# Metamodel-based importance sampling for structural reliability analysis

V. Dubourg<sup>a,b,\*</sup>, B. Sudret<sup>c</sup>, F. Deheeger<sup>b</sup>

<sup>a</sup>Clermont Université, IFMA, EA 3867, Laboratoire de Mécanique et Ingénieries, BP 10448, F-63000 Clermont-Ferrand

<sup>b</sup>Phimeca Engineering, Centre d'Affaires du Zénith, 34 rue de Sarliève, F-63800 Cournon d'Auvergne

<sup>c</sup>ETH Zürich – Institute of Structural Engineering – Chair of Risk, Safety & Uncertainty Quantification, Wolfgang-Pauli-Strasse 15 CH-8093 Zürich

# Abstract

Structural reliability methods aim at computing the probability of failure of systems with respect to some prescribed performance functions. In modern engineering such functions usually resort to running an expensive-to-evaluate computational model (*e.g.* a finite element model). In this respect simulation methods which may require  $10^{3-6}$  runs cannot be used directly. *Surrogate models* such as quadratic response surfaces, polynomial chaos expansions or Kriging (which are built from a limited number of runs of the original model) are then introduced as a substitute of the original model to cope with the computational cost. In practice it is almost impossible to quantify the error made by this substitution though. In this paper we propose to use a Kriging surrogate of the performance function as a means to build a quasi-optimal importance sampling density. The probability of failure is eventually obtained as the product of an *augmented* probability computed by substituting the metamodel for the original performance function and a *correction term* which ensures that there is no bias in the estimation even if the meta-model is not fully accurate. The approach is applied to analytical and finite element reliability problems and proves efficient up to 100 basic random variables.

*Keywords:* structural reliability, importance sampling, metamodeling error, Kriging, random fields, active learning, rare events

<sup>\*</sup>Corresponding author

Email addresses: dubourg@phimeca.com (V. Dubourg), sudret@ibk.baug.ethz.ch (B. Sudret), Preprint submitted to Probabilistic Engineering Mechanics February 19, 2013

# 1. Introduction

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

$$p_{f} \equiv \mathbb{P}\left(\left\{g\left(\boldsymbol{X}\right) \leq 0\right\}\right) = \int_{\mathcal{D}_{f} = \left\{\boldsymbol{x} \in \mathbb{R}^{n} : g(\boldsymbol{x}) \leq 0\right\}} f_{\boldsymbol{X}}\left(\boldsymbol{x}\right) \, \mathrm{d}\boldsymbol{x}$$
(1)

Introducing the failure indicator function  $\mathbb{1}_{g\leq 0}$  being equal to one if  $g(\boldsymbol{x}) \leq 0$  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  $f_{\boldsymbol{X}}$  of the random vector  $\boldsymbol{X}$ . This convenient definition allows one to derive the Monte Carlo estimator which reads:

$$\widehat{p}_{f \,\mathrm{MC}} \equiv \widehat{\mathbb{E}}_{\boldsymbol{X}} \left[ \mathbb{1}_{g \leq 0} \left( \boldsymbol{X} \right) \right] = \frac{1}{N} \sum_{k=1}^{N} \mathbb{1}_{g \leq 0} \left( \boldsymbol{x}^{(k)} \right)$$
(2)

where  $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(N)}\}\$  is a set of samples from the random vector  $\boldsymbol{X}$ . This estimator is asymptotically unbiased and convergent, although the convergence rate is low ( $\propto N^{-1/2}$ ). This makes 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.

In order to reduce the number of simulation runs, different alternatives to the bruteforce Monte Carlo method have been proposed and might be classified as follows. One first approach consists in replacing the original performance function g by a *surrogate*  $\tilde{g}$  which is much faster to evaluate. Various surrogates have been used amongst which are: quadratic response surfaces (Bucher and Bourgund, 1990; Kim and Na, 1997; Das and Zheng, 2000), *support vector machines* (Hurtado, 2004; Deheeger and Lemaire, 2007; Bourinet et al., 2011),

francois.deheeger@gmail.com (F. Deheeger)

*neural networks* (Papadrakakis and Lagaros, 2002) and *Kriging* (Kaymaz, 2005; Bichon et al., 2008). Nevertheless, it is often difficult or even impossible to quantify the error made by such a substitution. The well-known first- and second-order reliability methods (FORM/SORM), based on Taylor series expansions somewhat differ from these surrogate-based approaches because of their mathematical background (Breitung, 1984; Ditlevsen and Madsen, 1996). But in practice they feature the same limitation: the assumptions (mostly the unicity of the so-called *most probable failure point*) they are built on may not hold and it is difficult to validate them.

From another point of view, variance reduction techniques have been proposed in order to make Monte Carlo simulation more efficient. Importance sampling (Rubinstein and Kroese, 2008) aims at concentrating the Monte Carlo samples in the vicinity of the limit-state surface, *e.g.* around the most probable failure point (also known as design point) obtained by a preliminary FORM analysis (Melchers, 1989). Subset simulation (Au and Beck, 2001; Ching et al., 2005a,b) computes the failure probability as a product of conditional probabilities, each of them being estimated by Markov Chain Monte Carlo simulation. All these approaches reveal robust, although they are often too much computationally demanding to be implemented in industrial cases. As a summary the current practice for evaluating probabilities of failure in case of computationally demanding performance functions relies on the substitution of the limit-state function by a metamodel for which no general error estimation is usually available.

In this paper, a new hybrid approach combining importance sampling and an adaptive metamodeling technique is proposed. First, a Kriging surrogate of the limit-state function is built and adaptively refined. Then, the probabilistic prediction provided by the Kriging surrogate is used to build up a quasi-optimal importance sampling density. As a result the probability of failure is computed as the product of two terms, namely one obtained by sampling the *surrogate* limit-state function, and the other one being a correction factor computed from the *original* limit-state function.

The paper is organized as follows. Section 2 recalls the basic of Kriging and introduces the probabilistic classification function. Section 3 presents the construction of a quasi-optimal

importance sampling density derived from this function and the associated estimator of the failure probability. Section 4 introduces an adaptive refinement technique of this importance sampling density function so as to make the algorithm as parsimonious as possible and discusses the implementation details. Section 5 eventually provides different application examples includent a finite element reliability analysis problem.

# 2. Probabilistic classification using Kriging

Metamodels may be defined as a (statistics-based) model of (physics-based) computational model. Indeed a metamodel (or response surface) is built from a *design of experiments* (DOE), *i.e.* a set of computer experiments denoted by  $\mathcal{X} = \{x_1, \ldots, x_m\}$ , where  $\{x_i, i = 1, \ldots, m\}$  belong to the support  $\mathcal{D}_x$  of X. In this paper we make use of Kriging (Sacks et al., 1989; Welch et al., 1992; Santner et al., 2003) which is also known as *Gaussian process modeling*. The unique feature of Kriging is that it provides a built-in error estimate, namely the Kriging variance. This allows the development of adaptive algorithms in which the DOE is enriched iteratively based on in-fill criteria derived from the Kriging variance.

#### 2.1. Gaussian-process based prediction

Kriging assumes that the performance function g is a sample path of an underlying Gaussian process (GP) denoted by G that may be cast as follows:

$$G(\boldsymbol{x}) = \boldsymbol{f}(\boldsymbol{x})^{\mathsf{T}} \boldsymbol{\beta} + Z(\boldsymbol{x})$$
(3)

where  $\boldsymbol{f}(\boldsymbol{x})^{\mathsf{T}} \boldsymbol{\beta}$  denotes the mean of the GP which corresponds to a classical linear regression model on a given functional basis  $\{f_i, i = 1, \ldots, p\} \in \mathcal{L}_2(\mathcal{D}_{\boldsymbol{x}}, \mathbb{R})$  and  $Z(\boldsymbol{x})$  denotes a zeromean stationary GP with a constant variance  $\sigma_G^2$ . It is fully defined by its autocovariance function which reads:

$$C_{GG}(\boldsymbol{x}, \boldsymbol{x}') = \sigma_G^2 R(\boldsymbol{x} - \boldsymbol{x}', \boldsymbol{\ell})$$
(4)

where  $\ell$  is a vector of parameters defining R. The most widely used class of autocorrelation functions is the *anisotropic squared exponential* model:

$$R(\boldsymbol{x} - \boldsymbol{x}', \boldsymbol{\ell}) = \exp\left(-\sum_{k=1}^{n} \left(\frac{x_k - x'_k}{\ell_k}\right)^2\right)$$
(5)

