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Derivative-based sensitivity indices based on polynomial chaos expansions

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Global sensitivity analysis has emerged in the last 15 years as a powerful tool for improving the understanding of complex environmental, industrial or civil systems. In many fields of applied and engineering sciences indeed, computer simulation models are now inescapable. The increasing computer power which is available through large clusters of CPUs has made it possible to develop models with increasing fidelity (*e.g.* accounting for physical couplings) at the price of an increasing number of input parameters. In practice most of the parameters (corresponding for instance to initial or boundary conditions for evolutionary systems) are not well known. A probabilistic approach is then suitable for modelling the uncertainties about these parameters. Then the question of the relative impact of these uncertainties onto the model predictions naturally arises.

Global sensitivity analysis aims at determining which input parameters of the model (resp. which combination of input parameters) have the greatest influence on the variability of the model output [1]. Several methods are now well established depending on the type of information that is required:

- Screening methods [2,3] aim at finding which parameters have no influence on the model output at a low computational cost.
- Variance-based sensitivity indices such as the Sobol' indices aim at describing how the variance of the model output can be decomposed in terms of contributions of each input parameters or combinations thereof [4].
- Distribution-based sensitivity indices quantify how much the distribution of the output changes when some input parameters are fixed [5,6].
- Derivative based sensitivity indices that have been recently proposed in [7,8] may be viewed as a generalization of Morris importance measure.

In the context of industrial applications the computation budget, *i.e.* the number of affordable runs of the computational model that is allowed to evaluate the sensitivity indices is rather low, typically less than 1,000. Thus the classical Monte Carlo-based estimators of the various sensitivity indices listed above are not applicable.

In this paper we will concentrate on the last category of indices, namely the derivative-based sensitivity indices. Consider a random vector \mathbf{X} of dimension M with independent components and joint probability density function $f_{\mathbf{X}}$. Let us denote by $Y = \mathcal{M}(\mathbf{X})$ the random response of the simulation model of interest. The derivative based sensitivity indices (DGSM) are defined by:

$$\nu_j = \mathbb{E} \left[\left(\frac{\partial \mathcal{M}}{\partial x_j}(\mathbf{X}) \right)^2 \right] \quad (1)$$

In order to efficiently compute them efficiently a *polynomial chaos expansion* of the model output is used [9]:

$$Y = \sum_{\alpha \in \mathbb{N}^M} a_{\alpha} \Psi_{\alpha}(\mathbf{X}) \quad (2)$$

where $\Psi_{\alpha}(\mathbf{X})$ are multivariate orthonormal polynomials with respect to the probability measure associated with random vector \mathbf{X} . In the present paper we use *sparse* polynomial chaos expansions whose basis functions are selected using the Least Angle regression algorithm [10,11].

The accuracy of the sparse polynomial chaos expansion is checked by a leave-one-out cross-validation procedure. Once a sufficient accuracy has been obtained, the PC expansion is post-processed in order to compute the derivative-based sensitivity indices. The very polynomial nature of the expansion makes it possible to compute *analytically* the derivatives of the PC expansions.

The proposed approach is illustrated on several application examples that have been addressed in the recent literature, especially in [8,12]. The convergence of the indices as a function of the global leave-one-out mean square error is checked.

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