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On the use of derivatives in the PC-based non-intrusive global sensitivity and uncertainty analysis applied to high-dimensional distributed models

Conference Abstract

Uncertainty quantification (UQ) is an important step in analysis and validation of results in numerical modeling. In practice, this implies the uncertainty in a design function (Quantity of Interest (QoI)) to be characterized, given an uncertainty in the model inputs. The UQ methods are recently applied in the field of computational fluid dynamics [5, 2] involving the distributed-parameter nonlinear flow models. The set of inputs for such models is often high-dimensional, since it may include the distributed (spatially, temporally) initial and boundary conditions, source terms and/or fields of model coefficients. Due to the nonlinearity, a possible use of the linearized variants (tangent linear model) for uncertainty propagation is often limited. A special feature of the distributed systems with regard to UQ is that, sometimes, no edge between 'influential' and 'non-influential' inputs can be defined. Thus, the size of the 'influential' subset (active set) remains quite significant.

One possible option to deal with strong nonlinearity and large uncertainties is to use the polynomial chaos (PC) expansion. The straightforward implementation of the PC method is rarely possible, however. The 'intrusive' implementation of the PC approach leads to computationally feasible algorithms, but implies the development of 'spectral' counterparts of existing models [7], which requires a significant development effort. Besides, the accuracy of such surrogate models is often questionable. Non-intrusive methods of different nature (involving the PC approach) involve constructing the response surface by running the existing models [3, 6]. It is clear, however, that the possible number of runs may be bounded due to limitations in available computational resources.

The idea of using the gradient information seems particularly useful for CFD models involved in variational data assimilation, because for such models the adjoint model is available. The gradient-enhanced method for computing the PC expansion have received attention recently, e.g. [8, 1], etc. Here the gradient (first derivative of the design function) is used as a data in a specially defined cost-function to be minimized. This approach, often referred as 'regression', has certain drawbacks. In particular, the solvability of the regression problem depends on the condition number of its system matrix, which is proportional to the size of the sought vector of the PC coefficients $b = \{b_0, b_{i_1}, b_{i_1 i_2}, \dots, b_{i_1 \dots i_p}\}$, given by the formula

$$M = \frac{(N+p)!}{N!\,p\,!}, \tag{1}$$

where N is the size of the active set, and p is the chosen order of polynomials. Let us also note that the computational cost of solving the regression problem rapidly grows with the size of the active set and, starting from a certain point, may become a major computational bottleneck.

In contrast, here we present an explicit method for estimating the PC coefficients using the derivatives of the design function of any order, which may be regarded as a generalization of the 'projection' method [4]. The key feature of this approach is that the accuracy of the estimated PC coefficients depends on the 'statistical conditioning', which is independent on the size of b. In addition, we suggest an improved variant of the derivative-based global sensitivity measure suggested in [9].

Let us define the design function $\varepsilon(\xi)$ dependent on the input uncertainties ξ, and consider its PC expansion using 'probabilistic' Hermite polynomials H in the form

$$\varepsilon(\xi) = b_0 H_0 + \sum_{i_1=1}^{N} b_{i_1} H_1(\xi_{i_1}) + \sum_{i_1=1}^{N} \sum_{i_2=1}^{i_1} b_{i_1 i_2} H_2(\xi_{i_1}, \xi_{i_2}) + \sum_{i_1=1}^{N} \sum_{i_2=1}^{i_1} \sum_{i_3=1}^{i_2} b_{i_1 i_2 i_3} H_3(\xi_{i_1}, \xi_{i_2}, \xi_{i_3}) + ...+$$

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$$+\sum_{i_1=1}^{N}\sum_{i_2=1}^{i_1}\cdots\sum_{i_p=1}^{i_{p-1}} b_{i_1 i_2 \ldots i_p} H_p(\xi_{i_1}, \xi_{i_2}, \ldots, \xi_{i_p}). \tag{2}$$

The main results are collected in two theorems:

Theorem 1. For the coefficients b_0, $\{b_i\}$, $\{b_{ij}\}$, $\{b_{ijk}\}$, $i = 1, \ldots, N$, $1 \le j < i$, $1 \le k < j$ of the expansion (2), the following expressions hold:

$$b_0 = E[\varepsilon(\xi)], \tag{3}$$

$$\beta_i b_i = E[H_1(\xi_i)\varepsilon(\xi)] = E\left[H_0 \frac{\partial \varepsilon(\xi)}{\partial \xi_i}\right], \tag{4}$$

$$\beta_{ij} b_{ij} = E\left[H_2(\xi_i, \xi_j)\varepsilon(\xi)\right] = E\left[H_1(\xi_i)\frac{\partial \varepsilon(\xi)}{\partial \xi_j}\right] = E\left[H_0 \frac{\partial^2 \varepsilon(\xi)}{\partial \xi_i \partial \xi_j}\right], \tag{5}$$

$$\beta_{ijk} b_{ijk} = E\left[H_3(\xi_i, \xi_j, \xi_k)\varepsilon(\xi)\right] = E\left[H_2(\xi_i, \xi_j)\frac{\partial \varepsilon(\xi)}{\partial \xi_k}\right] = E\left[H_1(\xi_i)\frac{\partial^2 \varepsilon(\xi)}{\partial \xi_j \partial \xi_k}\right] =$$

$$= E\left[H_0 \frac{\partial^2 \varepsilon(\xi)}{\partial \xi_i \partial \xi_j \partial \xi_k}\right], \tag{6}$$

where β are constants.

