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Robust minimax design from costly simulations

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ABSTRACT: Design of complex physical systems most often relies on numerical simulations that may be extremely costly. In this paper, design is formalized as the optimization of a performance index with respect to *control variables*. Uncertainty is modeled via a vector of *environmental variables* that can take any value in a known compact set and may have an adverse effect on performance. In this context, the determination of a robust design requires the continuous minimax optimization of black-box functions. An algorithm combining Kriging-based optimization with relaxation is presented, which makes it possible to find approximate solutions to such problems on a limited computational budget. The design of a vibration absorber is presented as an illustrative example.

1 INTRODUCTION

Most real-life computer-aided design problems require costly simulations of knowledge-based models, which may involve, e.g., partial differential equations, complicated boundary conditions, several types of physics, etc. In such a context, one single simulation of the model for a given value of the parameters to be optimized may cost such a significant amount of computational resources that the budget for simulations is severely limited. This has given rise to a large number of contributions involving surrogate models, i.e., models that are cheaper to simulate than the initial knowledge-based model yet capture significant features of this model and are used to facilitate optimization. A particularly interesting approach is based on Kriging (developed about sixty years ago in the context of geostatistics (Matheron 1963) and still the object of much research under various names. One of the advantages of Kriging-based surrogate modeling is that the prediction of the output of the complex model by the surrogate model is provided with an estimate of its quality. This has made it possible to develop a particularly efficient method for global optimization known under the name of EGO (Efficient Global Optimization) (Jones 2001). EGO optimization has become a reference in the context of optimal design based on complex simulations, e.g., in the automotive industry.

Most often, it is unrealistic to assume that the design problem translates into the optimization of a deterministic function with respect to control parameters because uncertainty must be taken into account, so EGO cannot be used directly. In this communication, we present an approach for applying Kriging to worst-case design. We assume that performance is described by a scalar function of two vector arguments. The first is a vector of *control variables*, assumed to belong to some known compact set and the second is a vector of *environmental variables*, which encapsulates all the sources of uncertainty against which the design should be made robust. This second vector is also assumed to belong to some known compact set. The purpose of robust design is then to find the best feasible control vector for the worst feasible environmental conditions.

Remarkably few methods seem to have been devoted to such a problem of minimax optimization when performance is costly-to-evaluate. This communication presents a method that we recently developed (Marzat, Walter, & Piet-Lahanier 2012) based on a relaxation procedure (Shimizu & Aiyoshi 1980). By combining two optimization subproblems via EGO, it becomes possible to compute an approximate solution to the minimax problem from a limited number of evaluations of the performance function. The practical applicability of the method is demonstrated on a realistic robust mechanical design problem.

2 MINIMAX OPTIMIZATION FOR BLACK-BOX FUNCTIONS

Before presenting the new algorithm, MiMaReK (for MiniMax Optimization via Relaxation and Kriging), we recall the fundamentals of Kriging-based optimization.

2.1 Kriging-based optimization

The problem to be solved is finding

$$\hat{\mathbf{x}} = \arg \min_{\mathbf{x} \in \mathbb{X}} f(\mathbf{x}), \quad (1)$$

where $f(\cdot)$ is a function from $\mathbb{X} \subset \mathbb{R}^d \rightarrow \mathbb{R}$, \mathbf{x} a d -dimensional vector of real variables and \mathbb{X} a known compact set. Assume that $f(\cdot)$ has already been evaluated at \mathbf{x}_i , for $i = 1, \dots, n$, and let $\mathcal{X}_n = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ and $\mathbf{f}_n = [f(\mathbf{x}_1), \dots, f(\mathbf{x}_n)]^T$. Based on these data, Kriging (Matheron 1963) builds a surrogate approximation of $f(\cdot)$, by modeling it as a Gaussian Process (GP) $F(\cdot)$. In this paper, for the sake of simplicity, $F(\cdot)$ is assumed to be a zero-mean GP with covariance function $\text{cov}(\cdot, \cdot)$, though additional parametric priors may also be employed (Santner, Williams, & Notz 2003). The covariance function is usually modeled as

