

Global sensitivity analysis in high dimensions with partial least squares-driven PCEs

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ABSTRACT: We develop an efficient method for the computation of variance-based sensitivity indices using a recently introduced latent-variable-based polynomial chaos expansion, which is particularly suitable for high dimensional problems. By back-transforming the surrogate from its latent variable space-basis to the original input variable space-basis, we derive analytical expressions for these sensitivities that only depend on the model coefficients. Thus, once the surrogate model is built, the variance-based sensitivities can be computed at negligible computational cost as no additional sampling is required. The accuracy of the method is demonstrated with a numerical experiment of an elastic truss.

1. INTRODUCTION

Surrogate models have received much attention due to their potential of alleviating computational cost in applications requiring elaborate and expensive numerical models, see e.g. Hastie et al. (2001); Forrester et al. (2008); Sudret (2012). The general concept of surrogate modelling techniques is to establish an abstract, parametrized input-output-relation which has similar properties as the original model. The parameters of the surrogate model are determined based on a finite set of original model evaluations such as to maximize similarity between the surrogate and the original model according to a suitable criterion. Subsequently, the surrogate model can be used to cheaply approximate the original model and compute statistics of the output or a quantity of interest derived thereof. In addition to prediction, surrogates are also useful in efficiently

performing model sensitivity analysis - an otherwise typically computationally intensive task.

The main contribution of this work is the derivation of global, variance-based sensitivity measures for the model output from the coefficients of a recently introduced surrogate format called partial least squares-driven polynomial chaos expansions (PLS-PCE) (Papaioannou et al., 2018). PLS-PCE allows for the application of polynomial chaos expansions (PCE) in very high dimensions. Publications by Sudret (2008) and Konakli and Sudret (2016) have derived such sensitivity measures from the model coefficients of conventional PCEs (Xiu and Karniadakis, 2002) and polynomial-based canonical decompositions (Chevreuil et al., 2015), respectively. The paper is structured as follows: In chapter 2, we review the PLS-PCE surrogate model, its construction and some important properties. In chapter 3, we give a brief introduction to variance-based sensitivity analysis and its appli-

cation in the context of polynomial basis surrogate models. In chapter 4, we develop the methodology to compute sensitivities based on the model coefficients. In chapter 5, we demonstrate the new method based on two numerical examples and in chapter 6 we provide some concluding remarks.

2. PARTIAL LEAST SQUARES AND POLYNOMIAL CHAOS

Let \mathbf{X} be a random vector on the outcome space \mathbb{R}^d with joint CDF $F_{\mathbf{X}}$ whose elements are mutually independent and $\mathcal{Y}(\mathbf{X}) = Y \in \mathbb{R}$. If Y is square-integrable, i.e. $\mathbb{E}_{\mathbf{X}}[\mathcal{Y}(\mathbf{X})^2] < \infty$, it belongs to a Hilbert space \mathcal{H} with inner product of any two functions $g, h \in \mathcal{H}$

$$\begin{aligned} \langle g(\mathbf{X}), h(\mathbf{X}) \rangle_{\mathcal{H}} &= \mathbb{E}_{\mathbf{X}}[g(\mathbf{X})h(\mathbf{X})] \\ &= \int_{\mathbb{R}^d} g(\mathbf{x})h(\mathbf{x})f_{\mathbf{X}}(\mathbf{x})d\mathbf{x}, \end{aligned} \quad (1)$$

where $f_{\mathbf{X}}(\mathbf{x})$ is the joint PDF of \mathbf{X} . g and h are orthogonal if

$$\langle g(\mathbf{x}), h(\mathbf{x}) \rangle_{\mathcal{H}} = \mathbb{E}_{\mathbf{X}}[g(\mathbf{X})h(\mathbf{X})] = 0. \quad (3)$$