The best linear unbiased estimation (BLUE) (Santner et al., 2003) of G at point  $\boldsymbol{x}$  is shown to be a Gaussian random variate  $\widehat{G}(\boldsymbol{x}) \sim \mathcal{N}\left(\mu_{\widehat{G}}(\boldsymbol{x}), \sigma_{\widehat{G}}(\boldsymbol{x})\right)$  where:

$$\mu_{\widehat{G}}(\boldsymbol{x}) = \boldsymbol{f}(\boldsymbol{x})^{\mathsf{T}} \,\widehat{\boldsymbol{\beta}} + \boldsymbol{r}(\boldsymbol{x})^{\mathsf{T}} \,\mathbf{R}^{-1} \left(\boldsymbol{y} - \mathbf{F} \,\widehat{\boldsymbol{\beta}}\right)$$

$$\sigma_{\widehat{G}}^{2}(\boldsymbol{x}) = \sigma_{G}^{2} \,\left(1 - \boldsymbol{r}(\boldsymbol{x})^{\mathsf{T}} \,\mathbf{R}^{-1} \,\boldsymbol{r}(\boldsymbol{x}) + \boldsymbol{u}(\boldsymbol{x})^{\mathsf{T}} \,(\mathbf{F}^{\mathsf{T}} \,\mathbf{R}^{-1} \,\mathbf{F})^{-1} \,\boldsymbol{u}(\boldsymbol{x})\right)$$
(6)

Here  $\boldsymbol{y} = \langle g(\boldsymbol{x}_1), \ldots, g(\boldsymbol{x}_m) \rangle^{\mathsf{T}}$  is the vector of observations computed from the DOE  $\mathcal{X}$ ; **R** is their correlation matrix defined by  $R_{ij} = R(\boldsymbol{x}_i - \boldsymbol{x}_j, \boldsymbol{\ell})$ ,  $i, j = 1, \ldots, m; \boldsymbol{r}(\boldsymbol{x})$  is the vector of cross-correlations between the observations and the prediction  $(r_i(\boldsymbol{x}) = R(\boldsymbol{x} - \boldsymbol{x}_i, \boldsymbol{\ell}), i =$  $1, \ldots, m)$ ; **F** is the so-called regression matrix defined by  $F_{ij} = f_j(\boldsymbol{x}_i), i = 1, \ldots, m, j =$  $1, \ldots, p$ . Finally, the generalized least-squares solution  $\hat{\boldsymbol{\beta}}$  and the vector  $\boldsymbol{u}(\boldsymbol{x})$  respectively read:

$$\widehat{\boldsymbol{\beta}} = (\mathbf{F}^{\mathsf{T}} \mathbf{R}^{-1} \mathbf{F})^{-1} \mathbf{F}^{\mathsf{T}} \mathbf{R}^{-1} \boldsymbol{y} \qquad \boldsymbol{u}(\boldsymbol{x}) = \mathbf{F}^{\mathsf{T}} \mathbf{R}^{-1} \boldsymbol{r}(\boldsymbol{x}) - \boldsymbol{f}(\boldsymbol{x})$$
(7)

At this stage one can easily prove that  $\mu_{\widehat{G}}(\boldsymbol{x}_i) = g(\boldsymbol{x}_i)$  and  $\sigma_{\widehat{G}}(\boldsymbol{x}_i) = 0$  for  $i = 1, \ldots, m$ , thus meaning that the Kriging surrogate *interpolates* the observations. Given a choice for the regression and correlation models, the optimal set of parameters  $\boldsymbol{\beta}^*$ ,  $\boldsymbol{\ell}^*$  and  $\sigma_{G}^{2*}$  can then be inferred using the *maximum likelihood principle* applied to the single observation of the GP sample path grouped into the vector  $\boldsymbol{y}$ . This inference problem turns into an optimization problem that can be solved analytically for both  $\boldsymbol{\beta}^*$  and  $\sigma_{G}^{2*}$  assuming  $\boldsymbol{\ell}^*$  is known. Thus the problem is solved in two steps: the maximum likelihood estimation of  $\boldsymbol{\ell}^*$ is first solved by a global optimization algorithm which in turns allows one to evaluate the optimal  $\boldsymbol{\beta}^*$  and  $\sigma_{G}^{2*}$ . Implementation details can be found in Welch et al. (1992); Lophaven et al. (2002).

#### 2.2. Probabilistic classification function

Kriging provides both a surrogate of the limit-state function  $g(\boldsymbol{x})$  which is denoted by  $\mu_{\widehat{G}}(\boldsymbol{x})$  and an epistemic prediction uncertainty which is characterized by the Kriging variance  $\sigma_{\widehat{G}}^2(\boldsymbol{x})$ . A common practice in the field of Kriging-based reliability analysis consists in using the mean prediction as a surrogate (*i.e.*  $\widetilde{g}(\boldsymbol{x}) \equiv \mu_{\widehat{G}}(\boldsymbol{x})$ ) for computing the failure probability by means of any Monte Carlo sampling technique. Indeed, despite the Kriging variance is

often used for improving the accuracy of the metamodel in the vicinity of the limit-state surface (see *e.g.* Bichon et al., 2008; Echard et al., 2011), the proper estimation of the failure probability is performed on the mean prediction only. In this paper it is proposed to use the complete probabilistic prediction, see Picheny (2009) for a similar idea. Let us introduce for this purpose the following *probabilistic classification function*:

$$\pi(\boldsymbol{x}) \equiv \mathcal{P}\left[\widehat{G}(\boldsymbol{x}) \le 0\right]$$
(8)

In this expression, the probability measure  $\mathcal{P}[\bullet]$  refers to the Gaussian nature of the Kriging predictor  $\widehat{G}(\boldsymbol{x}) \sim \mathcal{N}(\mu_{\widehat{G}}(\boldsymbol{x}), \sigma_{\widehat{G}}(\boldsymbol{x}))$  and shall not be confused with the probability measure  $\mathbb{P}(\bullet)$  associated with the random vector  $\boldsymbol{X}$  in Eq. (1). Thanks to the Gaussian nature of the Kriging predictor, the probabilistic classification function rewrites:

$$\pi(\boldsymbol{x}) = \Phi\left(\frac{0 - \mu_{\widehat{G}}(\boldsymbol{x})}{\sigma_{\widehat{G}}(\boldsymbol{x})}\right) \text{ if } \boldsymbol{x} \notin \mathcal{X}$$
(9)

For points in the experimental design for which the prediction variance is equal to zero, the above function reads:

$$\pi(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{x} \in \mathcal{X}, \ g(\boldsymbol{x}) \leq 0 \\ 0 & \text{if } \boldsymbol{x} \in \mathcal{X}, \ g(\boldsymbol{x}) > 0 \end{cases}$$
(10)

It shall be again emphasized that  $\pi(\mathbf{x})$  is *not* the sought failure probability. It may be interpreted as the probability that the predictor  $\widehat{G}(\mathbf{x})$  (for some prescribed deterministic  $\mathbf{x}$ ) is negative with respect to the epistemic uncertainty.

# 3. Metamodel-based importance sampling

Picheny (2009) proposes to use the probabilistic classification function  $\pi$  (see Eq. (9)) as a surrogate for the original indicator function  $\mathbb{1}_{g\leq 0}$ , so that the failure probability is rewritten from its definition in Eq. (1) as follows:

$$p_{f\varepsilon} \equiv \int_{\mathbb{R}^n} \pi(\boldsymbol{x}) f_{\boldsymbol{X}}(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \mathbb{E}_{\boldsymbol{X}} \left[ \pi(\boldsymbol{X}) \right]$$
(11)

It is argued here that this quantity does not equal the failure probability because it sums the aleatory uncertainty in the random vector X and the epistemic uncertainty in the prediction

 $\widehat{G}$ . This is the reason why  $p_{f\varepsilon}$  will be referred to as the *augmented failure probability* in the sequel. 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 4), it is impossible to quantify the contribution of each source of uncertainty in  $p_{f\varepsilon}$ . This remark motivates the approach introduced in this section where the probabilistic classification function is used in conjunction with importance sampling in order to build a new estimator of the failure probability.

