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AN UNIFIED ENRICHMENT STRATEGY FOR RELIABILITY-BASED DESIGN OPTIMIZATION USING ADAPTIVE KRIGING AND ZERO-ORDER ALGORITHMS

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Abstract. *The optimal design of complex engineering systems is a necessary task in a challenging industrial environment. Constrained optimization frameworks properly take charge of the engineering requirements by considering uncertainties in the constraint and identifying the optimal compound of design parameters among the admissible ones. However, this procedure is often very time-consuming and requires a significant number of calls 3rd party solvers, especially when dealing with probabilities of rare events. The specific objective of this work is to propose a new unified enrichment strategy based on Adaptive Kriging and zero-order (gradient-free) optimization algorithms to identify efficiently the solution of Reliability-Based Design Optimization problems when using Monte Carlo Simulation based methods to assess reliability. This enables the parallel operation of the reliability computation and the optimization. As a result, the proposed procedure provides a significant improvement in the refinement of the Kriging surrogate around the most reliable design solution within an affordable computational-time cost.*

Keywords: Reliability-based design optimization (RBDO), Surrogate-assisted RBDO, Active learning, Adaptive Kriging, Zero-order algorithm, Evolutionary algorithm.

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1 INTRODUCTION

1.1 General considerations

In a demanding industrial environment, the optimal design of complex engineering systems is a must. Structural design must comply with different specifications, such as performance, durability, cost, and safety, to mention a few. However, real mechanical systems show uncertainties in practice. Those should be explicitly accounted for to fully capture the variability of the random parameters and achieve optimal performance. To this effect, constrained optimization frameworks properly take charge of the engineering requirements by considering uncertainties in the constraint and identifying the optimal solution among the admissible ones [1]. Thus, the goal relies upon finding the optimal compound of design parameters with respect to the specified mechanical strength constraint. However, computing the latter is often very time-consuming for industrial applications, requiring a significant number of calls to non-explicit mechanical models, especially when dealing with probabilities of rare events. The active field of research of Reliability-based design optimization (RBDO) counts an ever-increasing number of contributions [2]. Notwithstanding, their effectiveness is so far limited for high target reliability levels or high dimensional problems because of their highly associated computing time. A challenge needs to be tackled: the reduction of the number of failure probability assessments in order to limit the number of mechanical model calculations.

1.2 Motivation and objective

In this context, the specific objective of this work is to propose a new unified enrichment strategy based on Adaptive Kriging (AK) and zero-order (gradient-free) optimization algorithms to handle efficiently the solution of RBDO problems when using Monte Carlo simulation-based methods to assess the reliability. The goal is to classify efficiently a Monte Carlo sample based on machine-learning separators defined in an augmented-domain [3]. This enables the parallel operation of the reliability computation calculated by Monte Carlo simulation (MCS) and the optimization. As a result, the combination of the evolutionary algorithm with the proposed generalized learning metric available for both reliability and optimization provides a significant improvement in the refinement of the Kriging surrogate around the most reliable design solution within an affordable computational-time cost. This evidence is supported in the paper by a showcase of the algorithm's performance and effectiveness for a numerical engineering benchmark.

2 BACKGROUND

2.1 Literature context

Reliability-Based Design Optimization (RBDO) has become a crucial aspect of engineering design. It seeks to optimize the performance of a system while ensuring a desired level of its reliability. In recent years, this active field of research has counted an ever-increasing number of contributions. To date, a wide variety of methods exist in the literature to tackle the problem, namely *two-level-*, *mono-level-*, *decoupled-*, and *metamodel-* approaches [4, 5]; and according to the technique used for reliability analysis into *approximation-based* methods and *simulation-based* methods [6, 2]. One of the most common approaches is the so-called two-level method, in which the reliability analysis is performed in the first step to estimate the failure probability of the system using first- or second-order reliability methods (FORM or SORM), which are efficient but may not provide accurate results for complex systems; and the optimization is performed in the second step to find the optimal design parameters. In recent years, advanced reliability methods such as *Monte Carlo simulation* and *subset simulation* have been used to overcome the limitations of traditional reliability methods. In this context, most of the recent literature has emphasized the effective use of *metamodel-assisted* approaches to enhance performances, for which the computational cost of some complex engineering models is reduced by an inexpensive surrogate [7]. Specifically, several Kriging-assisted approaches have been proposed in the literature for nested loops RBDO problems, in which the time-consuming limit-state functions (LSF) are replaced with Kriging model, [8, 9, 10]. The use of Kriging (a.k.a. Gaussian Process) for RBDO is motivated by its ability to model the underlying relationships between inputs and outputs of a system with a high degree of accuracy. Kriging provides a probabilistic estimate of the system's response, which can be used to evaluate the reliability of the design. Moreover, Kriging is particularly well-suited for RBDO applications because it can handle deterministic and stochastic inputs and model non-linear relationships between inputs and outputs. Besides, the use of *meta-heuristics*, such as genetic algorithms and particle swarm optimization, has become popular in RBDO due to their ability to handle complex design spaces and non-linear objectives. These algorithms are particularly well-suited for problems where the gradients of the objective function are not available or difficult to calculate. Recently, a growing body of literature has investigated the effectiveness of the combined use of Kriging and gradient-free optimization algorithms in RBDO in optimizing the reliability of a variety of engineering systems [11, 12, 13]. These methods have the advantage of being able to provide a probabilistic estimate of the response of the system. However, they are often computationally intensive, which makes them less suitable for large-scale optimization problems. Therefore, there is still much room for improvement in this area, and further research is needed to develop more efficient and effective methods for RBDO.

