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Prediction of physical fields under linear constraint

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Abstract

Numerical simulation in computational fluid dynamics (CFD) is crucial for modeling complex physical phenomena, but it is time-consuming and resource-intensive, largely due to the fine meshes needed to capture detailed flow features. These costs increase when multiple simulations are required, such as for uncertainty quantification. In this context, metamodels offer an efficient solution to predict results, such as physical fields, from a limited number of simulations.

Predicting physical fields is particularly challenging due to their high dimensionality, which is associated with the size of the mesh. A field can contain thousands or even millions of data points, making it difficult to manage effectively in a predictive model. Additionally, these fields must adhere to physical constraints, such as conservation equations, to ensure the physical validity of the results. Therefore, it is essential to develop supervised methods capable of addressing both the high dimensionality and the associated physical constraints. In this work, we will consider the problem of building metamodels for physical fields under linear constraints that can be formulated as a multi-output regression problem with linear constraints :

$$\begin{cases} \text{find } \mathbf{f} = [\mathbf{f}_1^T, ..., \mathbf{f}_Q^T]^T \text{ such that } \mathbf{y} = \mathbf{f}(\mathbf{x}), \\ \mathcal{F}[\mathbf{f}(\mathbf{x})] = \sum_{j=1}^{Q} \alpha^j(\mathbf{x}) \mathbf{f}^j(\mathbf{x}) = \mathbf{c}(\mathbf{x}). \end{cases} \tag{1}$$

where $\mathbf{x}$ is the input parameter and $\mathbf{y}$ is the output of the code, which is concatenation of the scalar field values computed over a given mesh from a vector or tensor field. The constraint under consideration deals with the relationships between scalar fields and depends on the input parameters.

Previous research has tackled dimensionality reduction for field prediction by combining dimensionality reduction techniques with regression models [2], [3]. In [2], they proposed a framework that involves using linear principal component analysis (PCA) to project the outputs into low-dimensional space and applying independant Gaussian process (GP) regression on the coordinates, as they are uncorrelated. [3] extended the framwork to handle more complex data, such when a linear subspace fail to give a faithful representation of the data, by introducing non linear dimensionality reduction techniques. However, explicit consideration of physical constraints or simultaneous modeling of multiple high-dimensional physical fields has not been thoroughly explored.

Constrained Gaussian process: In the litterature, Gaussian Process regression has gained popularity for metamodelling due to its flexibility and capability to provide uncertainty on prediction. The use of Gaussian Process for physical problems has led the machine learning community to develop methods for incorporating constraints into GPs. Since then, various approach have been developped, ranging from conditionning the GP on data points using Bayes' rule, to encode linear constraints into the kernel by restricting to solutions of linear operator matrices [1]. Thus, we propose to use the parametrisation approach to constraint the GP regression in the reduced space under assumption that the output projection and reconstruction preserves linear constraint. So consider the problem of imposing a linear onstraint on a vector-valued Gaussian process $\mathbf{f} \sim \mathcal{GP}(\boldsymbol{\mu}_f(\mathbf{x}), \mathbf{K}_f(\mathbf{x}, \mathbf{x}'))$, $\boldsymbol{\mu}_f(\cdot) : \mathbb{R}^D \mapsto \mathbb{R}^P, \mathbf{K}_f(\cdot, \cdot) : \mathbb{R}^D \times \mathbb{R}^D \mapsto \mathbb{R}^P \times \mathbb{R}^P$ defined by the following linear operator:

$$\mathcal{L}[\mathbf{f}] = \mathbf{0} \tag{2}$$

The parametrization approach is based first on the principle of stability of Gaussian Processes under linear transformations, and then uses this principle to impose constraints on a linear operator, ensuring that the constraint is satisfied regardless of the underlying function. This technique involves considering that the function $\mathbf{f}$ is related to another function $\mathbf{g}$ via an operator $\mathcal{G} : \mathbb{R}^s \mapsto \mathbb{R}^P$. The operator is conditioned, and a GP prior is placed on $\mathbf{g} \sim \mathcal{GP}(\boldsymbol{\mu}_g(\mathbf{x}), \mathbf{K}_g(\mathbf{x}, \mathbf{x}'))$, from which the prior on $\mathbf{f}$ is derived :

$$\boldsymbol{\mu}_f(\mathbf{x}) = \mathcal{G}_{\mathbf{x}}[\boldsymbol{\mu}_g] \qquad \mathbf{K}_f(\mathbf{x}, \mathbf{x}') = \mathcal{G}_{\mathbf{x}} \mathbf{K}_g \mathcal{G}_{\mathbf{x}'}^T$$

PCA and constrained GP: To address the high dimensionality problem and ensure prediction under linear constraints for physical fields, we propose combining PCA with constrained GP regression, following the parametrization approach. The linearity of PCA is leveraged to validate the aforementioned hypothesis, meaning that the projection and reconstruction procedure of the data preserve the constraint. This implies that by ensuring the prediction of the weights using constrained GP, we can predict fields under constraints.

We validate this framework through a case study involving the prediction of a constrained tensor field derived from CFD simulations using the CFD code TrioCFD, developed in CEA, demonstrating its effectiveness in preserving constraints and predicting physically meaningful fields.

Short biography (PhD student)

Nassouradine Mahamat Hamdan is a PhD Student in CEA Saclay and is directed by Prof. Sébastien Da Veiga at ENSAI CREST. He obtained a Master's degree in Applied Mathematics from the University of Reims-Champagne Ardenne, specializing in scientific computing.

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References

[1] A. WIlls et Thomas B.Shon C. Jidling, N. Wahlstrom. Linearly constrained Gaussian processes. *31st Conference on Neural Information Processing Systems (NIPS 2017), Long Beach, CA, USA.*, pages 2–5, 2017.

[2] Dave Higdon, James Gattiker, Brian Williams, and Maria Rightley. Computer model calibration using high-dimensional output. *Journal of the American Statistical Association*, 103(482):570–583, 2008.

[3] Wei Xing, Akeel A Shah, and Prasanth B Nair. Reduced dimensional gaussian process emulators of parametrized partial differential equations based on isomap. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 471(2174):20140697, 2015.

A new paradigm for global sensitivity analysis

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Current theory of global sensitivity analysis, based on a nonlinear functional ANOVA decomposition of the random output, is limited in scope—for instance, the analysis is limited to the output's variance and the inputs have to be mutually independent—and leads to sensitivity indices the interpretation of which is not fully clear, especially interaction effects. Alternatively, sensitivity indices built for arbitrary user-defined importance measures have been proposed but a theory to define interactions in a systematic fashion and/or establish a decomposition of the total importance measure is still missing. It is shown that these important problems are solved all at once by adopting a new paradigm. By partitioning the inputs into those causing the change in the output and those which do not, arbitrary user-defined variability measures are identified with the outcomes of a factorial experiment at two levels, leading to all factorial effects without assuming any functional decomposition. To link various well-known sensitivity indices of the literature (Sobol indices and Shapley effects), weighted factorial effects are studied and utilized.

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General Sensitivity Indices for Hilbert Space-Valued Random Variables

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This paper introduces a familly of generalized sensitivity index for Hilbert space-valued random variables, extending the framework of global sensitivity analysis (GSA) to accommodate more complex output spaces. The need for this work stems from the growing complexity of computer models in various scientific and engineering fields, where understanding the influence of inputs on outputs is crucial but often challenging due to computational constraints.

We build on recent advancements in dependence measures [1] and propose new sensitivity indices that quantifie the influence of a real-valued input X on a Hilbert space-valued output Y. This generalization allows for a more thorough analysis of complex systems, accommodating outputs that may be functional or high-dimensional.

The paper begins by establishing the mathematical framework, defining the conditional law and conditional expectation for Hilbert space-valued random variables. We then introduce the concept of equivalent random variables, which is central to the definition of our sensitivity index.

To address the crucial issue of estimation for this proposed generalized sensitivity indices, Λ_φ, we propose an estimation method based on rank statistics, inspired by the work of Gamboa et al. [3] and following the approach introduced by Chatterjee [2]. This method provides advantages over traditional estimation techniques, particularly in terms of computational efficiency and the capability to estimate multiple indices simultaneously.

The rank-based estimation approach uses the ranks of the input and output variables to approximate the sensitivity index. This is particularly advantageous for Hilbert space-valued outputs, as it avoids the complexities associated with direct estimation in high-dimensional spaces.

The estimation procedure involves computing the ranks of the X_i values from a sample of n observations (X_i, Y_i), ordering the Y_i values according to these ranks, and constructing the estimator for Λ_ϕ based on the differences between consecutive ordered $Y_{(R_i)}$ values. This rank-based approach is computationally efficient, allows simultaneous estimation of multiple sensitivity indices, and is robust to outliers and non-linear relationships. Under appropriate conditions, the estimator is consistent and asymptotically normal, providing a basis for constructing confidence intervals and

hypothesis tests.

We provide a detailed analysis of the statistical properties of this estimator, including consistency and asymptotic normality results. These theoretical guarantees support the reliability of the proposed estimation method in practical applications.

Furthermore, we conduct numerical experiments to compare the performance of our rank-based estimator with traditional methods. These experiments demonstrate its efficiency and accuracy across a range of scenarios, including those with complex, high-dimensional outputs.
Our work contributes to the field of GSA by offering a rigorous and implementable tool for analyzing the sensitivity of complex, Hilbert space-valued outputs. The proposed index and its estimation method provide a means of understanding input-output relationships in high-dimensional and functional settings, with potential applications in various scientific and engineering disciplines.

References:

[1] Ansari, J., Langthaler, P. B., Fuchs, S., & Trutschnig, W. (2023). Quantifying and estimating dependence via sensitivity of conditional distributions. arXiv. doi:10.48550/ARXIV.2308.06168. Retrieved from `https://arxiv.org/abs/2308.06168`

[2] Chatterjee, S. (2021). A New Coefficient of Correlation. *Journal of the American Statistical Association*, 116(536), 2009–2022. doi:10.1080/01621459.2020.1758115. Retrieved from `https://www.tandfonline.com/doi/full/10.1080/01621459.2020.1758115`

[3] Gamboa, F., Gremaud, P., Klein, T., & Lagnoux, A. (2022). Global sensitivity analysis: A novel generation of mighty estimators based on rank statistics. *Bernoulli*, 28(4). doi:10.3150/21-BEJ1421. Retrieved from `https://projecteuclid.org/journals/bernoulli/volume-28/issue-4/Global-sensitivity-analysis--A-novel-generation-of-mighty-estimators/10.3150/21-BEJ1421.full`

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Reduced-space Bayesian optimization of process flowsheets

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Mathematical models are essential for evaluating and optimizing the performance of complex processes, providing insights into key performance indicators (KPIs) such as cost, efficiency, and environmental impact. However, these models often function as black-box systems, where underlying equations and derivative information are unavailable, making optimization challenging. This is particularly true for commercially available simulators that rely on steady-state models and heuristic rules, which complicate the identification of optimal process configurations. In such cases, data-driven optimization techniques, like Bayesian Optimization (BO), become highly valuable.

Bayesian Optimization (BO) is well-suited for handling expensive, black-box models (Brochu et al., 2010). However, BO may be challenged by high-dimensional problems. In this context, Global Sensitivity Analysis (GSA) can help identify the most influential variables that drive variability in the objective function (Saltelli et al., 2010). By quantifying both individual and interaction effects, GSA can reduce the variable set to only the critical ones (Kucherenko, 2013), improving BO efficiency. The integration of BO with GSA still faces challenges in balancing computational efficiency and solution accuracy, particularly when applied to complex simulation-based models. Additionally, surrogate-based models, while faster to evaluate, may not fully capture the true objective function, leading to suboptimal solutions.

In this work, we compare simulation-based and surrogate-based Bayesian optimization (Triantafyllou et al., 2024). For the simulation-based methods, we first apply Bayesian Optimization (BO) to the full set of decision variables. Next, we incorporate GSA as a dimensionality reduction step, followed by BO on the reduced variable set. For the surrogate-based approaches, we begin by using GSA to identify the key variables that significantly influence the objective function. These variables are then used to train feed-forward neural networks (ANNs), resulting in simpler, lower-dimensional surrogate models. We then optimize the ANNs using two different approaches: BO and mixed integer programming (MIP) with a big-M reformulation of ReLU ANNs (Triantafyllou et al., 2024; Ceccon et al., 2022).

The performance of both simulation-based and surrogate-based methods is evaluated using two benchmark case studies with different flowsheet simulators: (a) plasmid DNA production in SuperPro Designer with 18 decision variables, and (b) dimethyl ether (DME) production in Aspen HYSYS with 14 decision variables. Generally, simulation-based methods yield superior solutions since they evaluate the true objective function at each step, whereas surrogate-based approaches optimize an approximation (ANN) of the true objective function. This can lead to the ANN having optima that differ from the true objective function both globally and locally (Figure 1). However, the Bayesian optimization of the ANN (GSA-ANN-BO) consistently demonstrates the fastest execution times, achieving reductions of two to three orders of magnitude compared to simulation-based BO, without accounting for the time taken for initial sampling. This makes it particularly advantageous for real-time and resource-constrained optimization tasks, where computational efficiency is critical without a significant loss in solution quality.