Theorem 2. The expectation of the squared gradient is given by the series

$$E\left[\left(\frac{\partial \varepsilon(\xi)}{\partial \xi_i}\right)^2\right] = \tilde{\beta}_i b_i^2 + \sum_{j=1}^{i} \tilde{\beta}_{ij} b_{ij}^2 + \sum_{j=1}^{i}\sum_{k=1}^{j} \tilde{\beta}_{ijk} b_{ijk}^2 + ..., \tag{7}$$

where $\tilde{\beta} \ge \beta$ are constants.

Proof of these theorems is based on the PC expansion formulation given in [10].

Theorem 1 gives explicit expressions for computing the PC expansion coefficients using derivatives. In practice, their direct use is not possible for a small sample size L. Thus, these expressions are complemented with an efficient (relatively cheap) explicit filtering procedure which allows the major part of the sampling error to be removed. The suggested technique is useful for filtering the second and third order PC coefficients, which form a square and a cube, respectively, whereas its extension for higher-order tensors is not feasible in its present form. Let us note, however, that for the expected size of the active set, using polynomials of $p > 3$ seems quite unlikely anyway.

Theorem 2 provides a basis for improving the upper-bound estimate on the 'total effect' global sensitivity indices. The original estimate suggested in [9] reads as follows:

$$\mathcal{S}_i^T \; Var(\varepsilon(\xi)) < E\left[\left(\frac{\partial \varepsilon(\xi)}{\partial \xi_i}\right)^2\right]. \tag{8}$$

For a given sample of size L, this estimate can be improved by using

$$\mathcal{S}_i^T \; \overline{Var}(\varepsilon(\xi)) < \frac{1}{L}\sum_{i=1}^{L}\left(\frac{\partial \varepsilon(\xi^{(l)})}{\partial \xi_i}\right)^2 - \sum_{j=1}^{i}(\tilde{\beta}_{ij} - \beta_{ij}) b_{ij}^2 - \sum_{j=1}^{i}\sum_{k=1}^{j}(\tilde{\beta}_{ijk} - \beta_{ijk}) b_{ijk}^2 - ..., \tag{9}$$

where $\overline{Var}$ stands for the sample variance and $b_{ij}, b_{ijk}, ...$ are the estimated PC expansion coefficients based on this sample. The explicit estimation of b is not expensive even for large enough N; thus (9) should be preferred to (8).

