ASYMPTOTIC NORMALITY OF JOINT METAMODEL-BASED SOBOL' INDEX ESTIMATORS

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ABSTRACT

This paper proposes two joint metamodel-based Sobol' index estimators and investigates their asymptotic properties. The numerical evaluation corroborates the theoretical results and highlights the impact of the combination of training sample size and Monte Carlo sample size on the estimators' performance.

1 INTRODUCTION

Sobol' indices are widely used in global sensitivity analysis for assessing the input parameters' impact on the model output (Sobol' 1990; Saltelli and Annoni 2010), with successful applications in epidemiological modeling, defect detection in manufacturing, pollutant transport modeling, etc. Estimating Sobol' indices can be computationally demanding, especially when the input space dimensionality is high. Many Monte Carlo (MC)-based estimators have emerged to efficiently estimate Sobol' indices; see, e.g., Tarantola et al. (2007), Saltelli et al. (2010), and Mazo (2021). However, MC-based estimators can be inefficient when the simulation model is computationally expensive to evaluate. In recent years, research on metamodel-based Sobol' index estimators has attracted increasing attention; see, e.g., Marrel et al. (2012), Janon et al. (2014), and Hart et al. (2017). Thanks to efficient metamodeling techniques and suitable experimental designs, it is possible to construct an accurate metamodel using a relatively small training sample generated by a limited number of simulation runs for the purpose of Sobol' index estimation.

While point estimates of Sobol' indices can serve as a measure of the importance of input variables, it is arguably equally important to quantify the uncertainty associated with these estimates. Non-asymptotic uncertainty quantification methods based on bootstrapping and empirical distributions have been proposed; see, e.g., Storlie et al. (2009), Marrel et al. (2009), and Janon et al. (2014). On the other hand, Janon et al. (2014) investigated the asymptotic normality of metamodel-based Sobol' index estimators for deterministic simulation models. For stochastic simulation models, Mazo (2021) conducted an asymptotic analysis for MC-based Sobol' index estimators. However, the asymptotic properties of metamodel-based estimators for a stochastic simulation model have rarely been explored. To the best of our knowledge, this work is among the first to investigate the asymptotic normality of metamodel-based Sobol' index estimators for a stochastic simulation model.

In this paper, we propose joint metamodel-based Sobol' index estimators which rely on estimation of both the mean and variance functions implied by a stochastic simulation experiment. We prove the estimators' asymptotic normality, based on which asymptotic confidence intervals can be constructed for uncertainty quantification. The rest of the paper is organized as follows. Section 2 briefly introduces Sobol' indices and proposes two joint metamodel-based Sobol' index estimators. Section 3 presents the theoretical

analysis of the proposed estimators. Section 4 presents numerical experiments for performance evaluations and verifies the theoretical results.

2 JOINT METAMODEL-BASED ESTIMATION

This section briefly reviews Sobol' indices for global sensitivity analysis and proposes two joint metamodel-based Sobol' index estimators. Given the input vector $X = (X_1, X_2, \ldots, X_p)^\top \in \mathcal{X} \subset \mathbb{R}^p$, we consider a stochastic simulation model of the form $\mathcal{Y} = f(X, \varepsilon)$, where f is some real-valued function and ε represents the uncertainty inherent to the simulation model. For any subset $u \subset \{1, 2, \ldots, p\}$, define X_u as the subset of entries in X with indices in u; e.g., for $u = \{1, 2\}$, $X_u = (X_1, X_2)$. Define $X_{-u} := X \backslash X_u$. The Sobol' index of X_u quantifies the contribution of the input variable(s) in X_u towards the variance of the model output $\mathcal{Y}$, based on the following functional variance decomposition: $\text{Var}_{X,\varepsilon}(\mathcal{Y}) = V_\varepsilon(\mathcal{Y}) + \sum_{i=1}^p \sum_{|J|=i}(V_J(\mathcal{Y}) + V_{J\varepsilon}(\mathcal{Y}))$, where $V_i(\mathcal{Y}) = \text{Var}_{X_i}(\mathbb{E}_{X_{-i},\varepsilon}(\mathcal{Y} \mid X_i))$, $V_\varepsilon(\mathcal{Y}) = \text{Var}_\varepsilon(\mathbb{E}_X(\mathcal{Y} \mid \varepsilon))$, $V_{ij}(\mathcal{Y}) = \text{Var}_{X_i,X_j}\left(\mathbb{E}_{X_{-\{i,j\}},\varepsilon}(\mathcal{Y} \mid X_i, X_j)\right) - V_i(\mathcal{Y}) - V_j(\mathcal{Y})$, $i \neq j$, $V_{i\varepsilon}(\mathcal{Y}) = \text{Var}_{X_i,\varepsilon}(\mathbb{E}_{X_{-i}}(\mathcal{Y} \mid X_i, \varepsilon)) - V_i(\mathcal{Y}) - V_\varepsilon(\mathcal{Y})$, and so on. Following Mazo (2021), the Sobol' index of X_u for a stochastic simulation model is defined as

$$S^{X_u} = \frac{\text{Var}_{X_u}(\mathbb{E}_{X_{-u},\varepsilon}(\mathcal{Y} \mid X_u))}{\text{Var}_{X,\varepsilon}(\mathcal{Y})}, \quad u \subset \{1, 2, \ldots, p\}. \tag{1}$$

The value of S^{X_u} is between 0 and 1, and a larger value indicates greater importance of the input variable(s) in X_u to Y. The Sobol' index given in (1) can be estimated via different methods, e.g., the pick-freeze scheme (Gamboa et al. 2016), which amounts to running the simulation model at inputs $(X_{u,i}, X_{-u,i})$ and $(X'_{u,i}, X_{-u,i})$ for $i \in \mathbb{N}^+$, where $X_{u,i}$ and $X_{-u,i}$ are MC samples of X_u and X_{-u}, and $X'_{u,i}$ is an independent copy of $X_{u,i}$. When the simulation model is computationally expensive to evaluate, Janon et al. (2014), Hart et al. (2017), and Castellan et al. (2020) showed that metamodeling can facilitate efficient estimation of the Sobol' indices by only performing simulation runs to build a metamodel and evaluating the metamodel for Sobol' index estimation using a MC sample of input vectors.

Following Marrel et al. (2012), we consider joint metamodel-based Sobol' index estimation for stochastic simulation models. Denote by $Y_m(X) := \mathbb{E}_\varepsilon(\mathcal{Y} \mid X)$ the mean function and $Y_d(X) := \text{Var}_\varepsilon(\mathcal{Y} \mid X)$ the variance function, which are defined on the probability space $(\Omega_X, \mathcal{F}_X, \mathbb{P}_X)$. We can rewrite Equation (1) as

$$S^{X_u} = \frac{\text{Var}_{X_u}(\mathbb{E}_{X_{-u}}(Y_m \mid X_u))}{\text{Var}_X(Y_m) + \mathbb{E}_X(Y_d)}, \tag{2}$$

