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Optimization Under Uncertainty Using Derivatives and Kriging Surrogate Models

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Abstract: In this article the use of optimizations and surrogate models for the propagation of mixed aleatory/epistemic uncertainties in a robust optimization problem is demonstrated. Specifically, this work focuses on strategies applicable for models where input parameters can be divided into a set of variables containing only aleatory uncertainties and a set with only epistemic uncertainties. With the input parameters divided in this way, uncertainty due to the epistemic variables is propagated via a constrained optimization approach, while the uncertainty due to aleatory variables is propagated via sampling. A statistics-of-intervals approach is proposed in which the constrained optimization results are treated as a random variable and multiple optimizations are performed to quantify the aleatory uncertainty. In order to reduce the total number of optimizations required, a Kriging surrogate is employed to model the variation of the optimization results with respect to the aleatory variables, and exhaustive sampling is performed on this surrogate to determine the desired statistics for each robust optimization iteration. This approach makes robust optimization under mixed aleatory/epistemic uncertainty possible while at the same time keeping the computational cost for these types of problems manageable.

Keywords: Optimization Under Uncertainty, Robust Design Optimization, Aleatory and Epistemic Uncertainties, Kriging Surrogate Model, Gradient-based Optimization.

1 Introduction and Motivation

Many real-world problems involve input data that is noisy or uncertain, due to measurement or modeling errors, approximate modeling parameters [1], manufacturing tolerances [2], in-service wear-and-tear, or simply the unavailability of information at the time of the decision [3]. These imprecise or unknown inputs are important in the design process and need to be quantified in some fashion. To this end, uncertainty quantification (UQ) has emerged as an important area in modern computational engineering. Today, it is no longer sufficient to predict specific objectives using a particular physical model with deterministic inputs. Rather, a probability distribution function (PDF) or interval bound of the simulation objectives is required depending on whether aleatory or epistemic uncertainties are involved [4]. Uncertainty characterized by inherent randomness is called aleatory uncertainty (or type A, or irreducible uncertainty). In contrast, epistemic uncertainty (or type B, or reducible uncertainty) represents a lack of knowledge about the appropriate value to use for a quantity [5]. Epistemic uncertainty may or may not be modeled probabilistically and regulatory agencies and design teams are increasingly being asked to specifically characterize and quantify epistemic uncertainty and separate its effect from that of aleatory uncertainty [6].

Deterministic optimization tools are also widely used in engineering practice, however, engineering designs do not operate exactly at their design point due to physical variability in the environment. These small variations can deteriorate the performance of deterministically optimized designs. It is, therefore, necessary to account for these uncertainties in the optimization process using optimization under uncertainty (OUU) techniques, which implies that UQ is used in the optimization loop instead of a deterministic simulation. While there are some post-optimality criteria that provide insight into the sensitivity of an optimal design to parameter perturbations (for example, gradients and Hessians), these criteria only provide a local measure of sensitivity at the optimal design point. In many engineering system design applications, broader measures of objective and constraint function sensitivity are often needed. Statistical measures, such as mean value, standard deviation, and probability of failure can provide such information. Thus, it is a natural extension for engineers to incorporate statistical measures directly into the design optimization process. Beginning with the seminal works of Beale [7], Dantzig [8], and Tintner [9], OUU has experienced rapid development in both theory and algorithms. Dantzig considers planning under uncertainty as one of the most important open problems in optimization [10, 11]. Good overviews of the state of the art in the field of OUU are provided by Beyera *et al.* [12], Sahinidis [10], Giunta *et al.* [13] and Li [14].

An important subfield in OUU is robust optimization (RO) [15, 16] which can be divided into robust design based methods and reliability-based methods [17]. Robust design improves the quality of a product by minimizing the effect of the causes of variation without eliminating these causes. The objective here is to optimize the mean performance and minimize its variation, while maintaining feasibility with probabilistic constraints; hence robust design concentrates on the probability distribution near the mean values. The ability to identify and catalog overly conservative design margins resulting from applying safety factors on top of other safety factors, for example, is an important application for robust design, which is being increasingly viewed as an enabling technology for design of aerospace, civil, and automotive structures subject to uncertainty [18, 19, 20, 21, 22]. The reliability-based methods, on the other hand, are predominantly used for risk analysis by computing the probability of failure of a system. Thus, reliability approaches concentrate on the rare events at the tails of the probability distribution.

