Control variate Monte Carlo estimators based on sparse polynomial chaos expansions

Hui Duan[1] and Giray Ökten[1]

[1] Department of Mathematics, Florida State University, Tallahassee, USA

Abstract

We introduce two control variate Monte Carlo estimators where the control is based on the truncated sparse polynomial chaos expansion of the function in hand. We use the control variate estimators to estimate the lower and upper Sobol' indices in some applications, and compare them numerically with some of the best Monte Carlo estimators in the literature. The results suggest that in computationally expensive problems where a low-order polynomial chaos expansion is not an accurate approximation of the model but highly correlated with it, the control variate estimators are either the best or among the best in terms of efficiency.

Keywords

Control variate; Monte Carlo; Bayesian polynomial chaos; Sobol' sensitivity indices

1. Introduction

Global sensitivity analysis, uncertainty analysis via Monte Carlo methods, and surrogate models are among the methods highlighted for modeling uncertainties in the grand challenge of "integrated treatment of modeling uncertainty" in socio-environmental systems modeling by Elsawah et al. (2020). In this paper we introduce two control variate Monte Carlo estimators where the control is based on Bayesian polynomial chaos expansion (PCE) (Babacan et al., 2009) of the given model. The control variate estimators can be adjusted for use in uncertainty analysis, or in global sensitivity analysis, which is considered in this paper.

Consider a situation where the model at hand is expensive to sample from, and the computationally feasible surrogate model is not a sufficiently accurate description of the model. If the surrogate model is highly correlated with the actual model, even if it is not sufficiently accurate, then control variate Monte Carlo estimators based on the surrogate model could offer a remedy. The surrogate models we consider in this paper are based on truncated Bayesian PCE, but our methodology applies to any surrogate model. We will use numerical results to compare the efficiency of the new control variate estimators with the best Monte Carlo estimators according to Puy et al. (2022), when they are used to estimate Sobol' sensitivity indices. The Sobol' sensitivity indices are one of the popular methods in decision making in the social, economic and environmental modeling community (Saltelli et al., 2006).

In the numerical results we consider two problems. The first one is the SIR (susceptible, infectious, and/or recovered) model; a model commonly used in the mathematical modeling of infectious diseases. The second one is the Stiefel canonical distance model, which is used in computer vision and medical imaging (Chakraborty & Vemuri, 2019). The numerical results show that the control variate estimators have better or similar efficiency

Contact G. Ökten at okten@math.fsu.edu

Cite this article as:
Duan, H., and Ökten, G.
Control variate Monte Carlo estimators based on sparse polynomial chaos expansions
Socio-Environmental Systems Modelling, vol. 5, 18568, 2023, doi:10.18174/sesmo.18568

Socio-Environmental Systems Modelling
An Open-Access Scholarly Journal
http://www.sesmo.org

in estimating lower and upper Sobol' indices compared to some of the best Monte Carlo algorithms of Puy et al. (2022). It is important to emphasize that the efficiency advantages of the control variate estimators are realized in the aforementioned scenario: when the original model is computationally expensive, and simple surrogate models are not accurate.

The paper is organized as follows. In Section 2 we briefly introduce the ANOVA decomposition of functions and Sobol' sensitivity indices, and introduce the Monte Carlo estimators that will be used in the numerical results. In Section 3 we describe how Sobol' indices can be estimated using PCE. In Section 4 we introduce the control variate Monte Carlo estimators and in Section 5 we present the numerical results. We conclude in Section 6.

2. Global sensitivity analysis

Here we review some of the background material from global sensitivity analysis, in particular, the Sobol' sensitivity indices. Consider a square-integrable function $f(\mathbf{x})$ defined on $(0,1)^d$, where $\mathbf{x} = (x_1, \cdots, x_d)$, and let $D = \{1,2,\cdots,d\}$ be the index set. The ANOVA decomposition of $f(\mathbf{x})$ is

$$f(\mathbf{x}) = \sum_{u \subseteq D} f_u(\mathbf{x}^u),$$

where $f_u(\mathbf{x}^u)$ is the component function that only depends on $\mathbf{x}^u$. For the empty set, we have $f_\emptyset = \int f(\mathbf{x})d\mathbf{x}$.

If we assume $\mathbf{x}$ has a uniform distribution on $(0,1)^d$, we can write

$$\mathbb{E}[f(\mathbf{x})] = \int f(\mathbf{x})d\mathbf{x} = \mu,$$

and

$$\mathrm{Var}(f(x)) = \sigma^2 = \int f^2(\mathbf{x})d\mathbf{x} - \mu^2,$$

where the integrals are over $(0,1)^d$. Similarly, the variance for the component function f_u is

$$\sigma_u^2 = \int f_u^2(\mathbf{x})d\mathbf{x} - \left(\int f_u(\mathbf{x})d\mathbf{x}\right)^2 = \int f_u^2(\mathbf{x})d\mathbf{x},$$

since the integral of f_u is zero, if $u \neq \emptyset$.

The ANOVA decomposition is orthogonal, which implies the following relationship between the variances of f and its component functions f_u:

$$\sigma^2 = \sum_{u \subseteq D} \sigma_u^2$$

The Sobol' sensitivity indices for the subset u are defined as

$$\underline{S}_u = \frac{1}{\sigma^2}\sum_{v \subseteq u} \sigma_v^2 = \frac{\underline{\tau}_u}{\sigma^2} \text{ and } \bar{S}_u = \frac{1}{\sigma^2}\sum_{v \cap u \neq \emptyset} \sigma_v^2 = \frac{\bar{\tau}_u}{\sigma^2},$$

where $\underline{S}_u$ is called the lower Sobol' sensitivity index (or, the main effect) and $\bar{S}_u$ is called the upper Sobol' sensitivity index (or, the total effect).

Another interpretation of the Sobol' indices is in terms of the variance and expectation of conditional distributions,

$$\underline{\tau}_u = \mathrm{Var}(\mathbb{E}[f(\mathbf{x}) \mid \mathbf{x}^u])$$
$$\bar{\tau}_u = \mathbb{E}[\mathrm{Var}(f(\mathbf{x}) \mid \mathbf{x}^{-u})],$$

where $-u$ is the complement of u.

Sobol' (1993) showed that $\underline{S}_u$ and $\bar{S}_u$ can be written as multidimensional definite integrals,

$$\underline{S}_u = \frac{1}{\sigma^2}\left(\int f(\mathbf{x}^u, \mathbf{x}^{-u}) f(\mathbf{x}^u, \mathbf{z}^{-u}) d\mathbf{x} d\mathbf{z}^{-u} - \mu^2\right)$$
$$\bar{S}_u = \frac{1}{2\sigma^2}\int [f(\mathbf{x}^u, \mathbf{x}^{-u}) - f(\mathbf{z}^u, \mathbf{x}^{-u})]^2 d\mathbf{x} d\mathbf{z}^u,$$

which can be estimated using the Monte Carlo method (the domain of the integrals are the domains of the vectors $(\mathbf{x}, \mathbf{z}^{-u})$ and $(\mathbf{x}, \mathbf{z}^u)$, respectively). Several Monte Carlo estimators for $\underline{S}_u$, $\bar{S}_u$ have been introduced in the literature since then. Based on extensive numerical results, Puy et al. (2022) conclude that in general the most efficient estimators are those introduced by Jansen (1999), Owen (2013), Janon et al. (2014), and Azzini et al. (2020).

