Adaptive Design of Experiments for Sobol Indices Estimation Based on Quadratic Metamodel

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Abstract. Sensitivity analysis aims to identify which input parameters of a given mathematical model are the most important. One of the well-known sensitivity metrics is the Sobol sensitivity index. There is a number of approaches to Sobol indices estimation. In general, these approaches can be divided into two groups: Monte Carlo methods and methods based on metamodeling. Monte Carlo methods have well-established mathematical apparatus and statistical properties. However, they require a lot of model runs. Methods based on metamodeling allow to reduce a required number of model runs, but may be difficult for analysis. In this work, we focus on metamodeling approach for Sobol indices estimation, and particularly, on the initial step of this approach — design of experiments. Based on the concept of D-optimality, we propose a method for construction of an adaptive experimental design, effective for calculation of Sobol indices from a quadratic metamodel. Comparison of the proposed design of experiments with other methods is performed.

Keywords: Active learning · Global sensitivity analysis · Sobol indices · Adaptive design of experiments · D-optimality

1 Introduction

Understanding the behaviour of complex mathematical models of complex physical systems is a crucial point for an engineering practice. Discovering knowledge about the most important parameters of the model and learning parameters dependency structure allow to understand better the system behind the model and reveal the way to optimize its performance.

Given some mathematical model, the *sensitivity analysis* tries to find the input parameters which variability has strong effect on the model output and to evaluate this effect quantitatively; to determine how the parts of the model interplay, how the model relates to the real world (see [1]). One of the common metrics to evaluate the sensitivity is a *Sobol sensitivity index*. A lot of Monte Carlo methods were developed for estimation of Sobol indices: direct Monte

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Carlo simulation, FAST [2], SPF scheme [3] and others. However, these methods require a lot of runs of the analysed model and, therefore, are impractical for a number of industrial applications.

On the other hand, metamodeling methods for Sobol indices estimation allow to reduce the necessary number of model runs. In metamodeling approach, in general, we replace the original model by an approximating *metamodel* (also known as *surrogate model* or *response surface*) which is more computationally efficient and has known internal structure. Approaches based on metamodels consist of the following steps: generation of experimental design and training sample, construction of metamodel and calculation of sensitivity indices using the constructed model. Note that for the last step we can use both prediction based on the constructed model and knowledge about its internal structure, *e.g.* values of its estimated parameters.

This work is devoted to construction of adaptive experimental designs for effective calculation of Sobol indices, *i.e.* calculation using the minimal number of model runs.

There are several approaches related to the experimental design construction for sensitivity analysis problems. Most of them are associated with a uniform (in some sense) space filling design, *e.g.* Latin Hypercube, Sobol sequences and others. These approaches are highly flexible, since specified structure of the analysed model is not required for them. However, these designs, in general, are not optimal in the sense of the fastest convergence of sensitivities to their true values.

Unlike space-filling designs, we try to construct an effective design and, therefore, we make assumptions on the model structure. We assume that the analysed model is quadratic one with a white noise. Although we consider only this simple case, the obtained results can be generalized to a wider class of models, including Polynomial Chaos Expansions and others.

In the above assumptions, we investigate asymptotic behaviour (with respect to the increasing design size) of the proposed estimate for sensitivity index based on quadratic metamodel, prove its asymptotic normality and introduce an optimality criterion for designs. Based on this criterion, we propose a procedure for construction of an effective adaptive experimental design and compare it with other designs.

The paper is organized as follows: in section 2, we review the definition of sensitivity indices and describe their calculation based on quadratic metamodel. In section 3, asymptotic behaviour of index estimate is considered. In section 4, we introduce optimality criterion and propose the procedure for construction of an adaptive experimental design. In section 5, experimental results are given.

2 Calculation of Sensitivity Indices Using Quadratic Metamodel

2.1 Sensitivity Indices

Consider a mathematical 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) features*, $y \in \mathbb{R}^1$ is an *output feature* and $\mathscr{X}$ is *a design space*.