since $\text{Var}_{X_u}(\mathbb{E}_{X_{-u},\varepsilon}(\mathcal{Y} \mid X_u)) = \text{Var}_{X_u}(\mathbb{E}_{X_{-u}}(Y_m \mid X_u))$ and $\text{Var}_{X,\varepsilon}(\mathcal{Y}) = \text{Var}_X(Y_m) + \mathbb{E}_X(Y_d)$. Consider estimating Y_m and Y_d by metamodels $\widetilde{Y}_{m,\mathcal{T}_N}$ and $\widetilde{Y}_{d,\mathcal{T}_N}$, where $\mathcal{T}_N$ denotes a training sample, $\{(X_i, \mathcal{Y}_i)\}_{i=1}^n$, to obtain the metamodels, n denotes the training sample size, N denotes the MC sample size for metamodel evaluations, and $n \to \infty$ as $N \to \infty$. As Janon et al. (2014) showed for deterministic simulation models, there exist some relationships between n and N to make the metamodel-based Sobol' index estimators consistent. Assume that the training sample $\mathcal{T}_N$ is defined on the probability space $(\Omega_Z, \mathcal{F}_Z, \mathbb{P}_Z)$. The metamodels $\widetilde{Y}_{m,\mathcal{T}_N}$ and $\widetilde{Y}_{d,\mathcal{T}_N}$ are defined on the product space $(\Omega_Z \times \Omega_X, \sigma(\mathcal{F}_Z \times \mathcal{F}_X), \mathbb{P}_Z \otimes \mathbb{P}_X)$. In particular, given a fixed $\omega \in \Omega_Z$, $\widetilde{Y}_{m,\mathcal{T}_N(\omega)}$ and $\widetilde{Y}_{d,\mathcal{T}_N(\omega)}$ are defined on the probability space $(\Omega_X, \mathcal{F}_X, \mathbb{P}_X)$. Since Y_m and Y_d are unavailable, we adopt $\widetilde{Y}_{m,\mathcal{T}_N}$ and $\widetilde{Y}_{d,\mathcal{T}_N}$ for Sobol' index estimation. Define $\widetilde{Y}_{m,\mathcal{T}_N,i} := \widetilde{Y}_{m,\mathcal{T}_N}((X_{u,i}, X_{-u,i}))$, $\widetilde{Y}^X_{m,\mathcal{T}_N,i} := \widetilde{Y}_{m,\mathcal{T}_N}((X'_{u,i}, X_{-u,i}))$, $\widetilde{Y}_{d,\mathcal{T}_N,i} := \widetilde{Y}_{d,\mathcal{T}_N}((X_{u,i}, X_{-u,i}))$, and $\widetilde{Y}^{(X)}_{m,\mathcal{T}_N,i} := \widetilde{Y}_{m,\mathcal{T}_N}((X'_{u,i}, X'_{-u,i}))$ for $i \in \mathbb{N}^+$, where $X'_{-u,i}$ is an independent copy of $X_{-u,i}$. Based on (2), we propose two estimators to be detailed next.

The First Sobol' Index Estimator. The first estimator of S^{X_u} in (2) is devised by noting that $\text{Var}_{X_u}(\mathbb{E}_{X_{-u}}(Y_m \mid X_u)) = \text{Cov}(Y_m((X_u, X_{-u})), Y_m((X'_u, X_{-u})))$, where X'_u is an independent copy of X_u; see Lemma 2.2 of Janon et al. (2014). Based on the outputs $\{\widetilde{Y}_{m,\mathcal{T}_N,i}, \widetilde{Y}^X_{m,\mathcal{T}_N,i}, \widetilde{Y}_{d,\mathcal{T}_N,i}\}_{i=1}^N$ from evaluating the mean and variance metamodels,

the first estimator can be given as

$$\widetilde{S}^{X_u}_{\mathcal{T}_N} = \frac{\frac{1}{N}\sum_{i=1}^N \widetilde{Y}_{m,\mathcal{T}_N,i}\widetilde{Y}^X_{m,\mathcal{T}_N,i} - \left(\frac{1}{N}\sum_{i=1}^N \widetilde{Y}_{m,\mathcal{T}_N,i}\right)\left(\frac{1}{N}\sum_{i=1}^N \widetilde{Y}^X_{m,\mathcal{T}_N,i}\right)}{\frac{1}{N}\sum_{i=1}^N \widetilde{Y}^2_{m,\mathcal{T}_N,i} - \left(\frac{1}{N}\sum_{i=1}^N \widetilde{Y}_{m,\mathcal{T}_N,i}\right)^2 + \frac{1}{N}\sum_{i=1}^N \widetilde{Y}_{d,\mathcal{T}_N,i}}. \tag{3}$$

The Second Sobol' Index Estimator. There exist alternative estimators of the numerator on the right-hand side of (2); see, e.g., Table 2 in Saltelli et al. (2010). We study one of them in this paper. Define $\widetilde{Y}^{(X)}_{m,\mathcal{T}_N,i} := \widetilde{Y}_{m,\mathcal{T}_N}((X'_{u,i}, X'_{-u,i}))$. Based on the outputs $\{\widetilde{Y}_{m,\mathcal{T}_N,i}, \widetilde{Y}^X_{m,\mathcal{T}_N,i}, \widetilde{Y}^{(X)}_{m,\mathcal{T}_N,i}, \widetilde{Y}_{d,\mathcal{T}_N,i}\}_{i=1}^N$ from evaluating the metamodels, we can obtain the second estimator as

$$\widetilde{T}^{X_u}_{\mathcal{T}_N} = \frac{\frac{1}{N}\sum_{i=1}^N \widetilde{Y}_{m,\mathcal{T}_N,i}(\widetilde{Y}^X_{m,\mathcal{T}_N,i} - \widetilde{Y}^{(X)}_{m,\mathcal{T}_N,i})}{\frac{1}{N}\sum_{i=1}^N \widetilde{Y}^2_{m,\mathcal{T}_N,i} - \left(\frac{1}{N}\sum_{i=1}^N \widetilde{Y}_{m,\mathcal{T}_N,i}\right)^2 + \frac{1}{N}\sum_{i=1}^N \widetilde{Y}_{d,\mathcal{T}_N,i}}. \tag{4}$$

Our analysis of the two metamodel-based estimators given in (3) and (4) is detailed in the next section. It is worthwhile studying the following two estimators given the knowledge of the true mean and variance functions $Y_m(\cdot)$ and $Y_d(\cdot)$:

$$S^{X_u}_N = \frac{\frac{1}{N}\sum_{i=1}^N Y_{m,i}Y^X_{m,i} - \left(\frac{1}{N}\sum_{i=1}^N Y_{m,i}\right)\left(\frac{1}{N}\sum_{i=1}^N Y^X_{m,i}\right)}{\frac{1}{N}\sum_{i=1}^N Y^2_{m,i} - \left(\frac{1}{N}\sum_{i=1}^N Y_{m,i}\right)^2 + \frac{1}{N}\sum_{i=1}^N Y_{d,i}}, \tag{5}$$

and

$$T^{X_u}_N = \frac{\frac{1}{N}\sum_{i=1}^N Y_{m,i}(Y^X_{m,i} - Y^{(X)}_{m,i})}{\frac{1}{N}\sum_{i=1}^N Y^2_{m,i} - \left(\frac{1}{N}\sum_{i=1}^N Y_{m,i}\right)^2 + \frac{1}{N}\sum_{i=1}^N Y_{d,i}}, \tag{6}$$

where the two estimators above are defined analogously to those in (3) and (4) but with the outputs from evaluating the metamodels replaced by those from evaluating the true mean and variance functions.

3 ASYMPTOTIC ANALYSIS

This section investigates the asymptotic normality of the estimators proposed in Section 2. We first show that this property holds true for the estimators that are based on the true mean and variance functions under a bounded moment condition. Then, we investigate when the asymptotic normality holds true if the true mean and variance functions are unavailable and are replaced by the metamodels.

3.1 Analysis of the Sobol' Index Estimators Using the True Mean and Variance Functions

This subsection analyzes the asymptotic normality of the Sobol' index estimators given in (5) and (6) when the true mean and variance functions, $Y_m(X)$ and $Y_d(X)$, are available. For ease of notation, we write Y_m and Y_d hereafter. The analysis relies on Assumption 1 below.

Assumption 1 $\mathbb{E}_X\left(Y_m^4\right) < \infty$ and $\mathbb{E}_X\left(Y_d^2\right) < \infty$.

Proposition 1 Under Assumption 1, $\sqrt{N}\left(S^{X_u}_N - S^{X_u}\right) \xrightarrow[N\to\infty]{d} \mathcal{N}(0, \sigma_S^2)$ in $(\Omega_X, \mathcal{F}_X, \mathbb{P}_X)$, where

$$\sigma_S^2 = \text{Var}_X\left(\left(Y_m - \mathbb{E}_X\left(Y_m\right)\right)\left(Y_m^X - \mathbb{E}_X\left(Y_m\right)\right) - S^{X_u}\left(\left(Y_m - \mathbb{E}_X\left(Y_m\right)\right)^2 + Y_d\right)\right)\left(\text{Var}_{X,\varepsilon}\left(\mathcal{Y}\right)\right)^{-2}. \tag{7}$$