A mixed aleatory/epistemic UQ typically relies on a nested sampling strategy (or second-order probability). Although the required number of samples grows extremely fast, these strategies are conceptually easy to understand and are capable of separating the effects of each type of uncertainty [23, 24]. For nested strategies, samples are first drawn from the epistemic variables; and for each set of epistemic variables, the distribution of the output due to the aleatory variables is determined using sampling of the aleatory variables. The simplest approach for this is the Monte-Carlo (MC) method [25] for which a large number of independent calculations need to be computed. The number of samples required for the epistemic uncertainty grows exponentially fast with the number of epistemic variables [23], which rapidly results in prohibitively high computational cost, especially for complex high-fidelity physics-based simulations. To alleviate some of the cost, surrogates can be created as a function of all variables and samples extracted according to a nested strategy. For relatively low dimensions, this strategy can be effective and, when combined with gradient-enhancement, could be applied to problems of moderate dimension [26]. However, once the number of epistemic variables increases sufficiently, surrogate-based approaches will again become prohibitively expensive as the required number of training points increases exponentially fast for an accurate surrogate model known as "curse of dimensionality". In order to address this concern, combinations of sampling and optimization approaches have been explored [24, 27]. The idea is that for mixed aleatory/epistemic problems, the goal of the uncertainty quantification is to produce a region in which the function is contained with a specific level of confidence, known as a P-Box [23]. The bounds of the confidence interval of the output distribution must itself be an interval in order to account for the epistemic uncertainties. Because only the bounds of this box are required, the sampling with respect to the epistemic variables can be replaced by one maximization and one minimization problem.

In principle, these mixed sampling/optimization approaches may be posed in two ways: determining intervals of statistics and determining statistics of intervals. The first approach can be viewed as an optimization under uncertainty problem with the metric of the optimization defined as a relevant statistic of the aleatory distribution, such as the mean and variance, bounds on a confidence interval, or a reliability index [28, 24]. For each step in the optimization, the aleatory uncertainty is quantified, and the relevant statistic of the distribution is calculated and used as the objective function for the optimization. In the statistics-of-interval approach, on the other hand, an optimization problem can be posed for each set of aleatory variables, and repeated optimization evaluations can be used to determine the relevant statistics of the interval [27]. Using adjoint capabilities [29, 30] gradient-based optimization methods can be used, assuming that the global extrema in the epistemic design space can be found this way, reducing the cost of each optimization and ensuring very good scaling as the number of epistemic variables increases. To reduce the number of required optimizations for low statistical errors, a surrogate model of the optimization results can be constructed with respect to the aleatory variables which can then be sampled exhaustively, ensuring that fewer optimizations are required to characterize the statistics of the interval accurately.

The outline of this paper is as follows. Section 2 describes the employed OUU approach for mixed aleatory/epistemic uncertainties in detail. Application results of the presented approach are given in Section 3 and Section 4 concludes this paper.

2 Optimization Under Uncertainty With Mixed Aleatory/Epistemic Uncertainty

A conventional constrained optimization problem for an objective function, J, that is a function of input variables, D, state variables, $q(D)$, and simulation outputs, $f(D) = F(q(D), D)$, can be written as

$$\begin{array}{lrcl} \min\limits_{D} & J & = & J(f, q, D) \\ s.t. & 0 & = & R(q, D) \\ & 0 & \leq & g(f, q, D). \end{array} \tag{1}$$

Here, the state equation residuals, R, are expressed as an equality constraint, and other system constraints, g, are represented as inequality constraints. In the case where the input variables are precisely known, all functions of D are deterministic. However, given uncertainties in D all functions in equation (1) can no longer be treated deterministically.

For this work, the design variables are assumed to have only aleatory or only epistemic uncertainty. Let α represent the variables associated with aleatory uncertainties and β represent variables with epistemic uncertainties. The design variables $D = (D_\alpha, D_\beta)$ are considered to be either the mean values of aleatory uncertainties which are assumed to be statistically independent and normally distributed with $\alpha \sim \mathcal{N}(D_\alpha, \sigma_D^2)$, or the midpoint of bounds on epistemic uncertainties with $\beta \in I(D)$ where $I(D) = [D_\beta - s_D, D_\beta + s_D]$. These are reasonable and realistic assumptions for geometric shape variables subject to manufacturing tolerances, or for input flow conditions subject to random fluctuations, or other such input variables. One could also derive equations for correlated and/or non-normally distributed aleatory variables; however, the analysis and resulting equations become more complex [31] and are beyond the scope of this paper.

In order to account for both types of uncertainty, sampling is performed for the aleatory variables while optimization is performed over the epistemic variables as described in the introduction. Let $f(D) = f(\alpha, \beta)$ represent the output of interest of a simulation then the optimization can be represented mathematically as follows

$$f_{max}(\alpha) = \max_{\beta \in I(D)} f(\alpha, \beta) \tag{2}$$

$$f_{min}(\alpha) = \min_{\beta \in I(D)} f(\alpha, \beta). \tag{3}$$

The functional outputs f_{max} and f_{min} can now be treated as random variables, since the inputs α are random variables with associated distributions. In the remainder of this paper the subscript *ext* (for extrema) will be used as a placeholder for either *max* or *min*. To characterize the probability distribution of f_{ext}, one must extract repeated samples of f_{ext} according to the underlying PDF of α. Each sampling entails solving the appropriate optimization problem, equation (2) or (3), for the specified sample of α. For these optimizations an L-BFGS [32, 33] algorithm that can utilize function and gradient information is used in this work, thereby reducing the cost of each optimization and ensuring excellent scaling in the number of variables with epistemic uncertainties.

