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Computing derivative-based global sensitivity measures using polynomial chaos expansions

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ABSTRACT

In the field of computer experiments sensitivity analysis aims at quantifying the relative importance of each input parameter (or combinations thereof) of a computational model with respect to the model output uncertainty. Variance decomposition methods leading to the well-known Sobol' indices are recognized as accurate techniques, at a rather high computational cost though. The use of polynomial chaos expansions (PCE) to compute Sobol' indices has allowed to alleviate the computational burden though. However, when dealing with large dimensional input vectors, it is good practice to first use screening methods in order to discard unimportant variables. The *derivative-based global sensitivity measures* (DGSMs) have been developed recently in this respect. In this paper we show how polynomial chaos expansions may be used to compute analytically DGSMs as a mere post-processing. This requires the analytical derivation of derivatives of the orthonormal polynomials which enter PC expansions. Closed-form expressions for Hermite, Legendre and Laguerre polynomial expansions are given. The efficiency of the approach is illustrated on two well-known benchmark problems in sensitivity analysis.

1. Introduction

Nowadays, the increasing computing power allows one to use numerical models to simulate or predict the behavior of physical systems in various fields, *e.g.* mechanical engineering [1], civil engineering [2], chemistry [3], etc. The considered systems usually lead to highly complex models with numerous input factors (possibly tens to hundreds [4,5]) that are required to represent all the parameters driving the system's behavior, *e.g.* boundary and initial conditions, material properties, external excitations, etc. In practice these input factors are often not perfectly known, since they are obtained from possibly noisy measurements, or simply by expert judgment. In order to take into account the uncertainty, probabilistic approaches have been developed in the last two decades, in which the model input parameters are represented by random variables. Then the input uncertainties are propagated through the computational model and the distribution, moments or probability of exceeding prescribed thresholds may be computed [6,7].

In this context, sensitivity analysis (SA) examines the sensitivity of the model output with respect to the input parameters, *i.e.* how the output variability is affected by the uncertain input factors [8–10]. The use of SA is common in various fields: engineering [2,11,1,12], chemistry [3], nuclear safety [13], economy [14], biology [15], and medicine [16], among others. One can traditionally classify SA into *local* and *global* sensitivity analyses. The former aims at assessing the output sensitivity to small input perturbations around a selected *reference value*, *e.g.* the mean value of the input random vector, or the so-called *design point* in reliability analysis [17]. The latter aims at assessing the overall or average influence of input parameters onto the output. Local SA has the disadvantage of being related to a fixed nominal point in the input space, and the interaction between the inputs is not accounted for [18]. In contrast, global SA techniques take into account the input interactions and are not based on the choice of a reference point but account for the whole input space, usually at a larger computational cost though.

The most common sensitivity analysis methods found in the literature are the method of Morris [19], FAST [20–22] and variance decomposition methods originally investigated in [23–28]. Usually standard Monte Carlo simulation (MCS) or quasi Monte Carlo (QMC) techniques are employed for estimating the sensitivity indices in all these approaches. This requires a large number of model evaluations though, which becomes unaffordable when complex systems are investigated. To overcome this problem, metamodels (also called *surrogate models* or emulators) are usually used in order to carry out the Monte Carlo simulation [29,30]. In particular, polynomial chaos expansions (PCE) have been recognized as a versatile tool for building surrogate models and for conducting reliability and sensitivity analyses, as originally shown in [31–33]. Using PCE,

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variance-based sensitivity analysis becomes a mere post-processing of the polynomial coefficients once they have been computed.

More recently, a new gradient-based technique has been proposed for screening unimportant factors. The so-called *derivative-based global sensitivity measures* (DGSM) are shown to be upper bounds of the total Sobol' indices while being less computationally demanding [34,35,18,36]. Although the computational cost of this technique is reduced compared to the variance-based technique [18], its practical computation still relies on sampling techniques, *e.g.* the Monte Carlo simulation.

In this paper we investigate the potential of polynomial chaos expansions for computing derivative-based sensitivity indices and allow for an efficient screening procedure. The paper is organized as follows: the classical derivation of Sobol' indices and their link to derivative-based sensitivity indices is summarized in Section 2. The machinery of polynomial chaos expansions and the link with sensitivity analysis is developed in Section 3. The computation of the DGSM based on PC expansions is then presented in Section 4, in which an original method for computing the derivatives of orthogonal polynomials is presented. Finally two numerical tests are carried out in Section 5.

2. Derivative-based global sensitivity measures

2.1. Variance-based sensitivity measures

Global sensitivity analysis (SA) aims at quantifying the impact of input parameters onto the output quantities of interest. One input factor is considered insignificant (unessential) when it has little or no effect on the output variability. In practice, screening out the insignificant factors allows one to reduce the dimension of the problem, *e.g.* by fixing the unessential parameters.

