# Adaptive Kriging for Simulation-based Design under Uncertainty
## *Development of Metamodels in Augmeted Input Space and Adaptive Tuning of Their Characteristics*

Alexandros A. Taflanidis[1,2] and Juan Camilo Medina[1]
[1]*Department of Aerospace and Mechanical Engineering, University of Notre Dame, Notre Dame, IN, U.S.A*
[2]*Department of Civil and Environmental Engineering & Earth Sciences, University of Notre Dame, Notre Dame, IN, U.S.A*

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Abstract: This investigation focuses on design-under-uncertainty problems that employ a probabilistic performance as objective function and consider its estimation through stochastic simulation. This approach puts no constraints on the computational and probability models adopted, but involves a high computational cost especially for design problems involving complex, high-fidelity numerical models. A framework relying on kriging metamodeling to approximate the system performance in an augmented input space is considered here to alleviate this cost. A sub region of the design space is defined and a kriging metamodel is built to approximate the system response (output) with respect to both the design variables and the uncertain model parameters (random variables). This metamodel is then used within a stochastic simulation setting (addressing uncertainties in the model parameters) to approximate the system performance when estimating the objective function for specific values of the design variables. This information is then used to search for a local optimum within the previously established design sub domain. Only when the optimization algorithm drives the search outside this domain, a new metamodel is generated. The process is iterated until convergence is established and an efficient sharing of information across these iterations is established to adaptively tune characteristics of the kriging metamodel.

# 1 INTRODUCTION

In any engineering design application, the performance predictions for the system under consideration involve some level of uncertainty, stemming from the incomplete knowledge about the system itself and its environment (Schuëller and Jensen, 2008). Explicitly accounting for these uncertainties is exceptionally important for providing optimal configurations that exhibit robust performance and a probability logic approach provides a rational and consistent framework for this task (Jaynes, 2003). In this setting, the objective function corresponds to the expected value (probabilistic integral) of some chosen performance measure over the adopted probability distributions.

For complex systems, this probabilistic integral can rarely be calculated or accurately approximated analytically, and stochastic simulation (i.e. Monte Carlo) based techniques are emerging as a popular approach due to their general applicability as well as the possibility of exploiting advances in parallel/distributed computing (Royset and Polak, 2004, Taflanidis and Beck, 2008). A challenge related to this approach is, though, the significant computational cost involved to estimate the objective function (Spall, 2003).

An alternative framework, relying on surrogate modeling to approximate the system performance, is developed here to alleviate this burden. Kriging (Sacks, 1989, Lophaven, 2002) is utilized as surrogate model since it has been proven highly efficient for approximating complex response functions while simultaneously providing gradient information. Though, metamodeling approaches for design optimization under uncertainty are typically implemented for (i) approximating the objective function in the design space (Gasser and Schueller, 1997) (metamodel is used to guide optimization) or for (ii) approximating the system performance for specific design configurations (Gavin and Yau, 2007) (metamodel is used to calculate the objective function for these design configurations), a different approach is investigated here by considering an

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augmented input space. The approach is similar to the ideas in (Dubourg et al., 2011), a study that was constrained, though, to reliability based design optimization problems and investigated implementation within the entire design domain (gradually converging to smaller subsets). Here, a sub region of the design space is defined and a kriging metamodel is built to approximate the system response with respect to both the design variables and the uncertain model parameters. High-fidelity model evaluations are obtained at properly selected support points, and the kriging model is then developed employing this information. This metamodel is then used within a stochastic simulation setting to approximate the system performance when estimating the objective function and its gradient for specific values of the design variables, where the stochastic simulation is ultimately established with respect to the random model parameters. This information (i.e. estimate of objective function and gradient) is then used to search for a local optimum within the previously established design sub domain. Only when the optimization algorithm drives the search outside this sub domain, a new metamodel is generated, and the process is iterated until convergence is obtained. This framework provides great computational savings, since the high-fidelity model is only utilized for calculating the response for the chosen support points (as long as the design choices remain within the initial sub domain).

Additionally, an adaptive tuning of some characteristics of the kriging metamodel is established by sharing information across the iterations of the numerical optimization. For selecting the basis functions of the metamodel, a recently developed probabilistic global sensitivity analysis (Jia and Taflanidis, 2011) is seamlessly integrated, quantifying the importance of each model parameter and design variables towards the overall probabilistic performance. Higher order basis functions are assigned to the more important variables, contributing to increased approximation accuracy. Furthermore, an hybrid, adaptive sampling approach is developed for selecting the support points (design of experiments, DoE), populating more densely those regions in the random variable space that have higher contribution to the integrand quantifying the probabilistic performance. This DoE leads to a kriging model with enhanced accuracy in those regions, something that ultimately improves the accuracy of the objective function estimates. The overall framework is demonstrated with an example considering the optimization of semi-active dampers for a half-car model. Within this example the influence of explicitly including the kriging prediction error in the evaluation of the performance function is investigated.

## 2 PROBLEM FORMULATION

Consider a system with design vector $\mathbf{x}=[x_1\ x_2\ \dots\ x_{n_x}] \in X \subset \mathbb{R}^{n_x}$, where $X$ is the admissible design space, and uncertain model parameters (random variables) $\boldsymbol{\theta}=[\theta_1\ \theta_2\ \dots\ \theta_{n_\theta}] \in \Theta \subset \mathbb{R}^{n_\theta}$, where $\Theta$ denotes the set of their possible values. A Probability Density Function (PDF) $p(\boldsymbol{\theta})$, which incorporates our available knowledge about the system is assigned to these parameters. Let $\mathbf{z}(\mathbf{x},\boldsymbol{\theta}) \subset \mathbb{R}^{n_z}$ be the response vector of the system model dependent upon both $\mathbf{x}$ as well as $\boldsymbol{\theta}$, and let $h(\mathbf{x},\boldsymbol{\theta}): \mathbb{R}^{n_x} \times \mathbb{R}^{n_\theta} \to \mathbb{R}$ be the performance function characterizing the favorability of that response. The probabilistic performance is then given by the expected value under $p(\boldsymbol{\theta})$

$$H(\mathbf{x}) = \int_{\Theta} h(\mathbf{x},\boldsymbol{\theta})\, p(\boldsymbol{\theta})\, d\boldsymbol{\theta} \tag{1}$$

and corresponds to the objective function for a robust to uncertainties design. Assuming that lower values for $h(\mathbf{x},\boldsymbol{\theta})$ correspond to more favorable performance (i.e. $h(\mathbf{x},\boldsymbol{\theta})$ represents a cost function) the robust to uncertainties design problem is

$$\mathrm{x}^* = \arg\min_{\mathbf{x}\in X} H(\mathbf{x}) \tag{2}$$

where any deterministic constraints have been incorporated in the definition of the admissible design space $X$.

Utilizing stochastic simulation and sample set $\{\boldsymbol{\theta}^j : j = 1,...,N\}$ from a proposal density $q(\boldsymbol{\theta})$ the objective function in Eq. (1) is estimated as

$$\hat{H}(\mathbf{x}) = \frac{1}{N}\sum_{j=1}^{N} h(\mathbf{x},\boldsymbol{\theta}^j)\frac{p(\boldsymbol{\theta}^j)}{q(\boldsymbol{\theta}^j)} \tag{3}$$

where the proposal density is chosen to improve the accuracy of the approximation by concentrating the computational effort in regions of the model parameter space that have higher contribution to the integrand defining the probabilistic performance, an idea corresponding to the concept of importance sampling (IS) (Robert and Casella, 2004). The optimal design in Eq. (2) is then solved by substituting the approximation of Eq. (3) as the objective function. This leads to a challenging

simulation-based optimization problem because of the existence of an unavoidable estimation error, the high computational cost associated with each objective function evaluation (requiring $N$ evaluations of the system model response) and the inability to obtain gradient information for problem with complex, black-box models (Taflanidis and Beck, 2008). This paper considers an approach, utilizing kriging metamodeling for approximating the model response, that addresses these problems.