Nonetheless, because of the expense of these optimizations, strategies to reduce the number of samples and thus the computational cost associated with sampling must be employed. For this work, a surrogate is created for f_{ext} as a function of the aleatory variables, which enables the extraction of a large number of samples in order to obtain accurate statistics for very low computational cost. Because the number of aleatory variables used here is relatively small, the required number of training points for an accurate surrogate is small, necessitating only a small amount of optimizations. Because the optimization results are viewed as general random variables, any surrogate can be used to represent the aleatory dependence of the variables. A

Kriging surrogate model is employed in this work. The details of the construction of this particular Kriging model, which can utilize gradient and Hessian information and employs a dynamic training point selection, is described in previously published papers [34, 35, 36, 37, 38]. The center of the Kriging domain is prescribed by the mean value of α, D_α, and the boundary is taken to be two standard deviations σ_D away in all aleatory input dimensions. This implies that for the normally distributed input variables α more than 97 % of all MC samples fall within the Kriging domain and the less accurate extrapolation capabilities of the Kriging surrogate model only need to be used for a small fraction of the samples. Since the purpose of this article is a robust optimization and not the accurate prediction of the tail statistics this approach leads to very reasonable results as demonstrated in Section 3.

The deterministic optimization problem (1) can now be rewritten. The objective function can be written in terms of mean values of the functional outputs, $\bar{f}_{ext}$, and typically also becomes a function of the variances, $\mathrm{Var}_{f_{ext}}$, for example, for robust design optimizations objective functions are typically of the form given by equation (5). The state equation residual equality constraint, R, needs to be satisfied for all values of α and β. The inequality constraints can be cast into a probabilistic statement such that the probability that the constraints are satisfied is greater than or equal to a desired or specified probability, P_k. This statement can be transformed [39] into a constraint involving mean values and standard deviations (also called moment matching formulation [40]) and the entire OUU problem can be expressed as [31, 41]

$$\begin{array}{lrcl} \min\limits_{\alpha,\beta} & \mathcal{J} & = & \mathcal{J}(\bar{f}_{ext}, \mathrm{Var}_{f_{ext}}, q, \alpha, \beta) \\ s.t. & 0 & = & R(q,\alpha,\beta) \\ & 0 & \leq & g(\bar{f}_{ext}, q, \alpha, \beta) - k\sigma_g, \end{array} \tag{4}$$

where k is the number of standard deviations, σ_g, that the constraint g must be displaced in order to achieve P_k. A simple way to define an objective function for robust design optimization problems is to linearly combine the mean and variance of the simulation output using some user specified weights w_i

$$\mathcal{J} = w_1 \bar{f}_{ext} + w_2 \,\mathrm{Var}_{f_{ext}}. \tag{5}$$

One could even treat this as a multi-objective optimization problem [42, 43, 44] and use well-known techniques to determine the Pareto frontier of this robust design optimization problem.

The software package Ipopt (Interior Point OPTimizer) [45] for large-scale nonlinear optimization with constraints is used for the solution of the OUU problem given by equation (4). This package also allows users to impose bound constraints on the design variables. The required gradient information is obtained as follows. The gradient of the objective function, $\mathcal{J}$, given by equation (5) with respect to design variables associated with aleatory uncertainties is given by

$$\frac{d\mathcal{J}}{dD_\alpha} = \frac{\partial \mathcal{J}}{\partial \bar{f}_{ext}} \frac{d\bar{f}_{ext}}{dD_\alpha} + \frac{\partial \mathcal{J}}{\partial \mathrm{Var}_{f_{ext}}} \frac{d\mathrm{Var}_{f_{ext}}}{dD_\alpha} \tag{6}$$

where it is straightforward to calculate $\frac{\partial \mathcal{J}}{\partial \bar{f}_{ext}}$ and $\frac{\partial \mathcal{J}}{\partial \mathrm{Var}_{f_{ext}}}$. A Kriging surrogate is built to calculate $\bar{f}_{ext}$ and $\mathrm{Var}_{f_{ext}}$ using N training points for each of which one has to calculate f_{ext} by solving an optimization problem as given by equation (2) or (3). This Kriging surrogate is then sampled extensively $\tilde{N}$ times for inputs α^k, $k = 1, \ldots, \tilde{N}$ chosen based on their underlying probability distribution function [in this case $\alpha \sim D_\alpha + \sigma_D Z$ with $Z \sim \mathcal{N}(0,1)$] with the Kriging predictions represented by $\hat{f}_{ext}(\alpha^k)$. The mean of the simulation output can then be approximated by

