Metamodel-based importance sampling for the simulation of rare events

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ABSTRACT: In the field of structural reliability, the Monte-Carlo estimator is considered as the reference probability estimator. However, it is still untractable for real engineering cases since it requires a high number of runs of the model. In order to reduce the number of computer experiments, many other approaches known as reliability methods have been proposed. A certain approach consists in replacing the original experiment by a surrogate which is much faster to evaluate. Nevertheless, it is often difficult (or even impossible) to quantify the error made by this substitution. In this paper an alternative approach is developed. It takes advantage of the kriging meta-modeling and importance sampling techniques. The proposed alternative estimator is finally applied to a finite element based structural reliability analysis.

1 INTRODUCTION

Reliability analysis consists in the assessment of the level of safety of a system. Given a probabilistic model (a random vector $X$ with probability density function (PDF) $f$) and a performance model (a function $g$), it makes use of mathematical techniques in order to estimate the system’s level of safety in the form of a failure probability. A basic approach, which makes reference, is the Monte-Carlo simulation technique that resorts to numerical simulation of the performance model through the probabilistic model. Failure is usually defined as the event $F = \{g(X) \leq 0\}$, so that the failure probability is defined as follows:

$$p_f = \mathbb{P}(F) = \mathbb{P}(\{g(X) \leq 0\}) = \int_{g(x) \leq 0} f(x) \, dx$$  \hspace{1cm} (1)

Introducing the failure indicator function $\mathbb{I}_{g \leq 0}$ being equal to one if $g(x) \leq 0$ and zero otherwise, the failure probability turns out to be the mathematical expectation of this indicator function with respect to the joint probability density function $f$ of the random vector $X$. The Monte-Carlo estimator is then derived from this convenient definition. It reads:

$$\hat{p}_{f,MC} = \mathbb{E}[\mathbb{I}_{g \leq 0}(X)] = \frac{1}{N} \sum_{k=1}^{N} \mathbb{I}_{g \leq 0}(x^{(k)})$$  \hspace{1cm} (2)

where $\{x^{(1)}, \ldots, x^{(N)}\}$, $N \in \mathbb{N}^*$ is a set of samples of the random vector $X$. According to the central limit theorem, this estimator is asymptotically unbiased and normally distributed with variance:

$$\sigma^2_{\hat{p}_{f,MC}} = \mathbb{V}[\hat{p}_{f,MC}] = \frac{p_f(1-p_f)}{N}$$  \hspace{1cm} (3)

In practice, this variance is compared to the unbiased estimate of the failure probability in order to decide whether it is accurate enough or not. The coefficient of variation is defined as $\delta_{\hat{p}_{f,MC}} = \sigma_{\hat{p}_{f,MC}}/\hat{p}_{f,MC}$. Given $N$, this coefficient dramatically increases as soon as the failure event is too rare ($p_f \to 0$) and proves that the Monte-Carlo estimation technique intractable for real world engineering problems for which the performance function involves the output of an expensive-to-evaluate black box function – e.g. a finite element code. Note that this remark is also true for too frequent events ($p_f \to 1$) as the coefficient of variation of $1-\hat{p}_{f,MC}$ exhibits the same property.

In order to reduce the number of simulation runs, a large set of other approaches known as reliability methods have been proposed. They might be classified as follows.

A first approach consists in replacing the original experiment by a surrogate which is much faster to evaluate. Among such approaches, there are the well-known first and second order reliability methods (e.g. Ditlevsen and Madsen [1996], Lemaire [2009]), quadratic response surfaces (Bucher and Bourgund [1990]) and the more recent meta-models such as support vector machines...
2 ADAPTIVE PROBABILISTIC CLASSIFICATION USING MARGIN META-MODELS

A meta-model means to a model what the model itself means to the real-world. Loosely speaking, it is the model of the model. As opposed to the model, its construction does not rely on any physical assumption about the phenomenon of interest but rather on statistical considerations about the coherence of some scattered observations that result from a set of experiments. This set is usually referred to as a design of experiments (DOE): \( X = \{x_1, \ldots, x_m\} \). It should be carefully selected in order to retrieve the largest amount of statistical information about the underlying functional relationship over the input space \( \mathcal{D}_x \). Here, we attempt to build a meta-model for the failure indicator function \( g \leq 0 \). In the statistical learning theory (Vapnik 1995) this is referred to as a classification problem.