Note, that if g and h can be written as products of univariate functions of the components of \mathbf{X} , the following holds:

$$\langle g(\mathbf{x}), h(\mathbf{x}) \rangle_{\mathcal{H}} = \prod_{i=1}^d \mathbb{E}_{X_i}[g_i(X_i)h_i(X_i)]. \quad (4)$$

2.1. Polynomial Chaos Expansion

Given a complete and orthonormal basis of \mathcal{H} , $\{h_i(\mathbf{X}), i \in \mathbb{N}\}$, Y may be expressed as a linear combination of the basis functions:

$$Y = \mathcal{Y}(\mathbf{X}) = \sum_{i=0}^{\infty} a_i h_i(\mathbf{X}). \quad (5)$$

Then, since $Y \in \mathcal{H}$, the approximation

$$\widehat{Y}_p = \widehat{\mathcal{Y}}(\mathbf{X}) = \sum_{i=0}^p a_i h_i(\mathbf{X}) \quad (6)$$

asymptotically ($p \rightarrow \infty$) converges to Y in the mean-square sense. Henceforth, without loss of generality, we will consider the case $F_{\mathbf{X}} =$

Φ_d , where Φ_d denotes the d -variate independent standard-normal CDF. If the joint PDF of \mathbf{X} is known, one can express \mathbf{X} as a function of standard normal random variables through an isoprobabilistic transformation (Rosenblatt, 1952). Then, one can construct an orthonormal polynomial basis of \mathcal{H} using products of one-dimensional normalized Hermite polynomials

$$\Psi_{\mathbf{k}}(\mathbf{X}) = \prod_{i=1}^d \psi_{k_i}(X_i) \quad (7)$$

where $\{\psi_i(X), i \in \mathbb{N}\}$ are the normalized (probabilist) Hermite polynomials and $\mathbf{k} = (k_1, \dots, k_d) \in \mathbb{N}^d$. The PCE reads

$$\widehat{Y}_p = \sum_{|\mathbf{k}| \leq p} a_{\mathbf{k}} \Psi_{\mathbf{k}}(\mathbf{X}) \quad (8)$$

and the number of basis functions P is given combinatorially in terms of the dimensions d and the largest considered polynomial order p :

$$P = \binom{d+p}{p}. \quad (9)$$

The coefficients \mathbf{a} are computed through a projection of \mathcal{Y} onto the space spanned by $\{h_i, i = 0, \dots, P-1\}$, where the projection can be transformed into an equivalent ordinary least squares (OLS) problem (Berveiller et al., 2006). Equation (9) indicates a fast growth of the associated regression problem with increasing dimension d , rendering PCEs intractable for high-dimensional problems. Sparse PCE methods have been proposed to relax this constraint by solving a modified, \mathcal{L}_1 -regularized least-squares problem, which penalizes the number of terms in the expansion and thus reduces P (Blatman and Sudret, 2011), also known under the term 'compressive sampling/sensing'. Nevertheless, the computation of a sparse PCE still requires computing the entirety of all possible basis elements which can become a second (combinatorial) bottleneck in addition to the solution of the regression problem.

2.2. Basis adaptation

In order to address this problem, one may rotate the PCE representation onto a new basis defined by

the new variables $\mathbf{Z} = \mathbf{Q}^T \mathbf{X}$, where $\mathbf{Q} \in \mathbb{R}^{d \times d}$ and $\mathbf{Q}^T \mathbf{Q} = \mathbf{I}$. Then, an equivalent PCE representation is given by (Tipireddy and Ghanem, 2014)

$$\hat{Y}_p^{\mathbf{Q}} = \sum_{|\mathbf{k}| \leq p} b_{\mathbf{k}} \Psi_{\mathbf{k}}(\mathbf{Z}) = \sum_{|\mathbf{k}| \leq p} b_{\mathbf{k}} \Psi_{\mathbf{k}}(\mathbf{Q}^T \mathbf{X}). \quad (10)$$

