# Effective Design for Sobol Indices Estimation Based on Polynomial Chaos Expansions

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**Abstract.** Sobol' indices are a common metric of dependency in sensitivity analysis. It is used as a measure of confidence of input variables influence on the output of the analyzed mathematical model. We consider a problem of selection of experimental design points for Sobol' indices estimation. Based on the concept of $D$-optimality, we propose a method for constructing an adaptive design of experiments, effective for the calculation of Sobol' indices from Polynomial Chaos Expansions. We provide a set of applications that demonstrate the efficiency of the proposed approach.

**Keywords:** Design of experiment · Sensitivity analysis · Sobol indices · Polynomial chaos expansions · Active learning

## 1 Introduction

Computational models play an important role in different areas of human activity [1–3]. Over the past decades, they have become more complex, and there is an increasing need for special methods for the analysis of computational models. *Sensitivity analysis* is an important tool for investigation of computational models.

*Sensitivity analysis* tries to find how different model input parameters influence the model output, what are the most influential parameters and how to evaluate such effects quantitatively [4]. Sensitivity analysis allows to better understand the behavior of computational models. Particularly, it allows us to separate all input parameters into *important (significant)*, *relatively important* and *unimportant (nonsignificant)* ones. Important parameters, *i.e.* parameters whose variability has a strong effect on the model output, need to be controlled more accurately. Complex computational models often suffer from over-parameterization. By excluding unimportant parameters, we can potentially improve model quality, reduce parametrization (which is of great interest in the field of meta-modeling) and computational costs [26].

Sensitivity analysis includes a wide range of metrics and techniques *e.g.* the Morris method [5], linear regression-based methods [6], variance-based methods [7]. Among others, *Sobol' (sensitivity) indices* are a common metric to evaluate the influence of model parameters [10]. Sobol' indices describe the portion of the output variance explained by different input parameters and combinations thereof. This method is especially useful for the case of nonlinear computational models [11].

There are two main approaches to evaluation of Sobol' indices. *Monte Carlo approach* (Monte Carlo simulation, FAST [12], SPF scheme [13] and others) is relatively robust [8], but requires large number of model runs, typically in the order of $10^4$ for an accurate estimation of each index. Thus, it is impractical for a number of industrial applications, where each model evaluation is computationally costly.

*Metamodeling approaches* for Sobol' indices estimation allows one to reduce the necessary number of model runs [6,9]. Following this approach, we replace the original computational model by an approximating *metamodel* (also known as *surrogate model* or *response surface*) which is computationally efficient and has a clear internal structure [26]. The approach consists of the following general steps: selection of *the design of experiment (DoE)* and generation of *the training sample set*, construction of the metamodel based on the training samples, including quality assessment and evaluation of Sobol' indices (or any other measure) using the constructed metamodel. Note that the evaluation of indices may be either based on known internal structure of the metamodel or via Monte Carlo simulation on the metamodel itself.

In general, a metamodeling approach is more computationally efficient than a crude Monte Carlo approach, since the cost (in terms of the number of runs of the costly computational model) reduces to that of the training set (in general, a few dozens to a few hundreds). However, this approach may be nonrobust and its accuracy is more difficult for analysis. Indeed, although procedures like *cross-validation* [14,26] allow to estimate the quality of metamodels, the accuracy of complex statistics (*e.g.* Sobol' indices), derived from metamodels, has a complicated dependency on the metamodels structure and quality (see *e.g.* confidence intervals for Sobol' indices estimates [15] in case of Gaussian Processes metamodel [16–18] and bootstrap-based confidence intervals in case of polynomial chaos expansions [19]).

In this paper, we consider a problem of a design construction for a particular metamodeling approach: how to select the experimental design for building a polynomial chaos expansion for further evaluation of Sobol' indices, that is effective in terms of the number of computational model runs?

Space-filling designs are commonly used for sensitivity analysis. Methods like Monte Carlo sampling, *Latin Hypercube Sampling (LHS)* [20] or sampling in FAST method [12] try to fill "uniformly" the input parameters space with *design points* (*point*s are some realizations of parameters values). These sampling methods are *model free*, as they make no assumptions on the computational model.

In order to speed up the convergence of indices estimates, we assume that the computational model is close to its approximating metamodel and exploit knowledge of the metamodel structure. In this paper, we consider *Polynomial Chaos Expansions (PCE)* as a metamodel that is commonly used in engineering and other applications [21]. PCE approximation is based on a series of polynomials (Hermite, Legendre, Laguerre etc.) that are orthogonal w.r.t. the probability distributions of corresponding input parameters of the computational model. It allows to calculate Sobol' indices analytically from the expansion coefficients [22, 23].

In this paper, we address the problem of design of experiments construction for evaluating Sobol' indices from a PCE metamodel. Based on asymptotic considerations, we propose an adaptive algorithm for design and test it on a set of applied problems. Note that in [33], we investigated the adaptive design algorithm for the case of a quadratic metamodel (see also [34]). In this paper, we extend the results for the case of a generalized PCE metamodel and provide more examples, including real industrial applications.

The paper is organized as follows: in Sect. 2, we review the definition of sensitivity indices and describe their estimation based on PCE metamodels. In Sect. 3, asymptotic behavior of indices estimates is obtained. In Sect. 4, we introduce an optimality criterion and propose a procedure for constructing the experimental design. In Sect. 5, we provide experimental results, applications and benchmark with other methods of design construction.

## 2 Sensitivity Indices and PCE Metamodels

### 2.1 Sensitivity Indices

Consider a computational model $y = f(\mathbf{x})$, where $\mathbf{x} = (x_1, \ldots, x_d) \in \mathscr{X} \subset \mathbb{R}^d$ is a vector of *input variables* (or *parameters* or *features*), $y \in \mathbb{R}^1$ is an *output variable* and $\mathscr{X}$ is *a design space*. The model $f(\mathbf{x})$ describes the behavior of some physical system of interest.

We consider the model $f(\mathbf{x})$ as a black-box: no additional knowledge on its inner structure is assumed. For the selected *design of experiments* $X = \{\mathbf{x}_i \in \mathscr{X}\}_{i=1}^n \in \mathbb{R}^{n \times d}$ we can obtain a set of model responses and form *a training sample*

$$L = \{\mathbf{x}_i, y_i = f(\mathbf{x}_i)\}_{i=1}^n \triangleq \{X \in \mathbb{R}^{n \times d}, Y = f(X) \in \mathbb{R}^n\}, \tag{1}$$

which allows us to investigate properties of the computational model.

Assume there is a prescribed probability distribution $\mathscr{H}$ with independent marginal distributions on the design space $\mathscr{X}$ ($\mathscr{H} = \mathscr{H}_1 \times \ldots \times \mathscr{H}_d$). This distribution represents the uncertainty and/or variability of the input variables, modelled as a random vector $\boldsymbol{X} = \{X_1, \ldots, X_d\}$ with independent components. In these settings, the model output becomes stochastic variable $\boldsymbol{Y} = f(\boldsymbol{X})$.