$$\text{cov}(F(\mathbf{x}_i), F(\mathbf{x}_j)) = \sigma_F^2 R(\mathbf{x}_i, \mathbf{x}_j), \quad (2)$$

where σ_F^2 is the GP variance and $R(\cdot, \cdot)$ is a parametric correlation function. The widely-used correlation function adopted here is the *power exponential correlation function*,

$$R(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\sum_{k=1}^d \left|\frac{\mathbf{x}_i(k) - \mathbf{x}_j(k)}{\theta_k}\right|^{p_k}\right), \quad (3)$$

where the parameters $0 < p_k \leq 2$ reflect the smoothness of the approximation (the smoothest one being obtained for $p_k = 2$), while the parameters θ_k are scale factors. Other correlation functions may also be employed (Rasmussen & Williams 2006).

Under these hypotheses, Kriging provides a continuous interpolation of the data that is the best linear unbiased predictor of the value taken by $f(\cdot)$ at any $\mathbf{x} \in \mathbb{X}$,

$$\hat{F}(\mathbf{x}) = \mathbf{r}(\mathbf{x})^T \mathbf{R}^{-1} \mathbf{f}_n, \quad (4)$$

where

$$\begin{cases} \mathbf{R}_{|ij} = R(\mathbf{x}_i, \mathbf{x}_j) \\ \mathbf{r}(\mathbf{x}) = [R(\mathbf{x}, \mathbf{x}_1), \dots, R(\mathbf{x}, \mathbf{x}_n)]^T \end{cases} \quad (5)$$

This surrogate model is much less costly to evaluate than the original function $f(\cdot)$. An important property of Kriging is that the *variance of the prediction error*, which quantifies confidence on the prediction (4), is

readily computed as

$$\hat{\sigma}^2(\mathbf{x}) = \sigma_F^2 (1 - \mathbf{r}(\mathbf{x})^T \mathbf{R}^{-1} \mathbf{r}(\mathbf{x})). \quad (6)$$

Variance will be small near already sampled values of \mathbf{x} and much higher where the black-box function is less well known. An interesting application is the development of Kriging-based optimization algorithms that sample iteratively new points in \mathbb{X} where the function should be evaluated to enhance the estimate of the global optimum (Jones 2001). One of these strategies is *Efficient Global Optimization* (EGO) (Jones, Schonlau, & Welch 1998), which proceeds as indicated in Algorithm 1.

Algorithm 1 EGO

1. Choose \mathcal{X}_n and compute \mathbf{f}_n .
 2. Fit a Kriging model on \mathcal{X}_n and \mathbf{f}_n via (4) and (5).
 3. Find $f_{\min}^n = \min_{i=1, \dots, n} \{y(\mathbf{x}_i)\}$.
 4. Find $\hat{\mathbf{x}}_{n+1} = \arg \max_{\mathbf{x} \in \mathbb{X}} \text{EI}(\mathbf{x}, f_{\min}^n, \hat{F}, \hat{\sigma})$.
 5. If $n = n_{\max}$ or $\{\max_{\mathbf{x} \in \mathbb{X}} \text{EI}\} < \varepsilon_{\text{EI}}$, then return f_{\min}^n as an optimal solution. Else, append $\hat{\mathbf{x}}_{n+1}$ to \mathcal{X}_n and $f(\hat{\mathbf{x}}_{n+1})$ to \mathbf{f}_n and go to Step 2 with $n \leftarrow n + 1$.
-