$$\bar{f}_{ext} \approx \frac{1}{\tilde{N}} \sum_{k=1}^{\tilde{N}} \hat{f}_{ext}(\alpha^k) \tag{7}$$

and the derivative can be approximated at the same time with little computational overhead via [46]

$$\frac{d\bar{f}_{ext}}{dD_\alpha} \approx \frac{1}{\tilde{N}} \sum_{k=1}^{\tilde{N}} \frac{d\hat{f}_{ext}(\alpha^k)}{d\alpha^k} \frac{d\alpha^k}{dD_\alpha} = \frac{1}{\tilde{N}} \sum_{k=1}^{\tilde{N}} \frac{d\hat{f}_{ext}(\alpha^k)}{d\alpha^k}, \tag{8}$$

where it is straightforward to calculate $\frac{d\hat{f}_{ext}(\alpha^k)}{d\alpha^k}$ from the Kriging surrogate model [47, 46]. Similarly, the variance and its derivative can be approximated as

$$\mathrm{Var}_{f_{ext}} \approx \left(\frac{1}{\tilde{N}}\sum_{k=1}^{\tilde{N}} \hat{f}^2_{ext}(\alpha^k)\right) - \bar{f}^2_{ext} \tag{9}$$

$$\frac{d\mathrm{Var}_{f_{ext}}}{dD_\alpha} \approx \left(\frac{2}{\tilde{N}}\sum_{k=1}^{\tilde{N}} \hat{f}_{ext}(\alpha^k)\frac{d\hat{f}_{ext}(\alpha^k)}{d\alpha^k}\right) - 2\bar{f}_{ext}\frac{d\bar{f}_{ext}}{dD_\alpha}. \tag{10}$$

The gradient of the objective function, $\mathcal{J}$, with respect to design variables associated with epistemic uncertainties is also given by equation (6) if D_α is replaced with D_β. However, it is not trivial to calculate $\frac{d\bar{f}_{ext}}{dD_\beta}$ and $\frac{d\mathrm{Var}_{f_{ext}}}{dD_\beta}$ where D_β represents midpoints of epistemic uncertainty intervals since moving the midpoint will lead, in general, to different extrema for the training points and thus to a different Kriging surrogate which when sampled leads to different values of $\bar{f}_{ext}$ and $\mathrm{Var}_{f_{ext}}$. In contrast, the aleatory gradient was easy to obtain since one only has to take into account how the sample points change while being able to reuse the same Kriging surrogate. The approach for now is to use the approximations

$$\frac{d\bar{f}_{ext}}{dD_\beta} \approx \left.\frac{df_{ext}}{dD_\beta}\right|_{D_\alpha} \qquad \frac{d\mathrm{Var}_{f_{ext}}}{dD_\beta} \approx 0 \tag{11}$$

that is the derivative of f_{ext} with respect to D_β at the mean values of the aleatory uncertainty variables α. This derivative is, in general, non-zero since for the epistemic optimizations the extreme value is typically encountered on the interval bound. The variances for the problems studied in this paper are much smaller than the mean values which allows the neglection of $\frac{d\mathrm{Var}_{f_{ext}}}{dD_\beta}$. The following section will demonstrate that the presented approach can lead to successful robust optimizations.

3 Robust Optimization of a Transonic Airfoil

The steady inviscid flow over a transonic NACA 0012 airfoil is considered as a flow example which is described in more detail in Mani and Mavriplis [48, 49]. The computational mesh has about 20,000 triangular elements. The non-dimensionalized pressure contours for an angle of attack of 1.25 degrees and a free-stream Mach number of 0.755 are shown in Figure 1 leading to a lift and drag coefficient of $C_l = 0.268$ and $C_d = 0.00521$, respectively.

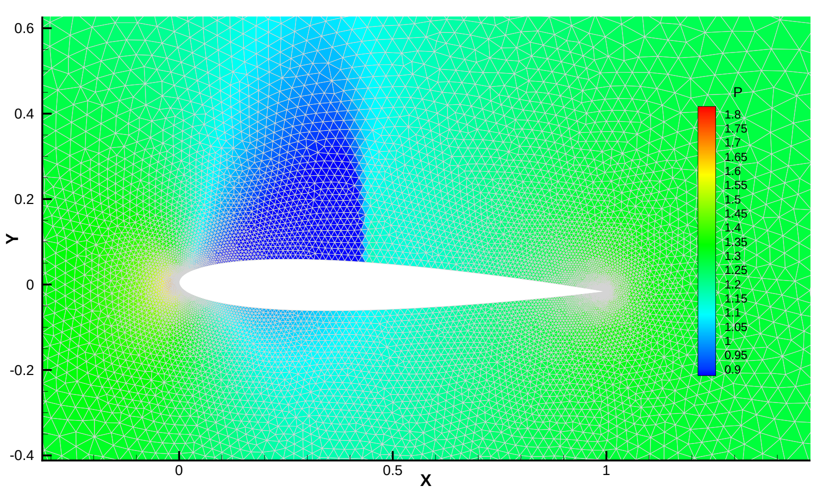

Figure 1: Non-dimensionalized pressure contours and mesh for angle of attack of 1.25 degrees and a free-stream Mach number of 0.755.