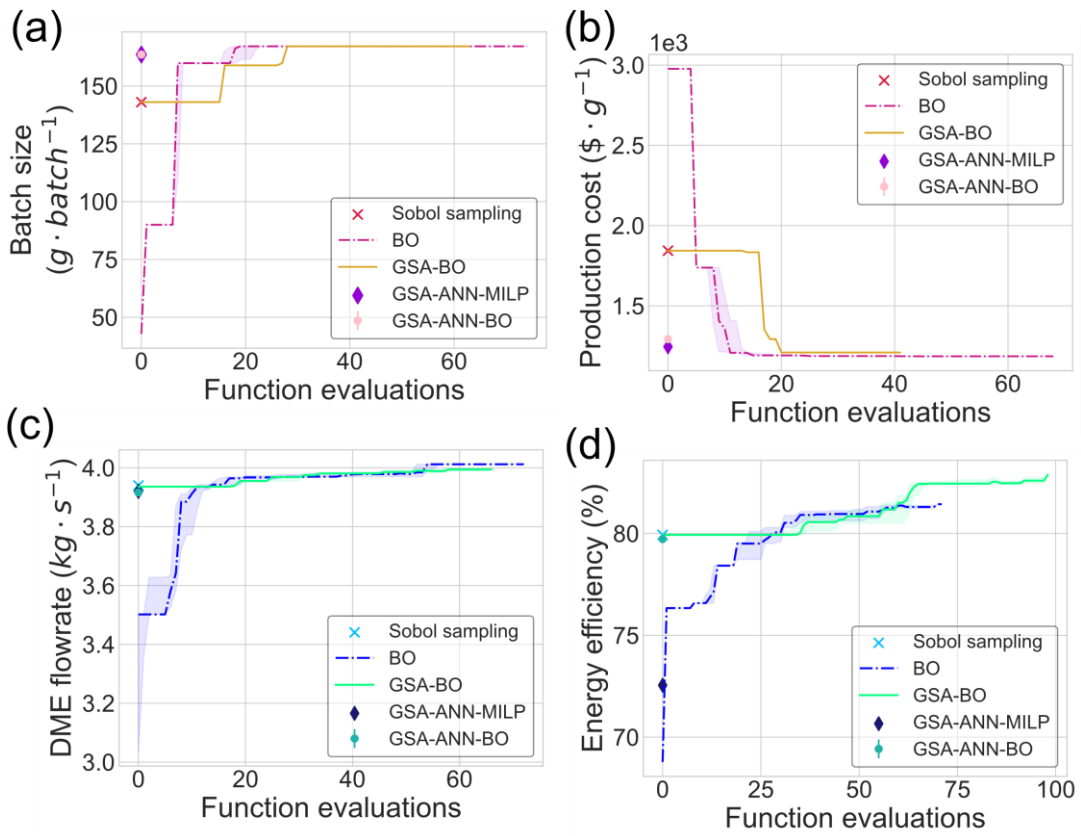

Figure 1. Overview of the optimization methods applied to manufacturing process optimization across the SuperPro Designer (a, b) and Aspen HYSYS (c, d) case studies (adapted from Triantafyllou et al., 2024). The simulation-based approaches include pure Bayesian optimization (BO) and Bayesian optimization combined with global sensitivity analysis (GSA-BO). The surrogate-based approaches consist of GSA-enhanced neural networks optimized using mixed-integer linear programming (GSA-ANN-MILP) and Bayesian optimization of GSA-enhanced neural networks (GSA-ANN-BO). For the Bayesian optimization methods, the plots display the median values along with confidence intervals (1st and 3rd quartiles) based on 10 random seed runs. The best value identified using Sobol sampling is also shown for comparison.

References :

[1] E. Brochu, V.M. Cora, N. De Freitas, "A tutorial on Bayesian optimization of expensive cost functions, with application to active user modeling and hierarchical reinforcement learning," arXiv preprint arXiv:1012.2599, 2010.

[2] A. Saltelli, P. Annoni, I. Azzini, F. Campolongo, M. Ratto, S. Tarantola, "Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index," Comput. Phys. Commun., 181(2):259-270, 2010.

[3] S. Kucherenko, "SobolHDMR: a general-purpose modeling software," Synthetic Biology, 191-224, 2013.

[4] N. Triantafyllou, B. Lyons, A. Bernardi, B. Chachuat, C. Kontoravdi, M.M. Papathanasiou, "Comparative assessment of simulation-based and surrogate-based approaches to flowsheet optimization using dimensionality reduction," Comput. Chem. Eng., 189:108807, 2024.

[5] F. Ceccon, J. Jalving, J. Haddad, A. Thebelt, C. Tsay, C.D. Laird, R. Misener, "OMLT: Optimization & machine learning toolkit," J. Mach. Learn. Res., 23(349):1-8, 2022.

Greedy packing algorithms with relaxation

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Following [1], we consider various relaxations of the greedy-packing algorithm for the construction of nested designs (or design sequence) on a given compact set X. The standard, non-relaxed, greedy-packing algorithm guarantees 50% packing and covering efficiency for each design in the sequence [2]. However, it places many design points close to the boundary of X, and a first form of relaxation aims at countering this effect and relies on boundary avoidance [3]: bounds on packing and covering efficiencies are still available, and an improvement in covering performance is observed in practice.

Relaxation can also include some randomness, with bounds on packing and covering efficiencies that can be set arbitrarily close to 50%. Compared to the now popular determinant point processes, the construction of a design of given size n is straightforward (but its stochastic properties are much more difficult to analyse).

When X is the hypercube $[0,1]^d$, the construction can take projections onto canonical subspaces into account, with the generation of random Latin hypercube (Lh) designs as a special case.

Greedy minimisation of the energy for an isotropic kernel K is also a form of relaxed greedy packing: here, each of the n design points present at iteration n has an influence on choice of the next point x_{n+1}. The kernel can be singular, which induces a strong repulsive property between points. It can also be positive definite and define a correlation function for a random process on X, with Matérn kernels as special cases. When the correlation length tends to zero fast enough, the sequence of nested designs is then asymptotically 50% packing and covering optimal.

Finally, the practical implementation of the methods above requires the usage of a big but finite candidate set where points are selected sequentially, which is sometimes a significant limitation: for example, generating a random n-point Lh design in $[0,1]^d$ requires a candidate set with n^d points, which is prohibitively large. A method is proposed which does not have this limitation and selects the coordinates one at a time for each new design point in the sequence (without any guarantee on the packing and covering efficiencies, however).

References:

[1] L. Pronzato and A.A. Zhigljavsky, "Quasi-uniform designs with asymptotically optimal and near-optimal uniformity constant", *J. of Approximation Theory*, **294**:105931, 2023 (hal-03494864, arXiv:2112.10401).

[2] T.F. Gonzalez, "Clustering to minimize the maximum intercluster distance", *Theoretical Computer Science*, **38**:293–306, 1985.

[3] A. Nogales Gómez, L. Pronzato and M.-J. Rendas, "Incremental space-filling design based on coverings and spacings: improving upon low discrepancy sequences", *J. of Statistical Theory and Practice*, **15**:77, 2021 (hal-02987983).

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Co-active subspace methods for adjacent computer models

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Active subspace methods have become a popular tool for global sensitivity analysis and dimension reduction for a computer model [1]. In this talk, we discuss an elegant generalization of traditional active subspace methods to perform a joint analysis of two "adjacent" computer models [2]. This approach allows us to define co-active direction, joint sensitivity indices (co-activity), and a scalar metric called "concordance" which measures the alignment (or non-alignment) of the gradient spaces of the two functions. An algorithm, based on [3], permits fast computation and implemented in a publicly available R package.

References:

[1] Constantine PG. Active subspaces: Emerging ideas for dimension reduction in parameter studies. Society for Industrial and Applied Mathematics; 2015 Mar 18.

[2] Rumsey K.N., Hardy Z.K., Ahrens C, Vander Wiel S. "Co-Active Subspace Methods for the Joint Analysis of Adjacent Computer Models." Technometrics (2024; in production).

[3] Rumsey K.N., Francom D, and Vander Wiel S. "Discovering Active Subspaces for High-Dimensional Computer Models." Journal of Computational and Graphical Statistics (2023): 1-13

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Robust Bayesian Analysis with information geometry and Perturbed-Law based sensitivity Indices

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Abstract

In modern science and engineering, computational models are popular tools for assessing the behavior of physical systems. They may be seen as maps associating some input parameters to quantities of interest (QoI) related to the response of the system under study. Despite their increasing fidelity, computational models remain simplified representations of the real system, and their input parameters are often not perfectly known. As a result, the QoI predicted by such models are tainted with uncertainties.

Bayesian inference constitutes a coherent framework for quantifying uncertainties and updating them by taking into account all available information. This framework is based on a probabilistic description of uncertainties and relies on the definition of a *prior* distribution, which encodes a state of knowledge about some input parameters before making any observations. Then, this prior state of knowledge can be updated through the derivation of a *posterior* distribution, which summarizes all the available information once new data have been observed. In particular, the general framework of Bayesian inference can be applied to inverse problems, in order to update uncertainties of input parameters of computational models from noisy and limited observation data.

The selection of the prior distribution is of utmost importance in the framework of Bayesian inference. This even constitutes a common criticism directed at Bayesian inference. The prior enables the integration of both qualitative and quantitative information related to parameters, including diverse sources such as past experiments, data taken from existing literature, or beliefs of one or several analysts (*i.e.*, expert judgment). Hence, encoding such various information into a single probability distribution appears as a non-trivial task. In this context, the field of Robust Bayesian Analysis, introduced in the early 90s, provides theoretical and computational foundations for the analysis of the influence of the choice of the prior on Bayesian inference results [1,2]. It aims at quantifying the range of variation of a given QoI by assuming that the prior belongs to a set of probability distributions, which represents all the possible choices for the prior.

More recently, a new Uncertainty Quantification (UQ) branch, named Robustness Analysis, has emerged in the field of sensitivity analysis [3,4]. It aims at measuring the impact of the choice of an input distribution, by studying variations of a QoI with respect to this choice. In particular, an interesting method is given by Perturbed-Law based Indices (PLI), originally introduced in the field of reliability analysis [5,6]. These sensitivity indices are simply defined by the relative variation of the QoI, for a given perturbation of the input distribution. In the recent literature, PLI have been proposed for various types of QoI, including failure probabilities [5,6], quantiles [4] or superquantiles [3].

We propose to study the influence of the choice of the prior distribution, through the definition of PLI dedicated to Bayesian inference. The definition of the proposed PLI is based on the recent work of [4], which provides a formal and coherent framework for perturbing input distributions. Such a framework is based on concepts taken from information geometry, notably the Fisher distance on manifolds of probability distributions.

Furthermore, we show that the proposed PLI can be reformulated as the relative variation of some failure probabilities, by using the so-called BUS (*Bayesian Updating with Structural reliability methods*) framework introduced in [7], which establishes an equivalence between Bayesian inference and a reliability analysis problem. Such a reformulation of the proposed PLI is particularly appealing from a computational point of view, since it allows the use of estimation techniques tailored for PLI of failure probabilities [5,6]. As a result, the proposed PLI are estimated through a reverse importance sampling mechanism [5].

The proposed approach is applied to various Bayesian inverse problems with varying complexity. The results suggest that the proposed Bayesian PLI enable to identify the parameters for which the choice of the prior has a significant impact on Bayesian inference results. Moreover, results underline that the proposed approach remains feasible in the case of Bayesian inverse problems with nonlinear models and possibly high-dimensional inputs.

References:

[1] J. O. Berger, "Robust Bayesian analysis: sensitivity to the prior", *Journal of Statistical Planning and Inference*, **25**:303–328, 1990.

[2] F. Ruggeri, D. R. Insua, J. Martín, "Robust Bayesian Analysis", *Handbook of Statistics*, **25**:623–667, 2005.

[3] B. Iooss, V. Vergès, V. Larget, "BEPU robustness analysis via perturbed-law based sensitivity indices", *ANS Best Estimate Plus Uncertainty International Conference (BEPU 2020)*, 2020.

[4] C. Gauchy, J. Stenger, R. Sueur, B. Iooss, "An Information Geometry Approach to Robustness Analysis for the Uncertainty Quantification of Computer Codes", *Technometrics*, **64**(1):80–91, 2022.

[5] P. Lemaître, E. Sergienko, A. Arnaud, N. Bousquet, F. Gamboa, B. Iooss, "Density modification-based reliability sensitivity analysis", *Journal of Statistical Computation and Simulation*, **85**:1200–1223, 2015.

[6] R. Sueur, N. Bousquet, B. Iooss, J. Bect, "Perturbed-Law based sensitivity indices for sensitivity analysis in structural reliability", *Proceedings of the 8th International Conference on Sensitivity Analysis of Model Output (SAMO2016)*, 2016.

[7] D. Straub, I. Papaioannou, "Bayesian Updating with Structural Reliability Methods", *Journal of Engineering Mechanics, American Society of Civil Engineers (ASCE)*, **141**(3):04014134, 2015.

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Third Moment Method for Sensitivity Estimation of Failure Probability with respect to Distribution Parameters

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Structural reliability analysis is a crucial part of designing systems that can withstand uncertainty in loading and material properties. Reliability methods provide solutions for evaluating failure probabilities, which can be highly sensitive to input variables. Understanding how changes in input variables affect failure probability is essential for optimization and safety enhancement.

Two kinds of sensitivity analysis of failure probability have been investigated with respect to deterministic and random parameters. The sensitivity measure considered herein is the sensitivity analysis of failure probability with respect to distribution parameters, with the sensitivity index defined as the partial derivative of failure probability with respect to the distribution parameters. Most of existing methods for computing such partial derivative have been developed as the post-processing step of an existing strategy for reliability analysis. Based on first-order reliability method (FORM) and second-order reliability method (SORM), the sensitivity of failure probability is computed with the aid of the so-called design point [1, 2]. Identifying the design point in highly nonlinear problems is challenging, making this sensitivity analysis method unsuitable for such cases. Another approach is simulation methods, such as the crude Monte Carlo Simulation [3], Importance Sampling [4], Lines Sampling [5] and Subset Simulation [6]. A key advantage of simulation methods is that the samples generated for estimating failure probability can be post-processed for sensitivity analysis without the need for additional structural analyses. However, the accuracy of failure probability relies greatly on the quality of sample generation, leading to a significant drop in computational efficiency for small failure probability problems. To decrease the number of structural analyses, surrogate models are adopted with combination of the simulation methods for sensitivity analysis, such as the Kriging model [7]. Although computational efficiency can be enhanced with the help of surrogate models, this introduces new challenges related to the construction of the surrogate model. In summary, the effectiveness of sensitivity analysis methods is significantly affected by the underlying reliability analysis techniques used. The method of moments [8] has been widely used for reliability analysis, demonstrating both efficiency and accuracy in addressing nonlinear problems and those with small failure probabilities. A sensitivity estimation framework based on the method of moments was proposed [9], focusing on methods that utilize the first, second, and fourth moments. Building on this approach, an analytical sensitivity estimation method using the fourth moment has been developed, with inputs modeled as normal random variables.

The present work introduces a third-moment method for estimating the partial derivatives of failure probability with respect to the mean, standard deviation, and skewness of input random variables. Assuming the variables are independent, the sensitivity index is formulated using the third-moment reliability index. An efficient numerical algorithm is developed, enabling the sensitivity index to be computed as a byproduct of the reliability analysis. Numerical examples demonstrate that the proposed method accurately estimates the sensitivity of failure probability with respect to the mean and standard

deviation. Additionally, for random variables with small positive or negative skewness, the sensitivity of failure probability with respect to skewness can be reliably estimated.

