On the construction of adaptive design of experiments for the approximation of complex computer code behaviors

Jean Baccou
Institut de Radioprotection et de Sûreté Nucléaire,
Laboratoire de Micromécanique et d'Intégrité des Structures (IRSN-CNRS-UM),
B.P. 3, 13115 Saint Paul-Lez-Durance, France
jean.baccou@irsn.fr

The analysis of the behavior of complex computer codes is a key topic in many industrial applications. When taking into account uncertainties, it is for example crucial to ensure that a system cannot deviate from its reference state and lead to unsafe conditions. From a methodological point of view, a computer code can be interpreted as an objective function $f : X \in \mathcal{D} \subset \mathbb{R}^d \mapsto y \in \mathbb{R}^{\tilde{d}}$ where X stands for the vector of input parameters and y is the response of interest. The relevance of the mathematical treatment essentially relies on the choice of the set of input values called design of experiments (DoEs) where the objective function is evaluated. There exists many approaches to construct such designs. The first one is based on the exploration of the whole input set [1]. However, when the computational budget is limited, this strategy is not satisfactory in the case of objective functions exhibiting heterogeneous behaviors for example. It is then more efficient to refine the design in regions of interest (such as high variation zones) where extra information is required to specify the code response behavior. It leads to adaptive DoEs. Their construction first relies on a modeling of the code response from a DoE with few evaluations then on the optimization of an infill criterion that provides the new evaluations to perform according to the type of regions of interest. This process is applied sequentially in order to update and improve the model at each iteration.
In this work, we describe several developments related to the construction of adaptive DoEs. They are all based on a modelling in the frame of Gaussian processes which is very popular for the analysis of computer experiments [2]. After an overview on existing approaches to handle the construction of adaptive DoEs, we introduce two recent contributions. The first one is related to the treatment of optimization problems involving complex computer codes [3]. The second one deals with the analysis of computer code responses exhibiting heterogeneous behaviors [4]. All these developments are illustrated on several test cases coming from IRSN nuclear studies.

Joint work with: C. Chevalier (UniNE), N. Garland (IRSN), D. Ginsbourger (UniBE/IDIAP), J. Liandrat (ECM/I2M), S. Marmin (IRSN), Y. Monerie (UM), F. Perales (IRSN)

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