Adaptive Designs of Experiments for Accurate Approximation of Target Regions

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Abstract

This paper addresses the issue of designing experiments for a metamodel that needs to be accurate for a certain level of the response value. Such situation is encountered in particular in constrained optimization and reliability analysis. Here, we propose an iterative strategy to build designs of experiments, which is based on an explicit trade-off between reduction of global uncertainty and exploration of the regions of interest. The method is illustrated on several test-problems. It is shown that a substantial reduction of error can be achieved in the crucial regions, with reasonable loss on the global accuracy. The method is finally applied to a reliability analysis problem; it is found that the adaptive designs significantly outperform classical space-filling designs.

1. Introduction

In the past decades, the use of *metamodeling* techniques has been recognized to efficiently address the issues of prediction and optimization of expensive-to-compute numerical simulators or black-box functions [1,2]. A metamodel (or surrogate model) is an approximation to system response constructed from its value at a limited number of selected input values, the *design of experiments* (DoE). The choice of the DoE is crucial for the accuracy of the metamodel approximation. Furthermore, in many engineering problems, the total number of function evaluations is drastically limited by computational cost; hence, it is of crucial interest to develop methods for selecting efficiently the experiments.

In this paper, we focus on a particular application where metamodels are used in a way that their accuracy is crucial for certain level-sets. Such situation appears in particular in two popular frameworks:

(1) In constrained optimization, the constraint function often relies on expensive calculations. For instance, a typical structural optimization formulation is to minimize a

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weight function such that the maximum stress, computed by finite element analysis, does not exceed a certain value. When using a metamodel to approximate the constraint, it is of utmost importance that the approximation error is minimal along the contour line that separates the admissible designs from infeasible ones.

(2) In reliability analysis, a metamodel is often used to propagate the uncertainty of random input variables to the performance function of a system [3,4]. In particular, the probability of failure of the system can be computed using sampling techniques (i.e. Monte-Carlo Simulations, MCS), by counting the number of samples that are above a certain threshold. The contour line of the response equal to the threshold must be known accurately to discriminate between samples.

The objective of the present work is to provide a methodology to construct a design of experiments such that the metamodel accurately approximates the vicinity of a contour line. Mourelatos et al. [5] used a combination of global and local metamodels to first detect the critical regions and then obtain a locally accurate approximation. Ranjan et al. [6] proposed a modified version of the EGO algorithm to sequentially explore the domain region along a contour line. Vasquez et al. [7] proposed an iterative strategy to minimize the classification error when computing a probability of failure based on Kriging. In this paper, we present an alternative criterion to choose sequentially the experiments, based on an explicit trade-off between the exploration of the target region (on the vicinity of the contour line) and reduction of the global uncertainty (prediction variance) in the metamodel.

The paper is organized as follow: in Section 2, the Kriging model and the framework of design of experiments are described. In Section 3, the original criterion of selecting experiments is presented, followed by its associated sequential strategy to derive designs of experiments. Results are presented for various analytical examples in Section 4. Finally, the criterion is applied to estimating the probability of failure.

2. Kriging Metamodel and Design of Experiments

Let us first introduce some notations. We denote y the response of numerical simulator or function that is to be studied:

$$\begin{array}{rccc} y: & D \subset \mathbb{R}^d & \rightarrow & \mathbb{R} \\ & \mathbf{x} & \mapsto & y(\mathbf{x}) \end{array} \tag{1}$$

where $\mathbf{x} = \{x_1, \ldots, x_d\}^T$ is a d-dimensional vector of input variables. In order to build a metamodel, the response y is observed at n distinct locations $\mathbf{X}$:

$$\begin{aligned} \mathbf{X} &= \left[\mathbf{x}^1, ..., \mathbf{x}^n\right] \\ \mathbf{Y} &= \left\{y\left(\mathbf{x}^1\right), ..., y\left(\mathbf{x}^n\right)\right\} = y(\mathbf{X}) \end{aligned} \tag{2}$$

In Eq. (2), choosing $\mathbf{X}$ is called the *design of experiments* (DoE), and $\mathbf{Y}$ is observations. Since the response y is expensive to evaluate, we approximate it by a simple model M, called the *metamodel* or *surrogate model*, based on hypothesis on the nature of y and on its observations $\mathbf{Y}$ at the points of the DoE. In this paper, we present a particular metamodel, Universal Kriging (UK), then we discuss some important issues about the choice of the design of experiments.

2.1 Universal Kriging Model

The main hypothesis behind the Kriging model is to assume that the true function y is one realization of a Gaussian process Y:

$$y(\mathbf{x}) = Y(\mathbf{x}, \omega) \tag{3}$$

where ω belongs to the underlying probability space Ω. In the following we use the notation $Y(\mathbf{x})$ for the process and $Y(\mathbf{x}, \omega)$ for one realization. For Universal Kriging, Y is of the form:

$$Y(\mathbf{x}) = \sum_{j=1}^{p} \beta_j f_j(\mathbf{x}) + Z(\mathbf{x}) \tag{4}$$

where f_j are linearly independent known functions, and Z is a Gaussian process with zero mean and covariance k with known correlation structure and parameters.

Under such hypothesis, the best linear unbiased estimator (BLUE) for y, knowing the observations $\mathbf{Y}$, is given by the following equation:

$$\begin{aligned} m_K(\mathbf{x}) &= E\left[Y(\mathbf{x}) \middle| Y(\mathbf{X}) = \mathbf{Y} \right] \\ &= \mathbf{f}(\mathbf{x})\hat{\boldsymbol{\beta}} + \mathbf{c}(\mathbf{x})^T \mathbf{C}^{-1}\left(\mathbf{Y} - \mathbf{F}\hat{\boldsymbol{\beta}}\right) \end{aligned} \tag{5}$$

where $\mathbf{f}(\mathbf{x}) = [f_1(\mathbf{x}), \ldots, f_p(\mathbf{x})]$ is $1 \times p$ vector of bases, $\hat{\boldsymbol{\beta}} = \{\hat{\beta}_1, \ldots, \hat{\beta}_p\}^T$ is $p \times 1$ vector of estimates of $\boldsymbol{\beta}$, $\mathbf{c}(\mathbf{x}) = [\mathrm{cov}(\mathbf{x}, \mathbf{x}^1), \ldots, \mathrm{cov}(\mathbf{x}, \mathbf{x}^n)]^T$ is $n \times 1$ vector of covariance, $\mathbf{C} = [\mathrm{cov}(\mathbf{x}^i, \mathbf{x}^j)]_{1 \le i, j \le n}$ is $n \times n$ covariance matrix, and $\mathbf{F}^T = [\mathbf{f}^T(\mathbf{x}^1), \ldots, \mathbf{f}^T(\mathbf{x}^n)]$ is $p \times n$ matrix of bases. In Eq. (5), $\hat{\boldsymbol{\beta}}$ is the vector of generalized least square estimates of $\boldsymbol{\beta}$:

$$\hat{\boldsymbol{\beta}} = \{\hat{\beta}_1, \ldots, \hat{\beta}_p\}^T = \left(\mathbf{F}^T \mathbf{C}^{-1} \mathbf{F}\right)^{-1} \mathbf{F}^T \mathbf{C}^{-1} \mathbf{Y} \tag{6}$$

In addition, the Kriging model provides an estimate of the accuracy of the mean predictor, the Kriging prediction variance:

$$s_K^2(\mathbf{x}) = \sigma^2 - \mathbf{c}(\mathbf{x})^T \mathbf{C}^{-1} \mathbf{c}(\mathbf{x}) + \left(\mathbf{f}(\mathbf{x})^T - \mathbf{c}(\mathbf{x})^T \mathbf{C}^{-1} \mathbf{F}\right)\left(\mathbf{F}^T \mathbf{C}^{-1} \mathbf{F}\right)^{-1}\left(\mathbf{f}(\mathbf{x})^T - \mathbf{c}(\mathbf{x})^T \mathbf{C}^{-1} \mathbf{F}\right)^T \tag{7}$$

where σ^2 is the process variance. For details of derivations, see for instance [8, 9]. Note that the Kriging variance in Eq. (7) does not depend on the observations $\mathbf{Y}$, but only on the design of experiments.