Hereafter, we define a margin meta-model as a meta-model that is able to give a probabilistic prediction of the response quantity of interest whose spread (i.e. variance) depends on the lack of information brought by the DOE. It is thus reducible by bringing more observations into the DOE. In other words, this is an epistemic (reducible) source of uncertainty. To the authors’ knowledge, there exist only two families of such margin-meta-models: the probabilistic support vector machines \( \text{P-SVM} \) by Platt (1999) and Gaussian-Process- (or kriging-) based classification (Santner et al. 2003). The present paper makes use of the kriging meta-model, but the overall concept could easily be extended to \( \text{P-SVM} \). The theoretical aspects of the kriging prediction are briefly introduced in the following subsection before it is applied to the classification problem of interest.

2.1 Gaussian-process based prediction

The Gaussian-Process based prediction (also known as kriging) theory is detailed in the book by Santner et al. (2003). In essence, kriging assumes that the performance function \( g \) is a sample path of an underlying Gaussian stochastic process \( G \) that would read as follows:

\[
G(x) = f(x)^T \beta + Z(x)
\]

where:

- \( f(x)^T \beta \) denotes the mean of the GP which corresponds to a classical linear regression model on a given functional basis \( \{f_i, i = 1, \ldots, p\} \in L^2(\mathcal{D}_x, \mathbb{R}) \);
- \( Z(x) \) denotes the stochastic part of the GP which is modelled as a zero mean, constant variance \( \sigma^2_g \), stationary Gaussian process with a given symmetric positive definite autocorrelation model. It is fully defined by its autocovariance function which reads (\( (x, x') \in \mathcal{D}_x \times \mathcal{D}_x \)):

\[
C_{GG}(x, x') = \sigma^2_G R(||x - x'||, \ell)
\]

where \( \ell \) is a vector of parameters defining \( R \).

The most widely used class of autocorrelation functions is the anisotropic squared exponential model:

\[
R(||x - x'||, \ell) = \exp \left( \sum_{k=1}^{n} \frac{-(x_k - x'_k)^2}{\ell_k^2} \right)
\]

The best linear unbiased estimation of \( G \) at point \( x \) is shown (Santer et al. 2003; Severini 2005, Chap. 8) to be the following Gaussian random variate:

\[
\tilde{G}(x) = G(x) |\{g(x_1), \ldots, g(x_m)\} \sim N\left(\mu_G(x), \sigma^2_G(x)\right)
\]

with moments:

\[
\mu_G(x) = f(x)^T \hat{\beta} + r(x)^T R^{-1} (Y - F \hat{\beta})
\]

\[
\sigma^2_G(x) = \sigma^2_G \left(1 - \left[ \frac{f(x)}{r(x)} \right]^T \left[ \begin{array}{c} \text{0} \\ F \end{array} \right]^T R^{-1} \left[ \begin{array}{c} f(x) \\ r(x) \end{array} \right] \right)
\]

where we have introduced \( r, R \) and \( F \) such that:

\[
r_i(x) = R(||x - x_i||, \ell), \quad i = 1, \ldots, m
\]

\[
R_{ij} = R(||x_i - x_j||, \ell), \quad i = 1, \ldots, m, \quad j = 1, \ldots, m
\]

\[
F_{ij} = f_i(x_j), \quad i = 1, \ldots, p, \quad j = 1, \ldots, m
\]

At this stage it can easily be proven that \( \mu_G(x_i) = g(x_i) \) and \( \sigma^2_G(x_i) = 0 \) for \( i = 1, \ldots, m \), thus meaning the kriging surrogate is an exact interpolator.
Given a choice for the regression and correlation models, the optimal set of parameters $\beta^\star$, $\ell^\star$ and $\sigma_{G}^{2\star}$ can then be inferred using the maximum likelihood principle applied to the unique sparse observation of the GP sample path grouped in the vector $y = \{g(x_{i}), i = 1, \ldots, m\}$. This inference problem turns into an optimization problem that can be solved analytically for both $\beta^\star$ and $\sigma_{G}^{2\star}$ assuming $\ell^\star$ is known. Thus, the problem is solved in two steps: the maximum likelihood estimation of $\ell^\star$ is first solved by a global optimization algorithm which in turns gives the optimal values of $\beta^\star$ and $\sigma_{G}^{2\star}$.

