Uncertainty Quantification with Aleatory and Epistemic Parameters

Sebastian Garreis

Technische Universität München, Fakultät für Mathematik,
Lehrstuhl für Mathematische Optimierung (M1), Prof. Dr. Michael Ulbrich

Elitenetzwerk Bayern

Abstract

Uncertainty Quantification (UQ) covers the problem of characterizing and quantifying the uncertainty of a *quantity of interest* that depends on uncertain parameters. In many technical applications this quantity is the result of a complex numerical simulation and, therefore, computing it can be expensive. The simplest methods for uncertainty quantification use, however, *sampling*, where the quantity of interest is calculated for many different realizations of the parameters. This becomes very expensive for a large number of parameters and a desired high accuracy. Thus, one can use more efficient methods like surrogate models, algorithms from nonlinear optimization or model order reduction in order to accelerate the procedure. Some of them are presented in this poster.

Basic Problem

We consider a simulation with uncertain input parameters and computable real-valued output. When treating uncertainties one can distinguish between two types:

- **Aleatory Uncertainties:** Random variables α_i ($i \in [m]$) written into a *random vector* $\alpha \in \mathbb{R}^m$ with a given distribution $\mathbb{P}_\alpha$ (induced probability measure on $\mathbb{R}^m$).
- **Epistemic Uncertainties:** Interval-bounded parameters written into a vector $\beta \in \mathbb{R}^n$ with corresponding lower and upper bounds $b^l, b^u \in \mathbb{R}^n$. The parameter β_j ($j \in [n]$) lies in the interval $I_j = [b^l_j, b^u_j]$, for short: $\beta \in I := \{\beta \in \mathbb{R}^n : b^l \le \beta \le b^u\}$.
- **Generalized epistemic parameters:** In the context of simulations with partial differential equations (PDEs) it can be useful to generalize the epistemic parameters to an element $f \in U$ of a reflexive Banach space U. The nonempty, bounded, closed and convex subset $U_{\text{ad}} \subset U$ is then the feasible set for f.

Generally speaking, a simulation fed with parameters α and f has an output Q (the **quantity of interest**) given by the at least weakly sequentially continuous function

$$Q : \mathbb{R}^m \times U \to \mathbb{R}, \quad (\alpha, f) \mapsto Q(\alpha, f).$$

In the context of simulations Q can be the *reduced objective functional* as known from optimization with PDEs.

Question: How can the uncertainty of the simulation output $Q(\alpha, f)$ be characterized and quantified if $\mathbb{P}_\alpha$ and U_{ad} are given?

UQ with one Type of Parameters

At first, we propose some methods for UQ for the case that only one type of uncertainty is present in the problem.

UQ with Aleatory Parameters

If the quantity of interest $Q = Q(\alpha)$ depends only on aleatory parameters α, it can be viewed as a real-valued random variable provided Q is a measurable (e. g. continuous) function. Then one would like to estimate stochastic quantities of $Q(\alpha)$ like the mean or variance or e. g. approximate the distribution function. There are basically two different types of methods that perform this task: sampling-based statistical and surrogate-based stochastic methods.

Sampling techniques like Monte-Carlo (MC) methods calculate the quantity of interest for many different realizations of α. The obtained "samples" can be explored statistically. As computing Q can be expensive, these methods can be accelerated by **surrogate models** for Q built from a few exact samples. This can be e. g. polynomial interpolation or regression. These can also be integrated analytically to obtain quadrature rules for approximating intergrated stochastic quantities of $Q(\alpha)$. Another often used surrogate is **kriging** – a statistical interpolation method which can accelerate a MC method significantly as can be seen in figure 1.

UQ with Epistemic Parameters

In the case that $Q = Q(f)$ depends only on (generalized) epistemic parameters f, it can also be viewed as epistemic if Q is weakly sequentially continuous. This is an easy conclusion of the extreme and intermediate value theorems. Therefore, it is necessary to determine the corresponding interval endpoints, defined by

$$q_{\text{min}} := \min_{f \in U_{\text{ad}}} Q(f) \quad \text{and} \quad q_{\text{max}} := \max_{f \in U_{\text{ad}}} Q(f).$$

This is a typical **optimization** task with an easy-to-handle feasible set I (constrained qualifications are fullfilled, vertices are known), but also some difficulties:

- One looks for *global extrema*. Techniques for global optimization are, however, very expensive. More efficient nonlinear optimizers can only find local extrema.
- *Convexity* of Q is useful for global minimization but can be used for (in high dimensions inefficient) global maximization only in the case $U_{\text{ad}} = I$ [2].

Sampling strategies can approximate the global extrema if Q is continuous. If Q is at least once continuously differentiable one can use **gradient-based nonlinear optimization methods** which are much more efficient than sampling. In the case of a simulation, the **adjoint-state method** allows fast computation of the gradient. Local optimizers can sometimes find the desired global extrema [3], possibly by using multiple starting points. This approach can also be used for only Lipschitz-continuous functions Q using a subgradient-based method from **nonsmooth optimization** [2].

Uncertainty Quantification with Mixed Parameters

Now we present methods for the case of mixed aleatory and epistemic parameters. Therefore, $Q = Q(\alpha, f)$ depends again on both types of parameters.