The coordinate transformation allows for the construction of PCEs along dominant directions of the problem input space, where these directions are defined by linear combinations of the original variable vector \mathbf{X} , the coefficients of which are stored in the rows of \mathbf{Q} . Then, by retaining only the $m < d$ most dominant directions in \mathbf{Q} , one obtains a matrix \mathbf{Q}_m and the corresponding PCE reads

$$\hat{Y}_p^{\mathbf{Q}_m} = \sum_{|\mathbf{k}_m| \leq p} b_{\mathbf{k}_m} \Psi_{\mathbf{k}_m}(\mathbf{Q}_m^T \mathbf{X}), \quad (11)$$

where $\mathbf{k}_m \in \mathbb{N}^m$. In the following we discuss briefly how the most dominant directions can be identified based on set of original function evaluations via partial least squares (PLS) and how to find the adapted PCE coefficients.

2.3. Partial least squares-based PCE

The basic idea of PLS is to find a relationship between variables \mathbf{X} and Y based on N observations of both quantities (Papaioannou et al., 2018). $\mathcal{X} \in \mathbb{R}^{N \times d}$ stores observations from \mathbf{X} and $\mathcal{Y} \in \mathbb{R}^{N \times 1}$ stores the corresponding responses, standard PLS sequentially identifies latent components $\mathbf{t}_i \in \mathbb{R}^{N \times 1}$ such that they are maximally correlated with \mathcal{Y} . After determining each \mathbf{t}_i , standard PLS assumes a linear relationship between \mathbf{t}_i and \mathcal{Y} and evaluates the corresponding coefficient b_i of \mathbf{t}_i by OLS. After each sequence, the matrices \mathcal{X} and \mathcal{Y} are deflated by the contribution of the i -th PLS-component. Components are extracted until a certain error criterion is met, which can be formulated e.g. through the norm of the residual response vector or via cross-validation.

Nonlinear PLS in turn relaxes the assumption of a linear relationship between the latent component and the response. This introduces an additional loop into the algorithm for running a Newton-Raphson procedure, which iterates between the current latent component and the response. In the context of PCE the nonlinear relationship between the

$\{\mathbf{t}_i\}_{i=1, \dots, m}$ and the response is a one-dimensional Hermite polynomial expansion. The coefficients of the PLS-driven PCE can be computed simultaneously with the latent variable structure as a byproduct of the PLS algorithm. Ultimately, the nonlinear PCE-driven PLS algorithm, which is detailed in Papaioannou et al. (2018), identifies m latent components. For each component, it returns the direction \mathbf{r}_i and the 1-dimensional PCE along this direction which is defined by its polynomial order q_i and the coefficient vector \mathbf{a}_i . The PLS-PCE reads

$$\hat{Y}_m^{\text{PLS}} = b_0 + \sum_{i=1}^m (\mathbf{a}^i)^T \boldsymbol{\psi}^{q_i} [(\mathbf{r}_i)^T \tilde{\mathbf{X}}], \quad (12)$$

where $b_0 = \widehat{\mathbb{E}}[Y]$, $\boldsymbol{\psi}^{q_i}(\mathbf{X})$ is a vector function assembling the evaluations of the one-dimensional Hermite polynomials up to order q_i and $\tilde{\mathbf{X}} = \mathbf{X} - \boldsymbol{\mu}_{\mathcal{X}}$, where $\boldsymbol{\mu}_{\mathcal{X}}$ is the columnwise sample mean of the training data \mathcal{X} .