We denote by $M(\mathbf{x})$ the Gaussian process conditional on the observations $\mathbf{Y}$:

$$\left(M(\mathbf{x})\right)_{\mathbf{x} \in D} = \left(Y(\mathbf{x}) / Y(\mathbf{X}) = \mathbf{Y}\right)_{\mathbf{x} \in D} = \left(Y(\mathbf{x}) / obs\right)_{\mathbf{x} \in D} \tag{8}$$

The Kriging model provides the distribution of M at a prediction point $\mathbf{x}$:

$$M(\mathbf{x}) \sim N\left(m_k(\mathbf{x}), s_k^2(\mathbf{x})\right) \tag{9}$$

The Kriging mean m_K interpolates the function $Y(\mathbf{x})$ at the design of experiment points:

$$m_K\left(\mathbf{x}^i\right) = Y\left(\mathbf{x}^i\right),\ 1 \le i \le n \tag{10}$$

The Kriging variance is null at the observation points $\mathbf{x}^i$, and greater than zero elsewhere:

$$s_K^2(\mathbf{x}^i) = 0 \qquad 1 \le i \le n$$
$$s_K^2(\mathbf{x}) > 0 \qquad \mathbf{x} \ne \mathbf{x}^i \tag{11}$$

Besides, the Kriging variance function increases with the distance of **x** to the observation points. Figure 1 shows a Kriging model with a first-order trend and five equally-spaced observations along with the confidence intervals, which is calculated from $m_K \pm 2s_K$. Note that due to the interpolating property of UK, the prediction variance is null at the observation points.

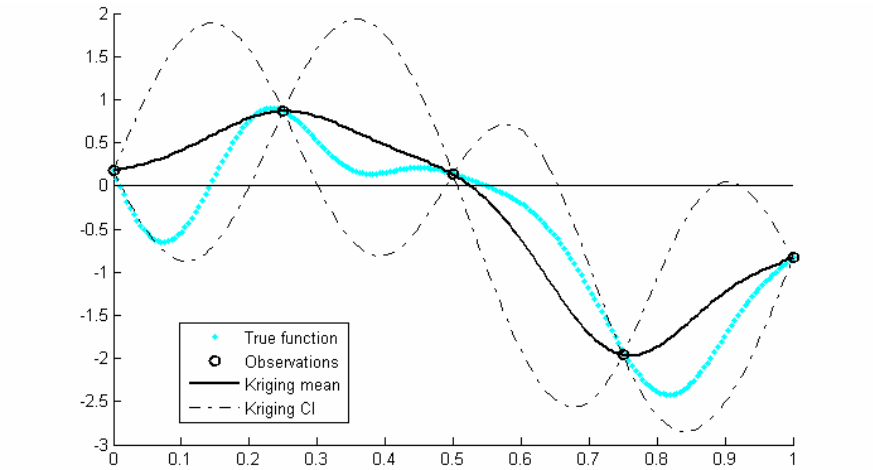


Figure 1: Example of Kriging model. The confidence intervals are $m_K \pm 2s_K$. The DoE consists of five points equally spaced in [0, 1]. The trend is a first order polynomial.

2.2 Design of Experiments

Choosing the set of experiments **X** plays a critical role in the accuracy of the metamodel and the subsequent use of the metamodel for prediction. In this section, we detail three families of design of experiments: classical designs, optimal designs, and sequential designs.

(i) Classical (space-filling) designs

The first family of DoE consists of designs based on geometric considerations. Full-factorial designs and central-composite designs belong to this category [10]. Although these designs ensure a reasonable space-filling property in low dimensions, they require a large number of observations in high dimensions, making them impractical for computationally expensive problems.

A popular alternative to the geometrical designs is Latin Hypercube sampling (LHS) [11]. LHS is a random DoE that insures uniformity of the marginal distributions of the input variables. LHS can also be optimized using several criteria; for instance, the maximum minimum distance between sampling points. Other space-filling strategies include maximum-entropy designs, low-discrepancy sequences, etc. [12]. Figure 2 shows three different DoEs (full-factorial, central composite, and LHS designs) for two-dimensional domain.

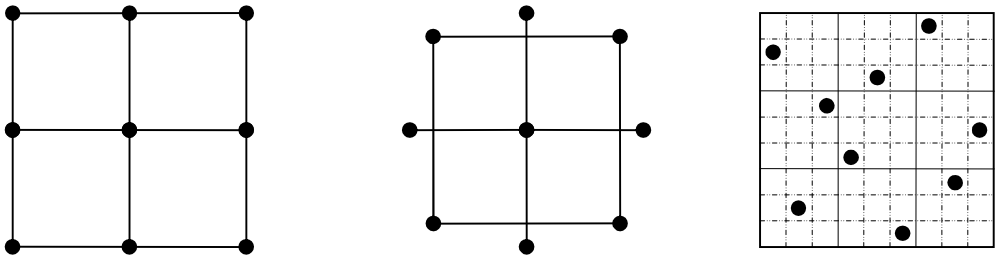


Figure 2: Full-factorial, central composite, and LHS designs with 9 points

(ii) Optimal designs (model-dependent designs)

DoE using optimal design theory has originally been developed in the frame of linear regression [13, 14]. The idea of optimal design theory is to choose the observation points in order to maximize the quality of statistical inference. A- and D-optimality aim at minimizing the uncertainty in the parameters of the metamodel. In the framework of linear regression, D-optimal designs minimize the volume of the confidence ellipsoid of the coefficients, while A-optimal designs minimize its perimeter. Formally, the A- and D-optimality criteria are, respectively, the trace and determinant of Fisher's information matrix.

For non-parametric metamodels such as Kriging, no criterion of this type is available. Instead, a natural alternative is to take advantage of the prediction variance associated with the metamodel. The prediction variance allows us to build measures that reflect the overall accuracy of the Kriging. Two different criteria are available: the integrated mean square error (IMSE) and maximum mean square error (MMSE) [15, 16]:

$$\mathrm{IMSE} = \int_D \mathrm{MSE}(\mathbf{x})\,\mathrm{d}\mu(\mathbf{x}) \tag{12}$$

$$\mathrm{MMSE} = \max_{\mathbf{x}\in D}\left[\mathrm{MSE}(\mathbf{x})\right] \tag{13}$$

where $\mu(\mathbf{x})$ is an integration measure and

$$\mathrm{MSE}(\mathbf{x}) = E\left[\left(y(\mathbf{x}) - M(\mathbf{x})\right)^2\right] \tag{14}$$

When no modeling error is involved, the MSE coincides with the prediction variance s_K^2. Note that the above criteria are often called I-criterion and G-criterion, respectively, in the regression framework. The IMSE is a measure of the average accuracy of the metamodel, while the MMSE measures the 'risk' of large error in prediction.