Variance-based SA relies upon the decomposition of the output variance into contributions of different components, *i.e.* marginal effects and interactions of input factors. Consider a numerical model $Y=\mathcal{M}(\boldsymbol{X})$ where the input vector $\boldsymbol{X}$ contains M independent input variables $\boldsymbol{X}=\{X_1,\ldots,X_M\}$ with uniform distribution over the unit-hypercube $\mathcal{H}^M$ and Y is the scalar output. The *Sobol' decomposition* reads [23]:

$$Y=\mathcal{M}(\boldsymbol{X})=\mathcal{M}_0+\sum_{i=1}^{M}\mathcal{M}_i(X_i)+\sum_{1\le i<j\le M}\mathcal{M}_{i,j}(X_i,X_j)+\cdots+\mathcal{M}_{1,\ldots,M}(X_1,\ldots,X_M) \tag{1}$$

in which $\mathcal{M}_0=\mathbb{E}[\mathcal{M}(\boldsymbol{X})]$ is a constant term and each summand $\mathcal{M}_{i_1,\ldots,i_s}(X_{i_1},\ldots,X_{i_s})$ is a function of the variables $\{X_{i_1},\ldots,X_{i_s}\}, s\le M$. For the sake of conciseness we introduce the following notation for the subset of indices:

$$\mathbf{u}\overset{\text{def}}{=}\{i_1,\ldots,i_s\} \tag{2}$$

and denote by $\boldsymbol{X}_{\mathbf{u}}$ the subvector of $\boldsymbol{X}$ that consists of the variables indexed by $\mathbf{u}$. Using this set notation, Eq. (1) rewrites:

$$Y\overset{\text{def}}{=}\mathcal{M}_0+\sum_{\mathbf{u}\subset\{1,\ldots,M\},\,\mathbf{u}\neq\mathbf{0}}\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}}), \tag{3}$$

in which $\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})$ is the summand including the subset of parameters $\boldsymbol{X}_{\mathbf{u}}$. According to [23], a unique decomposition requires the orthogonality of the summands, *i.e.*:

$$\mathbb{E}[\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})\,\mathcal{M}_{\mathbf{v}}(\boldsymbol{X}_{\mathbf{v}})]=\int_{\mathcal{H}^M}\mathcal{M}_{\mathbf{u}}(\boldsymbol{x}_{\mathbf{u}})\,\mathcal{M}_{\mathbf{v}}(\boldsymbol{x}_{\mathbf{v}})\,\mathrm{d}\boldsymbol{x}=0,\quad \mathbf{u}\neq\mathbf{v} \tag{4}$$

In particular each summand shall be of zero mean value. Accordingly the variance of the response $Y=\mathcal{M}(\boldsymbol{X})$ reads:

$$D\overset{\text{def}}{=}\mathrm{Var}[Y]=\sum_{\mathbf{u}\subset\{1,\ldots,M\},\,\mathbf{u}\neq\mathbf{0}}\mathrm{Var}[\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})]. \tag{5}$$

In this expansion $\mathrm{Var}[\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})]$ is the contribution of summand $\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})$ to the output variance.

The *Sobol' sensitivity index* $S_{\mathbf{u}}$ for the subset of variables $\boldsymbol{X}_{\mathbf{u}}$ is defined as follows [24]:

$$S_{\mathbf{u}}\overset{\text{def}}{=}\frac{D_{\mathbf{u}}}{D}=\frac{\mathrm{Var}[\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})]}{D} \tag{6}$$

The *total sensitivity index* for subset $\boldsymbol{X}_{\mathbf{u}}$ is given by [24]

$$S_{\mathbf{u}}^T\overset{\text{def}}{=}\frac{D_{\mathbf{u}}^T}{D}=\sum_{\mathbf{v}\supset\mathbf{u}}\frac{\mathrm{Var}[\mathcal{M}_{\mathbf{v}}(\boldsymbol{X}_{\mathbf{v}})]}{D} \tag{7}$$

where the sum is extended over all sets $\mathbf{v}=\{j_1,\ldots,j_t\}$ which contains $\mathbf{u}$. It represents the total amount of uncertainty apportioned to the subset of variables $\boldsymbol{X}_{\mathbf{u}}$. For instance, for a single variable $X_i,\ i=1,\ldots,M$ the *first order* Sobol' sensitivity index reads:

$$S_i=\frac{\mathrm{Var}[\mathcal{M}_i(X_i)]}{D}, \tag{8}$$

and the total Sobol' sensitivity index reads:

$$S_i^T=\sum_{\mathbf{v}\ni i}\frac{\mathrm{Var}[\mathcal{M}_{\mathbf{v}}(\boldsymbol{X}_{\mathbf{v}})]}{D}. \tag{9}$$

S_i and S_i^T respectively represent the sole and total effect of the factor X_i on the system's output variability. The smaller S_i^T is, the less important the factor X_i is. In the case when $S_i^T\ll 1$, say $S_i^T\approx 1$–5%, X_i is considered as unimportant (unessential or insignificant) and may be replaced in the analysis by a deterministic value.