This study offers three key innovations: (1) It is the first to provide a comprehensive investigation of the third moment method for sensitivity estimation. (2) It includes a detailed numerical algorithm based on the dimension reduction method, where all required inputs are obtained as byproducts of the reliability analysis. (3) It explores the derivative of failure probability with respect to skewness through practical examples.

References :

[1] P. Bjerager and S. Krenk, "Parametric sensitivity in first order reliability theory", *J. Eng. Mech.,* **115 (7)**: 1577-1582, 1989.

[2] I. Enevoldsen and J. D. Sørensen, "Reliability-based optimization of series systems of parallel Systems", J. Struct. Eng., **119 (4)**: 1069-1084, 1993.buzdethod", J. Struct. Eng., **119(4):** 1069-1084, 1993.

[3] N. Metropolis and S. Ulam, "The Monte Carlo method", American Statist. Associa., **44 (247)**: 335-341, 1949.

[4] R. Melchers, "Importance sampling in structural systems", Struct. Saf. **6 (1)**: 3-10, 1989.

M. A. Valdebenito, H. A. Jensen, H. Hernández, L. Mehrez, "Sensitivity estimation of failure probability applying line sampling", Reliab. Eng. Sys. Saf., **171**: 99–111, 2018.

[5] K. M. Zuev, J. L. Beck, S.K. Au, L. S. Katafygiotis, "Bayesian post-processor and other enhancements of subset simulation for estimating failure probabilities in high dimensions", Comput. Struct., **92**: 283-296, 2012.

[6] V. Dubourg and B. Sudret, "Meta-model-based importance sampling for reliability sensitivity analysis", Struct. Saf., **49**: 27-36, 2014.

[7] Y. G. Zhao and Z. H. Lu, "Structural reliability: approaches from perspectives of statistical moments", Wiley, 2021. doi:10.1002/9781119620754.

[8] Z. Z. Lu, J.W. Song, S. F. Song, Z. F. Yue, J. Wang, "Reliability sensitivity by method of moments", Appl. Math. Model, **34(10)**: 2860-2871, 2010.

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Learning signals defined on graphs with optimal transport and Gaussian process regression

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Abstract

In computational physics, machine learning has now emerged as a powerful complementary tool to explore efficiently candidate designs in engineering studies. In this context, we would like to be able to easily predict fields defined on meshes corresponding to new geometries without the need for costly simulations. While some methods like Graph Neural Networks [4] are intrinsically designed to predict signals defined on graphs or point clouds, a natural question is the extension of general scalar output regression models to such complex outputs. Changes between input geometries in terms of both size and adjacency structure in particular make this transition non-trivial. Another key challenge is the obtention of predictive uncertainties, which is crucial to certify the quality of results, to assist sequential design of experiments or to plug the models into Bayesian optimization workflows.

In this work, we propose an innovative strategy for Gaussian process regression where inputs are large and sparse graphs with continuous node attributes and outputs are signals defined on the nodes of the associated inputs. The methodology relies on the combination of regularized optimal transport [3], dimension reduction techniques [2], and the use of Gaussian processes [5] indexed by graphs. It extends previous work on Gaussian processes with Sliced Wasserstein Weisfeiler Lehman graph kernels [1] previously limited to scalar outputs. In addition to enabling signal prediction, the main point of our proposal is to come with confidence intervals on node values.

We illustrate the efficiency of the method with regression tasks involving large graphs from mesh-based simulations in computational fluid dynamics and mechanics [1]. Train datasets are made up of a few hundred graphs with their respective 2D/3D coordinates, where adjacency matrices vary between several inputs, and output fields represent physical quantities of interest on the nodes such as the pressure or the temperature. In Figure 1, we show predictions and associated uncertainties for two test samples of a problem in computational mechanics.

[1] Datasets: https://plaid-lib.readthedocs.io/en/latest/source/data_challenges.html

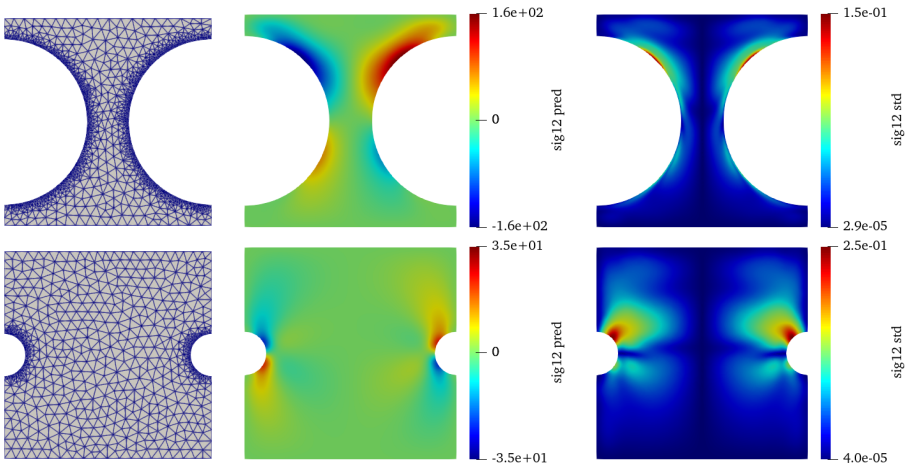

Figure 1: Predictions for two test meshes from the Tensile2d dataset (top and bottom lines). From left to right: the input mesh, the predicted field and the posterior standard deviation of the Gaussian process regression.

Short biography (PhD student)

I have a double Master's degree in Mathematics and Computer Science for Data Science (MIDS) from the University Paris Cité (formerly Diderot).
This thesis is a joint work between the Ecole polytechnique and Safran Tech.
It is part of the ANR SAMOURAI (ANR-20-CE46-0013).

References

[1] Raphaël Carpintero Perez, Sébastien Da Veiga, Josselin Garnier, and Brian Staber. Gaussian process regression with sliced Wasserstein Weisfeiler-Lehman graph kernels. In *Proceedings of The 27th International Conference on Artificial Intelligence and Statistics*, pages 1297–1305, 2024.

[2] Katiana Kontolati, Dimitrios Loukrezis, Dimitrios G Giovanis, Lohit Vandanapu, and Michael D Shields. A survey of unsupervised learning methods for high-dimensional uncertainty quantification in black-box-type problems. *Journal of Computational Physics*, 464:111313, 2022.

[3] Gabriel Peyré, Marco Cuturi, et al. Computational optimal transport: With applications to data science. *Foundations and Trends® in Machine Learning*, 11(5-6):355–607, 2019.

[4] Tobias Pfaff, Meire Fortunato, Alvaro Sanchez-Gonzalez, and Peter Battaglia. Learning mesh-based simulation with graph networks. In *International Conference on Learning Representations*, 2020.

[5] Christopher Ki Williams and Carl Edward Rasmussen. *Gaussian processes for machine learning*. MIT press, 2006.

Sensitivity Analysis in Systems Biology Research: New Perspectives and Considerations

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Utilising ordinary differential equation (ODE) models within systems biology (SB) allows for a more comprehensive representation of biological systems and their dynamics on a global scale, which may not be feasible with higher-order representations. By "global-scale dynamics," we refer to the ability of ODE models to capture the behaviour of entire biological systems over time, considering interactions across multiple scales—from molecular to cellular, and even organ-level processes [1]. For instance, an ODE model of the cardiovascular system might simultaneously account for the dynamics of heart muscle contraction, blood flow through arteries, and the regulation of blood pressure by the nervous system. This integrated approach enables researchers to understand how changes at the molecular level, such as alterations in ion channel function, can affect overall heart function and lead to systemic conditions like hypertension or heart failure. SB research in recent years has focused on the personalisation of these models in order to negate the need for invasive tests and predict patient outcomes.

The personalisation process utilises ODE models as virtual representations of specific biological processes [2], such as predicting a patient's metabolic response to a meal, personalising medical treatment based on tumour growth, or identifying cardiac pathophysiology through abnormal parameter values. The personalisation problem has gained popularity alongside the rise of the "digital twin" concept [3]. In drug discovery and the development of less invasive medical tests, the ability to personalise ODE models to inform medical decisions and predictions is increasingly crucial. With the adoption of such practices in the medical field, it is essential to quantify the uncertainty associated with any information inferred from these models. In the personalisation problem, the focus is often on a select set of model outputs that correspond to the available experimental data, which are used to calibrate the model parameters. In order to identify which parameters can be used to inform medical decisions one often performs a global sensitivity analysis [4]. In doing this the influential input parameters present themselves which are responsible for causing the largest variation in the outputs. However, this talk examines if this is sufficient enough for personalisation.

Figure 1 is a proposal for the personalisation of a standard ODE based systems biology model which emphasises the recursive nature of the personalisation process. For example, once a personalisable subset of parameters have been obtained, if said subset does not contain the biomarkers (input parameters), one must work with clinicians to establish what additional data can be obtained for a patient and thus GSA and subset selection can be iterated. In order to obtain a subset of input parameters which are likely to be identifiable. From figure 1 we propose that the personalisation process should be a largely offline process to obtain the best case personalisable set of input parameters. This stage is informed by GSA and subset selection methods. Then one performs an uncertainty analysis to examine if the parameter bounds prescribed are sufficient. Once we subsequently begin to constrain the model with experimental data, to personalise the model, this stage involves the optimisation and calibration of the model parameter values. Also, one can then begin to examine the practical identifiability of the model parameters which allows one to examine the uniqueness of the personalisable subset of model parameters given noisy clinical data.

The proposed workflow below defines a novel approach to quantifying the uncertainty associated with systems biology.

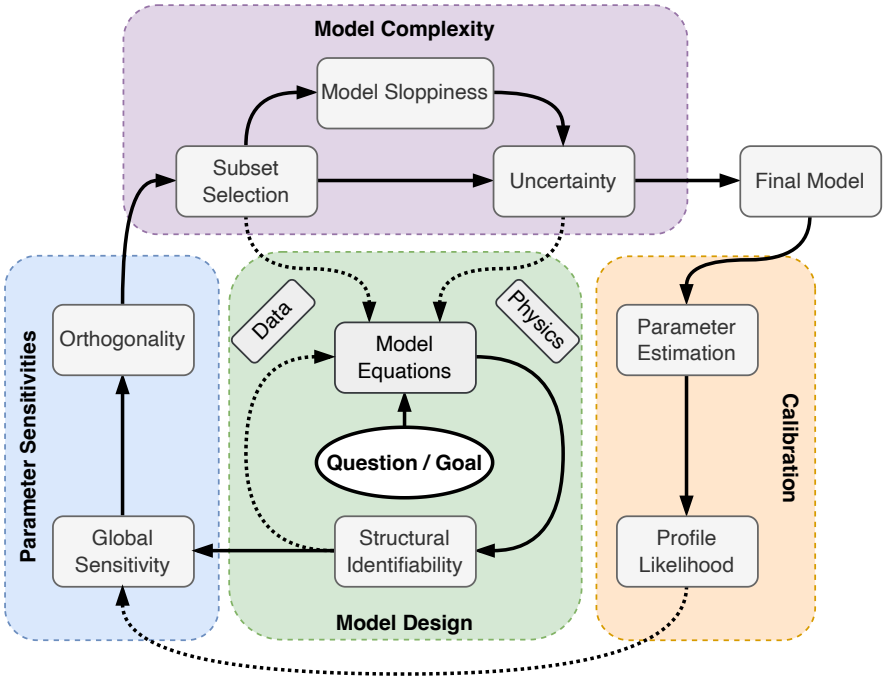

Figure 1: **The Personalisation Process**: Schematic highlighting the vital uncertainty quantification and sensitivity analysis stages involved in the personalisation of a systems biological model.

Conclusion/Main Contribution

In this talk, we propose and evaluate an extended workflow, centred on performing a comprehensive global sensitivity analysis, to improve the personalisation of models of systems biology. We compare this novel approach with previous personalisation methodologies, emphasising new considerations and highlighting the importance of offline model investigations involving global sensitivity analysis to ensure that the identified parameters are both identifiable and experimentally informative. The talk concludes with a discussion of the key challenges associated with sensitivity analysis in systems biology research.

References:

[1] Rangamani, P., & Iyengar, R. (2008). Modelling cellular signalling systems. Essays in Biochemistry, 45, 83-94.
[2] Guzzi, R., Colombo, T., & Paci, P. (2018). Inverse problems in systems biology: A critical review. Systems Biology, 69-94.
[3] Niederer, S. A., Sacks, M. S., Girolami, M., & Willcox, K. (2021). Scaling digital twins from the artisanal to the industrial. Nature Computational Science, 1(5), 313-320.
[4] Qian, G., & Mahdi, A. (2020). Sensitivity analysis methods in the biomedical sciences. Mathematical Biosciences, 323, 108306.

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Quantile oriented Shapley effect via projected random forest

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Global Sensitivity Analysis (GSA) is an important tool to better understand the behavior of black box models. Among the numerous methods for GSA, variance-based approaches have received much attention (Sobol' indices introduced in [1]). Only a few papers focus on Quantile Oriented Sensitivity Analysis (QOSA), which can help in analysing the behavior of the response at different quantile levels [2 , 3, 4, 5]. In [6], we introduced a new estimation procedure of QOSA indices based on the notion of projected random forest [7], with the initial random forest built from a criterion designed for quantiles: the pinball loss also known as quantile loss [8], with theoretical guarantees. Although informative, QOSA indices suffer from the drawback that they do not obey, even in the framework of independent inputs, any analogue to the variance decomposition offered by Sobol' indices through the theorem of Hoeffding [9]. This is the main reason why [5] introduced new indices based on the Shapley values [10]. While [11] introduced Shapley effects as variance-based measure importance, [12] suggested to adapt the value function to reach information on quantiles. In the present work, we propose to estimate the so-called quantile-oriented Shapley effects (QOSE) by combining the projection [7] of random forests built with from the quantile oriented criterion we introduced in [6], as far as arguments from Lundberg et al. Algorithm [13]. We implement our estimation procedure on both analytical examples and real data.