Optimal designs are *model-dependent*, in the sense that the optimality criterion is determined by the choice of the metamodel. In regression, A- and D-criteria depend on the choice of the basis functions, while in Kriging, the prediction variance s_K^2 depends on the linear trend, the covariance structure, and parameter values. However, one may notice that none of the criteria depends on the response values at the design points.

(iii) Adaptive designs

The previous DoE strategies choose all the points of the design before computing any observation. It is also possible to build the DoE sequentially, by choosing a new point as a function of the other points and their corresponding response values. Typically, the new point achieves a maximum on some criterion; for instance, the sequential DoE can be built by making at each step a new observation so that the prediction variance becomes maximal.

Williams et al. [17] use a Bayesian approach to derive sequential IMSE designs. Jones et al. (1998) derive sequential designs for the optimization of deterministic simulation models (the well-known EGO algorithm), by choosing at each step the point that maximizes the expected improvement, a functional that represents a compromise between exploration of unknown regions and local search [18].

A particular advantage of sequential strategies over other DoEs is that they can integrate the information given by the first k observation values to choose the $(k+1)^{th}$ training point. In this paper, the objective is to accurately fit a function when it is close to a given level-set. It is then evident that the DoE needs to be built according to the observation values, hence sequentially.

3. Weighted IMSE Criterion

In this section, we present a variation of the IMSE criterion, adapted to the problem of fitting a function accurately for a certain level-set. The controlling idea of this work is that the surrogate does not need to be globally accurate, but only in some critical regions, which are the vicinity of the target contour line.

3.1 Target region defined by an indicator function

The IMSE criterion is convenient because it sums up the uncertainty associated with the Kriging model over the entire domain D. However, when one is more interested in predicting Y accurately in the vicinity of a contour line $\mathbf{x} = y^{-1}(T)$ (T a constant), such a criterion is not suitable since it weights all points in D according to their Kriging variance, which does not depend on the observations $\mathbf{Y}$, and hence does not favor zones with respect to properties concerning their y values but only on the basis of their position with respect to DoE.

We propose to change the integration domain from D to a neighborhood of $y^{-1}(T)$ in order to learn y accurately near the contour line. We define a *region of interest* $\mathbf{X}_{T,\varepsilon}$ (parameterized by ε) as the subset in D whose image is within the bounds T-ε and T+ε:

$$\mathbf{X}_{T,\varepsilon} = y^{-1}\left([T-\varepsilon, T+\varepsilon]\right) = \left\{\mathbf{x} \in D \middle| y\left(\mathbf{x}\right) \in [T-\varepsilon, T+\varepsilon]\right\} \tag{15}$$

Figure 3 illustrates one-dimensional function with the region of interest being at T = 0.8. Note that the target region consists of two distinct sets.

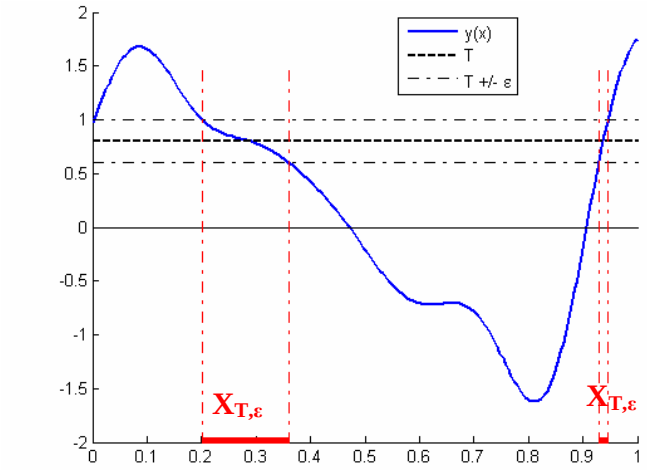


Figure 3: One-dimensional illustration of the target region. The level-set T is equal to 0.8, and ε to 0.2. The target region consists of two distinct sets.

With the region of interest, the reduced IMSE criterion is defined as follow:

$$\mathrm{IMSE}_W = \int_{X_{T,\varepsilon}} \mathrm{MSE}(\mathbf{x})\,\mathrm{d}\mathbf{x} = \int_D \mathrm{MSE}(\mathbf{x}) 1_{[T-\varepsilon \;\; T+\varepsilon]}[y(\mathbf{x})]\,\mathrm{d}\mathbf{x} \tag{16}$$

where $1_{[T-\varepsilon \; T+\varepsilon]}[y(\mathbf{x})]$ is the indicator function, equal to 1 when $y(\mathbf{x}) \in [T-\varepsilon \quad T+\varepsilon]$ and 0 elsewhere.

Finding a design that minimizes IMSE_W would make the metamodel accurate in the subset $\mathbf{X}_{T,\varepsilon}$, which is exactly what we want. Weighting the IMSE criterion over a region of interest was pointed by Box and Draper in [19]. However, the notable difference here is that this region is unknown by the user.

Now, we can adapt the criterion in the context of Kriging modeling, where y as a realization of a Gaussian process Y (see Section 2.1). Thus, IMSE_W is defined with respect to the event ω:

$$\int_D \mathrm{MSE}(\mathbf{x}) 1_{[T-\varepsilon \;\; T+\varepsilon]}[Y(\mathbf{x},\omega)]\,\mathrm{d}\mathbf{x} = I(\omega) \tag{17}$$

To come back to a deterministic criterion, we consider the expectation of $I(\omega)$, conditionally to the observations (which is the best approximation in the L^2 sense):

$$\begin{aligned} \mathrm{IMSE}_W &= E\left[I(\omega) \middle| obs \right] \\ &= E\left[\int_D \mathrm{MSE}(\mathbf{x}) 1_{[T-\varepsilon \;\; T+\varepsilon]}[Y(\mathbf{x})]\,\mathrm{d}\mathbf{x} \middle| obs \right] \end{aligned} \tag{18}$$

Since the quantity inside the integral is positive, we can commute the expectation and the integral:

$$\begin{aligned}\mathrm{IMSE}_W &= \int_D \mathrm{MSE}(\mathbf{x}) E\left[1_{[T-\varepsilon \quad T+\varepsilon]}[Y(\mathbf{x})] \middle| obs\right] \mathrm{d}\mathbf{x} \\ &= \int_D \mathrm{MSE}(\mathbf{x}) E\left[1_{[T-\varepsilon \quad T+\varepsilon]}[M(\mathbf{x})]\right] \mathrm{d}\mathbf{x} \\ &= \int_D \mathrm{MSE}(\mathbf{x}) W(\mathbf{x}) \mathrm{d}\mathbf{x}\end{aligned} \tag{19}$$

According to Eq. (19), the reduced criterion is simply the average of the MSE weighted by the function $W(\mathbf{x})$. Besides, $W(\mathbf{x})$ is simply the probability that the response is inside the interval $[T-\varepsilon \quad T+\varepsilon]$. Indeed:

$$W(\mathbf{x}) = E\left[1_{[T-\varepsilon \quad T+\varepsilon]}[M(\mathbf{x})]\right] = P\left(M(\mathbf{x}) \in [T-\varepsilon \quad T+\varepsilon]\right) \tag{20}$$

For the Kriging model, we have:

$$M(\mathbf{x}) \sim N\left(m_k(\mathbf{x}), s_k^2(\mathbf{x})\right) \tag{21}$$

We can obtain a simple analytical form for $W(\mathbf{x})$:

$$W(\mathbf{x}) = \int_{T-\varepsilon}^{T+\varepsilon} g_{N\left(m_k(\mathbf{x}), s_k^2(\mathbf{x})\right)}(u)\, du \tag{22}$$

where $g_{N(m_K(\mathbf{x}),\sigma_K^2(\mathbf{x}))}(u)$ is the probability density function (PDF) of $M(\mathbf{x})$. By integrating the PDF we obtain:

$$W(\mathbf{x}) = \Phi\left(\frac{T+\varepsilon-m_k(\mathbf{x})}{s_k(\mathbf{x})}\right) - \Phi\left(\frac{T-\varepsilon-m_k(\mathbf{x})}{s_k(\mathbf{x})}\right) \tag{23}$$

where Φ is the cumulative distribution function (CDF) of the standard normal distribution.