This iterative algorithm replaces the initial optimization problem (1) by the repeated optimization of a much easier-to-compute function called *Expected Improvement* (EI at Step 4), which is given (Schonlau, Welch, & Jones 1996) by

$$\begin{aligned} \text{EI}(\mathbf{x}, f_{\min}^n, \hat{F}, \hat{\sigma}) &= \left(f_{\min}^n - \hat{F}(\mathbf{x})\right) \Phi\left(\frac{f_{\min}^n - \hat{F}(\mathbf{x})}{\hat{\sigma}(\mathbf{x})}\right) \\ &\quad + \hat{\sigma}(\mathbf{x}) \phi\left(\frac{f_{\min}^n - \hat{F}(\mathbf{x})}{\hat{\sigma}(\mathbf{x})}\right), \end{aligned} \quad (7)$$

where ϕ and Φ are respectively the probability density and cumulative distribution functions of the normal distribution with zero mean and unit standard deviation. EI is simple and fast to evaluate, since it only involves the Kriging linear prediction (4) and standard deviation, trivially computed from the variance (6). It could thus be optimized at each step via an auxiliary algorithm to be chosen (DIRECT (Jones, Perttunen, & Stuckman 1993) in our experiments). Latin Hypercube Sampling (LHS) (Montgomery 2008) is used for initialization at Step 1, a usual heuristic being to draw ten points per dimension of \mathbb{X} . EGO

stops when the number of evaluations of $f(\cdot)$ becomes greater than the budget allotted n_{\max} , or when the expected improvement obtained at Step 4 gets lower than ε_{EI} . Variations of EGO can be found in (Sasena 2002, Huang, Allen, Notz, & Zeng 2006, Villemon-teix, Vazquez, & Walter 2009), and convergence results in (Vazquez & Bect 2010, Bull 2011).

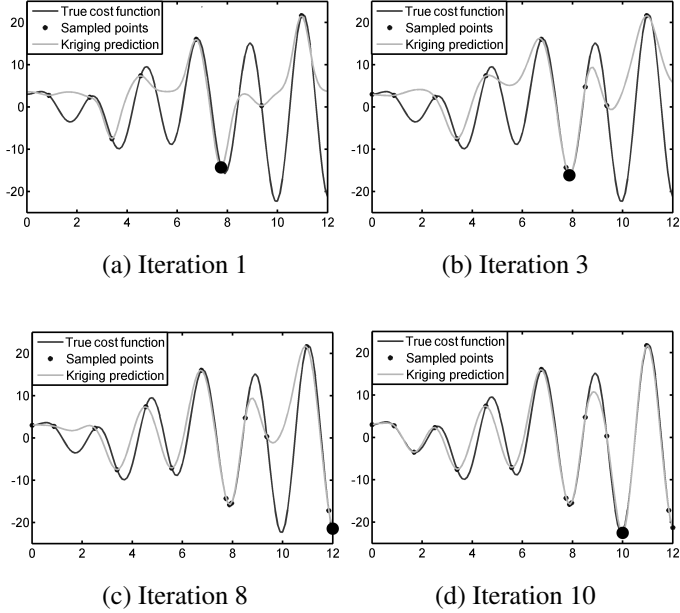


Figure 1: Minimization by EGO (big dot: current estimated global minimizer)

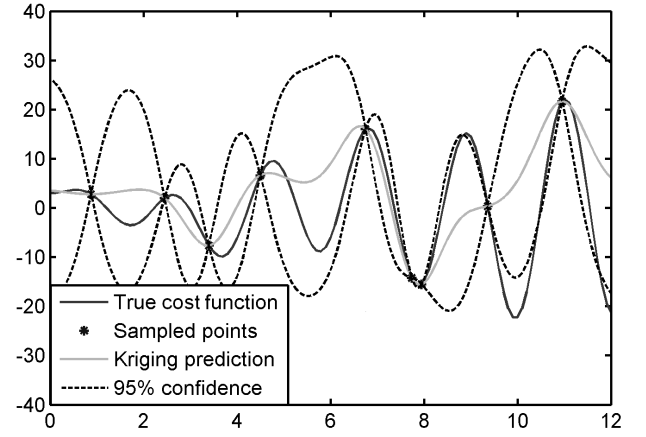
The potential of EGO is illustrated in Figure 1 for a one-dimensional test case with multiple local optimizers. The initial sampling consists of 8 points chosen randomly, which leads to an adverse situation where many local optimizers of the actual cost function have not been sampled. After a few iterations of EGO, the global optimum is nevertheless spotted. The Kriging interpolation has also improved with the sequential acquisition of new samples. Figure 2 displays the corresponding 95% confidence intervals, computed as $[\hat{F}(\mathbf{x}) - 2\hat{\sigma}(\mathbf{x}), \hat{F}(\mathbf{x}) + 2\hat{\sigma}(\mathbf{x})]$.

