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Ensemble Kalman Filters and geometric characterization of sensitivity spaces for uncertainty quantification in optimization

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Abstract

We present an original framework for uncertainty quantification (UQ) in optimization. It is based on a cascade of ingredients with growing computational complexity for both forward and reverse uncertainty propagation. The approach is merely geometric. It starts with a complexity-based splitting of the independent variables and the definition of a parametric optimization problem. Geometric characterization of global sensitivity spaces through their dimensions and relative positions by the principal angles between global search subspaces bring a first set of information on the impact of uncertainties on the functioning parameters on the optimal solution. Joining the multi-point descent direction and the quantiles on the optimization parameters permits to define the notion of Directional Extreme Scenarios (DES) without sampling of large dimension design spaces. One goes beyond DES with Ensemble Kalman Filters (EnKF) after the multi-point optimization algorithm is cast into an ensemble simulation environment. This formulation accounts for the variability in large dimension. The UQ cascade ends with the joint application of the EnKF and DES leading to the concept of Ensemble Directional Extreme Scenarios (EDES) which provides more exhaustive possible extreme scenarios knowing the Probability Density Function of our optimization parameters. A final interest of the approach is that it provides an indication of the size of the ensemble which must be considered in the EnKF. These ingredients are illustrated on an history matching problem.

Keywords: EnKF; Uncertainty quantification; Principal angles; Inverse problems; History matching; Extreme scenarios

1. Introduction

Forward and backward uncertainty propagation [1–3] are obviously of great importance. For instance, taking into account manufacturing uncertainties is of utmost importance for a design procedure to be efficient as it is impossible to make sure that the final product will exactly correspond to the design specifications. In shape optimization, for instance, either in mono or multidisciplinary frameworks, this uncertainty is rarely accounted for [4,5].

This question can be formulated through both forward and backward uncertainty propagation. Indeed, manufacturing uncertainties can be prescribed through probability density functions of the design parameters (often coming as characteristics of the product manufacturing process) [6,7]. They can also be introduced through uncertainties on the performances of a design (or other observations).

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1.1. Context of the work

We consider a generic situation where the simulation aims at predicting a given quantity of interest j (e.g. the maximum value of a variable in a given area) and there are a few functioning $\mathbf{u}$ and several control parameters $\mathbf{x}$ involved. The ranges of the functioning parameters define the global operating/functioning conditions of a given design. This splitting of the independent variables in two sets is important for the rest of the paper.

The literature on uncertainty quantification (UQ) is huge. In short, in our situation, forward propagation aims at defining a probability density function for j knowing those of $\mathbf{x}$ and $\mathbf{u}$ [8–10]. This can be done, for instance, through Monte Carlo simulations or a separation between deterministic and stochastic features using Karhunen–Loeve theory (polynomial chaos theory belongs to this class) [11–15]. Examples of shape optimization with polynomial chaos and surrogate models during optimization to address the issue of functional evaluations are given in [16,17].

Backward propagation aims at reducing models bias or calibrating models parameters knowing the probability density function of j (or other constraints and observations) [18–20]. This can be seen as a minimization problem and Kalman filters [21] give, for instance, an elegant framework for this inversion assimilating the uncertainties on the observations.

Our aim is to propose a geometric framework to address, in our particular situation, the curse of dimensionality of existing approaches related to the explosion of their computational complexity due to the sampling necessary to access probabilistic information (momentum), even if this can be improved with intelligent sampling techniques [22,23]. The different ingredients presented here can be applied with either high-fidelity or reduced order models, when available [24–27]. Low-order models are often used instead of the full models to overcome the computational complexity of UQ.

After the splitting of the independent variables mentioned above, we define a multi-point formulation to account for the variability on $\mathbf{u}$. This is feasible because the size of $\mathbf{u}$ is assumed small. We define a global sensitivity space using the sensitivities of j with respect to $\mathbf{x}$ for the multi-point problem. Once this space built, we analyze the dimension of its free generator subspace. Previous works have shown how to perform this task and how to use this information for adaptive sampling and robust optimization [28,29].

The next step is to analyze the impact of different modeling or discretizations on the results. Different models or solution procedures lead to different sensitivity spaces. Beyond their respective dimensions, principal angles [30–33] between the respective sensitivity spaces permit to measure the deviation due such changes. The dimensions of the spaces and the angles are interesting measures for both the epistemic and aleatory uncertainties. Indeed, suppose that, at given modeling procedure, the dimensions of the sensitivity spaces remain unchanged when enriching the sampling of the functioning parameter range, this stability would be a first indication of a low level of sensitivity of the simulations with respect to this parameter. Once this is established, principal angles between subspaces permit to analyze both the impact of a given evolution of the modeling on the sensitivity spaces or an enrichment of our sampling. Eventually, constant dimension and low angles will clearly indicate a situation of low uncertainty.

These ingredients can be used in a context of multi-point robust analysis of a system to define worst-case scenarios for its functioning. To this end we combine a multi-point sensitivity with the probabilistic features of the control parameters through their quantiles [6,34]. These ingredients permit to define the concept of Directional Extreme Scenarios (DES) without a sampling of large dimension design spaces.

Ensemble Kalman filters (EnKF) [21,35–39] permit to go beyond the directional uncertainty quantification concept when accounting for the uncertainties in large dimension. It also permits backward uncertainty propagation assimilating the uncertainty on the functional and constraints during the design. We propose to cast our multi-point optimization problem into the ensemble formulation. The geometric uncertainty quantification construction ends with the joint application of the EnKF and DES leading to the concept of Ensemble Directional Extreme Scenarios (EDES) which provides exhaustive possible extreme scenarios knowing the probability density function of the optimization parameters and this without any sampling of a large dimensional parameter space. Finally, the geometric information on the global sensitivity spaces provides lower bounds on the size of the ensemble which must be considered in the EnKF.

1.2. Summary of this work ingredients and calculation complexity

To summarize this work will propose a cascade of ingredients to account for uncertainties avoiding any sampling of large dimensional spaces. We insist on the fact a sampling is only necessary for the functioning parameters $\mathbf{u}$ range