Assuming that the function $f(\boldsymbol{X})$ is square-integrable with respect to distribution $\mathscr{H}$ (*i.e.* $\mathbb{E}[f^2(\boldsymbol{X})] < +\infty$)), we have the following unique Sobol' decomposition of $\boldsymbol{Y} = f(\boldsymbol{X})$ [10] given by

$$f(\boldsymbol{X}) = f_0 + \sum_{i=1}^{d} f_i(X_i) + \sum_{1 \le i \le j \le d} f_{ij}(X_i, X_j) + \ldots + f_{1\ldots d}(X_1, \ldots, X_d),$$

which satisfies:

$$\mathbb{E}[f_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}}) f_{\mathbf{v}}(\boldsymbol{X}_{\mathbf{v}})] = 0, \text{ if } \mathbf{u} \ne \mathbf{v},$$

where $\mathbf{u}$ and $\mathbf{v}$ are index sets: $\mathbf{u}, \mathbf{v} \subset \{1, 2, \ldots, d\}$.

Due to orthogonality of the summands, we can decompose the variance of the model output:

$$D = \mathbb{V}[f(\boldsymbol{X})] = \sum_{\substack{\mathbf{u} \subset \{1,\ldots,d\}, \\ \mathbf{u} \ne \mathbf{0}}} \mathbb{V}[f_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})] = \sum_{\substack{\mathbf{u} \subset \{1,\ldots,d\}, \\ \mathbf{u} \ne \mathbf{0}}} D_{\mathbf{u}},$$

In this expansion $D_{\mathbf{u}} \triangleq \mathbb{V}[f_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})]$ is the contribution of summand $f_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})$ to the output variance, also known as *partial variance*.

**Definition 1.** *The sensitivity index (Sobol' index) of variable set $\boldsymbol{X}_{\mathbf{u}}$, $\mathbf{u} \subset \{1, \ldots, d\}$ is defined as*

$$S_{\mathbf{u}} = \frac{D_{\mathbf{u}}}{D}. \tag{2}$$

The sensitivity index describes the amount of the total variance explained by the uncertainties in the subset of model input variables $\boldsymbol{X}_{\mathbf{u}}$.

*Remark 1.* In this paper, we consider only sensitivity indices of type $S_i \triangleq S_{\{i\}}, i = 1, \ldots, d$, called *first-order* or *main effect sensitivity indices*.

## 2.2   Polynomial Chaos Expansions

Consider a set of multivariate polynomials $\{\Psi_{\boldsymbol{\alpha}}(\boldsymbol{X}), \ \boldsymbol{\alpha} \in \mathscr{L}\}$ that consists of polynomials $\Psi_{\boldsymbol{\alpha}}$ having the form of tensor product

$$\Psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) = \prod_{i=1}^{d} \psi_{\alpha_i}^{(i)}(X_i), \ \boldsymbol{\alpha} = \{\alpha_i \in \mathbb{N}, \ i = 1, \ldots, d\} \in \mathscr{L},$$

where $\psi_{\alpha_i}^{(i)}$ is a univariate polynomial of degree $\alpha_i$ belonging $i$-th family (*e.g.* Legendre polynomials, Jacobi polynomials, etc.), $\mathbb{N} = \{0, 1, 2, \ldots\}$ is the set of nonnegative integers, $\mathscr{L}$ is some fixed set of multi-indices $\boldsymbol{\alpha}$.

Suppose that univariate polynomials $\{\psi_{\alpha}^{(i)}\}$ are orthogonal w.r.t. $i$-th marginal of the probability distribution $\mathscr{H}$, *i.e.* $\mathbb{E}[\psi_{\alpha}^{(i)}(X_i)\psi_{\beta}^{(i)}(X_i)] = 0$ if $\alpha \ne \beta$ for $i = 1, \ldots, d$. Particularly, Legendre polynomials are orthogonal w.r.t. standard uniform distribution; Hermite polynomials are orthogonal w.r.t. Gaussian distribution. Due to independence of $\boldsymbol{X}$'s components, we obtain that multivariate polynomials $\{\Psi_{\boldsymbol{\alpha}}\}$ are orthogonal w.r.t. the probability distribution $\mathscr{H}$ *i.e.* $\mathbb{E}[\Psi_{\boldsymbol{\alpha}}(\boldsymbol{X})\Psi_{\boldsymbol{\beta}}(\boldsymbol{X})] = 0$ if $\boldsymbol{\alpha} \ne \boldsymbol{\beta}$.

Provided $\mathbb{E}[f^2(\boldsymbol{X})] < +\infty$, the spectral polynomial chaos expansion of $f$ reads

$$f(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^d} c_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{X}), \tag{3}$$

where $\{c_{\boldsymbol{\alpha}}\}$ are coefficients.

In the sequel we consider a PCE approximation $f_{PC}(\boldsymbol{X})$ of the model $f(\boldsymbol{X})$ obtained by truncating the infinite series to a finite number of terms:

$$\hat{y} = f_{PC}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha} \in \mathscr{L}} c_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{X}). \tag{4}$$

By enumerating the elements of $\mathscr{L}$ we will also use the alternative form of (4):

$$\hat{y} = f_{PC}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha} \in \mathscr{L}} c_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) \triangleq \sum_{j=0}^{P-1} c_j \Psi_j(\boldsymbol{X}) = \mathbf{c}^T \boldsymbol{\Psi}(\boldsymbol{X}), \ \ P \triangleq |\mathscr{L}|,$$

where $\mathbf{c} = (c_0, \ldots, c_{P-1})^T$ is a column vector of coefficients and $\boldsymbol{\Psi}(\mathbf{x})\colon \mathbb{R}^d \to \mathbb{R}^P$ is a mapping from the design space to *the extended design space* defined as a column vector function $\boldsymbol{\Psi}(\mathbf{x}) = (\Psi_0(\mathbf{x}), \ldots, \Psi_{P-1}(\mathbf{x}))^T$. Note that index $j = 0$ corresponds to multi-index $\boldsymbol{\alpha} = \mathbf{0} = \{0, \ldots, 0\}$ *i.e.*

$$c_{j=0} \triangleq c_{\boldsymbol{\alpha}=\mathbf{0}}, \ \Psi_{j=0} \triangleq \Psi_{\boldsymbol{\alpha}=\mathbf{0}} = const.$$

The set of multi-indices $\mathscr{L}$ is determined by *the truncation scheme*. In this work, we use hyperbolic truncation scheme [24], which corresponds to

$$\mathscr{L} = \{\boldsymbol{\alpha} \in \mathbb{N}^d : \|\boldsymbol{\alpha}\|_q \ \le p\}, \ \|\boldsymbol{\alpha}\|_q \triangleq \left( \sum_{i=1}^{d} \alpha_i^q \right)^{1/q},$$

where $q \in (0, 1]$ is a fixed parameter and $p \in \mathbb{N} \backslash \{0\} = \{1, 2, 3, \ldots\}$ is a fixed maximal total degree of polynomials. Note that in case of $q = 1$, we have $P = \frac{(d+p)!}{d!p!}$ polynomials in $\mathscr{L}$ and smaller $q$ leads to a smaller number of polynomials.