2.2 RBDO problem formulation

In the setup of an RBDO problem, a general formulation of the problem reads (see e.g. [3]):

$$\boldsymbol{d}^* = \arg\min_{\boldsymbol{d}\in\mathbb{D}_{\boldsymbol{d}}} \mathfrak{c}(\boldsymbol{d}) : \mathbb{P}\Big(\mathfrak{g}_k(\boldsymbol{X_d}, \boldsymbol{X_p}) \leq 0\Big) \leq \overline{\mathcal{P}}_{f_k} \quad k = 1, \dots, n_h \tag{1}$$

In this formulation, the cost function $\mathfrak{c}(\boldsymbol{d})$ needs to be minimized with respect to the unknown design variables $\boldsymbol{d} = \{d_1, \dots, d_{n_d}\} \in \mathbb{D}_{\boldsymbol{d}} \subset \mathbb{R}^{n_d}$ in order to fulfill the *hard constraints* describing the system's performance. The latter is mathematically expressed by some *limit-state functions* denoted by $\mathfrak{g}_k\big(\boldsymbol{X_d}, \boldsymbol{X_p}\big)$. The failure occurs for any realization of $\boldsymbol{d}$ that generates $\mathfrak{g}_k\big(\boldsymbol{X_d}, \boldsymbol{X_p}\big) \leq 0$. Moreover, the probabilistic constraint $\mathbb{P}\Big(\mathfrak{g}_k(\boldsymbol{X_d}, \boldsymbol{X_p}) \leq 0\Big)$ is required to not exceed a fixed threshold probability $\overline{\mathcal{P}}_{f_k}$ (e.g., from 10^{-2} to 10^{-8} for rare event estimation). The computational definition of the failure probability takes the form of the following integral:

$$P_{f_k} = \mathbb{P}\Big(\mathfrak{g}_k(\boldsymbol{X_d}, \boldsymbol{X_p}) \leq 0\Big) = \int_{\mathbb{F}=\{\boldsymbol{x}\in\mathbb{X}:\mathfrak{g}_k(\boldsymbol{x})\leq 0\}} f_{\boldsymbol{X}}(\boldsymbol{x})\mathrm{d}\boldsymbol{x}, \tag{2}$$

where $\mathbb{F} = \{\boldsymbol{x} \in \mathbb{X} : \mathfrak{g}_k(\boldsymbol{x}) \leq 0\}$ is the *failure domain* and $\mathcal{S}_0 = \{\boldsymbol{x} \in \mathbb{X} : \mathfrak{g}_k(\boldsymbol{x}) = 0\}$ is the *limit-state surface*. $\mathbb{X} = \{\boldsymbol{X_d}, \boldsymbol{X_p}\}$ is the vector of the random variables which is constituted by: $\boldsymbol{X_d} \sim f_{\boldsymbol{X}|\boldsymbol{d}} : \boldsymbol{X_d} = \{x_{\boldsymbol{d},1}, \dots, x_{\boldsymbol{d},n_d}\}$ that is the vector of the random variables depending on the design variables $\boldsymbol{d}$, whereas $\boldsymbol{X_p} \sim f_{\boldsymbol{X}|\boldsymbol{p}} : \boldsymbol{X_p} = \{x_{\boldsymbol{p},1}, \dots, x_{\boldsymbol{p},n_p}\}$ are other random variables of the underlying problem that do not depend on $\boldsymbol{d}$.