Jansen (1999) introduced the following estimator for the upper Sobol' index

$$\bar{S}_u^{\text{jansen}} = \frac{\frac{1}{2N}\sum_{i=1}^{N} \left(f(\mathbf{x}_i) - f(\mathbf{z}_i^u, \mathbf{x}_i^{-u})\right)^2}{\sigma^2}, \tag{1}$$

where $\boldsymbol{x}_i$ and $\mathbf{z}_i$ are two independent vectors from the uniform distribution. Owen (2013) proposed an estimator for the lower Sobol' index that uses three independent input vectors

$$\underline{S}_u^{\text{owen}} = \frac{\frac{1}{N}\sum_{i=1}^{N} \left(f(\mathbf{x}_i) - f(\mathbf{y}_i^u, \mathbf{x}_i^{-u})\right)\left(f(\mathbf{x}_i^u, \mathbf{z}_i^{-u}) - f(\mathbf{z}_i)\right)}{\sigma^2}. \tag{2}$$

Janon et al. (2014) introduced estimators for both lower and upper Sobol' indices:

$$\underline{S}_u^{\text{janon}} = \frac{\frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_i) f(\mathbf{x}_i^u, \mathbf{z}_i^{-u}) - f_0^2}{\frac{1}{N}\sum_{i=1}^{N} \frac{f(\mathbf{x}_i)^2 + f(\mathbf{x}_i^u, \mathbf{z}_i^{-u})^2}{2} - f_0^2}, \tag{3}$$

$$\bar{S}_u^{\text{janon}} = 1 - \frac{\frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_i) f(\mathbf{z}_i^u, \mathbf{x}_i^{-u}) - \left(\tilde{f}_0\right)^2}{\frac{1}{N}\sum_{i=1}^{N} \frac{f(\mathbf{x}_i)^2 + f(\mathbf{z}_i^u, \mathbf{x}_i^{-u})^2}{2} - \left(\tilde{f}_0\right)^2}, \tag{4}$$

where $f_0 = \frac{1}{N}\sum_{i=1}^{N} \frac{f(\mathbf{x}_i) + f(\mathbf{x}_i^u, \mathbf{z}_i^{-u})}{2}$ and $\tilde{f}_0 = \frac{1}{N}\sum_{i=1}^{N} \frac{f(\mathbf{x}_i) + f(\mathbf{z}_i^u, \mathbf{x}_i^{-u})}{2}$. Likewise, Azzini et al. (2020) introduced the following estimators for the Sobol' indices:

$$\underline{S}_u^{\text{az}} = \frac{2\sum_{i=1}^{N} \left(f(\mathbf{x}_i^u, \mathbf{z}_i^{-u}) - f(\mathbf{z}_i)\right)\left(f(\mathbf{x}_i) - f(\mathbf{z}_i^u, \mathbf{x}_i^{-u})\right)}{\sum_{i=1}^{N} \left(f(\mathbf{x}_i) - f(\mathbf{z}_i)\right)^2 + \left(f(\mathbf{x}_i^u, \mathbf{z}_i^{-u}) - f(\mathbf{z}_i^u, \mathbf{x}_i^{-u})\right)^2}, \tag{5}$$

$$\bar{S}_u^{\text{az}} = \frac{\sum_{i=1}^{N} [f(\mathbf{z}_i) - f(\mathbf{x}_i^u, \mathbf{z}_i^{-u})]^2 + [f(\mathbf{x}_i) - f(\mathbf{z}_i^u, \mathbf{x}_i^{-u})]^2}{\sum_{i=1}^{N} [f(\mathbf{x}_i) - f(\mathbf{z}_i)]^2 + [f(\mathbf{x}_i^u, \mathbf{z}_i^{-u}) - f(\mathbf{z}_i^u, \mathbf{x}_i^{-u})]^2}. \tag{6}$$

3. Estimating Sobol' sensitivity indices using polynomial chaos expansion

If f is approximated by its polynomial chaos expansion (PCE), then its Sobol' sensitivity indices can be computed very efficiently as observed by Lemieux & Owen (2002) and Sudret (2008). Consider the truncated PCE of f

$$f_p(\mathbf{x}) = \sum_{i=0}^{P-1} k_i \Psi_i(\mathbf{x}), \tag{7}$$

where p is the truncated order and Ψ_i are the orthonormal polynomials. The number of terms in the summation is $P = \binom{d+p}{d}$. Suppose that the input $\mathbf{x}$ follows the uniform distribution and the basis $\{\Psi_i\}_{i=0}^{P-1}$ are multidimensional Legendre polynomials. Let $\{\phi_i\}_{i=0}^{P-1}$ be the one-dimensional Legendre polynomials. Let $\Psi_i = \Psi_{\alpha^{\mathrm{i}}}$, where α^i is a d-dimensional index vector with nonnegative integer entries. Each multidimensional polynomial can be expressed as the product of one-dimensional polynomials,

$$\Psi_{\alpha^i}(\mathbf{x}) = \prod_{j=1}^{d} \phi_{\alpha_j^{\mathrm{i}}}(x_j).$$

Define the set

$$\mathcal{A}_u = \left\{ i : \alpha_j^i > 0 \text{ for every } j \in u, \text{ and } \alpha_j^i = 0 \text{ otherwise } \right\}.$$

Then the ANOVA component f_u can be written as a sum of polynomial basis functions with indices in $\mathcal{A}_u$,

$$f_u(\mathbf{x}_u) = \sum_{i \in \mathcal{A}_u} k_i \Psi_{\alpha^i},$$

and

$$\sigma_u^2 = \sum_{i \in \mathcal{A}_u} k_i^2 .$$

Define the lower subset with truncated order p as

$$\underline{\mathcal{A}}_{u,p} = \left\{ i : i < P, \text{ and } \exists j \in u \text{ where } \alpha_j^i > 0, \text{ and } \alpha_j^i = 0 \text{ for every } j \in -u \right\},$$

and the upper subset as

$$\bar{\mathcal{A}}_{u,p} = \left\{ i : i < P, \text{ and } \exists j \in u \text{ where } \alpha_j^i > 0 \right\}.$$

The PCE-based lower Sobol' sensitivity index of u is given by

$$\underline{S}_u^{\text{pce}} \approx \frac{\sum_{i \in \underline{\mathcal{A}}_{u,p}} \hat{k}_i^2}{\sigma^2} = \frac{\sum_{i \in \underline{\mathcal{A}}_{u,p}} \hat{k}_i^2}{\sum_{i=1}^{P} \hat{k}_i^2}, \tag{8}$$

and the PCE-based upper Sobol' sensitivity index of u is given by

$$\bar{S}_u^{\text{pce}} \approx \frac{\sum_{i \in \bar{\mathcal{A}}_{u,p}} \hat{k}_i^2}{\sigma^2} = \frac{\sum_{i \in \bar{\mathcal{A}}_{u,p}} \hat{k}_i^2}{\sum_{i=1}^{P} \hat{k}_i^2}, \tag{9}$$

where $\hat{k}_i$ the estimated values for k_i.

