Bayesian calibration for the quantification of conditional uncertainty of input parameters in chained numerical models

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Abstract

Numerical models have become essential tools to study complex physical systems. The accuracy and robustness of their predictions is generally affected by different sources of uncertainty (numerical, epistemic). In this work, we deal with the uncertainty of the parameters of a multiphysics simulation composed of several numerical models coupled together in order to treat the various aspects of the physical system. The application motivating this work is part of the study of nuclear fuel behavior in pressurized water reactors. More specifically, we are interested in a model of fuel fission gas behavior chained upstream to a thermal model. As each of the two models has its own uncertain parameters, our objective is to calibrate the input parameters $\theta \in \mathbb{R}^p \, (p \geq 1)$ of the gas model conditionally on the value of the input parameter of the thermal model, namely the fuel conductivity $\lambda \in \mathbb{R}$. To do so, we set out a nonparametric Bayesian method, called GP-LinCC method, and based on several assumptions that are consistent with both the physical and numerical models. First, the functional dependence $\theta(\lambda)$ is assumed to be a realization of a Gaussian process prior whose hyperparameters are estimated from the set of experimental data. Then, assuming that the gas model is a linear function of $\theta(\lambda)$, the Bayesian machinery allows us to compute analytically the posterior predictive distribution of $\theta(\lambda)$ for any set of realizations of the conductivity λ. The application of GP-LinCC method on our data and the shape of $\theta(\lambda)$ thus obtained illustrates the interest of such a conditional parameter calibration approach in multiphysics simulation.

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Hoeffding-ANOVA decomposition of functions with dependent random inputs

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Abstract:

The ability to uniquely decompose square-integrable functions of dependent random inputs into a sum of functions of every possible subset of variables is key in the field of sensitivity analysis. Many approaches have been proposed in the literature, that either approximate such a decomposition or rely on rather restrictive assumptions on the probabilistic structure of the inputs. However, such a decomposition is achievable under two reasonable assumptions:

- Non-perfect functional dependence between the inputs;
- Non-degenerate stochastic dependence structure;

Under those assumptions, it is possible to show that the space of real-valued square-integrable functions admits a coalitional direct-sum decomposition. For the task of variance decomposition, it leads to the definition of novel sensitivity indices, which generalize the well-known Sobol' indices. Furthermore, this result allows for an intuitive definition for interaction and dependence effects. This talk is dedicated to presenting this result, discussing its implications, and highlighting the challenges to come for an practical implementation.

Short biography – After graduating from ENSAI and Rennes 1 University in 2020, I started a CIFRE PhD track in 2021 at EDF R&D and Institut de Mathématiques de Toulouse, working on the development of interpretability methods for ML models. My research interests are at the crossroads between sensitivity analysis and explainable artificial intelligence methods, and more specifically applied cooperative game theory and probability measure perturbations.

- Titre : « Combination of Optimization-free Kriging Models for High-Dimensional problems »

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- Abstract :

Kriging metamodeling (also called Gaussian Process regression) is a popular approach to predict the output of a function based on few observations. The Kriging method involves length-scale hyperparameters whose optimization is essential to obtain an accurate model and is typically performed using maximum likelihood estimation (MLE).

However, for high-dimensional problems, the hyperparameter optimization is problematic and often fails to provide correct values. This is especially true for Kriging-based design optimization where the dimension is often quite high, and building a good Kriging model becomes challenging. Several methods address this issue by reducing the dimension of the problem, for instance by embedding the design space into a lower dimensional space, or by considering simplifying hypothesis such as additive models. These methods generally suppose a particular form for the underlying functions to be predicted, and thus, there performances are very problem dependent.

In this presentation, we present a new method for building high-dimensional surrogate models which avoids the hyperparameter optimization by combining Kriging sub-models with randomly chosen length-scales. Contrarily to other approaches, it does not rely on dimension reduction techniques and it provides a closed-form expression for the model. Thus, this method is easily generalizable to various problems and computationally cheap. We present a recipe to determine a suitable sampling scheme length-scales for the random length-scales of the sub-models. We also present how we compute the weights in the combination. Finally, we introduce a method to access the predicted variance of the combination. We show for a high-dimensional test problem and a real-world application that our combination is more accurate than the classical Kriging approach using MLE.