Proof. Define

$$U_i := \left(\left(Y_{m,i} - \mathbb{E}_X\left(Y_m\right)\right)\left(Y_{m,i}^X - \mathbb{E}_X\left(Y_m\right)\right), Y_{m,i} - \mathbb{E}_X\left(Y_m\right), Y_{m,i}^X - \mathbb{E}_X\left(Y_m\right), \left(Y_{m,i} - \mathbb{E}_X\left(Y_m\right)\right)^2, Y_{d,i}\right), \tag{8}$$

and $\overline{U}_N := N^{-1} \sum_{i=1}^{N} U_i$. Define $\mu := \left(\text{Cov}\left(Y_m, Y_m^X\right), 0, 0, \text{Var}_X\left(Y_m\right), \mathbb{E}_X\left(Y_d\right) \right)$. We have $\sqrt{N}(\overline{U}_N - \mu) \xrightarrow[N \to \infty]{d} \mathcal{N}(0, \Gamma)$, where Γ is the variance-covariance matrix of U_1. Let $\psi_S(x, y, z, a, b) = (x - yz)/(a - y^2 + b)$, and $S_N^{X_u} = \psi_S(\overline{U}_N)$ according to (5). Since

$$\nabla \psi_S = \left(\frac{1}{a - y^2 + b}, -\frac{z}{a - y^2 + b} + \frac{2y(x - yz)}{(a - y^2 + b)^2}, -\frac{y}{a - y^2 + b}, -\frac{x - yz}{(a - y^2 + b)^2}, -\frac{x - yz}{(a - y^2 + b)^2} \right),$$

we have $\nabla \psi_S(\mu) = \left(\text{Var}_{X,\varepsilon}\left(\mathcal{Y}\right)^{-1}, 0, 0, -\text{Var}_{X,\varepsilon}\left(\mathcal{Y}\right)^{-1} S^{X_u}, -\text{Var}_{X,\varepsilon}\left(\mathcal{Y}\right)^{-1} S^{X_u} \right)$. It follows that

$$\nabla \psi_S(\mu) \Gamma \nabla \psi_S^\top(\mu) = \text{Var}_X \left((Y_m - \mathbb{E}_X\left(Y_m\right))\left(Y_m^X - \mathbb{E}_X\left(Y_m\right)\right) - S^{X_u} \left((Y_m - \mathbb{E}_X\left(Y_m\right))^2 + Y_d \right) \right) \left(\text{Var}_{X,\varepsilon}\left(\mathcal{Y}\right) \right)^{-2}.$$

Assumption 1 ensures the validity of $\nabla \psi_S(\mu) \Gamma \nabla \psi_S^\top(\mu)$. The proof is complete by applying the Delta method with $\sigma_S^2 = \nabla \psi_S(\mu) \Gamma \nabla \psi_S^\top(\mu)$. $\qquad\square$

Similarly, we can show that the asymptotic normality holds true for the estimator given in (6).

Proposition 2 Under Assumption 1, $\sqrt{N}\left(T_N^{X_u} - S^{X_u}\right) \xrightarrow[N \to \infty]{d} \mathcal{N}(0, \sigma_T^2)$ in $(\Omega_X, \mathcal{F}_X, \mathbb{P}_X)$, where

$$\sigma_T^2 = \text{Var}_X \left((Y_m - \mathbb{E}_X\left(Y_m\right))\left(Y_m^X - Y_m^{(X)}\right) - S^{X_u} \left((Y_m - \mathbb{E}_X\left(Y_m\right))^2 + Y_d \right) \right) \left(\text{Var}_{X,\varepsilon}\left(\mathcal{Y}\right) \right)^{-2}. \tag{9}$$

Proof. The proof is similar to that of Proposition 1. Define

$$U_i := \left((Y_{m,i} - \mathbb{E}_X\left(Y_m\right))\left(Y_{m,i}^X - \mathbb{E}_X\left(Y_m\right)\right), (Y_{m,i} - \mathbb{E}_X\left(Y_m\right))\left(Y_{m,i}^{(X)} - \mathbb{E}_X\left(Y_m\right)\right), \right.$$

$$\left. (Y_{m,i} - \mathbb{E}_X\left(Y_m\right))^2, Y_{m,i}^X - \mathbb{E}_X\left(Y_m\right), Y_{d,i} \right),$$

and $\overline{U}_N := N^{-1} \sum_{i=1}^{N} U_i$. Define $\mu := \left(\text{Cov}\left(Y_m, Y_m^X\right), 0, \text{Var}_X\left(Y_m\right), 0, \mathbb{E}_X\left(Y_d\right) \right)$. We have $\sqrt{N}(\overline{U}_N - u) \xrightarrow[N \to \infty]{d} \mathcal{N}(0, \Gamma)$, where Γ is the variance-covariance matrix of U_1. Let $\psi_S(x, y, z, a, b) = (x - y)/(z - a^2 + b)$, and $T_N^{X_u} = \psi_S(\overline{U}_N)$ according to (6). Since

$$\nabla \psi_S = \left(\frac{1}{z - a^2 + b}, -\frac{1}{z - a^2 + b}, -\frac{x - y}{(z - a^2 + b)^2}, \frac{2a(x - y)}{(z - a^2 + b)^2}, -\frac{xy}{(z - a^2 + b)^2} \right),$$

we have $\nabla \psi_S(u) = \left(\text{Var}_{X,\varepsilon}\left(\mathcal{Y}\right)^{-1}, \text{Var}_{X,\varepsilon}\left(\mathcal{Y}\right)^{-1}, -\text{Var}_{X,\varepsilon}\left(\mathcal{Y}\right)^{-1} S^{X_u}, 0, -\text{Var}_{X,\varepsilon}\left(\mathcal{Y}\right)^{-1} S^{X_u} \right)$, and it follows that

$$\nabla \psi_S(\mu) \Gamma \nabla \psi_S^\top(\mu) = \text{Var}_X \left((Y_m - \mathbb{E}_X\left(Y_m\right))\left(Y_m^X - Y_m^{(X)}\right) - S^{X_u} \left((Y_m - \mathbb{E}_X\left(Y_m\right))^2 + Y_d \right) \right) \left(\text{Var}_{X,\varepsilon}\left(\mathcal{Y}\right) \right)^{-2}.$$

Assumption 1 ensures the validity of $\nabla \psi_S(\mu) \Gamma \nabla \psi_S^\top(\mu)$. The proof is complete by applying the Delta method with $\sigma_T^2 = \nabla \psi_S(\mu) \Gamma \nabla \psi_S^\top(\mu)$. $\qquad\square$

As the estimators given in (5) and (6) are unbiased, we are interested in which one may have a lower asymptotic variance. Define $V := (Y_m - \mathbb{E}_X\left(Y_m\right))\left(Y_m^X - \mathbb{E}_X\left(Y_m\right)\right) - S^{X_u}\left((Y_m - \mathbb{E}_X\left(Y_m\right))^2 + Y_d \right)$. Then we have $\sigma_S^2 = \text{Var}_X\left(V\right)/\left(\text{Var}_{X,\varepsilon}\left(\mathcal{Y}\right)\right)^2$, and

$$\sigma_T^2 = \text{Var}_X \left((Y_m - \mathbb{E}_X\left(Y_m\right))\left(\mathbb{E}_X\left(Y_m\right) - Y_m^{(X)}\right) + V \right) \left(\text{Var}_{X,\varepsilon}\left(\mathcal{Y}\right) \right)^{-2}$$

$$= \sigma_S^2 + \frac{\text{Var}_X \left((Y_m - \mathbb{E}_X\left(Y_m\right))\left(\mathbb{E}_X\left(Y_m\right) - Y_m^{(X)}\right) \right) + 2\,\text{Cov}\left((Y_m - \mathbb{E}_X\left(Y_m\right))\left(\mathbb{E}_X\left(Y_m\right) - Y_m^{(X)}\right), V \right)}{\left(\text{Var}_{X,\varepsilon}\left(\mathcal{Y}\right) \right)^2}. \tag{10}$$

A closer examination reveals that the sign of the second term on the right-hand side of (10) is indeterminate. In fact, the relationship between σ_S^2 and σ_T^2 is example dependent; see Section 4 for more details.

3.2 Analysis of the Joint Metamodel-based Sobol' Index Estimators

This subsection investigates the asymptotic normality of the two joint metamodel-based estimators $\widetilde{S}_{\mathcal{T}_N}^{X_u}$ and $\widetilde{T}_{\mathcal{T}_N}^{X_u}$, respectively given in (3) and (4), when the true mean and variance functions are unavailable.