# 3.1. Importance sampling

Importance sampling (IS) consists in computing the mathematical expectation of the failure indicator function with respect to a biased PDF which favors the failure event of interest (Rubinstein and Kroese, 2008). The so-called *instrumental density* denoted by h is assumed to dominate  $\mathbb{1}_{q\leq 0} f_{\mathbf{X}}$ , meaning that:

$$\forall \boldsymbol{x} \in \mathcal{D}_{\boldsymbol{x}}, \ h(\boldsymbol{x}) = 0 \Rightarrow \mathbb{1}_{g \le 0}(\boldsymbol{x}) \ f_{\boldsymbol{X}}(\boldsymbol{x}) = 0$$
(12)

Given this instrumental density, the definition of the failure probability in Eq. (1) may be rewritten as follows:

$$p_f = \int_{\mathbb{R}^n} \mathbb{1}_{g \le 0}(\boldsymbol{x}) \, \frac{f_{\boldsymbol{X}}(\boldsymbol{x})}{h(\boldsymbol{x})} \, h(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} \equiv \mathbb{E}_h\left[\mathbb{1}_{g \le 0}(\boldsymbol{X}) \frac{f_{\boldsymbol{X}}(\boldsymbol{X})}{h(\boldsymbol{X})}\right]$$
(13)

In this expression, the expectation  $\mathbb{E}_h[\cdot]$  is now computed with respect to the instrumental density h. The above definition of the failure probability easily leads to the *importance* sampling estimator:

$$\widehat{p}_{f\,\mathrm{IS}} \equiv \frac{1}{N} \sum_{k=1}^{N} \mathbb{1}_{g \leq 0} \left( \boldsymbol{x}^{(k)} \right) \, \frac{f_{\boldsymbol{X}}(\boldsymbol{x}^{(k)})}{h(\boldsymbol{x}^{(k)})} \tag{14}$$

where  $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(N)}\}$  is a set of samples drawn from the instrumental density 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:

$$\operatorname{Var}\left[\widehat{p}_{f\,\mathrm{IS}}\right] = \frac{1}{N-1} \left( \frac{1}{N} \sum_{k=1}^{N} \mathbb{1}_{g \le 0}(\boldsymbol{x}^{(k)}) \frac{f(\boldsymbol{x}^{(k)})^2}{h(\boldsymbol{x}^{(k)})^2} - \widehat{p}_{f\,\mathrm{IS}}^2 \right)$$
(15)

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

$$h^*(\boldsymbol{x}) = \frac{\mathbb{1}_{g \le 0}(\boldsymbol{x}) f(\boldsymbol{x})}{\int \mathbb{1}_{g \le 0}(\boldsymbol{x}) f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}} = \frac{\mathbb{1}_{g \le 0}(\boldsymbol{x}) f(\boldsymbol{x})}{p_f}$$
(16)

However this instrumental PDF is not implementable in practice because it involves the sought failure probability  $p_f$  in its denominator. The art of importance sampling consists in building an instrumental density which is *quasi-optimal*.

# 3.2. A metamodel-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 *design point* obtained by FORM in the space of the independent standardized random variables. Au and Beck (1999) resort to a kernel smoothing approximation of the optimal instrumental PDF built from a set of failed samples obtained by a Markov-chain-Monte-Carlo-based algorithm.

In this paper, it is proposed to use the probabilistic classification function in Eq. (9) as a surrogate for the real indicator function in the optimal instrumental PDF in Eq. (16). Hence, the proposed quasi-optimal PDF reads as follows:

$$\widehat{h^*}(\boldsymbol{x}) = \frac{\pi(\boldsymbol{x}) f(\boldsymbol{x})}{\int \pi(\boldsymbol{x}) f(\boldsymbol{x}) d\boldsymbol{x}} = \frac{\pi(\boldsymbol{x}) f(\boldsymbol{x})}{p_{f\varepsilon}}$$
(17)

where  $p_{f\varepsilon}$  is the augmented failure probability which has been already defined in Eq. (11). For the sake of illustration, this quasi-optimal instrumental PDF is compared to the optimal (although impractical) one in Figure 1 using a two-dimensional limit state function introduced by Der Kiureghian and Dakessian (1998).

#### 3.3. The metamodel-based importance sampling estimator

Choosing the proposed quasi-optimal instrumental PDF (*i.e.* substituting  $\hat{h}^*$  for h in Eq. (13)) leads to the following new expression of the failure probability:

$$p_f = \int \mathbb{1}_{g \le 0}(\boldsymbol{x}) \frac{f(\boldsymbol{x})}{\hat{h^*}(\boldsymbol{x})} \, \hat{h^*}(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = p_{f\varepsilon} \, \int \frac{\mathbb{1}_{g \le 0}(\boldsymbol{x})}{\pi(\boldsymbol{x})} \, \hat{h^*}(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} \equiv p_{f\varepsilon} \, \alpha_{\mathrm{corr}} \tag{18}$$



(a) The optimal instrumental PDF  $h^*$ . (b) The proposed quasi-optimal instrumental PDF  $\hat{h^*}$ .

Figure 1: Comparison of the instrumental PDFs on the two-dimensional example from Der Kiureghian and Dakessian (1998)  $(g(X_1, X_2) = 5 - X_2 - \frac{1}{2}(X_1 - 0.1)^2, X_i \sim \mathcal{N}(0, 1), i = 1, 2)$ 

where we have introduced  $\alpha_{\text{corr}} \equiv \mathbb{E}_{\widehat{h^*}} \left[ \frac{\mathbb{1}_{g \leq 0}(X)}{\pi(X)} \right]$ . This means that the failure probability is equal to the product of the augmented failure probability  $p_{f \varepsilon}$  and a correction factor  $\alpha_{\text{corr}}$ . This correction factor is defined as the expected ratio between the real indicator function  $\mathbb{1}_{g \leq 0}$  and the probabilistic classification function  $\pi$ . Thus, if the Kriging prediction is fully accurate, the correction factor is equal to one and the failure probability is identical to the augmented failure probability (optimality of the proposed estimator). On the other hand, in the more general case where the Kriging prediction is not fully accurate, the correction factor modifies the augmented failure probability accounting for the epistemic uncertainty.

The two terms in Eq. (18) may now be estimated using Monte Carlo simulation:

$$\widehat{p}_{f\varepsilon} = \frac{1}{N_{\varepsilon}} \sum_{i=1}^{N_{\varepsilon}} \pi(\boldsymbol{x}^{(i)}) \qquad \widehat{\alpha}_{\text{corr}} = \frac{1}{N_{\text{corr}}} \sum_{j=1}^{N_{\text{corr}}} \frac{\mathbb{1}_{g \le 0}(\boldsymbol{h}^{(j)})}{\pi(\boldsymbol{h}^{(j)})}$$
(19)

where the first  $N_{\varepsilon}$ -sample set is generated from the original PDF  $f_{\mathbf{X}}$ , and the second  $N_{\text{corr}}$ sample set is generated from the quasi-optimal instrumental PDF  $\hat{h^*}$ . Due to the expression of the latter (see Eq.(17)), Markov chain Monte Carlo simulation (Robert and Casella, 2004) is used. The present implementation makes use of a revised version of the so-called *modified Metropolis-Hastings sampler* of Au and Beck (2001). In order to ensure that the samples used in Eq. (19) are independent, we use the so-called *thinning procedure* which consists in keeping only one sample every t states of the chain (say t = 10).

According to the central limit theorem, the two estimates in Eq.(19) are unbiased and normally distributed. Their respective variance denoted by  $\sigma_{\varepsilon}^2$  and  $\sigma_{\text{corr}}^2$  may be easily derived as in Eq. (15). Finally, the proposed estimator of the failure probability simply reads as follows:

$$\widehat{p}_{f\,\mathrm{metaIS}} = \widehat{p}_{f\,\varepsilon}\,\widehat{\alpha}_{\mathrm{corr}} \tag{20}$$

It is important to note that both terms in Eq. (20) are independent, since they rely upon sampling according to two independent PDFs. Based on this remark, it is shown in Appendix A that for reasonably small values of the coefficients of variation  $\delta_{\hat{p}_{f\varepsilon}}$  and  $\delta_{\hat{\alpha}_{corr}}$  of the two estimators  $\hat{p}_{f\varepsilon}$  and  $\hat{\alpha}_{corr}$  (say 1% to 10%), the coefficient of variation of the proposed estimator approximately reads:

$$\delta_{\hat{p}_{f \text{ metalS}}} \approx_{\delta_{\varepsilon}, \delta_{\text{corr}} \ll 1} \sqrt{\delta_{\hat{p}_{f_{\varepsilon}}}^2 + \delta_{\hat{\alpha}_{\text{corr}}}^2}$$
(21)

#### 4. Adaptive refinement of the probabilistic classification function

The efficiency of the approach mostly relies on the optimality of the instrumental PDF  $\hat{h^*}$ . Thus it is proposed here to adaptively refine the probabilistic classification function so that the quasi-optimal instrumental PDF  $\hat{h^*}$  converges towards its optimal counterpart  $h^*$ .

# 4.1. Refinement strategy

There exists a relatively large literature about the adaptive refinement of a Kriging prediction for accurate classification (or level-set approximation), see *e.g.* Oakley (2004); Lee and Jung (2008); Bichon et al. (2008); Vazquez and Bect (2009); Picheny et al. (2010); Echard et al. (2011). They all rely on the definition of a so-called *in-fill criterion* which is maximum or minimum in the region of interest, namely the region where the sign of the predicted performance function is the most uncertain. The interested reader may find the expressions for all these criteria together with a discussed comparison on two analytical examples in a recent paper by Bect et al. (2012).

