Reliability Engineering and System Safety 149 (2016) 130–136

Contents lists available at ScienceDirect

Reliability Engineering and System Safety

journal homepage: www.elsevier.com/locate/ress

Active learning surrogate models for the conception of systems with multiple failure modes

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ARTICLE INFO

Article history:
Received 2 June 2015
Received in revised form
13 December 2015
Accepted 19 December 2015
Available online 13 January 2016

Keywords:
Computer experiments
Gaussian Processes
System reliability
Sequential design

ABSTRACT

Due to the performance and certification criteria, complex mechanical systems have to taken into account several constraints, which can be associated with a series of performance functions. Different software are generally used to evaluate such functions, whose computational cost can vary a lot. In conception or reliability analysis, we thus are interested in the identification of the boundaries of the domain where all these constraints are satisfied, at the minimal total computational cost. To this end, the present work proposes an iterative method to maximize the knowledge about these limits while trying to minimize the required number of evaluations of each performance function. This method is based first on Gaussian process surrogate models that are defined on nested sub-spaces, and second, on an original selection criterion that takes into account the computational cost associated with each performance function. After presenting the theoretical basis of this approach, this paper compares its efficiency to alternative methods on an example.

1. Introduction

The conception (or risk assessment) of complex mechanical systems has to take into account a series of constraints. Such constraints can be due to certification criteria, performance objectives, cost limitations, and so on. In this context, the role of simulation has kept increasing for the last decades, as one should be able to predict if a given configuration of the system is likely to fulfil these constraints without having to build it and to test it experimentally. In many cases, the computation of these constraints is associated with a series of computer software, whose physics can vary a lot. For instance, in the car industry, the conception of a new vehicle can be subjected to constraints on its size and weight, which are rather easy to compute, but also on its emergency stopping distance, its crash or aerodynamic resistance, which can be much more difficult to evaluate.

To be more precise, let us consider a particular system, $\mathcal{S}$, which design is supposed to be characterized by a vector of d parameters, $\boldsymbol{x} = (x_1, \ldots, x_d) \in \mathbb{R}^d$. It is assumed that the system constraints can be evaluated from the computation of $N \geq 1$ performance functions, $\{g_n, 1 \leq n \leq N\}$, which respective numerical cost (in CPU time for instance), C_n, are supposed to be sorted in an ascending order:

$$C_1 \leq C_2 \leq \cdots \leq C_N. \tag{1}$$

Thus, the conception domain, which is denoted by Ω and which defines the set of admissible designs for the considered system, can be written as:

$$\Omega = \bigcap_{n=1}^{N} \Omega_n, \quad \Omega_n = \{\boldsymbol{x} \in \mathbb{R}^d, \quad g_n(\boldsymbol{x}) \leq 0\}. \tag{2}$$

Such a domain is a key element to perform optimizations of the system restricted to admissible design solutions, while being closely linked to reliability analysis prospects, as its complementary, $\mathbb{R}^d \backslash \Omega$, corresponds to the failure domain of the system. Hence, for the last decades, the identification of Ω, or of its boundary, $\partial\Omega$, has motivated the development of several methods, which can be sorted in two main categories: the direct and the indirect methods. Among the direct methods, the first-order or second-order reliability methods (FORM/SORM) approximate $\partial\Omega$ as a linear or a second-order polynomial function [9,14,13,4]. When confronted to applications where the limit state is multimodal or is strongly non-linear, alternative methods based on more advanced approximations have been introduced, such as support vector machines (SVM) techniques [19,17,11] and methods based on generalized least-squares linear regression [18,10].

On the other hand, the indirect methods focus on the approximation of the performance functions to deduce in a second step the searched boundary. Among these methods, the Gaussian process regression (GPR) method, or kriging, keeps playing a major role, which is due to its ability to provide a robust approximation of $\partial\Omega$, that is to say for which precision can be quantified [15,12,16,7].

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http://dx.doi.org/10.1016/j.ress.2015.12.017
0951-8320/

Based on this very efficient tool, the idea of this paper is to present a sequential sampling strategy to minimize the uncertainties about boundary $\partial\Omega$, at the minimal computational budget. In particular, the proposed strategy will take into account the computational costs associated with the evaluation of each function, $\{C_1, \ldots, C_N\}$.

The outline of this work is as follows. First, Section 2 presents the theoretical bases of the Gaussian process regression (GPR) and its use for the identification of limit states. The proposed method is then introduced in Section 3. Then, the efficiency of the method is illustrated on an analytic example in Section 4.