2.2 Black-box continuous minimax optimization

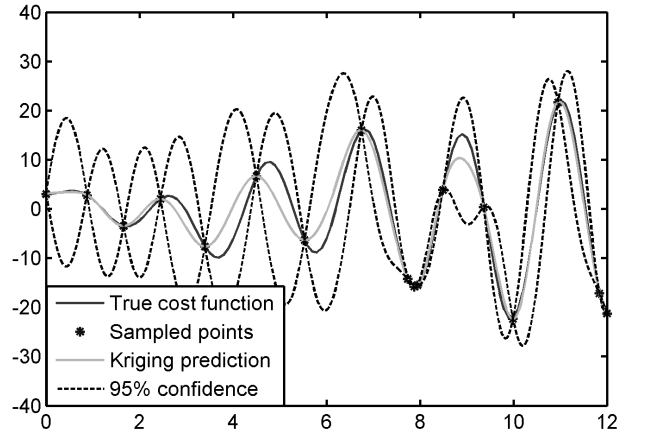
Design is now formalized as the optimization of a performance index y with respect to a vector \mathbf{x}_c of *control variables*. Uncertainty is modeled via a vector \mathbf{x}_e of *environmental variables* that can take any value in a known compact set and may have an adverse effect on performance. Optimal design then boils down to finding a feasible value of \mathbf{x}_c that optimizes y for the worst feasible value of \mathbf{x}_e . This can be written as the continuous minimax optimization problem

$$\{\hat{\mathbf{x}}_c, \hat{\mathbf{x}}_e\} = \arg \min_{\hat{\mathbf{x}}_c \in \mathbb{X}_c} \max_{\hat{\mathbf{x}}_e \in \mathbb{X}_e} y(\mathbf{x}_c, \mathbf{x}_e), \quad (8)$$

where $y(\mathbf{x}_c, \mathbf{x}_e)$ is evaluated through costly numerical simulations and where \mathbb{X}_c and \mathbb{X}_e are feasible spaces for \mathbf{x}_c and \mathbf{x}_e , assumed to be known compact sets.



(a) Iteration 2



(b) Iteration 10

Figure 2: Confidence intervals for Kriging prediction

This is a delicate issue, especially when the simulation budget is severely limited. Previous theoretical work on continuous minimax optimization has focused on the development of algorithms for functions with a closed-form expression, which is not assumed to be the case here. Few algorithms applicable to functions known only through numerical simulation have been reported. Most of them are based on evolutionary optimization (Parsopoulos & Vrahatis 2002, Viana, Kotinda, Rade, & Steffen Jr 2008, Cramer, Sudhoff, & Zivi 2009, Zhou & Zhang 2010, Lung & Dumitrescu 2011), which is usually extremely demanding in terms of function evaluations.

The procedure described in Algorithm 2 aims at finding an approximate minimax solution by iteratively relaxing the infinite set \mathbb{X}_e into a finite one \mathcal{R}_e . It has been shown in (Shimizu & Aiyoshi 1980) to converge to the minimax solution in a finite number of steps under realistic hypotheses.

Relaxation is achieved at Step 2, where the function to be minimized is the maximum of the performance index over the *finite* set \mathcal{R}_e . Steps 2 and 3 leave open the choice of the optimization algorithms to be employed. Since the performance index is evaluated via costly simulations, the algorithm should be able to cope with a restricted simulation budget.