# 3 DESIGN OPTIMIZATION THROUGH KRIGING IN AUGMENTED SPACE

The augmented input space for development of the kriging metamodel is defined as a tensor product between the design and uncertain spaces $X \otimes \Theta$, whereas to improve accuracy of the metamodel a smaller set of the design domain is considered instead of the entire domain, establishing the iterative approach

$$\mathbf{x}_{k+1} = G_{krig}(\mathbf{x}_k \mid \{\boldsymbol{\theta}^j\}_k) \tag{4}$$

where the function $G_{krig}$ represents the kriging-based optimization recursive relations and the notation $\{\boldsymbol{\theta}^j\}_k$ is used to denote the sample set (in the stochastic simulation) used within the $k^{th}$ iteration. Note that this sample set will ultimately change from iteration to iteration so that there is no dependence of the solution on the sample set used, an approach corresponding to the concept of exterior sampling (Spall, 2003). The design sub-domain in the $k^{th}$ iteration, also known as trust region, of the optimization algorithm will be denoted $X_k$ herein.

Thus, the input vector $\mathbf{y}$ for the kriging metamodel is composed of the design and uncertain model parameter vectors $\mathbf{y}=[\mathbf{x}\ \boldsymbol{\theta}]$ whereas the output vector corresponds to the system response vector $\mathbf{z}(\mathbf{x},\boldsymbol{\theta})$. Note that the computational complexity of the performance evaluation model for estimating $h(\mathbf{x},\boldsymbol{\theta})$ based on $\mathbf{z}(\mathbf{x},\boldsymbol{\theta})$ is typically small for most practical engineering applications. Establishing an approximation for $\mathbf{z}(\mathbf{x},\boldsymbol{\theta})$, and then using the actual performance evaluation model to estimate $h(\mathbf{x},\boldsymbol{\theta})$ circumvents one level of approximations and can ultimately offer significant improvements in accuracy (Jin et al., 2001). This approach further allows, as will be demonstrated in the illustrative example, the explicit consideration of the local kriging prediction error within the definition of the performance function.

The kriging model ultimately will provide an approximation for the response vector $\bar{\mathbf{z}}(\mathbf{y}) = \bar{\mathbf{z}}(\mathbf{x},\boldsymbol{\theta})$, and through this, an approximation to the performance function is established, denoted by $\bar{h}(\mathbf{y}) = \bar{h}(\mathbf{x},\boldsymbol{\theta})$. Simultaneously, gradient information can be also obtained for both of these quantities as will be demonstrated in the next section. Using this information the numerical optimization scheme $G_{krig}$ can be formulated. In this step, the objective function and its gradient are approximated as

$$H_{krig}(\mathbf{x}) = \int_{\Theta} \bar{h}(\mathbf{x},\boldsymbol{\theta})\, p(\boldsymbol{\theta})\, d\boldsymbol{\theta} \tag{5}$$

$$\begin{aligned} \nabla H_{krig}(\mathbf{x}) &= \nabla\left(\int_{\Theta} \bar{h}(\mathbf{x},\boldsymbol{\theta})\, p(\boldsymbol{\theta})\, d\boldsymbol{\theta}\right) \\ &= \int_{\Theta} \nabla\left(\bar{h}(\mathbf{x},\boldsymbol{\theta})\, p(\boldsymbol{\theta})\, d\boldsymbol{\theta}\right) = \int_{\Theta} p(\boldsymbol{\theta}) \nabla \tilde{h}(\mathbf{x},\boldsymbol{\theta})\, d\boldsymbol{\theta} \end{aligned} \tag{6}$$

where for obtaining the second equation we assume that the functions $\bar{h}(\mathbf{x},\boldsymbol{\theta})p(\boldsymbol{\theta})$ and $(\partial \bar{h}(\mathbf{x},\boldsymbol{\theta})/\partial x_i)\, p(\boldsymbol{\theta})$ are continuous in the domain $X \times \Theta$ and bounded, thus the differentiation and the expectation operators can commute (Spall, 2003). These probabilistic integrals can be then evaluated through stochastic simulation, leading to

$$\hat{H}_{krig}(\mathbf{x}) = \frac{1}{N} \sum_{j=1}^{N} \hat{h}(\mathbf{x},\boldsymbol{\theta}^j) \frac{p(\boldsymbol{\theta}^j)}{q_k(\boldsymbol{\theta}^j)} \tag{7}$$

$$\nabla \hat{H}_{krig}(\mathbf{x}) = \frac{1}{N} \sum_{j=1}^{N} \nabla \hat{h}(\mathbf{x},\boldsymbol{\theta}^j) \frac{p(\boldsymbol{\theta}^j)}{q_k(\boldsymbol{\theta}^j)} \tag{8}$$

where the notation $q_k(\boldsymbol{\theta})$ is used herein to represent the ability to choose the proposal density different at each iteration of the numerical optimization (more details on this later). Due to the computational efficiency of the kriging metamodel a large number of samples can be utilized within this setting to yield high accuracy for the stochastic simulation estimates.

Utilizing this information, especially the gradient approximation in Eq. (6), an appropriate gradient-based algorithm is adopted to establish a local search within $X_k$. Two possible outcomes can occur for this optimization: (i) converge to a local optimum within $X_k$ or (ii) reach the boundary of the search domain, which means that the local search should stop to

avoid extrapolations. The latter prompts the optimization algorithm to advance to the next iteration $\mathbf{x}_{k+1}$, and generate a new kriging model if the overall optimization has not converged. Note that the local search optimization identifying the optimal solution within $X_k$ has evidently its own inner iterations, but we are interested here in the iterations of the exterior optimization algorithm characterized by Eq. (4).

# 4 ADAPTIVE KRIGING

## 4.1 Review of Kriging Metamodeling

For forming the kriging metamodel a database with $n$ observations is utilized that provides information for the **y-z** pair. For this purpose $n$ samples for $\{\mathbf{y}^l\ l=1,\ldots,n\}$, also known as *support points*, are created and the model response $\mathbf{z}(\mathbf{y}^l)$ is evaluated for each of them. Using this dataset the kriging model is then obtained, providing ultimately approximation for each response quantity

$$z_i(\mathbf{y}) = \bar{z}_i(\mathbf{y}) + \bar{\varepsilon}_i(\mathbf{y}) \tag{9}$$

where $\bar{z}_i$ stands for the mean prediction whereas $\bar{\varepsilon}_i$ is a Gaussian variable with zero mean and standard deviation $\sigma_i(\mathbf{y})$ (Lophaven, 2002). The fundamental building blocks of kriging are the $n_p$ dimensional basis vector, $\mathbf{f}(\mathbf{y})$, and the correlation function $R(\mathbf{y}^j,\mathbf{y}^k)$. Selection of the former will be discussed later whereas for the latter the popular generalized exponential correlation is used

$$R(\mathbf{y}^j,\mathbf{y}^k) = \prod_{i=1}^{n_y} \exp[-s_i \,|\, \mathbf{y}_i^j - \mathbf{y}_i^k \,|^{s_{n_y+1}}] \qquad \mathbf{s} = [s_1 \ \cdots \ s_{n_y+1}] \tag{10}$$

