^{(2)}_i, \theta_1 \right)^T \right) \times f \left( X^{(1)}_i, X^{(2)}_{i,u}, r_{u \setminus u_0} \left( X^{(1)}_{i,w \setminus u} | X^{(1)}_{i,u \setminus u_0} \right), \theta_2 \right) - f \left( X^{(2)}_i, \theta_2 \right)^T \right),
\]
and
\[
\mathbb{E}\left( \Sigma_u^{\text{tot}}(\theta_1, \theta_2) \right) = \Sigma_u^{\text{tot}}(\theta_1, \theta_2).
\]

If \(m \to +\infty\), then we have
\[
\Sigma_u^{\text{tot}}(\theta_1, \theta_2) \overset{P}{\to} \Sigma_u^{\text{tot}}(\theta_1, \theta_2).
\]

**Proof.** The proof is an application of Theorem 2 bearing in mind Proposition 7. \(\square\)

We then deduce new estimators of the covariances of SFs in Corollary 6 and the variances of SFs in Corollary 7 for the multivariate response models and the single response models, respectively.

**Corollary 6** Let \(X_i^{(1)}, X_i^{(2)}\) \(i = 1, 2, \ldots, m\) be two independent samples of size \(m\) from \(X\). Assume that (A1)-(A4) hold.

(i) The MVU estimator of \(\Sigma_u\) is given by
\[
\hat{\Sigma}_u := \frac{1}{4m} \sum_{i=1}^{m} \left[ f\left(X_i^{(1)}\right) - f\left(X_i^{(2)}\right) \right]
\]
\[
\times \left[ f\left(X_i^{(1)}, X_i^{(1)}\right) - f\left(X_i^{(2)}, X_i^{(1)}\right) \right]
\]
\[
\times \left[ f\left(X_i^{(2)}, X_i^{(2)}\right) - f\left(X_i^{(2)}, X_i^{(2)}\right) \right]
\]
\[
\times \left[ f\left(X_i^{(1)}, \theta_1\right) - f\left(X_i^{(2)}, \theta_1\right) \right],
\]
and
\[
\mathbb{E}\left( \hat{\Sigma}_u \right) = \Sigma_u,
\]

(ii) The MVU estimator of \(\Sigma_u^{\text{tot}}\) is given by
\[
\hat{\Sigma}_u^{\text{tot}} := \frac{1}{4m} \sum_{i=1}^{m} \left[ f\left(X_i^{(1)}\right) - f\left(X_i^{(2)}\right) \right]
\]
\[
\times \left[ f\left(X_i^{(1)}, X_i^{(1)}\right) - f\left(X_i^{(2)}, X_i^{(1)}\right) \right]
\]
\[
\times \left[ f\left(X_i^{(2)}, X_i^{(2)}\right) - f\left(X_i^{(2)}, X_i^{(2)}\right) \right]
\]
\[
\times \left[ f\left(X_i^{(1)}, \theta_2\right) - f\left(X_i^{(2)}, \theta_2\right) \right],
\]
and
\[
\mathbb{E}\left( \hat{\Sigma}_u^{\text{tot}} \right) = \Sigma_u^{\text{tot}},
\]

**Proof.** Obvious using Corollary 5. \(\square\)
It is worth noting that when one is only interested in the total dSIs, the estimator $\Sigma^\text{tot}_u$ given by (99) becomes

$$
\frac{1}{2m} \sum_{i=1}^{m} \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2)} \right) \right] = \frac{1}{2m} \sum_{i=1}^{m} \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2)} \right) \right].
$$

Corollary 7 Let $X_i^{(1)}$, $X_i^{(2)}$, $i = 1, 2, \ldots, m$ be two independent samples of size $m$ from $X$. Assume that (A1)-(A4) hold and $n = 1$.

(i) The MVU estimator $\Sigma_u^\text{m}$ becomes

$$
\Sigma_u^\text{m} := \frac{1}{2m} \sum_{i=1}^{m} \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2)} \right) \right].
$$

(ii) The MVU estimator $\Sigma^\text{tot}_u$ becomes

$$
\Sigma^\text{tot}_u := \frac{1}{4m} \sum_{i=1}^{m} \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2)} \right) \right]^2 + \frac{1}{4m} \sum_{i=1}^{m} \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2)} \right) \right]^2.
$$

Proof. Obvious using Corollary 6 with $n = 1$.

When one is only interested in the total dSIs, the estimator $\Sigma^\text{tot}_u$ given by (102) becomes

$$
\frac{1}{2m} \sum_{i=1}^{m} \left[ f \left( X_i^{(1)} \right) - f \left( X_i^{(2)} \right) \right]^2.
$$

To estimate the dGSIs and dSIs when the dependency functions are invertible (A4), we have to

- replace in Theorem 3 the estimators of the cross-covariances of SFs, that is, $\Sigma^\text{m}_u(\theta_1, \theta_2)$ and $\Sigma_u^\text{tot}(\theta_1, \theta_2)$ from Theorem 2 with $\Sigma^\text{m}_u(\theta_1, \theta_2)$ and $\Sigma_u^\text{tot}(\theta_1, \theta_2)$ from Corollary 5, respectively.
- replace in Theorem 4 the estimators of the covariances of SFs $\Sigma_u^\text{m}$ and $\Sigma_u^\text{tot}$ from Corollary 2 with $\Sigma_u^\text{m}$ and $\Sigma_u^\text{tot}$ from Corollary 6, respectively.
- replace in Corollary 4 the estimators of the variances of SFs $\Sigma_u^\text{m}$ and $\Sigma_u^\text{tot}$ from Corollary 3 with $\Sigma_u^\text{m}$ and $\Sigma_u^\text{tot}$ from Corollary 7, respectively.

It is worth noting that the estimators of dGSIs and dSIs obtained after these replacements share the same statistical properties with the former estimators. It comes out from this section that when the inverse of the dependency function, that is, $r_u^{-1}$ is available, we can estimate the dGSIs and dSIs without using the innovation variables $Z_{w-1}$.
6. Analytical test cases

In this section, we illustrate our approach by means of analytical test cases, which allow for underlying some theoretical properties of the new indices.