Algorithm 2 MiniMax optimization via Relaxation

1. Pick $\mathbf{x}_c^{(1)} \in \mathbb{X}_c$, set $\mathcal{R}_c = \{\mathbf{x}_c^{(1)}\}$ and $i = 1$.
 2. Compute $\mathbf{x}_c^{(i)} = \arg \min_{\mathbf{x}_c \in \mathbb{X}_c} \left\{ \max_{\mathbf{x}_e \in \mathcal{R}_c} y(\mathbf{x}_c, \mathbf{x}_e) \right\}$
 3. Compute $\mathbf{x}_e^{(i+1)} = \arg \max_{\mathbf{x}_e \in \mathbb{X}_e} y(\mathbf{x}_c^{(i)}, \mathbf{x}_e)$
 4. If $y(\mathbf{x}_c^{(i)}, \mathbf{x}_e^{(i+1)}) - \max_{\mathbf{x}_e \in \mathcal{R}_c} y(\mathbf{x}_c^{(i)}, \mathbf{x}_e) < \varepsilon$ then return $\{\mathbf{x}_c^{(i)}, \mathbf{x}_e^{(i+1)}\}$ as an approximate solution to the initial minimax problem (8). Else, append $\mathbf{x}_e^{(i+1)}$ to \mathcal{R}_c , increment i by 1 and go to Step 2.
-

MiMaReK (Marzat, Walter, & Piet-Lahanier 2012) combines minimax optimization via relaxation with Kriging-based optimization, by using two independent Kriging models at Steps 2 and 3 of Algorithm 2. The first one depends only on \mathbf{x}_c , and interpolates the function $\max_{\mathbf{x}_e \in \mathcal{R}_c} \{y(\mathbf{x}_c, \mathbf{x}_e)\}$. The second one depends only on \mathbf{x}_e and interpolates $y(\mathbf{x}_c^{(i)}, \mathbf{x}_e)$. Two initial designs should thus be built (e.g., by LHS), one from \mathbb{X}_c and one from \mathbb{X}_e . To save computation time, they can be reused at each new call to Steps 2 and 3. This is especially useful at Step 2, where the computation of the optimized function requires to pick the maximum over all the elements \mathbf{x}_e in \mathcal{R}_c . Only one additional evaluation per sample in \mathbb{X}_c is then needed when the same design is used.

The parameters of the complete procedure are finally the stopping threshold ε and the parameters of the two EGO procedures, namely the budget of evaluations n_{\max} and stopping threshold ε_{EI} . These budget constraints are taken into account at each iteration of the global procedure, which means that at most $(\dim \mathcal{R}_c + 1) \cdot n_{\max}$ evaluations of the black-box function are allowed during one iteration of the main loop (i.e., the sequence of Steps 2, 3 and 4 of Algorithm 2). Note that the set \mathcal{R}_c is extended by one element at each iteration (Step 4), which implies that the number of evaluations grows linearly with the number of iterations of the main loop. Note that the relaxation procedure yields a suboptimal minimax solution even if it is interrupted before the threshold ε is reached, which may be used to limit the total number of iterations.

3 ROBUST DESIGN OF A VIBRATION ABSORBER

The optimal design of a vibration absorber for a structure with an uncertain forcing frequency is a classical benchmark problem, initially proposed in (Randall 1978). It can be formalized as a minimax optimization problem, for which various algorithms, ranging

from analytical optimization to evolutionary strategies, have already been employed (Pennestri 1998, Viana, Kotinda, Rade, & Steffen Jr 2008, Brown & Singh 2011). The results found in these papers are very similar, which make it possible to use them as reference solutions to assess the behavior of the procedure advocated in the present paper.

The system is described in Figure 3. A primary structure with mass m_1 is subjected to a sinusoidal force of amplitude X_0 and unknown frequency ω . The amplitude of the resulting harmonic motion of m_1 is denoted by X_1 . A smaller structure with mass m_2 is used to compensate for the oscillations generated by this disturbance through a viscous damping action. The design problem is to determine the characteristics of this damper so as to be robust to the worst case of forcing frequency.