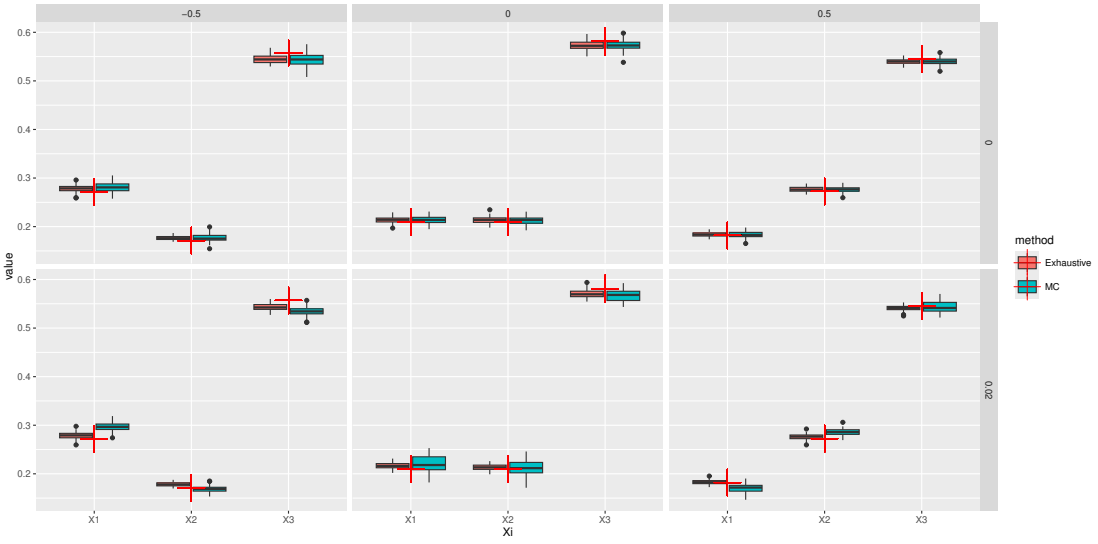

Figure 1: Box-plot on toy example with 100 repetitions. Red cross is ground truth. Red box is estimation from exhaustive search, blue box is our Monte-Carlo approximation result.

Model setting in Fig. 1:

$Y = \boldsymbol{\beta}^\intercal \boldsymbol{X}$, with $\boldsymbol{\beta} = (1,1,1)^\intercal$. $\boldsymbol{X} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ with $\boldsymbol{\mu} = (0,0,0)^\intercal, \boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \sigma_2^2 & \rho\sigma_2\sigma_3 \\ 0 & \rho\sigma_2\sigma_3 & \sigma_3^2 \end{pmatrix}, \sigma_1 = \sigma_2 = 1, \sigma_3 = 2, \rho = -0.5, 0, 0.5$. Sample size $n = 2000$.

References:

[1] Sobol' I. M., "Sensitivity estimates for nonlinear mathematical models", *Mathematical Modelling and Computational Experiments*, **1**(4):407–414, 1993.

[2] Thomas Browne, Jean-Claude Fort, Bertrand Iooss, Loïc Le Gratiet, "Estimate of quantile-oriented sensitivity indices", *hal-01450891*, 2017.

[3] Véronique Maume-Deschamps and Ibrahima Niang, "Estimation of quantile oriented sensitivity indices", *Statistics & Probability Letters*, **134**:122–127, 2018.

[4] Zdeněk Kala, "Quantile-oriented global sensitivity analysis of design resistance", *Journal of Civil Engineering and Management*, **25**(4):297–305, 2019.

[5] Kévin Elie-Dit-Cosaque and Véronique Maume-Deschamps, "Random forest based quantile-oriented sensitivity analysis indices estimation", *Computational Statistics* , **39**(4):1747–1777, 2024.

[6] Ri Wang, Véronique Maume-Deschamps, Clémentine Prieur, "Quantile oriented sensitivity analysis with random forest based on pinball loss", *hal-04606380*, 2024.

[7] Clément Bénard, Gérard Biau, Sébastien Da Veiga, Erwan Scornet, "SHAFF: Fast and consistent SHApley eFfect estimates via random Forests", *International Conference on Artificial Intelligence and Statistics*, PMLR, **151**:5563-5582, 2022.

[8] Bhat Harish S., Nitesh Kumar, Garnet J. Vaz. "Towards scalable quantile regression trees", *2015 IEEE International Conference on Big Data (Big Data)*, IEEE, 53–60, 2015.

[9] Hoeffding Wassily, "A Class of Statistics with Asymptotically Normal Distribution." *The Annals of Mathematical Statistics*, **19**(3): 293–325, 1948.

[10] Shapley Lloyd S., "A value for n-person games", *Contribution to the Theory of Games*, **2**:307–317, 1953.

[11] Owen, Art B., "Sobol'indices and Shapley value", *SIAM/ASA Journal on Uncertainty Quantification*, **2**(1):245–251, 2014.

[12] Kévin Elie-Dit-Cosaque and Véronique Maume-Deschamps, "On quantile oriented sensitivity analysis", *arXiv:2102.05895*, 2021

[13] Lundberg Scott M. and Su-In Lee, "A Unified Approach to Interpreting Model Predictions", *Advances in Neural Information Processing Systems*, **30**:4765–4774, 2017.

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Surrogate-based active learning for Sobol' indices estimation with dependent inputs

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Abstract

Sensitivity analysis is a pivotal technique in numerous scientific and engineering disciplines, employed to quantify the influence of input uncertainties on model outputs. One of the most frequently employed methodologies for global sensitivity analysis is the computation of Sobol indices [1], which provide a measure of the contribution of each input variable to the output variance. However, the computation of Sobol indices is frequently a time-consuming process due to the necessity for extensive sampling from the original simulation model. The computational burden can be alleviated by using surrogate models, such as Gaussian Process (GP) models [2], which substitute the original code with a statistical regression model that is computationally efficient. However, the accuracy of the estimated Sobol indices is contingent upon the quality of the fitted metamodel, which in turn depends on the design of computer experiments (DoE) used for its training.

The objective of this work is to discuss techniques of active learning to guarantee the quality of the metamodel. Our goal is to improve the efficiency and accuracy of Sobol indices estimation by optimising the DoE used to fit GP metamodels. This process requires the initial DoE to be augmented with points that are deemed most impactful according to an acquisition function. Our approach relies on the use of Derivative-based Global Sensitivity Measures (DGSM) [3] or its variants to derive a relevant acquisition function. We will explore these techniques in the context of complex inputs, which may include groups of dependent random vectors and functional inputs. The various adopted strategies will be tested numerically on a range of examples, from toy functions to real-world problems. In particular, the method will be applied to the digital twin of a French vineyard catchment (Beaujolais region) with the aim of designing a vegetative filter strip and reducing the transfer of water, sediment, and pesticides from the fields to the river [4, 5].

Short biography (PhD student)

I hold a Master's degree in Applied Mathematics from the University of Lyon. I am a second-year PhD student at École Centrale de Lyon and INRAE Lyon, supervised by Céline Helbert and Claire Lauvernet. The objective of my thesis is to develop active learning methods that can

handle complex input data, with applications to water quality modeling. The research is part of the MARQUISE project from the French National program LEFE (Les Enveloppes Fluides et l'Environnement) and the european Water4All AQUIGROW project (Water Security for the Planet). This thesis is also supported by the CIROQUO consortium.

References

[1] I. Sobol. "Sensitivity Estimates for Nonlinear Mathematical Models". In: 1993. (Visited on 09/05/2023).

[2] Carl Edward Rasmussen and Christopher K. I. Williams. *Gaussian Processes for Machine Learning (Adaptive Computation and Machine Learning)*. The MIT Press, 2005. ISBN: 026218253X.

[3] I.M. Sobol' and S. Kucherenko. "Derivative based global sensitivity measures and their link with global sensitivity indices". In: *Mathematics and Computers in Simulation* 79.10 (2009), pp. 3009–3017. ISSN: 0378-4754. DOI: 10.1016/j.matcom.2009.01.023.

[4] V. Gouy et al. "Ardières-Morcille in the Beaujolais, France: A research catchment dedicated to study of the transport and impacts of diffuse agricultural pollution in rivers". In: *Hydrological Processes* 35.10 (2021), e14384. DOI: 10.1002/hyp.14384.

[5] F. Veillon, N. Carluer, C. Lauvernet, and M. Rabotin. "BUVARD-MES : Un outil en ligne pour dimensionner les zones tampons enherbées afin de limiter les transferts de pesticides vers les eaux de surface". In: *50e congrès du Groupe Français des Pesticides* (NAMUR, May 18–20, 2022). in french. 2022.

New results on Generalized Hoeffding decomposition of numerical models

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Additive functional decomposition of arbitrary functions of random elements, under the form of *high-dimensional model representations* (HDMR) [1] is crucial for global sensitivity analysis [2] and more generally understanding black-box models. Formally, for random inputs $X = (X_1, \dots, X_d)^\top$, and an output $G(X)$, it amounts to finding the unique decomposition

$$G(X) = \sum_{A \in D} G_A(X_A), \tag{1}$$

where $D = \{1, \dots, d\}$, D is the set of subsets of D, and $G_A(X_A)$ are functions of the subset of input $X_A = (X_i)_{i \in A}$. Whenever the X_i are assumed to be mutually independent, such a decomposition is known as *Hoeffding's decomposition*. It is well known to allow the derivation of meaningful Sobol' indices for the analysis of the output variance, among others. Whenever the inputs are not assumed to be mutually independent, several generalizing approaches have been proposed in the literature [3-7], but at the price of imposing restrictive assumptions on the correlation structure or lacking interpretability.

Our recent works [8] hightlights the necessity of proposing a new framework at the cornerstone of probability theory, functional analysis, and abstract algebra to understand how Hoeffding's decomposition can be generalized in a more broader way to dependent inputs. By viewing random variables as measurable functions, we prove that a unique decomposition such as (1), for square-integrable black-box outputs $G(X)$, is indeed possible under two fairly reasonable assumptions on the inputs:

1. Non-perfect functional dependence;
2. Non-degenerate stochastic dependence.

While the first condition, extending non-multicolinearity, appears to very classical, the second condition can be understood through the prism of angles between subspaces of L^2, using a generalized notion of covariance between such subspaces. This originates from the following fomal rationale. Denote σ_X the σ-algebra generated by X, and $L^2\sigma_X$ the space of square-integrable σ_X-measurable real-valued functions (real-valued functions of X). From the proposed framework, defining a decomposition such as in (1) equates to defining a direct-sum decomposition of $L^2\sigma_X$ of the form

$$L^2\sigma_X = \bigoplus_{A \in D} V_A,$$

where V_A are some linear vector subspaces of functions of X_A, which can be completely characterized.

In addition, novel sensitivity indices based on this generalized decomposition can be proposed, along with theoretical arguments to justify their relevance. They first highlight that the popular SHAP method to decompose predictions is theoretically sound if and only if the inputs are mutually

independent. Besides, they lead to four new indices for quantifying the importance of inputs, based on the variance decomposition of $G(X)$. They allow the disentanglement of effects due to interactions and the effects due to the dependence structure. Such indices will be discussed, and a first illustration of the generalized decomposition involving Bernoulli random inputs, typically used in failure tree modeling in the industrial world, will be presented.

References:

[1] H. Rabitz and O. Alis, General foundations of high-dimensional model representations", *Journal of Mathematical Chemistry*, 25: 1572-8897, 1999.

[2] S. Da Veiga and F. Gamboa and B. Iooss and C. Prieur, "Basics and Trends in Sensitivity Analysis: Theory and Practice in R", SIAM, 2021.

[4] J. Hart and P.A. Gremaud, "An approximation theoretic perspective of Sobol' indices with dependent variables", *International Journal for Uncertainty Quantification*, 8, 2018

[5] G. Chastaing and F. Gamboa and C. Prieur, "Generalized Hoeffding-Sobol decomposition for dependent variables - application to sensitivity analysis", *Electronic Journal of Statistics*, 6: 2420-2448, 2012

[6] G. Hooker, "Generalized Functional ANOVA Diagnostics for High-Dimensional Functions of Dependent Variables", *Journal of Computational and Graphical Statistics*, 16: 709-732, 2007.

[7] F.Y. Kuo and I.H. Sloan and G.W. Wasilkowski and H. Woźniakowski, "On decompositions of multivariate functions", *Mathematics of Computation*, 79: 953–966, 2009.

[8] G. Peccati, "Hoeffding-ANOVA decompositions for symmetric statistics of exchangeable observations", *The Annals of Probability*, 32: 1796–1829, 2004.

[2] M. Il Idrissi and N. Bousquet and F. Gamboa and B. Iooss and J.-M. Loubes, "Hoeffding decomposition of black-box models with dependent inputs", arXiv:2310.06567, 2023.

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Sensitivity analysis for nuclear waste repository safety assessment considering heterogeneities of the host rock

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The simulation and understanding of potential radionuclide release scenarios and the transport of radionuclides through the host rock is a crucial component of the safety assessment of radioactive waste repositories in deep geological formations. In this study, we present our approach to use Geostatistical and Global Sensitivity Analysis techniques to optimize models with regard to host rock retardation mechanisms.
The aim is to evaluate parameter relevance for geological and geochemical modeling to enable prioritization of the most significant ones with respect both to future experimental and modelling resource assignments. Sorption onto mineral surfaces is an important retardation process for radionuclide migration through host rock and groundwater systems. Thus, a realistic parameterization of the geological as well as geochemical models is essential. There, heterogeneities of the host rock and the high complexity of the associated geochemistry pose challenges.

We developed a modular workflow with the following consecutive steps:

- Geostatistical simulation of a large number of realizations of the host rock based on real samples. This allows a quantitative statement to be made about the statistical dispersion of the mineralogical composition of the host rock.
- Determining the minerals exposed along potential and existing pathways for radionuclides dissolved in aqueous fluids.
- Geochemical simulation based on mechanistic calculations of the solid/liquid distribution coefficients K_d [1]. The input data is composed of the relevant mineralogical composition of the host rock, the composition of the aqueous fluids and thermodynamic sorption data (surface complexation models and ion exchange).
- The input data described above as well as the calculated K_d values are feeding a Sensitivity Analysis. Main effects and interactions are evaluated using the HDMR (High Dimensional Model Representation) and CUSUNORO (Cumulative sum of reordered normalized output) techniques [2, 3].

The workflow is implemented in Python. The geostatistical simulation is based on the truncated multi-Gaussian approach [4]. For the geochemical simulation, GWB (The Geochemist's Workbench) with a Python plug-in is used [5]. Additionally, a user-friendly toolbox is developed that supports the Global

Sensitivity Analysis by incorporating techniques such as regression methods, ANOVA (Analysis of Variance), and graphical methods.
In our workflow, the sensitivity analysis is an essential tool for evaluating and simplifying the geostatistical and geochemical models, thus saving costs and computing time. In addition, our workflow provides information about the ability of the host rock of a potential repository to retain radionuclides. Thanks to the uncertainty analysis, information can also be provided about the reliability of this statement.