Reference prior construction for Bayesian inference applied to seismic fragility curve estimation

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Abstract

Seismic fragility curves of mechanical structures are key quantities of interest for probabilistic seismic risk assessment studies. They express the probability of failure of the mechanical structure conditional to a scalar value derived from the seismic ground motions, coined intensity measure (IM). Evaluation of these curves can be carried out by using Monte Carlo methods and mechanical numerical simulations with artificial seismic signals. Nevertheless, when resorting to a complex and detailed modeling, the number of data available is limited due to the calculation burden, making estimation of those curves challenging.

The Bayesian viewpoint makes it possible to learn more efficiently the parameters which determine the fragility curves. It avoids the generation of unrealistic samples – which is common with classical methods – and which can lead to degenerate curves such as unit step functions for example. With a small dataset, it is known that the choice of prior has a significant influence on the posterior distribution. In practice, however, its definition requires information that is not necessarily available or difficult to justify, so it may be debatable.

Reference prior theory provides answers to this problem. It relies on the maximization of an objective criterion that is based on a mutual information metric. To support the prior choice, we propose an enrichment of this criterion with a wider range of mutual information measures which we prove to be asymptotically maximized by the Jeffreys' prior. We then suggest an implementation of this prior in the context of seismic fragility curve estimation. The posterior distributions of the parameter of interest are compared both theoretically and numerically with the ones obtained with classical priors from the literature.

While our results show the robustness of Jeffreys' prior which outperforms the ones of the literature, they highlight the sensitivity of the estimates with respect to the chosen prior. Also, by investigating different IMs (Peak Ground Acceleration vs. Pseudo Spectral Acceleration), we unveil degenerative phenomena that may happen when using an IM that is correlated to the structure response and may be difficult to handle by any non-informative prior.

Our conclusion emphasizes the importance of an appropriate and objective construction for the prior in Bayesian studies.

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Optimization on Riemannian Manifolds for Uncertainty Quantification

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Abstract

Uncertainty quantification (UQ) is the study of a quantity of interest (QoI) defined on the output Y of a numerical model G when the inputs $X_1, ..., X_d$ are considered to be random variables with reference laws $\pi_{1,0}, ..., \pi_{d,0}$. In this domain, robustness analysis (RA) aims to examine to what extend the QoI is robust to the choice of a particular probabilistic model π_i for an uncertain input X_i. This robustness can be assessed by searching the maximal change generated on the QoI when perturbing the law $\pi_{i,0}$ of the input X_i. This approach is hence based on the resolution of an optimisation problem, in the following form:

$$\max_{\pi_i \in \Lambda_i} \mathrm{QoI}(\pi_i) \quad (\star).$$

This implies to define Λ_i the set of all possible perturbed laws upon which one searches the maximum output perturbation. This, in turn, relies on a specific metric to quantify the magnitude of a perturbation of π_i around the reference law $\pi_{i,0}$. In the OF-PLI paradigm, the metric adopted to do so is based on the Fisher matrices of a family of distributions parametrized by Θ and the Fisher-Rao geodesic distance it defines: $d_F(\theta_0, \theta)$, where $\theta_0 \in \Theta$ are the parameters associated to $\pi_{i,0}$, and θ those of the perturbed law. This way of measuring a perturbation of the input law does not depend on a particular representation of the parametric family in which π lies [3]. The QoI under study can be either the quantile q^α or the superquantile Q^α of the output Y defined as

$$q^\alpha = \inf\{t \in \mathbb{R} \mid \mathbb{P}(Y \leq t) \geq \alpha\} \quad \text{and} \quad Q^\alpha = \mathbb{E}\left[Y | Y \geq q^\alpha\right].$$

The impact of the input perturbation is then summarized by the following index:

$$S_i(\theta) = \frac{\mathrm{QoI}(\theta) - \mathrm{QoI}(\theta_0)}{\mathrm{QoI}(\theta_0)}.$$

In this setting, Θ endowed with the Fisher metric is a Riemannian manifold, and $(\star)$ becomes a Riemannian optimization problem.