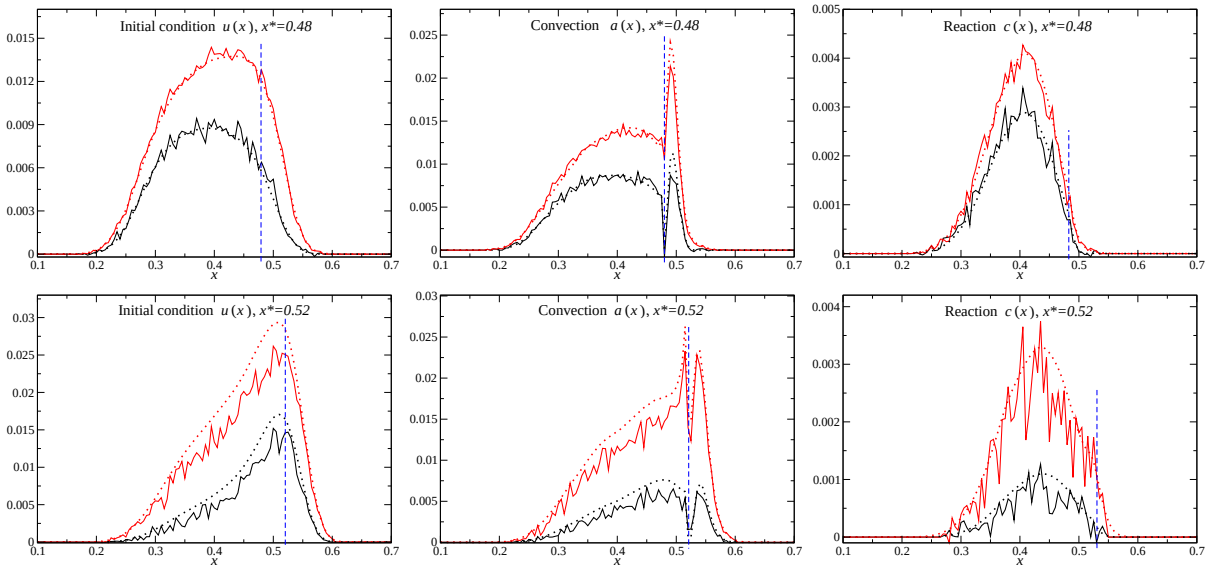

Figure 1: Fist-order 'main-effect' (in black) and 'total-effect' (in red) global sensitivity indices by direct Monte-Carlo (in solid lines) and using the gradient-based upper-bound estimates (in dashed lines).

Numerical experiments have been performed for the 1D generalized Burger's equation. The flow forecast error at the chosen spatial point averaged over the given time interval is considered as the design function $\varepsilon(\xi)$, which depends on the uncertainties ξ in the initial conditions $u(x)$ and distributed convection $a(x)$, diffusion $d(x)$ and reaction $c(x)$ coefficients. The discretized Burger's equation contains $n = 200$ nodes in space, therefore the size of the complete input vector is equal to $N = 800$. After considering the 'total effect' sensitivity indices $\mathcal{S}_i^T$ (see Fig.1), the active set of size $N' = 200$ is defined. The sample of design functions and gradients of size $L = 400$ is computed first. For the active set the third-order PC expansion is constructed, then a histogram is built using the meta-model ((see Fig.2)). The results show that taking into account the second- and third-order interactions allows the essential non-gaussian features in the probability distribution of $\varepsilon(\xi)$ to be revealed (as compared to the first-order approximation, which is gaussian by definition). One can note that the second-order interactions mainly contribute to the skewness, whereas the third-order interactions - into kurtosis.

In conclusion, the presented method [3] is an essential non-intrusive tool for the global sensitivity and uncertainty analysis, designed for high-dimensional distributed-parameter models (i.e. those governed by the partial differential equations). The size of the active set in such models could remain quite significant, which means that a low-order PC expansion (say $p \leq 3$) can only be afforded. Our method belongs to the group of 'projection' methods, allowing the explicit estimation of the PC expansion coefficients. The novelty is that it allows the derivatives of any order to be used (not only the gradient but, also, the second-order derivative or Hessian, for example), in combination with the explicit filtering procedure. The advantage of the method (in contrast with regression methods) is that the sample size (L) required for estimating the PC coefficients does not depend on the size of the active set (N).

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[3] The presented material is a summary of the paper submited and currently under review in *Computer Methods in Applied Mechanics and Engineering*.

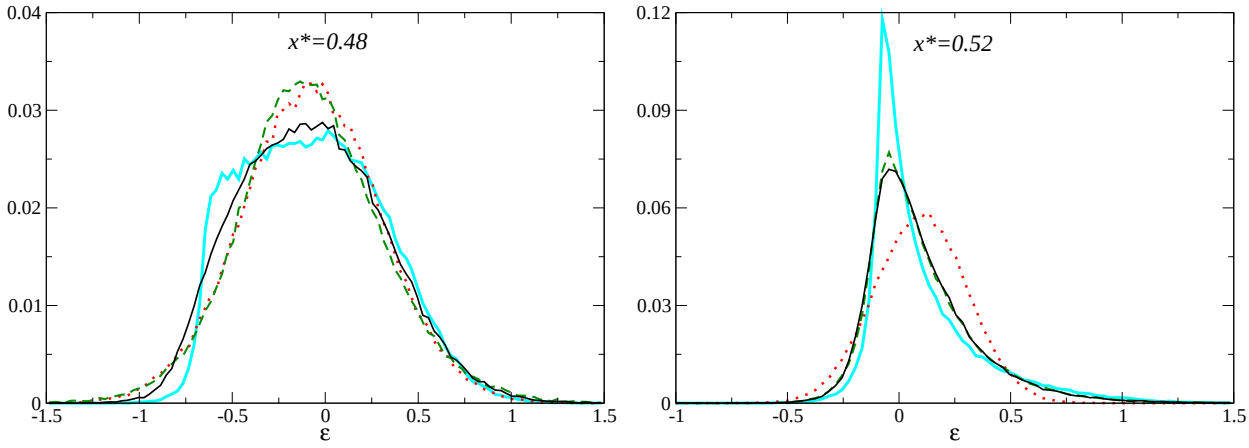

Figure 2: Distribution of $\varepsilon(\xi)$ (histograms), for $L = 400$. Solid pale (light blue) line - the reference histogram by Monte Carlo for large sample, dotted (red) line - using first-order meta-model, dashed (green) line - using second-order meta-model and solid (black) - using third-order meta-model.

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