There is a number of strategies for calculating the expansion coefficients $c_{\boldsymbol{\alpha}}$ in (4). In this paper, *the least-square (LS)* minimization method is used [25]. Expansion coefficients are calculated via minimization of the approximation error on the training sample $L = \{\mathbf{x}_i, y_i = f(\mathbf{x}_i)\}_{i=1}^{n}$:

$$\hat{\mathbf{c}}_{LS} = \arg \min_{\mathbf{c} \in \mathbb{R}^P} \frac{1}{n} \sum_{i=1}^{n} \left[ y_i - \mathbf{c}^T \boldsymbol{\Psi}(\mathbf{x}_i) \right]^2. \tag{5}$$

### 2.3   PCE Post-processing for Sensitivity Analysis

Consider a PCE model $f_{PC}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha} \in \mathscr{L}} c_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) = \sum_{j=0}^{P-1} c_j \Psi_j(\boldsymbol{X})$. According to [22], we have an explicit form of Sobol' indices (main effects) for model $f_{PC}(\boldsymbol{X})$:

$$S_i(\mathbf{c}) = \frac{\sum_{\boldsymbol{\alpha} \in \mathscr{L}_i} c_{\boldsymbol{\alpha}}^2 \mathbb{E}[\Psi_{\boldsymbol{\alpha}}^2(\boldsymbol{X})]}{\sum_{\boldsymbol{\alpha} \in \mathscr{L}_*} c_{\boldsymbol{\alpha}}^2 \mathbb{E}[\Psi_{\boldsymbol{\alpha}}^2(\boldsymbol{X})]}, \ i = 1, \ldots, d, \tag{6}$$

where $\mathscr{L}_* \triangleq \mathscr{L}\backslash\{\mathbf{0}\}$ and $\mathscr{L}_i \subset \mathscr{L}$ is the set of multi-indices $\boldsymbol{\alpha}$ such that only the index on the $i$-th position is nonzero: $\boldsymbol{\alpha} = \{0,\ldots,\alpha_i,\ldots,0\}$, $\alpha_i \in \mathbb{N}$, $\alpha_i > 0$.

Suppose for simplicity that the multivariate polynomials $\{\Psi_{\boldsymbol{\alpha}}(\boldsymbol{X}),\ \boldsymbol{\alpha} \in \mathscr{L}\}$ are not only orthogonal but also normalized w.r.t. distribution $\mathscr{H}$:

$$\mathbb{E}[\Psi_{\boldsymbol{\alpha}}(\boldsymbol{X})\Psi_{\boldsymbol{\beta}}(\boldsymbol{X})] = \delta_{\boldsymbol{\alpha}\boldsymbol{\beta}}, \tag{7}$$

where $\delta_{\boldsymbol{\alpha}\boldsymbol{\beta}}$ is the Kronecker symbol, *i.e.* $\delta_{\boldsymbol{\alpha}\boldsymbol{\beta}} = 1$ if $\boldsymbol{\alpha} = \boldsymbol{\beta}$, otherwise $\delta_{\boldsymbol{\alpha}\boldsymbol{\beta}} = 0$. Then (6) takes the form

$$S_i(\mathbf{c}) = \frac{\sum_{\boldsymbol{\alpha}\in\mathscr{L}_i} c_{\boldsymbol{\alpha}}^2}{\sum_{\boldsymbol{\alpha}\in\mathscr{L}_*} c_{\boldsymbol{\alpha}}^2},\ i = 1,\ldots,d. \tag{8}$$

Thus, (8) gives a simple expression for the calculation of Sobol' indices for PCE metamodels. If the original model of interest $f(\boldsymbol{X})$ is close to its PCE approximation $f_{PC}(\boldsymbol{X})$, then we can use the expression for indices (8) with estimated coefficients (5) to approximate Sobol' indices of the original model:

$$\hat{S}_i = S_i(\hat{\mathbf{c}}) = \frac{\sum_{\boldsymbol{\alpha}\in\mathscr{L}_i} \hat{c}_{\boldsymbol{\alpha}}^2}{\sum_{\boldsymbol{\alpha}\in\mathscr{L}_*} \hat{c}_{\boldsymbol{\alpha}}^2},\ i = 1,\ldots,d, \tag{9}$$

where $\hat{\mathbf{c}} \triangleq \hat{\mathbf{c}}_{LS}$.

## 3   Asymptotic Properties

In this section, we consider asymptotic properties of the indices estimates in Eq. (9) if the coefficients (5) are estimated on noisy data. Unlike (3), the original model is supposed to be the truncated PC with Gaussian noise:

$$f(\mathbf{x}) = f_{PC}(\mathbf{x}) + \varepsilon = \sum_{j=0}^{P-1} c_j \Psi_j(\mathbf{x}) + \varepsilon = \mathbf{c}^T \boldsymbol{\Psi}(\mathbf{x}) + \varepsilon, \tag{10}$$

where $\varepsilon \sim N(0,\sigma^2)$ is i.i.d. Gaussian noise. Let $\hat{\mathbf{c}}_n$ be the LS estimate (5) of the true coefficients vector $\mathbf{c}$ based on the training sample $L = \{\mathbf{x}_i, y_i = f(\mathbf{x}_i)\}_{i=1}^n$. In this section and further, if some variable has index $n$, then this variable depends on the training sample (1) of size $n$; and all expectations and variances are w.r.t. Gaussian noise.

Define *information matrix* $A_n \in \mathbb{R}^{P\times P}$ as

$$A_n = \sum_{i=1}^n \boldsymbol{\Psi}(\mathbf{x}_i)\boldsymbol{\Psi}^T(\mathbf{x}_i), \tag{11}$$

and assume that $A_n$ is not degenerate, *i.e.* $\det A_n \neq 0$. Then, using standard results for linear regression coefficients [26,27], we have

$$\mathbb{E}_{\varepsilon}[\hat{\mathbf{c}}_n] = \mathbf{c},\ \mathbb{V}_{\varepsilon}[\hat{\mathbf{c}}_n] = \sigma^2 A_n^{-1}$$

and
$$\hat{\mathbf{c}}_n - \mathbf{c} \sim \mathcal{N}(0, \ \sigma^2 A_n^{-1}). \tag{12}$$

The following theorem allows to establish asymptotic properties of the indices estimate based on the model (10) while new examples are added to the training sample.