Optimization problems appear in a very wide range of mathematical domains, from fundamental to applied mathematics as well as in engineering or other applied sciences [4]. This class of problems can be defined in a very general way, in the usual language of set theory, as the search for the maximum value of an objective function f over a set E on which f is defined. This basic formulation does not require any additional assumption on E nor on f. In practice, optimization methods are all based on a more specific knowledge of E and f, and different branches of the optimization domain are linked to the hypothesis one can make on both the objective function and the optimization domain. For example, gradient descent is a class of commonly used algorithms that require the differentiability of f. Here we will focus on the case where E is a manifold endowed with a certain metric, and try to see how it can be useful (or even necessary) to take this structure into account to solve an optimization problem on E [1], [2], [5]. Moreover, we will explain the difficulty of the Riemannian optimization approach for $(\star)$ in addition to the fact that S_i cannot be computed explicitly. Therefore, this approach must be adapted to $(\star)$ with a suitable statistical sampling method.

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Field uncertainties estimation through [hyper]parameters sampling using Bayesian inference

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Abstract

Inverse problems arise in many application fields whenever we want to infer a quantity from (potentially indirect, sparse and noisy) observations [3]. An usual approach to solve inverse problems is the Bayesian inference which provides the full posterior distribution of the quantity of interest thanks to a Markov–Chain Monte Carlo sampling [2].

In this work, we are interested in estimating an infinite dimensional physical field, which is parametrized to consider a finite dimensional MCMC algorithm. We focus on a way to avoid overconfidence on the parametrization by means of hyperparameters sampling. In our formulation, the use of a naive random walk leads to inaccurate results. Indeed, the prior law of the parameters is highly stretched along the hyperparameters and induces a strong dependency of the sampling to the current state chain. This problem is commonly known as hierarchical sampling in the MCMC community [1]. Different sampling strategies are presented to solve this issue.

The method is applied to a seismic tomography inversion, where we infer a seismic wave velocity field with the first-arrival traveltimes at given locations. More realistic predictions than when fixing the hyperparameters at constant values are obtained. Moreover, this method allows for various field shapes, while keeping the implementation computationally tractable.

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Gaussian process regression for high dimensional graph inputs

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Abstract

In the design phases of new product parts, numerical simulation is now omnipresent to predict the behavior and performance of such parts, thus allowing to find the right characteristics (geometry, material types, etc) to achieve the desired specifications. To reduce the computational cost of the optimization in the design phase, the most used approach is based on the construction of statistical regression models commonly called meta-models.
We use Gaussian process regression to be able to predict physical quantities with uncertainty quantification. The inputs of the regression model are meshes seen as graphs with a large number of nodes (which can vary between different graphs) having continuous attributes. This requires the definition of a kernel between such graphs.

The definition of kernels between graphs is not new, and there are a number of comprehensive reviews on the subject [1]. Unfortunately, state of the art kernels have an extremely penalizing complexity with respect to the number of nodes and are mainly applied to graphs with discretely labeled vertices/edges. In addition, many kernels are not positive definite.

The proposed approach consists in two steps. The first one is to find a node embedding that maps the graph to a point cloud thanks to Weisfeiler Lehman iterations. Then, point clouds are compared using optimal transport, and more specifically the Sliced Wasserstein distance, that guarantees the positive definiteness needed when using Gaussian process regression.
We illustrate the performance of the kernel for two tasks: classification of small graphs coming from bioinformatics, and regression for high dimensional graphs coming from fluid and solid mechanics.

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Simulation d'événements rares pour des marches aléatoires sur des graphes finis

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Abstract

On souhaite estimer la probabilité qu'une trajectoire de processus de Markov déterministe par morceaux (PDMP) atteigne une région cible de son espace d'états avant une date fixée. On s'intéresse en particulier au cas où la région cible est rarement visitée et donc où la probabilité cible est faible. Exemple typique : le PDMP modélise un système industriel dynamique et la région cible correspond à la défaillance du système.

Un estimateur de variance nulle de la probabilité cible peut être construit à l'aide d'une méthode d'échantillonnage préférentiel à condition de connaître la "fonction committor" du processus [2]. Celle-ci correspond à la probabilité d'atteindre la région cible sachant l'état actuel de la trajectoire. Inaccessible en pratique, un des enjeux principaux de ma thèse est de déterminer comment approcher efficacement cette fonction committor.