The model is defined as a "black box": its internal structure is unknown, but for the selected *design of experiment* $X = \{\mathbf{x}_i\}_{i=1}^n \in \mathbb{R}^{n\times d}$ we can get a set of model responses and form a *training sample* $L = \{\mathbf{x}_i, y_i = f(\mathbf{x}_i)\}_{i=1}^n$, which allows us to investigate properties of this model.

Let there be given some probability distribution on the design space $\mathscr{X}$ with independent components, and let $\mathbf{x}_\Omega = (x_{i_1}, \ldots, x_{i_p})$ be some subset of input features.

Definition 1. *Sensitivity index of feature set x_Ω is defined as*

$$S_\Omega = \frac{\mathbb{V}(\mathbb{E}(y|x_\Omega))}{\mathbb{V}(y)}, \tag{1}$$

where $\mathbb{E}$ and $\mathbb{V}$ denote a mathematical expectation and a variance.

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

Remark 2. In practice, in order to simulate the variability of input features if no additional information is available, independent uniform distributions are often used with the borders, obtained from physical considerations.

2.2 Metamodeling Approach

Consider calculation of sensitivity indices using the quadratic (meta)model. The model can be represented as

$$y = \alpha_0 + \sum_{i=1}^d \alpha_i x_i + \sum_{i,j=1,\, i\le j}^d \beta_{ij} x_i x_j, \tag{2}$$

where α_i and β_{ij} are coefficients of the model.

This model can be rewritten as $y = \boldsymbol{\varphi}(\mathbf{x})\boldsymbol{\theta}$, where $\boldsymbol{\theta} = (\alpha_1, \ldots, \alpha_d, \beta_{12}, \ldots, \beta_{(d-1)d}, \beta_{11}, \ldots, \beta_{dd}, \alpha_0) \in \mathbb{R}^q$, $q = d + \frac{d(d-1)}{2} + d + 1$ and

$$\boldsymbol{\varphi}(\mathbf{x}) = (x_1, \ldots, x_d,\ x_1x_2, \ldots, x_{d-1}x_d,\ x_1^2, \ldots, x_d^2,\ 1). \tag{3}$$

As it was mentioned above, the variability of input features is often modeled via uniform distribution on some interval. Without loss of generality, we assume that $x_i \sim U([-1,1])$, $i = 1, \ldots, d$. Following [4], it is easy to calculate the analytical expressions for sensitivity indices for the quadratic model (2) with uniformly distributed features.

Proposition 1. *Let x_i be i.i.d. and $x_i \sim U([-1,1])$ for $i = 1, \ldots, d$, then the sensitivity indices for the quadratic model (2) have the following form:*

$$S_k = \frac{\frac{1}{3}\alpha_k^2 + \frac{4}{45}\beta_{kk}^2}{\frac{1}{3}\sum_{i=1}^d \alpha_i^2 + \frac{1}{9}\sum_{i,j=1,\, i<j}^d \beta_{ij}^2 + \frac{4}{45}\sum_{i=1}^d \beta_{ii}^2}, \quad k = 1, \ldots, d. \tag{4}$$

Assuming that the original model $f(\mathbf{x})$ is well approximated by some quadratic model, we can obtain an estimate for the sensitivity index S_i of original model using analytical expression for indices (4). Taking into account the results of Proposition 1, we can propose the following procedure for indices estimation:

1. Generate an experimental design $X = \{\mathbf{x}_i\}_{i=1}^n \in \mathbb{R}^{n\times d}$,
2. Simulate the original mathematical model on this design,
3. Form the training sample $L = \{\mathbf{x}_i, y_i = f(\mathbf{x}_i)\}_{i=1}^n$,
4. Construct a quadratic model based on this training sample,
5. Calculate sensitivity indices using estimated coefficients α_i and β_{ij}.

In this paper, we focus on construction of an effective experimental design for this procedure. Note that since $S_k = \psi(\boldsymbol{\alpha}, \boldsymbol{\beta})$ is a nonlinear function of the parameters $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, then the existing approaches to the construction of experimental designs, which are effective for estimating α_i and β_{ij} (D-, IV-criterion, see [8]), are not effective for the considered case.