2. Surrogate models for system reliability

The Gaussian process regression is based on the assumption that each performance function, g_n, $1 \le n \le N$, can be seen as a sample path of a stochastic process, which is supposed to be Gaussian for the sake of tractability. By conditioning this Gaussian process by a set of $Q \ge 1$ code evaluations, $\mathcal{S}^{\text{learn}} = \{(\boldsymbol{x}^{(q)}, g_n(\boldsymbol{x}^{(q)})), 1 \le q \le Q\}$, it is possible to define very interesting predictors for the value of g_n in any non-computed point of the input space. These predictors of functions g_n at any $\boldsymbol{x}$ in $\mathbb{R}^d$, which are respectively denoted by $\widehat{g}_n(\boldsymbol{x})$, are Gaussian by construction, $\widehat{g}_n(\boldsymbol{x}) \sim \mathcal{N}(\widehat{\mu}_n(\boldsymbol{x}), \widehat{\sigma}_n^2(\boldsymbol{x}))$, and we refer to [15,16] for further details about the expression of the conditioned means, $\widehat{\mu}_n(\boldsymbol{x})$, and standard deviations, $\widehat{\sigma}_n^2(\boldsymbol{x})$. Such a predictor interpolates in the sense that, for all $1 \le q \le Q$,

$$\mathbb{P}(\widehat{g}_n(\boldsymbol{x}^{(q)}) = g_n(\boldsymbol{x}^{(q)})) = 1. \tag{3}$$

It is moreover sequentially improved: for all $\boldsymbol{x}$ in $\mathbb{R}^d$, the higher is Q, the smaller the integrated mean square error (IMSE), $\mathbb{E}\left[\int_{\mathbb{R}^d} (g_n(\boldsymbol{x}) - \widehat{g}_n(\boldsymbol{x}))^2 d\boldsymbol{x}\right]$, is supposed to be. Under the assumption that $\widehat{\mu}_n$ is a good predictor of g_n, a good approximation of $\partial\Omega$ is therefore given by the elements of $\mathbb{R}^d$ such that $\mathbb{P}(\widehat{g}_n(\boldsymbol{x}) \le 0) = \mathbb{P}(\widehat{g}_n(\boldsymbol{x}) \ge 0) = 1/2$, which yields:

$$\partial\Omega_n \approx \widehat{\partial\Omega}_n = \left\{\boldsymbol{x} \in \mathbb{R}^d, \quad \widehat{\mu}_n(\boldsymbol{x})\right\} = 0. \tag{4}$$

Function $\widehat{\sigma}_n$ can then be used to quantify the precision of such an approximation $\widehat{\partial\Omega}_n$, as the smaller $\widehat{\sigma}_n(\boldsymbol{x})$ is, the more chance there is for $g_n(\boldsymbol{x})$ and $\widehat{\mu}_n(\boldsymbol{x})$ to be close. Improving the knowledge about $\widehat{\partial\Omega}_n$ amounts therefore at adding new points $\boldsymbol{x}^{(n),\star}$ to the learning set $\mathcal{S}^{\text{learn}}$, which have to be chosen according to a specific criterion to minimize the total computational cost for a given precision. Such new points are generally chosen iteratively such that:

$$\boldsymbol{x}^{(n),\star} = \arg \max_{\boldsymbol{x} \in \mathbb{R}^d,\, \widehat{\mu}_n(\boldsymbol{x}) = 0} \widehat{\sigma}_n(\boldsymbol{x}), \tag{5}$$

that is to say where the expected value of g_n is the closest to the threshold ($\widehat{\mu}_n(\boldsymbol{x}) = 0$) with the largest uncertainty. Solving the problem defined by Eq. (5) being complex, two adaptations have been proposed to provide a balance between exploration and exploitation. On the first hand, the Efficient Global Reliability Analysis (EGRA) method (see [3] for further details) replaces such a constrained maximization of the standard deviation $\widehat{\sigma}_n$, by the unconstrained maximization of a learning function called Expected Feasibility Function, EF, which writes:

$$\text{EF}(\boldsymbol{x}, n) = \mathbb{E}\left[\epsilon(\boldsymbol{x}) - \min\left(|\widehat{g}_n(\boldsymbol{x})|, \epsilon(\boldsymbol{x})\right)\right], \tag{6}$$

where ϵ is a function chosen to focus the search in the immediate vicinity of $\partial\Omega_n$ (for instance, ϵ can be chosen proportional to $\widehat{\sigma}_n$). Details on the implementation and the maximization of function EF can be found in [3]. On the other hand, the Active learning and Kriging-based Monte-Carlo Simulation (AK-MCS) method (see [6]) proposes a discrete adaptation of the optimization problem defined by Eq. (5):

$$\boldsymbol{x}^{(n),\star} \approx \arg \min_{\boldsymbol{z} \in \{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(\nu)}\}} \frac{|\widehat{\mu}_n(\boldsymbol{z})|}{\widehat{\sigma}_n(\boldsymbol{z})}, \tag{7}$$

where $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(\nu)}\}$ is a set of ν vectors that are randomly chosen in $\mathbb{R}^d$. Therefore, both former methods realize a trade-off between exploration of each boundary $\partial\Omega_n$ of Ω_n and global uncertainty reduction, at a relatively small numerical cost.