As Eqn. (8) and Eqn. (9) show, the computational cost of using the truncated PCE to estimate the Sobol' index is mainly from estimating the PCE coefficients k_i. A popular method of estimating these coefficients is regression. One drawback of the regression based methods is that as the truncation level p or the dimension of the vector $\mathbf{x}$ increases, the number of coefficients to estimate increases drastically. A solution is to use sparse regression and only consider a small number of basis functions and estimate the corresponding coefficients. A survey of sparse polynomial chaos expansions is given by Lüthen et al. (2021). Here we will use the Bayesian PCE approach introduced in Babacan et al. (2009).

4. Control variate Monte Carlo estimators based on Bayesian polynomial chaos expansion

Consider the problem of estimating $\mathbb{E}[Y]$ with the control variate Monte Carlo method, where we assume there is another random variable C, called the control, with known mean μ_C, and C&Y are correlated.

The control variate estimator for $\mathbb{E}[Y]$ is given by

$$Y(\beta) = Y - \beta(C - \mu_C), \tag{10}$$

where β is a constant with optimal value (the value that minimizes the variance of $Y(\beta)$)

$$\beta^* = \frac{\mathrm{Cov}(Y, C)}{\mathrm{Var}(C)}. \tag{11}$$

In practice, β^* is estimated from the data. We then estimate $E[Y]$ using the sample mean of $Y(\beta)$

$$\hat{\theta} = \frac{1}{N}\sum_{n=1}^{N} \left(Y_n - \beta^*(C_n - \mu_C)\right), \tag{12}$$

where $Y_1, C_1, \dots, Y_N, C_N$ is a random sample of size N from Y and C.

In Fox & Ökten (2021), the control C was chosen as the (truncated) PCE expansion of Y. Here we will use Bayesian PCE as the control. Let $Y(\beta) = f^{cv}, Y = f$, and $C = f_p$. The general form of these estimators is

$$f^{cv}(\mathbf{x}) = f(\mathbf{x}) - \beta^*\left(f_p(\mathbf{x}) - \mathbb{E}[f_p]\right), \tag{13}$$

where p is the truncation order, and $f_p(\mathbf{x})$ is the truncated PCE where the coefficients k_i in Eqn. (7) are obtained using the Bayesian PCE method. If we know the truncated PCE f_p exactly, which means knowing the coefficients k_i in Eqn. (7) exactly, then the optimal β^* equals to one.

In practice, we estimate $f_p(\mathbf{x})$ as

$$\hat{f}_p(\mathbf{x}) = \sum_{i=0}^{P-1} \hat{k}_i \Psi_i(\mathbf{x}),$$

where $\hat{k}_i$ is obtained using regression. Another way to obtain $\hat{k}_i$ is to use the Monte Carlo method. In that case, the optimal β converges to one from below as the Monte Carlo sample size goes to infinity. For details see Fox & Ökten (2021).

We next introduce two control variate estimators, called cv1 and cv2, where each estimator has two versions, one for lower and one for upper Sobol' index.

The first control variate estimator, cv1

For the lower Sobol' index, cv1 uses Owen's three-parameter estimator for $\underline{\tau}_u$. The cv1 estimator for $\underline{\tau}_u$, denoted by $\underline{\tau}_u^{cv1}$, takes $Y = \underline{\tau}_u^{\text{owen}}$ and $C = \underline{\tau}_{u,p}^{\text{owen}}$ in Eqn. (10):

$$\underline{\tau}_u^{cv1}(\mathbf{x}, \mathbf{y}^u, \mathbf{z}) = \underline{\tau}_u^{\text{owen}}(\mathbf{x}, \mathbf{y}^u, \mathbf{z}) - \underline{\beta}^*\left(\underline{\tau}_{u,p}^{\text{owen}}(\mathbf{x}, \mathbf{y}^u, \mathbf{z}) - \mathbb{E}\left[\underline{\tau}_{u,p}^{\text{owen}}\right]\right) \tag{14}$$

where

$$\underline{\tau}_u^{\text{owen}} = \left(f(\mathbf{x}) - f(\mathbf{y}^u, \mathbf{x}^{-u})\right)\left(f(\mathbf{x}^u, \mathbf{z}^{-u}) - f(\mathbf{z})\right),$$

and

$$\underline{\tau}_{u,p}^{\text{owen}} = \left(\hat{f}_p(\mathbf{x}) - \hat{f}_p(\mathbf{y}^u, \mathbf{x}^{-u})\right)\left(\hat{f}_p(\mathbf{x}^u, \mathbf{z}^{-u}) - \hat{f}_p(\mathbf{z})\right).$$

The lower Sobol' index then can be estimated from

$$\underline{S}_u^{cv1} = \frac{\underline{\tau}_u^{cv1}(\mathbf{x}, \mathbf{y}^u, \mathbf{z})}{\sigma^2}.$$

The expectation of control is $\mathbb{E}\left[\underline{\tau}_{u,p}^{\text{owen}}\right] = \sum_{i \in \mathcal{A}_{u,p}} \hat{k}_i^2$, from Eqn. (8). The optimal $\underline{\beta}^*$ is estimated by using sample covariance and sample variance of the simulated data using Eqn. (11).

To estimate the upper Sobol' index, cv1 uses Jansen's estimator for $\bar{\tau}_u$. The cv1 estimator for $\bar{\tau}_u$ is

$$\bar{\tau}_u^{cv1}(\mathbf{x}, \mathbf{z}^u) = \bar{\tau}_u^{\text{jansen}}(\mathbf{x}, \mathbf{z}^u) - \bar{\beta}^*\left(\bar{\tau}_{u,p}^{\text{jansen}}(\mathbf{x}, \mathbf{z}^u)\right) - E\left[\bar{\tau}_{u,p}^{\text{jansen}}\right]\Big), \tag{15}$$

where

$$\bar{\tau}_u^{\text{jansen}}(\mathbf{x},\mathbf{z}^u)=\frac{1}{2}\left(f(\mathbf{x})-f(\mathbf{z}^u,\mathbf{x}^{-u})\right)^2$$
$$\bar{\tau}_{u,p}^{\text{jansen}}(\mathbf{x},\mathbf{z}^u)=\frac{1}{2}\left(\hat{f}_p(\mathbf{x})-\hat{f}_p(\mathbf{z}^u,\mathbf{x}^{-u})\right)^2.$$

The upper Sobol' index is estimated from

$$\bar{S}_u^{cv1}=\frac{\bar{\tau}_u^{cv1}(\mathbf{x},\mathbf{z}^u)}{\sigma^2}.$$

The expectation of control is $\mathbb{E}\left[\bar{\tau}_{u,p}^{\text{jansen}}\right]=\sum_{i\in\bar{\mathcal{A}}_{u,p}}\hat{k}_i^2$ from Eqn. (9). The optimal $\bar{\beta}^*$ is estimated similarly using Eqn. (11).