3 Asymptotic Approximation

In this section, we consider asymptotic properties of our indices estimates if the original model is quadratic with Gaussian noise:

$$y = \boldsymbol{\varphi}(\mathbf{x})\boldsymbol{\theta} + \varepsilon, \text{ where } \varepsilon \sim N(0, \sigma^2). \tag{5}$$

Rewrite the formula (4) for sensitivity index using $\boldsymbol{\lambda} = A\boldsymbol{\theta}$:

$$S_k = \frac{\lambda_k^2 + \lambda_{kk}^2}{\sum_{i=1}^d \lambda_i^2 + \sum_{i,j=1,\, i<j}^d \lambda_{ij}^2 + \sum_{i=1}^d \lambda_{ii}^2}\ k = 1, \ldots, d, \tag{6}$$

where $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_d, \lambda_{12}, \ldots, \lambda_{(d-1)d}, \lambda_{11}, \ldots, \lambda_{dd}) \in \mathbb{R}^{q-1}$, $q = d + \frac{d(d-1)}{2} + d + 1$, normalization matrix $A = [diag(\sqrt{1/3}, \ldots, \sqrt{1/3}, \sqrt{4/45}, \ldots, \sqrt{4/45}, \sqrt{1/9}, \ldots, \sqrt{1/9}), zeros(q-1, 1)] \in \mathbb{R}^{(q-1)\times q}$ consists of a diagonal matrix and a column of zeros; kk denotes the index of the term, corresponding to the squared value of the k-th feature.

Let us assume that the training sample $L = \{\mathbf{x}_i, y_i = f(\mathbf{x}_i)\}_{i=1}^n$ is given, where $X = \{\mathbf{x}_i\}_{i=1}^n \in \mathbb{R}^{n\times d}$ is *a design matrix*. Let $\hat{\boldsymbol{\theta}}_{\text{OLS}}$ be the Ordinary Least Square estimate of the model parameter $\boldsymbol{\theta}$ based on this training sample, then the estimated index $\hat{S}_k$ has the form:

$$\hat{S}_k = \frac{\hat{\lambda}_k^2 + \hat{\lambda}_{kk}^2}{\sum_{i=1}^d \hat{\lambda}_i^2 + \sum_{i,j=1,\, i<j}^d \hat{\lambda}_{ij}^2 + \sum_{i=1}^d \hat{\lambda}_{ii}^2},\ \ k = 1, \ldots, d, \tag{7}$$

where $\hat{\boldsymbol{\lambda}} = A\hat{\boldsymbol{\theta}}_{\text{OLS}}$.

Using standard results for a linear regression (see [5]), it is not difficult to prove the following proposition.

Proposition 2. *Let $\Psi = \boldsymbol{\varphi}(X) \in \mathbb{R}^{n\times q}$ be an extended design matrix for the training sample in the case of quadratic model, the matrix $\Psi^T\Psi$ is invertible, then*

$$\mathbb{V}(\hat{\boldsymbol{\lambda}}) = \mathbb{V}(A\hat{\boldsymbol{\theta}}) = A\cdot\mathbb{V}(\hat{\boldsymbol{\theta}})\cdot A^T = \sigma^2 A(\Psi^T\Psi)^{-1}A^T,$$

$$\mathbb{E}\hat{\boldsymbol{\lambda}} = A\boldsymbol{\theta} = \boldsymbol{\lambda},$$

$$\hat{\boldsymbol{\delta}} = \hat{\boldsymbol{\lambda}} - \boldsymbol{\lambda} \sim \mathcal{N}(0, \sigma^2 A(\Psi^T\Psi)^{-1}A^T).$$