When interested in identifying the boundary of the intersection of domains $(\Omega_n)_{1 \le n \le N}$, a very simple strategy would be to use either the EGRA or the AK-MCS iterative method to train each model g_n to sufficient accuracy, and then identify space $\Omega = \Omega_1 \cap \cdots \cap \Omega_N$, as:

$$\Omega = \left\{\boldsymbol{x} \in \mathbb{R}^d, \quad \max_{1 \le n \le N} g_n(\boldsymbol{x}) \le 0\right\} \approx \left\{\boldsymbol{x} \in \mathbb{R}^d, \quad \max_{1 \le n \le N} \widehat{\mu}_n(\boldsymbol{x}) \le 0\right\}. \tag{8}$$

However, it is clear that such a procedure can lead to many useless evaluations of the performance functions. For instance, if $\Omega_1 \subset \Omega_2$, no evaluations of g_2 are needed to analyse the boundary of Ω. To limit the number of calls to performance functions that have little or no influence on the definition of $\partial\Omega$, it would seem interesting to directly apply the EGRA or the AK-MCS methods to the composite function $g^{\max} = \max_{1 \le n \le N} g_n$. However, it appears that such an approach is affected by several problems. Indeed, even if functions g_n are regular, $g^{\max}$ is generally highly irregular and its modeling by a GPR-based surrogate model can be difficult and lead to additional expense. Hence, instead of working on the aggregation of the performance functions, it appears to be more efficient to still consider the approximations of each performance function g_n by a GPR-based surrogate model, and choose a selection criterion that is adapted to the system case. To this end, let $n^\star$ be the index such that, for all $\boldsymbol{x}$ in $\mathbb{R}^d$,

$$n^\star(\boldsymbol{x}) = \arg \max_{1 \le n \le N} \widehat{\mu}_n(\boldsymbol{x}). \tag{9}$$

Therefore, it has been proposed in [2] and [8] to choose the new evaluation point, $\boldsymbol{x}^\star$, such that $\boldsymbol{x} \mapsto \text{EF}(\boldsymbol{x}, n^\star(\boldsymbol{x}))$ is maximal, or such that :

$$\boldsymbol{x}^\star = \arg \min_{\boldsymbol{z} \in \{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(\nu)}\}} \frac{|\widehat{\mu}_{n^\star(\boldsymbol{z})}(\boldsymbol{z})|}{\widehat{\sigma}_{n^\star(\boldsymbol{z})}(\boldsymbol{z})}, \tag{10}$$

to accurately adapt the EGRA and the AK-MCS procedures to the system case, respectively. At this new point $\boldsymbol{x}^\star$, only the true performance function, $\boldsymbol{x} \mapsto g_{n^\star(\boldsymbol{x})}(\boldsymbol{x})$, has to be computed, such that only a small number of calls to true performance functions that have little influence on $\partial\Omega$ should be made.

It can be noticed that such pointwise strategies do not take into account in their selection criteria the fact that the new evaluation point will bring additional information on its neighbourhood. In contract, Stepwise Uncertainty Reduction (SUR) approaches [1] propose to choose the new evaluation point in order to minimize the expected value of a well-chosen measure of the uncertainty about the search domain. For instance, if we denote by $\mathbb{V}(\Omega, m)$ the variance of the volume of Ω, which is conditioned by all the available code evaluations at step m, then the new point, $\boldsymbol{x}^*$, can be chosen such that:

$$(\boldsymbol{x}^*, n^*) = \arg \min_{\boldsymbol{x}^{m+1} \in \mathbb{R}^d, 1 \le n \le N} \mathbb{E}\left[\mathbb{V}(\Omega, m+1) | g_n(\boldsymbol{x}^{m+1}) = \widehat{g}_n(\boldsymbol{x}^{m+1})\right]. \tag{11}$$

Such methods based on global measures of uncertainty of Ω have been shown to outperform pointwise approaches for the identification of excursion set on a series of applications based on a single performance function [1]. In spite of recent algorithmic developments [5], the main drawback of these methods is the fact