In order to perform a robust lift-constrained drag minimization under mixed aleatory/epistemic uncertainty one shape design variable on the upper surface and one on the lower surface which control the magnitude of Hicks-Henne sine bump functions [50] are allowed to vary. The resulting deformation of the mesh is calculated via a linear tension spring analogy [51, 48]. Both shape design variables are assumed to have epistemic uncertainties due to manufacturing tolerances. A zero value corresponds to the original NACA 0012 airfoil and $s_{D_{u,l}}$ is taken to be 0.005. Figure 2 shows the original NACA 0012 airfoil and the airfoils resulting from design variable values of ± 0.005. The angle of attack and free-stream Mach number

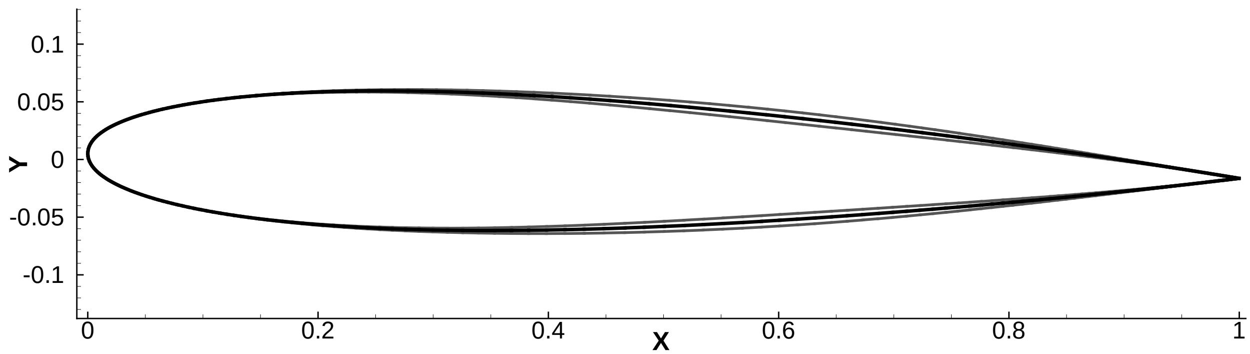

Figure 2: NACA 0012 airfoil (black) and airfoils resulting from design variable values of ± 0.005 (gray).

are assumed to have aleatory uncertainties which are both modeled with normal distributions. The mean values are given by the design variable values, D_{AoA} and D_M, and the standard deviations are prescribed as $\sigma_{D_{AoA}} = 0.1$ and $\sigma_{D_M} = 0.01$, respectively. A robust optimization problem as given by equation (4) can be posed by using

$$\mathcal{J} := \bar{C}_{d_{max}} + \sigma^2_{C_{d_{max}}} \tag{12}$$

as objective function and

$$g := \bar{C}_{l_{min}} - C_l^* \qquad \sigma_g := \sigma_{C_{l_{min}}} \tag{13}$$

as inequality constraint to maintain a target lift coefficient of $C_l^* = 0.6$. Box constraints on all four design variables are used to prevent the generation of invalid geometries from the mesh movement algorithm and solver robustness issues. They are chosen as follows:

$$D_{u,l} \in [-0.025, 0.025] \qquad D_{AoA} \in [0, 1.85] \qquad D_M \in [0.6, 0.78] \tag{14}$$

Because of the expense of the CFD simulation, the exact mixed aleatory/epistemic uncertainty results can not easily be calculated through either nested sampling or exhaustive sampling of optimization results. In order to provide validation for the OUU framework with mixed aleatory/epistemic uncertainty the uncertainty propagations of aleatory and epistemic variables are validated separately against exhaustive sampling. First, optimization is used to propagate the epistemic uncertainties within the problem. For this test, the aleatory variables are fixed at their mean value taken to be $D_{AoA} = 1.25$ and $D_M = 0.755$, and optimization is performed over the epistemic variables $D_u = D_l = 0$ to determine the associated intervals for the output functions of interest. The interval produced through optimization is validated by performing Latin hypercube sampling (with 500 samples plus the corners of the domain) over the epistemic variables, again with the aleatory variables fixed at their mean values. The excellent agreement can be seen in Table 1. Note that the optimizations only took a few function and gradient evaluation each.

Table 1: Validation of epistemic uncertainty propagation.