6.1. Linear function without explicit interaction \( (d = 3, \ n = 1) \)

The linear function, that is,

\[
\mathbf{f}(\mathbf{X}) = \mathbf{X}_1 + \mathbf{X}_2 + \mathbf{X}_3,
\]

includes three inputs \( \mathbf{X} \sim \mathcal{N} \left( \mathbf{0}, \begin{bmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 & \rho_{13}\sigma_1\sigma_3 \\ \rho_{12}\sigma_1\sigma_2 & \sigma_2^2 & \rho_{23}\sigma_2\sigma_3 \\ \rho_{13}\sigma_1\sigma_3 & \rho_{23}\sigma_2\sigma_3 & \sigma_3^2 \end{bmatrix} \right) \). A dependency function of \( (\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3) \) is given by \( (\mathbf{X}_2, \mathbf{X}_3) = r_1(\mathbf{X}_1, \mathbf{Z}_2, \mathbf{Z}_3) \) where

\[
\begin{align*}
\mathbf{X}_2 &= \frac{\rho_{12}\sigma_2}{\sigma_2} \mathbf{X}_1 + \sqrt{1 - \rho_{12}^2} Z_2 \\
\mathbf{X}_3 &= \frac{\rho_{13}\sigma_3}{\sigma_3} \mathbf{X}_1 + \frac{\sigma_2(\rho_{23} - \rho_{12}\rho_{13})}{\sigma_2\sqrt{1 - \rho_{12}^2}} Z_2 + \sqrt{\frac{1 - \rho_{12}^2 - \rho_{13}^2 - \rho_{23}^2 + 2\rho_{12}\rho_{13}\rho_{23}}{1 - \rho_{12}^2}} Z_3,
\end{align*}
\]

\( Z_j \sim \mathcal{N}(0, \sigma_j^2) \), \( j = 2, 3 \), and \( Z_2, Z_3, X_1 \) are independent. Therefore, an equivalent representation of \( f \) is

\[
g_1(\mathbf{X}_1, \mathbf{Z}_2, \mathbf{Z}_3) = \left( 1 + \frac{\rho_{12}\sigma_2}{\sigma_1} + \frac{\rho_{13}\sigma_3}{\sigma_1} \right) \mathbf{X}_1 + \left( \sqrt{1 - \rho_{12}^2} + \frac{\sigma_3(\rho_{23} - \rho_{12}\rho_{13})}{\sigma_2\sqrt{1 - \rho_{12}^2}} \right) Z_2 + \sqrt{\frac{1 - \rho_{12}^2 - \rho_{13}^2 - \rho_{23}^2 + 2\rho_{12}\rho_{13}\rho_{23}}{1 - \rho_{12}^2}} Z_3.
\]

Using such equivalent representation of \( f \), we have the following dSIs of \( \mathbf{X}_1 \) and \( (\mathbf{X}_1, \mathbf{X}_2) \)

\[
\begin{align*}
dS_1 &= dS_{T_1} = \frac{(\sigma_1 + \rho_{12}\sigma_2 + \rho_{13}\sigma_3)^2}{\sum_{j=1}^3 \sigma_j^2 + 2\rho_{12}\sigma_1\sigma_2 + 2\rho_{13}\sigma_1\sigma_3 + 2\rho_{23}\sigma_2\sigma_3}, \\
dS_{12} &= dS_{T_{12}} = \frac{(1 - \rho_{12}^2) (\sigma_1 + \rho_{12}\sigma_2 + \rho_{13}\sigma_3)^2 + (\sigma_2 (1 - \rho_{12}^2) + \sigma_3(\rho_{23} - \rho_{12}\rho_{13}))^2}{(1 - \rho_{12}^2) \left( \sum_{j=1}^3 \sigma_j^2 + 2\rho_{12}\sigma_1\sigma_2 + 2\rho_{13}\sigma_1\sigma_3 + 2\rho_{23}\sigma_2\sigma_3 \right)},
\end{align*}
\]

respectively. Using the same reasoning and bearing in mind that \( R_{\min} = 3 \), we made use of two more equivalent representations of \( f \) to obtain other results. When using \( g_2(\mathbf{X}_2, \mathbf{Z}_3, \mathbf{Z}_1) \), we have

\[
\begin{align*}
dS_2 &= dS_{T_2} = \frac{(\sigma_2 + \rho_{12}\sigma_1 + \rho_{23}\sigma_3)^2}{\sum_{j=1}^3 \sigma_j^2 + 2\rho_{12}\sigma_1\sigma_2 + 2\rho_{13}\sigma_1\sigma_3 + 2\rho_{23}\sigma_2\sigma_3}, \\
dS_{23} &= dS_{T_{23}} = \frac{(1 - \rho_{23}^2) (\sigma_2 + \rho_{12}\sigma_1 + \rho_{23}\sigma_3)^2 + (\sigma_3 (1 - \rho_{23}^2) + \sigma_1(\rho_{13} - \rho_{12}\rho_{23}))^2}{(1 - \rho_{23}^2) \left( \sum_{j=1}^3 \sigma_j^2 + 2\rho_{12}\sigma_1\sigma_2 + 2\rho_{13}\sigma_1\sigma_3 + 2\rho_{23}\sigma_2\sigma_3 \right)},
\end{align*}
\]

Likewise, when using \( g_3(\mathbf{X}_3, \mathbf{Z}_1, \mathbf{Z}_2) \), we have

\[
\begin{align*}
dS_3 &= dS_{T_3} = \frac{(\sigma_3 + \rho_{13}\sigma_1 + \rho_{23}\sigma_2)^2}{\sum_{j=1}^3 \sigma_j^2 + 2\rho_{12}\sigma_1\sigma_2 + 2\rho_{13}\sigma_1\sigma_3 + 2\rho_{23}\sigma_2\sigma_3}, \\
dS_{31} &= dS_{T_{31}} = \frac{(1 - \rho_{13}^2) (\sigma_3 + \rho_{13}\sigma_1 + \rho_{23}\sigma_2)^2 + (\sigma_1 (1 - \rho_{13}^2) + \sigma_2(\rho_{12} - \rho_{13}\rho_{23}))^2}{(1 - \rho_{13}^2) \left( \sum_{j=1}^3 \sigma_j^2 + 2\rho_{12}\sigma_1\sigma_2 + 2\rho_{13}\sigma_1\sigma_3 + 2\rho_{23}\sigma_2\sigma_3 \right)}.
\end{align*}
\]
6.2. Portfolio model (d = 4, n = 1)

We consider the model given by

$$f(X) = X_1 X_2 + X_3 X_4,$$

with $$(X_1, X_2) \sim N_2 \left(0, \begin{bmatrix} \sigma_1^2 & \rho_{12} \sigma_1 \sigma_2 \\ \rho_{12} \sigma_1 \sigma_2 & \sigma_2^2 \end{bmatrix} \right)$$;

$$(X_3, X_4) \sim t \left(0, \nu, \begin{bmatrix} \sigma_3^2 & \rho_{34} \sigma_3 \sigma_4 \\ \rho_{34} \sigma_3 \sigma_4 & \sigma_4^2 \end{bmatrix} \right), \nu > 4$$ and $$(X_1, X_2)$$ is independent of $$(X_3, X_4)$$.