2.2 Probabilistic classification function

A surrogate-based reliability analysis simply consists of replacing the performance function $g$ by its metamodel $\hat{G}$. Again, this metamodel may be a first- or second-order Taylor expansion of the limit-state surface $g = 0$ at a so-called design point (Ditlevsen and Madsen, 1996, FORM/SORM), a polynomial response surface (Bucher and Bourgund, 1990), a neural networks based prediction (Papadrakakis and Lagaros, 2002), or a kriging based prediction (Bichon et al., 2008). This surrogate may not be fully accurate and it is difficult or even impossible to quantify the error made by substitution on the final failure probability of interest.

In this paper as in the work by Picheny (2009), it is proposed to use the complete probabilistic prediction provided by the kriging meta-model instead of the sole mean prediction (e.g. as in Bichon et al., 2008). Indeed, since the probabilistic distribution of the prediction is fully characterized, the probability that the prediction is negative may be expressed in closed-form and reads as follows:

\[
P \left[ \hat{G}(x) \leq 0 \right] = \Phi \left( \frac{0 - \mu_{\hat{G}}(x)}{\sigma_{\hat{G}}(x)} \right)
\]

Note that this latter quantity is not the sought failure probability $P_{f}$, this is simply the probability that the prediction $\hat{G}$ at some deterministic vector $x$ is negative.

Picheny (2009) proposes then to use this probabilistic classification function as a surrogate for the real failure indicator function, and uses crude Monte-Carlo simulation to estimate the failure probability. A different use is proposed in the next section.

Figure 1 illustrates the concepts introduced in this section on a basic structural reliability example from Der Kiureghian and Dakuessian (1998). This example involves two independent standard Gaussian random variates $X_1$ and $X_2$, and the performance function reads:

\[
g(x_{1}, x_{2}) = b - x_{2} - \kappa (x_{1} - c)^{2}
\]

where $b = 5$, $\kappa = 0.5$ and $c = 0.1$. In subfigure 1(a) the limit-state function $g(x) = 0$ is represented by the black dash-dot line. The red minusses ($g \leq 0$) and blue plusses ($g > 0$) represent the initial DOE from which the kriging meta-model is built. The mean prediction’s limit-state $\mu_{\hat{G}}(x) = 0$ is represented by the dashed black line. It can be seen that the meta-model is not fully accurate since the green triangle $x^{0}$ (among others) is misclassified. Indeed, $x^{0}$ is safe according to the real performance function $g$, but it fails according to the mean prediction of the meta-model $\mu_{\hat{G}}$. The probabilistic classification function makes a smoother decision possible: $x^{0}$ fails with a 60% probability w.r.t. the epistemic uncertainty in the random prediction $\hat{G}(x^{0}) \sim \mathcal{N}(\mu_{\hat{G}}(x^{0}), \sigma_{\hat{G}}(x^{0}))$. Note also that the red and blue points in the DOE fails with probabilities 100% and 0% (safe) respectively due to the interpolating property of the kriging metamodel.

Subfigure 1(a) is the one-dimensional illustration of the three classification strategies for the vector $x^{0}$. The deterministic decision function is an heaviside function centered in zero, and the probabilistic classification is a smoother Gaussian cumulative density function.

2.3 Refinement of the probabilistic classification function

In this subsection, a strategy is proposed in order to refine the probabilistic classification function so that it tends towards the real indicator function $\mathbb{1}_{\mathcal{X}_{\mathcal{M}}}$. First, let the margin of uncertainty $\mathbb{M}$ be defined as follows:

\[
\mathbb{M} = \{ x : -k \sigma_{\hat{G}}(x) \leq \hat{G}(x) \leq +k \sigma_{\hat{G}}(x) \}
\]

where $k$ might be chosen as $k = \Phi^{-1}(97.5\%) = 1.96$ meaning a 95% confidence interval onto the prediction of the limit-state surface is chosen. Such a 95% confidence margin is illustrated in Subfigure 1(a) as the area bounded below by the blue line (2.5% confidence level) and above by the red line (97.5% confidence level). The points that are located in this margin have an uncertain sign, the others being either failed or safe with a confidence level greater than 97.5%.