3. GLOBAL SENSITIVITY ANALYSIS

3.1. Variance-based sensitivity analysis

The idea behind variance-based sensitivity analysis for model outputs Y is to decompose the response variance $\mathbb{V}[Y]$ into partial variances, that are attributable to variable combinations in the input \mathbf{X} . If X is jointly uniform on $[0, 1]$ and its components are independent, this is accomplished by projecting Y onto a unique, orthogonal basis w.r.t. the uniform joint density (which is generalizable to other standard distribution types through an isoprobabilistic transformation). The representation of Y is then the Sobol'-Hoeffding decomposition (Sobol', 1993), which reads:

$$f(\mathbf{X}) = f_0 + \sum_{i=1}^d f_i(X_i) + \sum_{i=1}^d \sum_{j=i+1}^d f_{ij}(X_i, X_j) + \dots + f_{12\dots d}(\mathbf{X}). \quad (13)$$

Here f_0 is a constant, the f_i are a univariate functions of X_i , the f_{ij} are bivariate functions of X_i and X_j etc.. Each summand in equation (13) represents the influence of a distinct variable subset of \mathbf{X} , $\mathbf{X}_{\mathcal{A}}$ and due to the orthogonality property, the partial variance associated with \mathcal{A} is given immediately by

$\mathbb{V}[f_{\mathcal{A}}]$. The Sobol' index is then the ratio of the partial variance due to $f_{\mathcal{A}}$ and the total variance (Sobol', 1993):

$$S_{Y,\mathcal{A}} = \mathbb{V}[f_{\mathcal{A}}]/\mathbb{V}[Y]. \quad (14)$$

The total-effect index S^T (Homma and Saltelli, 1996) is the ratio of the sum of all partial variances associated with variable combinations of which $\mathbf{X}_{\mathcal{A}}$ is a subset:

$$S_{Y,\mathcal{A}}^T = \sum_{\mathcal{A} \subseteq \mathcal{B}} \mathbb{V}[f_{\mathcal{B}}]/\mathbb{V}[Y]. \quad (15)$$

That is, the Sobol' index measures the influence of a given subset of input variables without considering their interaction with variables outside the subset while the total-effect index takes these interactions into account.

3.2. PCE-based sensitivity analysis

A core feature of representing a response $Y \in \mathcal{H}$ as \hat{Y} with an orthogonal basis of \mathcal{H} lies in the simplicity of finding statistical properties of \hat{Y} and thus - if the model accurately represents Y - approximating statistics of Y . Given the model representation (8) with P terms, e.g. the first two moments can be computed as

$$\mathbb{E}[\hat{Y}] = a_0, \quad \mathbb{V}[\hat{Y}] = \sum_{i=1}^{P-1} a_i^2. \quad (16)$$

Moreover, Sudret (2008) showed that the indices $S_{\hat{Y},\mathcal{A}}$ and $S_{\hat{Y},\mathcal{A}}^T$ of representation (8) can also be found merely by postprocessing its coefficients \mathbf{a} . For a given subset of the input variables denoted by the index set \mathcal{A} , we define a boolean index vector $\mathcal{I}^{\mathcal{A}} \in \{0,1\}^d$ s.t. $\mathcal{I}_i^{\mathcal{A}} = 0$ if $i \notin \mathcal{A}$ and $\mathcal{I}_i^{\mathcal{A}} = 1$ if $i \in \mathcal{A}$. In the same way, we define such an index vector for the j -th row of \mathbf{k}_j s.t. $\mathcal{I}_i^{k_j} = 0$ if $k_{ij} = 0$ and $\mathcal{I}_i^{k_j} = 1$ if $k_{ij} > 0$. Then, the PCE-based sensitivity indices read (Sudret, 2008):

$$\hat{S}_{\hat{Y},\mathcal{A}} = \frac{1}{\mathbb{V}[\hat{Y}]} \sum_{\substack{\mathcal{I}^{\mathcal{A}} = \mathcal{I}^{k_j} \\ 1 \leq j \leq P-1}} a_j^2, \quad \hat{S}_{\hat{Y},\mathcal{A}}^T = \frac{1}{\mathbb{V}[\hat{Y}]} \sum_{\substack{\mathcal{I}^{\mathcal{A}} \subseteq \mathcal{I}^{k_j} \\ 1 \leq j \leq P-1}} a_j^2. \quad (17)$$

