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A comparison of three metamodel-based methods for global sensitivity analysis: GP modelling, HDMR and LAR-gPC

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Abstract

Three metamodel-based method are compared for computing the Sobol' indices of models featuring uncertain input parameters, namely Gaussian Process (GP) modelling, High-Dimensional Model Representation (HDMR) and Least Angle Regression-based generalized Polynomial Chaos expansions (LAR-gPC). The approaches are applied to the computation of the Sobol' indices of several test functions featuring 3-50 input random variables. The computational costs and convergence rates associated with each scheme are compared. Eventually the strengths and weaknesses of each technique are highlighted and discussed.

Keywords: global sensitivity analysis; metamodels; Sobol' indices; high-dimensional model representation; polynomial chaos expansion; Gaussian process modelling; Least Angle Regression

Global sensitivity analysis aims at quantifying the relative importance of uncertain input variables onto the response of a mathematical model of a physical system. ANOVA-based indices such as the Sobol' indices are well-known in this context (Sobol', 1993). These indices are usually computed by direct Monte Carlo or quasi-Monte Carlo simulation, which may reveal hard to apply for computationally demanding industrial models. As an alternative, it is possible to replace the model with an analytical approximation which may be evaluated at a negligible cost. Such an approximation is usually referred to as a response surface or a metamodel in the literature. In this context, all the computational effort is focused on the metamodel fitting.

Many kinds of metamodels have been proposed in order to perform sensitivity analysis, see for instance the comparative study in Storlie et al. (2009). The present paper is dedicated to three specific techniques, namely GP modelling, HDMR and LAR-gPC. Gaussian Process (GP) modelling relies upon the assumption that the response of the model under consideration is a sample path of an underlying Gaussian random field. Such a stochastic framework is a way to represent the epistemic uncertainty associated with the prediction of the model at an untried set of input parameters. A nice feature of the method is that it provides a metamodel together with confidence intervals on the predictions. A Bayesian formulation of GP modelling as well as analytical formulae for computing the Sobol' indices may be found in Oakley and O'Hagan (2004); Marrel et al. (2009).

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The so-called High-Dimensional Model Representation (HDMR) method has been devised in Rabitz et al. (1999). It consists in approximating the functions arising from the ANOVA decomposition of the model response, up to a given interaction order. Such an approach leads to neglect those ANOVA components that involve a high number of input parameters, according to the so-called *sparsity-of-effects principle* (Montgomery, 2004) which states that most models are principally governed by main effects and low-order interactions. The use of metamodels made of orthogonal polynomials has been proposed in Li et al. (2002) to represent the ANOVA functions. In this setup, the Sobol' indices may be computed by elementary operations on the coefficients that appear in the various representations. A procedure for automatically selecting the polynomial degrees has been implemented in the GUI-HDMR Matlab toolbox (Ziehn and Tomlin, 2009).

Lastly, an adaptive strategy based on the polynomial chaos (PC) expansion of the model response has been detailed in Blatman (2009); Blatman and Sudret (2009), namely LAR-gPC (for Least Angle Regression-based generalized PC). This scheme is similar to HDMR since it is also based on a representation in terms of orthogonal polynomials. Nonetheless, the PC scheme relies upon a direct approximation of the whole model response rather than its ANOVA components. As in HDMR, the Sobol' indices may be computed analytically from the PC coefficients (Sudret, 2008). The LAR-gPC method allows the analyst to build up a *sparse* PC approximation of the response, i.e. a representation which contains a small number of nonzero terms. Thus the few related coefficients may be evaluated using a low number of model evaluations, i.e. at a reduced computational cost. Precisely, the significant PC terms are iteratively selected using the Least Angle Regression (LAR) algorithm (Efron et al., 2004). This adaptive selection of PC terms is coupled to an automatic enrichment of the experimental design, i.e. the set of realizations of the random input variables at which the model has to be evaluated.

The GP modelling, HDMR and LAR-gPC methods are applied to the computation of the Sobol' indices of several test functions (whose evaluation is inexpensive) featuring 3-50 input random variables. In this purpose, *quasi-random* computer experimental designs with size varying from 256 to 4,096 are used. The computational costs and convergence rates associated with each scheme are compared. Eventually the strengths and weaknesses of each technique are highlighted and discussed.

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