Then for the set of $n$ observations with input matrix $\mathbf{Y}=[\mathbf{y}^1 \ \ldots \ \mathbf{y}^n]^T$ and corresponding output matrix $\mathbf{Z}=[\mathbf{z}^1 \ \ldots \ \mathbf{z}^n]^T$, we define the basis matrix $\mathbf{F}=[\mathbf{f}(\mathbf{y}^1) \ \ldots \ \mathbf{f}(\mathbf{y}^n)]^T$ and the correlation matrix $\mathbf{R}$ with the $jk$-element defined as $R(\mathbf{y}^j,\mathbf{y}^k)$, $j,k=1, \ldots, n$. Also for every new input **y,** we define the correlation vector $\mathbf{r}(\mathbf{y})=[R(\mathbf{y},\mathbf{y}^1) \ \ldots \ R(\mathbf{y},\mathbf{y}^n)]^T$ between the input and each of the elements of $\mathbf{Y}$. The kriging mean prediction for vector $\mathbf{z}$ is given by (Lophaven, 2002)

$$\bar{\mathbf{z}}^T(\mathbf{y}) = \mathbf{f}(\mathbf{y})^T\boldsymbol{\alpha}^* + \mathbf{r}(\mathbf{y})^T\boldsymbol{\beta}^*$$
$$\boldsymbol{\alpha}^* = (\mathbf{F}^T\mathbf{R}^{-1}\mathbf{F})^{-1}\mathbf{F}^T\mathbf{R}^{-1}\mathbf{Z};\ \boldsymbol{\beta}^* = \mathbf{R}^{-1}(\mathbf{Z}-\mathbf{F}\boldsymbol{\alpha}^*) \tag{11}$$

Through the proper tuning of the parameters $\mathbf{s}$ of the correlation function, kriging can efficiently approximate very complex functions. The optimal selection of $\mathbf{s}$ is based on the Maximum Likelihood Estimation (MLE) principle, where the likelihood is defined as the probability of the $n$ observations, and maximizing this likelihood with respect to $\mathbf{s}$ ultimately corresponds to the optimization problem

$$\mathbf{s}^* = \arg\min_{\mathbf{s}} \left[ |\mathbf{R}|^{\frac{1}{n}} \sum_{i=1}^{n} \tilde{\sigma}_i^2 \right] \tag{12}$$

where $|.|$ stands for determinant of a matrix and $\tilde{\sigma}_i^2$, $i = 1,.., n_z$ correspond to the diagonal elements of matrix $(\mathbf{Z}\text{-}\mathbf{F}\boldsymbol{\alpha}^*)^T\mathbf{R}^{-1}(\mathbf{Z}\text{-}\mathbf{F}\boldsymbol{\alpha}^*)$. Beyond the mean kriging predictions the error can be also explicitly considered in the optimization as will be illustrated in the example considered later. This requires estimation of the prediction error variance $\sigma_i^2(\mathbf{y})$ for $z_i$ and input $\mathbf{y}$ which is given by

$$\sigma_i^2(\mathbf{y}) = \tilde{\sigma}_i^2[1 + \mathbf{u}^T(\mathbf{F}^T\mathbf{R}^{-1}\mathbf{F})^{-1}\mathbf{u} - \mathbf{r}(\mathbf{y})^T\mathbf{R}^{-1}\mathbf{r}(\mathbf{y})] \qquad \mathbf{u} = \mathbf{F}^T\mathbf{R}^{-1}\mathbf{r}(\mathbf{y}) - \mathbf{f}(\mathbf{y}) \tag{13}$$

Gradient information can be also easily derived by differentiating directly Eqs. (11) and (13) and noting that vectors $\boldsymbol{\alpha}^*$ and $\boldsymbol{\beta}^*$ are independent of $\mathbf{y}$. For example, for the mean kriging predictions, and denoting $\mathbf{J}_f$ and $\mathbf{J}_r$ are the Jacobian matrices with respect to $\mathbf{y}$ of $\mathbf{f}$ and $\mathbf{r}$, respectively, this leads to

$$\nabla\bar{\mathbf{z}}^T = \mathbf{J}_f(\mathbf{y})^T\boldsymbol{\alpha}^* + \mathbf{J}_r(\mathbf{y})^T\boldsymbol{\beta}^* \tag{14}$$

## 4.2 Adaptive Formulation

In the proposed framework, a kriging approximation is developed in the augmented input space by sharing information across the iterations of the optimization algorithm described through Eq. (4). Within such a setting, the focus is on the adaptive Design of Experiments (DoE) to select the support points as well as the adaptive selection of the polynomial order of basis functions.

To formalize these concepts, let $\mathbf{x}_k$ denote the design variable vector that has been identified at the end of the $k^{th}$ iteration of the numerical optimization of Eq. (4). Evaluation of the approximation to the system performance will be also available for $\mathbf{x}_k$, $\{\bar{h}(\mathbf{x}_k,\boldsymbol{\theta}^j); j=1,\ldots,N\}$ for the sample set $\{\boldsymbol{\theta}^j\}_k$ used to estimate the objective function through Eq. (7). A localized box-bounded design sub-domain (trust region) is then defined $X_k$; this domain is centered on $\mathbf{x}_k$ and has an appropriate length for each design variable (defining the length vector $\mathbf{L}_k$) that

ultimately prescribes the upper and lower bounds for the design vector $\mathbf{x}_k^l$ and $\mathbf{x}_k^u$, respectively. Any appropriate technique may be adopted for selecting the length vector $\mathbf{L}_k$ (Rodríguez et al., 2000). A relevant recommendation for this is that the length is gradually reduced as iterations progress to regions closer to a minimum, where one needs higher accuracy approximations. A kriging metamodel is then established within sub-domain $X_k$ for the augmented input vector $\mathbf{y}$ and then used within the optimization given in Eq. (4).

### 4.2.1 Design of Experiments

Space filling techniques or adaptive design of experiments (Wang and Shan, 2007, Picheny et al., 2010) are commonly preferred for the design of experiments in kriging metamodeling applications. However, the former may not provide the necessary accuracy in regions of importance, while the latter may significantly increase the computational cost for selecting the support points. Therefore, a hybrid DoE is proposed in this investigation instead.

Due to their distinct nature, the two different components of the input vector $\mathbf{y}$ have different characteristics/demands related to their accuracy. For instance, in the case of $\mathbf{x}$, accurate approximations are needed within the entire domain $X_k$ since the metamodel is ultimately used to compare different design choices within this entire domain to converge towards the optimal design configuration. This indicates that a space filling technique should be considered and Latin hypercube sampling (LHS) is adopted here for this purpose.

On the other hand, for $\boldsymbol{\theta}$ an accurate approximation is needed over the domain in the uncertain model parameters space $\Theta$ that provides higher contribution towards the integrand in the evaluation of the objective function. Thus for $\boldsymbol{\theta}$ a target region DoE is needed and an approach with minimal computational overhead is developed here for this purpose. The basis of the approach is the approximation of the target region as the important region for the integrand of the objective function through the definition of the auxiliary density

$$\pi(\boldsymbol{\theta}\,|\,\mathbf{x}) = \frac{|\,h(\mathbf{x},\boldsymbol{\theta})\,|\,p(\boldsymbol{\theta})}{\hat{H}_{krig}(\mathbf{x})} \propto |\,h(\mathbf{x},\boldsymbol{\theta})\,|\,p(\boldsymbol{\theta}) \qquad (15)$$

Since this requires knowledge of $h(\mathbf{x},\boldsymbol{\theta})$ an approximation is established considering the density $\bar{\pi}(\boldsymbol{\theta}\,|\,\mathbf{x})$, for which $h(\mathbf{x},\boldsymbol{\theta})$ is replaced by the kriging prediction $\bar{h}(\mathbf{x},\boldsymbol{\theta})$.