4. GLOBAL SENSITIVITY ANALYSIS VIA PLS-PCE

Here we derive expressions for $S_{\hat{Y}}$ and $S_{\hat{Y}}^T$ for \hat{Y} of the form (12). Note, that the sensitivity indices of any latent variable component Z_i can be obtained immediately as

$$S_{\hat{Y}_m^{\text{PLS}},Z_i} = S_{\hat{Y}_m^{\text{PLS}},Z_i}^T = \sum_{j=1}^{q_i} (\mathbf{a}^i)_j^2 / \sum_{i=1}^m \sum_{j=1}^{q_i} (\mathbf{a}^i)_j^2. \quad (18)$$

The partial variances contributed by each of the latent components, which are given in the numerators of equation (18) serve as a measure for the relevance of the respective components of the PLS-transformed random vector \mathbf{Z} . Here, we are interested in computing sensitivities of \hat{Y}_m^{PLS} to the original input vector \mathbf{X} . To this end, we will derive the equivalent standard PCE format of \hat{Y}_m^{PLS} . (Buet-Golfouse, 2015) provide the following multinomial theorem for a normalized probabilist's Hermite polynomial of order k (Theorem 4):

$$\begin{aligned} \psi^j(\mathbf{s}^T \mathbf{X}) &= \sum_{|\mathbf{k}|=j} \sqrt{\frac{j!}{k_1! \cdot k_2! \cdot \dots \cdot k_d!}} \prod_{l=1}^d s_l^{k_l} \psi^l(X_l) \\ &= \sum_{|\mathbf{k}|=j} \sqrt{\frac{j!}{k_1! \cdot k_2! \cdot \dots \cdot k_d!}} \prod_{l=1}^d s_l^{k_l} \Psi_{\mathbf{k}}(\mathbf{X}), \end{aligned} \quad (19)$$

under the condition that $\|\mathbf{s}\|=1$. Within the context of PLS-based PCE, the vector \mathbf{s} is given by a PLS direction \mathbf{r}_i . Asymptotically, the sample mean is zero, i.e.

$$\lim_{N \rightarrow \infty} \boldsymbol{\mu}_{\mathcal{X}} = \mathbf{0}$$

and Papaioannou et al. (2018) prove that

$$\lim_{N \rightarrow \infty} \|\mathbf{r}_i\| = 1 \quad i = 2, \dots, m,$$

while $\|\mathbf{r}_1\|=1$ always. That is, in the asymptotic limit we can use identity (19) to write

$$\hat{Y}_m^{\text{PLS}} = b_0 + \sum_{i=1}^m \sum_{|\mathbf{k}| \leq q_i} \mathbf{a}_{|\mathbf{k}|}^i \sqrt{|\mathbf{k}|!} \frac{r_{i1}^{k_1} \cdot r_{i2}^{k_2} \cdot \dots \cdot r_{id}^{k_d}}{\sqrt{k_1! \cdot k_2! \cdot \dots \cdot k_d!}} \Psi_{\mathbf{k}}(\mathbf{X}). \quad (20)$$

In practice, the sample mean decays towards 0 relatively fast, such that the approximation error introduced by neglecting the variable centering in equation (20) is typically orders of magnitude smaller than the leading error introduced by the surrogate model itself. The error due to $\|\mathbf{r}_i\| \neq 1$ grows with the number of included components m (with $m = 1$, the representation is exact since $\|\mathbf{r}_1\| = 1$ always). It is possible to derive exact expressions with respect to both non-zero sample mean and non-unit-length component directions based on expanding the Hermite polynomials into a suitable Taylor series and applying a well-known product theorem for Hermite polynomials of scaled variables. Equation (20) is merely a linear combination of m standard PCEs each representing a latent component in standard PCE format such that we can write