Let $\hat{t}_i \triangleq 2\lambda_i\hat{\delta}_i + \hat{\delta}_i^2$, $\hat{t}_{ij} \triangleq 2\lambda_{ij}\hat{\delta}_{ij} + \hat{\delta}_{ij}^2$, $\hat{t}_{ii} \triangleq 2\lambda_{ii}\hat{\delta}_{ii} +$ $+\, \hat{\delta}_{ii}^2$, $i, j = 1, \ldots, d$, $i \leq j$, and

$$\hat{\mathbf{t}} = (\hat{t}_1, \ldots, \hat{t}_d, \hat{t}_{12}, \ldots, \hat{t}_{(d-1)d}, \hat{t}_{11}, \ldots, \hat{t}_{dd}) \in \mathbb{R}^{q-1}. \tag{8}$$

Let us rewrite formula (7) for estimated sensitivity index in the form

$$\hat{S}_k(\hat{\mathbf{t}}) = \frac{\lambda_k^2 + \lambda_{kk}^2 + \hat{t}_k + \hat{t}_{kk}}{\sum_{i=1}^d(\lambda_i^2 + \hat{t}_i) + \sum_{i,j=1,\, i<j}^d(\lambda_{ij}^2 + \hat{t}_{ij}) + \sum_{i=1}^d(\lambda_{ii}^2 + \hat{t}_{ii})}.$$

The following theorem allows to establish asymptotic properties of this index estimate while new examples are added to the training sample. In this theorem, if some variable has index n, then this variable depends on the training sample of size n.

Theorem 1. *1. Let new points are being added iteratively to experimental design so that*

$$\frac{1}{n}\Psi_n^T\Psi_n \underset{n\to+\infty}{\longrightarrow} \Sigma, \text{ where } \Sigma = \Sigma^T,\ \det\Sigma > 0. \tag{9}$$

2. Let $\mathbf{t} = (t_1, \ldots, t_d, t_{12}, \ldots, t_{(d-1)d}, t_{11}, \ldots, t_{dd}) \in \mathbb{R}^{q-1}$, $\mathbf{S}(\mathbf{t}) = (S_1(\mathbf{t}), \ldots, S_d(\mathbf{t}))$, where for $k = 1, \ldots, d$

$$S_k(\mathbf{t}) = \frac{\lambda_k^2 + \lambda_{kk}^2 + t_k + t_{kk}}{\sum_{i=1}^d(\lambda_i^2 + t_i) + \sum_{i,j=1,\, i<j}^d(\lambda_{ij}^2 + t_{ij}) + \sum_{i=1}^d(\lambda_{ii}^2 + t_{ii})}.$$

$$G = \left(\frac{\partial\mathbf{S}}{\partial\mathbf{t}}\right)\Bigg|_{\mathbf{t}=\mathbf{0}},\quad \Lambda = diag(\lambda_1, \ldots, \lambda_{q-1}) \tag{10}$$

and holds

$$\det(B\Sigma^{-1}B^T) \neq 0 \tag{11}$$

where $B = G\Lambda A$, **then**

$$\sqrt{n}(\hat{\mathbf{S}}_n - \mathbf{S}) \underset{n\to+\infty}{\xrightarrow{\mathfrak{D}}} \mathcal{N}(0, 4\sigma^2 B\Sigma^{-1}B^T). \tag{12}$$

Proof. 1. From Proposition 2 we obtain

$$\sqrt{n}\,\hat{\boldsymbol{\delta}}_n \underset{n\to+\infty}{\xrightarrow{\mathfrak{D}}} \mathcal{N}(0, \sigma^2 A\Sigma^{-1}A^T), \tag{13}$$

$$\sqrt{n}\,\hat{\boldsymbol{\delta}}_n^2 \underset{n\to+\infty}{\xrightarrow{\mathfrak{D}}} 0. \tag{14}$$

Using Slutsky's theorem ([6]) we obtain from (13) and (14) for $\hat{\mathbf{t}}$:

$$\sqrt{n}\,\hat{\mathbf{t}} \underset{n\to+\infty}{\xrightarrow{\mathfrak{D}}} \mathcal{N}(0, 4\sigma^2\Lambda(A\Sigma^{-1}A^T)\Lambda^T). \tag{15}$$

2. Applying δ-method ([7]) on expansion of $\hat{\mathbf{S}}(\hat{\mathbf{t}}) = (\hat{S}_1(\hat{\mathbf{t}}), \ldots, \hat{S}_d(\hat{\mathbf{t}}))$ and asymptotically small parameter $\hat{\mathbf{t}}$, we obtain required expression (12).