The following decomposition is key to our analysis of the first joint metamodel-based estimator $\widetilde{S}_{\mathcal{T}_N}^{X_u}$:

$$\sqrt{N}\left(\widetilde{S}_{\mathcal{T}_N}^{X_u} - S^{X_u}\right) = \sqrt{N}\left(\widetilde{S}_{\mathcal{T}_N}^{X_u} - \widetilde{S}^{X_u}\right) + \sqrt{N}\left(\widetilde{S}^{X_u} - S^{X_u}\right), \tag{11}$$

where $\widetilde{S}^{X_u} := \mathrm{Var}_{X_u}\left(\mathbb{E}_{X_{-u}}\left(\widetilde{Y}_{m,\mathcal{T}_N} \mid X_u\right)\right) / \left(\mathrm{Var}_X\left(\widetilde{Y}_{m,\mathcal{T}_N}\right) + \mathbb{E}_X\left(\widetilde{Y}_{d,\mathcal{T}_N}\right)\right)$ which is similar as S^{X_u} given in (2), but with the true mean and variance functions replaced by the respective metamodels built on the given data set $\mathcal{T}_N$. A decomposition similar to (11) holds true for the second estimator $\widetilde{T}_{\mathcal{T}_N}^{X_u}$ as well. We next investigate the properties of $\sqrt{N}\left(\widetilde{S}_{\mathcal{T}_N}^{X_u} - \widetilde{S}^{X_u}\right)$ and $\sqrt{N}\left(\widetilde{S}^{X_u} - S^{X_u}\right)$ in light of (11). Let us start with some technical conditions.

Assumption 2 For almost every $\omega \in \Omega_Z$, $\delta_{m,\mathcal{T}_N(\omega)} := \widetilde{Y}_{m,\mathcal{T}_N(\omega)} - Y_m \xrightarrow[N\to\infty]{\mathcal{L}^2} c$, where c is some constant.

Assumption 3 For almost every $\omega \in \Omega_Z$, $\mathbb{E}_X\left(\widetilde{Y}_{d,\mathcal{T}_N(\omega)}\right) \xrightarrow[N\to\infty]{} \mathbb{E}_X(Y_d)$.

Assumption 3′ For almost every $\omega \in \Omega_Z$, $\delta_{d,\mathcal{T}_N(\omega)} := \widetilde{Y}_{d,\mathcal{T}_N(\omega)} - Y_d \xrightarrow[N\to\infty]{\mathcal{L}^2} 0$.

We note that Assumptions 2 and 3′ can be fulfilled by well-known metamodeling techniques under mild conditions. For instance, Kohler et al. (2003) showed that kernel smoothing is strongly universally consistent under some assumptions, i.e., $\mathbb{E}_X(|\widetilde{Y}_{m,\mathcal{T}_N} - Y_m|^2) \xrightarrow[N\to\infty]{a.s.} 0$ and $\mathbb{E}_X(|\widetilde{Y}_{d,\mathcal{T}_N} - Y_d|^2) \xrightarrow[N\to\infty]{a.s.} 0$ with respect to $(\Omega_Z, \mathcal{F}_Z, \mathbb{P}_Z)$. Rather than examining a particular metamodeling technique (e.g., kernel smoothing, Gaussian process), we focus on the asymptotic analysis of the metamodel-based estimators under some sufficient conditions on the metamodels. We first examine $\widetilde{S}^{X_u}$ defined in (11).

Proposition 3 Under Assumptions 1 to 3, $\widetilde{S}^{X_u} \xrightarrow[N\to\infty]{} S^{X_u}$ for almost every $\omega \in \Omega_Z$.

Proof. Under Assumption 2 and by the Cauchy–Schwarz inequality, we have

$$\left|\mathbb{E}_X\left(\widetilde{Y}_{m,\mathcal{T}_N(\omega)}\right) - \mathbb{E}_X(Y_m + c)\right| \leq \left(\mathbb{E}_X\left(\left|\delta_{m,\mathcal{T}_N(\omega)} - c\right|^2\right)\right)^{\frac{1}{2}} \xrightarrow[N\to\infty]{} 0.$$

It follows that $\mathbb{E}_X\left(\widetilde{Y}_{m,\mathcal{T}_N(\omega)}\right) \xrightarrow[N\to\infty]{} \mathbb{E}_X(Y_m) + c$. On the other hand, by the continuity of the L_2 norm,

$$\left|\left(\mathbb{E}_X\left(\widetilde{Y}_{m,\mathcal{T}_N(\omega)}^2\right)\right)^{\frac{1}{2}} - \left(\mathbb{E}_X\left((Y_m + c)^2\right)\right)^{\frac{1}{2}}\right| \leq \left(\mathbb{E}_X\left(\left(\delta_{m,\mathcal{T}_N(\omega)} - c\right)^2\right)\right)^{\frac{1}{2}} \xrightarrow[N\to\infty]{} 0,$$

which implies that $\mathbb{E}_X\left(\widetilde{Y}_{m,\mathcal{T}_N(\omega)}^2\right) \xrightarrow[N\to\infty]{} \mathbb{E}_X\left((Y_m + c)^2\right)$. Hence,

$$\mathrm{Var}_X\left(\widetilde{Y}_{m,\mathcal{T}_N(\omega)}\right) = \mathbb{E}_X\left(\widetilde{Y}_{m,\mathcal{T}_N(\omega)}^2\right) - \mathbb{E}_X\left(\widetilde{Y}_{m,\mathcal{T}_N(\omega)}\right)^2 \xrightarrow[N\to\infty]{} \mathbb{E}_X\left((Y_m + c)^2\right) - \mathbb{E}_X\left((Y_m + c)\right)^2 = \mathrm{Var}_X(Y_m).$$

Also, we have

$$\mathbb{E}_{X_u}\left(\left|\mathbb{E}_{X_{-u}}\left(\widetilde{Y}_{m,\mathcal{T}_N(\omega)}-Y_m-c\mid X_u\right)\right|^2\right)=\int_{X_u}\left|\mathbb{E}_{X_{-u}}\left(\delta_{m,\mathcal{T}_N(\omega)}-c\mid X_u\right)\right|^2 d\mu_{X_u}$$

$$\leq\int_{X_u}\mathbb{E}_{X_{-u}}\left(\left|\delta_{m,\mathcal{T}_N(\omega)}-c\right|^2\mid X_u\right)d\mu_{X_u}=\mathbb{E}_X\left(\left|\delta_{m,\mathcal{T}_N(\omega)}-c\right|^2\right)\xrightarrow[N\to\infty]{}0,$$

which yields

$$\mathbb{E}_{X_{-u}}\left(\widetilde{Y}_{m,\mathcal{T}_N(\omega)}\mid X_u\right)\xrightarrow[N\to\infty]{\mathcal{L}^2}\mathbb{E}_{X_{-u}}\left(Y_m\mid X_u\right)+c, \tag{12}$$

and hence,

$$\mathrm{Var}_{X_u}\left(\mathbb{E}_{X_{-u}}\left(\widetilde{Y}_{m,\mathcal{T}_N(\omega)}\mid X_u\right)\right)\xrightarrow[N\to\infty]{}\mathrm{Var}_{X_u}\left(\mathbb{E}_{X_{-u}}\left(Y_m\mid X_u\right)\right).$$

Since $\mathrm{Var}_X(Y_m)+\mathbb{E}_X(Y_d)>0$, according to Assumption 3 and the quotient law for convergent sequences, for almost every $\omega\in\Omega_Z$, $\widetilde{S}^{X_u}=\mathrm{Var}_{X_u}\left(\mathbb{E}_{X_{-u}}\left(\widetilde{Y}_{m,\mathcal{T}_N(\omega)}\mid X_u\right)\right)/\left(\mathrm{Var}_X\left(\widetilde{Y}_{m,\mathcal{T}_N(\omega)}\right)+\mathbb{E}_X\left(\widetilde{Y}_{d,\mathcal{T}_N(\omega)}\right)\right)$ converges to $S^{X_u}=\mathrm{Var}_{X_u}\left(\mathbb{E}_{X_{-u}}\left(Y_m\mid X_u\right)\right)/\left(\mathrm{Var}_X(Y_m)+\mathbb{E}_X(Y_d)\right)$ as $N\to\infty$. $\square$

To analyze the term $\sqrt{N}(\widetilde{S}^{X_u}_{\mathcal{T}_N}-\widetilde{S}^{X_u})$ (respectively $\sqrt{N}(\widetilde{T}^{X_u}_{\mathcal{T}_N}-\widetilde{S}^{X_u})$) related to the first (resp. second) metamodel-based estimator in the decomposition shown in (11), we stipulate the following assumption.