3 METHODOLOGY

3.1 Surrogate-assisted approach with zero-order optimization algorithm

Solving Equation (1) requires many evaluations of the performance function $\mathfrak{g}_k\big(\boldsymbol{X_d}, \boldsymbol{X_p}\big)$. As discussed in Section 1, a well-established strategy to leverage the computation consists in substituting the original expensive computational model with an approximated and fast-to-evaluate surrogate model (a.k.a. metamodel or emulator). These metamodels are defined by a set of hyperparameters that must be calibrated. The use of a metamodel of the probability of failure covering the whole design space would require a huge and unaffordable design of experiments (DoE). Therefore, the LSF is approximated in this work by using a global Kriging surrogate model trained with a sequentially enriched set of model evaluations. To this aim, a new active learning (AL) metric is presented herein. The latter is meant to gather information from the optimization and the metamodel parameters, namely the Kriging mean and the Kriging variance. This means that the metamodel is adaptively and efficiently enriched only in regions that actually matter, i.e. where the optimal design parameters are likely to be found and in the vicinity of the limit state of a constraint. In particular, in the proposed method, a Genetic Algorithm (GA) is employed to search the global optimal solution of design parameters that satisfy the reliability constraints. This choice is a natural consequence of operating directly on the design space avoiding the computation of the objective function derivatives.

3.2 The implementation of the proposed algorithm

Exactly, GA is employed to solve the optimization problem defined in Equation (1) in order to acquire a global optimum solution. The evolution begins with randomly generated design individuals. The latter are also selected as the initial DoE to compute the global Kriging to classify whether a design solution belongs to the feasible region or not. At each iteration, a new generation is constructed starting from the previous one using the normalized fitness function $f(\boldsymbol{X_d})$ of Equation (3) that also represents the new solution set for the next algorithm iteration:

$$f(\boldsymbol{X_d}) = \frac{\mathfrak{c}^*(\boldsymbol{d}) + \mathbb{I}\big[\mathbb{P}(\hat{\mathfrak{g}}(\boldsymbol{X_d}) \leq 0) \leq \overline{\mathcal{P}}_{f_k}\big]}{2} \qquad \text{where : } \begin{cases} \mathbb{I} = 0 & \hat{\mathfrak{g}}(\boldsymbol{X_d}) > 0 \\ \mathbb{I} = 1 & \hat{\mathfrak{g}}(\boldsymbol{X_d}) \leq 0 \end{cases} \tag{3}$$

where $\mathfrak{c}^*(\boldsymbol{d})$ is the normalized cost in the interval $[0, 1]$, whereas $\mathbb{I}$ expresses the penalty factor used to identify the sign of the reliability constraint, i.e. whether a realization of the design parameters is located in the feasible region. It should be observed that the surrogate model is only used as a classification tool. To gradually improve the accuracy of the metamodel, if necessary, the enrichment is performed at the same time as conducting the optimization. This task is performed where the probabilistic constraints are likely to be violated and near the reliable optimum, by defining a newly Active Learning metric for which a new candidate sample $\boldsymbol{x}^{\text{new}}$ is added to the DoE as follows:

$$\boldsymbol{x}^{\text{new}} = \underset{\boldsymbol{x} \in \mathbb{X}}{\arg\min} \; U\big(\boldsymbol{X}(\boldsymbol{d}^{(i-gen)})\big) \tag{4}$$

where U is the learning function defined in [14] as:

$$U = \frac{|\mu_{\hat{\mathfrak{g}}}|}{\sigma_{\hat{\mathfrak{g}}}} \tag{5}$$

The major advantage with respect to the stopping criterion based on U is that now the number of enrichment is drastically reduced. This is because the condition $U \geq 2$ on the local MCS population is not met for each population. In other words, Equation (4) allows the selection of only one enrichment point per GA generation, which means adding only one call to the numerically demanding performance function at each generation, the one that is most likely to be misclassified (i.e., maximum error on $\hat{\mathfrak{g}}(\boldsymbol{X_d})$ sign estimation). The hard constraint is checked at each step estimating the failure probability by using the MCS and the Kriging model sequentially enriched. The algorithm loops until the stop condition associated with the optimality of the solution is reached, i.e. when the number of generations reaches the given maximum number. As a result, the combination of the evolutionary algorithm with the proposed generalized learning metric available for both reliability and optimization provides a significant improvement in the refinement of the Kriging surrogate around the most reliable design solution within an affordable computational-time cost. Finally, the outline of the algorithm reads as follows:

Algorithm 1 - Outline

Generate the initial random population: $\boldsymbol{d}^{(0-gen)} = \{d_1, \dots, d_{n_{\boldsymbol{d}}}\}$
Build the Kriging surrogate $\hat{\mathfrak{g}}_k^{(0)}(\boldsymbol{X_d})$ of the limit state function on $\boldsymbol{d}^{(0-gen)}$
while $n^{(i-gen)} \leq n^{(MAX-gen)}$ **do**
  for each $d_m \in \boldsymbol{d}^{(i-gen)}$ **do** sampling local Monte Carlo population
    Compute $\hat{P}_{f_k} = \mathbb{P}\Big(\hat{\mathfrak{g}}_k(\boldsymbol{X_d}) \leq 0\Big) = \frac{N_{\hat{\mathfrak{g}}\leq 0}}{N_{MCS}}$
  end for
  Evaluation of the fitness function $f(\boldsymbol{X_d})$ defined in Equation (3)
  Selection $n_{\boldsymbol{d}}/2$ parent pairs from for crossover
  Generate a new population of $n_{\boldsymbol{d}}$ offspring
  Randomly mutate some points in the population to obtain $\boldsymbol{d}^{(i+1-gen)}$
  if $\hat{P}^-_{f_k} = \frac{N_{\hat{\mathfrak{g}}\leq 0 \& U \geq 2}}{N_{MCS}} < \hat{P}_{f_k} < \hat{P}^+_{f_k} = \frac{N_{\hat{\mathfrak{g}}\leq 0 \& U \geq 2} + N_{U \leq 2}}{N_{MCS}}$ **then**
    if $U\big(\boldsymbol{X}(\boldsymbol{d}^{(i+1-gen)})\big) < 2$ **then** $\boldsymbol{x}^{\text{new}} = \underset{\boldsymbol{x}\in\mathbb{X}}{\arg\min}\ U\big(\boldsymbol{X}(\boldsymbol{d}^{(i-gen)})\big)$
      $\text{DoE}^{(i+1-gen)} += \boldsymbol{x}^{\text{new}}$
      Update Kriging surrogate $\hat{\mathfrak{g}}_k^{(s)}(\boldsymbol{X_d})$ on $\text{DoE}^{(i+1-gen)}$
    end if
  end if
  $n^{(i-gen)} += 1$
end while

4 NUMERICAL CASE STUDY

4.1 A highly nonlinear limit-state surface

In this section, a 2-dimensional benchmark is investigated to illustrate and validate the strategy proposed in Section 3. This numerical example was presented first by Lee and Jung in [15] and consists of two performance functions. In this work, the only highly nonlinear limit-state function is taken into account in the calculations for the sake of simplicity:

$$\mathfrak{g}_1(\boldsymbol{X}_d) = -x_1 sin(4x_1) - 1.1x_2 sin(2x_2) \tag{6}$$

where $\boldsymbol{x}$ is the realization of the design random variable set $\boldsymbol{X}_d = \{x_1, x_2\}$ of two independent normal variables: $\boldsymbol{x_1} \sim \mathcal{N}(\mu_1, 0.1)$; $\boldsymbol{x_2} \sim \mathcal{N}(\mu_2, 0.1)$. And the design vector $\boldsymbol{d} = \{\mu_1, \mu_2\}$ is a set of parameters restrained in the following hyperrectangular design space:

$$\mathbb{D}_{\boldsymbol{d}} = [0; 3.7] \times [0; 4] \subset \mathbb{R}^2 \tag{7}$$

The optimization is performed in order to minimize the following quadratic objective function:

$$\mathfrak{c}(\boldsymbol{d}) = (\mu_1 - 3.7)^2 + (\mu_2 - 4)^2 \tag{8}$$

and the optimum must satisfy the probabilistic constraint:

$$P_{f_k} = \mathbb{P}\Big(\mathfrak{g}_k(\boldsymbol{X_d}) \leq 0\Big) \leq \overline{\mathcal{P}}_{f_k} \tag{9}$$

Table 1 summarizes all the parameters that have been used to set the algorithm options.

Parameters	Symbol	Value
Maximum number of generation	$n^{(MAX-gen)}$	200
Number of chromosomes in each population	n_{chr}	32
Crossover probability	p_c	0.7
Mutation probability	p_m	0.1
Number of samples of the input vector in each population	N_{MCS}	10^5
Threshold probability	$\overline{\mathcal{P}}_{f_k}$	10^{-4}

Table 1: Set of algorithm's parameters used in the numerical benchmark.