The density $\bar{\pi}(\boldsymbol{\theta}\,|\,\mathbf{x}_k)$ may be then taken to represent the region of importance for the kriging metamodel to be developed in the next iteration. An efficient approximation for this density can be established through sample set, denoted $\{\boldsymbol{\theta}^a\}_k$, that can be obtained utilizing the readily available evaluations of $\bar{h}(\mathbf{x}_k,\boldsymbol{\theta}^j)$ for the sample set $\{\boldsymbol{\theta}^j\}_k$ (established in the previous iteration) for the proposal density used in that iteration $q_k(\boldsymbol{\theta})$. Such samples can be obtained through rejection sampling by accepting the samples for which the following relationships holds (Medina and Taflanidis, 2014)

$$\frac{|\,\bar{h}(\mathbf{x}_k,\boldsymbol{\theta}^j)\,|\,p(\boldsymbol{\theta}^j)}{u^j q_k(\boldsymbol{\theta}^j)} > \max_j\left[\frac{|\,\bar{h}(\mathbf{x}_k,\boldsymbol{\theta}^j)\,|\,p(\boldsymbol{\theta}^j)}{q_k(\boldsymbol{\theta}^j)}\right] \qquad (16)$$

where $\{u^j; j=1,...,N\}$ are independent uniformly distributed random samples in range [0 1]. The sample set $\{\boldsymbol{\theta}^a\}_k$ corresponds to the samples of $\{\boldsymbol{\theta}^j\}_k$ for which the above equation holds and ultimately represents the region in the $\Theta$ space that contributes more towards the probabilistic performance for $\mathbf{x}_k$ and as such corresponds to a good approximation for the target region where higher accuracy is sought after in the kriging metamodel. Any sample-based density approximation approach can be utilized to approximate the target region utilizing these samples. This density will be denoted $f_k^s(\boldsymbol{\theta})$ herein.

Because of the importance of this approximation and ultimately of the number of samples in the set $\{\boldsymbol{\theta}^a\}_k$ for providing sufficient information for this approximation, a further modification is introduced to guarantee that a sufficient number of samples is available. Upon convergence to $\mathbf{x}_k$, an additional sample set, beyond the $N$ samples in $\{\boldsymbol{\theta}^j\}_k$, is generated to obtain a large sample set consisting of $N_p$ samples for which $\bar{h}(\mathbf{x}_k,\boldsymbol{\theta})$ is evaluated. The rejection sampling in Eq. (16) is then performed over this larger sample set. Given that evaluation of $\bar{h}(\mathbf{x}_k,\boldsymbol{\theta})$ involves a small computational effort this modification creates a small only additional burden, but guarantees that sufficient samples will be obtained to provide a good approximation of $f_k^s(\boldsymbol{\theta})$.

Finally it is important to consider that the kriging metamodel needs to have sufficient accuracy even in regions beyond this specific target region, since erroneous approximations in such regions can

impact the estimation result (these regions may become erroneously important because of such errors). This consideration leads to the following two stage *hybrid* DoE with the first stage aiming to obtain satisfactory global accuracy in the broader domain $\Theta$ and the second stage aiming to obtain higher accuracy in the target region. Initially (first stage) $n_1^s$ samples are obtained adopting a space filling approach (LHS) within the domain of importance based on $p(\boldsymbol{\theta})$ (for example 4-5 standard deviations away from the median values for each model parameters). Then, additional $n_2^s$ are obtained from the density approximation $f_k^s(\boldsymbol{\theta})$. The total number of support points is, thus, $n = n_1^s + n_2^s$.

### 4.2.2 Selection of Basis Functions

Another feature for the kriging approximation is the selection of basis functions. Typically polynomials of some lower order are used and then the important question is the exact polynomial order of the basis functions for each component of the input vector **y**. Selecting the same higher order for all components might reduce the accuracy of the kriging metamodel; ultimately components that exhibit higher sensitivity should have higher order associated with them but the optimization to identify the best basis function selection is in general a challenging task (Jia and Taflanidis, 2013). This challenge is circumvented here by integrating the global sensitivity analysis proposed recently by Jia and Taflanidis (2011), and selecting second order polynomial functions only for the most important components and linear polynomial functions for the rest.

For vector **y** this sensitivity analysis is established by considering the density function

$$\pi(\mathbf{y}) = \pi(\mathbf{x},\boldsymbol{\theta}) \propto |\, h(\mathbf{x},\boldsymbol{\theta}) \,|\, p(\boldsymbol{\theta}) p(\mathbf{x}) \qquad (17)$$

where $p(\mathbf{x})$ corresponds to a uniform density in $X_k$, and by comparing this density to the prior joint distribution $p(\boldsymbol{\theta})p(\mathbf{x})$ for each component of **y** separately (comparison of the marginal distributions). Bigger differences correspond to higher importance towards the overall probabilistic performance (Jia and Taflanidis, 2011). This comparison is efficiently performed utilizing samples for $\pi(\mathbf{y})$; such samples can be readily obtained utilizing the support points within $X_k$ from the second DoE stage, using again rejection sampling. They corresponds to the samples (out of the larger set of samples utilizing distribution $f_k^s(\boldsymbol{\theta})$ for $\boldsymbol{\theta}$) for which the following relationship holds

$$\frac{|\, h(\mathbf{x}^j,\boldsymbol{\theta}^j) \,|\, p(\boldsymbol{\theta}^j)}{u^j f_k^s(\boldsymbol{\theta}^j)} > \max_{j=1,\ldots,n_2^s} \left[ \frac{|\, h(\mathbf{x}^j,\boldsymbol{\theta}^j) \,|\, p(\boldsymbol{\theta}^j)}{f_k^s(\boldsymbol{\theta}^j)} \right] \qquad (18)$$

This approach leads to total of $N_s$ samples, denoted $\{y_i^s\}$ for each component of $y$, and to the following approximation for marginal distributions of interest utilizing kernel density approximation (Jia and Taflanidis, 2011)

$$\tilde{\pi}(y_i) = \frac{1}{N_s} \sum_{s=1}^{N_s} \left( \frac{1}{t_i} \left[ K\left( \frac{y_i - y_i^s}{t_i} \right) \right] \right) \qquad (19)$$

where $K$ is a Gaussian kernel and bandwidth $t_i$ is given by $1.06 \cdot N_s^{-1/5} \sigma_i$ with $\sigma_i$ corresponding to the standard deviation of the samples $\{y_i^s\}$.

The importance of the different model parameters (Jia and Taflanidis, 2011) is quantified based on the relative entropy of the marginal distributions, which utilizing the kernel density approximation can be calculated as

$$D\left(\pi(y_i) \,||\, p(y_i)\right) \approx \int_{b_{li}}^{b_{ui}} \tilde{\pi}(y_i) \log\left( \frac{\tilde{\pi}(y_i)}{p(y_i)} \right) dy_i \qquad (20)$$

where $b_{ui}$ and $b_{li}$ are the upper and lower bounds, respectively, for the sample set $\{y_i^s\}$ and the integral in this equation can be readily obtained through one-dimensional numerical integration.

A threshold $D_{\min}^{re}$ can be then set to determine the importance of the input vector components. Only if the value of relative entropy is larger than this threshold, then that particular parameter will be assigned a higher order basis function. This threshold is adaptively selected to correspond to a fraction of the highest relative entropy value. If the allowable percentage reduction of the maximum entropy among the entire input vector is $s_e^{re}$, then

$$D_{\min}^{re} = s_e^{re} \max_i \left[ D\left(\pi(y_i) \,||\, p(y_i)\right) \right] \qquad (21)$$

and this formulation ultimately leads to consideration of higher order basis functions for parameters that correspond to relative entropy values higher or equal to $s_e^{re}$ of the maximum entropy over the entire input vector.