Assumption 4 There exist $s_1,s_2>0$ and $C>0$ such that for almost every $\omega\in\Omega_Z$, $\mathbb{E}_X\left(|\widetilde{Y}_{m,\mathcal{T}_N(\omega)}|^{4+s_1}\right)<C$ and $\mathbb{E}_X\left(|\widetilde{Y}_{d,\mathcal{T}_N(\omega)}|^{2+s_2}\right)<C$, $\forall N\in\mathbb{N}^+$.

Proposition 4 Under Assumptions 2, 3′, and 4, for almost every $\omega\in\Omega_Z$, $\sqrt{N}\left(\widetilde{S}^{X_u}_{\mathcal{T}_N(\omega)}-\widetilde{S}^{X_u}\right)\xrightarrow[N\to\infty]{d}\mathcal{N}(0,\sigma_S^2)$, where σ_S^2 is defined in (7).

Proof. Define

$$\widetilde{U}_{\mathcal{T}_N(\omega),i}:=\left(\left(\widetilde{Y}_{m,\mathcal{T}_N(\omega),i}-\mathbb{E}_X\left(\widetilde{Y}_m\right)\right)\left(\widetilde{Y}^X_{m,\mathcal{T}_N(\omega),i}-\mathbb{E}_X\left(\widetilde{Y}_m\right)\right),\widetilde{Y}_{m,\mathcal{T}_N(\omega),i}-\mathbb{E}_X\left(\widetilde{Y}_m\right),\right.$$

$$\left.\widetilde{Y}^X_{m,\mathcal{T}_N(\omega),i}-\mathbb{E}_X\left(\widetilde{Y}_m\right),\left(\widetilde{Y}_{m,\mathcal{T}_N(\omega),i}-\mathbb{E}_X\left(\widetilde{Y}_m\right)\right)^2,\widetilde{Y}_{d,\mathcal{T}_N(\omega),i}\right),$$

and $\overline{\widetilde{U}}_{\mathcal{T}_N(\omega)}:=N^{-1}\sum_{i=1}^N\widetilde{U}_{\mathcal{T}_N(\omega),i}$. By Assumption 4, there exist $s'>0$ and $C'>0$ such that for almost every $\omega\in\Omega_Z$, $\mathbb{E}_X\left(\left\|\widetilde{U}_{\mathcal{T}_N(\omega),i}\right\|^{2+s'}\right)<C'$, $\forall N\in\mathbb{N}^+$. Then, we have

$$\mathbb{E}_X\left(\left\|\widetilde{U}_{\mathcal{T}_N(\omega),i}\right\|^2\mathbf{1}\left\{\left\|\widetilde{U}_{\mathcal{T}_N(\omega),i}\right\|>\varepsilon\sqrt{N}\right\}\right)\xrightarrow[N\to\infty]{}0,\forall\varepsilon>0,$$

and

$$\mathbb{E}_X\left(\left\|\widetilde{U}_{\mathcal{T}_N(\omega),i}\right\|^2\mathbf{1}\left\{\left\|\widetilde{U}_{\mathcal{T}_N(\omega),i}\right\|>\varepsilon\sqrt{N}\right\}\right)=\mathbb{E}_X\left(\frac{\left\|\widetilde{U}_{\mathcal{T}_N(\omega),i}\right\|^{2+s'}}{\left\|\widetilde{U}_{\mathcal{T}_N(\omega),i}\right\|^{s'}}\mathbf{1}\left\{\left\|\widetilde{U}_{\mathcal{T}_N(\omega),i}\right\|>\varepsilon\sqrt{N}\right\}\right)\leq\frac{C'}{\varepsilon^{s'}N^{s'/2}},$$

where $\mathbf{1}\{\cdot\}$ denotes the indicator function. Therefore, for each i, $\left\{\left\|\widetilde{U}_{\mathcal{T}_N(\omega),i}\right\|^2\right\}_{N\geq1}$ is uniformly integrable. By Assumptions 2 and 3′, $\widetilde{U}_{\mathcal{T}_N(\omega),i}\xrightarrow[N\to\infty]{\mathbb{P}}U_i$ (recall (8)), hence the same convergence holds true in L^2. As a result, the covariance matrices of $\widetilde{U}_{\mathcal{T}_N(\omega),i}$ converge to Γ. The rest of the proof follows by applying the Delta method as shown in the proof of Proposition 1. $\square$

Similarly, we have the following result for $\sqrt{N}\left(\widetilde{T}_{\mathcal{T}_N}^{X_u} - \widetilde{S}^{X_u}\right)$ in (11). The proof of Proposition 5 is in the same vein as that of Proposition 4 and is omitted for the sake of brevity.

Proposition 5 Under Assumptions 2, 3', and 4, for almost every $\omega \in \Omega_{\mathbf{Z}}$, $\sqrt{N}\left(\widetilde{T}_{\mathcal{T}_N(\omega)}^{X_u} - \widetilde{S}^{X_u}\right) \xrightarrow[N\to\infty]{d}$ $\mathcal{N}(0, \sigma_T^2)$, where σ_T^2 is defined in (9).

Finally, Theorem 1 gives a set of sufficient conditions for establishing the asymptotic normality of the two metamodel-based estimators given in (3) and (4). In addition to Assumptions 2, 3', and 4, we note that the convergence rates of the metamodels to the true mean and variance functions also play an important role.

Theorem 1 Define

$$
\begin{aligned}
C_{\delta, \mathcal{T}_N(\omega)} := & 2(\mathrm{Var}_X(Y_m))^{\frac{1}{2}}\left(\mathrm{Corr}\left(Y_m, \delta_{m,\mathcal{T}_N(\omega)}\right) - \frac{\mathrm{Var}_X(Y_m)}{\mathrm{Var}_{X,\varepsilon}(\mathcal{Y})}\cdot \mathrm{Corr}\left(Y_m, Y_m^X\right)\cdot \mathrm{Corr}\left(Y_m, \delta_{m,\mathcal{T}_N(\omega)}\right)\right) \\
& + \left(\mathrm{Var}_X\left(\delta_{m,\mathcal{T}_N(\omega)}\right)\right)^{\frac{1}{2}}\left(\mathrm{Corr}\left(\delta_{m,\mathcal{T}_N(\omega)}, \delta_{m,\mathcal{T}_N(\omega)}^X\right) - \frac{\mathrm{Var}_X(Y_m)}{\mathrm{Var}_{X,\varepsilon}(\mathcal{Y})}\cdot \mathrm{Corr}\left(Y_m, Y_m^X\right)\right),
\end{aligned}
$$

for almost every $\omega \in \Omega_{\mathbf{Z}}$, where $\mathrm{Corr}(A, B) = \mathrm{Cov}(A, B)/(\mathrm{Var}(A)\mathrm{Var}(B))^{1/2}$, given any L^2 random variables A and B of nonzero variance, and $\delta_{m,\mathcal{T}_N(\omega)}^X := \widetilde{Y}_{m,\mathcal{T}_N(\omega)}^X - Y_m^X$.

Assume that $C_{\delta, \mathcal{T}_N(\omega)}$ does not converge to 0 as $N \to \infty$ and Assumptions 2, 3' and 4 are fulfilled.

1. Suppose $\mathrm{Var}_X\left(\delta_{m,\mathcal{T}_N(\omega)}\right) = o\left(N^{-1}\right)$ and $\mathbb{E}_X\left(\delta_{d,\mathcal{T}_N(\omega)}\right) = o\left(N^{-1}\right)$ for almost every $\omega \in \Omega_{\mathbf{Z}}$, then for $\forall x \in \mathbb{R}$,

    $$
    \mathbb{P}_{\mathbf{Z}}\left(\omega \in \Omega_{\mathbf{Z}} : \limsup_{N\to\infty}\left|\mathbb{P}_X\left(\sqrt{N}\left(\widetilde{S}_{\mathcal{T}_N(\omega)}^{X_u} - \widetilde{S}^{X_u}\right)/\sigma_S \le x\right) - \Phi(x)\right| > \varepsilon\right) = 0, \forall \varepsilon > 0, \qquad (13)
    $$

    where $\Phi(x)$ is the standard normal cumulative density function.