$$\hat{Y}_m^{\text{PLS}} = b_0 + \sum_{|\mathbf{k}| \leq q_{\max}} c_{\mathbf{k}} \Psi_{\mathbf{k}}(\mathbf{X}), \quad (21)$$

where

$$q_{\max} = \max_{i \in \{1, \dots, m\}} (q_i). \quad (22)$$

The equivalent PCE coefficients \mathbf{c} then read

$$c_{\mathbf{k}} = \sum_{i=1}^m a_{|\mathbf{k}|}^i \sqrt{|\mathbf{k}|!} \prod_{l=1}^d \frac{r_{il}^{k_l}}{\sqrt{k_l!}}, \quad (23)$$

where $\{a_{|\mathbf{k}|}^i : q_i < |\mathbf{k}|\} = 0$. Thus, we can apply the standard post-processing defined by equations (17) to format (21) in order to obtain variance-based sensitivity indices as a function of the \mathbf{a}^i and \mathbf{r}_i only. We observe that the index set \mathbf{k} required for the PLS-PCE-based sensitivity indices is equivalent to that of a full PCE formulation of maximum polynomial order q_{\max} . Typically, the additional degrees of freedom emerging from the latent variable formulation (i.e. the \mathbf{r}_i) lead to significantly smaller required polynomial degrees in PLS-PCE compared to sparse and classical PCE models. That is, the computational bottleneck of computing \mathbf{k} can be relaxed significantly in most applications. Note, that the presented procedure can be extended to multivariate output straight-forwardly based on a similar formulation in combination with the PLS2 algorithm.

In the following, we demonstrate the new sensitivity indices by means of a numerical experiment.

5. NUMERICAL EXPERIMENT

We consider an elastic truss, which consists of 23 rods, where horizontal and diagonal rods have cross-sections A_1 , A_2 and Young's moduli E_1 , E_2 , respectively (Lee and Kwak, 2006). The truss sustains 6 vertical point loads $P_1 - P_6$. It is depicted in Figure 1 and the input variable definitions are provided in Table (1).

We compute Sobol' and total-effect indices

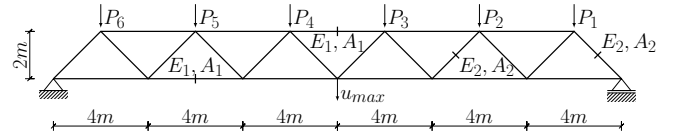


Figure 1: 2-D truss example.

Table 1: Input variable definitions of the truss example.

Random Variable	Distribution	Mean	Standard deviation
A_1 [m^2]	Log-Normal	$2 \cdot 10^{-3}$	$2 \cdot 10^{-4}$
A_2 [m^2]	Log-Normal	$1 \cdot 10^{-3}$	$1 \cdot 10^{-4}$
E_1, E_2 [Pa]	Log-Normal	$2.1 \cdot 10^{11}$	$2.1 \cdot 10^{10}$
$P_1 - P_6$ [N]	Gumbel	$5.0 \cdot 10^4$	$7.5 \cdot 10^4$

for the maximum truss deflection u_{\max} . Reference solutions are obtained via direct Monte Carlo (DMC) and with the estimators proposed in (Saltelli et al., 2010) using 10^6 independent samples (Figure 2). Moreover, we repeat the analysis 50 times to find the mean relative error (Figure 3) and its standard deviation (Figure 4), where the relative error for a quantity Q is defined as:

$$\epsilon_Q = \frac{|Q - Q_{\text{DMC}}|}{Q_{\text{DMC}}}. \quad (24)$$

The PLS-PCE-based sensitivities are compared both to the reference solution and results from two conventional polynomial basis surrogate models (sparse PCE according to Blatman and Sudret (2011) and low-rank approximations (LRA) according to Konakli and Sudret (2016)). Figure 2 indicates good agreement of the PLS-PCE-based