3.2 Target region defined by a Gaussian density

Defining the region of interest $\mathbf{X}_{T,\varepsilon}$ is convenient to understand the concepts and to derive the weight function. However, it might not correspond exactly to our objective. Indeed, if we consider an ideal case where the function is entirely known, the indicator function will yield a weight 1 to a point $\mathbf{x}$ where $G(\mathbf{x}) - T = \varepsilon$, but 0 if $G(\mathbf{x}) - T = \varepsilon + 10^{-9}$. Also, it will not discriminate between a point where the difference is equal to ε and another one where this difference is equal to zero.

Instead, we prefer a criterion that continuously increases the importance of the location when the response approaches the threshold. For instance, we can choose a triangular function (with a maximum at T) or a sigmoid function. Here, we choose to use the probability density function of a normal distribution which leads to a simple analytical form of the weight function.

Therefore, the Gaussian-based weight function is defined as

$$W(\mathbf{x}) = E\left[g_\varepsilon\left(M(\mathbf{x}) - T\right)\right] \tag{24}$$

where $g_\varepsilon(u)$ is the PDF of $N\left(0, \quad \sigma_\varepsilon^2\right)$.

When $M(\mathbf{x})$ stands for the Kriging model, we can obtain a simple form for the weight function:

$$W(\mathbf{x}) = \int_{-\infty}^{+\infty} g_\varepsilon(u-T) g_{N\left(m_k(\mathbf{x}), s_k^2(\mathbf{x})\right)}(u)\, du \tag{25}$$

Since g_ε is symmetric:

$$W(\mathbf{x}) = \int_{-\infty}^{+\infty} g_\varepsilon(T-u) g_{N\left(m_k(\mathbf{x}), s_k^2(\mathbf{x})\right)}(u)\, du \tag{26}$$

$W(\mathbf{x})$ is the convolution product of two Gaussian densities; hence, we deduce:

$$W(\mathbf{x}) = \frac{1}{\sqrt{2\pi\left(\sigma_\varepsilon^2 + \sigma_k^2(\mathbf{x})\right)}} e^{\left(-\frac{1}{2}\frac{\left(m_k(\mathbf{x})-T\right)^2}{\sigma_\varepsilon^2+\sigma_k^2(\mathbf{x})}\right)} \tag{27}$$

This new weight function depends on a single parameter σ_ε that allows us to select the size the domain of interest around the function. A large value of σ_ε would enhance space-filling, since the weight function would tend to a constant and the weighted IMSE to a uniform IMSE criterion. On the contrary, a small value would enhance the accuracy of the surrogate on a narrow region around the contour line of interest.

3.3 Illustration

We consider a one-dimensional case, where the function y to approximate is a realization of a Gaussian process with Gaussian covariance structure. y is defined on [0, 1]; the design of experiments consists of five observations equally spaced in this interval. The level-set of interest T is chosen as 1.3, and both σ_ε and ε are taken as 0.2. Figure 4 represents the true function, the Kriging metamodel and corresponding weights. The weight function in Eq. (23) is shown as "interval", while that in Eq. (27) is shown as 'Gaussian" in the figure.

Among the five observations, one is substantially closer to T than the others. As a consequence, the weight functions are large around this observation point. For the indicator-based weight function, the weights are null at the observation points, since on this example no observation is inside the target value interval. For the Gaussian-based weight, it is also very close to zero. For both functions, high weights are given to regions for which the actual function is inside the target interval. Both weight functions are also non-zero where the uncertainty is high, even if the Kriging mean is far from T (around x = 0.65 and 0.85).

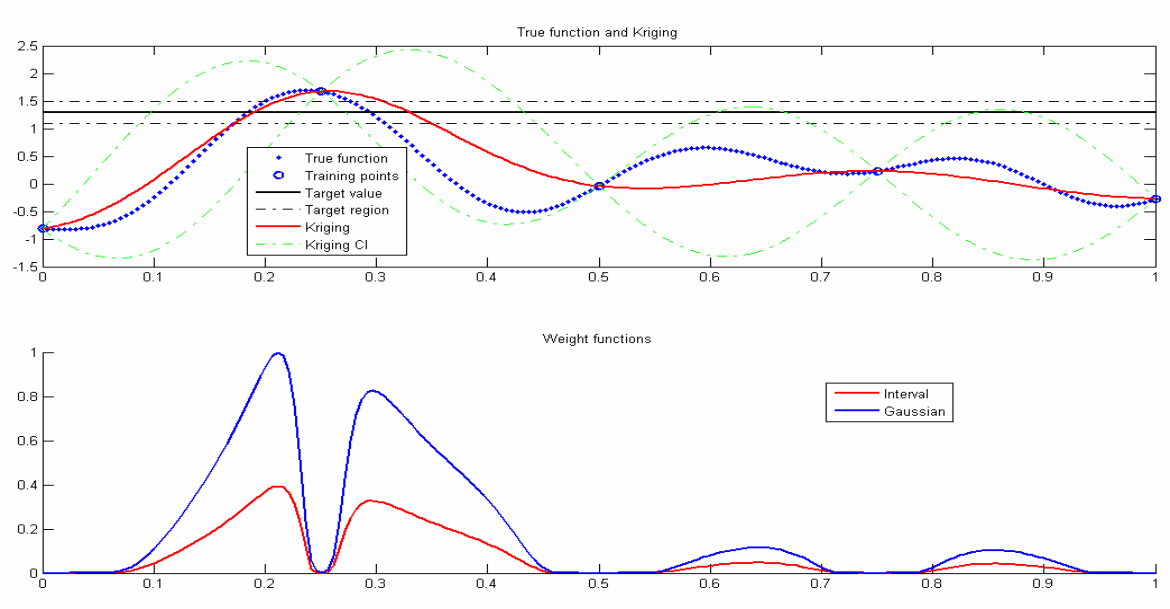


Figure 4: Illustration of the weights functions. Upper graph: true function, observations, Kriging mean and confidence intervals, and target region. Lower graph: weight functions. Both weights are large where the true function is inside the target region, but also in regions of high uncertainties (around x = 0.65 and 0.85).