2. Suppose $C_{\delta, \mathcal{T}_N(\omega)}$ converges to a constant $C \ne 0$ and there exists $\gamma \in \mathbb{R}$ so that $\mathrm{Var}_X\left(\delta_{m,\mathcal{T}_N(\omega)}\right) = (CN)^{-1}\gamma + o\left(N^{-1}\right)$ and $\mathbb{E}_X\left(\delta_{d,\mathcal{T}_N(\omega)}\right) = o\left(N^{-1}\right)$ for almost every $\omega \in \Omega_{\mathbf{Z}}$, then there is a constant γ' such that for $\forall x \in \mathbb{R}$,

    $$
    \mathbb{P}_{\mathbf{Z}}\left(\omega \in \Omega_{\mathbf{Z}} : \limsup_{N\to\infty}\left|\mathbb{P}_X\left(\sqrt{N}\left(\widetilde{S}_{\mathcal{T}_N(\omega)}^{X_u} - \widetilde{S}^{X_u} - \gamma'\right)/\sigma_S \le x\right) - \Phi(x)\right| > \varepsilon\right) = 0, \forall \varepsilon > 0. \qquad (14)
    $$

The convergence in (13) and (14) holds true for the second metamodel-based estimator $\widetilde{T}_{\mathcal{T}_N(\omega)}^{X_u}$, with σ_S replaced by σ_T.

Proof. We focus on the proof regarding the first metamodel-based estimator $\widetilde{S}_{\mathcal{T}_N(\omega)}^{X_u}$, as the proof regarding $\widetilde{T}_{\mathcal{T}_N(\omega)}^{X_u}$ can be given in the same vein and hence is omitted. Recall the decomposition in (11). Since $\sqrt{N}\left(\widetilde{S}_{\mathcal{T}_N(\omega)}^{X_u} - \widetilde{S}^{X_u}\right) \xrightarrow[N\to\infty]{d} \mathcal{N}(0, \sigma_S^2)$ in $(\Omega_X, \mathcal{F}_X, \mathbb{P}_X)$ for a fixed $\omega \in \Omega_{\mathbf{Z}}$ according to Proposition 4, if $\sqrt{N}\left(\widetilde{S}^{X_u} - S^{X_u}\right)$ goes to some constant κ, then for the fixed $\omega \in \Omega_{\mathbf{Z}}$, $\sqrt{N}\left(\widetilde{S}_{\mathcal{T}_N(\omega)}^{X_u} - S^{X_u}\right) \xrightarrow[N\to\infty]{d}$

$\mathcal{N}(\kappa, \sigma_S^2)$ in $(\Omega_X, \mathcal{F}_X, \mathbb{P}_X)$. Regarding $\sqrt{N}\left(\widetilde{S}^{X_u} - S^{X_u}\right)$, we have

$$
\begin{aligned}
\widetilde{S}^{X_u} - S^{X_u} &= \frac{\mathrm{Cov}\left(\widetilde{Y}_{m,\mathcal{T}_N(\omega)}, \widetilde{Y}^X_{m,\mathcal{T}_N(\omega)}\right)}{\mathrm{Var}_X\left(\widetilde{Y}_{m,\mathcal{T}_N(\omega)}\right) + \mathbb{E}_X\left(\widetilde{Y}_{d,\mathcal{T}_N(\omega)}\right)} - \frac{\mathrm{Cov}\left(Y_m, Y_m^X\right)}{\mathrm{Var}_{X,\varepsilon}(\mathcal{Y})} \\[2mm]
&= \frac{\mathrm{Cov}\left(Y_m, Y_m^X\right) + 2\,\mathrm{Cov}\left(Y_m, \delta^X_{m,N}\right) + \mathrm{Cov}\left(\delta_{m,\mathcal{T}_N(\omega)}, \delta^X_{m,\mathcal{T}_N(\omega)}\right)}{\mathrm{Var}_X(Y_m) + 2\,\mathrm{Cov}\left(Y_m, \delta_{m,\mathcal{T}_N(\omega)}\right) + \mathrm{Var}_X\left(\delta_{m,\mathcal{T}_N(\omega)}\right) + \mathbb{E}_X(Y_d) + \mathbb{E}_X\left(\delta_{d,\mathcal{T}_N(\omega)}\right)} - \frac{\mathrm{Cov}\left(Y_m, Y_m^X\right)}{\mathrm{Var}_{X,\varepsilon}(\mathcal{Y})} \\[2mm]
&= \frac{\mathrm{Var}_X\left(\delta_{m,\mathcal{T}_N(\omega)}\right)^{\frac{1}{2}} C_{\delta,\mathcal{T}_N(\omega)} - \mathrm{Var}_{X,\varepsilon}(\mathcal{Y})^{-1}\mathrm{Cov}\left(Y_m, Y_m^X\right)\mathbb{E}_X\left(\delta_{d,\mathcal{T}_N(\omega)}\right)}{\mathrm{Var}_X(Y_m) + 2\,\mathrm{Cov}\left(Y_m, \delta_{m,\mathcal{T}_N(\omega)}\right) + \mathrm{Var}_X\left(\delta_{m,\mathcal{T}_N(\omega)}\right) + \mathbb{E}_X(Y_d) + \mathbb{E}_X\left(\delta_{d,\mathcal{T}_N(\omega)}\right)}. \quad (15)
\end{aligned}
$$

Under the assumption that $C_{\delta,\mathcal{T}_N(\omega)}$ converges to some $C \neq 0$, the denominator of the right-hand side of (15) follows as

$$
\mathrm{Var}_X(Y_m) + 2\,\mathrm{Cov}\left(Y_m, \delta_{m,\mathcal{T}_N(\omega)}\right) + \mathrm{Var}_X\left(\delta_{m,\mathcal{T}_N(\omega)}\right) + \mathbb{E}_X(Y_d) + \mathbb{E}_X\left(\delta_{d,\mathcal{T}_N(\omega)}\right)
$$

$$
\leq \mathrm{Var}_X(Y_m) + \mathbb{E}_X(Y_d) + 2\left(\mathrm{Var}_X(Y_m)\,\mathrm{Var}_X\left(\delta_{m,\mathcal{T}_N(\omega)}\right)\right)^{\frac{1}{2}} + \mathrm{Var}_X\left(\delta_{m,\mathcal{T}_N(\omega)}\right) + \mathbb{E}_X\left(\delta_{d,\mathcal{T}_N(\omega)}\right)
$$

$$
= \mathrm{Var}_X(Y_m) + \mathbb{E}_X(Y_d) + o(1).
$$

Hence, Equation (15) can be written as

$$
\widetilde{S}^{X_u} - S^{X_u} = \frac{C_{\delta,\mathcal{T}_N(\omega)}\,\mathrm{Var}_X\left(\delta_{m,\mathcal{T}_N(\omega)}\right)^{\frac{1}{2}} - \mathrm{Var}_{X,\varepsilon}(\mathcal{Y})^{-1}\mathrm{Cov}\left(Y_m, Y_m^X\right)\mathbb{E}_X\left(\delta_{d,\mathcal{T}_N(\omega)}\right)}{\mathrm{Var}_X(Y_m) + \mathbb{E}_X(Y_d) + o(1)}.
$$

If $\mathrm{Var}_X\left(\delta_{m,\mathcal{T}_N(\omega)}\right) = o(N^{-1})$ and $\mathbb{E}_X\left(\delta_{d,\mathcal{T}_N(\omega)}\right) = o\left(N^{-1}\right)$, we have $\sqrt{N}\,\mathrm{Var}_X\left(\delta_{m,\mathcal{T}_N(\omega)}\right)^{\frac{1}{2}} = o(1)$ and $\sqrt{N}\mathbb{E}_X\left(\delta_{d,\mathcal{T}_N(\omega)}\right) = o\left(N^{-1/2}\right)$, thus $\sqrt{N}(\widetilde{S}^{X_u}_{\mathcal{T}_N(\omega)} - S^{X_u}) = o(1)$ and for almost every $\omega \in \Omega_Z$, $\sqrt{N}(\widetilde{S}^{X_u}_{\mathcal{T}_N(\omega)} - S^{X_u}) \xrightarrow[N\to\infty]{d} \mathcal{N}(0, \sigma_S^2)$. Hence, the convergence takes place in the product space $(\Omega_Z \times \Omega_X, \sigma(\mathcal{F}_Z \times \mathcal{F}_X), \mathbb{P}_Z \otimes \mathbb{P}_X)$, which leads to (13).