Method	$C_{l_{min}}$	$C_{l_{max}}$	$C_{d_{min}}$	$C_{d_{max}}$
Optimization	0.195	0.344	$3.56 \cdot 10^{-3}$	$6.90 \cdot 10^{-3}$
LHS Sampling	0.195	0.344	$3.56 \cdot 10^{-3}$	$6.90 \cdot 10^{-3}$

With the optimization portion of the method validated, the ability of the Kriging surrogate model to capture the aleatory variation of the output functions of interest is tested next. For this test, the original NACA 0012 airfoil is used (i.e. no epistemic uncertainty), and sampling from Kriging surrogates (build from a varying number of training points, N) is performed over the aleatory variables $D_{AoA} = 1.25$ and $D_M = 0.755$, respectively. In order to provide validation data, full non-linear MC (NLMC) sampling is performed over the aleatory variables, and both distributions are characterized by calculating statistics of interest using the same samples. For a reasonable trade-off between acquiring accurate statistics and computational cost for the NLMC, 3,000 samples are used. Because the epistemic variables for this test are fixed, each training point for the Kriging or sample point for the NLMC requires only a single CFD simulation. A summary of these comparisons can be found in Table 2.

Table 2: Comparison of NLMC and Kriging aleatory uncertainty propagation.

Method	$\bar{C}_l$	σ_{C_l}	$\bar{C}_d$	$\sigma^2_{C_d}$
NLMC ($\tilde{N} = 3000$)	0.269	$2.3 \cdot 10^{-2}$	$5.54 \cdot 10^{-3}$	$6.1 \cdot 10^{-6}$
Kriging ($N = 5$)	0.270	$2.2 \cdot 10^{-2}$	$5.65 \cdot 10^{-3}$	$7.5 \cdot 10^{-6}$
Kriging ($N = 13$)	0.269	$2.4 \cdot 10^{-2}$	$5.53 \cdot 10^{-3}$	$6.1 \cdot 10^{-6}$
Kriging ($N = 19$)	0.269	$2.3 \cdot 10^{-2}$	$5.54 \cdot 10^{-3}$	$6.1 \cdot 10^{-6}$

The Kriging model constructed from thirteen training points yields reasonable results for a fraction of the cost of a full NLMC simulation. Thus, all the required Kriging response surfaces for the actual robust optimization runs are constructed from thirteen training points and the sampling is performed using $\tilde{N} = 10^5$ latin hypercube samples to keep the statistical error small. Lastly, in Table 3 a comparison of NLMC and Kriging predictions is presented using the same 3,000 samples of optimization results for the initial airfoil and flow conditions ($D_u = D_l = 0$, $D_{AoA} = 1.25$ and $D_M = 0.755$) which demonstrates the good quality of the predictions of the proposed approach for statistics of the lift and drag coefficients.

Table 3: Comparison of NLMC and Kriging predictions for the initial guess.

	$\bar{C}_{l_{min}}$	$\sigma_{C_{l_{min}}}$	$\bar{C}_{d_{max}}$	$\sigma^2_{C_{d_{max}}}$
NLMC (3000 optimizations)	0.195	$2.1 \cdot 10^{-2}$	$7.22 \cdot 10^{-3}$	$7.9 \cdot 10^{-6}$
Kriging (13 optimizations)	0.195	$2.1 \cdot 10^{-2}$	$7.22 \cdot 10^{-3}$	$7.9 \cdot 10^{-6}$

Using the presented framework for the entire robust optimization gives the results presented in Table 4. The number of required optimization iterations for convergence (norm of gradient less than 10^{-4}) varies between 12 to 22 for all the presented cases.

Table 4: Robust optimization results with two shape design variables.

k	P_k	$\bar{C}_{d_{max}}$	$\sigma^2_{C_{d_{max}}}$	$\bar{C}_{l_{min}}$	$\sigma_{C_{l_{min}}}$	D_u	D_l	D_{AoA}	D_M
0	0.5000	$7.94 \cdot 10^{-3}$	$8.1 \cdot 10^{-6}$	0.600	$3.1 \cdot 10^{-2}$	$2.50 \cdot 10^{-2}$	$2.43 \cdot 10^{-2}$	1.85	0.711
1	0.8413	$9.95 \cdot 10^{-3}$	$1.1 \cdot 10^{-5}$	0.631	$3.4 \cdot 10^{-2}$	$2.50 \cdot 10^{-2}$	$2.28 \cdot 10^{-2}$	1.85	0.730
2	0.9772	$1.36 \cdot 10^{-2}$	$1.0 \cdot 10^{-5}$	0.657	$2.3 \cdot 10^{-2}$	$2.49 \cdot 10^{-2}$	$2.40 \cdot 10^{-2}$	1.84	0.736
Deterministic		$1.36 \cdot 10^{-3}$	-	0.600	-	$1.76 \cdot 10^{-2}$	$2.06 \cdot 10^{-2}$	1.58	0.734

One can see that the average drag increases as the desired probability, P_k, of maintaining the target lift coefficient of $C_l^* = 0.6$ is increased. The principal mechanism of achieving this higher probability is to increase the mean Mach number. Note that a deterministic lift-constrained drag minimization yields a minimal drag of $C_d = 1.36 \cdot 10^{-3}$ at a Mach number of 0.734 and a lower angle of attack of 1.58 degrees. In Table 5 a comparison of NLMC and Kriging predictions using the same 3,000 samples for the optimal design with $k = 1$ is presented which demonstrates the quality of the predictions for statistics of the lift and drag coefficients.