We are in presence of two groups of variables ($$K = 2$$) if the correlations $$\rho_{12} \neq 0$$ and $$\rho_{34} \neq 0$$.

A dependency function of $$(X_1, X_2)$$ is given by

$$X_2 = r_1(X_1, Z_2) = \frac{\rho_{12}}{\sigma_1} X_1 + \sqrt{1 - \rho_{12}^2} Z_2$$

with $$X_1 \sim \mathcal{N}(0, \sigma_1^2)$$ and $$Z_2 \sim \mathcal{N}(0, \sigma_2^2)$$. Likewise a dependency function $X_4 = r_3(X_3, Z_4)$ is given by (see Lemma 2)

$$r_3(X_3, Z_4) = \frac{\rho_{34}}{\sigma_3} X_3 + \sqrt{1 - \rho_{34}^2} (\nu \sigma_3^2 + X_3^2) Z_4,$$

with $$X_3 \sim t(0, \nu, \sigma_3^2)$$ and $$Z_4 \sim t(0, \nu + 1, \sigma_2^2)$$. Thus, a first equivalent representation of the model is given by

$$g_{13}(X_1, Z_2, X_3, Z_4) = \frac{\rho_{12}}{\sigma_1} X_1^2 + \sqrt{1 - \rho_{12}^2} Z_2 X_1 + \frac{\rho_{34}}{\sigma_3} X_3^2 + \sqrt{1 - \rho_{34}^2} (\nu \sigma_3^2 + X_3^2) Z_4 X_3.$$

Using such equivalent representation of $$f$$, we have the following dSIs of $$X_1$$, $$(X_1, X_2)$$, $$X_3$$, $$(X_3, X_4)$$ and $$(X_1, X_3)$$

$$dS_1 = 2\frac{\rho_{12}^2 \sigma_1^2 \sigma_2^2}{D}, \quad dS_{T_1} = dS_{T_2} = dS_{T_{12}} = \frac{\sigma_2^2 \sigma_3^2 (1 + \rho_{12}^2)}{D},$$

$$dS_3 = \frac{\rho_{34}^2 \sigma_2^2 \sigma_4^2 D}{D(\nu - 4)(\nu - 2)^2},$$

$$dS_5 = dS_{T_3} = \frac{\rho_{34}^2 \sigma_2^2 \sigma_4^2 4(\nu - 2)(\nu - 4) + \nu (\nu - 4)}{D(\nu - 1)(\nu - 2)(\nu - 4)},$$

respectively with

$$D = \sigma_1^2 \sigma_2^2 (1 + \rho_{12}^2) + \rho_{34}^2 \sigma_3^2 \sigma_4^2 4(\nu - 2) - \nu (\nu - 4) + \sigma_4^2 \sigma_4^2 (1 - \rho_{34}^2) \frac{\nu (\nu - 4) + 6(\nu - 2)}{(\nu - 1)(\nu - 2)(\nu - 4)}.$$

Using the remaining equivalent representations of $$f$$ (i.e., $$R_{\min} = 4$$), we obtain

$$dS_2 = dS_1, \quad dS_{T_2} = dS_{T_1}, \quad dS_{23} = dS_{13}, \quad dS_{T_{23}} = 1,$$

$$dS_4 = dS_3, \quad dS_{T_4} = dS_{T_3}, \quad dS_{14} = dS_{13}, \quad dS_{T_{14}} = 1,$$

$$dS_{24} = dS_{13}, \quad dS_{T_{24}} = 1.$$
6.3. Functional outputs: dynamic model ($d = 2, n = 1$)

The following dynamic model includes two inputs $X \sim N\left(0, \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}\right)$, and it is defined as follows:

$$f(X, t) = (X_1 + X_2 + aX_1X_2)(2 - \alpha(t)) + \left(X_1^2 + \sqrt{2}X_2\right)(-1 + \alpha(t)),$$

with $a \in \mathbb{R}$, $t \in [0, 365]$ and $\alpha(t) \in \mathbb{R}$. When $a = 0$ there is no explicit interaction between $X_1$ and $X_2$.

To illustrate the difference between both types of dGSIs, we suppose that we have observed the model outputs at $t \in \{t_1, t_2\}$ with $\alpha(t_1) = 1$ and $\alpha(t_2) = 2$. Using the dependency functions $X_2 = r_1(X_1, Z_2) = \rho X_1 + \sqrt{1 - \rho^2}Z_2$ and $X_1 = r_2(X_2, Z_1) = \rho X_2 + \sqrt{1 - \rho^2}Z_1$ with $Z_j \sim N(0, 1)$ and $j = 1, 2$, Figure 1 shows the two types of dGSIs.

![Graphs showing different types of dGSIs](image)

**Figure 1.** First-type, prime second-type and second-type dGSIs for different values of the correlation between the two inputs and for $a = -2, 0$.

The first figure (top-left panel) shows the first-type and second-type dGSIs, and we can see
that both types of dGSIs give the same ranking of inputs for negative values of the correlation. In absence of correlation or dependencies \( (\rho = 0) \), \( X_1 \) and \( X_2 \) have the same effect according to the first-type dGSIs although the second-type dGSIs identify \( X_2 \) as the most influential input. When \( \rho > 0.5 \), the first-type dGSIs show that \( X_2 \) is the most important input while the second-type dGSIs show that both inputs have the same total effects. The second figure (top-right panel) compares the prime second-type and the second-type total dGSIs, and the results are similar to those of the first figure. The third figure (bottom-left panel) compares the first-order dGSIs of the first and second types, and we can see that both types of dGSIs give contrary (single) importance of inputs for positive values of correlation. In the last figure, the first-type and second-type dGSIs give the same ranking of inputs except for \( \rho = 0 \). As different raking of inputs can happen using one or another dGSIs, and knowing that the second-type dGSIs (dGSI\(^2\)) account for the correlation among SFs, we should prefer such indices in practice.