If $\mathrm{Var}_X\left(\delta_{m,\mathcal{T}_N(\omega)}\right) = (CN)^{-1}\gamma + o(N^{-1})$ and $\mathbb{E}_X\left(\delta_{d,\mathcal{T}_N(\omega)}\right) = o\left(N^{-1}\right)$, we have $\sqrt{N}\,\mathrm{Var}_X\left(\delta_{m,\mathcal{T}_N(\omega)}\right)^{1/2} \xrightarrow[N\to\infty]{} \sqrt{\gamma/C}$ and $\sqrt{N}\mathbb{E}_X\left(\delta_{d,\mathcal{T}_N(\omega)}\right) \xrightarrow[N\to\infty]{} 0$, thus there exists $\gamma' \in \mathbb{R}$ such that for almost every $\omega \in \Omega_Z$, $\sqrt{N}(\widetilde{S}^{X_u} - S^{X_u}) \xrightarrow[N\to\infty]{} \gamma'$, and $\sqrt{N}(\widetilde{S}^{X_u}_{\mathcal{T}_N(\omega)} - S^{X_u}) \xrightarrow[N\to\infty]{d} \mathcal{N}(\gamma', \sigma_S^2)$. The resulting convergence takes place in the product space $(\Omega_Z \times \Omega_X, \sigma(\mathcal{F}_Z \times \mathcal{F}_X), \mathbb{P}_Z \otimes \mathbb{P}_X)$, which results in (14). The proof is complete. $\quad\square$

4 NUMERICAL EVALUATION

In this section, we numerically evaluate the efficiency of the Sobol' index estimators given in (3) to (6) and verify the theoretical results. We consider the Ishigami function which is a classical example for evaluating global sensitivity analysis approaches (Ishigami and Homma 1990; Marrel et al. 2012):

$$
Y = f(X_1, X_2, X_3) = \sin(X_1) + 7\sin(X_2)^2 + 0.1X_3^4 \sin(X_1), \quad (16)
$$

where X_i's are independent and uniformly distributed in $[-\pi, \pi]$, $i = 1, 2, 3$. To make model (16) a stochastic one, we treat X_1 and X_2 as the input variables and X_3 as the random variable that incurs stochastic noise. The true mean and variance functions follow from (16) as

$$
Y_m(x_1, x_2) = \left(1 + \frac{\pi^4}{50}\right)\sin(x_1) + (\sin(x_2))^2, \; Y_d(x_1, x_2) = \pi^8\left(\frac{1}{900} - \frac{1}{2500}\right)(\sin(x_1))^2, \; \text{for } x_i \in [-\pi, \pi].
$$

We are interested in obtaining point estimates and confidence interval estimates for the first-order Sobol' indices of X_1 and X_2. The true values are available in this case, which are respectively $S^{X_1} = 0.3139$ and $S^{X_2} = 0.4424$.

Experimental settings. Obtaining the joint metamodel-based Sobol' index estimators given in (3) and (4) requires metamodel construction and MC sampling to evaluate the metamodels. Regarding the metamodel construction, we adopt the following iterative procedure proposed by Marrel et al. (2012) for estimating the mean and variance functions. Specifically, we first generate a training sample of size n via Latin hypercube sampling (LHS) and build a standard Gaussian process (GP) model (denoted as $GP_{m,1}$) for estimating the mean function. Next, taking the squared residuals based on $GP_{m,1}$, we construct a metamodel (denoted as $\hat{V}_1$) for approximating the variance function. We then construct a heteroscedastic GP model (denoted as $GP_{m,2}$) for the mean function estimation, with the noise variances being estimated by $\hat{V}_1$. Finally, the squared residuals are calculated based on $GP_{m,2}$ to construct another metamodel (denoted as $\hat{V}_2$) for the ultimate variance function estimation. We adopt the resulting $GP_{m,2}$ and $\hat{V}_2$ as $\widetilde{Y}_{m,\mathcal{T}_N}$ and $\widetilde{Y}_{d,\mathcal{T}_N}$ in the subsequent Sobol' index estimation. We consider two variants of this iterative procedure in terms of constructing the variance metamodels $\hat{V}_1$ and $\hat{V}_2$, via either GP modeling (referred to as "Variant 1") or kernel smoothing (referred to as "Variant 2"). Variant 2 seems to enhance numerical stability in implementation. For MC evaluations, we use LHS to draw a sample of size N for model evaluations. Similar designs such as Sobol' quasi-random sequences are also suggested by Saltelli et al. (2010) for MC-based Sobol' index estimation.

Performance metrics. To assess the accuracy of the metamodels $\widetilde{Y}_{m,\mathcal{T}_N}$ and $\widetilde{Y}_{d,\mathcal{T}_N}$, we use the predictivity coefficient Q_2 (Marrel et al. 2012). For a given metamodel $\widetilde{Y}$, $Q_2(\widetilde{Y}) := 1 - \sum_{i=1}^{N}(Y_i - \widetilde{Y}_i)^2 / \sum_{i=1}^{N}\left(N^{-1}\sum_{i=1}^{N}Y_i - Y_i\right)^2$, where recall that N denotes the MC sample size, $\widetilde{Y}_i$ denotes the metamodel prediction at input X_i, and Y_i is the corresponding true function value. The closer $Q_2(\widetilde{Y})$ to 1, the higher the accuracy of the metamodel $\widetilde{Y}$.

For performance evaluation, we perform R independent macro-replications. The root mean squared error (RMSE), standard deviation, and bias of Sobol' index estimators given in (3) and (4) are calculated across the macro-replications. Specifically, RMSE $:= \sqrt{R^{-1}\sum_{i=r}^{R}\left(\widetilde{S}_r^{X_u} - S^{X_u}\right)^2}$, where $\widetilde{S}_r^{X_u}$ is a given estimator of S^{X_u} obtained on the rth macro-replication. To assess the asymptotic normality, we examine the empirical coverage of the asymptotic confidence interval (referred to as CI) with the target level set to 0.95. The confidence interval CI_r based on the two estimators on the rth macro-replication is given by $\widetilde{S}_{\mathcal{T}_N,r}^{X_u}$ (resp. $\widetilde{T}_{\mathcal{T}_N,r}^{X_u}$) $\pm 1.96\widetilde{\sigma}_{S,r}$ (resp. $\widetilde{\sigma}_{T,r}$) $/\sqrt{N}$, where $\widetilde{S}_{\mathcal{T}_N,r}^{X_u}$ and $\widetilde{T}_{\mathcal{T}_N,r}^{X_u}$ denote the joint metamodel-based estimators, and $\widetilde{\sigma}_{S,r}$ and $\widetilde{\sigma}_{T,r}$ are the MC-based estimators of σ_S and σ_T obtained on the rth macro-replication; to ease notation, we write $\widetilde{\sigma}_S$ and $\widetilde{\sigma}_T$ hereinafter. The empirical coverage is calculated as $R^{-1}\sum_{r=1}^{R}\mathbf{1}\left\{S^{X_u} \in CI_r\right\}$.

Results. We first examine the two estimators constructed using the true mean and variance functions, $S_N^{X_u}$ and $T_N^{X_u}$, given in (5) and (6). The results are obtained based on $R = 2000$ macro-replications. Figure 1 shows the empirical coverage of the CIs built based on Propositions 1 and 2. We see that as the MC sample size N increases, for $S_N^{X_u}$ and $T_N^{X_u}$ ($u = 1, 2$), the empirical coverage meets and slightly overshoots the target level. The results corroborate Propositions 1 and 2. Table 1 displays the CI widths (rescaled by $\sqrt{N}$) and the RMSE of $S_N^{X_u}$ and $T_N^{X_u}$ for $u = 1, 2$. Since the rescaled CI widths are equal to $3.92\widetilde{\sigma}_S$ (resp. $3.92\widetilde{\sigma}_T$), we see from Table 1 that the Sobol' index of X_1, estimated by the second estimator $T_N^{X_1}$, has a smaller variance, while the first estimator $S_N^{X_2}$ is better at estimating the index of X_2. We have the same observation regarding the RMSEs of the two estimators. Therefore, neither estimator dominates the other, and one can adopt different estimators for estimating Sobol' indices of different input variables for higher statistical accuracy.

For evaluating the joint metamodel-based Sobol' index estimators, we perform $R = 100$ macro-replications. Table 2 presents the average Q_2 values across the macro-replications and the RMSEs of

Table 1: The confidence interval widths (rescaled by $\sqrt{N}$) and the RMSEs of $S_N^{X_u}$ and $T_N^{X_u}$ given in (5) and (6) obtained with an MC sample size $N = 10^6$.