We also define the probability that a point $x \in \mathcal{D}_{k}$ belongs to this margin of uncertainty. Due to the Gaussian nature of the prediction, this probability may also be expressed in closed-form and reads as follows:

\[
P[x \in \mathbb{M}] = \Phi \left( \frac{k \sigma_{\hat{G}}(x) - \mu_{\hat{G}}(x)}{\sigma_{\hat{G}}(x)} \right) - \Phi \left( -\frac{k \sigma_{\hat{G}}(x) - \mu_{\hat{G}}(x)}{\sigma_{\hat{G}}(x)} \right)
\]

Then, finding the point that maximizes this quantity on the support of the PDF of $X$ will finally bring the best improvement point in the DOE. Starting with this statement, many authors in the kriging literature
In this paper, as in Dubourg et al. (2011), a slightly different strategy is proposed in order to add several points in the DOE. The proposed criterion $P]\text{\hat{g}}(x_0]) = 0.00\text{.}$ can be used in order to generate $N$ (say $N = 10^4$) samples from the pseudo-PDF $c$. These samples are expected to be highly concentrated around the maxima of the criterion $\mathbb{P}(x \in \mathbb{M})$, and in the vicinity of the predicted limit-state $\mu_\mathbb{G}(x_0) = 0$ where the sign of $\mathbb{G}$ is the most uncertain. This large candidate population can then be reduced to a smaller one that condensates its statistical properties by means of a $K$-means clustering algorithm (MacQueen, 1967). The $K$ ($K$ being given) cluster centers uniformly span the margin $\mathbb{M}$ and may be added to the DOE in order to enrich the prediction of the performance function in the vicinity of the limit-state and thus reduce the margin of uncertainty.

3 META-MODEL-BASED IMPORTANCE SAMPLING

Picheny (2009) proposes to use the probabilistic classification function as a surrogate for the real indicator function, so that the failure probability is rewritten from its definition in Eq. (1) as follows:

$$p_f = \int \mathbb{P}[\mathbb{G}(x) \leq 0] f(x) dx \equiv \mathbb{E}_f [\mathbb{P}[\mathbb{G}(X) \leq 0]]$$

It is argued here that this latter quantity does not equal the failure probability of interest because it sums the aleatory uncertainty in the random vector $X$ and the epistemic uncertainty in the prediction $\mathbb{G}$. This is the reason why $p_f$ will hereafter be referred to as the augmented failure probability. As a matter of fact, even if the epistemic uncertainty in the prediction can be reduced (e.g. by enriching the DOE as proposed in section 2.3), it is impossible to quantify the contribution of each source of uncertainty a posteriori.
This remark motivates the approach introduced in this section where the probabilistic classification function is used in conjunction with the importance sampling technique in order to build a new estimator of the failure probability.

3.1 Importance sampling

According to [Rubinstein and Kroese (2008)], importance sampling (IS) is the most efficient variance reduction technique. This technique consists in computing the mathematical expectation of the failure indicator function according to a biased PDF which favors the failure event of interest. This PDF is called the instrumental density.

Given an instrumental density $h$, such that $h$ dominates $\mathbb{I}_{g \leq 0}$, the definition of the failure probability of Eq. (1) may be rewritten as follows:

$$p_f = \int_{g(x) \leq 0} \frac{f(x)}{h(x)}\, dx = \mathbb{E}_h \left[ \mathbb{I}_{g \leq 0}(X) \frac{f(X)}{h(X)} \right]$$  \hspace{1cm} (20)

where the subscript $h$ on the expectation operator is added to recall that $X$ is therefore distributed according to $h$. Note that the domination requirement of $h$ over $\mathbb{I}_{g \leq 0}$ simply means that:

$$\forall x \in \mathcal{D}_X, \quad h(x) = 0 \Rightarrow \mathbb{I}_{g \leq 0}(x) f(x) = 0$$  \hspace{1cm} (21)

so that the so-called likelihood ratio $\ell(x) = f(x)/h(x)$ is finite for any given $x \in \mathcal{D}_X$.

