Adaptive kriging meta-models for the simulation of rare events by importance sampling

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1 Context of the Ph.D thesis

In structural mechanics, design optimization is the decision-making process that aims at finding the best set of design variables; namely, the one that minimizes some cost model while satisfying some performance model requirements. Due to the inconsistency between these two objectives, the optimal solutions often lie on the boundaries of the admissible space. Such solutions are rather sensitive to the uncertainties either in the model parameters (aleatory) or in the model itself (epistemic). A first alternative to *deterministic design optimization* (DDO) is the *partial safety factor* (PSF) approach which copes with uncertainties through the application of safety coefficients specified in the codes of practice. Nevertheless, it is often argued that such approaches do not permit a tuning of the reliability level and might thus lead to overdesign. *Reliability-based design optimization* (RBDO) is a more optimal approach as it accounts explicitly for the uncertainties along the optimization process.

Based on a probabilistic model of the model input parameters $\boldsymbol{X}$, the deterministic performance constraint is transformed into a probabilistic constraint and one aims at finding the optimal set of hyperparameters in the joint *probability density function* (PDF) $f_{\boldsymbol{X}}(\boldsymbol{x} \mid \boldsymbol{\theta})$ that minimizes $c(\boldsymbol{\theta})$. This reads:

$$\boldsymbol{\theta}^* = \arg \min_{\boldsymbol{\theta} \in \mathcal{D}_{\boldsymbol{\theta}}} c\left(\boldsymbol{\theta}\right) \;:\; \begin{cases} f_i\left(\boldsymbol{\theta}\right) \leq 0,\; i = 1, \ldots, n_c \\ \mathbb{P}\left(g_l\left(\boldsymbol{X}\left(\boldsymbol{\theta}\right)\right) \leq 0\right) \leq P_{f\,l}^0,\; l = 1, \ldots, n_p \end{cases} \tag{1}$$

In this formulation, c is the objective function to be minimized with respect to the design variables $\boldsymbol{\theta} \in \mathcal{D}_{\boldsymbol{\theta}}$, while satisfying to n_c deterministic soft constraints $\{f_i,\; i = 1, \ldots, n_c\}$ bounding the so-called *admissible design space* defined by the analyst. A *deterministic design optimization* (DDO) problem would simply require additional performance functions $\left\{g_l,\; l = 1, \ldots, n_p\right\}$ describing system failure with respect to the specific code of practice. As opposed to the previous soft constraints, these functions often involve the output of an expensive-to-evaluate black-box function $\mathcal{M}$. RBDO differs from DDO in the sense that these constraints are wrapped into n_p probabilistic constraints $\left\{\mathbb{P}\left(g_l\left(\boldsymbol{X}\right) \leq 0\right) \leq P_{f\,l}^0,\; l = 1, \ldots, n_p\right\}$. $P_{f\,l}^0$ is the minimum safety requirement expressed here in the form of an acceptable *probability of failure* which may be different for each performance function g_l. Such probabilities of failure are conveniently defined in terms of the following multidimensional integrals:

$$P_{f\,l}\left(\boldsymbol{\theta}\right) = \mathbb{P}\left(g_l\left(\boldsymbol{X}\left(\boldsymbol{\theta}\right)\right) \leq 0\right) = \int_{g_l(\boldsymbol{x}) \leq 0} f_{\boldsymbol{X}}\left(\boldsymbol{x} \mid \boldsymbol{\theta}\right) \mathrm{d}\boldsymbol{x}, \quad l = 1, \ldots, n_p \tag{2}$$

These latter quantities are known to be expensive-to-evaluate when both the performance model involves the output of a high-fidelity computer code, and the system to be designed tends to become highly reliable – which is the purpose of the optimization process.

The purpose of the Ph.D thesis is to propose a computational strategy that is able to solve the RBDO problem efficiently when the performance model involves the output of an expensive-to-evaluate black-box function – *e.g.* a nonlinear finite-element model. This is the reason why the so-called *variance reduction* (Rubinstein and Kroese, 2008) techniques have been explored.

2 Contributions

The presentation will review some contributions to the field of reliability-based design whose common purpose is to provide a computational strategy that is able to solve the problem in Eq. (1) within a reasonable amount of time.

To do so, we first resort to an approximation of the expensive-to-evaluate performance model and try to *quantify* and *reduce* the error introduced by such an approximation. The so-called meta-model is built from a set of observations (a design of experiments) of the real performance model using the kriging technique (Lophaven et al., 2002; Santner et al., 2003). One interesting fact about kriging is that it provides a probabilistic (Gaussian) prediction which is convenient to elaborate refinement techniques as reviewed in the sequel.

The first contribution is a sampling alternative to the conventional global optimization schemes used for the adaptive refinement of kriging predictions. It basically consists in considering the so-called *in-fill criteria* (denoted by C) like the ones proposed in *e.g.* Oakley (2004) or Picheny et al. (2010) as improper PDFs for the improvement points **C**. Indeed it is assumed that:

$$\boldsymbol{C} \sim \frac{C(\boldsymbol{c})\, w(\boldsymbol{c})}{\int C(\boldsymbol{x})\, w(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}} \propto C(\boldsymbol{c})\, w(\boldsymbol{c}) \tag{3}$$

where w is a weighting PDF used to ensure that the normalizing integral is finite. Different weighting PDFs might be used depending on the space of interest: *e.g.* $w(x) = f_{\boldsymbol{X}}(\boldsymbol{x})$. A Markov chain Monte-Carlo technique known as slice sampling (Neal, 2003) is then used in order to generate a population of candidate points distributed according to this improper PDF. The resulting population is finally reduced to its K cluster centers for evaluation and refinement of the kriging prediction.

Another contribution that will be developped in the presentation concerns an alternative to crude substitution for metamodel-based reliability analysis. Here, we propose to use the kriging probabilistic prediction in order to build a non-parametric quasi-optimal importance sampling density (Rubinstein and Kroese, 2008) suited for the efficient estimation of low probabilities in possibly high-dimensional spaces where the kriging strategy is known to lose efficiency. In addition to the failure probability estimator, we derive its sensitivities *w.r.t.* the parameters $\boldsymbol{\theta}$ in the joint PDF of the random input $\boldsymbol{X}$ based on the work by Song et al. (2009).

3 About the authors

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