References :

[1] Stockmann, M., et al. "Smart K_d-values, their uncertainties and sensitivities-Applying a new approach for realistic distribution coefficients in geochemical modeling of complex systems." *Chemosphere* 187 (2017): 277-285.
[2] Li, Genyuan, and Herschel Rabitz. "General formulation of HDMR component functions with independent and correlated variables." *Journal of mathematical chemistry* 50 (2012): 99-130.
[3] Borgonovo, Emanuele, and Elmar Plischke. "Sensitivity analysis: A review of recent advances." *European Journal of Operational Research* 248.3 (2016): 869-887.
[4] Beucher, Hélène, and Didier Renard. "Truncated Gaussian and derived methods." *Comptes Rendus Geoscience* 348.7 (2016): 510-519.
[5] Bethke, Craig M. *Geochemical and biogeochemical reaction modeling*. Cambridge university press, 2022.

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On one dimensional weighted Poincaré inequalities for Global Sensitivity Analysis

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The principle of global sensitivity analysis (GSA) is to quantify the influence of input variables (viewed as independent random variables) on the output of a multivariate function, often expensive to evaluate. (Total) Sobol indices, although commonly used for this purpose, are numerically expensive to estimate. Through *Poincaré inequalities*, they can be upper bounded by using DGSM (Derivative Global Sensitivity Measures), which are cheaper to compute (see [2]). This makes DGSM cost-effective alternatives for identifying non-influential variables.

In the preprint [1], we develop the use of *weighted Poincaré inequalities* in dimension 1 for GSA. These are similar to the classical ones but include a non-negative weight introduced in the right-hand side of the inequality. The use of weights is sometimes necessary for certain probability distributions that do not satisfy a classical Poincaré inequality (e.g., the Cauchy distribution) and provides an additional degree of freedom to enhance the precision of the upper bounds.

A first work on the use of weights in GSA was proposed in [4]. Their weight is specifically adapted for linear phenomena. Indeed, the underlying weighted Poincaré inequality is saturated (i.e. becomes an equality) for linear functions. We extend their approach by constructing a weight from any suitable monotonic (non-linear) function and developing a numerical method for estimating it. In particular, our algorithm can be used to generate:

- data-driven weights from estimators of the *main effects* (functions representing the individual influence of each variable), when they are monotonic. We establish results on stability and consistency for such weights.
- non-vanishing weights that, somewhat similar to that emphasized in [3], ensure the existence of the so-called *Poincaré chaos* and provide as well sharp lower bounds for total Sobol indices.

We illustrate the relevance of our approach through analytic toy models and a standard application for a simplified flood model (see Figure 1). For instance, Figure 2 displays total Sobol indices, along with their upper and lower bounds, of the four most influential variables – Q (a truncated Gumbell variable), K_s (a truncated normal one), Z_v and H_d (triangular ones)– of the maximal overflow of a river, whose expression is omitted here. For these variables, we compare our results with the unweighted ones derived in [2,3], observing in the weighted cases an important improvement for the upper bounds, as well as a notable gain for the lower bounds.

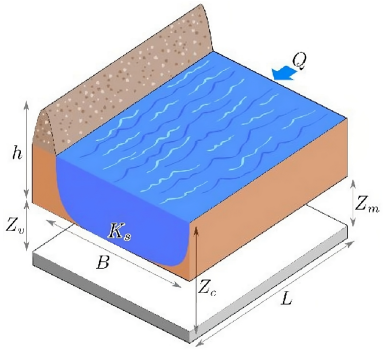

Figure 1: A dyke, a river and variables for flood modeling.

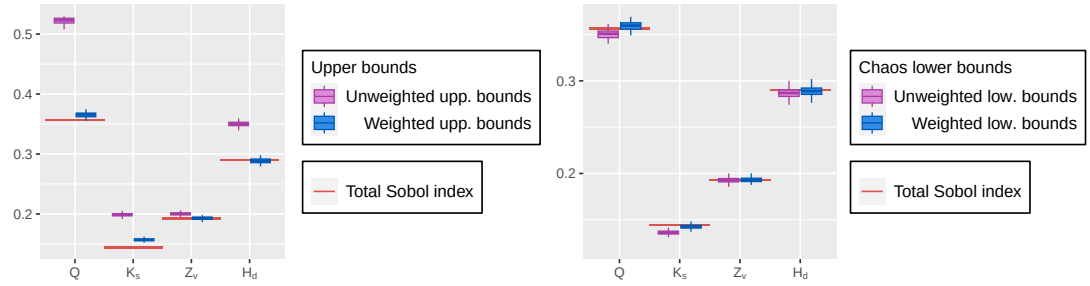

Figure 2: Total Sobol indices and several estimations of their:
(**left**) upper bounds with/without a weight, (**right**) lower bounds with/without a weight, associated with variables Q, K_s, Z_v and H_d in the maximal overflow of a river.

References:

[1] D. Heredia, A. Joulin and O. Roustant. "On one dimensional weighted Poincaré inequalities for global sensitivity analysis", Preprint 2024. Available in Arxiv soon.

[2] O. Roustant, F. Barthe and B. Iooss. "Poincaré inequalities on intervals – application to sensitivity analysis", *Electron. J. Stat.*, **11**(2):3081–3119, 2017.

[3] O. Roustant, F. Gamboa and B. Iooss. "Parseval inequalities and lower bounds for variance-based sensitivity indices", *Electron. J. Stat.*, **14**:386–412, 2020.

[4] S. Song, Z. Tong, L. Wang, S. Kucherenko, and Z. Lu. "Derivative-based new upper bound of Sobol' sensitivity measure", *Reliab. Eng. Syst. Saf.*, **187**:142–148, 2018.

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Hoeffding HDMR, Sobol' HDMR and the Shapley Value

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Let $y = f(\boldsymbol{x})$ be the quantity of interest, function of some predictors $\boldsymbol{x} = (x_1, \ldots, x_d)$, also called features or inputs. We denote $\mathcal{D} = (1, \ldots, d)$, $\mathcal{D}_{+i}$ any subset of $\mathcal{D}$ that contains the label $i \in \mathcal{D}$. We aim at assessing how sensitive is y to the x variables. To do so, it is convenient to refer to some high-dimensional model representation (hdmr) of f to assess the contribution of each input variable to y.

The first hdmr we consider is the one of W. Hoeffding [1], that is,

$$f(\boldsymbol{x}) = f_0^H + \sum_{i_1=1}^{d} f_{i_1}^H(x_{i_1}) + \sum_{i_2>i_1}^{d} f_{i_1,i_2}^H(x_{i_1}, x_{i_2}) + \cdots + f_{1\ldots d}^H(x_1, \ldots, x_d) \tag{1}$$

where, $f_0^H = \mathbb{E}[f(\boldsymbol{x})]$ and $f_{\boldsymbol{\alpha}}^H = \sum_{\beta\subseteq\alpha}(-1)^{|\boldsymbol{\alpha}|-|\boldsymbol{\beta}|}\mathbb{E}[f(\boldsymbol{x})|\boldsymbol{x}_\beta]$, $\boldsymbol{\alpha} \subseteq \mathcal{D}$. Hoeffding hdmr is always unique but the summands are only orthogonal if the x-variables are independent of each other. Otherwise, it is not obvious to infer how the input variables contribute to $f(\boldsymbol{x})$ or to its variance $\mathbb{V}[f(\boldsymbol{x})]$ given that they can contribute alone or mutually (due to correlations and interactions). L. Shapley [5] derived some statistic $\phi_i(\boldsymbol{x})$ to assess the fair contribution of x_i to y. By fair, it is meant that mutual contributions are equally shared among the cooperating variables. It results that,

$$f(\boldsymbol{x}) = f_0^H + \sum_{i=1}^{d} \phi_i(\boldsymbol{x}) \tag{2}$$

and it can be shown that $\phi_i(\boldsymbol{x}) = \sum_{\alpha\subseteq\mathcal{D}_{+i}} \dfrac{f_\alpha^H(\boldsymbol{x}_\alpha)}{|\alpha|}$. Besides, by denoting $\boldsymbol{\phi} = (\phi_1, \ldots, \phi_d)$ and $C = \mathrm{Cov}(\boldsymbol{\phi})$ the covariance matrix of $\boldsymbol{\phi}$, one obtains the variance-based Shapley value [3] as follows, $Sh_i = \sum_{j=1}^{d} C_{i,j}$.

The second hdmr we consider is the one of I.M. Sobol' [6], that stipulates that for any $\boldsymbol{u} \sim \mathcal{U}(0,1)^d$, we can write,

$$g(\boldsymbol{u}) = g_0 + \sum_{i_1=1}^{d} g_{i_1}(u_{i_1}) + \sum_{i_2>i_1}^{d} g_{i_1,i_2}(u_{i_1}, u_{i_2}) + \cdots + g_{1\ldots d}(u_1, \ldots, u_d) \tag{3}$$

with the summands orthogonal to each other by imposing that $\int_0^1 g_\alpha(\boldsymbol{x}_\alpha)\mathrm{d}u_{i_k} = 0$, $\forall i_k \in \boldsymbol{\alpha}$. The hierarchical Rosenblatt transformation (RT) [4] provides the link between $\boldsymbol{u}$ and $\boldsymbol{x}$, as follows,

$$\begin{cases} u_{i_1} = F_{i_1}(x_{i_1}) \\ u_{i_2} = F_{i_2|i_1}(x_{i_2}|x_{i_1}) \\ \vdots \\ u_{i_d} = F_{i_d|\sim i_d}(x_{i_d}|\boldsymbol{x}_{\sim i_d}) \end{cases} \tag{4}$$

where $(i_1, \ldots, i_d)$ is an arbitrary ordering of the set $(1, \ldots, d)$, F_{i_1} is the marginal cumulative density function (cdf) of x_{i_1}, $F_{\alpha|\beta}$ is the conditional cdf of $\boldsymbol{x}_\alpha$ on $\boldsymbol{x}_\beta$ with $\alpha \cap \beta = \emptyset$. Obviously, $y = f(\boldsymbol{x}) = g(\boldsymbol{u})$, but neither the RT is unique (unless the variables be independent of each other) and nor the Sobol' hdmr.

We note that only $g_0 = f_0^H$ and $g_{i_1}(F_{i_1}^{-1}(u_{i_1})) = f_{i_1}^H(x_{i_1})$ when the inputs are not independent. From the Sobol' hdmr in Eq.(3) it is possible to compute the following variance-based sensitivity

indices [2],

$$S_{x_{i_1}} = \frac{\mathbb{V}\left[\mathbb{E}\left[y|u_{i_1}\right]\right]}{\mathbb{V}\left[y\right]} = \frac{\mathbb{V}\left[g_{i_1}(u_{i_1})\right]}{\mathbb{V}\left[y\right]}, \tag{5}$$

$$ST^{ind}_{x_{i_d}} = \frac{\mathbb{E}\left[\mathbb{V}\left[y|\boldsymbol{u}_{\sim i_d}\right]\right]}{\mathbb{V}\left[y\right]} = \frac{\sum_{\alpha \subseteq \mathcal{D}_{+i_d}} \mathbb{V}\left[g_\alpha(u_\alpha)\right]}{\mathbb{V}\left[y\right]}, \tag{6}$$

$$S^{ind}_{x_{i_d}} = \frac{\mathbb{V}\left[\mathbb{E}\left[y|u_{i_d}\right]\right]}{\mathbb{V}\left[y\right]} = \frac{\mathbb{V}\left[g_{1\ldots d}(u_1,\ldots,u_d)\right]}{\mathbb{V}\left[y\right]}, \tag{7}$$

$$ST_{x_{i_1}} = \frac{\mathbb{E}\left[\mathbb{V}\left[y|\boldsymbol{u}_{\sim i_1}\right]\right]}{\mathbb{V}\left[y\right]} = \frac{\sum_{\alpha \subseteq \mathcal{D}_{+i_1}} \mathbb{V}\left[g_\alpha(u_\alpha)\right]}{\mathbb{V}\left[y\right]}, \tag{8}$$

$S_{x_{i_1}}$ is the amount of variance explained by x_{i_1} alone including its cooperative contribution due to its dependence on $\boldsymbol{x}_{\sim i_1}$ while $S^{ind}_{x_{i_d}}$ is the one of x_{i_d} that does not account for the mutual contribution. $ST_{x_{i_1}}$ is the amount of variance explained by x_{i_1} including all its mutual contributions (i.e. interactions+correlations) with $\boldsymbol{x}_{\sim i_1}$ while $ST^{ind}_{x_{i_d}}$ does not take into account contributions due to the dependences of x_{i_d} on $\boldsymbol{x}_{\sim i_d}$.

In my talk I will discuss the pros and the cons of the different approaches to analyze model responses or any given dataset and I will show some examples.

References

[1] W. Hoeffding. A class of statistics with asymptotically distribution. *Annals of Mathematics and Statistics*, 19:293–325, 1948.

[2] T. A. Mara and W. E. Becker. Polynomial chaos expansionfor sensitivity analysis of model output with dependent inputs. *Reliability Engineering and System Safety*, 214:107795, 2021.

[3] A. B. Owen and C. Prieur. Sobol' indices and shapley value. *J. of Uncertainty Quantification*, 2:245–251, 2014.

[4] M. Rosenblatt. Remarks on the multivariate transformation. *Annals of Mathematics and Statistics*, 43:470–472, 1952.

[5] L. S. Shapley. *A value for n-person games*, chapter Contribution to the Theory of Games II (Annals of Mathematics Studies 28), pages 307–317. Princeton University Press,, Princeton, NJ, 1953.

[6] I. M. Sobol'. Sensitivity estimates for nonlinear mathematical models. *Math. Mod. and Comput. Exp.*, 1:407–414, 1993.