The latter definition of the failure probability easily leads to the establishment of the importance sampling estimator which reads as follows:

$$\hat{p}_{f\text{IS}} = \mathbb{E}_f \left[ \mathbb{I}_{g \leq 0}(X) \right] = \frac{1}{N} \sum_{k=1}^{N} \mathbb{I}_{g \leq 0}(x^{(k)}) \frac{f(x^{(k)})}{h(x^{(k)})}$$  \hspace{1cm} (22)

where $\{x^{(1)}, \ldots, x^{(N)}\}$, $N \in \mathbb{N}^*$ is a set of samples from $h$. According to the central limit theorem, this estimation is unbiased and its quality may be measured by means of its variance of estimation which reads:

$$\text{Var} \left[ \hat{p}_{f\text{IS}} \right] = \frac{1}{N-1} \left( \frac{1}{N} \sum_{k=1}^{N} \mathbb{I}_{g \leq 0}(x^{(k)}) \left( \frac{f(x^{(k)})}{h(x^{(k)})} \right)^2 - \hat{p}_{f\text{IS}}^2 \right)$$  \hspace{1cm} (23)

Rubinstein and Kroese (2008) show that this variance is zero (optimality of the IS estimator) when the instrumental PDF is chosen as:

$$h^*(x) = \frac{\mathbb{I}_{g \leq 0}(x) f(x)}{\int_{g \leq 0}(x) f(x)\, dx} = \frac{\mathbb{I}_{g \leq 0}(x) f(x)}{p_f}$$  \hspace{1cm} (24)

However this instrumental PDF is not implementable in practice because it involves the sought failure probability in its denominator. There exists infinitely many PDF $h$ that allows to significantly reduce the variance of estimation though.

3.2 A meta-model-based approximation of the optimal instrumental PDF

Different strategies have been proposed in order to build quasi-optimal instrumental PDF suited for specific estimation problems. For instance, Melchers (1989) uses a standard normal PDF centered onto the most probable failure point (MPFP) in the space of the independent standard Gaussian random variables $U = T(X)$ in order to estimate a failure probability. Although this approach may lose accuracy as soon as the MPFP is not unique, Cannamela et al. (2008) use a kriging prediction of the performance function $g$ in order to build an instrumental PDF suited for the estimation of extreme quantiles of the random variate $G = g(X)$.

Here, it is proposed to use the probabilistic classification function in Eq. (13) as a surrogate for the real indicator function in the optimal instrumental PDF in Eq. (24). The proposed quasi-optimal PDF thus reads as follows:

$$\hat{h}^*(x) = \frac{\mathbb{P} \left[ \hat{G}(x) \leq 0 \right] f(x)}{\mathbb{P} \left[ \hat{G}(x) \leq 0 \right] f(x)\, dx} = \frac{\mathbb{I}_{g \leq 0}(x) f(x)}{p_{f\text{\epsilon}}}$$  \hspace{1cm} (25)

where $p_{f\text{\epsilon}}$ is the augmented failure probability which has been already defined in Eq. (19). This quasi-optimal instrumental PDF is compared to its impractical optimal counterpart in Figure 2 using the example of Section 2.2.

3.3 The meta-model-based importance sampling estimator

Choosing the proposed quasi-optimal instrumental PDF in Eq. (25) in the importance sampling definition of the failure probability in Eq. (20) leads to the following new definition:

$$p_f = \int_{g \leq 0} \frac{f(x)}{h^*(x)} \hat{h}^*(x)\, dx$$  \hspace{1cm} (26)

$$= p_{f\text{\epsilon}} \int \mathbb{I}_{g \leq 0}(x) \hat{h}^*(x)\, dx$$  \hspace{1cm} (27)

$$= p_{f\text{\epsilon}} \alpha_{\text{corr}}$$  \hspace{1cm} (28)

where we have introduced:

$$\alpha_{\text{corr}} \equiv \mathbb{E}_{\hat{h}^*} \left[ \frac{\mathbb{I}_{g \leq 0}(X)}{\mathbb{P} \left[ \hat{G}(X) \leq 0 \right]} \right]$$  \hspace{1cm} (29)

This means that the failure probability is now defined as the product between the augmented failure probability $p_{f\text{\epsilon}}$ and a correction factor $\alpha_{\text{corr}}$. This correction factor is defined as the expected ratio between the real
The calculation of the coefficient of variation of the final estimator $\hat{p}_{f_{\text{metal}}} \in P$ will be detailed in a forthcoming paper.