**Theorem 1.** *1. Let us assume that there is an infinite sequence of points in the design space $\{\mathbf{x}_i \in \mathcal{X}\}_{i=1}^{\infty}$, such that*

$$\frac{1}{n} A_n = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{\Psi}(\mathbf{x}_i) \boldsymbol{\Psi}^T(\mathbf{x}_i) \underset{n \to +\infty}{\longrightarrow} \Sigma, \tag{13}$$

*where $\Sigma \in \mathbb{R}^{P \times P}$: $\Sigma = \Sigma^T$, $\det \Sigma > 0$, and new design points be added successively from this sequence to the design of experiments $X_n = \{\mathbf{x}_i\}_{i=1}^n$.*
*2. Let the sensitivity indices vector-function be defined by its components (8):*

$$\mathbf{S}(\boldsymbol{\nu}) = (S_1(\boldsymbol{\nu}), \dots, S_d(\boldsymbol{\nu}))^T$$

*and $\hat{\mathbf{S}}_n \triangleq \mathbf{S}(\hat{\mathbf{c}}_n)$, where $\hat{\mathbf{c}}_n$ is defined by (5).*
*3. Assume that for the true coefficients $\mathbf{c}$ of the model (10):*

$$\det(B \Sigma^{-1} B^T) \neq 0, \tag{14}$$

*where $B$ is the matrix of partial derivatives defined as*

$$B \triangleq B(\mathbf{c}) = \left. \frac{\partial \mathbf{S}(\boldsymbol{\nu})}{\partial \boldsymbol{\nu}} \right|_{\boldsymbol{\nu} = \mathbf{c}} \in \mathbb{R}^{d \times P} \tag{15}$$

*then*

$$\sqrt{n} \left( \mathbf{S}(\hat{\mathbf{c}}_n) - \mathbf{S}(\mathbf{c}) \right) \underset{n \to +\infty}{\overset{\mathfrak{D}}{\longrightarrow}} \mathcal{N}(0, \sigma^2 B \Sigma^{-1} B^T). \tag{16}$$

*Proof*

1. Condition (13) implies that $\det A_n \neq 0$ starting from some $n_0$. Therefore, (12) holds true for $n \geq n_0$. Now, consider only $n \geq n_0$.
2. From (12) and (13) we have

$$\sqrt{n}(\hat{\mathbf{c}}_n - \mathbf{c}) \sim \mathcal{N}(0, \ \sigma^2 (A_n/n)^{-1}) \underset{n \to +\infty}{\overset{\mathfrak{D}}{\longrightarrow}} \mathcal{N}(0, \ \sigma^2 \Sigma^{-1}).$$

3. Applying $\delta$-method [28] on vector-function $\mathbf{S}(\boldsymbol{\nu})$ at point $\boldsymbol{\nu} = \mathbf{c}$, we obtain required expression (16).

*Remark 2.* Note that the elements of $B$ have the following form

$$b_{i\boldsymbol{\beta}} \triangleq \frac{\partial S_i}{\partial c_{\boldsymbol{\beta}}} = \begin{cases} \frac{2c_{\boldsymbol{\beta}} \sum_{\boldsymbol{\alpha} \in \mathscr{L}_*} c_{\boldsymbol{\alpha}}^2 - 2c_{\boldsymbol{\beta}} \sum_{\boldsymbol{\alpha} \in \mathscr{L}_i} c_{\boldsymbol{\alpha}}^2}{\left( \sum_{\boldsymbol{\alpha} \in \mathscr{L}_*} c_{\boldsymbol{\alpha}}^2 \right)^2}, & \text{if } \boldsymbol{\beta} \in \mathscr{L}_i, \\ 0, & \text{if } \boldsymbol{\beta} = \mathbf{0} \triangleq \{0, \dots, 0\}, \\ \frac{-2c_{\boldsymbol{\beta}} \sum_{\boldsymbol{\alpha} \in \mathscr{L}_i} c_{\boldsymbol{\alpha}}^2}{\left( \sum_{\boldsymbol{\alpha} \in \mathscr{L}_*} c_{\boldsymbol{\alpha}}^2 \right)^2}, & \text{if } \boldsymbol{\beta} \notin \mathscr{L}_i \cup \mathbf{0}, \end{cases} \tag{17}$$

where $i = 1, \ldots, d$ and multi-index $\boldsymbol{\beta} \in \mathscr{L}$. The elements of $B$ can be also represented as

$$b_{i\boldsymbol{\beta}} \triangleq \frac{\partial S_i}{\partial c_{\boldsymbol{\beta}}} = \frac{-2c_{\boldsymbol{\beta}}}{\sum_{\boldsymbol{\alpha} \in \mathscr{L}_*} c_{\boldsymbol{\alpha}}^2} \times \begin{cases} S_i - 1, & \text{if } \boldsymbol{\beta} \in \mathscr{L}_i, \\ 0, & \text{if } \boldsymbol{\beta} = \mathbf{0} \triangleq \{0, \ldots, 0\}, \\ S_i, & \text{if } \boldsymbol{\beta} \notin \mathscr{L}_i \cup \mathbf{0}, \end{cases} \qquad (18)$$

*Remark 3.* We can see that the theorem conditions do not depend on the type of orthonormal polynomials.

## 4   Design of Experiments Construction

### 4.1   Preliminary Considerations

Taking into account the results of Theorem 1, the limiting covariance matrix of the indices estimates depends on

1. Noise variance $\sigma^2$,
2. True values of PC coefficients $\mathbf{c}$, defining $B$,
3. Experimental design $X$, defining $\Sigma$.

   If we have a sufficiently accurate approximation of the original model, then in the above assumptions, the asymptotic formula (16) allows to evaluate the quality of the experimental design. Indeed, generally speaking the smaller the norm of the covariance matrix $\|\sigma^2 B \Sigma^{-1} B^T\|$, the better the estimation of the sensitivity indices. Theoretically, we could use this formula for constructing an experimental design that is effective for calculating Sobol' indices: we could select designs that minimize the norm of the covariance matrix. However, there are some problems when proceeding this way:

– The first one relates to the selection of the specific functional for minimization. Informally speaking, we need to choose "the norm" associated with the limiting covariance matrix.
– The second one refers to the fact that we do not know the true values of the PC model coefficients, defining $B$; therefore, we will not be able to accurately evaluate the quality of the design.

   The first problem can be solved in different ways. A number of statistical criteria for design optimality ($D$-, $I$-optimality and others, see [29]) are known. Similar to the work [33], we use the $D$-optimality criterion, as it a provides computationally efficient procedure for design construction. $D$-optimal experimental design minimizes the determinant of the limiting covariance matrix. If the vector of the estimated parameters is normally distributed then $D$-optimal design allows to minimize the volume of the confidence region for this vector.

   The second problem is more complex. The optimal design for estimating sensitivity indices that minimizes the norm of limiting covariance matrix depends on the true values of the indices, so it can be constructed only if these true values are known. However, in this case design construction makes no sense.

The dependency of the optimal design for indices evaluation on the true model parameters is a consequence of the nonlinearity of the indices estimates w.r.t. the PC model coefficients. In order to underline this dependency, the term "*locally D*-optimal design" is commonly used [30]. In these settings, there are several approaches, which are usually associated with either some assumptions about the unknown parameters, or adaptive design construction [30]. We use the latter approach.