The second control variate estimator, cv2

The cv2 estimator has a slightly different form than Eqn. (10), and it is a *biased* estimator. The cv2 estimator for $\underline{\tau}_u$ is

$$\underline{\tau}_u^{cv2}=Y-(C-\mathbb{E}[C])+\left(\mathbb{E}\left[\underline{\tau}_{u,p}^{\text{owen}}\right]-\mathbb{E}[C]\right) \tag{16}$$

where $Y=\underline{\tau}_u^{\text{owen}}$, and

$$C=\left(f(\mathbf{x})-f(\mathbf{y}^u,\mathbf{x}^{-u})\right)\left(\hat{f}_p(\mathbf{x}^u,\mathbf{z}^{-u})-\hat{f}_p(\mathbf{z})\right)+\left(\hat{f}_p(\mathbf{x})-\hat{f}_p(\mathbf{y}^u,\mathbf{x}^{-u})\right)\left(f(\mathbf{x}^u,\mathbf{z}^{-u})-f(\mathbf{z})\right)$$
$$-\left(\hat{f}_p(\mathbf{x})-\hat{f}_p(\mathbf{y}^u,\mathbf{x}^{-u})\right)\left(\hat{f}_p(\mathbf{x}^u,\mathbf{z}^{-u})-\hat{f}_p(\mathbf{z})\right).$$

If the bias term, $\mathbb{E}\left[\underline{\tau}_{u,p}^{\text{owen}}\right]-\mathbb{E}[C]$ equals zero, then $\mathbb{E}\left[\underline{\tau}_u^{\text{cv2}}\right]=\mathbb{E}\left[\underline{\tau}_u^{\text{owen}}\right]=\underline{\tau}_u$. Observe that if $\hat{f}_p\approx f$, then $C\approx\mathbb{E}\left[\underline{\tau}_{u,p}^{\text{owen}}\right]$ and the bias term is small.

The cv2 estimator for $\bar{\tau}_u$ is

$$\bar{\tau}_u^{cv2}=Y-(C-\mathbb{E}[C])+\left(\mathbb{E}\left[\bar{\tau}_{u,p}^{\text{jansen}}\right]-\mathbb{E}[C]\right) \tag{17}$$

where $Y=\bar{\tau}_u^{\text{jansen}}$, and

$$C=\left(f(\mathbf{x})-f(\mathbf{z}^u,\mathbf{x}^{-u})\right)\left(\hat{f}_p(\mathbf{x})-\hat{f}_p(\mathbf{z}^u,\mathbf{x}^{-u})\right)-\frac{1}{2}\left(\hat{f}_p(\mathbf{x})-\hat{f}_p(\mathbf{z}^u,\mathbf{x}^{-u})\right)^2.$$

If the bias $\mathbb{E}\left[\bar{\tau}_{u,p}^{\text{jansen}}\right]-\mathbb{E}[C]$ is zero then cv2 is an unbiased estimator for $\bar{\tau}_u$.

The corresponding estimators for lower and upper Sobol' indices are obtained by dividing τ^{cv2} values by σ^2. Estimators in the form of cv2 were used by Fox & Ökten (2021) where C was based on PCE, and by Kucherenko et al. (2015) where C was based on first order ANOVA terms.

4.1 Complexity analysis

Define the efficiency of a Monte Carlo algorithm **B** as

$$E_B=\sigma_B^2\times t_B, \tag{18}$$

where σ_B^2 is the variance of the estimator, and t_B is the complexity of the algorithm which is measured in terms of function evaluations or computing time.

Here we will consider the unbiased control variate estimator cv1, which is based on Eqn. (13), and let t_B be the number of function evaluations in the estimator. We assume the truncated PCE expansion f_p is known exactly, which implies $\beta^*=1$. Fox & Ökten (2021) showed that $\mathrm{Cov}(f,f_p)=\mathrm{Var}(f_p)$ in this case. Then

$$\mathrm{Var}(f^{cv})=\mathrm{Var}(f)+\mathrm{Var}(f_p)-2\mathrm{Cov}\left(f,(f_p-\mathbb{E}[f_p])\right)=\mathrm{Var}(f)-2\mathrm{Cov}(f,f_p)+\mathrm{Var}(f_p)=\mathrm{Var}(f)-\mathrm{Var}(f_p).$$

Let F be the cost of one function evaluation of f, and F_p the cost of one function evaluation of f_p. The control variate method cv1 uses Owen's estimator for estimating the lower Sobol' index (Eqn. (14)), where four function evaluations of f , and four truncated Bayesian PCE function evaluations of f_p are needed. Then the total cost is $4(F + F_p)$. For the upper Sobol' index, cv1 uses Jansen's estimator and thus two function evaluations and two Bayesian PCE function evaluations (Eqn. (15)) for a total cost of $2(F + F_p)$.

The efficiency of Owen's estimator for estimating the lower Sobol' index is

$$E_{\text{owen}} = 4F \times \text{Var}(f),$$

and the efficiency cv1 is

$$\begin{aligned} E_{cv} &= \left(\text{Var}(f) - \text{Var}(f_p)\right) \times \left(4F + 4F_p\right) \\ &= 4F \times \text{Var}(f) - 4F \times \text{Var}(f_p) + 4F_p\left(\text{Var}(f) - \text{Var}(f_p)\right) \\ &= E_{\text{owen}} - 4F \times \text{Var}(f_p) + 4F_p\left(\text{Var}(f) - \text{Var}(f_p)\right). \end{aligned}$$

The efficiency of Jansen's estimator is

$$E_{\text{jansen}} = 2F \times \text{Var}(f),$$

and the efficiency of cv1 is

$$\begin{aligned} E_{cv} &= \left(\text{Var}(f) - \text{Var}(f_p)\right) \times \left(2F + 2F_p\right) \\ &= 2F \times \text{Var}(f) - 2F \times \text{Var}(f_p) + 2F_p\left(\text{Var}(f) - \text{Var}(f_p)\right) \\ &= E_{\text{jansen}} - 2F \times \text{Var}(f_p) + 2F_p\left(\text{Var}(f) - \text{Var}(f_p)\right). \end{aligned}$$

Therefore if $\text{Var}(f_p) \approx \text{Var}(f)$ we expect the control variate estimators to have better (smaller) efficiency than that of Owen and Jansen.