## 4.3 Optimization under Uncertainty with Adaptive Kriging

### 4.3.1 Considerations for Implementation Across Iterations

For the proposed implementation of kriging across the iterations of the numerical optimization the following questions need to still be answered: (a) How is the IS density $q_k(\boldsymbol{\theta})$ for the estimations in Eqs. (7) and (8) established? (b) How is convergence evaluated? (c) What are the recommendations for the selection of the length vector $\mathbf{L}_k$ defining the trust region?

Starting with the IS density, this density may be selected based on the information from the sample set $\{\boldsymbol{\theta}^a\}_k$ from distribution $\pi(\boldsymbol{\theta}|\mathbf{x}_k)$ which corresponds actually to the optimal IS density for design configuration $\mathbf{x}_k$ (Robert and Casella, 2004). The density $\pi(\boldsymbol{\theta}|\mathbf{x}_k)$ is expected to provide a satisfactory accuracy for the entire domain $X_k$ if, as discussed previously, $\mathbf{x}_k$ provides an adequate representation about the behavior of the integrand for different design configurations within $X_k$. Recall that exploiting the efficiency of the kriging metamodel, a large number of samples $N$ can be used in this case for the stochastic-simulation-based evaluation of the objective function and its gradient, described in Eqs. (7) and (8), respectively. As such, no special attention needs to be placed on a highly efficient IS formulation; improvement in accuracy is primarily sought after by adopting a larger number of $N$, though considerable advantages are also expected from the IS implementation. For example, a simple parametric density approximation can be implemented, although more advanced approaches have been also recently proposed (Medina and Taflanidis, 2014).

Moving now to the convergence of the algorithm, this is established when the new identified optimum $\mathbf{x}_k^*$ is a local optimum of the trust region $X_k$. To further improve the quality of the obtained solution, a second optimization stage is proposed: upon convergence, the number of support points is increased to establish a higher accuracy kriging metamodel and the optimization described by Eq. (4) is repeated. This allows the use of smaller number of support points $n = n_1^s + n_2^s$ in the initial iterations, until convergence is established. Ultimately we are not concerned with obtaining high accuracy estimates for the kriging metamodel at the initial iterations; establishing an approximate descend direction in the design domain towards the optimal design is sufficient (greedy optimization approach).

Finally, with respect to the length vector selection $\mathbf{L}_k$, initially it can be considered as a specific fraction $s_1^l$ of the design domain $X$, i.e. $\mathbf{L}_1 = s_1^l X$. At each iteration a specific reduction, $s^r$, of this proportionality can be implemented leading to selection $s_k^l = (s^r)^{k-1} s_1^l$ and $\mathbf{L}_k = s_k^l X$. Upon initial convergence, a further reduction by $s_f^r$ can be established to localize the search around the candidate optimum. Figure 1 provides an example of how the algorithm progresses through the design space. The squares are the trust regions $X_k$ for each iteration. The gray dots show the intermediate steps needed to find a local optimum within the trust region (only using evaluations of the kriging model). The dash-dot line shows the second stage of the optimization that starts when the first stage has encountered an interior point local optimum. This stage has a significantly more reduced length and the number of support points within the domain is increased in order to improve the accuracy of the kriging model near the optimum point.

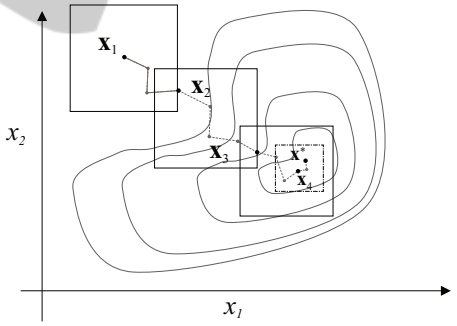


Figure 1: Evolution of trust region.

### 4.3.2 Algorithm for Adaptive Kriging Implementation

When combining the previous ideas, one can formulate the following optimization algorithm utilizing adaptive kriging. First, define the bounded design space $X$, the starting point of the algorithm $\mathbf{x}_1$, the number of support points for the hybrid DoE approach, $n_1^s$ and $n_2^s$, respectively, as well as the respective numbers when the second optimization stage (convergence) has been reached, $n_1^f$ and $n_2^f$. Select the number of samples $N$ for the estimation of the objective function and its gradient utilizing

stochastic simulation, the number of samples $N_p$ for which $\bar{h}(\mathbf{x}_k,\boldsymbol{\theta})$ will be obtained, the allowable percentage entropy reduction for the basis function formulation $s_e^{re}<1$. Finally choose the fraction parameter $s_1^l$ defining the initial trust region as well as its reduction $s^r$ per iteration and the final reduction upon convergence $s_f^r$.

At iteration $k$ of the numerical optimization algorithm [Eq. (4)] perform the following steps:

Step 1 (trust region definition): Define box-bounded search domain $X_k$ centered around $\mathbf{x}_k$ with length vector given by $\mathbf{L}_k=(s^r)^{k-1}s_1^l X$. If convergence has been established (last iteration) further reduce length vector by $s_f^r$. Adjust (truncate) trust region if it exceeds the design domain bounds $X$.

Step 2 (support points): Employing the hybrid DoE for $\boldsymbol{\theta}$, obtain $n_1^s$ ($n_1^f$ if convergence has been established) samples using a space filling approach (LHS) in the region of importance for $p(\boldsymbol{\theta})$, then obtain $n_2^s$ ($n_2^f$ if convergence has been established) samples from density $f_k^s(\boldsymbol{\theta})$ [$p(\boldsymbol{\theta})$ in first iteration]. For $\mathbf{x}$ obtain $n=n_1^s+n_2^s$ ($n=n_1^f+n_2^f$ if convergence has been established) samples using a space filling approach (LHS) in $X_k$.

Step 3 (Evaluation of model response). For all the support points evaluate the model response $\{\mathbf{z}(\mathbf{x}^j,\boldsymbol{\theta}^j);\ j=1,\ldots,n\}$ and ultimately the system performance function $\{h(\mathbf{x}^j,\boldsymbol{\theta}^j);j=1,\ldots,n\}$.

Step 4 (Selection of basis functions): Based on the evaluations on the performance function on the support points from the second stage $\{h(\mathbf{x}^j,\boldsymbol{\theta}^j);j=1,\ldots,n_s^2\}$, obtain samples from $\pi(\mathbf{x},\boldsymbol{\theta})$ through rejection sampling as in Eq. (18). Then calculate the entropy for each component of the output vector $D(\pi(y_i)\|p(y_i))$ using the approximation in Eq. (20) obtained through these samples. Consider higher order (quadratic) basis functions only for components of the input vector with relative entropy higher than the value given by Eq. (21) and lower order (linear) basis functions for the rest.

Step 5 (kriging model): employing the information in steps 1-4, build the kriging model in augmented input space through the approach discussed in Section 4.1.

Step 6 (trust region local optimum): Simulate set of $N$ samples from distribution $q_k(\boldsymbol{\theta})$ [$p(\boldsymbol{\theta})$ in first iteration] and perform optimization described by Eq. (4) utilizing estimations in Eqs. (7) and (8), employing a gradient based algorithm. Identify local optimum $\mathbf{x}_k^*$.