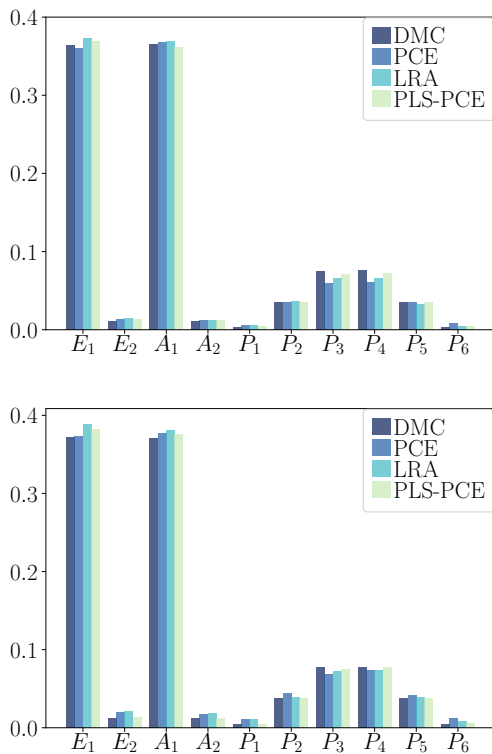


Figure 2: Sobol' (left) and total-effect (right) indices of u_{max} obtained with $N = 2^5$ model evaluations.

sensitivities with the reference solution. Figure 3 shows all three surrogate-based sensitivity indices are estimated with similar mean relative error and convergence rate as N increases. Nevertheless, the proposed PLS-PCE-based approach leads to smaller errors compared to the other surrogate approaches in small sample sizes. Figure 4 indicates the same for the relative error variance.

6. CONCLUSION

This paper facilitates the computation of variance-based sensitivity indices from PLS-PCE surrogate models without requiring any additional original or surrogate model evaluations. A multinomial theorem for Hermite polynomials is applied to derive expressions for the sensitivity measures of the PLS-PCE model based on the model coefficients in an approximate way. Asymptotically, i.e. with the number of samples $N \rightarrow \infty$, the presented estimates for the Sobol' and the total-effect indices are exact. The sensitivities have been computed for an elastic truss model and match the DMC-based reference solution up to relative errors of $\approx 1\%$. The