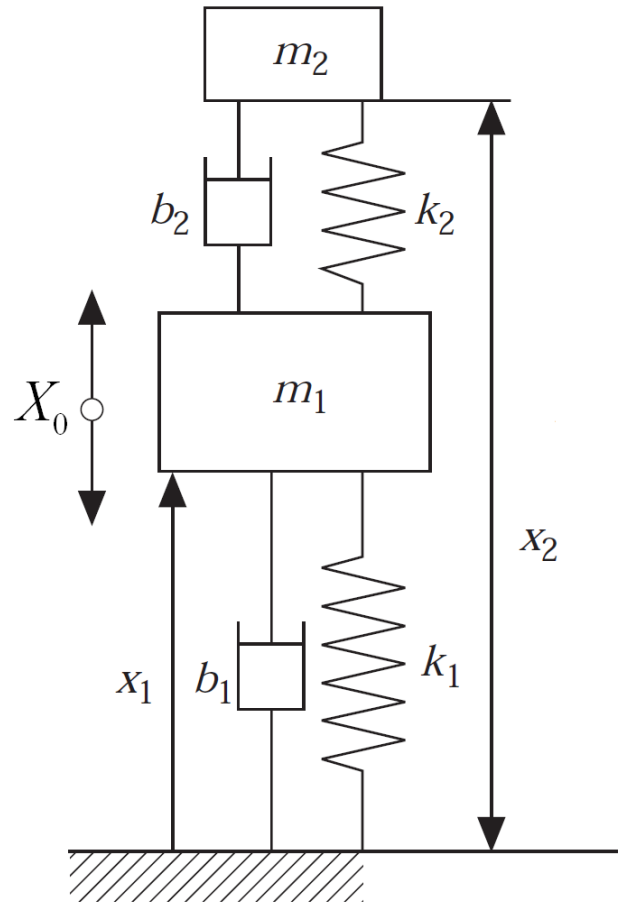


Figure 3: Vibration absorber

The performance index to be optimized is the normalized maximum displacement of the primary structure, which can be expressed (see (Randall 1978, Pennestri 1998)) as

$$y = \frac{k_1 X_1}{X_0} = \frac{1}{Z} \sqrt{\left(1 - \frac{\beta^2}{T^2}\right)^2 + 4 \left(\frac{\zeta_2 \beta}{T}\right)^2}, \quad (9)$$

where

$$Z^2 = \left[\frac{\beta^2}{T^2} (\beta^2 - 1) - \beta^2 (1 + \mu) - 4 \frac{\zeta_1 \zeta_2 \beta^2}{T} + 1 \right]^2 + 4 \left[\frac{\zeta_1 \beta^3}{T^2} + \frac{\zeta_2 \beta^3 (1 + \mu) - \zeta_2 \beta}{T} - \zeta_1 \beta \right]^2. \quad (10)$$

These definitions involve the reduced variables

$$\omega_i = \sqrt{\frac{k_i}{m_i}}, \quad \zeta_i = \frac{b_i}{2\sqrt{k_i m_i}}, \quad \beta = \frac{\omega}{\omega_1}, \quad T = \frac{\omega_2}{\omega_1}, \quad \mu = \frac{m_2}{m_1}. \quad (11)$$

The parameters of the main system are fixed to $\mu = 0.1$, $\zeta_1 = 0.1$ and $\omega_1 = 100$. The control variables to be determined are ζ_2 and T , while the environmental variable to the effect of which the optimization should be robust is β . The design problem can thus be written as the search for

$$\left\{ \widehat{\zeta}_2, \widehat{T}, \widehat{\beta} \right\} = \min_{\zeta_2, T} \max_{\beta} y. \quad (12)$$

Following (Randall 1978, Pennestri 1998, Brown & Singh 2011), we assume that $\zeta_2 \in [0, 1]$, $T \in [0, 2]$ and $\beta \in [0, 2.5]$. Note that, in spite of the analytical character of the performance index, it is considered here as a black-box.