As an introduction to the proposed strategy, it is argued that the available approximation of the optimal instrumental PDF after m observations, say  $\hat{h}^*(\boldsymbol{x}) \propto \pi(\boldsymbol{x}) f_{\boldsymbol{X}}(\boldsymbol{x})$ , is an interesting trade-off criterion because it takes large values in regions (i) where the sign of the predicted performance function is supposed to be negative due to  $\pi(\boldsymbol{x})$ , and (ii) where the probability density function  $f_{\boldsymbol{X}}$  is maximum. As a consequence, it is proposed to replace the step of optimization of the in-fill criterion by a sampling step, as proposed in Dubourg et al. (2011). This is achieved by considering the in-fill criterion as an improper PDF. The algorithm proceeds as follows:

- 1. Sample a large population (say  $10^4$  samples) from the weighted in-fill criterion (here  $\hat{h^*}$ ) using a MCMC simulation technique such as the modified Metropolis-Hastings sampler.
- 2. Reduce this population to its K clusters' center (K being prescribed, see Section 5) using the K-means clustering algorithm (MacQueen, 1967).
- 3. Evaluate the performance function on the K clusters' center.
- 4. Enrich the former experimental design with these K new observations.
- 5. Update the Kriging prediction and loop back to step 1 until some target accuracy is achieved, see Section 4.2.

The proposed sampling-based refinement strategy allows one to refine the prediction from a batch of optimal points instead of a single best point. It thus solves the problem of locally optimal points. Indeed, the in-fill criteria proposed in the literature commonly features several optima thus meaning that there does *not* exist a single best point. In the proposed strategy all the *maxima* are interpreted as modes of the improper PDF  $\pi(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x})$  and this leads to local concentrations of points close to these modes in Step #1. The K-means clustering algorithm used in the second step reduces the population generated in the first step to the most significant modes. Note also that this approach allows one to perform several computations of the performance model in a distributed manner (*i.e.* on a high performance computing platform).

In a similar fashion, the very first experimental design is obtained by clustering a crude

Monte Carlo sample of X (of size  $10^4$  as for the other iterations). Alternatively one may use a latin hypercube design (LHS), see McKay et al. (1979).

#### 4.2. Stopping criterion

Finally a metric is required to check the optimality of the probabilistic classification function. This metric may then be used as a stopping criterion for the previously detailed refinement strategy thus making it *adaptive*. The metric is based on a cross-validation procedure. Cross-validation techniques are classically used for model selection (see *e.g.* Stone, 1974). Basically, the design of experiments  $\mathcal{X} = \{\boldsymbol{x}_i, i = 1, \ldots, m\}$  is split into a learning subset  $\mathcal{X}_L$  and a validation subset  $\mathcal{X}_V$  such that  $\mathcal{X}_L \cap \mathcal{X}_V = \emptyset$  and  $\mathcal{X}_L \cup \mathcal{X}_V = \mathcal{X}$ . The model is then built using the learning subset  $\mathcal{X}_L$  (hence denoted by  $\tilde{g}_{\mathcal{X}_L}$ ) and validated by comparing the predicted values  $\tilde{g}_{\mathcal{X}_L}(\boldsymbol{x})$  and the real values  $g(\boldsymbol{x})$  onto the validation subset  $\boldsymbol{x} \in \mathcal{X}_V$ . The *leave-one-out* technique is a special case where the learning subset is defined as  $\mathcal{X}_L = \mathcal{X} \setminus \boldsymbol{x}_i$ . In a regression context, Allen (1971) propose to use a leave-one-out estimate of the mean squared error referred to as the *predicted residual sum of squares*:

$$PRESS = \frac{1}{m} \sum_{i=1}^{m} \left( \tilde{g}_{\mathcal{X} \setminus \boldsymbol{x}_i}(\boldsymbol{x}_i) - g(\boldsymbol{x}_i) \right)^2$$
(22)

The metric proposed in this paper is a kind of leave-one-out estimate of the correction factor in Eq. (18), namely:

$$\widehat{\alpha}_{\text{corr LOO}} = \frac{1}{m} \sum_{i=1}^{m} \frac{\mathbb{1}_{g \le 0}(\boldsymbol{x}_i)}{\mathcal{P}\left[\widehat{G}_{\mathcal{X} \setminus \boldsymbol{x}_i}(\boldsymbol{x}_i) \le 0\right]}$$
(23)

where  $\widehat{G}_{\mathcal{X}\setminus \boldsymbol{x}_i}$  is the *i*-th leave-one-out Kriging prediction of the performance function built from the DOE  $\mathcal{X}$  without the *i*-th sample  $\boldsymbol{x}_i$ . This quantity should be estimated using a minimal number of samples (say  $m \geq 30$ ) so that it is sufficiently accurate.

The reason for introducing this leave-one-out estimate of  $\hat{\alpha}_{corr}$  is the following. In the early steps of the refinement procedure, the Kriging predictor is not accurate enough to evaluate the failure probability by means of Eq. (20) efficiently. Thus it would be ineffective to waste costly evaluations of the true limit-state function to compute the true correction factor in Eq. (19).

On the contrary, the leave-one-out estimate  $\hat{\alpha}_{\text{corr LOO}}$  in Eq. (23) makes use only of the *available observations* in the experimental design only, so that it is fast to evaluate. As discussed earlier in Section 3.3, a sufficient accuracy is reached when the estimate in Eq. (23) gets close to one because it means that the probabilistic classification function converges towards the failure indicator function. Consequently the instrumental PDF  $\hat{h}^*$  converges towards its optimal counterpart  $h^*$ . It is thus proposed to use  $\hat{\alpha}_{\text{corr LOO}}$  as an indication to stop the refinement strategy. Precisely, the iterative enrichment of  $\mathcal{X}$  is stopped if  $\hat{\alpha}_{\text{corr LOO}}$  is in the order of magnitude of 1, say between 0.1 and 10. Note that in the case of high dimensional and/or highly nonlinear problems, the size of the DOE may be limited to, say  $m_{\text{max}} = 1000$ , for computational efficiency.

It may happen that a leave-one-out estimate of the Kriging variance  $\sigma_{\widehat{G}_{X\setminus x_i}}^2(\boldsymbol{x}_i)$  gets close or even equal to zero. This is problematic because the ratio in Eq. (23) might not be defined in such cases. Indeed, if the mean prediction  $\mu_{\widehat{G}_{X\setminus x_i}}(\boldsymbol{x}_i)$  is positive, the probabilistic classification function in the denominator equals zero and it may cause an exception. It is argued that this variance should never be exactly zero (the Kriging variance equals zero only at the samples in the DOE, here  $\mathcal{X} \setminus \boldsymbol{x}_i$ ), so that it is proposed to bound the probabilistic classification function above a reasonably low value (say the machine precision,  $\varepsilon_{\rm M} \approx 10^{-16}$ ).

# 4.3. Summary of the implementation

The purpose of this section is to summarize the proposed metamodel-based importance sampling algorithm. The flowchart of the algorithm is given in Figure 4.3. It is essentially divided in three independent steps, two of which could potentially be run in parallel.

First, the algorithm only requires the choice of a targeted coefficient of variation  $\delta_{\text{target}}$  for the final estimate  $\hat{p}_{f \text{ metaIS}}$  and the number K of points that should be added at each refinement iteration. Note that the user may also want to limit the total number of calls to the original limit-state function through the  $N_{\text{max}}$  parameter.



Figure 2: Flowchart of the proposed metamodel-based importance sampling algorithm

Then, the first step of the algorithm is to build a reasonably accurate approximation of the probabilistic classification function that will bring a significant variance reduction for the final importance-sampling-based estimate of the failure probability. Note that this step is optional in the case the analysis is resumed from an existing DOE.

The two other steps are independent and might be run in parallel. They consist in using Monte Carlo simulation for the estimation of the two terms  $\hat{\alpha}_{corr}$  and  $\hat{p}_{f\varepsilon}$  defining the

proposed estimator  $\hat{p}_{f \text{ metaIS}}$ , see Section 3. In the current implementation, we targeted the same coefficient of variation  $\delta_{\varepsilon} = \delta_{\text{corr}} = \delta_{\text{target}}/\sqrt{2}$  for the two estimators. It could also be possible to implement these two steps in two independent threads that would communicate between each other and decide whether to stop the simulation or not based on the estimate of the final coefficient of variation. It should also be pointed out that it is easier to reduce the estimation variance on the augmented failure probability than the one on the correction factor because the former only depends on the Kriging surrogate.

# 5. Application examples

In this section, the proposed strategy is applied to a number of structural reliability problems for the sake of illustration. The first examples involve simple analytical limit-state functions and can thus be used to validate the implementation of the proposed strategy. The last example involves a more sophisticated nonlinear finite element model coupled with a high dimensional stochastic model so as to prove the applicability of the strategy to industrial problems.