7. Conclusion

We have derived general dependency functions, including empirical ones, for most type of dependencies inferred on input variables such as complex mathematical models under constraints and/or input variables under constraints. Combining such dependency functions with a model of interest, we have proposed dependent generalized sensitivity indices and dependent sensitivity indices of any subset of input variables for the multivariate and/or functional outputs (including spatio-temporal models and dynamic models) and the single response models, respectively. Our indices are consistent with raking input variables using the total-effect index and are well-suited for models with discrete and/or continuous variables. We provided consistent estimators of dGSIs and dSIs and their asymptotic distributions by distinguishing the case where the dependency function is invertible and when one uses the distribution of the innovation variables.

Analytical test cases confirmed that our first-order indices of any subset of inputs are less than the total indices. In the case of the dynamic model, it came out that the second-type dGSIs, which account for the correlations among the components of sensitivity functionals, and the first-type dGSIs can give different ranking of inputs variables. Therefore, we should prefer the second-type dGSIs in practice. Moreover, it came out that the sum of the main-effect indices can be greater than one. In next future, it is interesting to i) investigate new approach for which the main-effect sensitivity indices sum up to one; ii) investigate the development of an emulator for complex models with only the most influential dependent variables.
Appendix A  Proof of Lemma 1

Consider the variable \( Y_k = \Phi^{-1}(F_k(X_k)) \) if \( X_k \) is continuous and \( Y_k = \Phi^{-1}(\tau_{F_k}(X_k, U_k)) \) otherwise. It is well-known that \( Y_k \) follows the standard normal distribution with \( k = 1, \ldots, d \), and \( Y = (Y_j, Y_{-j}) \) has the same copula as \( X \) ([41]), as \( \Phi^{-1} \circ F_k \) (resp. \( \Phi^{-1} \circ \tau_{F_k} \)) is a strictly increasing transformation on the range of \( X_k \). Therefore, \( Y \sim N_d(0, \mathcal{R}) \). Knowing that the dependency function of \( Y \) is given by \( Y_{-j} = \left[ \mathcal{C}[Y_j, Z^2] \right] \) (see [34]), the result follows using the inverse transformation of the form \( X_k = F_k^{-1} \circ \Phi(Y_k) \).

Appendix B  Proof of Lemma 2

Using the same reasoning as in Appendix A, we can see that \( Y \sim t_d(\nu, 0, \mathcal{R}) \) with \( Y = T_k^{-1}(F_k(X_k)) \) for continuous variable \( X_k \) and \( Y_k = T_k^{-1}(\tau_{F_k}(X_k, U_k)) \) otherwise. We then have to derive the dependency function of \( Y \) to obtain the result, and it is done below.

As \( Y \sim t_d(\nu, 0, \mathcal{I}) \Longleftrightarrow \mathcal{L}Y \sim t_d(\nu, 0, \mathcal{R}) \) with \( \mathcal{L} \) the Cholesky factor of \( \mathcal{R} \), we have to show that

\[
\begin{bmatrix}
Y_{j0} \\
Y_{w1} \\
\vdots \\
Y_{wd-1}
\end{bmatrix}
\sim t_d(\nu, 0, \mathcal{I}).
\]

For a multivariate \( t \)-distribution \( Y \sim t_d(\nu, 0, \mathcal{I}) \), it is known that \( Y_{w_{k-1}} | y_{j0}, y_{w1}, \ldots, y_{w_{k-2}} \sim t\left(\nu + k - 1, 0, \frac{\nu + y_{j0}^2 + \sum_{j=1}^{k-2} y_{wj}^2}{\nu + k - 1}\right) \) (see [25] for more details). Thus, it is sufficient to show that \( Y_{w_{k-1}} | y_{j0}, z_{w1}, \ldots, z_{w_{k-2}} \sim t\left(\nu + k - 1, 0, \frac{\nu + y_{j0}^2 + \sum_{j=1}^{k-2} y_{wj}^2}{\nu + k - 1}\right) \) with \( k = 2, \ldots, d \). The recurrence reasoning leads to the following steps.

First, we can see that \( Y_{w_{1}} | y_{j0} \sim t\left(\nu + 1, 0, \frac{\nu + y_{j0}^2}{\nu + 1}\right) \), as \( Z_{w1} \sim t(\nu + 1, 0, 1) \).

Second, in one hand, we suppose that \( Y_{w_{d-2}} | y_{j0}, z_{w1}, \ldots, z_{w_{d-3}} \sim t\left(\nu + d - 2, 0, \frac{\nu + y_{j0}^2 + \sum_{i=1}^{d-3} y_{wi}^2}{\nu + d - 2}\right) \), and we can write

\[
Y_{w_{d-2}} | y_{j0}, z_{w1}, \ldots, z_{w_{d-3}} \overset{d}{=} \sqrt{\frac{\nu + y_{j0}^2 + \sum_{i=1}^{d-3} y_{wi}^2}{\nu + d - 2}} Z_{w_{d-2}},
\]

as \( Z_{w_{d-2}} \sim t(\nu + d - 2, 0, 1) \). The above equation means that for any realization \( z_{w_{d-2}} \) of \( Z_{w_{d-2}} \), there exists a realization \( y_{w_{d-2}} \) of \( Y_{w_{d-2}} \) such that

\[
y_{w_{d-2}} = \sqrt{\frac{\nu + y_{j0}^2 + \sum_{i=1}^{d-3} y_{wi}^2}{\nu + d - 2}} z_{w_{d-2}} \implies y_{w_{d-2}}^2 = \frac{\nu + y_{j0}^2 + \sum_{i=1}^{d-3} y_{wi}^2}{\nu + d - 2} (z_{w_{d-2}})^2.
\]
In the other hand, it comes from the dependency model that

\[
Y_{w_{d-2}}\mid y_{j_0}, z_{w_1}, \ldots, z_{w_{d-3}} \overset{d}{=} \sqrt{\frac{(\nu + y_{j_0}^2) \prod_{i=1}^{d-3} (\nu + i + (z_{w_i})^2)}{\prod_{i=1}^{d-2} (\nu + i)}} Z_{w_{d-2}}.
\]