The original NACA 0012, the deterministically and robustly ($k = 2$) optimized airfoils are all shown in Figure 3. One can see that the robustly optimized airfoil looks different from the deterministically optimized one especially along the lower surface.

Table 5: Comparison of NLMC and Kriging predictions for the optimal design obtained for $k = 1$.

	$\bar{C}_{d_{max}}$	$\sigma^2_{C_{d_{max}}}$	$\bar{C}_{l_{min}}$	$\sigma_{C_{l_{min}}}$
NLMC (3000 optimizations)	$9.95 \cdot 10^{-3}$	$1.0 \cdot 10^{-5}$	0.636	$4.0 \cdot 10^{-2}$
Kriging (13 optimizations) ($\tilde{N} = 3000$)	$1.02 \cdot 10^{-2}$	$4.9 \cdot 10^{-6}$	0.634	$3.3 \cdot 10^{-2}$
Kriging (13 optimizations) ($\tilde{N} = 10^5$)	$9.95 \cdot 10^{-3}$	$1.1 \cdot 10^{-5}$	0.631	$3.4 \cdot 10^{-2}$

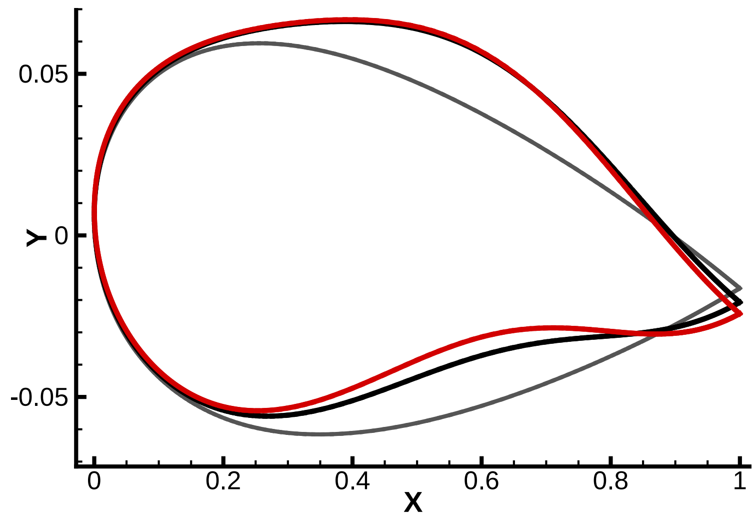

Figure 3: The original NACA 0012 at $\alpha = 1.25$ (gray) as well as the deterministically (black), and robustly ($k = 2$, red) optimized airfoils.

In order to demonstrate the scalability of the framework the number of epistemic design variables is increased from two to six. Therefore, three shape design variables are placed on the upper surface and three on the lower surface (at 40%, 60%, and 80% chord) and Figure 4 shows the original NACA 0012 airfoil and the airfoils resulting from perturbations of all six shape design variables of ± 0.005. The box constraints to

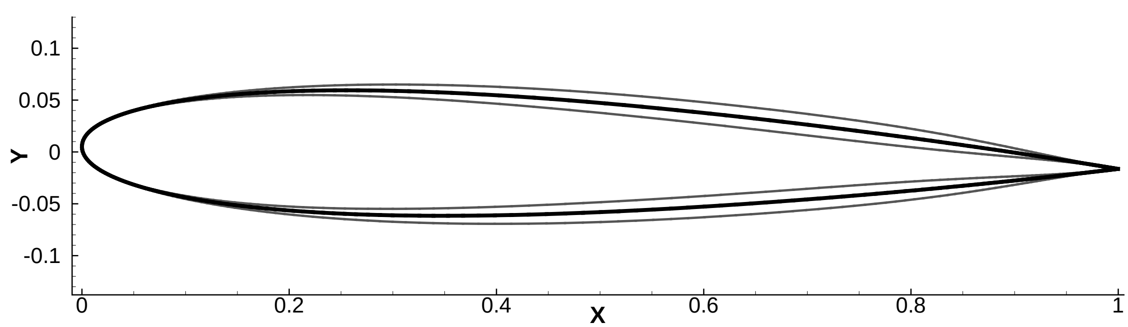

Figure 4: The NACA 0012 airfoil (in black) and airfoils resulting from perturbations of ± 0.005 (in gray).