In the case of adaptive designs, new design points are generated sequentially based on current estimate of the unknown parameters. This allows to avoid a priori assumptions on these parameters. However, this approach has a problem with a confidence of the solution found: if at some step of design construction parameters estimates are significantly different from their true values, then the design, which is constructed based on these estimates, may lead to new parameters estimates, which are also different from the true values.

In practice, during the construction of adaptive design, the quality of the approximation model and assumptions on non-degeneracy of results can be checked at each iteration and one can control and adjust the adaptive strategy.

### 4.2   Adaptive Algorithm

In this section, we introduce the adaptive algorithm for constructing a design of experiments that is effective to estimate sensitivity indices based on the asymptotic $D$-optimality criterion (see the algorithm scheme and Fig. 1). As it was discussed, the main idea of the algorithm is to minimize the confidence region for indices estimates. At each iteration, we replace the limiting covariance matrix by its approximation based on the current PC coefficients estimates.

As for initialization, we suppose that there is some *initial design*, and we require that this initial design is non-degenerate, *i.e.* such that the initial information matrix $A_0$ is nonsingular (det $A_0 \neq 0$). In addition, at each iteration the non-degeneracy of the matrix $B_i A_i^{-1} B_i^T$, related to the criterion to be minimized, is checked.
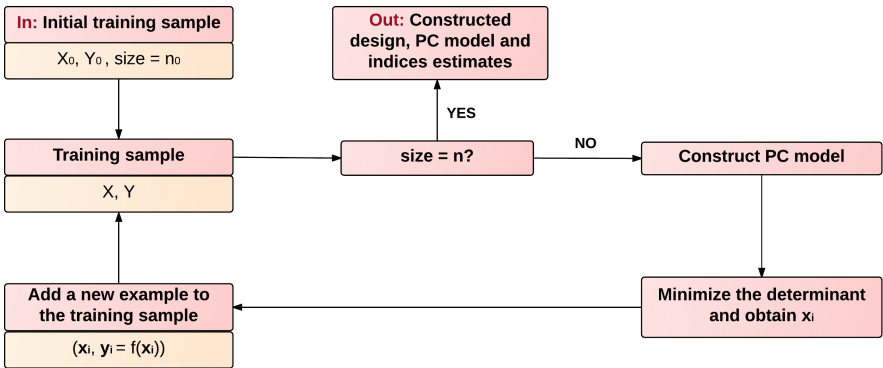


**Fig. 1.** Adaptive algorithm for constructing an effective experimental design to evaluate PC-based Sobol' indices

**Goal:** Construct an effective experimental design for the calculation of sensitivity indices

**Parameters:** initial and final numbers of points $n_0$ and $n$ in the design; set of candidate design points $\Xi$.

**Initialization:**

– initial training sample $\{X_0, Y_0\}$ of size $n_0$, where design $X_0 = \{\mathbf{x}_i\}_{i=1}^{n_0} \subset \Xi$ defines a non-degenerate information matrix $A_0 = \sum_{i=1}^{n_0} \boldsymbol{\Psi}(\mathbf{x}_i)\boldsymbol{\Psi}^T(\mathbf{x}_i)$;
– $B_0 = B(\hat{\mathbf{c}}_0)$, obtained using the initial estimates of the coefficients of PC model, see (15), (17), (18);

**Iterations:** for all $i$ from 1 to $n - n_0$:

– $\mathbf{x}_i = \arg\min_{\mathbf{x}\in\Xi} \det\left[B_{i-1}(A_{i-1} + \boldsymbol{\Psi}(\mathbf{x})\boldsymbol{\Psi}^T(\mathbf{x}))^{-1}B_{i-1}^T\right]$
– $A_i = A_{i-1} + \boldsymbol{\Psi}(\mathbf{x}_i)\boldsymbol{\Psi}^T(\mathbf{x}_i)$
– Add the new sample point $(\mathbf{x}_i, y_i = f(\mathbf{x}_i))$ to the training sample and update current estimates $\hat{\mathbf{c}}_i$ of the PCE model coefficients
– Calculate $B_i = B(\hat{\mathbf{c}}_i)$

**Output:** The design of experiment $X = X_0 \cup X_{add}$, where $X_{add} = \{\mathbf{x}_k\}_{k=1}^{n-n_0}$

### 4.3   Details of the Optimization Procedure

The idea behind the proposed optimization procedure is analogous to the idea of the Fedorov's algorithm for constructing optimal designs [31].

In order to simplify the optimization problem, we use two well-known identities:

– Let $M$ be some nonsingular square matrix, $\mathbf{t}$ and $\mathbf{w}$ be vectors such that $1 + \mathbf{w}^T M^{-1}\mathbf{t} \neq 0$, then

$$(M + \mathbf{t}\mathbf{w}^T)^{-1} = M^{-1} - \frac{M^{-1}\mathbf{t}\mathbf{w}^T M^{-1}}{1 + \mathbf{w}^T M^{-1}\mathbf{t}}. \tag{19}$$

– Let $M$ be some nonsingular square matrix, $\mathbf{t}$ and $\mathbf{w}$ be vectors of appropriate dimensions, then

$$\det(M + \mathbf{t}\mathbf{w}^T) = \det(M) \cdot (1 + \mathbf{w}^T M^{-1}\mathbf{t}). \tag{20}$$

Define $D \triangleq B(A + \boldsymbol{\Psi}(\mathbf{x})\boldsymbol{\Psi}^T(\mathbf{x}))^{-1}B^T$, then applying (19), we obtain

$$\det(D) = \det\left[BA^{-1}B^T - \frac{BA^{-1}\boldsymbol{\Psi}(\mathbf{x})\boldsymbol{\Psi}^T(\mathbf{x})A^{-1}B^T}{1 + \boldsymbol{\Psi}^T(\mathbf{x})A^{-1}\boldsymbol{\Psi}(\mathbf{x})}\right]$$

$$\triangleq \det\left[M - \mathbf{t}\mathbf{w}^T\right], \tag{21}$$

where $M \triangleq BA^{-1}B^T$, $\mathbf{t} \triangleq \frac{BA^{-1}\boldsymbol{\Psi}(\mathbf{x})}{1+\boldsymbol{\Psi}^T(\mathbf{x})A^{-1}\boldsymbol{\Psi}(\mathbf{x})}$, $\mathbf{w} \triangleq BA^{-1}\boldsymbol{\Psi}(\mathbf{x})$. Assuming that matrix $M$ is nonsingular and applying (20), we obtain

$$\det(D) = \det(M) \cdot (1 - \mathbf{w}^T M^{-1}\mathbf{t}) \rightarrow \min$$

The resulting optimization problem is

$$\mathbf{w}^T M^{-1} \mathbf{t} \to \max \tag{22}$$

or explicitly

$$\frac{(\boldsymbol{\Psi}^T(\mathbf{x}) A^{-1}) B^T (B A^{-1} B^T)^{-1} B (A^{-1} \boldsymbol{\Psi}(\mathbf{x}))}{1 + \boldsymbol{\Psi}^T(\mathbf{x}) A^{-1} \boldsymbol{\Psi}(\mathbf{x})} \to \max_{\mathbf{x} \in \Xi}. \tag{23}$$

## 5   Benchmark

In this section, we validate the proposed algorithm on a set of computational models of different input dimensions. Three analytic problems and two industrial problems based on finite element models are considered. Input parameters (variables) of the considered models have independent uniform and independent normal distributions. For some models, independent gaussian noise is added to their outputs.