5. Numerical results

In this section, we first compare the PCE and Bayesian PCE methods when they are used to estimate the integral of two test functions: Ishigami and Morris functions. The Ishigami function (Ishigami & Homma, 1990) is defined as

$$f(\mathbf{x}) = \sin(x_1) + a\sin^2(x_2) + bx_3^4\sin(x_1),$$

where $\mathbf{x} = (x_1, x_2, x_3) \sim U[-\pi, \pi]^3$. In our numerical results we take $a = 7, b = 0.1$.

The Morris function (Morris, 1991) is

$$Y = \beta_0 + \sum_{i=1}^{20} \beta_i X_i + \sum_{i<j}^{20} \beta_{ij} X_i X_j + \sum_{i<j<k}^{20} \beta_{ijk} X_i X_j X_k + \sum_{i<j<k<l}^{20} \beta_{ijkl} X_i X_j X_k X_l$$

where

$$X_i = \begin{cases} 2(1.1x_i/(x_i + 0.1) - 0.5) & \text{if } i = 3,5,7 \\ 2(x_i - 0.5) & \text{otherwise} \end{cases}$$

and $x_i \sim U(0,1)$. The coefficients β_i are:

$$\begin{cases} \beta_i = 20 & \text{for } i = 2, \dots, 10 \\ \beta_{ij} = -15 & \text{for } i, j = 1, \dots, 6 \\ \beta_{ijk} = -10 & \text{for } i, j, k = 1, \dots, 5 \\ \beta_{ijkl} = 5 & \text{for } i, j, k, l = 1, \dots, 4. \end{cases}$$

The remaining coefficients are given by $\beta_0 = 0,\ \beta_i = (-1)^i$ and $\beta_{ij} = (-1)^{i+j}$.

To compare PCE and Bayesian PCE numerically we will estimate the relative error of each method which is defined as

$$\epsilon = \frac{\mathbb{E}\left[f(\mathbf{x}) - \hat{f}_p(\mathbf{x})\right]^2}{\mathrm{Var}[f(\mathbf{x})]},$$

where $f(\mathbf{x})$ is the exact function evaluation and $\hat{f}_p(\mathbf{x})$ is the estimated truncated PCE for Ishigami and Morris functions. We use the package UQLab (Marelli & Sudret, 2014) to compute the PCE and Bayesian PCE. For the truncation level we use $p = 6$ for the Ishigami function and $p = 3$ for the Morris function. We estimate ϵ via Monte Carlo simulation

$$\hat{\epsilon} = \frac{M-1}{M}\left[\frac{\sum_{i=1}^{M}\left(f(\mathbf{x}^{(i)}) - \hat{f}_p(\mathbf{x}^{(i)})\right)^2}{\sum_{i=1}^{M}(f(\mathbf{x}^{(i)}) - \hat{\mu})^2}\right],$$

where $\mathbf{x}^{(i)}, i = 1, \ldots, M$ is a random sample of size M, and $\hat{\mu} = \frac{1}{M}\sum_{i=1}^{M} f\left(\mathbf{x}^{(i)}\right)$ is the sample mean of the function evaluations.

Fig. 1 plots the relative error of PCE and Bayesian PCE against the sample size M. The Bayesian PCE has smaller error than PCE for smaller sample sizes, and as the sample size increases the error becomes similar. These results explain our motivation to develop control variate estimators for Sobol' indices based on Bayesian PCE.

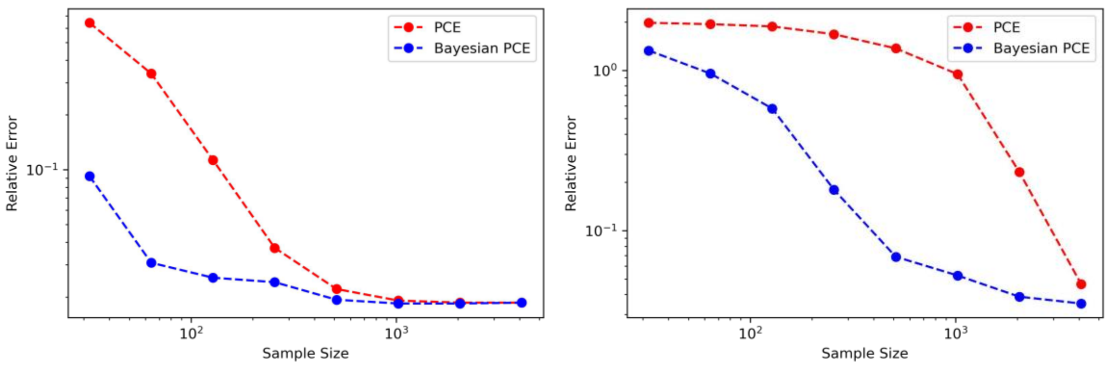

Figure 1: Relative error of PCE and Bayesian PCE using Sobol' sequence (left: Ishigami function, right: Morris function).

In the rest of this section we will consider two problems; an SIR model and the Stiefel canonical distance model. Building an accurate PCE model for these problems is computationally expensive: the truncation level has to be relatively large and the function evaluations are expensive. We will use our control variate estimators based on a Bayesian PCE with truncation level two ($p = 2$) to estimate the Sobol' indices. We will compare the control variate estimators with (i) the *pure* Bayesian PCE approach where one computes the Sobol' indices from Eqns. (8) and (9), (ii) the estimators of Owen, Janon, Azzini. Since we are comparing a mix of unbiased and biased estimators, we cannot use sample variance as a measure of error: the biased estimators may have a small sample variance but large actual error. Instead we use the mean square error (MSE):

$$\mathrm{MSE} = \frac{1}{K}\sum_{k=1}^{K}\left(\hat{S}^{(k)} - S\right)^2,$$

where S is the "exact" solution obtained from a large Monte Carlo simulation, and $\hat{S}^{(1)}, \ldots, \hat{S}^{(K)}$ are K independent estimates for S. Consequently, we define the efficiency of a Monte Carlo estimator B as $E_B = \mathrm{MSE}_B \times t_B$, where t_B is the computing time. For the control variate methods, the computing time also includes the time for estimating the Bayesian PCE coefficients k_i. [1]

[1] There could be a scenario where one computes the Bayesian PCE and f_P, and then computes Sobol' sensitivity indices many times. In a situation like that, one might consider computing the PCE coefficients as a part of the initialization, and not include the computing time in the efficiency calculations. That would make the control variate estimators more efficient than what is reported here.

We use randomized quasi-Monte Carlo methods[2] to generate the estimates $\hat{S}^{(1)}, \dots, \hat{S}^{(K)}$, where each estimate $\hat{S}^{(k)}$ is obtained using the first 500 Sobol' vectors of the corresponding sequence, setting the sample size $N = 500$ in the definition of the Monte Carlo estimators in Sections 2 and 4.