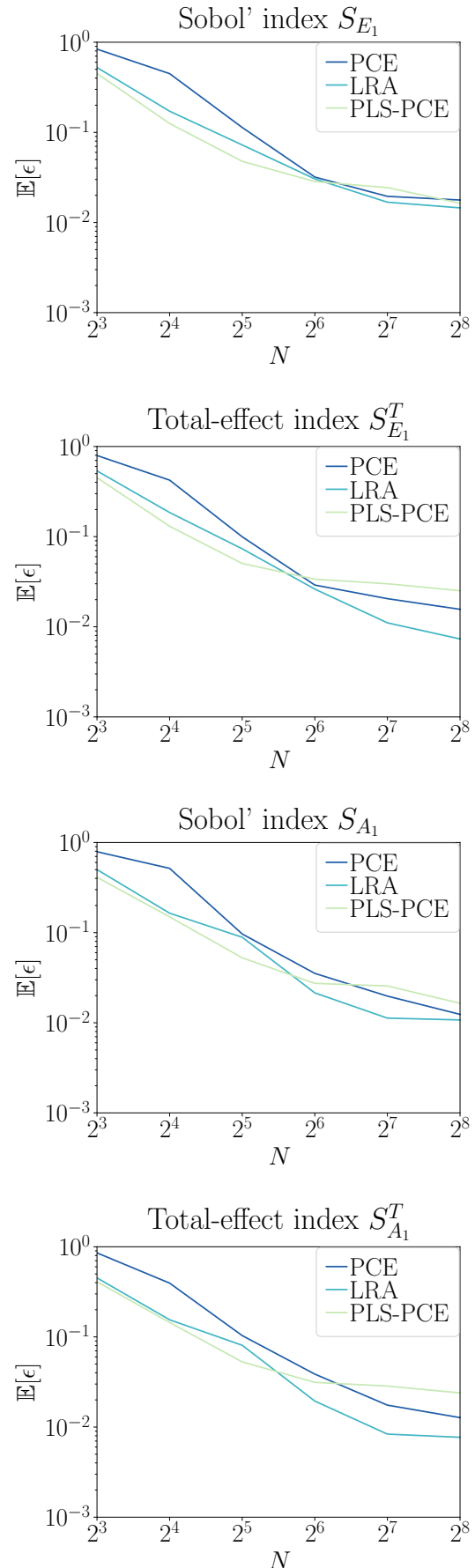


Figure 3: Mean relative errors for the two most influential inputs E_1 and A_1 , computed with sparse PCE, LRA and PLS-PCE.

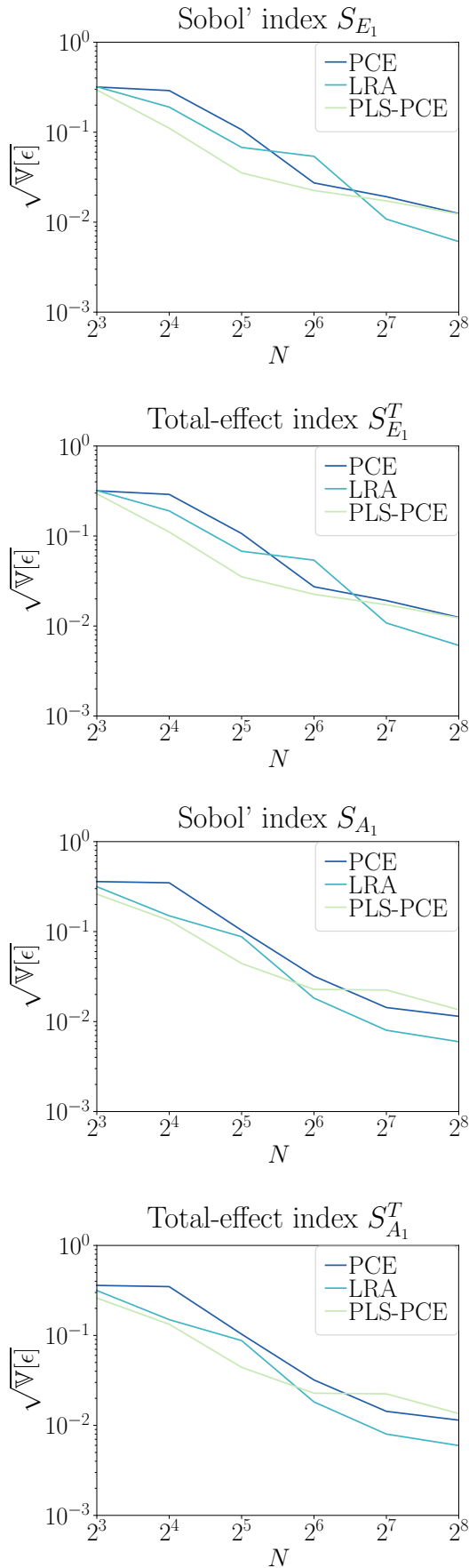


Figure 4: Relative error standard deviation for the two most influential inputs E_1 and A_1 , computed with sparse PCE, LRA and PLS-PCE.

results were compared with the ones obtained with sparse PCE and LRA surrogates and the proposed approach led to smaller relative errors at small sample sizes. In a future work, we plan to extend the formulation to yield exact estimators for the non-asymptotic case with non-zero input sample mean and non-normal basis vectors defining the latent components, i.e. for the case where $\mu_X = 0$ and $\|\mathbf{r}_i\| \neq 1$.

7. ACKNOWLEDGMENT

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