At first, we form non-degenerate random initial design, and then we use various techniques to add new design points iteratively. We compare our method for design construction (denoted as **Adaptive for SI**) with the following methods:

– **Random** method iteratively adds new design points randomly from the set of candidate design points $\Xi$;
– **Adaptive D-opt** iteratively adds new design points that maximize the determinant of the information matrix (11): $\det A_n \to \max_{\mathbf{x}_n \in \Xi}$ [31]. The resulting design is optimal, in some sense, for estimation of the coefficients of a PCE model. We compare our method with this approach to prove that it gives some advantage over usual $D$-optimality. Strictly speaking, $D$-optimal design is not iterative but if we have an initial training sample then the sequential approach seems natural generalization of a common $D$-optimal designs.
– **LHS**. Unlike other considered designs, this method is not iterative as a completely new design is generated at each step. This method uses Latin Hypercube Sampling, as it is common to compute PCE coefficients.

The metric of design quality is **the mean error** defined as the distance between estimated and true indices $\sqrt{\sum_{i=1}^{d} (S_i - \hat{S}_i^{\mathrm{run}})^2}$ averaged over runs with different random initial designs (200–400 runs). We consider not only *mean* error but also its *variance*. Particularly, we use Welch's t-test [32] to ensure that the difference of mean distances is statistically significant for the various methods considered. Note that lower p-values correspond to greater confidence.

In all cases, we assume that the truncation set (retained PCE terms) was selected before the experiment.

### 5.1   Analytic Functions

Two analytic functions with uniformly distributed input variables are considered, namely Sobol and Wing Weight functions. Independent gaussian noise is added to their outputs to simulate random errors due to measurement uncertainty.

*The Sobol' function* is commonly used for benchmarking methods in global sensitivity analysis

$$f(\mathbf{x}) = \prod_{i=1}^{d} \frac{|4x_i - 2| + c_i}{1 + c_i},$$

where $x_i \sim \mathcal{U}(0, 1)$. In our case, parameters $d = 3$, $c = (0.0, 1.0, 1.5)$ are used. Independent gaussian noise is added to the output of the function. The standard deviation of noise is 0 (without noise), 0.2 and 1.4 that corresponds to 0 %, 28 % and 194 % of the function standard deviation due to given uncertainty of the inputs. Analytical expressions for its sensitivity indices are available in [10].

*The Wing Weight function* models the weight of aircraft wing [35]

$$f(\mathbf{x}) = 0.036 S_w^{0.758} W_{fw}^{0.0035} \left(\frac{A}{\cos^2(\Lambda)}\right)^{0.6} q^{0.006} \lambda^{0.04} \left(\frac{100 t_c}{\cos(\Lambda)}\right)^{-0.3} (N_z W_{dg})^{0.49} + S_w W_p,$$

where 10 input variables and their distributions are defined as: $S_w \sim \mathcal{U}(150, 200)$, wing area $(ft^2)$; $W_{fw} \sim \mathcal{U}(220, 300)$, weight of fuel in the wing (lb); $A \sim \mathcal{U}(6, 10)$, aspect ratio; $\Lambda \sim \mathcal{U}(-10, 10)$, quarter-chord sweep (degrees); $q \sim \mathcal{U}(16, 45)$, dynamic pressure at cruise $(lb/ft^2)$; $\lambda \sim \mathcal{U}(0.5, 1)$, taper ratio; $t_c \sim \mathcal{U}(0.08, 0.18)$, aerofoil thickness to chord ratio; $N_z \sim \mathcal{U}(2.5, 6)$, ultimate load factor; $W_{dg} \sim \mathcal{U}(1700, 2500)$, flight design gross weight (lb); $W_p \sim \mathcal{U}(0.025, 0.08)$, paint weight $(lb/ft^2)$. Independent gaussian noise $\mathcal{N}(0, 5.0^2)$ is added to the output of the function.

*Experimental setup* for analytic functions is summarized in Table 1. In the experiments, we assume that the set of candidate design points $\Xi$ is a uniform grid in the $d$-dimensional hypercube. Note that $\Xi$ affects the quality of optimization.

## 5.2   Finite Element Models

*Case 1: Truss Model.* The deterministic computational model, originating from [36], resembles the displacement $V_1$ of a truss structure with 23 members as shown in Fig. 2.

   10 random variables are considered:

– $E_1$, $E_2$ (Pa) $\sim \mathcal{U}(1.68 \times 10^{11},\ 2.52 \times 10^{11})$;
– $A_1$ $(m^2) \sim \mathcal{U}(1.6 \times 10^{-3},\ 2.4 \times 10^{-3})$;
– $A_2$ $(m^2) \sim \mathcal{U}(0.8 \times 10^{-3},\ 1.2 \times 10^{-3})$;
– $P_1$ - $P_6$ (N) $\sim \mathcal{U}(3.5 \times 10^4,\ 6.5 \times 10^4)$;

   It is assumed that all the horizontal elements have perfectly correlated Young's modulus and cros-sectional areas with each other and so is the case with the diagonal members.
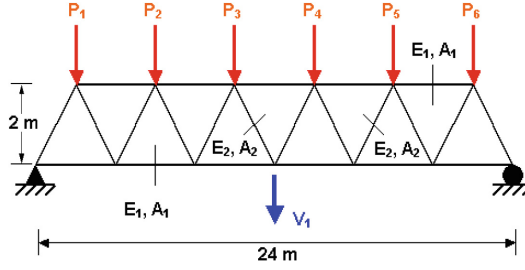
**Fig. 2.** Truss structure with 23 members

*Case 2: Heat Transfer Model.* We consider the two-dimensional stationary heat diffusion problem used in [37]. The problem is defined on the square domain $D = (-0.5, 0.5) \times (-0.5, 0.5)$ shown in Fig. 3a, where the temperature field $T(z)$, $z \in D$, is described by the partial differential equation:

$$-\nabla(\kappa(\mathbf{z})\nabla T(z)) = 500 I_A(z),$$

with boundary conditions $T = 0$ on the top boundary and $\nabla T \mathbf{n} = 0$ on the left, right and bottom boundaries, where $\mathbf{n}$ denotes the vector normal to the boundary; $A = (0.2, 0.3) \times (0.2, 0.3)$ is a square domain within $D$ and $I_A$ is the indicator function of $A$. The diffusion coefficient, $\kappa(z)$, is a lognormal random field defined by

$$\kappa(z) = \exp[a_k + b_k g(z)],$$

where $g(z)$ is a standard Gaussian random field and the parameters $a_k$ and $b_k$ are such that the mean and standard deviation of $\kappa$ are $\mu_\kappa = 1$ and $\sigma_\kappa = 0.3$, respectively. The random field $g(z)$ is characterized by an autocorrelation function $\rho(z, z') = \exp(-\|z - z'\|^2/0.2^2)$. The quantity of interest, $Y$, is the average temperature in the square domain $B = (-0.3, -0.2) \times (-0.3, -0.2)$ within $D$ (see Fig. 3a).