Therefore, we have the following equality

\[
\frac{(\nu + y_{j_0}^2) \prod_{i=1}^{d-3} (\nu + i + (z_{w_i})^2)}{\prod_{i=1}^{d-2} (\nu + i)} = \frac{\nu + y_{j_0}^2 + \sum_{i=1}^{d-3} y_{w_i}^2}{\nu + d - 2}.
\]

Third, as \( Z_{w_{d-1}} \sim t (\nu + d - 1, 0, 1) \), we have

\[
Y_{w_{d-1}}\mid y_{j_0}, z_{w_1}, \ldots, z_{w_{d-2}} \sim t \left( \nu + d - 1, 0, \frac{(\nu + y_{j_0}^2) \prod_{i=1}^{d-2} (\nu + i + (z_{w_i})^2)}{\prod_{i=1}^{d-1} (\nu + i)} \right)
\]

because

\[
\frac{(\nu + y_{j_0}^2) \prod_{i=1}^{d-2} (\nu + i + (z_{w_i})^2)}{\prod_{i=1}^{d-1} (\nu + i)} = \frac{\nu + y_{j_0}^2 + \sum_{i=1}^{d-3} y_{w_i}^2}{\nu + d - 2} \times \frac{\nu + d - 2 + (z_{w_{d-2}})^2}{\nu + d - 1}
\]

\[
= \frac{\nu + y_{j_0}^2 + \sum_{i=1}^{d-3} y_{w_i}^2}{\nu + d - 1} \times \left( 1 + \frac{(z_{w_{d-2}})^2}{\nu + d - 2} \right)
\]

\[
= \frac{\nu + y_{j_0}^2 + \sum_{i=1}^{d-3} y_{w_i}^2}{\nu + d - 1} \times \left( 1 + \frac{y_{j_0}^2 + \sum_{i=1}^{d-2} y_{w_i}^2}{\nu + y_{j_0}^2 + \sum_{i=1}^{d-1} y_{w_i}^2} \right)
\]

\[
= \frac{\nu + y_{j_0}^2 + \sum_{i=1}^{d-2} y_{w_i}^2}{\nu + d - 1},
\]

Appendix C  Proof of Proposition 2

For Point (i), we have to show that \((Y_u, Y_{\sim u}) \overset{d}{=} (Y_u, T_{\sim u} (r_u (T_u^{-1} (Y_u), Z, U))))\). For any measurable function \(h : \mathbb{R}^{[\mu_0]+n} \to \mathbb{C}\), we can write

\[
\mathbb{E} [h (Y_u, T_{\sim u} (r_u (T_u^{-1} (Y_u), Z, U)))] = \mathbb{E} [h (Y_u, T_{\sim u} (r_u (X_u, Z, U)))]
\]

\[
= \mathbb{E} [h (Y_u, T_{\sim j_0} (X_{\sim u}))]
\]

\[
= \mathbb{E} [h (Y_u, Y_{\sim u})] = \mathbb{E} [h (Y)],
\]

and Point (i) holds.

For Point (ii), first, using Point (i), we have \(|Y_{\sim u}| = T_{\sim u} (r_u (T_u^{-1} (|Y_u|), Z, U))\).

Second, we can see that \(S_j |Y_j| \overset{d}{=} Y_j\), and the result holds.

Appendix D  Proof of Corollary 1

Point (i) is a linear transformation, which is a particular case of Equation (12). Indeed, \(T_{\sim j} (X_{\sim j}) = \Sigma_{j \neq j_0} X_{\sim j} + \mu_{\sim j}\) and \(Y_j = T_j (X_j) = \Sigma_{j} X_{j} + \mu_{j}\).

Point (ii) is a particular case of (12) because \(T_{\sim j} = (T_{w_i}, i = 1, \ldots, d - 1)\).

Point (iii) is a particular case of (13) because \(T_{\sim j} = (T_{w_i}, i = 1, \ldots, d - 1)\).
Appendix E  Proof of Lemma 3

Consider any measurable and integrable function \( h : \mathbb{R}^n \to \mathbb{R} \).

For Point (i), bearing in mind the theorem of transfer, we can write

\[
\mathbb{E} \left[ h (f(X, \theta)) \mid X_{u_0}, X_{j_k}, \ldots, X_{j_m} \right] = \mathbb{E} \left[ h (f(X, X_{s}, r_s (X_{s}, Z), \theta)) \mid X_{u_0}, X_{j_k}, \ldots, X_{j_m} \right]
\]

For Point (ii), First, it is known from Proposition 1 that

\[
\text{Thus,}
\]

At the end of the first step (i.e., \( e_0 = 1 \)), \( B_k \) contains super-sets of \( \{j_k\} \) for all \( j_k \in \{1, \ldots, d_k\} \)

of the form \( (j_k, v_k) \) with \( v_k \in \{1, \ldots, d\} \setminus \{j_k\} \). For two super-sets \( (j_{1}, v_{1}) \) and \( (j_{2}, v_{2}) \), we have

\[
\{j_{1}, v_{1,1}, \ldots, v_{1,k_1}\} \neq \{j_{2}, v_{2,1}, \ldots, v_{2,k_2}\} \text{ for all } j \in \{1, \ldots, j_{0,k}\},
\]

and

\[
\{v_{j,1}, \ldots, v_{d_j,k_j}\} \neq \{v_{j,1}, \ldots, v_{d_j,k_j}\} \text{ for all } j \in \{j_{0,k} + 1 \ldots, d_k\}.
\]

Thus, \( \{u \subseteq \{1, \ldots, d_k\} : |u| = 1\} \subseteq B_k \).

Second, when \( e_0 = 2 \) (from iteration \( d_k + 1 \) to \( \frac{d_k(d_k-1)}{2} \)), we add the super-sets of \( \{j_{1}, j_{2}\} \) of the form \( (j_{1}, j_{2}, v_{1,k_1,k_2}) \), which were not in \( B_k \) at the end of the first step \( e_0 = 1 \). As for new two

super-sets, that is, \( (j_{1}, j_{2}, v_{1,k_1,k_2}), (j_{1}, j_{3}, v_{1,k_1,k_3}), \) we have \( \{j_{1}, j_{2}\} \neq \{j_{1}, j_{3}\}, \{j_{1}, j_{2}\} \neq \{j_{1}, v_{1}\}, \{j_{1}, v_{1}\} \neq \{j_{1}, j_{2}\}, \{j_{1}, v_{1}\} \neq \{j_{1}, j_{3}\}, \) the first two steps allow for obtaining \( \{u \subseteq \{1, \ldots, d_k\} : 1 \leq |u| \leq 2\} \subseteq B_k \).