5.1 SIR model

The SIR model is a commonly used model for disease dynamics

$$\frac{dS}{dt} = \delta N - \delta S - \gamma kIS, S(0) = S_0$$
$$\frac{dI}{dt} = \gamma kIS - (r+\gamma)I, I(0) = I_0$$
$$\frac{dR}{dt} = rI - \gamma R, R(0) = R_0$$

where $S(t), I(t)$and $R(t)$ are the number of susceptible, infectious and recovered individuals in a population of size $N = S(t) + I(t) + R(t)$. The parameters γ, k, r denote the infection coefficient, the interaction coefficient, and the recovery rate, respectively. δ denotes the birth and death rate, which are assumed to be equal here. We assume that the input $\theta = [\gamma, k, r, \delta]$ follows the uniform distribution on $(0,1)^4$. Consider the scalar response

$$y = \int_0^1 R(t,\theta)dt,$$

where $S_0 = 900,\ I_0 = 100,\ R_0 = 0.$ We want to estimate the sensitivity of y with respect to the parameters in θ.

We use 3,300,000 function evaluations to estimate the "exact" values for Sobol' indices using Janon's estimator as shown in Table 1. These are the values we use for the exact value in the MSE calculations.

Table 1: Sobol' indices for the SIR model

	S_1	S_2	S_3	S_4
lower Sobol'	0.0316	0.0303	0.8424	0.0488
upper Sobol'	0.0576	0.0575	0.8743	0.0611

Tables 2 and 3 display the efficiency of the control variate methods, and the Bayesian PCE method for truncation levels 2 through 5. There are four Sobol' indices that are estimated and there are four corresponding efficiencies given in the table rows. The last row displays the computing time for each estimator. Table 2 is for the lower Sobol' indices, and Table 3 for the upper. Among different Bayesian PCE methods, the one with truncation level $p = 3$ seems to be the most efficient (lower efficiency means better efficiency) approach in both tables. For the lower Sobol' indices, cv1 has slightly better efficiency in two cases than the optimal Bayesian PCE approach, and worse in the rest. cv2 is better than the optimal Bayesian PCE in one case, and worse in the others. The ratio of efficiency in favor of Bayesian PCE ranges from 0.6 to 5.9.

Table 2: Comparing efficiency of control variate methods and BPCE for estimating lower Sobol' indices: SIR model.

Methods	cv1($p=2$)	cv2($p=2$)	BPCE($p=2$)	BPCE($p=3$)	BPCE($p=4$)	BPCE($p=5$)
eff1	1.8e-04	7.5e-05	3.4e-05	3.1e-05	4.5e-05	6.5e-05
eff2	1.3e-04	6.8e-05	2.9e-05	2.7e-05	4.0e-05	6.2e-05
eff3	3.3e-04	2.2e-04	3.9e-04	3.5e-04	4.8e-04	7.1e-04
eff4	2.3e-06	1.3e-05	3.6e-06	4.1e-06	6.1e-06	9.9e-06
time	1.3746	1.3746	0.1523	0.2757	0.6493	1.2910

For the upper Sobol indices, both control variates estimators have better efficiency than the Bayesian PCE methods for all cases, except BPCE($p = 3$) versus cv2 for eff4. The factors of improvement favoring control methods range from 0.6 to 11.

[2] Linear scrambled Sobol' sequences with a random digital shift of Matoušek (1998).

Table 3: Comparing efficiency of control variate methods and BPCE for estimating upper Sobol' indices: SIR model.

Methods	cv1($p=2$)	cv2($p=2$)	BPCE($p=2$)	BPCE($p=3$)	BPCE($p=4$)	BPCE($p=5$)
eff1	3.7e-05	3.5e-05	1.7e-04	1.5e-04	1.9e-04	2.7e-04
eff2	4.6e-05	2.4e-05	1.8e-04	1.5e-04	2.1e-04	3.1e-04
eff3	6.0e-05	7.7e-05	1.9e-04	1.6e-04	2.2e-04	3.1e-04
eff4	5.1e-07	9.5e-06	4.7e-06	5.6e-06	1.2e-05	1.8e-05
time	0.4733	0.4733	0.1523	0.2757	0.6493	1.2910

Next we compare the control variate methods with the estimators of Owen, Janon, and Azzini. Tables 4 and 5 display the efficiency of the methods. Table 4 shows that Azzini's estimator has better efficiency for all cases, except the fourth Sobol' index, where cv1 is better, and Azzini's estimator has a tie with cv2. The next best estimator is cv2, although Janon's estimator has better efficiency than cv2 in one case.

Table 5 displays the efficiency values for estimating the upper Sobol' index. cv2 has better efficiency than Jansen, Janon, Azzini, in all cases except one. cv1 has the best efficiency for the fourth Sobol' index among all methods, and has better efficiency than Jansen, Janon, Azzini, for the remaining indices except for the second Sobol' index.

Table 4: Comparing efficiency of Monte Carlo estimators for estimating lower Sobol' indices: SIR model.

Methods	Owen	Janon	Azzini	cv1($p=3$)	cv2($p=3$)
eff1	1.6e-04	5.9e-03	3.8e-05	1.8e-04	7.5e-05
eff2	1.3e-04	5.2e-03	5.1e-05	1.3e-04	6.8e-05
eff3	4.7e-03	1.9e-04	1.0e-04	3.3e-04	2.2e-04
eff4	1.8e-05	5.9e-03	1.3e-05	2.3e-06	1.3e-05

Table 5: Comparing efficiency of Monte Carlo estimators for estimating upper Sobol' indices: SIR model.

Methods	Jansen	Janon	Azzini	cv1($p=3$)	cv2($p=3$)
eff1	7.7e-05	7.7e-05	1.4e-04	3.7e-05	3.5e-05
eff2	3.1e-05	3.1e-05	2.4e-05	4.6e-05	2.4e-05
eff3	1.4e-03	1.5e-03	1.1e-04	6.0e-05	7.7e-05
eff4	3.5e-06	3.1e-06	1.4e-05	5.1e-07	9.5e-06

Numerical results reported in Tables 2 and 3 indicate that overall Bayesian PCE with $p=3$ is the best method in terms of efficiency among the different truncation levels. Why are we not implementing the control variate methods cv1 and cv2 with this truncation level and instead use the suboptimal choice $p=2$? We assume there may not be sufficient computing resources for the user to conduct a numerical investigation of the optimal truncation level in a practical problem, and we propose using the least expensive non-linear model ($p=2$) in constructing the control variate estimators even though using the optimal BPCE will likely improve the control variate estimators.