"Intervals of Statistics" [1]

One approach is to view the output $Q(\alpha, f) = Q_f(\alpha)$ as a random variable parametrized by the epistemic parameters. Let then $S_\alpha(f)$ be a stochastic quantity of $Q_f(\alpha)$. Under certain conditions $S_\alpha(f)$ lies in a compact interval if $f \in U_{\text{ad}}$ [2]. Its endpoints

$$s_{\text{min}} := \min_{f \in U_{\text{ad}}} S_\alpha(f) \quad \text{and} \quad s_{\text{max}} := \max_{f \in U_{\text{ad}}} S_\alpha(f)$$

can be determined by optimization methods. As $S_\alpha(f)$ is normally not computable explicitly, one can use surrogate models like quadrature rules from interpolation or regression. For the convergence of the surrogate one needs Q to be analytic and for the application of optimization methods the surrogate should be enough differentiable.

"Statistics of Intervals" (SOI) [3]

The other way round one can view $Q(\alpha, f) = Q_\alpha(f)$ as a epistemic variable parametrized by the random vector α. If Q is weakly sequentially continuous, the interval endpoints

$$q_{\text{min}}(\alpha) := \min_{f \in U_{\text{ad}}} Q(\alpha, f) \quad \text{and} \quad q_{\text{max}}(\alpha) := \max_{f \in U_{\text{ad}}} Q(\alpha, f)$$

are continuous functions and thus random variables [2]. One can use the following algorithm to obtain statistics for these random variables:

Algorithm: SOI with kriging

1. Generate realizations $\left(a^{(k)}\right)_{k=1}^{N_\alpha} \subset \mathbb{R}^m$ of the random vector α.
2. Determine for some realizations $a^{(k_l)}$ the values $q_{\text{min}}\left(a^{(k_l)}\right)$ and $q_{\text{max}}\left(a^{(k_l)}\right)$ using an appropriate optimization method.
3. Determine approximations of $q_{\text{min}}\left(a^{(k)}\right)$ and $q_{\text{max}}\left(a^{(k)}\right)$ for the rest of the realizations by an appropriate surrogate model, e. g. kriging.
4. Explore the obtained data with statistical methods.

A result of the algorithm can be seen in figure 2.

Some Numerical Results

Kriging-enhanced Quasi-Monte-Carlo method

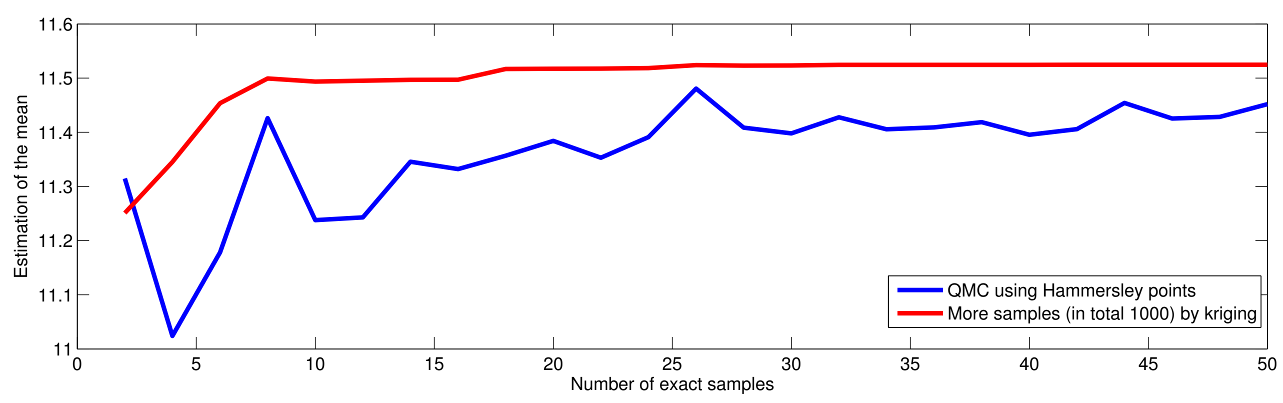

Figure 1: Comparison of a QMC method (blue) with a kriging-enhanced one (red) where more samples are computed by a kriging surrogate. For only 30 exact samples the improved method already gives a quite good approximation of the mean of $Q(\alpha)$.

Simulation of an elastic membrane with obstacle

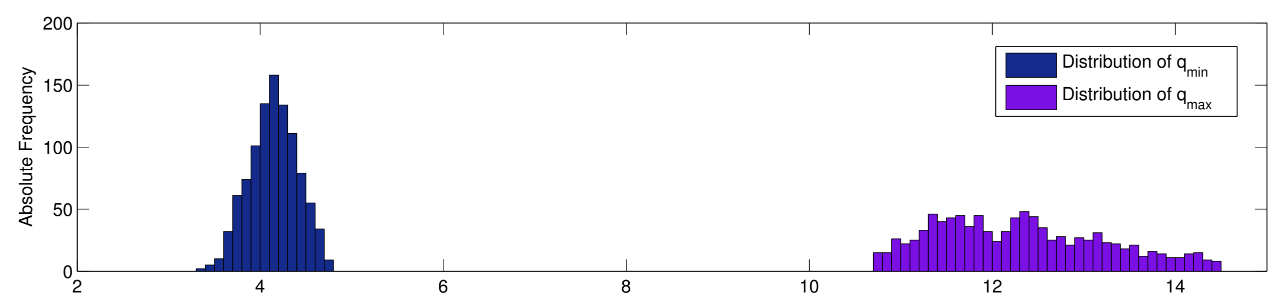

Figure 2: An elastic membrane with aleatory elasticity coefficients under an epistemic force held by an obstacle was simulated. The SOI-kriging-algorithm with a nonsmooth optimization method was used to determine statistics of the "compliance" of the membrane. A typical result can be seen above.

References

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