Third, we repeat that procedure up to \( e_0 = j_{0,k} - 1 \) to obtain

Appendix F  Proof of Lemma 4

Let’s start with Equation (29).

At the end of the first step (i.e., \( e_0 = 1 \)), \( B_k \) contains super-sets of \( \{j_k\} \) for all \( j_k \in \{1, \ldots, d_k\} \)
of the form \( (j_k, v_k) \) with \( v_k \in \{1, \ldots, d\} \setminus \{j_k\} \). For two super-sets \( (j_{1}, v_{1}) \) and \( (j_{2}, v_{2}) \), we have

\[
\{j_{1}, v_{1,1}, \ldots, v_{1,k_1}\} \neq \{j_{2}, v_{2,1}, \ldots, v_{2,k_2}\} \text{ for all } j \in \{1, \ldots, j_{0,k}\},
\]

and

\[
\{v_{j,1}, \ldots, v_{d_j,k_j}\} \neq \{v_{j,1}, \ldots, v_{d_j,k_j}\} \text{ for all } j \in \{j_{0,k} + 1 \ldots, d_k\}.
\]

Thus, \( \{u \subseteq \{1, \ldots, d_k\} : |u| = 1\} \subseteq B_k \).

Second, when \( e_0 = 2 \) (from iteration \( d_k + 1 \) to \( \frac{d_k(d_k-1)}{2} \)), we add the super-sets of \( \{j_{1}, j_{2}\} \) of the form \( (j_{1}, j_{2}, v_{1,k_1,k_2}) \), which were not in \( B_k \) at the end of the first step \( e_0 = 1 \). As for new two

super-sets, that is, \( (j_{1}, j_{2}, v_{1,k_1,k_2}), (j_{1}, j_{3}, v_{1,k_1,k_3}), \) we have \( \{j_{1}, j_{2}\} \neq \{j_{1}, j_{3}\}, \{j_{1}, j_{2}\} \neq \{j_{1}, v_{1}\}, \{j_{1}, v_{1}\} \neq \{j_{1}, j_{2}\}, \{j_{1}, v_{1}\} \neq \{j_{1}, j_{3}\}, \) the first two steps allow for obtaining \( \{u \subseteq \{1, \ldots, d_k\} : 1 \leq |u| \leq 2\} \subseteq B_k \).

Third, we repeat that procedure up to \( e_0 = j_{0,k} - 1 \) to obtain
{u \subseteq \{1, \ldots, d_k\} : 1 \leq |u| \leq j_{0,k} - 1} \subseteq B_k. These operations are possible because \( \binom{d_k}{e_0} \leq \binom{d_k}{j_{0,k}} \) for all \( e_0 = 1, \ldots, j_{0,k} - 1 \), and we avoid permutations \( (w_k) \) that bring replicated sets in both \( B_k \) and \( E_k \).

Fourth, the iterations \( \binom{d_k}{j_{0,k} - 1} < i \leq \binom{d_k}{j_{0,k}} \) (when possible) aim to add the remaining subsets of \( j_{0,k} \) elements.

Fifth, we have \( \{u \subseteq \{1, \ldots, d_k\} : |u| = j_{0,k} + 1\} \subseteq B_k \) because for any \( u_0 \subseteq \{1, \ldots, d_k\} \) with \( |u_0| = j_{0,k} + 1 \), there exists \( w_k^* \in \mathcal{P}_k \) such that \( \{w_{j_{0,k}+2,k}^*, \ldots, w_{d_k,k}^*\} \cap u_0 = \emptyset \). Indeed, the permutation \( w_k^* \) was included in \( \mathcal{P}_k \) when constructing all the subsets \( u \subseteq \{1, \ldots, d_k\} \) with \( |u| = d_k - j_{0,k} - 1 < j_{0,k} \) thanks to \( E_k \) and the fact that \( \binom{d_k}{j_{0,k} + 1} = \binom{d_k}{d_k - j_{0,k} - 1} \).

Finally, we use the same reasoning to obtain the results.

Equation (30) is obvious by construction (see Algorithm 1).

**Appendix G  Proof of Theorem 1**

For Point (i), first, for \( u_k \subseteq \{1, \ldots, d_k\} \) with \( |u_k| > 0 \), there exists \( w_k^* \in \mathcal{P}_k \) such that \( u_k = \{w_{1,k}^*, \ldots, w_{|u_k|,k}^*\} \) according to Lemma 4. Lemma 3 ensures the determination of the distribution of \( f \) given \( X_{u_k} \) using an equivalent representation of \( f \) associated with \( w_k^* \).

Second, for \( u := (u_0, u_2, \ldots, u_K) \) where \( u_0 \subseteq \emptyset, u_k \subseteq \{1, \ldots, d_k\} \) and \( |u_k| = j_{0,k} \) with \( k = 2, \ldots, K \), there exists only one permutation \( w_k^* \in \mathcal{P}_k \) such that \( u_k = \{w_{1,k}^*, \ldots, w_{|u_k|,k}^*\}, \forall k = 2, \ldots, K \). As i) only one representation of \( f \) associated with \( w_k^* \), \( k = 2, \ldots, K \) out of \( \prod_{k=2}^{K} \binom{d_k}{j_{0,k}} \) allows for determining the distribution of \( f \) given \( X_u \), and ii) we have \( R := \prod_{k=2}^{K} \binom{d_k}{j_{0,k}} \) possibilities of \( \{u_2, \ldots, u_K\} \) with \( |u_k| = j_{0,k} \), it is clear that we need \( R \) different representations of \( f \). The result follows because \( R \) is the highest number of possibilities of \( \{u_k \subseteq \{1, \ldots, d_k\}, k = 2, \ldots, K : |u_k| > 0\} \), and other possibilities are in the \( R \) representations (Lemma 4).

For Point (ii), suppose that \( R_{p_2 \ldots p_K} = \binom{d_k}{p_{k_0}} \). Bearing in mind Lemma 3 and Lemma 4, \( R_{p_2 \ldots p_K} \) equivalent representations of \( f \) are sufficient and necessary to assess the distribution of \( f \) given \( X_{u_{d_k}} \) for all \( u_{d_k} \subseteq \{1, \ldots, d_{k_0}\} \) with \( |u_{k_0}| \leq p_{k_0} \). With the same number of representation, we can assess the effect of other groups of variables because \( \binom{d_k}{p_k} \leq R_{p_2 \ldots p_K}, \forall k = 2, \ldots, K \).