#### 5.1. Analytical limit-state functions

# 5.1.1. Example 1: Influence of the dimension

This first structural reliability example is taken from Rackwitz (2001). It involves n independent lognormal random variates with mean value  $\mu = 1$  and standard deviation  $\sigma = 0.2$ . The performance function reads as follows:

$$g(\boldsymbol{x}) = \left(n + a \,\sigma \sqrt{n}\right) - \sum_{i=1}^{n} x_i \tag{24}$$

where a is set equal to 3 for the present application. The dimension of the problem is successively set equal to  $n = \{2, 50, 100\}$  to assess the influence of the dimension on the proposed estimator.

The results and performance of the proposed strategy are compared to that obtained by other state-of-the-art reliability methods in Table 1. It can first be seen that the FORM approximation becomes severely wrong when the dimension increases because of the curvature of the limit-state surface, as pointed out by Rackwitz (2001). Then, all Monte-Carlosimulation-based methods were tuned on purpose to reach a 2% target coefficient of variation (c.o.v.). Since this problem features a single design point, the design-point-based importance sampling strategy ( $P^*$ -IS) proposed by Melchers (1989) performs very well and yields unbiased estimates of the failure probability. Note however that the unicity of this point cannot be guaranteed in general. The number of calls required by this approach accounts for both the search for the design point ( $n_{\text{FORM}}$ ) and the importance sampling scheme ( $N_{\text{IS}}$ ). Eventually, meta-model-based importance sampling (Meta-IS) yields unbiased estimates of the failure probability with a significant variance reduction that makes it competitive with  $P^*$ -IS.

Method		Monte Carlo	FORM	$P^*$ -IS $^a$	$Meta-IS^b$
	N	500,000	31	31 + 8,600	12 + 100
n = 2	$p_f$	$4.98\times 10^{-3}$	$3.84\times10^{-3}$	$5.02\times 10^{-3}$	$5.03\times10^{-3}$
	C.o.V.	$<\!2\%$	_	$<\!2\%$	$<\!2\%$
n = 50	N	1,329,400	166	166 + 13,900	300 + 1,500
	$p_f$	$1.88\times 10^{-3}$	$1.54\times 10^{-4}$	$1.97\times 10^{-3}$	$1.95\times 10^{-3}$
	C.o.V.	$<\!\!2\%$	_	$<\!2\%$	$<\!2\%$
	N	$1,\!385,\!100$	316	316 + 18,800	600 + 2,000
n = 100	$p_f$	$1.80 \times 10^{-3}$	$4.20\times 10^{-5}$	$1.76\times 10^{-3}$	$1.74\times 10^{-3}$
	C.o.V.	${<}2\%$	_	$<\!\!2\%$	$<\!\!2\%$

 $^{a}N = n_{\rm FORM} + N_{\rm IS}$ 

 ${}^{b}N = m + N_{\text{corr}}.$ 

Table 1: Results for Example 1 (Rackwitz, 2001): 
$$g(\mathbf{X}) = (n + a \sigma \sqrt{n}) - \sum_{i=1}^{n} X_i;$$

Using the mean of the Kriging prediction obtained from the final DOE as a surrogate for the limit-state function in a crude Monte Carlo simulation results in the following probability estimates:  $4.69 \times 10^{-3}$ ,  $1.49 \times 10^{-3}$ ,  $1.21 \times 10^{-3}$  for n = 2, 50 and 100 respectively (and up to a 2% c.o.v). Despite these probabilities seem reasonably accurate *in the light of the reference*  results provided by Monte Carlo sampling, it must be noted that there is no proof they are in general. Detailed results regarding the application of metamodel-based importance sampling to this example are given in Table 2. Note that the correction factor increases with the dimension. In low dimension (n = 2) the Kriging surrogate almost exactly equals the performance function (at least in the vicinity of the limit-state surface) hence  $\hat{\alpha}_{corr} = 1$ and  $\hat{p}_{f \text{metalS}} = \hat{p}_{f\varepsilon}$  (no misclassification according to the sign of the surrogate  $\mu_{\hat{g}}$ ). In larger dimensions the surrogate loses accuracy, and the correction factor gets more and more important. The size of the DOE from which the Kriging prediction is built is given as the product between the number of refinement iterations and the number K of clusters' center added per iteration. K is chosen equal to the number of input random variables  $(n = \{2, 50, 100\}).$ 

n	2	50	100
m	6  imes 2	$6 \times 50$	$6 \times 100$
$\widehat{p}_{farepsilon}$	$5.03  imes 10^{-3}$	$1.97\times 10^{-3}$	$1.87\times 10^{-3}$
$\delta_{arepsilon}$	$\leq 1.41\%$	$\leq 1.41\%$	$\leq 1.41\%$
$N_{ m corr}$	100	1,500	2,000
$\widehat{\alpha}_{\mathrm{corr}}$	1	0.99	0.93
$\delta_{ m corr}$	0%	$\leq 1.41\%$	$\leq 1.41\%$
$m + N_{\rm corr}$	112	1,800	2,700
$\widehat{p}_{f \text{ metals}}$	$5.03  imes 10^{-3}$	$1.95\times 10^{-3}$	$1.74 \times 10^{-3}$
$\delta_{ m metaIS}$	$\leq 1.41\%$	$\leq 2\%$	$\leq 2\%$

Table 2: Detailed results for the application of metamodel-based importance sampling to Example 1 (Rackwitz, 2001):  $g(\mathbf{X}) = (n + a \sigma \sqrt{n}) - \sum_{i=1}^{n} X_i;$ 

Table 3 provides some additional information about the computational time required by the sampling-clustering-based refinement strategy detailed in Section 4.1.  $10^4$  samples from the refinement PDF are required in the present setup of the algorithm. These samples are generated here using the modified Metropolis-Hastings algorithm . The Markov chains are thinned by retaining one sample every 10 states. Hence this requires  $10^5$  evaluations of the probabilistic classification function  $\pi$  per refinement iteration. K-means clustering is used here to cluster K = n groups out of the 10<sup>4</sup> points generated in the previous step. The sampling time obviously increases with both the dimension n and the size of the experimental design because the Kriging surrogates becomes more and more expensive to evaluate. The clustering time depends on the size of the sample (fixed here equal to  $10^4$  for all runs) and the number of groups K. However, these computation times remain acceptable with respect to that required by a single evaluation of a finite-element-based limit-state function.

Refinement iteration		init.	2	3	4	5	6
	DOE size	2	4	6	8	10	12
n = 2	Sampling time (s)	<1	3	4	4	4	4
	Clustering time (s)	<1	<1	<1	<1	<1	<1
n = 50	DOE size	50	100	150	200	250	300
	Sampling time (s)	<1	9	18	28	36	54
	Clustering time (s)	6	3	5	5	6	6
	DOE size	100	200	300	400	500	600
n = 100	Sampling time (s)	<1	22	46	62	105	143
	Clustering time (s)	2	2	3	2	2	2

Table 3: Computational times required by the sampling/clustering-based refinement strategy on Example 1 using Matlab<sup>TM</sup> on an Intel<sup>®</sup> Core<sup>TM</sup> i5 CPU M560 @2.67GHz running Ubuntu Linux 10.04 LTS codename "Lucid Lynx".

# 5.1.2. Example 2: Multiple design points

A two-dimensional series system from the article by Au and Beck (1999) is taken as a second example for demonstrating the applicability of Meta-IS to limit-state surfaces featuring multiple design points. The limit-state function reads as follows:

$$g(x_1, x_2) = \min \left\{ \begin{array}{c} c - 1 - x_2 + \exp\left(-x_1^2/10\right) + (x_1/5)^4 \\ c^2/2 - x_1 x_2 \end{array} \right\}$$
(25)

where  $x_1$  and  $x_2$  are the realizations of two independent standard Gaussian random variates  $X_1$  and  $X_2$ . The limit-state surface features 3 design points whose coordinates are  $\boldsymbol{x}^{*(1)} = (0, c)^{\mathsf{T}}, \ \boldsymbol{x}^{*(2)} = (c/\sqrt{2}, c/\sqrt{2})^{\mathsf{T}}$  and  $\boldsymbol{x}^{*(3)} = (-c/\sqrt{2}, -c/\sqrt{2})^{\mathsf{T}}$ . Au and Beck (1999) focused on the two first design points and apparently omitted the third one without much consequence on the results they present though.

Comparative results are shown in Table 4. Single-design-point-based approaches are not used here since they would be mistaken by the 3 design points. Sampling-based approaches are tuned on purpose to reach a 5% c.o.v, except for Au and Beck's results which are reported from the original article. Crude Monte Carlo estimates are considered here as reference. The results of Au and Beck (1999) are averaged over the 5 runs of their algorithm in the case where they use N = 500 samples as read in Table 1 of the original article. The coefficients of variation are estimated empirically on each sample of the 5 probability estimates. Meta-IS yields unbiased estimates of the failure probability for all values of c because the Kriging surrogate captured the three design points. It can be seen that Meta-IS saves a significant amount of calls to the performance function with respect to the other sampling approaches. The failure probabilities estimated by crude Monte Carlo sampling on the means of the Kriging predictors for c = 3, 4 and 5 are respectively equal to  $\tilde{p}_f = 3.04 \times 10^{-3}$ ,  $1.05 \times 10^{-4}$ and  $7.05 \times 10^{-7}$  up to a 5% c.o.v.