5.2 Stiefel canonical distance model

We consider the distance model of a matrix and neighborhood under the canonical metric on Stiefel manifold,

$$\mathbf{St}_{n,k} := \{U \in \mathbb{R}^{n\times k} : U^T U = I_k\}.$$

Let $d_{\mathrm{st}}(\tilde{U}, V)$ be the Stiefel canonical distance between $\tilde{U}$ and V (see Edelman et al. (1998) for details), investigating the distribution of $d_{\mathrm{St}}(\tilde{U}, V)$ for $\tilde{U}$ around some given $U \in \mathbf{St}_{n,k}$ is useful for approximating the directional derivative of the Riemannian exponential on $\mathbf{St}_{n,k}$. Since this model involves sampling points on a manifold, which is nontrivial in general, we specify a strategy as follows.

For any point $\tilde{U}$ in a neighborhood of $U \in \mathbf{St}_{n,k}$ with orthogonal complement $U_\perp$, there is a unique skew symmetric matrix $A = -A^T \in \mathbb{R}^{k\times k}$ and a real matrix $B \in \mathbb{R}^{(n-k)\times k}$ such that

$$\tilde{U}(A,B) := [U \quad U_\perp] \exp\left(\begin{bmatrix} A & -B^T \\ B & 0 \end{bmatrix}\right) \begin{bmatrix} I_k \\ 0 \end{bmatrix}.$$

Here $\exp(\cdot)$ is matrix exponential. The lower triangular entries in A and all entries in B naturally give a parameterization of points around U. In the numerical results, we set $n = 5$ and $k = 2$, then there are 7 parameters $\mathbf{x} := (x_1, \cdots, x_7)$ that determine A, B as

$$A(\mathbf{x}) := \begin{bmatrix} 0 & -x_1 \\ x_1 & 0 \end{bmatrix}, B(\mathbf{x}) := \begin{bmatrix} x_2 & x_5 \\ x_3 & x_6 \\ x_4 & x_7 \end{bmatrix},$$

which further determines $\tilde{U}$ as $\tilde{U}(\mathbf{x}) := \tilde{U}(A(\mathbf{x}), B(\mathbf{x}))$. By generating independent samples $\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(N)}$ from uniform distribution on $(-1,1)^7$, and computing $d_{\mathrm{St}}(\tilde{U}(\mathbf{x}), V)$ (using the algorithm from Zimmermann (2017)) for each $\mathbf{x}^{(i)}$, we can approximate $\mathbb{E}[d_{\mathrm{St}}(\mathcal{N}, V)]$ on the neighborhood

$$\mathcal{N} := \{\tilde{U}(\mathbf{x}): \| \mathbf{x} \|_\infty \leq 1 \;\; d_{\mathrm{st}} (\tilde{U}(\mathbf{x}), U) = \| \mathbf{x} \|_2\}$$

via the sample mean.[3]

We use 4,950,000 function evaluations to estimate the "exact" values for the Sobol' indices for the inputs $x_1, \ldots, x_7$, where the output is $d_{\mathrm{St}}(\tilde{U}, V)$, using Janon's estimator. The results are shown in Table 6.

Table 6: Sobol' indices for Stiefel canonical distance model.

	S_1	S_2	S_3	S_4	S_5	S_6	S_7
lower Sobol'	0.1686	0.2106	0.1058	0.1596	0.1068	0.0316	0.0560
upper Sobol'	0.2366	0.2926	0.1544	0.2300	0.1754	0.0735	0.1243

Tables 7 and 8 display the efficiency of the control variate methods, and the Bayesian PCE method for truncation levels 2 through 5, and the computing times. There are seven Sobol' indices that are estimated. Table 7 presents the lower Sobol' indices, and Table 8 the upper ones. The Bayesian PCE with $p = 3$ seems to be the best method among the different Bayesian PCE methods for estimating the lower Sobol' indices. There is no clear distinction between cv1, cv2, and BPCE$(p = 3)$ methods in Table 7.

Table 7: Comparing efficiency of control variate methods and BPCE for estimating lower Sobol' indices: Stiefel canonical distance model.

Methods	cv1$(p = 2)$	cv2$(p = 2)$	BPCE$(p = 2)$	BPCE$(p = 3)$	BPCE$(p = 4)$	BPCE$(p = 5)$
eff1	5.5e-03	1.4e-03	1.7e-03	4.5e-04	1.8e-03	3.3e-02
eff2	6.9e-05	1.0e-03	3.6e-03	4.6e-04	2.5e-03	4.0e-02
eff3	4.6e-04	6.4e-04	3.8e-04	4.5e-04	1.9e-03	9.9e-03
eff4	1.5e-03	1.2e-03	1.2e-03	4.4e-04	4.0e-03	2.6e-02
eff5	2.6e-04	3.2e-04	3.3e-04	3.1e-04	1.2e-03	8.6e-03
eff6	1.1e-04	1.8e-04	5.9e-05	1.2e-04	6.4e-04	1.9e-03
eff7	3.7e-04	3.1e-04	3.2e-04	2.4e-04	9.6e-04	3.9e-03
time	5.3468	5.3469	3.7488	5.3001	27.5277	70.5805

Table 8: Comparing efficiency of control variate methods and BPCE for estimating lower Sobol' indices: Stiefel canonical distance model.

Methods	cv1$(p = 2)$	cv2$(p = 2)$	BPCE$(p = 2)$	BPCE$(p = 3)$	BPCE$(p = 4)$	BPCE$(p = 5)$
eff1	2.6e-03	2.3e-03	2.0e-03	1.6e-03	8.2e-03	2.4e-02
eff2	7.7e-04	1.4e-03	1.7e-03	2.2e-03	8.7e-03	2.4e-02
eff3	3.8e-04	8.8e-04	3.9e-03	2.4e-03	9.0e-03	3.8e-02
eff4	5.8e-04	1.4e-03	6.0e-03	4.4e-03	1.1e-02	4.9e-02
eff5	4.3e-04	6.9e-04	7.1e-03	3.6e-03	1.2e-02	7.2e-02
eff6	4.5e-04	5.9e-04	1.7e-03	1.2e-03	5.3e-03	3.9e-02
eff7	2.8e-04	2.8e-04	2.9e-03	2.1e-03	9.6e-03	6.2e-02
time	6.8774	6.8774	3.7488	5.3001	27.5277	70.5805

[3] Note that for a neighborhood different than the *N* here, one is expected to find an appropriate parameterization that describes such neighborhood with independent parameters in [−1, 1].

For the upper Sobol' indices, Bayesian PCE with $p = 3$ is again the best method among the different Bayesian PCE methods. From Table 8 we see that cv1 and cv2 have better efficiency than the optimal Bayesian PCE method in all cases except one. The factor of improvement favoring control variate methods range from 1.5 to 8.3.

Next we compare the efficiencies of the Monte Carlo estimators. Table 9 presents the results for the lower Sobol' indices, and Table 10 presents the upper indices. For the lower Sobol' indices, cv1 and cv2 have better efficiency than all the other methods, for all cases except one, where Azzini has the same result as cv1 for the fourth index. The efficiency ratio in favor of cv1 (efficiency of a method divided by efficiency of cv1) ranges from 0.97 to 1829, and the efficiency ratio in favor of cv2 ranges from 1.28 to 882. For the upper Sobol' indices, cv1 has better efficiency than Owen, Janon, and Azzini for all cases, and cv2 has better efficiency than Owen, Janon, and Azzini for all cases except the fifth index. The efficiency ratio in favor of cv1 ranges from 1.25 to 52, and the efficiency ratio in favor of cv2 ranges from 0.58 to 58.