**Appendix H  Proof of Proposition 3**

The proofs are straightforward. The results rely on the Hoeffding decomposition of an equivalent representation of \( f \) and the fact that for two positive semi-definite matrices \( A_1, A_2 \), the Loewner partial ordering, that is, \( A_1 \preceq A_2 \) implies \( \text{Tr}(A_1) \leq \text{Tr}(A_2) \) and \( ||A_1||_F \leq ||A_2||_F \). See [34] for more details.
Appendix I  Proof of Proposition 5

Without loss of generality, we suppose that the model \( f \) is centered, that is, \( \mathbb{E}[f(X^{(1)}, \theta)] = 0. \)

For Point (i), bearing in mind that \( X^{(1)} = (X^{(1)}_{\{o,s\}}, r_s(X^{(1)}_s, Z^{(1)}_{w-1})) \) and \( X^{(2)} = (X^{(2)}_{\{o,s\}}, r_s(X^{(2)}_s, Z^{(2)}_{w-1})) \), we can write

\[
\Sigma_u(\theta_1, \theta_2) = \mathbb{E}\left[ f^o_u(X^{(1)}_u, \theta_1)f^o_u(X^{(1)}_u, \theta_2)^T \right]
= \mathbb{E}\left[ f(X^{(1)}, \theta_1) | X^{(1)}_u \right]\mathbb{E}\left[ f(X^{(1)}, r_s(X^{(1)}_s, Z^{(1)}_{w-1}), \theta_2) | X^{(1)}_u \right]^T
= \mathbb{E}\left[ f(X^{(1)}, \theta_1) \right] \times \mathbb{E}\left[ f(X^{(1)}, r_s(X^{(1)}_s, Z^{(1)}_{w-1}), \theta_2) | X^{(1)}_u \right]^T
= \mathbb{E}\left[ f(X^{(1)}, \theta_1) f(X^{(1)}_{\{o,s\}} \cap u, X^{(2)}_{\{o,s\}} \setminus u, r_s(X^{(1)}_{w\cap u}, X^{(2)}_{w\cap u}, Z^{(1)}_{w-1\cap u}, Z^{(2)}_{w-1\cap u}), \theta_2) | X^{(1)}_u \right]^T.
\]

The derivation of Point (ii) is similar to the derivation of Point (i). Indeed, we have

\[
\Sigma_u^{tot}(\theta_1, \theta_2) = \mathbb{E}\left[ f^{tot}_u(X^{(1)}_{\{o,s\}}, Z^{(1)}_{w-1}, \theta_1)f^{tot}_u(X^{(1)}_{\{o,s\}}, Z^{(1)}_{w-1}, \theta_2)^T \right]
= \mathbb{E}\left[ f(X^{(1)}, \theta_1) f(X^{(1)}, \theta_2)^T \right]
- \mathbb{E}\left[ f(X^{(1)}, \theta_1) \right] \mathbb{E}\left[ f(X^{(1)}_{\{o,s\}}, r_s(X^{(1)}_s, Z^{(1)}_{w-1}), \theta_2) | X^{(1)}_{\{o,s\}} \setminus u, Z^{(1)}_{w-1\cap u} \right]^T
- \mathbb{E}\left[ f(X^{(1)}_{\{o,s\}}, r_s(X^{(1)}_s, Z^{(1)}_{w-1}), \theta_1) | X^{(1)}_{\{o,s\}} \setminus u, Z^{(1)}_{w-1\cap u} \right] \mathbb{E}\left[ f(X^{(1)}, \theta_2)^T \right]
+ \mathbb{E}\left[ f(X^{(1)}_{\{o,s\}}, r_s(X^{(1)}_s, Z^{(1)}_{w-1}), \theta_1) | X^{(1)}_{\{o,s\}} \setminus u, Z^{(1)}_{w-1\cap u} \right] \times \mathbb{E}\left[ f(X^{(1)}, \theta_2)^T \right]
= \mathbb{E}\left[ f(X^{(1)}, \theta_1)f(X^{(1)}, \theta_2)^T \right]
- \mathbb{E}\left[ f(X^{(1)}, \theta_1) f(X^{(2)}_{\{o,s\}} \cap u, X^{(1)}_{\{o,s\}} \setminus u, r_s(X^{(1)}_{w\cap u}, X^{(1)}_{w\cap u}, Z^{(1)}_{w-1\cap u}, Z^{(2)}_{w-1\cap u}), \theta_2)^T \right].
\]

bearing in mind Point (i).

Appendix J  Proof of Theorem 2

Using Proposition 5, the proofs of Points (i)-(iii) are straightforward. Indeed, by expanding the above expressions of the estimators, we obtain unbiased estimators, and by applying the law of large number, we obtain consistent estimators.

Appendix K  Proof of Corollary 2

First, the proposed estimators are unbiased and consistent by applying Theorem 2 where \( \theta_1 = \theta_2 = \theta_0 \) is a constant. Second, the MVU properties are due to the symmetric properties of such
estimators ([56]). Indeed, each estimator remains unchanged when one permutes $X_{i,(0,s)\cap u}^{(1)}$ with $X_{i,(0,s)\cap u}^{(2)}$ or $X_{i,(0,s)\setminus u}^{(1)}$ with $X_{i,(0,s)\setminus u}^{(2)}$ or $X_{i,s\cap u}^{(1)}$ with $X_{i,s\setminus u}^{(2)}$ or $X_{i,s\setminus u}^{(1)}$ with $Z_{i,w_{-1}\cap v}^{(2)}$ or $Z_{i,w_{-1}\setminus v}^{(1)}$ with $Z_{i,w_{-1}\setminus v}^{(2)}$. More details can be found in [30] (Theorems 2, 3).