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Sequential transport for density estimation and its applications

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Abstract

Transport-based methods are receiving growing interest because of their ability to sample easily from the approximated density. These methods aim at building a deterministic diffeomorphism $\mathcal{T}$, also called a transport map, which pushes forward an arbitrary reference probability density ρ_{ref} to a given target probability density π to be approximated. Typically, the transport map $\mathcal{T}$ is parameterized *e.g.* by invertible neural networks and fitted using variational methods of the form

$$\min_{\mathcal{T}\in\mathcal{M}} \mathrm{D}(\pi||\mathcal{T}_\sharp\,\rho_{\text{ref}}) \tag{1}$$

with a statistical divergence $\mathrm{D}(\cdot\,||\cdot)$, typically the (reversed) KL-divergence. An emerging strategy for this problem is to first estimate π by $\widetilde{\pi}$ and then to compute a map $\mathcal{T}$ which exactly pushes forward ρ_{ref} to $\widetilde{\pi}$, see [2, 1]. Among the infinitely many maps $\mathcal{T}$ which satisfy $\mathcal{T}_\sharp\,\rho_{\text{ref}} = \widetilde{\pi}$, the Knothe–Rosenblatt (KR) map is rather simple to evaluate since it requires only computing the cumulative distribution functions (CDFs) of the conditional marginals of $\widetilde{\pi}$. In general, problem (1) is difficult to solve when π is multimodal or when it concentrates on a low-dimensional manifold. The solution proposed in [1] consists in introducing an arbitrary sequence of bridging densities

$$\pi^{(1)}, \pi^{(2)}, \ldots, \pi^{(L)} = \pi, \tag{2}$$

with increasing complexity. The sequential strategy consists in building L transport maps $\mathcal{Q}_1, \ldots, \mathcal{Q}_L$ one after the other by solving

$$\min_{\mathcal{Q}_\ell\in\mathcal{M}} \mathrm{D}(\pi^{(\ell)}||(\mathcal{T}_{\ell-1}\circ\mathcal{Q}_\ell)_\sharp\,\rho_{\text{ref}}), \quad \text{where} \quad \mathcal{T}_{\ell-1} = \mathcal{Q}_1\circ\ldots\circ\mathcal{Q}_{\ell-1}. \tag{3}$$

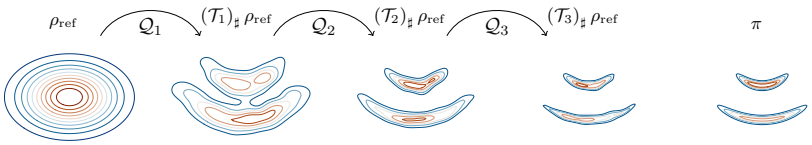

Figure 1: Visualization of the approximation of a bimodal density π (right) using $L = 3$ intermediate tempered densities estimated using SoS (4) and a Gaussian reference density ρ_{ref}.

For suitable statistical distances, so that $\mathrm{D}(\pi||\mathcal{T}_\sharp\rho) = \mathrm{D}(\mathcal{T}^\sharp\pi||\rho)$, these problems are equivalent to estimating the pullback density $(\mathcal{T}_{\ell-1})^\sharp\pi^{(\ell)}$ with an intermediate approximation $\rho^{(\ell)} = (\mathcal{Q}_\ell)_\sharp\,\rho_{\mathrm{ref}}$.

In our work, we contribute to this methodology as follows.

First, we employ Sum-of-Squares (SoS) densities to approximate the intermediate densities $\rho^{(\ell)}$ using α-divergences $\mathrm{D}_\alpha(\cdot||\cdot)$. We sequentially solve the variational density approximation problem as in Equation (3) with D_α as the statistical divergence and where

$$\rho^{(\ell)}(\boldsymbol{x}) = \left(\Phi(\boldsymbol{x})^\top A_\ell \Phi(\boldsymbol{x})\right)\rho_{\mathrm{ref}}(\boldsymbol{x}), \tag{4}$$

for some arbitrary orthonormal basis function Φ in $L^2(\rho_{\mathrm{ref}})$. Here, the positivity of the matrix $A_\ell \succeq 0$ ensures the density $\rho^{(\ell)}$ to be positive. Since the α-divergence is defined for general *unnormalized* densities, it is not necessary to know the normalizing constant of π beforehand. α-divergences $\mathrm{D}_\alpha(\cdot||\cdot)$ with parameter $\alpha \in \mathbb{R}$ include the Hellinger distance and KL-divergence, which have been used in previous works. The proposed SoS densities permit to efficiently normalize the estimated unnormalized density and to compute the KR map $\mathcal{Q}_\ell$ such that $(\mathcal{Q}_\ell)_\sharp\,\rho_{\mathrm{ref}} = \rho^{(\ell)}$. This combined use of α-divergence for performing SoS density estimation results in a *convex* optimization problems which can be efficiently solved using off-the-shelf toolboxes.

Second, we extend the methodology to the scenario where *only samples* $\boldsymbol{X}^{(1)}, \dots, \boldsymbol{X}^{(N)}$ from π are available, as opposed to *point-evaluations* of the target density π. In this scenario, we propose to use diffusion-based bridging densities $\pi^{(\ell)}(\boldsymbol{x})$ where the distribution follows a time–inversed diffusion process such as the Ornstein-Uhlenbeck process with time parameters $t_{\ell-1} \leq t_\ell$ and $t_L = 0$. This idea is at the root of diffusion models.

Third, we present a novel convergence analysis using the geometric properties of α-divergences. This analysis unifies and extends previous analyses proposed in [3, 1] and, more interestingly, it guides the choice of bridging densities. In particular, we show that a smart choice of β_ℓ for tempered densities or of t_ℓ for diffusion-based densities yield a convergence rate of $\mathcal{O}(1/L^2)$ with respect to the number of layer L.

Last, we give an outlook for using sequential measure transport to solve optimal transport problems, where we mitigate the difficulty of estimating the optimal coupling by a sequence of entropic regularized problems.

We demonstrate the capability of our proposed method in unsupervised learning, Bayesian inverse, and optimal transport problems in moderate dimensions.

Short biography (PhD student)

I am an electrical engineer, now pursuing a PhD in applied mathematics at the Université Grenoble Alpes while working at INRIA in the AIRSEA team. In my thesis, I work on estimation of densities using compositional methods and its applications.

References

[1] Tiangang Cui and Sergey Dolgov. Deep composition of tensor-trains using squared inverse Rosenblatt transports. *Foundations of Computational Mathematics*, September 2021. arXiv:2007.06968 [cs, math, stat].

[2] Sergey Dolgov, Karim Anaya-Izquierdo, Colin Fox, and Robert Scheichl. Approximation and sampling of multivariate probability distributions in the tensor train decomposition. *Statistics and Computing*, 30(3):603–625, May 2020.

[3] Josephine Westermann and Jakob Zech. Measure transport via polynomial density surrogates, November 2023. arXiv:2311.04172 [cs, math, stat].

Multi-output excursion set estimation applied to the calibration of a wind turbine numerical model

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Many industrial challenges involve excursion set estimation, which can be defined as identifying a set of feasible input values for black-box models. These input values must satisfy a constraint on the model's output, such as remaining below a specified threshold (e.g., [1]). A widely used approach to address this problem involves modeling the expensive black-box function as a realization of a Gaussian Process (GP). This surrogate model is constructed through a sequential Design of Experiments, with points selected in the design space $\mathbb{X} \subset \mathbb{R}^d$ based on the optimization of an acquisition criterion (see [2] for more details). The Bichon criterion [3] is a classical approach to excursion set estimation that offers a balanced trade-off between exploring the design space and exploiting known regions around the boundary of the excursion set.

In this work, we focus on the pre-calibration of a numerical model for wind turbines. The simulator, treated as a black-box model, takes system parameters (such as stiffness coefficients of various materials) as inputs and returns vibration frequencies and deformation eigenmodes as outputs in response to wind loads. The inputs are denoted by Θ, and the outputs by $\lambda_i(\Theta)$ for frequencies and $\mathrm{Mod}_i(\Theta)$ for modes, where $i \in 1, \ldots, p$, and p is the number of modes.

Our goal is to estimate the set of feasible input parameters that ensure the simulator's outputs match the experimentally observed data. More precisely, we aim to pre-calibrate the numerical model (Figure 1) by determining a set of feasible input parameters Θ for the simulator. These parameters must ensure that the vibration frequencies $\lambda_i(\Theta)$ and deformation modes $\mathrm{Mod}_i(\Theta)$ computed by the simulator are sufficiently close, within predefined thresholds, to the observed frequencies $\lambda_i^\star$ and modes $\mathrm{Mod}_i^\star$, derived from experimental data based on Operational Modal Analysis (OMA) (e.g., [3]).

Figure 1: Schematic diagram of the wind turbine simulator.

Mathematically, we focus on black-box models with vector-valued outputs $\boldsymbol{G} := (G_1, \ldots, G_p)$. The partial excursion sets are defined as follows:

$$\forall\, i \in \{1, \ldots, p\},\ \Gamma_i^\star := \{\mathbf{x} \in \mathbb{X}, G_i(\mathbf{x}) \leq T_i\}. \tag{1}$$

In [5], a criterion is proposed for estimating the intersection of partial excursion sets. In the context of our pre-calibration problem, knowing the input values that are feasible for all output components is insufficient. Therefore, this work aims to estimate the partial excursion sets for each output component simultaneously. This allows us to determine, for any given point in the design space, which output component exceeds its respective threshold.

We propose two natural extensions of the Bichon criterion: (1) Alternating Scal, which alternates optimization between components, and (2) Pareto Scal, which leverages Pareto solutions from the bi-objective optimization of the Bichon criteria. These two approaches use separate GP models for each output component. We also introduce a vector extension (Vect) of the Bichon criterion, based on minimizing the distances between each component of the GP and its respective threshold. This extension relies on a multi-output GP model that incorporates correlations between outputs (see [6]) and requires the computation of orthant probabilities in multivariate normal distributions.

The methodologies introduced above are compared across several analytical examples, considering 2 and 4 input components, and 2 output components. Subsequently, these methodologies are applied to the pre-calibration stage of the wind turbine simulation, exploring two different problem formulations based on two dissimilarity measures. The first focuses on the two primary deformation modes, while the second considers all deformation modes and all vibration frequencies.

Our results on both analytical examples and the wind turbine simulator pre-calibration demonstrate the effectiveness of our proposed strategies for estimating partial excursion sets. However, limitations associated with the covariance structure of the multi-output GP model suggest areas for future refinement.

References:

[1] M.R. El Amri, C. Helbert, O. Lepreux, M. Munoz Zuniga, C. Prieur, and D. Sinoquet. "Data-driven stochastic inversion via functional quantization.", *Statistics and Computing*, 30:525-541, 2020.

[2] V. Picheny, D. Ginsbourger, O. Roustant, R. T. Haftka, and N. Kim. "Adaptive designs of experiments for accurate approximation of a target region". *Journal of Mechanical Design*, 132(7), 071008-9. 2010.

[3] B.J. Bichon, M.S. Eldred, L. Painton Swiler, S. Mahadevan, and J.M. McFarland. "Efficient global reliability analysis for nonlinear implicit performance functions". *AIAA journal*, 46(10):2459-2468, 2008.

[4] R. Brincker, & C. Ventura, "Introduction to operational modal analysis". *John Wiley & Sons*, 2015

[5] T.O. Fossum, C. Travelletti, J. Eidsvik, D. Ginsbourger, and K. Rajan. "Learning excursion sets of vector-valued gaussian random fields for autonomous ocean sampling". *The annals of applied statistics*, 15(2):597-618, 2021.

[6] H. Liu, J. Cai, & Y.S. Ong. "Remarks on multi-output Gaussian process regression". *Knowledge-Based Systems*, 144, 102-121, 2018.

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Variational inference for approximate reference priors using neural networks

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Abstract

In Bayesian statistics, the choice of the prior distribution can have an important influence on the posterior and the parameter estimation. This is especially true if few data samples are available and if the prior is quite informative. The subjectivity intrinsic to the choice of the prior should be prohibited in cases with real safety and auditability issues, this is why we wish to define the prior by a "objective" criterion.

We utilize the reference prior theory formalized in [1], and extended, among others, in [4] and [5], which defines priors that maximize the mutual information $I_D(\cdot \mid N)$ with D being a divergence and N is the number of data samples. The mutual information can be interpreted as the difference between the prior and the posterior. Hence, these priors maximize the importance of the information provided by the data :

$$\pi^* \in \underset{\pi \text{ prior}}{\arg\max}\, I_D(\pi \mid N).$$

However, computing reference priors is a difficult task in general. We develop in this work a flexible algorithm based on variational inference which computes approximations of reference priors from a set of parametric distributions π_λ on the variable of interest θ. Using the approach of [2] and [3], we parameterize the prior by a neural network g with parameters λ and a simple latent variable ε :

$$\theta \sim \pi_\lambda \iff \theta = g(\lambda, \varepsilon) \quad \text{and} \quad \varepsilon \sim \mathbb{P}_\varepsilon.$$

The algorithm is not limited to the uni-dimensional case $\theta \in \mathbb{R}$ and is compatible with a larger class of dissimilarity measures, namely α-divergences [4] and not only with the Kullback-Leibler divergence.

We also propose a simple method to recover a relevant approximation of the parametric posterior distribution $\pi_\lambda(\theta \mid X)$ using Markov Chain Monte Carlo methods even if the density function of π_λ is not known in general.

We apply the algorithm on several statistical models of increasing complexity. We show the usefulness of this approach by recovering the Jeffreys prior, which is the asymptotic reference prior for the considered divergences. The performance of the algorithm is evaluated on the

prior distributions as well as the posterior distributions, jointly using variational inference and MCMC sampling. Finally, we also show that our algorithm can be used for related problems, such as the approximation of reference priors under moment constraints as theorized in [5].

Our results leave us confident that our algorithm can be transposed to various statistical inference problems to produce robust Bayesian estimates.

Short biography (PhD student)

The work presented here is the result of my current research internship, which takes place at the CEA, in Saclay. After my graduation from my Master's degree in mathematics and machine learning (master MVA, ENS Paris-Saclay), I will pursue with a PhD between the École polytechnique and the CEA, supervised by Josselin Garnier (CMAP), Cyril Feau and Baptiste Kerleguer (CEA) on the subject of multi-fidelity models, starting in November. The PhD thesis is funded by the CEA.

References

[1] James O. Berger, José M. Bernardo, and Dongchu Sun. The formal definition of reference priors. *The Annals of Statistics*, 37(2):905 – 938, 2009.

[2] Clément Gauchy, Antoine Van Biesbroeck, Cyril Feau, and Josselin Garnier. Inférence variationnelle de lois a priori de référence. In *Proceedings des 54èmes Journées de Statistiques (JdS)*. SFDS, 07 2023.

[3] Eric Nalisnick and Padhraic Smyth. Learning approximately objective priors. In *Proceedings of the 33rd Conference on Uncertainty in Artificial Intelligence (UAI)*. Association for Uncertainty in Artificial Intelligence (AUAI), 2017.