4. Sequential Strategy for Selecting Experiments

Without any observation, the weight function $W(\mathbf{x})$ is, by construction, a constant. Every time a new observation is performed, the weight function will more precisely discriminate the regions of interest from the others. Hence, the procedure to build an optimal DoE is necessarily iterative, as shown in Table 1:

Table 1: Procedure of the IMSE_w-based sequential DoE strategy

Create an initial DoE, $\mathbf{X}_\text{k}$, and generate observation $\mathbf{Y}_\text{k} = y(\mathbf{X})$

For i going **from** one **to** the total number of additional observations n:

Fit the Kriging model to the data $\left\{\mathbf{X}_{k+i-1}, \mathbf{Y}_{k+i-1}\right\}$

Find a new training point $\mathbf{x}_\text{new}$ that minimizes the criterion $\text{IMSE}_\text{w}\left(\left\{\mathbf{X}_k, \mathbf{x}_{new}\right\}\right)$

Compute the new observation $y_\text{new} = y(\mathbf{x}_\text{new})$

Update the DoE and observations:

$$\mathbf{X}_{k+i} = \left\{\mathbf{X}_{k+i-1}, \mathbf{x}_{new}\right\}$$

$$\mathbf{Y}_{k+i} = \left\{\mathbf{Y}_{k+i-1}, y_{new}\right\}$$

End of loop

The Kriging parameters can be reevaluated after every new observation, or only from the initial DoE before the iterative procedure. Note that reevaluating the parameters can

be problematic. Indeed, the algorithm will tend to make observations where the function value is close to the threshold *T*. The observations are then likely to have the same values, even if they are not close to each other. Hence, by reevaluating the model, there is a risk of finding a model 'flatter' than the true function.

Finding the new training point requires an inner optimization procedure. When the classical IMSE criterion is considered, the optimization can be expressed as:

$$\min_{\mathbf{x}_{new}\in D} \quad \mathrm{IMSE}\left(\mathbf{X}_{k+1}\right) = \mathrm{IMSE}\left(\left\{\mathbf{X}_k, \mathbf{x}_{new}\right\}\right) \tag{28}$$

where

$$\mathrm{IMSE}\left(\left\{\mathbf{X}_k, \mathbf{x}_{new}\right\}\right) = \int_D s_K^2\left(\mathbf{x}\middle|\left\{\mathbf{X}_k, \mathbf{x}_{new}\right\}\right)\mathrm{d}\mathbf{x} \tag{29}$$

$s_K^2\left(\mathbf{x}\middle|\left\{\mathbf{X}_k, \mathbf{x}_{new}\right\}\right)$ is the variance at $\mathbf{x}$ of the Kriging based on the design of experiments $\mathbf{X}$ augmented with the training point $\mathbf{x}_{new}$. Since the Kriging variance does not depend on the observation, there is no need to have $y(\mathbf{x}_{new})$ to compute the IMSE.

In contrast, the weighted IMSE depends on the observations through the weight function $W(\mathbf{x})$. Hence, when expressing the weighted IMSE as a function of $\mathbf{x}_{new}$, we update only the variance part under the integral and not the weight:

$$\mathrm{IMSE}_W\left(\mathbf{X}_k, \mathbf{Y}_k, \mathbf{x}_{new}\right) = \int_D s_k^2\left(\mathbf{x}\middle|\left\{\mathbf{X}_k, \mathbf{x}_{new}\right\}\right) W\left(\mathbf{x}\middle|\mathbf{X}_k, \mathbf{Y}_k\right)\mathrm{d}\mathbf{x} \tag{30}$$

Using this expression, we have the simple formulation for the inner optimization problem:

$$\min_{\mathbf{x}_{new}\in D} \quad \mathrm{IMSE}_W\left(\mathbf{X}_k, \mathbf{Y}_k, \mathbf{x}_{new}\right) \tag{31}$$

The above optimization problem may be, in practice, challenging. The problem dimension is the same with the design space dimension. The objective function can have many local optima and is expensive to compute. Indeed, for any candidate $\mathbf{x}_{\mathrm{new}}$, the Kriging model must be reevaluated (to obtain $s_K^2\left(\mathbf{x}\middle|\left\{\mathbf{X}_k, \mathbf{x}_{new}\right\}\right)$). Also, since the criterion is in integral form, it must be evaluated by numerical integration.

5. Numerical Examples

In this section, we evaluate the accuracy and efficiency of the method through numerical examples. We consider the fitting of realizations of random processes with known covariance structures. Hence, there is no modeling error when using a Kriging approximation; the error is only due to the lack of information.

5.1 Two-dimensional example

The first example is the approximation of a realization of a two dimensional isotropic Gaussian process with Gaussian covariance function. The design space is $[-1\ 1]^2$. For both numerical integration and optimization, the design space is divided by a 32×32 grid. We present the results for the following configurations:

- Target value *T* is chosen as 0.5
- Gaussian-based weight function is used, with parameter $\sigma_\varepsilon = 0.07$.
- Initial DoE consists of the four corners of the domain

16 points are added iteratively to the DoE as described in the previous section. The final results are presented in Figure 5.

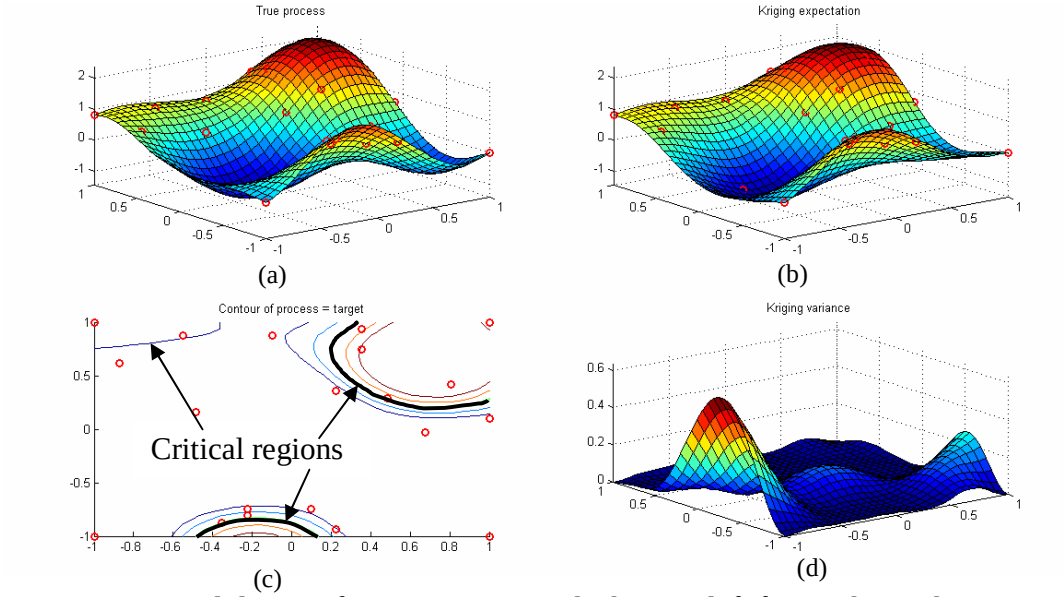
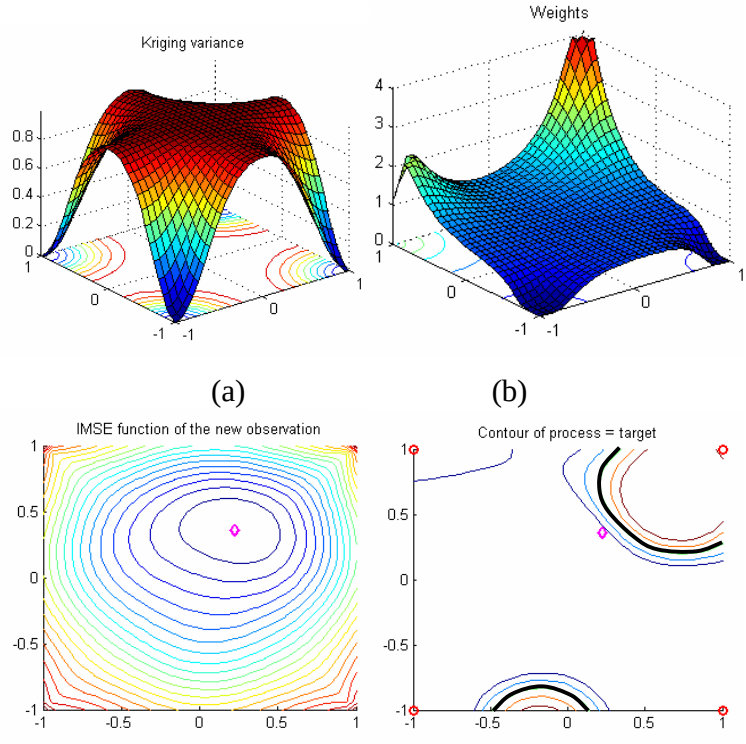