In the literature one can find different approaches for computing the total Sobol' indices, such as the Monte Carlo simulation (MCS) and the spectral approach. Refs. [23,24] proposed direct estimation of the sensitivity indices for subsets of variables using only the model evaluations at specially selected points. The approach relies on computing analytically the integral representations of $D_{\mathbf{u}}$ and $D_{\mathbf{u}}^T$ respectively defined in Eqs. (6) and (7).

Let us denote by $\overline{\mathbf{u}}$ the set that is complementary to $\mathbf{u}$, *i.e.* $\boldsymbol{X}=(\boldsymbol{X}_{\mathbf{u}},\boldsymbol{X}_{\overline{\mathbf{u}}})$. Let $\boldsymbol{X}$ and $\boldsymbol{X}'$ be vectors of independent uniform variables defined on the unit hypercube $\mathcal{H}^M$ and define $\boldsymbol{X}'=(\boldsymbol{X}'_{\mathbf{u}},\boldsymbol{X}'_{\overline{\mathbf{u}}})$. The partial variance $D_{\mathbf{u}}$ is represented as follows [25]:

$$D_{\mathbf{u}}=\iint\mathcal{M}(\boldsymbol{x})\mathcal{M}(\boldsymbol{x}_{\mathbf{u}},\boldsymbol{x}'_{\overline{\mathbf{u}}})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{x}'_{\overline{\mathbf{u}}}-\mathcal{M}_0^2 \tag{10}$$

The total variance $D_{\mathbf{u}}^T$ is given by [25]

$$D_{\mathbf{u}}^T=\frac{1}{2}\iint[\mathcal{M}(\boldsymbol{x})-\mathcal{M}(\boldsymbol{x}'_{\mathbf{u}},\boldsymbol{x}_{\overline{\mathbf{u}}})]^2\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{x}_{\overline{\mathbf{u}}} \tag{11}$$

A Monte Carlo algorithm is used to estimate the above integrals. For each sample point, one generates two M-dimensional samples $\boldsymbol{x}=(\boldsymbol{x}_{\mathbf{u}},\boldsymbol{x}_{\overline{\mathbf{u}}})$ and $\boldsymbol{x}'=(\boldsymbol{x}'_{\mathbf{u}},\boldsymbol{x}'_{\overline{\mathbf{u}}})$. The function is evaluated at three points $(\boldsymbol{x}_{\mathbf{u}},\boldsymbol{x}_{\overline{\mathbf{u}}})$, $(\boldsymbol{x}'_{\mathbf{u}},\boldsymbol{x}_{\overline{\mathbf{u}}})$ and $(\boldsymbol{x}_{\mathbf{u}},\boldsymbol{x}'_{\overline{\mathbf{u}}})$. Using N independent sample points, one computes the quantities of interest D, $D_{\mathbf{u}}$ and $D_{\mathbf{u}}^T$ by means of the following crude Monte Carlo estimators:

$$\mathcal{M}_0=\frac{1}{N}\sum_{i=1}^{N}\mathcal{M}(\boldsymbol{x}^{(i)}) \tag{12}$$

$$D+\mathcal{M}_0^2=\frac{1}{N}\sum_{i=1}^{N}[\mathcal{M}(\boldsymbol{x}^{(i)})]^2 \tag{13}$$

$$D_{\mathbf{u}}+\mathcal{M}_0^2=\frac{1}{N}\sum_{i=1}^{N}\mathcal{M}(\boldsymbol{x}^{(i)})\mathcal{M}(\boldsymbol{x}_{\mathbf{u}}^{(i)},\boldsymbol{x}_{\overline{\mathbf{u}}}^{(i)\prime}) \tag{14}$$

$$D_{\mathbf{u}}^T=\frac{1}{N}\sum_{i=1}^{N}\frac{1}{2}\left[\mathcal{M}(\boldsymbol{x}^{(i)})-\mathcal{M}\left(\boldsymbol{x}_{\mathbf{u}}^{(i)\prime},\boldsymbol{x}_{\overline{\mathbf{u}}}^{(i)}\right)\right]^2 \tag{15}$$

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