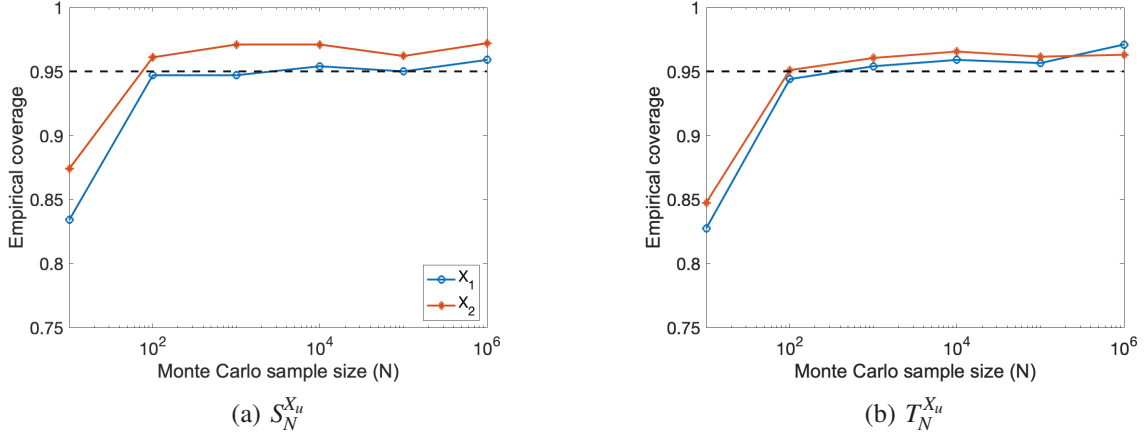|	$S_N^{X_1}$	$S_N^{X_2}$	$T_N^{X_1}$	$T_N^{X_2}$
Rescaled *CI* width	2.39	2.15	2.06	2.47
RMSE ($\times 10^{-4}$)	6.1	5.5	4.8	5.8

(a) $S_N^{X_u}$ (b) $T_N^{X_u}$

Figure 1: The empirical coverage of the asymptotic CIs for $S_N^{X_u}$ and $T_N^{X_u}$ as a function of the MC sample size N.

the first joint metamodel-based Sobol' index estimator $\widetilde{S}_{\mathcal{T}_N}^{X_1}$ obtained using the metamodels constructed via the two variants of the iterative fitting procedure. We observe that the variance metamodel obtained via Variant 1 has higher accuracy than that obtained via Variant 2, and the accuracy of the mean metamodels obtained via the two variants is comparable. Furthermore, the RMSEs of the resulting joint metamodel-based Sobol' index estimators are also comparable. This indicates that the mean metamodel is likely to play a dominating role in the joint metamodel-based Sobol' index estimation. We note that, as the training sample size n increases, the heteroscedastic GP model produced by Variant 1 for the mean function estimation becomes numerically unstable, rendering the Sobol' index estimation unreliable. Hence, we focus on Variant 2 in the rest of the study.

Table 2: Comparisons of $Q_2(\widetilde{Y}_{m,\mathcal{T}_N})$, $Q_2(\widetilde{Y}_{d,\mathcal{T}_N})$, and RMSE of $\widetilde{S}_{\mathcal{T}_N}^{X_1}$ produced by the two variants of the iterative fitting procedure.

N	n	$Q_2(\widetilde{Y}_{m,\mathcal{T}_N})$		$Q_2(\widetilde{Y}_{d,\mathcal{T}_N})$		RMSE of $\widetilde{S}_{\mathcal{T}_N}^{X_1}$	
		Variant 1	Variant 2	Variant 1	Variant 2	Variant 1	Variant 2
50	1000	0.99	0.99	0.88	0.47	0.082	0.087
100	1000	0.99	0.99	0.90	0.48	0.061	0.058
500	1000	0.99	0.99	0.89	0.48	0.033	0.027
1000	1000	0.99	0.99	0.90	0.49	0.026	0.021

    Table 3 shows the point estimation accuracy and the variability of the first metamodel-based estimator $\widetilde{S}_{\mathcal{T}_N}^{X_u}$ given in (3) for $u = 1, 2$. Since the results of the second estimator $\widetilde{T}_{\mathcal{T}_N}^{X_u}$ lead to similar conclusions, we omit them for the sake of brevity. We see from Table 3 that, for a fixed training sample size n, increasing N does not always lower the bias, as the accuracy of the metamodels is constrained by the given training sample. In contrast, the RMSE and the standard deviation of the joint metamodel-based estimator decrease

with N in most cases. While one may be inclined to increase N to improve the point estimation accuracy, we highlight that, once N becomes very large, the law of diminishing marginal returns emerges. To reduce the RMSE to a given level, a slight increase in the training sample size n can be more computationally efficient. We do not go into the details to economize on space.

Table 3: The RMSE, the standard deviation (std), and the bias of $\widetilde{S}_{\mathcal{T}_N}^{X_u}$ under different combinations of (N,n).

N	n	$\widetilde{S}_{\mathcal{T}_N}^{X_1}$			$\widetilde{S}_{\mathcal{T}_N}^{X_2}$		
		RMSE	std	bias	RMSE	std	bias
150	300	0.052	0.052	0.002	0.055	0.052	0.018
500	300	0.039	0.039	0.004	0.046	0.042	0.018
800	300	0.036	0.034	0.002	0.041	0.040	0.010
250	500	0.040	0.040	0.003	0.046	0.045	0.010
500	500	0.035	0.034	0.007	0.036	0.033	0.015
800	500	0.028	0.028	0.004	0.035	0.034	0.009
500	1000	0.027	0.027	0.002	0.030	0.027	0.012
800	1000	0.028	0.028	0.003	0.030	0.028	0.010
1000	1000	0.021	0.021	0.000	0.023	0.023	0.004
800	2000	0.021	0.021	0.000	0.023	0.022	0.003
1000	2000	0.021	0.021	0.002	0.023	0.022	0.007
1200	2000	0.020	0.020	0.002	0.018	0.017	0.006

Finally, we investigate the empirical coverage of the asymptotic confidence intervals obtained based on Theorem 1. Table 4 shows the combinations of (N,n) that help achieve the target coverage level. We see that, for the Sobol' index of X_1, both asymptotic CIs based on estimators $\widetilde{S}_{\mathcal{T}_N}^{X_1}$ and $\widetilde{T}_{\mathcal{T}_N}^{X_1}$ achieve the target coverage level using $N \approx 0.5n$. For the Sobol' index of X_2, the asymptotic CI based on $\widetilde{S}_{\mathcal{T}_N}^{X_2}$ achieves the target coverage level using $N \approx 0.2n$ while that based on $\widetilde{T}_{\mathcal{T}_N}^{X_2}$ achieves the target level using $N \approx 0.1n$. Without showing details, we mention some important observations made throughout the experiment. First, as n and N increase, the empirical coverage of the asymptotic CIs approaches the target level, which corroborates Theorem 1. Second, increasing or decreasing N does not always improve the empirical coverage, and the relationship between n and N is crucial to make the empirical coverage meets the target level. Our results echo those of Janon et al. (2014), who demonstrated that different metamodeling techniques require different combinations of (N,n) for the asymptotic CIs constructed to reach a prescribed target coverage level.

Table 4: The empirical coverage of the asymptotic CIs based on Thoerem 1 under different combinations of (N,n). The values in parentheses in Column "N" are those that lead to the corresponding empirical coverages closer to the target level at 0.95.

n	$\widetilde{S}_{\mathcal{T}_N}^{X_1}$		$\widetilde{S}_{\mathcal{T}_N}^{X_2}$		$\widetilde{T}_{\mathcal{T}_N}^{X_1}$		$\widetilde{T}_{\mathcal{T}_N}^{X_2}$	
	N	coverage	N	coverage	N	coverage	N	coverage
300	150	0.96	60	0.91	150	0.92	30	0.94
500	250	0.95	100	0.96	250 (100)	0.9 (0.93)	50	0.94
1000	500	0.97	200	0.97	500	0.94	100	0.95
1500	750 (650)	0.89 (0.94)	300	0.98	750	0.96	150	0.91
2000	1000	0.94	400	0.93	1000	0.93	200	0.96

In summary, while increasing the MC sample size N for obtaining the joint metamodel-based estimators is computationally convenient, our results suggest that setting N to an extremely large value given a fixed training sample is ineffective for improving the point estimation accuracy and the empirical coverage of the asymptotic confidence intervals.

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