Meta-IS is now run 30 times in the sole case where c = 3 in order to prove that *(i)* the estimator is unbiased, and that *(ii)* the c.o.v given in Eq. (21) is a sound estimate of its accuracy (see also Appendix A). The average of the 30 estimates of the failure probability is  $p_f = 3.36 \times 10^{-3}$  up to a 7% empirical c.o.v.) which is slightly larger than the target (5%) estimated by means of Eq. (21).

#### 5.1.3. Example 3: Concave limit-state surface

This structural reliability example was first proposed in the report by Der Kiureghian and de Stefano (1991). It was then used for benchmark purposes in the recent article by Bourinet et al. (2011). It consists in studying the failure of a two-degree-of-freedom damped oscillator under a white-noise base excitation. The probabilistic model is composed of n = 8

Method		Monte Carlo (ref)	Subset	Au and Beck $(1999)^{ab}$	$Meta-IS^{c}$
	N	120,000	300,000	100 + 500	44 + 600
c = 3	$p_f$	$3.35 \times 10^{-3}$	$3.48\times 10^{-3}$	$2.47\times 10^{-3}$	$3.54\times 10^{-3}$
	C.o.V.	$<\!5\%$	<3%	8%	$<\!5\%$
	N	4,620,000	500,000	100 + 500	64 + 600
c = 4	$p_f$	$8.68 \times 10^{-5}$	$8.34\times10^{-5}$	$6.51\times10^{-5}$	$8.60\times 10^{-5}$
	C.o.V.	$<\!5\%$	$<\!\!4\%$	10%	$<\!5\%$
	N	422,110,000	700,000	100 + 500	40 + 2,900
c = 5	$p_f$	$9.48 \times 10^{-7}$	$6.55\times 10^{-7}$	$6.54\times10^{-7}$	$9.17\times 10^{-7}$
	C.o.V.	$<\!5\%$	<5%	12%	$<\!5\%$

 $^{a}N = M + N_{\text{IS}}.$ 

<sup>b</sup>Averaged from Au and Beck (1999, Table 1, N = 500).

 $^{c}N = m + N_{\text{corr}}.$ 

Table 4: Results for Example 2 (Au and Beck, 1999):  $g(X_1, X_2) = \min \left\{ c - 1 - X_2 + \exp \left( -X_1^2/10 \right) + \left( X_1/5 \right)^4 ; c^2/2 - X_1 X_2 \right\};$ 

independent random variables whose distributions are defined in Table 5. The mean value of  $F_s$  is varied from 15.0 to 27.5 as in Bourinet et al. (2011). The limit-state function reads as follows:

$$g(\boldsymbol{x}) = F_s - p \, k_s \left[ \pi \, \frac{S_0}{4 \, \zeta_s \, \omega_s^3} \, \frac{\zeta_a \, \zeta_s}{\zeta_p \, \zeta_s \, (4 \, \zeta_a^2 + \theta^2) + \gamma \, \zeta_a^2} \, \frac{(\zeta_p \, \omega_p^3 + \zeta_s \, \omega_s^3) \, \omega_p}{4 \, \zeta_a \, \omega_a^4} \right]^{1/2} \tag{26}$$

It is characterized by a highly nonlinear limit-state surface around a single design point.

The adaptive refinement of the Kriging surrogate is initialized with  $K_0 = 32$  points and K = 16 new points are sequentially added until the leave-one-out estimate of the correction factor reaches a stable value between 0.1 and 10. The adaptive importance sampling scheme uses 100 Markov chains incremented in parallel and a 5% c.o.v. is targeted. Table 6 presents the results obtained on this example for the three values of  $\mu_{F_s}$ . For the sake of validation, the results yielded by the proposed metamodel-based importance sampling technique are compared with those obtained by subset sampling (using a sample size of  $10^5$  per step ) which is considered here as the reference. FORM results were obtained by Der Kiureghian and de Stefano (1991) and confirmed by Bourinet et al. (2011) using the iHLRF algorithm

Variable	Distribution	Mean	C.o.V.
$m_p$	Lognormal	1.5	10%
$m_s$	Lognormal	0.01	10%
$k_p$	Lognormal	1	20%
$k_s$	Lognormal	0.01	20%
$\zeta_p$	Lognormal	0.05	40%
$\zeta_s$	Lognormal	0.02	50%
$F_S$	Lognormal	$\{15, 21.5, 27.5\}$	10%
$S_0$	Lognormal	100	10%

Table 5: Probabilistic model for Example 3 (two-degree of freedom damped oscillator).

(Zhang and Der Kiureghian, 1995). It can be seen that the "bias" yielded by the FORM approximation is rather significant, especially when the probability of failure is small (up to one order of magnitude).

The results yielded by the proposed strategy are finally compared to those obtained by Bourinet et al.'s surrogate-based approach. From the computational cost point of view, it can be seen that (i) for the proposed strategy, the total number of calls to the original performance function is comparable with that required by their substitution approach, and that (ii) both approaches yield accurate estimates of the quantity of interest. However, it should again be noted that surrogate-based approaches do not yield statistically consistent results while Meta-IS does.

Meta-IS is run again for the sole case where  $\mu_{F_s} = 27.5$ . For this run, the adaptive refinement strategy of the experimental design is arbitrarily stopped after 10 iterations in order to prove (i) the ability of Meta-IS to provide unbiased estimates even from a coarse Kriging surrogate, and (ii) the importance of refining the surrogate to reduce the estimation variance. The experimental design now contains m = 176 points which is significantly less than the 480 points used in the first adaptive run. The failure probability estimated by subset simulation using the mean of the Kriging predictor yields  $\tilde{p}_f = 8.26 \times 10^{-10}$  up to a 7% c.o.v. It should be noted that this estimate is heavily biased (by 3 orders of magnitude)

$\mu_{F_s}$	values	$\mathbf{FORM}^{a}$	Subset (ref)	$\mathbf{SVM} + \mathbf{Subset}^a$	$\mathbf{Meta} extsf{-}\mathbf{IS}^{b}$
	N	$1,\!179$	300,000	1,719	464 + 200
15	$p_f$	$2.19\times 10^{-2}$	$4.63\times 10^{-3}$	$4.78\times10^{-3}$	$4.80\times10^{-3}$
	C.o.V.	_	$<\!\!3\%$	<4%	$<\!5\%$
21.5	N	2,520	500,000	2,865	336 + 400
	$p_f$	$3.50\times 10^{-4}$	$4.75\times10^{-5}$	$4.42\times10^{-5}$	$4.46\times 10^{-5}$
	C.o.V.	_	$<\!\!4\%$	<7%	$<\!5\%$
27.5	N	2,727	700,000	4,011	480 + 200
	$p_f$	$3.91\times 10^{-6}$	$3.47\times 10^{-7}$	$3.66\times 10^{-7}$	$3.76\times 10^{-7}$
	C.o.V.	_	$<\!5\%$	<10%	$<\!5\%$

<sup>a</sup>As computed by Bourinet et al. (2011).

 ${}^{b}N = m + N_{\text{corr}}.$ 

Table 6: Results for Example 3 (two-degree of freedom damped oscillator).

with respect to the reference solution provided in Table 6. This emphasize the fact that the crude substitution of surrogate model may be a hazardous practice in structural reliability analysis.

The augmented failure probability is  $p_{f\varepsilon} = 3.17 \times 10^{-8}$  (c.o.v.=4%). The correction factor estimated with  $N_{\rm corr} = 20,000$  samples equals  $\alpha_{\rm corr} = 4.21$  (c.o.v.=17%). Hence, the coarse but unbiased Meta-IS estimate of the failure probability is  $1.33 \times 10^{-7}$  (c.o.v.=17%). Note that the total computational cost (176 + 20,000) is much greater than that presented in Table 6 (480 + 200). As a conclusion, it appears more efficient to spend more time in enriching the DOE in order to obtain a more accurate Kriging predictor.

# 5.2. Nonlinear stability analysis of an imperfect shell roof



Figure 3: Illustration of the Scordelis-Lo shell roof example.