Figure 5: Optimal design after 16 iterations. The bottom left figure shows the contour lines of the true function at levels [T-2σ_ε, T-σ_ε, T, T+σ_ε, T+2σ_ε], which delimit the target regions; the bold line corresponds to the target contour. Most of the training points are chosen close to the target region. The Kriging variance (bottom right figure) is very small in these regions and large in non-critical regions.

Figure 5(a) is the plot of the true function, and Figure 5(b) is that of the Kriging mean. In the contour plot in Figure 5(c), it is shown that there are three critical regions; on two of them the function takes the value *T*, on the third region the response is lower but close to the threshold. After 16 iterations, the sequential strategy used five points to explore the first critical region, eight points to explore the second region, two points for the third region and one point for space-filling. As shown in Figure 5(d), the Kriging variance becomes small near the critical regions, while it is relatively large in the non-critical region.

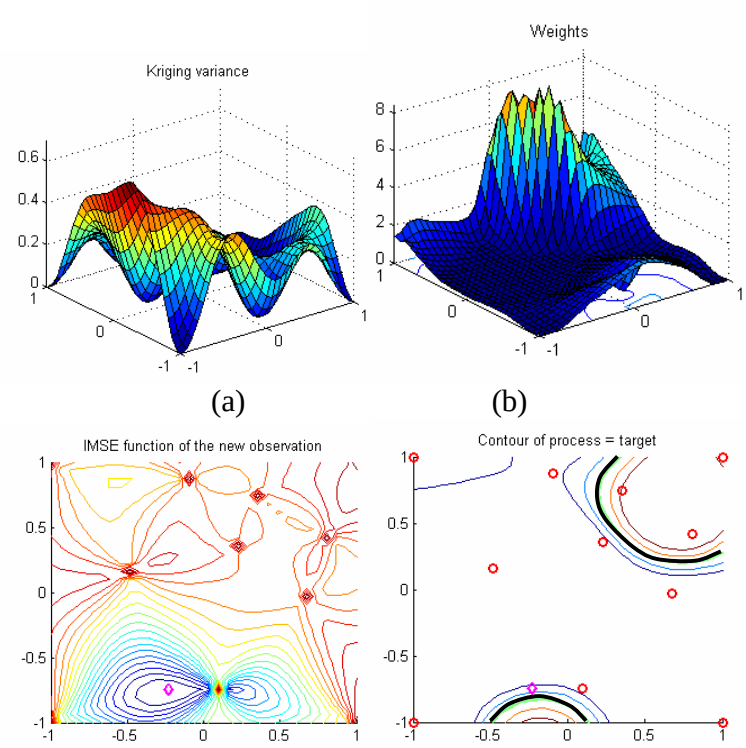
Figure 6 and (c) (d)
Figure 7 show the initial stage and the stage after adding eight observations. Initially, the prediction variance is constant, except at the vicinity of the corners, as shown in Figure 6(a). Since one corner has a response value close to the target, the weight is higher in that region (Figure 6(b)). Thus, a new observation is chosen closer to this corner than the others (Figure 6(c)). After eight iterations ((c) (d)
Figure 7), the weight function shows that the regions are already well identified. The new observation is not chosen where the weight is largest, but where both weight and variance are relatively large, that is on the critical region that is not well-explored yet.



(a) (b)

(c) (d)

Figure 6: Initial state. The weight function is almost uniform, except near the training points.



(a) (b)

(c) (d)

Figure 7: Optimization problem after 8 iterations. The weight function discriminates between critical and non-critical regions.

5.2 Six-dimensional example

In the second example, we consider a realization of a six-dimensional isotropic Gaussian process with Gaussian covariance function. The design space is $[-1\ 1]^6$. In order to limit the complexity (number of non-connected target regions) of the target region, we add a linear trend to the Gaussian process.

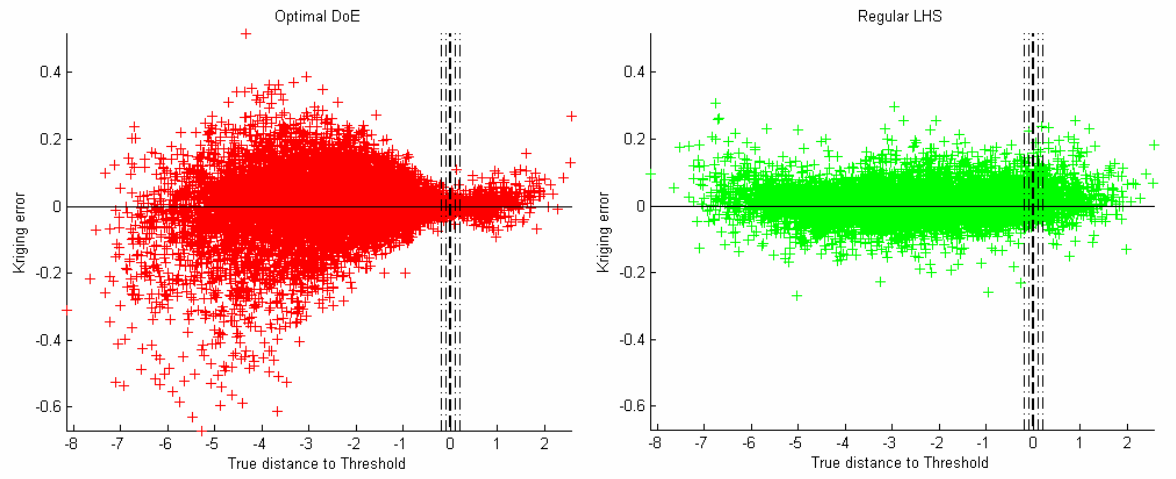
The weighted IMSE criterion is computed by Quasi Monte-Carlo integration. The integration points are chosen from a Sobol sequence [20] to ensure a good space filling property. At each step, the optimization is performed using the population-based optimizer CMA-ES [21].

We present the results for the following configurations:

- Target value is chosen as 2
- Gaussian-based weight function is used, with $\sigma_\varepsilon = 0.05$.
- Initial DoE consists of 20 points chosen from Latin-hypercube sampling (LHS)
- 70 points are added iteratively to the DoE.

For comparison purpose, we generate a classical space-filling DoE that consists of 90 LHS points with maximum minimum distance criterion.

First, we represent the error at 10,000 (uniformly distributed) data points (Figure 8). The classical space-filling DoE leads to a uniform error behavior, while the optimal DoE lead to large errors when the response is far from the target value, while small errors when it is close to the target.