4.2 Results

Figure 1 pictures the convergence of the algorithm from the initial stage on the left to the optimal solution on the right. In the plots, the dashed line represents the prediction of the Kriging mean, the blue stars are the enrichment points added to the original DoE, whereas the green crosses surrounded by the purple nebula are the GA chromosomes with their local Monte Carlo population generated during the optimization phases.

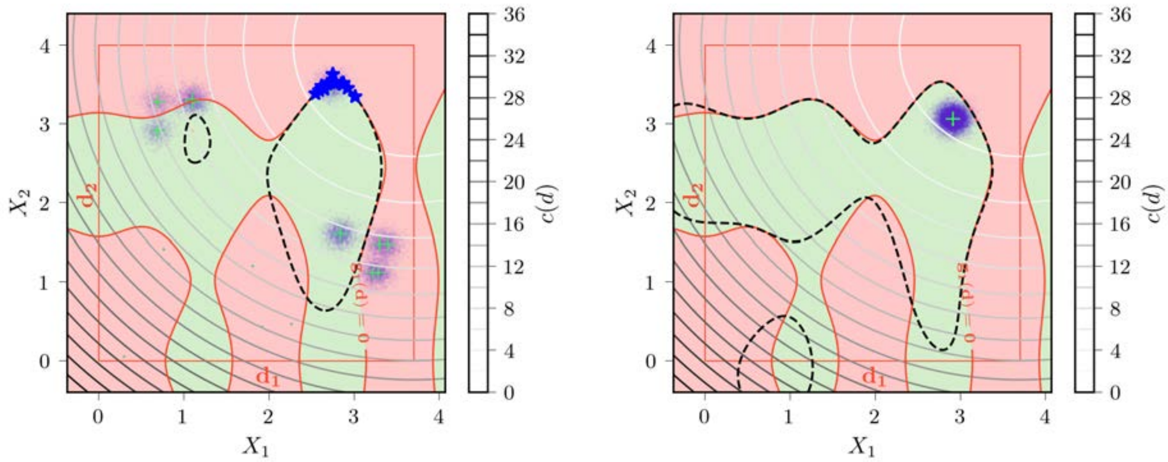

Figure 1: Convergence of the RBDO algorithm for the numerical example: on the left the initial stage of the algorithm and on the right the optimal solution.

As it is intuitive to expect, the accuracy of the Kriging surrogate prediction at the final stage of the algorithm is higher near the optimal solution. This is because most of the enrichment is performed in that region. Moreover, from the superposition of all the chromosomes in the final frame, it appears clear how the convergence of the algorithm is achieved. The performance of the proposed strategy with respect to other methods available in the literature is presented in Table 2. By employing the proposed algorithm based on the newly defined metric (Equation (4)), it can be obtained that the final optimum design is $\boldsymbol{d} = \{\mu_1 = 2.84; \mu_2 = 3.18\}$. This result is achieved within an affordable computational time. Specifically, only 26 calls to the performance function are required during the algorithm run, i.e. more than half of calls with respect to other referenced methods.

Method	μ_1	μ_2	cost	$\mathfrak{g}_1$-calls
Brute force*	2.84	3.23	1.330	10^7
PMA w/ Kriging*	2.82	3.30	1.260	90
Meta-RBDO*	2.81	3.25	1.350	80
$\arg\min_{\boldsymbol{x}\in\mathbb{X}} U\big(\boldsymbol{X}(\boldsymbol{d}^{(i-gen)})\big)$	2.84	3.18	1.414	26

Source(s): *cited from [3]

Table 2: Comparative results in terms of calls to the performance function for the numerical example.

5 CONCLUSIONS

The focus of this work is centered on the proposal of a new unified enrichment strategy for Reliability-Based Design Optimization. This metric allows the parallel operation of the reliability computation calculated by Monte Carlo simulation (MCS) and the optimization. From the investigated numerical engineering benchmark, it can be concluded how the combination of the evolutionary algorithm with the proposed generalized learning metric provides a significant improvement in the refinement of the Kriging surrogate around the most reliable design solution within an affordable computational-time cost with small number of model evaluations compared with existing methods.

The next steps for this research include the extension of this metric to more complex problems in order to be able to handle high-dimensional input spaces providing a probabilistic estimate of the response of the system. There is still much room for improvement and further research is needed to develop more efficient and effective methods for RBDO.

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