Step 7 (information for $\mathbf{x}_{k+1}$ and proposal density formulation for DoE); consider $\mathbf{x}_{k+1}=\mathbf{x}_k^*$ and evaluate the response and the performance function through the kriging approximation for $N_p$ samples. Obtain sample set $\{\boldsymbol{\theta}^a\}_{k+1}$ through Eq. (16) and establish $f_{k+1}^s(\boldsymbol{\theta})$.

Step 8 (IS proposal density for iteration $k+1$): Utilizing the same sample set $\{\boldsymbol{\theta}^a\}_{k+1}$ formulate the IS proposal density $q_{k+1}(\boldsymbol{\theta})$.

Step 9 (convergence check); if $\mathbf{x}_{k+1}$ is on the boundary of $X_k$ then convergence has not been established and proceed back to Step 1 and advance to $k$+1. If not, then convergence has been potentially attained and the second optimization stage needs to be implemented by repeating steps 1-6 with $n=n_1^f+n_2^f$ and $s_f^r$.

# 5 ILLUSTRATIVE EXAMPLE

The framework is illustrated next in an example considering the optimization of semi-active dampers for the suspension of a half-car nonlinear model riding on a rough road. The excitation (rough road) is modelled as a stochastic process (Verros et al., 2005) and the ride comfort and damper fatigue are considered as performance objectives, both estimated through their root mean square (RMS) statistics. The models adopted include various sources of nonlinearities and time-domain simulation is used to estimate the car response and ultimately RMS performance.

## 5.1 Numerical/Probability Model

The half-car model is shown in Figure 2. The chassis is represented as a rigid body connected to the tires at the ends by a combination of a spring and a dashpot. Furthermore, the tires are connected to the ground by another spring/dashpot combination. A detailed description of the numerical model considered may be found in (Medina and Taflanidis, 2014). Next a brief review is offered.

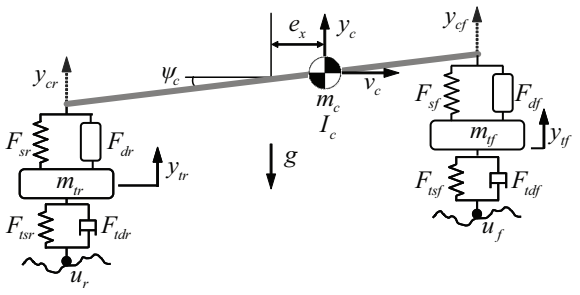


Figure 2: Half-car model schematic.

The model is developed by using small angle assumption. In this context, let $y_c$, $y_{tf}$, $y_{tr}$, and $\psi_c$ denote the vertical displacements of the chassis' center of mass, the front tire, the rear tire, and the angular displacement (pitch) of the chassis respectively. These correspond to the primary state variables for the system. The vertical displacement of the front and rear suspensions are denoted by $y_{cf}$ and $y_{cr}$ and can be easily calculated based on the primary state variables. To simplify notation the location of a given component is represented herein by subscript $o := \{f, r\}$ (either front or rear). For example, $y_{co}$ might correspond to any of the $y_{cr}$ or $y_{cf}$ discussed above.

For the spring, $F_{tso}$, and damper $F_{tdo}$, tire forces linear characteristics are assumed with spring constant $K_{to}$ and dashpot constant $C_{to}$. For the spring suspension force a linear and nonlinear (cubic term) component are assumed with spring constants $K_o^l$ and $K_o^n$, respectively. The semi-active suspension damper force is taken to correspond to an idealized skyhook damper

$$F_{do} = C_o^s \dot{y}_{so} - C_o^t \dot{y}_{to} \tag{22}$$

and all coefficients are taken as design variables, leading to definition of design variable vector as $\mathbf{x}=[C_f^t \quad C_r^s \quad C_r^t \quad C_r^s]^T$.

The road surface input $u_o$ is modeled as a zero-mean Gaussian stationary stochastic process with the Power Spectral Density $S(\Omega)$ proposed in (Verros et al., 2005), defined through parameter $\kappa_i$ representing the roughness coefficient whose value is defined by the International Standard Organization (ISO). A time-domain realization for $u_f$ and $u_r$ is obtained by using the spectral representation method assuming that the car drives with a constant horizontal velocity $v_c$.

Ultimately the system of equations describing the half-car dynamical model are

$$\begin{aligned} m_c\ddot{y}_c + F_{sf} + F_{df} + F_{sr} + F_{dr} &= m_c g \\ m_{tr}\ddot{y}_{tr} - F_{sr} - F_{dr} + F_{tsr} + F_{tdr} &= m_{tr} g \\ m_{tf}\ddot{y}_{tf} - F_{sf} - F_{df} + F_{tsf} + F_{tdf} &= m_{tf} g \\ I_c\ddot{\theta}_c + (F_{sf} + F_{df})(1-e_x)L - (F_{sr} + F_{dr})(1+e_x)L &= 0 \end{aligned} \tag{23}$$

where $g$ denotes gravity acceleration, $e_x$ is the eccentricity between the geometric center of the chassis and its center of mass, $L$ is the half-distance between the two suspensions, $m_c$, $m_{tf}$, $m_{tr}$ are masses for the chassis, the front, and rear tires respectively, and $I_c$ is the moment of inertia of the chassis. A numerical model for this dynamical system is developed in SIMULINK (Klee and Allen, 2007) and finally the response statistics (RMS) under the random road excitation are obtained through the time-domain simulation results by

$$RMS_c = \sqrt{\frac{1}{T}\int_0^T c^2(t)dt} \tag{24}$$

where $T=L_r/v_c$ and $L_r$ is the total length of the road considered. The computational burden for one simulation, that is one evaluation of the response, is on the average $3s$ on a $3.GHz$ Xeon CPU (care was taken to establish a model that balances between numerical accuracy and efficiency), meaning that an evaluation of the objective function within a stochastic simulation setting with $N$=600 samples takes half an hour.

All model parameters apart from $L$ are considered as uncertain, leading to $\boldsymbol{\theta}$ ultimately having 15 components, and Table 1 reviews the adopted probability models. In this Table $\mu$ corresponds to median, $cv$ to coefficient of variation and $\rho$ to correlation coefficient.

Table 1: Probability models adopted for the different model parameters.

| | | | |
|---|---|---|---|
| $m_c$ | Lognormal<br>$\mu$=580 kg, $cv$=0.2 | $m_{to}$ | Lognormal<br>$\mu$=40 kg, $cv$=0.2 |
| $I_c$ | Lognormal<br>$\mu$=1180 kg m$^2$, $cv$=0.2 | $v_c$ | Lognormal<br>$\mu$=60 km/h, $cv$=0.2 |
| $C_{to}$ | Lognormal<br>$\mu$=20 N s/m, $cv$=0.2 | $K_{to}$ | Lognormal<br>$\mu$=190 kN/m, $cv$=0.2 |
| $\kappa_i$ | Lognormal<br>$\mu$=64e-6 m$^2$/cycle<br>$cv$=0.1 | $K_o^l$<br>$K_o^n$ | Correlated Lognormal<br>$\mu$=23.5 kN/m, for $K_o^l$<br>$\mu$=435 kN/m$^3$, for $K_o^n$<br>$cv$=0.2, $\rho$=0.4 |
| $e_x$ | Uniform in [0.1 0.4] | $L$ | 4m (deterministic) |