(a) (b)

Figure 8: Comparison of error distribution for two DoEs: (a) optimal DoE and (b) classical LHS. The x-axis is the difference between the true function and the threshold, the y-axis is the error. Five vertical bars are drawn at $-2\sigma_\varepsilon$, $-\sigma_\varepsilon$, 0, $+\sigma_\varepsilon$ and $+2\sigma_\varepsilon$ for the target region. The error is on average smaller for the LHS design, but the optimal DoE reduces substantially the error in the target region.

In order to analyze the error in the target region, we draw the boxplots of the errors for the test points where responses are inside the domains $[-\sigma_\varepsilon, +\sigma_\varepsilon]$ and $[-2\sigma_\varepsilon, +2\sigma_\varepsilon]$ (Figure

9). Compared to the space-filling strategy, the optimal design reduces significantly the error. In particular, on both graphs the lower-upper quartiles interval is 2.5 times smaller for the optimal DoE.

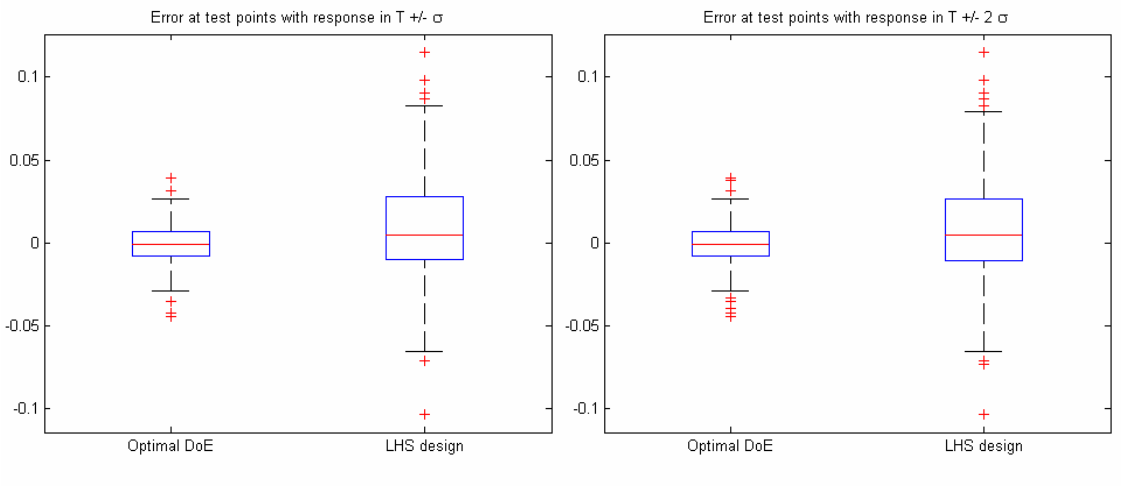


Figure 9: Boxplots of errors for the LHS and optimal designs for the test points where responses are inside the domains $[-\sigma_\varepsilon, +\sigma_\varepsilon]$ (left) and $[-2\sigma_\varepsilon, +2\sigma_\varepsilon]$ (right). Error at these points is a lot smaller for the optimal designs for both intervals.

6. Application to Probability of Failure Estimation

6.1 Probability of failure using metamodel

Failure of a system can usually be determined through a criterion, called a limit-state, G. The limit-state is defined such that the system is considered safe if $G \leq 0$, while failed otherwise. For instance, the limit-state of a structure can be defined as the difference between response, R, (e.g., maximum stress or strain) and capacity, C, (e.g., maximum allowable stress or strain):

$$G = R - C \tag{32}$$

Due to uncertainties in material properties and loadings, the limit-state often shows random distribution. When the limit-state is random, the safety of the system should be evaluated in terms of reliability or probability of failure. The probability of failure is defined as:

$$P_f = \text{Prob}\left(G \geq 0\right) \tag{33}$$

There are many methods for calculating the failure probability of a system [22-24]. Some of them use the relation between input random variables and the limit-state (e.g., first-order reliability method) and some consider the limit-state as a black-box (e.g., Monte-Carlo Simulations, MCS). MCS generates samples of the limit-state and calculates the number of failed samples [24]. The ratio between the numbers of failures and the total number of samples approximates the probability of failure of the system:

$$\hat{P}_f = \frac{1}{N}\sum_{i=1}^{N} \mathrm{I}\left[G \geq 0\right] \tag{34}$$

Where $\mathrm{I}[\alpha]$ is the indicator function, equals to 1 if α is true and 0 otherwise.

The accuracy of MCS strongly depends on the number of samples used, especially when the probability of failure is low. When the cost of simulation is high, engineers can afford to have only a small number of samples, which is not good enough to estimate the reliability with acceptable accuracy [25, 26]. Hence, using a metamodel to approximate the limit-state *G* is a natural solution to the lack of data; MCS is then performed on the metamodel that is inexpensive to evaluate.

Besides, the use of Kriging allows us to replace the indicator function by a continuous distribution:

$$\hat{P}_f = \frac{1}{N}\sum_{i=1}^{N} \Phi_k^{(i)}(0) \tag{35}$$

where $\Phi_k^{(i)}$ denotes the cumulative distribution function (CDF) of the Kriging model at x_i.

6.2 Adaptation of the weighted IMSE criterion

When approximating the limit-state, it is clear that a particular effort must be given to the regions where it is close to zero, since error in that region is likely to affect the probability estimate. Naturally, the critical region is where the value of limit state is close to zero.

However, substantial improvement can be given, by taking into account the distribution of the input variables. Indeed, let us consider the case of two distinct failure regions, one of it dominating the other (that is, the probability that the input falls onto the first region is much larger than the probability that it falls onto the other). Instead of learning indifferently the two critical regions, it will be more efficient to spend more computational effort on the one that will affect most the probability estimate. In the same sense, when learning a single critical region, it is efficient to learn it only where the samples are more likely to be.

To address this probability of input variables, we modify the weighted IMSE criterion by integrating the weighted MSE not with a uniform measure, but with the PDF of the input variables:

$$\mathrm{IMSE}_W = \int_D \mathrm{MSE}(\mathbf{x}) W(\mathbf{x}) \mathrm{d}\mu(\mathbf{x}) \tag{36}$$

where $\mu(\mathbf{x})$ is the joint PDF of the input variables.

6.3 Example

The limit state function is taken as a classical parametric function from the optimization literature (modification of the Camelback function [27]). The two-dimensional design space is given as $(u,v) \in [-1 \quad 1]$. Then, the performance function is defined as

$$f(u,v) = -\frac{1}{3.15}\left[\left(4 - 2.1\bar{u}^2 + \frac{1}{3}\bar{u}^4\right)\bar{u}^2 + \frac{2}{3}\bar{u}\bar{v} + \frac{16}{9}\left(-4 + \frac{16}{9}\bar{v}^2\right)\bar{v}^2\right] + 0.2717 \tag{37}$$

where $\bar{u} = u - 3/5$ and $\bar{v} = v - 9/40$.

Let U and V be independent Gaussian variables with zero mean and standard deviation taken at 0.28; i.e., $U,V \sim N\left(0,0.28^2\right)$. Then, the failure is defined when f becomes greater than 0.4. Thus, the limit state is defined as

$$G = f\left(U,V\right) - 0.4 \tag{38}$$

Figure 10 plots the performance function $f(u,v)$ and the contour line for $f(u,v) = 0.4$. Contour lines show that there are two failure regions, one dominating the other.