Table 9: Comparing efficiency of Monte Carlo estimators for lower Sobol' indices: Stiefel canonical distance model.

Methods	Owen	Janon	Azzini	cv1($p = 2$)	cv2($p = 2$)
eff1	5.6e-01	1.4e-02	5.8e-02	5.5e-03	1.4e-03
eff2	1.7e-03	1.3e-01	6.2e-03	6.9e-05	1.0e-03
eff3	1.5e-03	1.5e-01	8.6e-04	4.6e-04	6.4e-04
eff4	2.1e-03	1.3e-01	1.5e-03	1.5e-03	1.2e-03
eff5	4.2e-04	1.7e-01	2.0e-03	2.6e-04	3.2e-04
eff6	7.6e-04	1.6e-01	1.5e-03	1.1e-04	1.8e-04
eff7	1.3e-03	1.7e-01	1.5e-03	3.7e-04	3.1e-04

Table 10: Comparing efficiency of Monte Carlo estimators for upper Sobol' indices: Stiefel canonical distance model.

Methods	Jansen	Janon	Azzini	cv1($p = 2$)	cv2($p = 2$)
eff1	1.3e-01	1.4e-01	1.2e-01	2.6e-03	2.3e-03
eff2	3.3e-03	3.2e-03	1.1e-02	7.7e-04	1.4e-03
eff3	9.2e-04	8.1e-04	4.0e-03	3.8e-04	8.8e-04
eff4	8.2e-04	9.0e-04	7.2e-03	5.8e-04	1.4e-03
eff5	5.4e-04	5.6e-04	4.0e-03	4.3e-04	6.9e-04
eff6	1.5e-03	1.5e-03	2.0e-03	4.5e-04	5.9e-04
eff7	7.3e-04	6.8e-04	3.1e-03	2.8e-04	2.8e-04

6. Conclusions

Numerical results suggest the proposed control variate methods are competitive when function evaluation is expensive, and a low-order (B)PCE expansion is not a good approximation to the function. The Stiefel distance model is significantly more expensive than the SIR model, and control variate methods perform better compared to the SIR model. The control variate methods also perform better, in general, for upper Sobol' indices estimation than the lower indices. The reason is we use the less expensive Jansen's estimator in constructing the control for the upper indices, as opposed to Owen's estimator for the lower indices. One can develop control variate estimators using other estimators, or other surrogate models than (B)PCE, and explore the benefits of this approach in computationally expensive problems.

Acknowledgements

We thank Kyle Gallivan and Zhifeng Deng for their help with the Stiefel canonical distance model.

References

Azzini, I., Mara, T., & Rosati, R. (2020). Monte Carlo estimators of first-and total-orders Sobol' indices. arXiv preprint arXiv:2006.08232.

Babacan, S. D., Molina, R., & Katsaggelos, A. K. (2009). Bayesian compressive sensing using Laplace priors. IEEE Transactions on Image Processing, 19(1):53–63.

Chakraborty, R. & Vemuri, B. C. (2019). Statistics on the stiefel manifold: theory and applications. The Annals of Statistics, 47(1):415–438.

Edelman, A., Arias, T. A., & Smith, S. T. (1998). The geometry of algorithms with orthogonality constraints. SIAM Journal on Matrix Analysis and Applications, 20(2): 303–353.

Elsawah, S., Filatova, T., Jakeman, A. J., Kettner, A. J., Zellner, M. L., Athanasiadis, I. N., Hamilton, S. H., Axtell, R. L., Brown, D. G., Gilligan, J. M., et al. (2020). Eight grand challenges in socio-environmental systems modeling. Socio-Environmental Systems Modelling, 2: 16226.

Fox, J. & Ökten, G. (2021). Polynomial chaos as a control variate method. SIAM Journal on Scientific Computing, 43(3): A2268–A2294.

Ishigami, T. & Homma, T. (1990). An importance quantification technique in uncertainty analysis for computer models. In [1990] Proceedings. First International Symposium on Uncertainty Modeling and Analysis, pages 398–403. IEEE.

Janon, A., Klein, T., Lagnoux, A., Nodet, M., & Prieur, C. (2014). Asymptotic normality and efficiency of two Sobol' index estimators. ESAIM: Probability and Statistics, 18: 342–364.

Jansen, M. J. (1999). Analysis of variance designs for model output. Computer Physics Communications, 117(1-2):35–43.

Kucherenko, S., Delpuech, B., Iooss, B., & Tarantola, S. (2015). Application of the control variate technique to estimation of total sensitivity indices. Reliability Engineering & System Safety, 134: 251–259.

Lemieux, C. & Owen, A. B. (2002). Quasi-regression and the relative importance of the ANOVA components of a function. In Monte Carlo and Quasi-Monte Carlo Methods 2000. Springer, pp. 331–344.

Lüthen, N., Marelli, S., & Sudret, B. (2021). Sparse polynomial chaos expansions: Literature survey and benchmark. SIAM/ASA Journal on Uncertainty Quantification, 9(2): 593–649.

Marelli, S. & Sudret, B. (2014). Uqlab: A framework for uncertainty quantification in Matlab. In Vulnerability, uncertainty, and risk: quantification, mitigation, and management, pp. 2554–2563.

Matoušek, J. (1998). On the L2-discrepancy for anchored boxes. Journal of Complexity, 14(4): 527–556.

Morris, M. D. (1991). Factorial sampling plans for preliminary computational experiments. Technometrics, 33(2): 161–174.

Owen, A. B. (2013). Better estimation of small Sobol' sensitivity indices. ACM Transactions on Modeling and Computer Simulation (TOMACS), 23(2): 1–17.

Puy, A., Becker, W., Piano, S. L., & Saltelli, A. (2022). A comprehensive comparison of total-order estimators for global sensitivity analysis. International Journal for Uncertainty Quantification, 12(2): 1-18.

Saltelli, A., Ratto, M., Tarantola, S., & Campolongo, F. (2006). Sensitivity analysis practices: Strategies for model-based inference. Reliability Engineering & System Safety, 91(10-11): 1109–1125.

Sobol', I. M. (1993). Sensitivity analysis for non-linear mathematical models. Mathematical Modelling and Computational Experiment, 1: 407–414.

Sudret, B. (2008). Global sensitivity analysis using polynomial chaos expansions. Reliability Engineering & System Safety, 93(7): 964–979.

Zimmermann, R. (2017). A matrix-algebraic algorithm for the Riemannian logarithm on the Stiefel manifold under the canonical metric. SIAM Journal on Matrix Analysis and Applications, 38(2): 322–342.