The next section provides a method for construction of an experimental design for effective calculation of sensitivity indices.

4 Optimality Criterion and Procedure for Design Construction

Taking into account the results of Theorem 1, the limiting covariance matrix of the indices estimates depends on a) variance σ^2, b) true values of coefficients of quadratic model, defining B, c) experimental design, defining Σ.

In the above assumptions, the asymptotic formula (12) allows to evaluate the quality of the experimental design. Indeed, generally speaking the less covariance matrix norm $\|4\sigma^2 B \Sigma^{-1} B^T\|$ is, the less risk of sensitivity indices estimation is. However, there are two problems on the way of using this formula to construct effective designs. The first one relates to the choice of specific minimized functional for the limiting covariance matrix. The second one refers to the fact that we do not know true values of the coefficients of quadratic model, 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 (A-, C-, D-, I-optimality and others, see [8]) are known. In this work, we use D-optimality criterion. 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 complicated: the optimal design for estimation of sensitivity indices depends on the true values of these indices, and it can be constructed only if these true values are known.

There are several approaches to this problem. These approaches are usually associated with either some assumptions about the unknown parameters, or adaptive design construction (see [10]).

Particularly, the minimax-optimal criterion and the averaging-optimal (Bayesian optimal) criterion for design construction use the assumptions about the unknown parameters and allow to achieve design that is optimal in average and independent from the true values of the unknown parameters. However, in this case there is a problem of the choice of an a priori set of possible values (in case of minimax-optimal criterion) or an a priori distribution (in case of the averaged optimal criterion) for the unknown parameters.

On the other hand, in case of adaptive designs, new points are generated sequentially based on current estimate of the unknown parameters, which allows to avoid a priori assumptions on these parameters. However, in this case there is a problem with a confidence of the solution found: if on some step of design construction parameters estimates are very different from their true values, then the design, which is constructed on the basis of these estimates, may lead to new parameters estimates, which are also very different from the real values and so on. In practice, during the construction of adaptive design, assumptions on non-degeneracy of results can be checked at each iteration, and depending on the results one can adjust the current estimates.

In this paper, we propose an adaptive method for construction of design of experiment for calculation of sensitivity indices based on the asymptotic D-optimal criterion (see an algorithm below). As an initial condition, we require an original design to be non-degenerate, *i.e.* such that for an extended design matrix at the initial moment it holds that $\det(\Psi_0^T \Psi_0) \neq 0$. In addition, at each iteration the non-degeneracy of the matrix, defining the minimized criterion, is checked.

In Section 4.1 the details of the optimization procedure are given.

Goal: Construct experimental design for calculation of sensitivity indices
Parameters: initial n_0 and final n numbers of points in the design; set of possible design points Ξ.
Initialization:

- non-degenerate initial design $X_0 = \{\mathbf{x}_i\}_{i=1}^{n_0} \subset \Xi$;
- $\Phi_0 = \sum_{i=1}^{n_0} \boldsymbol{\varphi}(\mathbf{x}_i)\boldsymbol{\varphi}^T(\mathbf{x}_i)$;
- $B_0 = G_0 \Lambda_0 A$, where G_0 and Λ_0 (10) are obtained using the initial estimates of the coefficients of a quadratic model;

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

- $\mathbf{x}_{n_0+i} = \arg\min_{\mathbf{x}\in\Xi} \det\left[B_{i-1}(\Phi_{i-1} + \boldsymbol{\varphi}(\mathbf{x})\boldsymbol{\varphi}^T(\mathbf{x}))^{-1} B_{i-1}^T\right]$
- Calculate values G_i, Λ_i and $B_i = G_i \Lambda_i A$ using current estimates of the quadratic model coefficients
- $\Phi_i = \Phi_{i-1} + \boldsymbol{\varphi}(\mathbf{x}_{n_0+i})\boldsymbol{\varphi}^T(\mathbf{x}_{n_0+i})$

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

4.1 Optimization Details

The idea behind the optimization procedure in the proposed algorithm is analogous to the idea of the Fedorov algorithm for construction of optimal designs [9].