To facilitate solution of the problem, the random field $g(z)$ is represented using the Expansion Optimal Linear Estimation (EOLE) method [38]. By truncating the EOLE series after the first $M$ terms, $g(z)$ is approximated by

$$\hat{g}(z) = \sum_{i=1}^{M} \frac{\xi_i}{\sqrt{\ell_i}} \phi_i^T \mathbf{C}_{z\zeta}$$

In the above equation, $\{\xi_1, \ldots, \xi_M\}$ are independent standard normal variables; $\mathbf{C}_{z\zeta}$ is a vector with elements $\mathbf{C}_{z\zeta}^{(k)} = \rho(z, \zeta_k)$, where $\{\zeta_1, \ldots, \zeta_M\}$ are the points of an appropriately defined mesh in $D$; and $(\ell_i, \phi_i)$ are the eigenvalues and eigenvectors of the correlation matrix $\mathbf{C}_{\zeta\zeta}$ with elements $\mathbf{C}_{\zeta\zeta}^{(k,\ell)} = \rho(\zeta_k, \zeta_\ell)$, where $k, \ell = 1, \ldots, n$. We select $M = 53$ in order to satisfy

$$\sum_{i=1}^{M} \ell_i / \sum_{i=1}^{n} \ell_i \geq 0.99$$

(a) Finite-element mesh     (b) Temperature field realizations
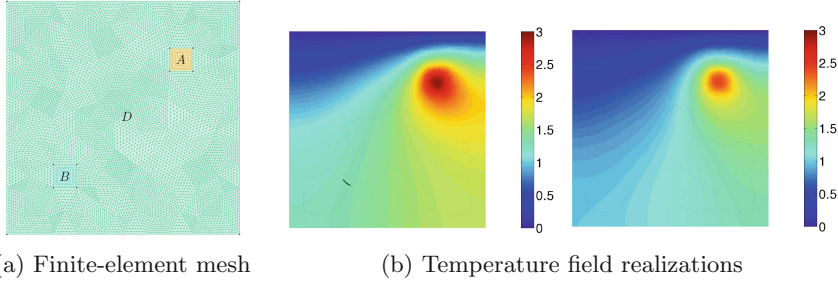
**Fig. 3.** Heat diffusion problem

The underlying deterministic problem is solved with an in-house finite-element analysis code. The employed finite-element discretization with triangular $T3$ elements is shown in Fig. 3a. Figure 3b shows the temperature fields corresponding to two example realizations of the diffusion coefficient.

*Experimental Setup.* For these finite element models, we assume that the set of candidate design points $\Xi$ is

– a uniform grid in the 10-dimensional hypercube for Truss model;
– LHS design with normally distributed variables in 53-dimensional space for Heat transfer model.

Experimental settings for all models are summarized in Table 1.

**Table 1.** Benchmark settings

| Characteristic | Sobol | WingWeight | Truss | Heat transfer |
|---|---|---|---|---|
| Input dimension | 3 | 10 | 10 | 53 |
| Input distributions | Unif | Unif | Unif | Norm |
| PCE degree | 9 | 4 | 4 | 2 |
| $q$-norm | 0.75 | 0.75 | 0.75 | 0.75 |
| Regressors number | 111 | 176 | 176 | 107 |
| Initial design size | 150 | 186 | 176 | 108 |
| Added noise std | (0, 0.2, 1.4) | 5.0 | — | — |

### 5.3   Results

Figures 4a, b, c, and 5 show results for analytic functions. Figures 6 and 7 present results for finite element models.
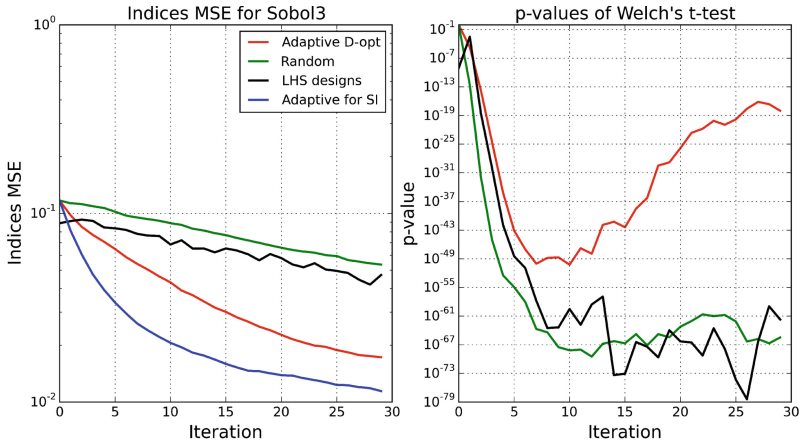
(a) Noise std: 0
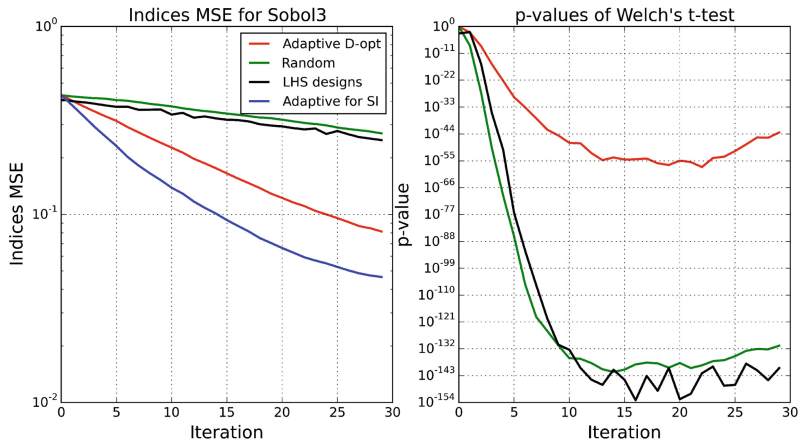
(b) Noise std: 0.2
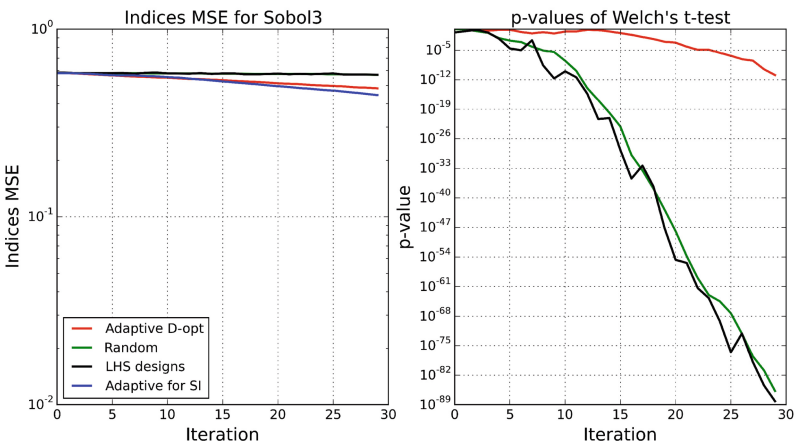
(c) Noise std: 1.4