Nous avons proposé en première partie de ma thèse une méthode adaptative d'approximation de la fonction committor lorsque le PDMP modélise un système "cohérent" [1]. Nous étendons à présent notre méthode à des PDMP plus généraux. La nouvelle méthode repose sur une approximation de l'évolution des modes de ce PDMP par une marche aléatoire sur un graphe fini. Pour cette marche aléatoire, on peut calculer explicitement les temps moyens d'atteinte de la région cible du graphe depuis chaque sommet. Ces temps moyens d'atteinte nous permettent ensuite de construire une approximation pertinente de la fonction committor.

On construit plus exactement une famille d'approximations de la fonction committor, conduisant à une famille paramétrique de distributions d'importance dont le paramètre est optimisé séquentiellement par entropie croisée. Ces distributions d'importance successives produisent des estimateurs de plus en plus fiables de la probabilité cible.

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Calibrating a 3D Finite Element Model of Tunnel Boring Machine Excavation Using Monitoring Data Through Bayesian Approaches

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Metropolises are facing the saturation of their mobility corridors, which has led to the implementation of new major infrastructure projects, such as tunnel construction. However, tunnel construction comes with risks, notably surface displacements caused by excavation work.

It is crucial to anticipate and monitor the extent of settlements to assess these risks and safeguard surface buildings. For this purpose, various prediction methods have been developed, encompassing empirical, analytical, and numerical approaches. Three-dimensional models based on the finite element method (FEM), incorporating realistic soil mechanical behaviours, are acknowledged as the most faithful to reality, but their complexity renders them computationally expensive processes.

The integration of elements of random uncertainty into FEM models can take the form of significant spatial variability in soil properties or even intrinsic epistemic uncertainties within the FEM model, such as the horizontality of strata or the incorporation of fictitious parameters like uniform pressure from the tunnel boring machine (TBM) on the ground. This incorporation of uncertainties compromises the reliability of model outcomes, which then risks deviating from observations derived from monitoring data.

With the aim of precisely adjusting the 3D FEM model using monitoring data, the central objective of this presentation will be to outline the fundamental issue of my research topic while shedding light on various adjustment methods from the state-of-the-art we would like to implement.

Conformal Prediction for surrogate modelling in the UQ framework

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Abstract

Conformal Prediction (CP) [5], has become an increasingly popular approach for performing a sort of Uncertainty Quantification of machine learning models. Assuming the minimal hypothesis of exchangeability of the dataset $\mathcal{D}$ (i.i.d for example), CP allows to build set prediction sets with formal probabilistic coverage guarantees. In the case of scalar outputs, this paradigm enables for any confidence level $\alpha \in (0, 1)$ to have *prediction intervals* and not only the point-output. After outlining some general principles of CP, we will present the full-conformal estimators followed by the more computationally-tractable split-conformal [3] and cross-conformal [1] methods. We will then sketch some ongoing work for evaluating the performance of metamodels of computer codes [2] by tuning CP with Gaussian Process regressors [4].

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Design of experiments for computer code calibration

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Résumé

In industry, computer codes are widely used to mimic the behavior of physical phenomena whose experimentation can be costly, difficult or even dangerous. These computer codes depend on parameters that need to be estimated in order to simulate the physical phenomenon. The designing of physical and numerical experiments to solve a calibration problem is crucial in a context where the physical phenomenon is modeled by an expensive computer code and the physical experiments are equally costly. Based on the classical Bayesian framework of Kennedy and O'Hagan (2001) we propose an algorithm for designing physical and numerical experiments. The first step is to choice the physical experiments. For this reason, we begin by presenting criteria for measuring the quality of a design of physical experiments. These criteria can be grouped into two categories : those based on the information matrix taken from the literature and those based on the exact a posteriori distribution we propose. The latter are better suited to the calibration problem, as they take into account uncertainties about the physical phenomenon and the calibration parameters. However, they are costly to evaluate, due to the use of Monte-Carlo procedures. The first challenge is to evaluate these criteria quickly, and the second is to solve the resulting optimization problem. For the former, we will present a fast calculation method without Monte-Carlo procedure, and for the latter, a variant of simulated annealing. These criteria on the design of physical experiments will be combined with an algorithm for the choice of numerical experiments from the literature to give a mixed algorithm for the calibration of computer codes. Numerical experiments on a toy case will be presented to assess and compare the performance of the algorithms.

Keywords : *Gaussian process, calibration, design of physical experiments, design of numerical experiments, information matrix, Kullback-Leibler divergence.*