In order to simplify the optimization problem, we need several identities:

- Let A be some non-singular square matrix, $\mathbf{u}$ and $\mathbf{v}$ be vectors such that $1 + \mathbf{v}^T A^{-1}\mathbf{u} \neq 0$, then

$$(A + \mathbf{u}\mathbf{v}^T)^{-1} = A^{-1} - \frac{A^{-1}\mathbf{u}\mathbf{v}^T A^{-1}}{1 + \mathbf{v}^T A^{-1}\mathbf{u}}. \qquad (16)$$

– Let A be some non-singular square matrix, $\mathbf{u}$ and $\mathbf{v}$ be vectors of appropriate dimensions, then

$$\det(A + \mathbf{u}\mathbf{v}^T) = \det(A)\dot{(}1 + \mathbf{v}^T A^{-1}\mathbf{u}). \tag{17}$$

Let $D = B(\Phi + \boldsymbol{\varphi}(\mathbf{x})\boldsymbol{\varphi}^T(\mathbf{x}))^{-1}B^T$, then applying (16) and (17), we obtain

$$\det(D) = \det\left[B\Phi^{-1}B^T - \frac{B\Phi^{-1}\boldsymbol{\varphi}(\mathbf{x})\boldsymbol{\varphi}^T(\mathbf{x})\Phi^{-1}B^T}{1 + \boldsymbol{\varphi}^T(\mathbf{x})\Phi^{-1}\boldsymbol{\varphi}(\mathbf{x})}\right]$$
$$= \det\left[M - \mathbf{u}\mathbf{v}^T\right], \tag{18}$$

where $M = B\Phi^{-1}B^T$, $\mathbf{u} = \frac{B\Phi^{-1}\boldsymbol{\varphi}(\mathbf{x})}{1+\boldsymbol{\varphi}^T(\mathbf{x})\Phi^{-1}\boldsymbol{\varphi}(\mathbf{x})}$, $\mathbf{v} = B\Phi^{-1}\boldsymbol{\varphi}(\mathbf{x})$. Assuming that matrix M is non-degenerate, we obtain

$$\det(D) = \det(M)\dot{(}1 - \mathbf{v}^T M^{-1}\mathbf{u}) \to \min$$

The resulting optimization problem is

$$\mathbf{v}^T M^{-1}\mathbf{u} \to \max \tag{19}$$

or

$$\frac{(\boldsymbol{\varphi}^T(\mathbf{x})\Phi^{-1})B^T(B\Phi^{-1}B^T)^{-1}B(\Phi^{-1}\boldsymbol{\varphi}(\mathbf{x}))}{1 + \boldsymbol{\varphi}^T(\mathbf{x})\Phi^{-1}\boldsymbol{\varphi}(\mathbf{x})} \to \max_{\mathbf{x}\in\Xi} \tag{20}$$

This problem is easier than the initial one and can be solved with one of the standard methods of optimization.

5 Experimental Results

5.1 Description of Experiments

This section describes the comparison of the proposed approach with some modifications and with other approaches. In the experiments, we assume that the set of possible design points Ξ is a uniform grid in the hypercube $[-1, 1]^d$. At first, we generated some non-degenerate random initial design, and then we used various techniques to add new points iteratively. The sizes of the initial and final designs were $n_0 = 30$ and $n = 60$ points. Normalized empirical quadratic risk was chosen as a metric of quality of the results, normalization coefficient was equal to σ^2/n_i, where n_i is a size of the design on the i-th iteration.

Methods for Testing. iterDoptSI: the proposed method; **iterDopt**: adding a point maximizing the determinant of the information matrix $|\Psi_n^T\Psi_n| \to \max_{x_n}$ (see [9]). The resulting design is in some sense optimal for estimation of the coefficients of a quadratic model; **rand**: adding a random point from the set of possible design points; **randunif**: adding a random point in the hypercube $[-1, 1]^d$.