[4] Antoine Van Biesbroeck. Generalized mutual information and their reference priors under csizar f-divergence, 2024.

[5] Antoine Van Biesbroeck. Properly constrained reference priors decay rates for efficient and robust posterior inference, 2024.

The universe of uncertainty that didn't hide

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In a series of recent papers [1, 2] we have offered global sensitivity analysis (GSA) [3] as the solution for the recently manifested problem of analytic variability in applied statistical and econometric work, commonly associated with the so-called "Garden of Forking Paths" [4, 5] that analysts engage with when setting up an investigation. Our title refers to the expression "A universe of uncertainty hiding in plain sight" [6] that has been used to comment on the results of multi-analysis studies displaying unexpected variability. In a sense, in our SAMO community of practitioners engaged in sensitivity analysis, this uncertainty was indeed always in plain sight – and was chased with an array of techniques going from efficient design of numerical experiments to setting-specific sensitivity analysis practices. Considering these practice as self-evident may constitute a sort of SAMO-specific bias, especially given the complex and nuanced relation that quantification sciences have with uncertainty across different disciplines, especially at the interfaces between science, society and policy [7]. Thus, we look at the issue of "analytic flexibility" discovered in this new context and reconnect it to how GSA has been taken up in several disciplines to test the quality of a quantification. In particular we recall early econometricians' works [8, 9] suggesting global sensitivity analysis (GSA) to test the robustness of a quantitative inference, and comment on the recommendations' slow take up [10] in both econometrics and other disciplines. We show how today a mature [11] GSA approach permits analysts to properly chart gardens of forking paths before venturing into one, or to make sense of a multi-analyst experiment after it has been done. GSA allows the "universe of uncertainty" hidden in multi-analyst studies to be unveiled (uncertainty quantification) and characterised (sensitivity analysis proper), especially in relation to pattern of strong dependencies of the inference upon high order interaction terms that appear to characterise the experimental settings of multi-analyst studies [12]. We illustrate our treatment of a a recent multi-analyst study from Breznau and co-workers [13], that we extend here to a different policy setting. We call our application of GSA to the garden of forking path a "modelling of the modelling process" [14, 15] (MOMP), detailing the differences between this and a more recent "multiverse analysis" [16]. We trace a path from global sensitivity analysis – often concerned with mostly parametric uncertainty – t0 MOMP – where the modelling process is opened up to investigation – to sensitivity auditing [17] where the policy dimensions of an analysis are questioned. We conclude offering a programming environment for these studies.

Bibliography

[1] A. Saltelli, A. Puy, A. Lachi, and N. Breznau. "Global sensitivity analysis unveils the hidden universe of uncertainty in multiverse studies". en-us. In: *OSF Meta ArXiv* (2024). DOI: 10.31222/osf.io/b67w9.

[2] A. Saltelli, N. Breznau, A. Lachi, and A. Puy. "Leamer Reloaded: A long-neglected suggestion to use global sensitivity analysis before publishing a quantification is rediscovered". In: *In progress* (2024).

[3] A. Saltelli, M. Ratto, T. Andres, F. Campolongo, J. Cariboni, D. Gatelli, M. Saisana, and S. Tarantola. *Global sensitivity analysis: the primer*. John Wiley & Sons, 2008.

[4] A. Gelman and E. Loken. "The garden of forking paths: Why multiple comparisons can be a problem, even when there is no "fishing expedition" or "p-hacking" and the research hypothesis was posited ahead of time". In: *Department of Statistics, Columbia University* 348.1-17 (2013), p. 3.

[5] J. L. Borges et al. "The garden of forking paths". In: *Collected fictions* 119 (1962).

[6] P. Engzell. "A universe of uncertainty hiding in plain sight". In: *Proceedings of the National Academy of Sciences* 120.2 (2023), e2218530120.

[7] I. Scoones and A. Stirling. *The Politics of Uncertainty*. Ed. by I. Scoones and A. Stirling. Abingdon, Oxon; New York, NY: Routledge, 2020. — Series: Pathways to sustainability: Routledge, 2020. DOI: 10.4324/9781003023845.

[8] E. E. Leamer. "Sensitivity analyses would help". In: *The American Economic Review* 75.3 (1985), pp. 308–313.

[9] P. Kennedy. *A guide to econometrics*. John Wiley & Sons, 2008.

[10] E. E. Leamer. "Tantalus on the Road to Asymptopia". In: *Journal of Economic Perspectives* 24.2 (2010), pp. 31–46.

[11] A. Saltelli, A. J. Jakeman, S. Razavi, and Q. Wu. "Sensitivity analysis: A discipline coming of age". In: *Environmental Modelling and Software* 146,105226 (2021). DOI: https://doi.org/10.1016/j.envsoft.2021.105226.

[12] A. Puy, P. Beneventano, S. A. Levin, S. Lo Piano, T. Portaluri, and A. Saltelli. "Models with higher effective dimensions tend to produce more uncertain estimates". In: *Science Advances* 8.eabn9450 (2022).

[13] N. Breznau, E. M. Rinke, A. Wuttke, H. H. Nguyen, M. Adem, J. Adriaans, A. Alvarez-Benjumea, H. K. Andersen, D. Auer, F. Azevedo, et al. "Observing many researchers using the same data and hypothesis reveals a hidden universe of uncertainty". In: *Proceedings of the National Academy of Sciences* 119.44 (2022), e2203150119.

[14] A. Saltelli and A. Puy. "What Can Mathematical Modelling Contribute to a Sociology of Quantification?" en. In: *Humanities and Social Sciences Communications* 10.213 (2023). DOI: 10.2139/ssrn.4212453.

[15] S. L. Piano, R. Sheikholeslami, A. Puy, and A. Saltelli. "Unpacking the modelling process via sensitivity auditing". In: *Futures* 144 (2022), p. 103041.

[16] S. Steegen, F. Tuerlinckx, A. Gelman, and W. Vanpaemel. "Increasing transparency through a multiverse analysis". In: *Perspectives on Psychological Science* 11.5 (2016), pp. 702–712.

[17] A. Saltelli, Â. Guimaraes Pereira, J. P. Van der Sluijs, and S. Funtowicz. "What do I make of your latinorum? Sensitivity auditing of mathematical modelling". In: *International Journal of Foresight and Innovation Policy* 9.2-3-4 (2013), pp. 213–234.

Democratizing global sensitivity analysis with a no-code web dashboard.

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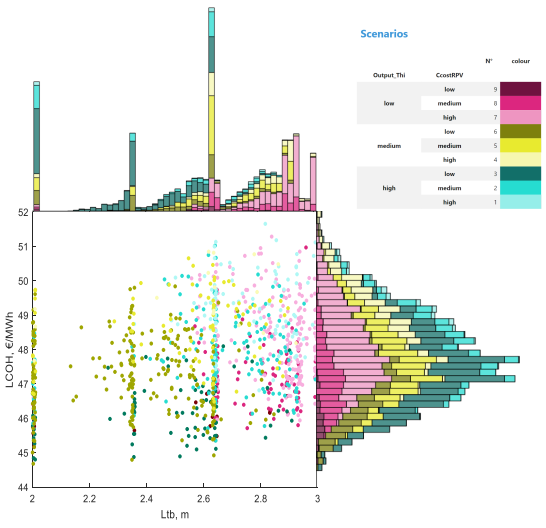
Global sensitivity analysis (GSA) is undoubtedly a valuable exercise to understand the behavior of a computational model and to devise an effective intervention. Moreover, policies and decisions that were based on a limited comprehension of uncertainty often turned out to be disastrous (5; 9; 1; 10). However, many factors contribute to **the near universal non-take-up** of GSA, including thematic complexity, implementation challenges, and computational costs (8). Furthermore, GSA lacks a visualization convention, which leads to the situation, where a majority of studies employing GSA compute the strength of the effects of input variables, but fail to examine their shape (2), which often can be critical for decision-making (3).

A hybrid sensitivity-uncertainty approach Simulation Decomposition (SimDec) was created to tackle the above challenges. At its core, it has an efficient computation of variance-based sensitivity indices (2), which further informs an intelligent visualization that transcribes multidimensional relationships onto a two-dimensional graph (3), all implemented in open-source packages and complemented by a no-code web dashboard freely accessible at https://simdec.io (6). SimDec as a method has been shown to provide added insights for the wide range of models from different fields (business, engineering, environment) and formulated in a variety of mathematical frameworks (4).



This conference presentation introduces the latest development in the SimDec dashboard: the two-output graphs. Its usefulness is demonstrated on the selected cases from operations research. The two-output graph consists of a scatterplot constructed for two arbitrary model outputs selected by the user, and the two corresponding histograms that show the marginal distributions of the two outputs. Further, the SimDec procedure is used to identify the most influential inputs for the first output and perform the decomposition by these inputs applied to the entire graph set: the scatterplot and the histograms become correspondingly color-coded.

The figure demonstrates the results of an optimization model for a heat exchanger of a nuclear district heating reactor (Saari et al.), in particular, the relationship between the two optimization outcomes, levelized cost of heat (*LCOH* on Y-axis) and the mechanical design characteristic (*Ltb* on X-axis), and their dependency on the two most influential input variables.

The optimization favors certain values of *Ltb* creating peaks in its distribution. *LCOH* slightly grows with larger *Ltb*. The inputs influence the mechanical design considerably, but not the LCOH, which is only slightly affected by the inputs.

Through the two-output graph on SimDec dashboard, the user acquires visual access to the multivariate input-output behavior of a model, supplied in an intuitive and interactive graphical format. The entire complexity of the GSA as a topic therefore remains behind the scenes, while being crucial in the process of creating meaningful graphics. Consequently, we believe that the dashboard has the potential to contribute in democratizing GSA, making its valuable functionality accessible for modelers even with limited mathematical training.

BIBLIOGRAPHY

[1] Hubbard, D. W. (2020). *The failure of risk management: Why it's broken and how to fix it.* John Wiley & Sons.

[2] Kozlova, M., Ahola, A., Roy, P. T., and Yeomans, J. S. (2023). Simple binning algorithm and simdec visualization for comprehensive sensitivity analysis of complex computational models. *arXiv preprint arXiv:2310.13446*.

[3] Kozlova, M., Moss, R. J., Yeomans, J. S., and Caers, J. (2024). Uncovering heterogeneous effects in computational models for sustainable decision-making. *Environmental Modelling & Software*, 171:105898.

[4] Kozlova, M. and Yeomans, J. S. (2024). *Sensitivity Analysis for Business, Technology, and Policymaking: Made Easy with Simulation Decomposition (SimDec).* Routledge, London, UK.

[5] Lo Piano, S., Lőrincz, M. J., Puy, A., Pye, S., Saltelli, A., Smith, S. T., and van der Sluijs, J. (2024). Unpacking the modeling process for energy policy making. *Risk Analysis*, 44(6):1273–1284.

[6] Roy, P. T. and Kozlova, M. (2024). Simulation decomposition in python. *Journal of Open Source Software*, 9(98):6713.

[Saari et al.] Saari, J., Kozlova, M., Suikkanen, H., Sermyagina, E., Hyvärinen, J., and Yeomans, J. S. Global sensitivity analysis of nuclear district heating reactor primary heat exchanger optimization. *Available at SSRN 4784218*.

[8] Saltelli, A., Aleksankina, K., Becker, W., Fennell, P., Ferretti, F., Holst, N., Li, S., and Wu, Q. (2019). Why so many published sensitivity analyses are false: A systematic review of sensitivity analysis practices. *Environmental modelling & software*, 114:29–39.

[9] Saltelli, A., Bammer, G., Bruno, I., Charters, E., Di Fiore, M., Didier, E., Nelson Espeland, W., Kay, J., Lo Piano, S., Mayo, D., et al. (2020). Five ways to ensure that models serve society: a manifesto.

[10] Savage, S. L. and Markowitz, H. M. (2009). *The flaw of averages: Why we underestimate risk in the face of uncertainty.* John Wiley & Sons.

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Reliability sensitivity analysis with failure samples obtained by Markov chain Monte Carlo simulation

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Reliability is an essential criterion for measuring the quality of many engineering structures. A highly reliable structure will have a low probability of failing and causing catastrophic results. To design highly reliable structures more efficiently, one must understand the influence that different uncertain factors have on failure probability. This is known as reliability sensitivity analysis, typically achieved via so-called Reliability Sensitivity Indices (RSIs). Traditional reliability sensitivity analysis uses partial derivatives of failure probability with respect to the distributional parameters of uncertain input variables, resulting in *local* RSIs corresponding to nominal parameter values. On the contrary, *global* reliability sensitivity analysis measures the average effect of uncertain factors on failure probability, averaged across their entire distribution.

The global RSI based on Safety/failure Classification of model output (StarComp) can effectively measure the average effects of uncertain model inputs on the failure of engineering structures. The StarComp RSI is defined through the difference between a specified input variable's failure-conditional Probability Density Function (PDF) and its unconditional PDF. These different PDFs are defined by classifying model outputs (and corresponding input variable sets) according to whether they indicate a failure state or not, i.e., whether the so-called limit state function is negative or positive. As StarComp unveils these failure-conditional PDFs, it provides insights into both the importance of input variables for reliability and the likelihood of failure associated with specific input values.

To estimate the StarComp RSI, the first step is to assess the input variables' failure-conditional PDF. An intuitive approach to achieve this task is crude Monte Carlo simulation (via a naive rejection sampling based on "fail" versus "safe"). However, such a crude Monte Carlo is not computationally efficient, especially for problems with small failure probabilities. From the perspective of Bayes' theorem, the failure-conditional PDF can also be considered as a posterior PDF, which can be simulated directly with widely-used Markov Chain Monte Carlo (MCMC) methods. However, due to the binary property of the failure indicator function (a.k.a. likelihood in the Bayesian setting), locating an initial sample in the failure domain is an essential step.

We propose a two-stage MCMC simulation method to simulate the failure-conditional PDF efficiently and then estimate the StarComp RSI. Its general idea is to find an initial failure sample in the first stage with a modified MCMC. The second stage runs a straightforward MCMC, starting from the initial failure sample, to explore the failure-conditional PDF. For problems with multiple failure domains, multiple random chains are simulated independently in the first stage to obtain multiple failure samples in different failure domains. Then, starting with each failure sample, the second stage runs multiple independent Markov chains to sample from the failure-conditional PDF across different failure domains. A set of weights is also constructed for the failure samples from different failure domains to estimate the failure-conditional PDF correctly.