prevent invalid meshes and flow convergence issues are as follows:

$$D_{1,6} \in [-0.01, 0.01] \qquad D_{2-5} \in [-0.02, 0.02] \qquad D_{AoA} \in [0, 1.85] \qquad D_M \in [0.6, 0.78] \tag{15}$$

where $D_{1,6}$ are the shape design variables closest to the trailing edge on the lower and upper surface, respectively. The robust optimization results are presented in Table 6. The number of required optimization iterations for convergence (again norm of gradient less than 10^{-4}) varies between 9 to 27 for all the presented cases. Again, the average drag and mean Mach number increase as the desired probability, P_k, of maintaining

Table 6: Robust optimization results with six shape design variables.

k	P_k	$\bar{C}_{d_{max}}$	$\sigma^2_{C_{d_{max}}}$	$\bar{C}_{l_{min}}$	$\sigma_{C_{l_{min}}}$	D_{AoA}	D_M
0	0.5000	$2.75 \cdot 10^{-3}$	$2.0 \cdot 10^{-8}$	0.600	$1.8 \cdot 10^{-2}$	1.75	0.600
1	0.8413	$2.87 \cdot 10^{-3}$	$2.3 \cdot 10^{-8}$	0.618	$1.8 \cdot 10^{-2}$	1.85	0.602
2	0.9772	$3.28 \cdot 10^{-3}$	$2.0 \cdot 10^{-7}$	0.640	$2.0 \cdot 10^{-2}$	1.85	0.623
3	0.9986	$5.60 \cdot 10^{-3}$	$5.5 \cdot 10^{-6}$	0.666	$2.2 \cdot 10^{-2}$	1.85	0.645
Deterministic		$1.21 \cdot 10^{-3}$	-	0.600	-	1.85	0.600

the target lift coefficient is increased.

In Table 7 a comparison of NLMC and Kriging predictions using the same $3,000$ samples for the optimal design with $k = 2$ is presented which demonstrates the quality of the predictions for statistics of the lift and drag coefficients.

Table 7: Comparison of NLMC and Kriging predictions for the optimal design with six shape design variables.

	$\bar{C}_{d_{max}}$	$\sigma^2_{C_{d_{max}}}$	$\bar{C}_{l_{min}}$	$\sigma_{C_{l_{min}}}$
NLMC (3000 optimizations)	$3.33 \cdot 10^{-3}$	$2.3 \cdot 10^{-7}$	0.640	$2.0 \cdot 10^{-2}$
Kriging (13 optimizations) ($\tilde{N} = 3000$)	$3.33 \cdot 10^{-3}$	$1.8 \cdot 10^{-7}$	0.640	$2.0 \cdot 10^{-2}$
Kriging (13 optimizations) ($\tilde{N} = 10^5$)	$3.28 \cdot 10^{-3}$	$2.0 \cdot 10^{-7}$	0.640	$2.0 \cdot 10^{-2}$

The original NACA 0012 as well as the deterministically and robustly ($k = 2$) optimized airfoils are all shown in Figure 5. Once again one can see that the robustly optimized airfoil looks different from the deterministically optimized one this time especially along the upper surface.

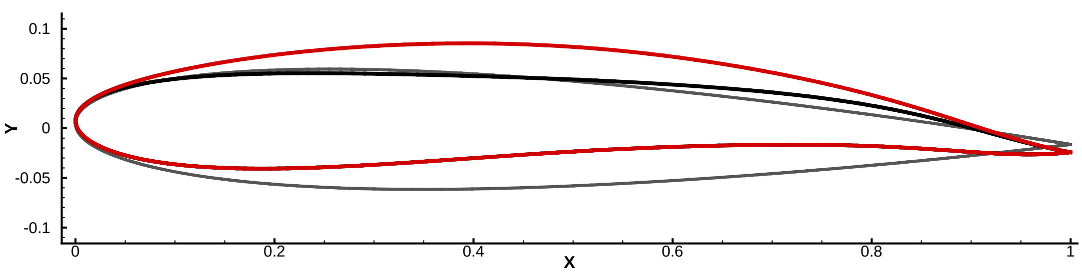

Figure 5: The original NACA 0012 at $\alpha = 1.25$ (gray) as well as the deterministically (black), and robustly ($k = 2$, red) optimized airfoils.

4 Conclusions

This article describes the use of gradient-based optimizations and Kriging surrogate models for the propagation of mixed aleatory/epistemic uncertainties for a robust lift-constrained drag minimization problem. Uncertainty due to epistemic variables is propagated via a constrained optimization approach, while the uncertainty due to aleatory variables is propagated via sampling of a Kriging surrogate model. This statistics-of-intervals approach makes robust optimization under mixed aleatory/epistemic uncertainty possible while at the same time keeping the computational cost for these types of problems manageable.

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