4 RELIABILITY ANALYSIS OF AN 8-HOLE PLATE

This structural reliability example is inspired from [Deheeger and Lemaire (2007)]. It concerns the reliability analysis of a 200 × 100 mm 8-hole plate illustrated in Figure 3. The diameter of the holes $\varnothing$ is set equal to 10 mm. Its left end is clamped both horizontally and vertically while its right end is subjected to a distributed line load with magnitude $q = 100$ MPa. Plain stress is assumed and the material is supposed to have a linear elastic behavior. The Poisson coefficient $\nu$ is set equal to 0.3. Due to the boundary conditions the Poisson effect is not the same on all the plate though. The Young’s modulus is modeled by an homogeneous lognormal random field with a mean $E = 200000$ MPa, a coefficient of variation $\delta_E = 25\%$ and assuming an isotropic squared exponential autocorrelation function with a 20 mm correlation length $\ell$. The two-dimensional random field is represented by a translated Karhunen-Loeve expansion discretized by means of a wavelet-Galerkin strategy proposed by [Phoon et al. (2002)]. The stochastic model involves 20 independent standard Gaussian random variates grouped in the vector $X$ to simulate the random field. The mechanical model is solved with Code_Aster [eDF, R&D Division (2006)] in order to retrieve the maximal Von Mises stress in the plate $P$. The performance function is then defined as follows:

$$g(x) = \sigma_0 - \max_{p \in P} \{ \sigma_{\text{Von Mises}}(p) \}$$  \hspace{1cm} (33)$$

with respect to an arbitrary threshold $\sigma_0 = 450$ MPa.
The proposed meta-model-based importance sampling procedure is applied to this structural reliability example. First an initial kriging predictor is built for the performance function $g$ using a 100-point DOE. These 100 points are uniformly generated within the $\beta_0$ radius hypersphere. Based on this initial prediction, the DOE refinement procedure introduced in Section 2.3 is used. $K = 100$ new points are added at each refinement iteration. The refinement procedure is stopped after 1000 estimations of the performance function. This may seem arbitrary but it is difficult to provide another stopping criterion for the refinement procedure – this needs further investigation. Then, the probabilistic classification function is defined with respect to the latest (finest) kriging prediction and it is used to compute the proposed estimator of the failure probability.

The results are provided in Table 1. They are compared to a reference solution obtained by subset simulation (Au and Beck, 2001), and the multi-FORM estimator from Der Kiureghian and Dakessian (1998) using FERUM v4.0 (Bourinet et al., 2009) implementations of these algorithms. FERUM is a Matlab toolbox for reliability analysis published under the General Public License. The estimate of the augmented failure probability is equal to $\hat{\gamma}_f = 2.85 \times 10^{-5}$, and the correction factor is equal to $\hat{\alpha}_{\text{corr}} = 0.412$. It means that the kriging predictor is rather accurate in that case. The probabilistic classification function is very close to its deterministic counterpart – and so is the instrumental importance sampling density $\hat{h}$.

5 Conclusion

Starting from the double premise that a surrogate-based reliability analyses does not permit to quantify the substitution error, and that the existing variance reduction techniques remain time-consuming when the performance function involves the output of an expensive-to-evaluate black box function, an hybrid strategy has been proposed. First, the probabilistic classification function was introduced, this function allows a smoother classification than its deterministic counterpart accounting for the epistemic uncertainty in the kriging prediction. Using this smoother classification function within an importance sampling framework then allowed to derive a meta-model-based importance sampling estimator. This estimator converges towards the theoretically impractical optimal importance sampling estimator and may provide a significant reduction of the estimation variance as illustrated in the example.

In the present paper, the refinement procedure that leads to the probabilistic classification function is stopped arbitrarily. Work is in progress in order to establish the best trade-off between the size of the DOE and the number of simulations required to estimate the correction factor $\alpha_{\text{corr}}$.

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