The mechanical model for this example is inspired by Scordelis and Lo (1961). It concerns the buckling analysis of a cylindrical shell roof whose dimensions are given in Figure 3. The longitudinal edges of the roof are free while its circumferential edges are supported by rigid diaphragms (radial displacement fixed to zero). Its constitutive material is assumed to have a nonlinear elastic Ramberg-Osgood material behavior. It is subjected to a constant surface load q and the structure is considered to fail if its critical buckling load  $q_{\rm cr}$  is less than a prescribed service load of magnitude  $q_0 = 0.18$  MPa, so that the associated performance function may be defined as follows:

$$g(\boldsymbol{\xi}) = q_{\rm cr}(\boldsymbol{\xi}) - q_0 \tag{27}$$

where  $\boldsymbol{\xi}$  denotes the outcome of the random vector  $\boldsymbol{\Xi}$  introduced in the sequel.

The critical buckling load  $q_{cr}$  is determined by means of the *asymptotic numerical method* (Cochelin, 1994) coupled with a 30 × 30 8-node Büchter-Ramm shell finite element mesh (Büchter et al., 1994) using the EVE finite element code. This academic software was initially developed by Cochelin (1994) and further developed by Noirfalise et al. (2008). The

stochastic model, inspired from Dubourg et al. (2009), involves four independent random fields defined over the roof surface. They describe respectively the initial shape imperfection  $\zeta$ , the material Young's modulus E, the material yield stress  $\sigma_y$  and the shell thickness h. The random shape imperfection is modeled as a linear combination of the three most critical Euler buckling modes' shape { $\mathcal{U}_k, k = 1, ..., 3$ }, so that it reads as follows:

$$\zeta(\boldsymbol{x},\,\theta) = \sum_{k=1}^{3} \Xi_{\zeta\,k} \,\mathcal{U}_k(x,\,\theta) \tag{28}$$

where  $\{\Xi_{\zeta k}, k = 1, \ldots, 3\}$  are three independent Gaussian random variates with mean  $\mu_{\zeta} = 0$  and standard deviation  $\sigma_{\zeta} \approx 9.5$  mm (see details in Dubourg (2011)). The other three random fields are assumed independent and lognormal with constant means  $\mu_h = 76$  mm,  $\mu_E = 200,000$  MPa and  $\mu_{\sigma_y} = 390$  MPa and c.o.v.  $\delta_h = 5\%$ ,  $\delta_E = 3\%$  and  $\delta_{\sigma_y} = 7\%$ . They are represented by three Karhunen-Loève expansions of three independent standard Gaussian random fields, whose sample paths are *translated* into lognormal sample paths, see Dubourg et al. (2009) for the mapping. These three Gaussian random fields are assumed to have the same isotropic squared exponential autocorrelation function with a correlation length  $\ell = 3,500$  mm. Due to the choice of this correlation function, the Fredholm integral equation involved in the Karhunen-Loève discretization scheme has no analytical solution. A so-called *wavelet-Galerkin* numerical procedure was thus used as detailed in Phoon et al. (2002). Each random field is simulated by means of 30 independent standard Gaussian random variates leading to a relative mean squared discretization error of 3.70%. Finally the complete stochastic model involves 93 independent random variables.

The reliability results are gathered in Table 7. The proposed importance sampling scheme leads to a failure probability in full agreement with the value obtained by subset simulation (as implemented in the FERUM toolbox v4.0 by Bourinet et al., 2009) which validates the proposed strategy. In this example the augmented failure probability  $\hat{p}_{f\varepsilon}$  is equal to 2.06 ×  $10^{-4}$  (with a c.o.v. of 5.70%), and the correction factor  $\hat{\alpha}_{corr}$  is equal to 0.641 (with a c.o.v. of 12.49%). The instrumental PDF is sampled here by means of the slice sampler of Neal (2003) which is another MCMC sampling technique (see also Dubourg, 2011, Appendix B). A multiple FORM analysis revealed the existence of 4 most probable failure configurations

Method	Subset (ref.)	Multi-FORM	Meta-IS
DOE size	-	-	$6 \times 93$
MPFP search	-	$\approx 10,000$	-
Simulations	20,000	-	9,464
$p_f$ estimates	$1.27\times 10^{-4}$	$1.22\times 10^{-4}$	$1.32\times 10^{-4}$
C.o.V.	12.36%	-	13.75%

Table 7: Comparative results for the shell roof example adapted from Dubourg et al. (2009).

identified by means of the restarted *i*-HLRF algorithm from Der Kiureghian and Dakessian (1998). These 4 failure modes corresponds to the 4 extreme cases for which the "demand" random field  $\zeta$  is maximal in the corner of the roof whereas the "capacity" random fields E,  $\sigma_y$  and h are minimal. The combination of these 4 failure modes in a series system then allowed to give a *Multi-FORM* approximation of the failure probability (third column in Table 7). In this case, the Ditlevsen's bounds coincide (up to the accuracy provided in Table 7). For the sake of illustration, one of the 4 most probable failure configurations is shown in Figure 4. This proves the ability of the proposed strategy to deal with reliability problems featuring multiple design points in a reasonably high dimension.

#### 6. Conclusion

Starting from the double premise that the usual surrogate-based reliability analyses do not permit to quantify the error made by using the metamodel instead of the original limitstate function, 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, a probabilistic classification function based on the post-processing of a Kriging prediction was introduced. This function allows a smoother classification than its deterministic counterpart (*i.e.* the indicator function of the failure domain) accounting for the epistemic uncertainty in the Kriging prediction. The probabilistic classification is then used to for-



Figure 4: One of the 4 most probable failure configurations.

mulate a quasi-optimal importance sampling density. Using elementary algebra the failure probability is recast as a product of two terms, namely the *augmented failure probability*  $p_{f\varepsilon}$  which is evaluated by means of the meta-model only, and a correction factor  $\alpha_{corr}$  that is computed from evaluations of the original limit-state function. In order to decide whether the Kriging surrogate is accurate enough, a leave-one-out estimate of  $\alpha_{corr}$  is used and the iterative refinement is stopped when it is in the order of magnitude of 1. Once the Kriging surrogate has been built, the two terms of the product defining the failure probability may be evaluated in parallel.

The method turned out to be efficient on various application examples, as shown in this paper and further detailed in Dubourg (2011). It can handle problems featuring a reasonably high number of random variables and multiple design points. Further work is in progress to include the proposed algorithm within a reliability-based design optimization framework.

### Acknowledgements

The first author is funded by a CIFRE grant from Phimeca Engineering S.A. subsidized by the ANRT (convention number 706/2008). The financial support from the French National Research Agency (ANR) through the KidPocket project (ANR Grant #xxx) is also gratefully acknowledged.

# Appendix A. Calculation of the coefficient of variation

The estimator in Eq. (20) is defined as the product of two estimators. Let us denote these two unbiased independent estimators as  $\hat{p}_1$ ,  $\hat{p}_2$  with variances  $\sigma_1^2$ ,  $\sigma_2^2$  for the sake of clarity. The calculation of the variance of the final estimator  $\hat{p} = \hat{p}_1 \hat{p}_2$  proceeds as follows. First, according to its definition, the variance reads:

$$\sigma_{\widehat{p}}^2 \equiv \operatorname{Var}\left[\widehat{p}\right] \equiv \mathbb{E}\left[\widehat{p_1}^2 \, \widehat{p_2}^2\right] - \mathbb{E}\left[\widehat{p_1} \, \widehat{p_2}\right]^2 \tag{A.1}$$

Since the two estimators  $\hat{p_1}$  and  $\hat{p_2}$  are independent, the variance also reads:

$$\sigma_{\widehat{p}}^2 = \mathbb{E}\left[\widehat{p_1}^2\right] \mathbb{E}\left[\widehat{p_2}^2\right] - \mathbb{E}\left[\widehat{p_1}\right]^2 \mathbb{E}\left[\widehat{p_2}\right]^2 \tag{A.2}$$

which may be further elaborated according to the König-Huyghens theorem:

$$\sigma_{\widehat{p}}^2 = \left(\mathbb{E}\left[\widehat{p_1}\right]^2 + \sigma_1^2\right) \left(\mathbb{E}\left[\widehat{p_2}\right]^2 + \sigma_2^2\right) - \mathbb{E}\left[\widehat{p_1}\right]^2 \mathbb{E}\left[\widehat{p_2}\right]^2 \tag{A.3}$$

Due to the unbiasedness of the estimators, one finally gets:

$$\sigma_{\hat{p}}^2 = (p_1^2 + \sigma_1^2) (p_2^2 + \sigma_2^2) - p_1^2 p_2^2$$
(A.4)

$$= \sigma_1^2 \sigma_2^2 + p_1^2 \sigma_2^2 + p_2^2 \sigma_1^2 \tag{A.5}$$

Denoting by  $\delta_i = \sigma_i/p_i$  the coefficients of variation of  $\hat{p}_i$ , i = 1, 2, the coefficient of variation of  $\hat{p} = \hat{p}_1 \hat{p}_2$  eventually reads:

$$\delta \equiv \frac{\sigma_{\hat{p}}}{p_1 \, p_2} = \sqrt{\delta_1^2 + \delta_2^2 + \delta_1^2 \, \delta_2^2} \tag{A.6}$$