Appendix L Proof of Theorem 3

For Point (i), according to the law of large numbers, we have

$$
\frac{1}{L} \sum_{\ell=1}^{L} \text{Tr} \left( \Sigma_u^{(0)}(\theta_{c}, \theta_{t}) \right) \xrightarrow{P} \int_{\Theta} \text{Tr} \left( \Sigma_u(\theta, \theta) \right) d\theta,
$$

$$
\frac{1}{L} \sum_{\ell=1}^{L} \text{Tr} \left( \Sigma_u^{tot}(\theta_{c}, \theta_{t}) \right) \xrightarrow{P} \int_{\Theta} \text{Tr} \left( \Sigma_u^{tot}(\theta, \theta) \right) d\theta \text{ and}
$$

$$
\frac{1}{L} \sum_{\ell=1}^{L} \text{Tr} \left( \Sigma(\theta_{c}, \theta_{t}) \right) \xrightarrow{P} \int_{\Theta} \text{Tr} \left( \Sigma(\theta, \theta) \right) d\theta. \text{ Point (i) holds by applying the Slutsky theorem.}
$$

Point (ii) is similar to Point (i) since

$$
\frac{1}{L} \sum_{\ell=1}^{L} \left\| \Sigma_u^{(0)}(\theta_{c}, \theta_{t}) \right\|_F \xrightarrow{P} \int_{\Theta} \left\| \Sigma_u(\theta, \theta) \right\|_F d\theta, \frac{1}{L} \sum_{\ell=1}^{L} \left\| \Sigma_u^{tot}(\theta_{c}, \theta_{t}) \right\|_F \xrightarrow{P} \int_{\Theta} \left\| \Sigma_u^{tot}(\theta, \theta) \right\|_F d\theta \text{ and}
$$

$$
\frac{1}{L} \sum_{\ell=1}^{L} \left\| \Sigma(\theta_{c}, \theta_{t}) \right\|_F \xrightarrow{P} \int_{\Theta} \left\| \Sigma(\theta, \theta) \right\|_F d\theta. \text{ Point (ii) holds.}
$$

Point (iii) is similar to Point (ii).

Appendix M Proof of Theorem 4

The results about the consistency are deduced from Theorem 3, as $\Theta = \{\theta_0\}$.

For the asymptotic distribution of Point (i), the central limit theorem (CLT) allows for writing

$$
\sqrt{m} \left( \text{Tr} \left( \Sigma_u \right) - \text{Tr} \left( \Sigma_u \right) \right) \xrightarrow{D} \mathcal{N} \left( 0, \mathbb{V} \left[ \text{Tr}(K(X)) \right] \right),
$$

and the Slutsky theorem gives

$$
\sqrt{m} \left( \frac{\text{Tr} \left( \Sigma_u \right)}{\text{Tr} \left( \Sigma \right)} - \frac{\text{Tr} \left( \Sigma_u \right)}{\text{Tr} \left( \Sigma \right)} \right) \xrightarrow{D} \mathcal{N} \left( 0, \frac{\mathbb{V} \left[ \text{Tr}(K(X)) \right]}{\mathbb{V} \left[ \text{Tr}(\Sigma) \right]^2} \right).
$$

The result holds because $\sqrt{m} \left( \frac{\text{Tr} \left( \Sigma_u \right)}{\text{Tr} \left( \Sigma \right)} - \frac{\text{Tr} \left( \Sigma_u \right)}{\text{Tr} \left( \Sigma \right)} \right)$ is asymptotically equivalent (in probability) to $\sqrt{m} \left( \frac{\text{Tr} \left( \Sigma_u \right)}{\text{Tr} \left( \Sigma \right)} - \frac{\text{Tr} \left( \Sigma_u \right)}{\text{Tr} \left( \Sigma \right)} \right)$ under the technical condition $m/M \to 0$ (see [30, 31] for more details). By replacing $\overline{\Sigma_u}$ with $\overline{\Sigma_u^{tot}}$, we have Point (i).

For Point (ii), the CLT implies

$$
\sqrt{m} \left( \text{Vec}(\overline{\Sigma_u}) - \text{Vec}(\overline{\Sigma_u}) \right) \xrightarrow{D} \mathcal{N} \left( 0, \mathbb{V} \left[ \text{Vec}(K(X)) \right] \right).
$$

The delta method gives

$$
\sqrt{m} \left( \text{Vec}(\overline{\Sigma_u})^T \text{Vec}(\overline{\Sigma_u}) - \text{Vec}(\overline{\Sigma_u})^T \text{Vec}(\overline{\Sigma_u}) \right) \xrightarrow{D} \mathcal{N} \left( 0, 4 \text{Vec}(\overline{\Sigma_u})^T \mathbb{V} \left[ \text{Vec}(K(X)) \right] \text{Vec}(\overline{\Sigma_u}) \right),
$$

and

$$
\sqrt{m} \left( \sqrt{\text{Vec}(\overline{\Sigma_u})^T \text{Vec}(\overline{\Sigma_u})} - \sqrt{\text{Vec}(\overline{\Sigma_u})^T \text{Vec}(\overline{\Sigma_u})} \right) \xrightarrow{D} \mathcal{N} \left( 0, \frac{\text{Vec}(\overline{\Sigma_u})^T \mathbb{V} [\text{Vec}(K(X))] \text{Vec}(\overline{\Sigma_u})}{\text{Vec}(\overline{\Sigma_u})^T \text{Vec}(\overline{\Sigma_u})} \right).$$
Using the same reasoning as for Point (i) under the technical condition $m/M \to 0$, we have the result, that is,

$$\sqrt{m} \left( \frac{\|\Sigma_u\|_F}{\|\Sigma\|_F} - \frac{\|\Sigma_u\|_F}{\|\Sigma\|_F} \right) \xrightarrow{\mathcal{D}} \mathcal{N} \left( 0, \frac{\text{Vec}(\Sigma_u)^T \mathbb{V} [\text{Vec}(K)] \text{Vec}(\Sigma_u)}{\text{Vec}(\Sigma_u)^T \text{Vec}(\Sigma_u) \|\Sigma\|_F^2} \right).$$

**Appendix N  Proof of Proposition 6**

Bearing in mind Equation (7), the proofs of Points (i)-(ii) are obtained by replacing $Z^{(2)}_{u \backslash v}$ (resp. $Z^{(1)}_{u \backslash v}$) of Proposition 5 with $r^{-1}_{u \backslash u_0} \left( X^{(4)}_{w \backslash u_0} | X^{(4)}_{w \backslash u_0} \right)$ (resp. $r^{-1}_{u \backslash u_0} \left( X^{(3)}_{w \backslash u_0} | X^{(3)}_{w \backslash u_0} \right)$, which is independent of $X^{(1)}$ and $X^{(2)}$.

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