Post-Optimal Design using Optimal Uncertainty Quantification

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Abstract:

The certification of the performance of an aircraft or a system is often formulated using statistical concepts, where the objective functions are the mean and standard deviation of the objective functions assigned to deterministic or worst-case scenarios. However, it is not enough to probe the system by performing a limited number of so-called "hero calculations", or even computing the mean performance and design margins by means of extensive sampling. Instead, it is imperative to be able to predict the system performance with rigorously quantified uncertainties. By rigorous we specifically mean that the performance measures (outputs) assigned to the design processes are certified by mathematically provable bounds, of which sharpness is not jeopardized by the aggregate of multiple sources of uncertainties. In this context, certification is understood as the process of guaranteeing that the probability of exceeding a given threshold a is below an acceptable tolerance ϵ, which is typically small. Namely, one wants to certify that $\mathbb{P}[F(\mathbf{X}) \geq a] \leq \epsilon$, where F is the performance function depending on some random parameters $\mathbf{X}$. The requirement of rigorous Uncertainty Quantification (UQ) is thus to assess carefully the extent to which the performance of the system is likely to deviate from its mean. Concentration-of-measure (CoM) inequalities are a powerful tool for rewording these needs into rigorous and precise mathematical terms, though they are seldom used in engineering applications. The CoM phenomenon refers to the observation that functions depending on a large number of variable parameters with controlled oscillations in each variable are almost constant. The fluctuations about these constant mean values are in addition certified by rigorous inequalities, the CoM inequalities. In this research, we shall mainly work with bounded-differences inequalities of McDiarmid's type, which bounds the fluctuations of a real function $F(\mathbf{X})$ away from its mean $\mathbb{E}\{F(\mathbf{X})\}$ without *a priori* knowledge of the probability distribution functions (PDFs) of the random variables $\mathbf{X}$. Assuming that the latter are independent, one has indeed for all $a > 0$ that:

$$\mathbb{P}[F(\mathbf{X}) \geq a] \leq \mathrm{e}^{-2\frac{(a-\mathbb{E}\{F(\mathbf{X})\})_+^2}{D_F^2}}, \tag{1}$$

where $x_+ := \max(0, x)$ and D_F is the so-called verification diameter of the function F [2]. The fact that this inequality does not require any information on the marginal PDFs of the random variables $\mathbf{X}$ is clearly an advantage in design processes of aircrafts, where experimental data may be scarce. In fact, Eq. 1 is not the optimal inequality which one can obtain given the same information. The tightest bounds can be found by worst-case and best-case approaches depicted in the Optimal Uncertainty Quantification (OUQ) framework [4].

The McDiarmid's inequality and optimal McDiarmid's inequality are in fact the supremum of a family of cumulative distribution functions with respect to the threshold a obtained through a numerical routine. More generally, the OUQ setting aims at finding the optimum value of the following optimization problem

$$F^{\dagger}(a) = \sup_{(f,\mu)\in\mathcal{A}} \mathbb{P}_{\mathbf{X}\sim\mu}[f(\mathbf{X}) \leq a], \tag{2}$$

where f is a real-valued function of a random variable $\mathbf{X}$ following the law μ that can be both unknown but known to be in some class $\mathcal{A}$. This can be done numerically by using the computer code *mystic* [3] for example. Thus, the points obtained by the numerical routine are imperfect and contain numerical errors. Given a numerical optimisation routine which can compute a numerical estimation of the ground truth supremum, one wishes to reconstruct this family with minimal error. In fact, it has been shown in [1] that the convergence of the proposed algorithm depends on the properties of the ground truth function. For instance, if this function is continuous, the convergence is uniform. But if it is piecewise continuous, the convergence is only in mean.

In many cases, the ground truth function f is not know exactly everywhere, or may be too costly to evaluate on-demand. Therefore, let f the unknown function to approximate. Given N observations of this function, we are looking for approximating f. In the Kriging framework, the approximation of f, denoted by f_N, assuming that there is no noise on the observations, is given by

$$f_N(\mathbf{X}) = \sum_{i=1}^{N} c_i K(\mathbf{X}, \mathbf{X}_i), \tag{3}$$

where K is a kernel, and c_i is chosen as $f_N(\mathbf{X}_i) = f(\mathbf{X}_i)$, for $i = 1, \ldots, N$. The main problem in the Kriging framework is the choice of the kernel K and more particularly the hyperparameters associated with it. For instance, if the kernel is the Gaussian kernel, that is $K(\mathbf{X}, \mathbf{Y}) = \exp(-\frac{||\mathbf{X}-\mathbf{Y}||^2}{\gamma^2})$, one has to determine the value of γ. This is the parametric point of view. The value of this parameter can be determined by, for instance, maximum a posteriori estimation or cross-validation. In the following, instead of only seeking to determine a parameter γ, we want to determine a whole function g so that $K(\mathbf{X}, \mathbf{Y}) = K_0(g(\mathbf{X}), g(\mathbf{Y}))$ with for example $K_0(\mathbf{X}, \mathbf{Y}) = \exp(-\frac{||\mathbf{X}-\mathbf{Y}||^2}{\gamma^2})$. This is the non-parametric point of view. In that respect, in order to find the function g, we define the accuracy measurement ρ as

$$\rho = \frac{||f_N - f_{N/2}||^2}{||f_{N/2}||^2}. \tag{4}$$

We will say that the kernel K is a good kernel if the number of observations can be halved without losing too much accuracy, that is when ρ is as close as possible to zero. Thus, g will correspond to the minimum of ρ obtained by an iterative process. This is the Kernel Flow algorithm [5]. An application to a 2D aerodynamic case has been done. The performance function is the lift-to-drag ratio of a RAE2822 wing profile where the input parameters are the Mach number and the angle of attack.

References

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Short biography – Luc Bonnet is a third-year PhD student in the computational fluid mechanics department at the French aerospace lab ONERA. He holds a Master's degree in Mechanical Engineering from ENS Paris-Saclay. His doctoral research mainly focuses on the certification of the performance of aircraft under uncertainty using rigorous mathematical tools. He received a thesis scholarship from the French government and ONERA.