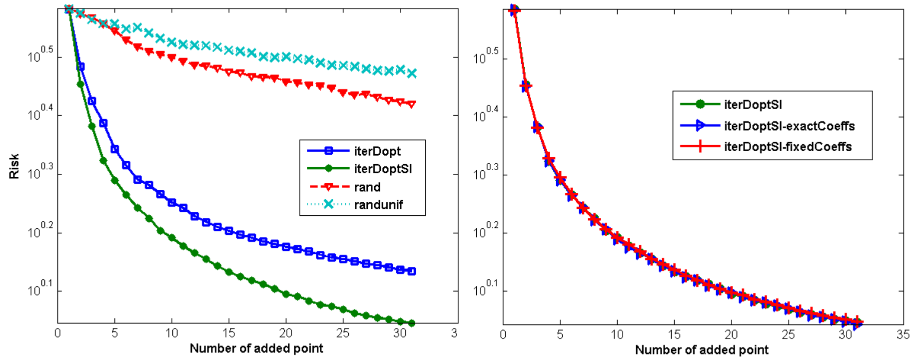

Fig. 1. Quadratic risk in case of different designs. 3-dimensional case

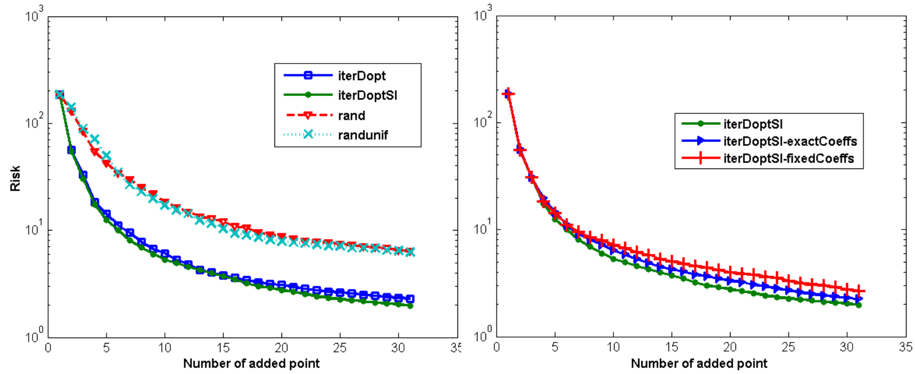

Fig. 2. Quadratic risk in case of different designs. 6-dimensional case

Additional Methods. iterDoptSI-exactCoeffs: variation of the proposed method, in which the estimates of quadratic model coefficients, which are used when adding next points, are replaced with their true values; **iterDoptSI-fixedCoeffs**: variation of the proposed method, in which the estimates of quadratic model coefficients, which are used when adding next points, are fixed to their initial values.

5.2 Description of Results

Figures 1 and 2 demonstrate the performance of different approaches in the case of 3 and 6-dimensional design space. They show the dependence of the normalized quadratic empirical risk on the number of iteration related to adding a new point to the design.

The presented figures illustrate that a) the proposed method **iterDoptSI** allows to get better results than the methods **iterDopt**, **rand** and **randunif**; b) if sensitivity indices are estimated accurately at initial moment, then the performances of the proposed method, **iterDoptSI-exactCoeffs** and **iterDoptSI-fixedCoeffs** are approximately the same, so one can use simplified computational schemes in which the evaluated indices are not updated at each iteration of Algorithm 4; c) method **iterDoptSI** is more efficient at low dimensions.

6 Conclusion

We proposed an asymptotic optimality criterion and method for construction of experimental design which is effective for calculation of sensitivity indices in case of noisy quadratic model. Comparison with other designs shows the superiority of the proposed method over competitors. The proposed approach can be generalized to arbitrary polynomial metamodel and arbitrary continuous distribution of input features. This will be the topic of our future works.

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