The results obtained with our procedure (640 evaluations of the function (9) were required) are indicated in Table 1, together with those reported in previous works. The algorithm was tuned with the parameters $\varepsilon = 10^{-4}$, $\varepsilon_{EI} = 10^{-6}$ and $n_{\max} = 20$ for both EGO algorithms. Figure 4.a shows the behavior of the performance index for the resulting tuning on the range of the environmental variable, while Figure 4.b compares our result with those from the literature around the location of the worst case. An adequate solution is thus found on this benchmark with the proposed strategy. For comparison, a similar design problem has been addressed in (Viana, Kotinda, Rade, & Steffen Jr 2008) using ant colony optimization, and required more than 10^4 evaluations. In (Randall 1978, Pennestri 1998, Brown & Singh 2011), the results were obtained based on the analytical properties of the performance index, which makes it difficult to extend these approaches to more complicated mechanical designs. MiMaReK, on the other hand, can deal with, e.g., multiphysics finite-element models with complicated boundary conditions.

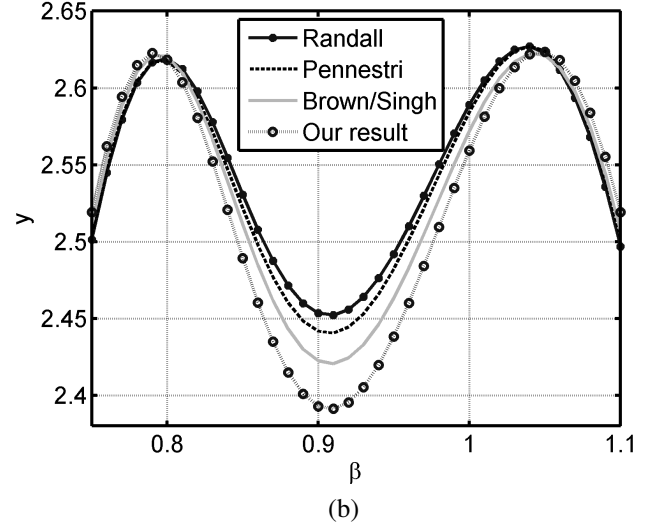
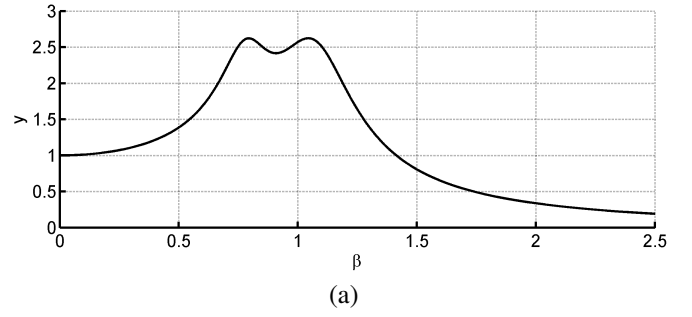


Figure 4: Performance with the estimated optimal design on the range of the environmental variable (a) and zoom near the worst-case value (b)

Table 1: Approximate minimax result obtained, compared to references

	$\widehat{\zeta}_2$	\widehat{T}	$\widehat{\beta}$	y_{\max}
Randall	0.204	0.861	1.038	2.6271
Pennestri	0.202	0.861	1.04	2.6272
Brown & Singh	0.1986	0.8619	1.043	2.6227
Our result	0.1978	0.8619	1.044	2.6229

4 CONCLUSIONS AND PERSPECTIVES

By combining EGO, a well-known global optimization procedure based on Kriging, with a relaxation procedure, one can handle complicated problems of optimal design under uncertainty. The performance index may take the form of a black-box function that can only be studied through costly numerical evaluations. A classical benchmark in mechanics has been used to compare the results provided by the new methodology with those of the literature. For the time being, constraints can only be incorporated in the definitions of \mathbb{X}_c and \mathbb{X}_e . The case of more complicated and possibly uncertain constraints remains to be investigated.

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