## 5.2 Performance Quantification and Adjustment for Kriging Error

The performance measure $h(\mathbf{x},\boldsymbol{\theta})$ is selected as the normalized linear combination of the fragilities related to the root mean square of the vertical acceleration at the center of mass $RMS_{ac}$, which in turn is a measure of passenger comfort, and of the root mean square of the suspension's damping forces at the rear and front of the car $RMS_{df}$, $RMS_{dr}$, respectively, which is a measure of suspension fatigue

$$h(\mathbf{x},\boldsymbol{\theta}) = \frac{1}{3}\sum_{i=ac,df,dr} \Phi\left[\frac{\ln RMS_i - \ln b_i}{\sigma_{bi}}\right] \quad (25)$$

where $\Phi[.]$ corresponds to the standard Gaussian Cumulative Distribution Function (CDF) – $b_i$ is the threshold related to each response quantity of interest, taken here as 1 m/s$^2$ for the acceleration, and 160 N in the damper forces, and $\sigma_{bi}$ is the coefficient of variation for the fragilities, assumed as 5% for all of them. The introduction of the fragilities through the CDF, can be also viewed as addressing unmodeled uncertainties (Taflanidis and Beck, 2010): rather than having a binary distinction of the performance, i.e. perform acceptably when the response is smaller than threshold $b_i$ and unacceptably when not. In this context each quantity within the sum in Eq. (25) corresponds equivalently to probability $P[RMS_i>b_i\varepsilon_i]$ with $\varepsilon_i$ having a lognormal distribution with median equal to one and logarithmic standard deviation $\sigma_{bi}$. Analytical integration of the influence of $\varepsilon_i$ leads ultimately to the CDF fragility expressions in Eq. (25). The objective function $H(\mathbf{x})$ is the average failure probability over the three different RMS response quantities and is constrained within the [0 1] range.

The kriging approximation is formulated directly for the log values of the RMS response, since these are the ones appearing in the performance function, thus $\mathbf{z}(\mathbf{x},\boldsymbol{\theta})=[\ln(RMS_{ac}) \ \ln(RMS_{df}) \ \ln(RMS_{dr})]^T$. Furthermore the prediction error stemming from the kriging metamodeling may be directly incorporated into the performance function definition, exploiting the equivalent representation discussed above. This is established by considering the following transformation of the probability $P[RMS_i>b_i\varepsilon_i]$

$$\begin{aligned} P[RMS_i > b_i\varepsilon_i] &= P[\ln(\varepsilon_i) \le \ln(RMS_i) - \ln(b_i)] \\ &= P[\ln(\varepsilon_i) \le \bar{z}_i + \bar{\varepsilon}_i - \ln(b_i)] \\ &= P[\ln(\varepsilon_i) - \bar{\varepsilon}_i \le \bar{z}_i - \ln(b_i)] = \Phi\left[\frac{\bar{z}_i - \ln(b_i)}{\sqrt{\sigma_i^2 + \sigma_{bi}^2}}\right] \end{aligned} \quad (26)$$

where $\bar{z}_i$ corresponds to the kriging approximation for $\ln(RMS_i)$ and the last equality is based on the fact that since $\ln(\varepsilon_i)$ and $\bar{\varepsilon}_i$ are zero mean independent Gaussian variables with variances, $\sigma_i^2$ and $\sigma_{bi}^2$, respectively, their sum (or difference in this case) is also a Gaussian variable with zero mean and variance $\sigma_i^2+\sigma_{bi}^2$. This leads to the following approximation to the performance function

$$\bar{h}(\mathbf{x},\boldsymbol{\theta}) = \frac{1}{3}\sum_{i=ac,df,dr} \Phi\left[\frac{\bar{z}_i - \ln(b_i)}{\sqrt{\sigma_i^2 + \sigma_{bi}^2}}\right] \quad (27)$$

The gradient of this expression will be also needed in the optimization and can be obtained by

$$\begin{aligned} \nabla\bar{h}(\mathbf{x},\boldsymbol{\theta}) &= \frac{1}{3}\sum_{i=ac,df,dr} \nabla\Phi\left[\frac{\bar{z}_i - \ln(b_i)}{\sqrt{\sigma_i^2 + \sigma_{bi}^2}}\right] \\ &= \frac{1}{3}\sum_{i=ac,df,dr}^{3} \phi\left[\frac{\bar{z}_i - \ln(b_i)}{\sqrt{\sigma_i^2 + \sigma_{bi}^2}}\right] f_g \\ f_g &= \left(\frac{\nabla\bar{z}_i}{\sqrt{\sigma_i^2 + \sigma_{bi}^2}} - \frac{(\bar{z}_i - \ln(b_i))}{(\sigma_i^2 + \sigma_{bi}^2)^{3/2}}\nabla\sigma_i^2\right) \end{aligned} \quad (28)$$

where $\phi[.]$ corresponds to the Gaussian Probability Density Function (PDF), and evaluation of all required gradients in the last equation was discussed in Section 4.

## 5.3 Numerical Details for Optimization

The design domains $X$ has upper bounds [400 4000 400 4000] N s/m , and lower bounds [0 0 0 0] N s/m . For the trust region definition, the length of the initial region $\mathbf{L}_1$ is initially selected as 20% of the design domain $X$ , i.e. $s_1^l = 0.2$ with a reduction in size of 5% with every iteration, i.e. $s^r = 0.95$ . When the optimization has reached the last stage, the reduction in the trust region is set to 50% or $s_f^r = 0.5$ . For the local search within $X_k$ a trust-region-reflective algorithm is adopted. For the local search an exterior sampling approach is

adopted (same samples are utilized within the trust-region-reflective algorithm) whereas, as discussed earlier, the overall implementation is formulated as interior sampling (different sample set is generated whenever the algorithm is initiated at the beginning of each local search/optimization).

The number of support points for the hybrid DoE approach is selected as $n_1^s = 200$ and $n_2^s = 700$ whereas the number of support points for the second optimization stage, for increasing the accuracy of the kriging approximation, is taken to be double these values. The number of samples for the estimates in Eqs. (7) and (8) for the local search is taken as $N$=2000 and increased to $N$=10000 in the second optimization stage. The total number of simulations for $\overline{h}(\mathbf{x}_k, \boldsymbol{\theta})$ to inform the selection of IS densities and the sampling density for the second stage of the DoE approach is set to $N_p$=10000. For the basis functions selection, the percentage reduction (defining the cut-off entropy with respect to the maximum entropy over the entire input vector) is set to $s_e^{re} = 0.4$.

Apart from the fully adaptive kriging implementation that additionally incorporates the kriging error in the objective function formulation, two additional cases are examined, leading to a total of three different optimization approaches considered. The first, denoted AK (adaptive kriging), and second, denoted AKE (adaptive kriging with error), correspond to the proposed algorithm that adaptively employs the probabilistic sensitivity analysis to select the order of the basis function for the kriging model, and also adopts the proposed hybrid DoE. The only difference is that the first approach does not include the kriging error in the objective function while the second one does. The former is established simply by taking $\nabla\sigma_i^2 = \sigma_i^2 = 0$ in Eqs. (27) and (28). The third approach, denoted LK (Latin Hypercube Kriging), employs the traditional sampling technique of LHC for both $\mathbf{x}$ and $\boldsymbol{\theta}$, uses quadratic basis functions for all the parameters of the kriging model, and does not include the kriging error in the objective function. This last configuration is the baseline case, where none of the proposed advances are employed.

To judge the quality of the obtained solutions, the optimization problem was additionally solved using the simultaneous perturbation stochastic approximation algorithm (Spall, 2003) coupled with the highly efficient adaptive IS formulation proposed recently by Medina and Taflanidis (2014). The optimal benchmark solution was found to be $\mathbf{x}^*$=[175.2 1645.3 190.1 1495.4] with respective performance $H(\mathbf{x}^*)$=0.066% whereas the total number of model evaluations needed to converge to this solution was close to 265000. This large computational effort should be attributed to the fact that the performance close to the optimum corresponds to a rare event (small failure probability) requiring a large number of samples for accurate approximation, even with implementation of an efficient adaptive IS scheme.