In practice usual target coefficients of variation  $\delta_{\text{target}}$  range from 1% to 10% so that:

$$\delta \approx \sqrt{\delta_1^2 + \delta_2^2}$$
 when  $\delta_1, \delta_2 \ll 1$  (A.7)

#### References

- Allen, D., 1971. The prediction sum of squares as a criterion for selecting prediction variables. Tech. Rep. 23, Dept. of Statistics, University of Kentucky.
- Au, S., Beck, J., 1999. A new adaptive importance sampling scheme for reliability calculations. Structural Safety 21 (2), 135–158.
- Au, S., Beck, J., 2001. Estimation of small failure probabilities in high dimensions by subset simulation. Prob. Eng. Mech. 16 (4), 263–277.
- Bect, J., Ginsbourger, D., Li, L., Picheny, V., Vazquez, E., 2012. Sequential design of computer experiments for the estimation of a probability of failure. Stat. Comput. 22 (3), 773–793.
- Bichon, B., Eldred, M., Swiler, L., Mahadevan, S., McFarland, J., 2008. Efficient global reliability analysis for nonlinear implicit performance functions. AIAA Journal 46 (10), 2459–2468.
- Bourinet, J.-M., Deheeger, F., Lemaire, M., 2011. Assessing small failure probabilities by combined subset simulation and support vector machines. Structural Safety 33 (6), 343–353.
- Bourinet, J.-M., Mattrand, C., Dubourg, V., 2009. A review of recent features and improvements added to FERUM software. In: Proc. ICOSSAR'09, Int Conf. on Structural Safety And Reliability, Osaka, Japan.
- Breitung, K., 1984. Asymptotic approximation for multinormal integrals. J. Eng. Mech. 110 (3), 357–366.
- Bucher, C., Bourgund, U., 1990. A fast and efficient response surface approach for structural reliability problems. Structural Safety 7, 57–66.
- Büchter, N., Ramm, E., Roehl, D., 1994. Three-dimensional extension of non-linear shell formulation based on the enhanced assumed strain concept. Int. J. Num. Meth. Eng. 37 (15), 2551–2568.
- Ching, J., Au, S., Beck, J., 2005a. Reliability estimation for dynamical systems subject to stochastic excitation using subset simulation with splitting. Comput. Methods Appl. Mech. Engrg. 194 (12-16), 1557–1579.
- Ching, J., Beck, J., Au, S., 2005b. Hybrid subset simulation method for reliability estimation of dynamical systems subject to stochastic excitation. Prob. Eng. Mech. 20 (3), 199–214.
- Cochelin, B., 1994. A path-following technique via an asymptotic-numerical method. Computers and Structures 53, 1181–1192.
- Das, P.-K., Zheng, Y., 2000. Cumulative formation of response surface and its use in reliability analysis. Prob. Eng. Mech. 15 (4), 309–315.
- Deheeger, F., Lemaire, M., 2007. Support vector machines for efficient subset simulations: <sup>2</sup>SMART method. In: Proc. 10th Int. Conf. on Applications of Stat. and Prob. in Civil Engineering (ICASP10), Tokyo, Japan.
- Der Kiureghian, A., Dakessian, T., 1998. Multiple design points in first and second-order reliability. Structural Safety 20 (1), 37–49.
- Der Kiureghian, A., de Stefano, M., 1991. Efficient algorithms for second order reliability analysis. J. Eng.

Mech. 117 (12), 2906–2923.

Ditlevsen, O., Madsen, H., 1996. Structural reliability methods. J. Wiley and Sons, Chichester.

- Dubourg, V., 2011. Adaptive surrogate models for reliability analysis and reliability-based design optimization. Ph.D. thesis, Université Blaise Pascal, Clermont-Ferrand, France.
- Dubourg, V., Bourinet, J.-M., Sudret, B., 2009. FE-based reliability analysis of the buckling of shells with random shape, material and thickness imperfections. In: Furuta, H., Frangopol, D., Shinozuka, M. (Eds.), Proc. 10th Int. Conf. Struct. Safety and Reliability (ICOSSAR'2009), Osaka, Japan.
- Dubourg, V., Sudret, B., Bourinet, J.-M., 2011. Reliability-based design optimization using kriging and subset simulation. Struct. Multidisc. Optim. 44 (5), 673–690.
- Echard, B., Gayton, N., Lemaire, M., 2011. AK-MCS: an active learning reliability method combining kriging and Monte Carlo simulation. Structural Safety 33 (2), 145–154.
- Hurtado, J., 2004. Structural reliability Statistical learning perspectives. Vol. 17 of Lecture notes in applied and computational mechanics. Springer.
- Kaymaz, I., 2005. Application of kriging method to structural reliability problems. Structural Safety 27 (2), 133–151.
- Kim, S.-H., Na, S.-W., 1997. Response surface method using vector projected sampling points. Structural Safety 19 (1), 3–19.
- Lee, T., Jung, J., 2008. A sampling technique enhancing accuracy and efficiency of metamodel-based RBDO: Constraint boundary sampling. Computers & Structures 86 (13-14), 1463–1476.
- Lophaven, S., Nielsen, H., Søndergaard, J., 2002. DACE, A Matlab Kriging Toolbox. Technical University of Denmark.
- MacQueen, J., 1967. Some methods for classification and analysis of multivariate observations. In: Le Cam, L.M. & Neyman, J. (Ed.), Proc. 5<sup>th</sup> Berkeley Symp. on Math. Stat. & Prob. Vol. 1. University of California Press, Berkeley, CA, pp. 281–297.
- McKay, M. D., Beckman, R. J., Conover, W. J., 1979. A comparison of three methods for selecting values of input variables in the analysis of output from a computer code. Technometrics 2, 239–245.
- Melchers, R., 1989. Importance sampling in structural systems. Structural Safety 6, 3–10.
- Neal, R., 2003. Slice sampling. Annals Stat. 31, 705–767.
- Noirfalise, C., Bourinet, J.-M., Fogli, M., Cochelin, B., 2008. Reliability analysis of the buckling of imperfect shells based on the Karhunen-Loève expansion. In: Proc. 8th World Cong. Comput. Mech. (WCCM8) and 5th Eur. Congress Comput. Meth. Appl. Sci. Eng. (ECCOMAS 2008), Venice, Italy.
- Oakley, J., 2004. Estimating percentiles of uncertain computer code outputs. J. Roy. Statist. Soc. Ser. C 53 (1), 83–93.
- Papadrakakis, M., Lagaros, N., 2002. Reliability-based structural optimization using neural networks and

Monte Carlo simulation. Comput. Methods Appl. Mech. Engrg. 191 (32), 3491–3507.

- Phoon, K., Huang, S., Quek, S., 2002. Simulation of second-order processes using Karhunen-Loève expansion. Computers & Structures 80 (12), 1049–1060.
- Picheny, V., 2009. Improving accuracy and compensating for uncertainty in surrogate modeling. Ph.D. thesis, University of Florida.
- Picheny, V., Ginsbourger, D., Roustant, O., Haftka, R., 2010. Adaptive designs of experiments for accurate approximation of a target region. J. Mech. Des. 132 (7), 071008.
- Rackwitz, R., 2001. Reliability analysis A review and some perspectives. Structural Safety 23, 365–395.
- Robert, C., Casella, G., 2004. Monte Carlo statistical methods  $(2^{nd} \text{ Ed.})$ . Springer Series in Statistics. Springer Verlag.
- Rubinstein, R., Kroese, D., 2008. Simulation and the Monte Carlo method. Wiley Series in Probability and Statistics. Wiley.
- Sacks, J., Welch, W., Mitchell, T., Wynn, H., 1989. Design and analysis of computer experiments. Stat. Sci. 4, 409–435.
- Santner, T., Williams, B., Notz, W., 2003. The Design and Analysis of Computer Experiments. Springer, New York.
- Scordelis, A. C., Lo, K. S., 1961. Computer analysis of cylindrical shells. ACI Journal 61, 539–561.
- Stone, M., 1974. Cross-validatory choice and assessment of statistical predictions. J. Royal Stat. Soc., Series B 36, 111–147.
- Vazquez, E., Bect, J., 2009. A sequential Bayesian algorithm to estimate a probability of failure. In: 15th IFAC Symposium on System Identification. IFAC, Saint-Malo.
- Welch, W., Buck, R., Sacks, J., Wynn, H., Mitchell, T., Morris, M., 1992. Screening, predicting, and computer experiments. Technometrics 34, 15–25.
- Zhang, Y., Der Kiureghian, A., 1995. Two improved algorithms for reliability analysis. In: Rackwitz, R., Augusti, G., Bori, A. (Eds.), Proc. 6th IFIP WG7.5 on Reliability and Optimization of Structural systems, Assisi, Italy. Chapman & Hall, London.