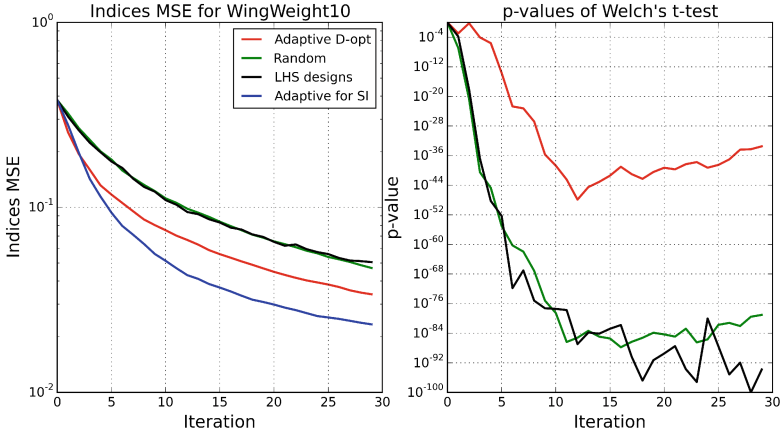**Fig. 4.** Sobol function. 3-dimensional input.

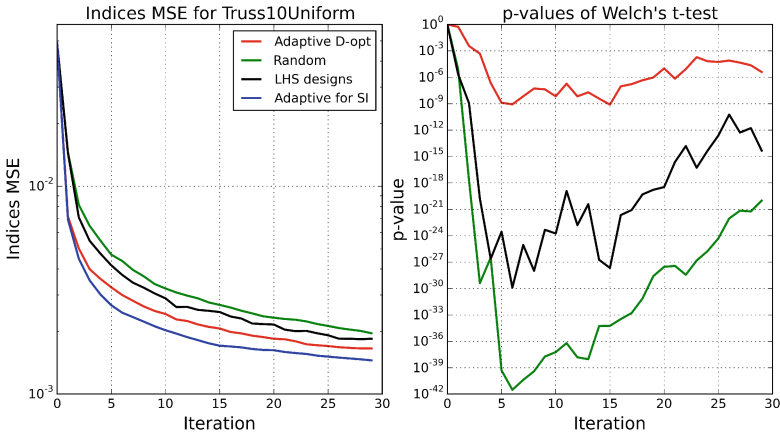**Fig. 5.** WingWeight function. 10-dimensional input



**Fig. 6.** Truss model. 10-dimensional input

In the presented experiments, the proposed method performs better than other considered methods in terms of the mean error of estimated indices. Particularly note its superiority over standard LHS approach that is commonly used in practice. The difference in mean errors is statistically significant according to Welch's t-test.

Comparison of Fig. 4a, b, c with different levels of additive noise shows that the proposed method is effective when the analyzed function is deterministic or when the noise level is *small*.

Because of robust problem statement and limited accuracy of the optimization, the algorithm may produce duplicate design points. Actually, it's a common situation for locally $D$-optimal designs [30]. If the computational model is deterministic, one may modify the algorithm, *e.g.* exclude repeated design points.
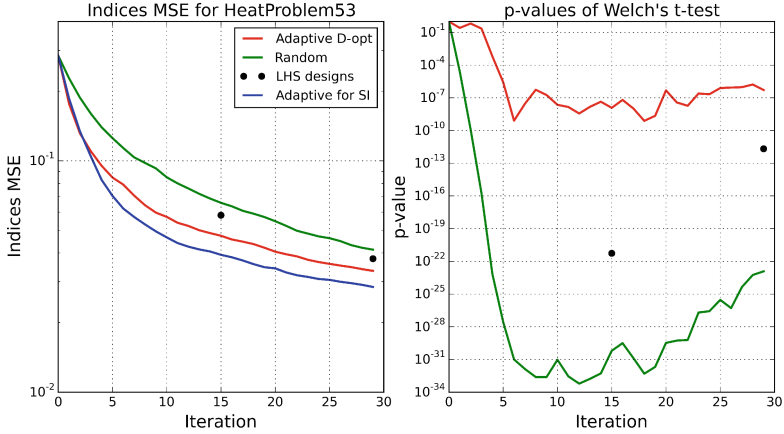
**Fig. 7.** Heat transfer model. 53-dimensional input

Although high dimensional optimization problems may be computationally prohibitive, the proposed approach is still useful in high dimensional settings. We propose to generate a uniform candidate set (*e.g.* LHS design of large size) and then choose its subset for the effective calculation of Sobol' indices using our adaptive method (see results for Heat transfer model on Fig. 7).

It should be noted that in all presented cases the specification of sufficiently accurate PCE model (reasonable values for degree and $q$-norm defining the truncation set) is assumed to be known *a priori* and the size of the initial training sample is sufficiently large. If we use an inadequate specification of the PCE model (*e.g.* quadratic PCE in case of cubic analyzed function), the method will perform worse in comparison with methods which do not depend on PCE model structure. In any case, usage of inadequate PCE models may lead to inaccurate results. That is why it is very important to control PCE model error during the design construction. For example, one may use *cross-validation* for this purpose [26]. Thus, if the PCE model error increases during design construction this may indicate that the model specification is inadequate and should be changed.

## 6   Conclusions

We proposed the design of experiments algorithm for evaluation of Sobol' indices from PCE metamodel. The method does not depend on a particular form of orthonormal polynomials in PCE. It can be used for the case of different distributions of input parameters of the analyzed computational models.

The main idea of the method comes from metamodeling approach. We assume that the computational model is close to its approximating PCE metamodel and exploit knowledge of a metamodel structure. This allows us to improve the evaluation accuracy. All comes with a price: if additional assumptions on the computational model to provide good performance are not satisfied, one may

expect accuracy degradation. Fortunately, in practice, we can control approximation quality during design construction and detect that we have selected inappropriate model. Note that from a theoretical point of view, our asymptotic considerations (w.r.t. the training sample size) simplify the problem of accuracy evaluation for the estimated indices.

Our experiments demonstrate: if PCE specification defined by the truncation scheme is appropriate for the given computational model and the size of the training sample is sufficiently large, then the proposed method performs better in comparison with standard approaches for design construction.

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