## 5.4 Results and Discussion

Results are reported in Table 2 for five different trials corresponding to different initial conditions $\mathbf{x}_1$ for the algorithm. In particular, the optimal solution $\mathbf{x}^*$, the total number of simulations of the system high-fidelity model till convergence is established, $N^{tot}$, the objective function value obtained through the use of the kriging metamodel, $\hat{H}_{krig}(\mathbf{x}^*)$, which is obtained directly from the optimization algorithm, as well as the objective function value obtained through the use of the actual system model, $\hat{H}(\mathbf{x}^* | \{\boldsymbol{\theta}^c\})$, are reported. For the latter the same sample set $\{\boldsymbol{\theta}^c\}$ (common random numbers) are used across all comparisons for each design problem to enable a consistent comparison (Spall, 2003). $N$=10000 samples are used in this comparison which facilitates a small coefficient of variation for $\hat{H}(\mathbf{x}^* | \{\boldsymbol{\theta}^c\})$, close to 4%. A three-fold comparison can be established based on these results: (i) Comparison between $\hat{H}_{krig}(\mathbf{x}^*)$ and $\hat{H}(\mathbf{x}^* | \{\boldsymbol{\theta}^c\})$ shows the accuracy of the kriging implementation, (ii) comparison of the $N^{tot}$ for different approaches shows the computational efficiency for convergence of the algorithm, (iii) comparison between $\hat{H}(\mathbf{x}^* | \{\boldsymbol{\theta}^c\})$ and the benchmark optimal solution of 0.0066% shows the robustness of the approach in converging to the true optimum.

The results for AKE demonstrate a remarkable *computational efficiency* and *robustness*. The identified solution $\mathbf{x}^*$ is always in the vicinity of the benchmark optimum solution and, more importantly, the attained performance is always comparable or even better than the benchmark performance. This is accomplished with a small number of model evaluations, not exceeding 7100 for any trial. Note that the differences between these trials are well expected since there is a strong dependence of the optimization approach on the initial conditions. Overall the reported efficiency corresponds to

tremendous computational savings (265000 simulations needed before), something that is accomplished primarily through the proposed formulation of the kriging metamodel in the augmented input space.

Table 2: Optimization results for different cases considered and different trials.

| Trial | $\mathbf{x}^*$ (Nm/s) | $N^{tot}$ | $\hat{H}_{krig}(\mathbf{x}^*)$ | $\hat{H}(\mathbf{x}^* \mid \{\boldsymbol{\theta}^c\})$ |
|---|---|---|---|---|
| AK (adaptive kriging) | | | | |
| 1 | [122.5 2121.1 142.8 1884.5] | 8817 | 0.025 % | 0.079 % |
| 2 | [161.3 1484.9 145.7 1725.3] | 6607 | 0.023 % | 0.091 % |
| 3 | [149.4 1780.3 168.6 1568.5] | 12046 | 0.020 % | 0.073 % |
| 4 | [125.6 2183.2 113.1 1656.2] | 3736 | 0.020 % | 0.113 % |
| 5 | [159.1 1541.0 160.2 1532.8] | 8698 | 0.022 % | 0.089 % |
| AKE (adaptive kriging with error) | | | | |
| 1 | [136.9 2091.9 154.5 1814.3] | 5721 | 0.054 % | 0.066 % |
| 2 | [159.4 1819 189.8 1521.3] | 4751 | 0.053 % | 0.063 % |
| 3 | [158.6 1886.3 153.6 1762.9] | 5512 | 0.059 % | 0.063 % |
| 4 | [173.1 1731.5 147.5 1808.1] | 7076 | 0.045 % | 0.064 % |
| 5 | [171.3 1847.5 170.1 1708.0] | 4703 | 0.059 % | 0.063 % |
| LK (Latin hypercube kriging) | | | | |
| 1 | [148.7 2649.4 195.1 1765.9] | 19778 | 0.024 % | 0.175 % |
| 2 | [220.3 2011.5 84.0 1860.4] | 19720 | 0.182 % | 0.279 % |
| 3 | [157.5 1838.1 145.3 2400.7] | 19153 | 0.026 % | 0.091 % |
| 4 | [189.9 1887.6 71.3 2174.7] | 18763 | 0.032 % | 0.119 % |
| 5 | [136.3 1937 306.3 859.2] | 19591 | 0.119 % | 0.191 % |

Moving now to the accuracy of the kriging implementation (still for AKE), assessed through the comparison between $\hat{H}_{krig}(\mathbf{x}^*)$ and $\hat{H}(\mathbf{x}^* \mid \{\boldsymbol{\theta}^c\})$, there is an overall good agreement. When compared against the accuracy of the kriging implementation when the prediction error is not included in the performance function estimate (compare the values of $\hat{H}_{krig}(\mathbf{x}^*)$ and $\hat{H}(\mathbf{x}^* \mid \{\boldsymbol{\theta}^c\})$ for AK) it is evident that the explicit consideration of that error provides significantly improved estimates, i.e., closer values of $\hat{H}_{krig}(\mathbf{x}^*)$ and $\hat{H}(\mathbf{x}^* \mid \{\boldsymbol{\theta}^c\})$.

The more interesting comparison is, however, between AKE and the alternative approaches (AK/LK) in terms of computational efficiency (comparison of $N^{tot}$ for same trial) and more importantly robustness (comparison of $\hat{H}(\mathbf{x}^* \mid \{\boldsymbol{\theta}^c\})$ for same trial). In all instances it is shown that the other two approaches do not share the robustness of the proposed AKE implementation, as they converge for some trials to a significantly suboptimal performance $\hat{H}(\mathbf{x}^* \mid \{\boldsymbol{\theta}^c\})$. The differences are perhaps more evident for LK and secondary for AK. This is an important result; it shows that a space-filling DoE, even though might provide a good global accuracy, leads to significant errors in regions of the model parameters that are of importance for the probabilistic performance and ultimately to erroneous identified optimal designs. Similarly ignoring the prediction error, not only decreases the accuracy of the estimated performance as argued in the previous paragraph, but, and perhaps more importantly, can provide erroneous optimal solutions. Even though calculation of this error does involve a higher computational burden compared to using only the mean kriging approximation (Jia and Taflanidis, 2013), it is evident that its explicit consideration provides significant enhancements that counteract this burden.

# 6 CONCLUSIONS

An adaptive implementation of kriging metamodeling was considered to reduce the computational burden associated with optimization under uncertainty problems adopting a simulation-driven (stochastic simulation) approach for evaluation of the objective function. Two important aspects for tuning of the kriging metamodel were adaptively addressed within this implementation by seamlessly sharing information across the iterations of the numerical optimization: (i) design of experiments (DoE) for selecting support points aimed at improving the accuracy over a targeted region, the one contributing most towards the probabilistic performance, and (ii) selection of the order of basis functions for the different inputs of the metamodel. Additionally, a novel implementation

was introduced formulating the kriging metamodel in the augmented model parameter and design variable space whereas the local prediction error associated with the kriging approximation was explicitly considered in the objective function estimation.

The illustrative example showed the computational efficiency (convergence with small number of evaluations of the high-fidelity system model) as well as robustness (convergence to solutions that are close to the true optimum) established through the proposed kriging implementation in the augmented input space. The proposed hybrid DoE for a targeted region was additionally shown to greatly enhance the accuracy of the kriging approximation and its ability to avoid converging to suboptimal solutions. Finally the explicit incorporation of the prediction error improved not only the accuracy of the estimated objective function through the kriging metamodel but also similarly supported a more robust optimization.

## ACKNOWLEDGEMENTS

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