Optimization Under Uncertainty Using Derivatives and Kriging Surrogate Models

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Abstract: In this paper a first-order moment method and a Kriging surrogate model are used for optimizations under uncertainty applied to two-dimensional lift-constrained drag minimizations. Given uncertainties in statistically independent, random, normally distributed input variables, the two approaches are used to propagate these uncertainties through the mathematical model in order to be able to optimize output statistics of interest.

Keywords: Optimization under uncertainty, uncertainty quantification, Kriging surrogate model, moment methods, gradient and Hessian.

1 Introduction and Motivation

In spite of the rapid advances and acceptance of numerical simulations, serious deficiencies remain in terms of accuracy, uncertainty, and validation for many applications. 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 uncertainty quantification (UQ) is used in the optimization loop instead of a deterministic simulation. As one might expect given the computational burden that is created both in optimization and in UQ alone when applied to realistic engineering applications, OUU becomes computationally expensive for all but the most trivial of problems. This is why OUU is considered as one of the most important open problems in optimization [1].

2 Preliminary Results

Moment methods can be a good choice for propagating uncertainties through the simulation process [2]. They are based on Taylor series expansions of the original non-linear objective function $\mathcal{J}(D)$ about the mean of the input, $\bar{D}$, given standard deviations σ_{D_j}, $j = 1, \ldots, M$. The resulting mean, $\bar{\mathcal{J}}$, and variance, $\mathrm{Var}_{\mathcal{J}}$, of the objective function are given to first order (MM1) by $\bar{\mathcal{J}} = \mathcal{J}(\bar{D})$ and $\mathrm{Var}_{\mathcal{J}} = \sum_{j=1}^{M} \left(\frac{d\mathcal{J}}{dD_j}\Big|_{\bar{D}} \sigma_{D_j} \right)^2$. A general optimization under uncertainty (OUU) problem can be expressed as

$$\begin{array}{lrcl} \min & \mathcal{F} & = & \mathcal{F}(\bar{\mathcal{J}}, \mathrm{Var}_{\mathcal{J}}, \bar{q}, \bar{D}) \\ s.t. & R(\bar{q}, \bar{D}) & = & 0 \\ & g(\bar{\mathcal{J}}, \bar{q}, \bar{D}) + k\sigma_g & \leq & 0, \end{array} \tag{1}$$

where k is the number of standard deviations, σ_g, that the inequality constraint, g, must be displaced such that the probability that g is satisfied is greater than a specified probability, P_k, and the equality constraint, R, is deemed satisfied at the mean values $\bar{D}$ and $\bar{q}(\bar{D})$. Note that MM1 requires first-order sensitivities to calculate $\mathrm{Var}_{\mathcal{J}}$ and σ_g. Thus, a gradient-based quasi-Newton optimization requires the Hessian to compute the objective function and constraint gradients.

A more accurate estimate of the required means and variances in (1) can be obtained by using a Kriging surrogate [2, 3]. One disadvantage of the Kriging method is the fact that one has to construct a separate response surface for each simulation output $\mathcal{J}$ and system constraint g. This will make this approach computationally more expensive than the MM1 method.

A robust lift-constrained drag minimization of the steady inviscid flow over a transonic NACA 0012 airfoil is considered by using $\mathcal{F} := \bar{C}_d + \mathrm{Var}_{C_d}$. The free-stream Mach number is 0.755 with an angle of attack of 1.25 degrees. Six shape design variables which control the magnitude of Hicks-Henne sine bump functions are allowed to vary and the resulting deformation of the mesh is calculated via a linear tension spring analogy. All six design variables are assumed to have aleatory uncertainties due to manufacturing tolerances which are modeled with the same normal distributions. A zero mean corresponds to the original NACA 0012 airfoil and the standard deviations are taken to be 0.005. The ability to calculate the gradient and Hessian for this problem and a robustness analysis of the lift coefficient, C_l, has been previously demonstrated [3]. In order to assess the quality of the predictions for the mean and variance of the different methods, a non-linear Monte-Carlo (NLMC) simulation with 3,000 latin hypercube samples is used for comparison in Table 1.

	$\bar{C}_l$	Var_{C_l}	$\bar{C}_d$	Var_{C_d}
NLMC	0.267	$8.7 \cdot 10^{-3}$	$5.95 \cdot 10^{-3}$	$5.8 \cdot 10^{-6}$
MM1	0.268	$6.6 \cdot 10^{-3}$	$5.21 \cdot 10^{-3}$	$3.6 \cdot 10^{-6}$
Kriging	0.267	$8.7 \cdot 10^{-3}$	$5.93 \cdot 10^{-3}$	$5.5 \cdot 10^{-6}$

Table 1: Comparison of NLMC, MM1, and Kriging predictions

The Kriging model (constructed from 49 sample points) yields reasonable answers for a fraction of the cost of a NLMC simulation. The difference to the MM1 predictions shows the non-linearities in the design space. Using the Kriging model for the entire robust optimization process (for the function, constraint, and gradient evaluation) yields the following results:

k	P_k	$\bar{C}_d$	Var_{C_d}	$\bar{C}_l$	σ_{C_l}
0	0.5000	$5.28 \cdot 10^{-3}$	$5.8 \cdot 10^{-6}$	0.268	0.093
1	0.8413	$7.30 \cdot 10^{-3}$	$7.9 \cdot 10^{-6}$	0.367	0.093
2	0.9772	$1.02 \cdot 10^{-2}$	$1.5 \cdot 10^{-5}$	0.451	0.092
3	0.9986	$1.92 \cdot 10^{-2}$	$2.8 \cdot 10^{-5}$	0.561	0.098

Table 2: Robust optimization results using Kriging predictions for different values of k

Just evaluating the optimal design obtained for $k = 2$ by using NLMC with 3000 sample points yields $\bar{C}_d = 1.02 \cdot 10^{-2}$, $\mathrm{Var}_{C_d} = 1.5 \cdot 10^{-5}$, $\bar{C}_l = 0.451$, and $\sigma_{C_l} = 0.091$ and shows again the excellent agreement between the Kriging results and a full NLMC.

3 Conclusion and Future Work

The final paper will have MM1 results which were omitted for brevity as well as more test cases.

References

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