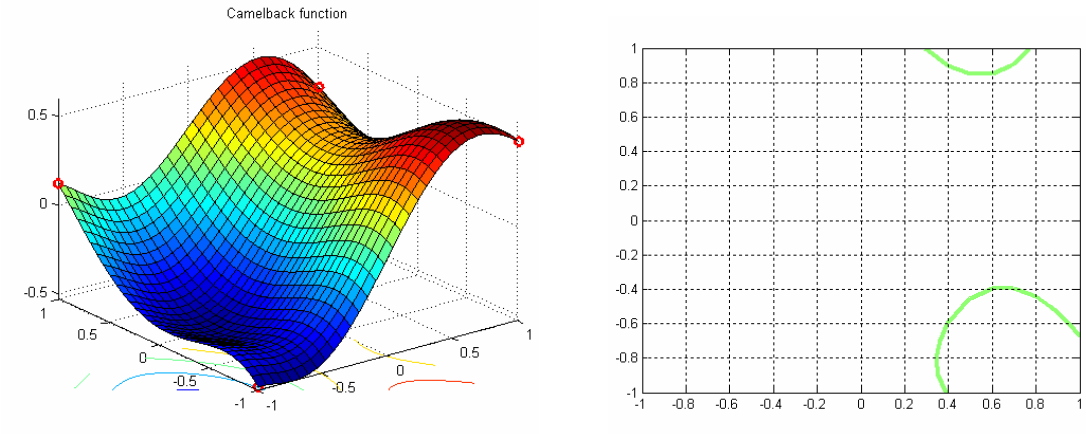


Figure 10: $f(u,v)$ function and contour lines for $f(u,v) = 0.4$. There are two failure regions, one (bottom right, right figure) dominating the other (top right).

For this example, we generate two optimal designs: the first is generated sequentially as described in Section 4, with uniform integration measure (Eq. (19)); the second is generated using the input distribution as integration measure (Eq.(36)). Both use the four corners of the domain as starting DoE and 12 iterations are performed. For comparison purpose, a 16-point full factorial design is also used. It is found that a Simple Kriging model (UK without linear trend) with isotropic Gaussian covariance function approximates well the function. The same (accurate) covariance parameters are used for the different DoEs.

Figure 11 draws the two optimal designs obtained and the full factorial designs. Both optimal designs concentrate the computational effort on the failure regions and the center of the domain. With uniform measure integration in Figure 11(a), the DoE achieve more space-filling than the other one. By taking the input distribution into account in Figure 11(b), we see that only two observations are used to explore the dominated critical region, while five are used for the most critical one. Besides, all five points are located relatively close to the center of the domain.

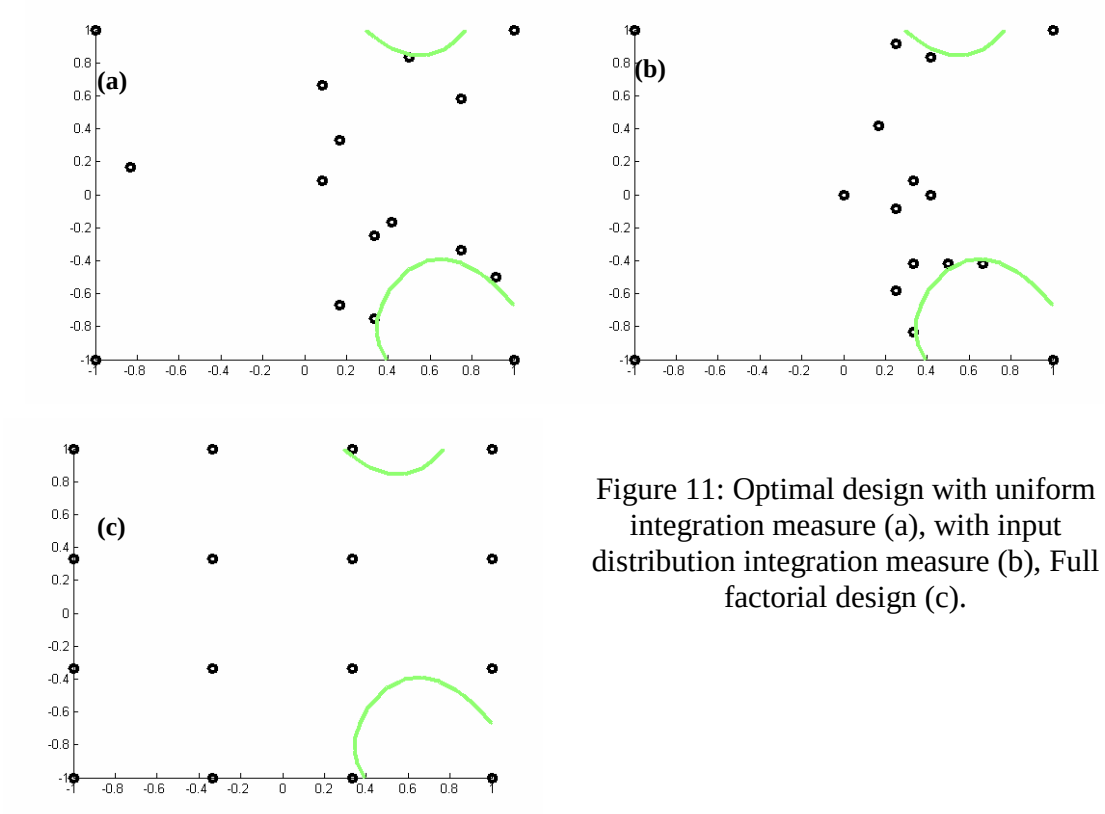


Figure 11: Optimal design with uniform integration measure (a), with input distribution integration measure (b), Full factorial design (c).

Finally, we perform 10^7 MCS on the three metamodels to compute the probability of failure estimates. 10^7 MCS are also performed directly on the test function to obtain the true probability of failure. Results are reported in Table 2. The full-factorial design leads to 36% error, while both optimal designs lead to a small error. Substantial improvement is obtained by taking the input distribution into account.

Table 2: Probability of failure estimates for the three DoEs and the actual function based on 10^7 MCS. The standard deviation of all estimates is of the order of 2×10^{-5}.

DoE	FF	Optimal without input distribution	Optimal with input distribution	Probability estimate based on 10^7 MCS
Probability of failure (%)	0.279	0.416	0.431	0.434
Relative error	35.6 %	4.1 %	0.6 %	

7. Conclusions

In this paper, we addressed the issue of choosing a design of experiments when the Kriging metamodel was used to approximate a function accurately around a particular level-set. This situation frequently occurs in constrained optimization and reliability analysis. We proposed a modified version of the classical IMSE criterion by weighting the prediction variance by the expected proximity to target values. The choice of a new

observation based on such criterion is a trade-off between exploration of the target region (on the vicinity of the contour line) and reduction of the global uncertainty (prediction variance) in the metamodel.

We applied our strategy to examples in two and six dimensions. In two dimensions, we showed that the sampling efficiently explored the target regions while ensuring space-filling. In six dimensions, we showed that compared to a classical space-filling design, the error reduction in the target region was of the order of five.

Finally, the method was tested for reliability estimation on an analytical example. An additional criterion was adapted to integrate the distribution of input random variables. It was found that both criterion-based strategies significantly outperformed space-filling designs, and taking into account the input distribution provides additional improvement. In this paper, the question of modeling error was not addresses. Future work will include a study on the effect of error in the Kriging parameters on the accuracy and efficiency of the method.

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