Checkerboard Partitioning for Third-Order Sensitivity Analysis: Application in Reactive Transport Modeling for Nuclear Waste Disposal

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Keywords: Third Order Sensitivity Analysis, Graphical Representation of Sensitivity, Nuclear Waste Disposal, Radionuclide Retention, Geochemical Modeling

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Towards Methodological Refinement of Power System Protection Testing via Statistical Design of Experiments

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The growing complexity of modern power systems calls for sophisticated protection functions in order to ensure the correct operation as well as the reliability, quality and security of supply. Testing the protection functions implemented in protection equipment/systems is, hence, a vital activity for ultimately preventing the potentially disruptive consequences of protection failures.

In general, any testing activity requires three main components:

1. **What to test**, i.e., the Device Under Test (DUT), whose ability to operate based on manufacturers' specification is tested under realizable power system conditions.
2. **Where to test**, i.e., the platform over which to conduct the tests, which is usually based on a real-time hardware-in-the-loop simulation test set-up to investigate the DUT behavior under close-to-operation conditions.
3. **How to test**, i.e., the methodology defining which and how many tests to conduct in each experiment, by deliberately varying different factors potentially having an impact on the system response.

In power system protection testing, while the first two components are well established, the testing methodologies are still less mature and quite fragmented, and are thus the focus of our work. Harmonization efforts have been produced by national and international standards, such as the IEC 60255-121:2014 standard [1], which was issued with the intent to address the lack of uniformity among testing methodologies, prevent misunderstandings among stakeholders, and produce a uniform procedure to evaluate and compare performance claims from different manufacturers. The testing methodology recommended by the IEC 60255-121:2014 standard [1] is implicitly based on a (replicated) full factorial design, which may not be compatible with the maximum number of tests that the operator can afford in each experiment. For example, the testing activity performed in [2] based on such full factorial design consisted of almost 100,000 tests; as only 5 tests per minute were possible, this translated into about 40 days of tests.

Power system operators often work in resource-saving contexts, and, not rarely, time/money considerations are adopted to justify the "arbitrary" or "convenient" selection of which and how many tests to perform. Such common practice can be overcome by the statistical Design Of Experiments (stat-DOE), which combines the strength of the classical DOE with the power of the statistical approach to aid in both properly laying out a resource-saving experimental plan and conducting robust statistical analysis of the data.

The stat-DOE was an integral part of the smart grid interoperability testing methodology proposed in [3]. The relevance of the stat-DOE was shown in [4], which applied the methodology of [3] for testing the interoperability of a metering infrastructure. However, in [4], a full factorial design was employed, which quickly undergoes the curse of dimensionality as the number of factors grows.

In [5], it was proposed to integrate the stat-DOE in the power system protection testing especially in resource-saving contexts. In particular, it was practically demonstrated how the stat-DOE can aid in the optimal selection of the tests and in the systematic investigation of the effect of different factors, it was proven the superiority of modern designs over classical designs (such as full and fractional factorial), and replicable guidelines were elaborated for the application of the stat-DOE in the performance testing of power system protection functions.

Leveraging on [5], we go one step further by showing how the stat-DOE can be employed to test the performance of different DUTs coming from different manufacturers. In our work, the DUTs are physical relays where the distance protection function is implemented, the latter being the

power system protection function most commonly adopted in transmission systems. The distance protection function, which is subject of the testing activity in our work, estimates the location of the fault on the transmission line based on the DUT internal fault location algorithm and using current and voltage measurements coming from the field.

Following the recommendations of the IEC 60255-121:2014 standard [1], various factors potentially affecting the DUT performance are considered, such as fault resistance, fault location, fault type and fault inception angle. Special attention is placed on the type of design used for the optimal selection of the tests to conduct, owing to the well-known challenges of time/money limitations often affecting the testing activity. The response measured to quantify the distance protection performance is the DUT operate time (i.e., the interval between the time at which the fault happens and the time at which the relay sends the trip signal). As the interest of the operator is, often, whether the DUT operate time exceeds a pre-defined threshold, the test results are also analyzed in terms of pass/fail outcomes.

By applying the stat-DOE workflow, we show how building a surrogate model of the fault location algorithm can be of practical use to validate the performance claims of different DUTs and hence detect potential internal inconsistencies in a cheap yet robust manner before the field implementation. Also, we demonstrate how the stat-DOE can effectively support the definition of pass/fail criteria based on specific requirements of the transmission system operators.

Although in the first place the purpose of the testing activity is usually not directly related to Sensitivity Analysis (SA), the operator may be interested in identifying which factors mainly drive the degradation of the DUT performance in order to support the definition of further experiments. By interpreting the test results in terms of pass/fail outcomes, we recast the problem into the "factor mapping" SA setting, and we recommend the operator to employ a simple statistical test for identifying the factors to which the DUT performance is most sensitive. If additional experiments are needed, this may instruct the operator e.g., to sample the most important factor(s) at more levels, and/or to neglect those which turned to have minimal impact on the DUT performance.

Overall, the attained results allow us to claim that integrating the stat-DOE into the testing activity of power system protection can overcome the limitations of the existing testing methodologies, and that, at a broader level, it can represent a common and standardized basis for ensuring replicability, robustness and objectivity of the testing activity.

References:

[1] International Electrotechnical Commission. Measuring relays and protection equipment – Part 121: Functional requirements for distance protection. 2014.

[2] A. Novikov, J. Jesus de Chavez, and M. Popov. Performance assessment of distance protection in systems with high penetration of PVs. In *2019 IEEE Milan PowerTech*, 1–6, 2019.

[3] I. Papaioannou, S. Tarantola, A. Lucas, E. Kotsakis, A. Marinopoulos, M. Ginocchi, M. Olariaga Guardiola, and M. Masera, Smart Grid Interoperability Testing Methodology. *Publications Office of the European Union*, 2018.

[4] N. Andreadou, A. Lucas, S. Tarantola, and I. Poursanidis, "Design of experiments in the methodology for interoperability testing: Evaluating AMI message exchange". *Applied Sciences*, 9(6), 2019.

[5] M. Ginocchi, T. Penthong, F. Ponci, and A. Monti, "Statistical design of experiments for power system protection testing: A case study for distance relay performance testing". *IEEE Access*, 12:27052–27072, 2024.

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Generic framework for decision-making models in risk analysis

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Abstract

As part of the reliability and risk assessment of complex and critical power generation systems (e.g., nuclear and hydropower plants), the operator must perform uncertainty analyses in order to provide safety margins to the safety and regulatory authorities. However, for a number of historical and methodological reasons, common engineering practices for safety and reliability assessment can vary between applications. For example, on the one hand, the study of accident scenarios in nuclear safety [3] is often based on the estimation of penalised quantile values provided by the Wilks' approach [8]. On the other hand, reliability analyses carried out in the hydropower sector (e.g., penstock reliability) rely on the estimation of (conditional) rare event probabilities to be compared with safety thresholds [1]. Finally, in other areas such as financial risk modelling, quantiles and superquantiles (also known as "value-at-risk" and "conditional value-at-risk") are the quantities of interest. Thus, in practice, a panel of *risk measures* can be defined and used [7]. More specifically, a set of four risk measures can be considered: quantiles, superquantiles, failure probabilities and buffered failure probabilities. These four risk measures have several theoretical properties that have been intensively studied [4, 5, 2]. However, the theoretical properties of the statistical estimators as well as the practical interest of these risk measures is still an area of research.

The aim of this paper is twofold. In a first step, an analysis of the theoretical properties and the theoretical links between these four risk measures is discussed in the light of practical desirability criteria. Furthermore, in the context of naive Monte Carlo estimation, asymptotic statistical properties of the estimators are analysed and illustrated by means of elementary toy cases. In a second step, a theoretical formulation of a risk analysis decision problem is proposed, in the spirit of [6], but extended to the panel of four risk measures discussed earlier. In addition, the impact of the different sources of uncertainty (e.g., on the input distribution) is taken into account. The limits of this approach will be explored, in particular with respect to the curse of dimension, or in a non-asymptotic framework where the available samples are of finite size.

Short biography (PhD student)

Marie Temple-Boyer graduated from *École Nationale des Ponts et Chaussées* in June 2023 and was awarded the "Agrégation de Mathématiques" in June 2024. She is now involved in a PhD

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References

[1] A. Ajenjo, E. Ardillon, V. Chabridon, S. Cogan, and E. Sadoulet-Reboul. Robustness evaluation of the reliability of penstocks combining line sampling and neural networks. *Reliability Engineering and System Safety*, 234:109192, 2023.

[2] J.-E. Byun and J. O. Royset. Data-driven optimization of reliability using buffered failure probability. *Structural Safety*, 98:102232, 2022.

[3] C. Charignon, J.-C. Lecoy, and J.-Y. Sauvage. CathSBI, a new methodology for the revised French LOCA rules. In *Proc. of the 11th International Topical Meeting on Nuclear Reactor Thermal Hydraulics, Operations and Safety (NUTHOS-11)*, Gyeongju, Korea, October 9-13, 2016.

[4] A. Mafusalov, A. Shapiro, and S. Uryasev. Estimation and asymptotics for buffered probability of exceedance. *European Journal of Operational Research*, 270:826–836, 2018.

[5] A. Mafusalov and S. Uryasev. Buffered Probability of Exceedance: Mathematical Properties and Optimization. *SIAM Journal on Optimization*, 28(2):1077–1103, 2018.

[6] G. Perrin, J. Reygner, and V. Chabridon. Enhancing Reliability Analysis with Limited Observations: A Statistical Framework for System Safety Margins. *hal.archives-ouvertes*, pages 1–49, 2024.

[7] R. T. Rockafellar and J. O. Royset. Engineering Decisions under Risk Averseness. *ASCE-ASME Journal of Risk and Uncertainty in Engineering Systems, Part A: Civil Engineering*, 1(2):1–12, 2015.

[8] S. S. Wilks. Determination of Sample Sizes for Setting Tolerance Limits. *The Annals of Mathematical Statistics*, 12(1):91–96, 1941.

Mollifiers to enhance gradient-based dimension reduction

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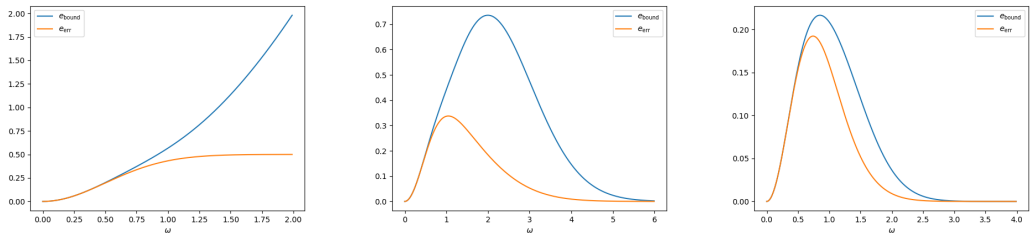
Abstract

Modern computational models for scientific and engineering applications typically involve a large number of input parameters and are expensive-to-evaluate both in time and resources. Replacing the model with an accurate and fast-to-evaluate surrogate (or approximation) offers a viable workaround in many applications. Approximating such high-dimensional functions with classical approximation tools such as polynomials, wavelets or neural networks is, however, a difficult task. This is even aggravated in the small sample regime where one only has access to a little number of model evaluations. One way to address this challenge is to reduce the input dimension beforehand. This consists in approximating the *model* $x \mapsto u(x)$ as the composition of two functions: a *feature map* $x \mapsto z = g(x)$ which extracts the relevant features of the input variables, and a *profile function* $z \mapsto f(z)$ which regresses the model output on the features. The feature map can be built by minimizing an upper bound of the reconstruction error $\min_f \mathbb{E}[(u(\boldsymbol{X}) - f \circ g(\boldsymbol{X}))^2]$ obtained with Poincaré-type inequalities. When the feature map is linear this strategy reduces to Active Subspace [4, 2]. The case of nonlinear feature maps has been studied in [1] for polynomial feature maps and in [3, 5] for diffeomorphism-based feature maps. The bound derived from Poincaré inequality is proportional to the L^2-norm of model gradients, therefore, this strategy works well for slowly varing functions for which the bound is tight. For oscillatory model with large gradient norms, however, the bound reveals too loose to build a meaningfull feature map and the method fails.

In this talk we demonstrate that working with a mollified version of the model $(u \star \rho_\sigma)$ is a good strategy to circumvent this issue as it allows to obtain sharper Poincaré error bounds and to reduce the dimension efficiently using gradient-based techniques. Here ρ_σ is the gaussian kernel with 0 mean and $\sigma^2 I_d$ covariance, $\star$ is the convolution operator and we call σ the mollifying parameter. We demonstrate that the reconstruction error when using a mollified version of the model can be bounded by the sum of two terms: one that vanishes when the mollifying parameter goes to zero and one that is proportional to the Poincaré error bound of the mollified model. This bound shows the trade-off between mollification and dimension reduction: for strongly mollified models the first term is large and the second one quite small and the other way around when the model is less mollified. Based on this result, we propose an iterative algorithm for dimension reduction. More precisely, we introduce a sequence $\sigma_1 > \sigma_2 > \ldots > \sigma_p \geq 0$ of decreasing mollifying parameters. Then at the first iteration we approximate a strongly mollified version of the model $u_1^* = u \star \rho_{\sigma_1}$ with a feature map g_1 and a profile function f_1. At the next interation the algorithm approximates a slightly less mollified version of the residual model $u_2^* = (u - f_1 \circ g_1) \star \rho_{\sigma_2}$ with a feature map g_2 and a profile function f_2. This proccess iterates p times and at the end the original model u is approximated by $\sum_{1 \leq i \leq p} f_i \circ g_i$.

Let us illustrate on some example the impact of the mollification step on the accuracy of Poincaré error bound. We consider the analytical toy model $u(x) = \sum_{i=1}^d a_i \sin(\omega_i x_i)$, where a_i, ω_i, x_i are

respectivelly the ith components of vectors $a \in \mathbb{R}^d, \omega \in \mathbb{R}^d, x \in \mathbb{R}^d$. We aim at approximating u by $f \circ g$ with g a projector onto $\{e_1, ..., e_d\}$ the canonical basis of $\mathbb{R}^d$. Here g is a linear feature map and $g = U^\top \sum_{i \in \tau} e_i e_i^\top$ where $\tau \subset \{1, \dots, d\}$, $\#\tau = m$ and $U = [e_i]_{i \in \tau} \in \mathbb{R}^{d \times m}$. In this framework, and for $\boldsymbol{X} \sim \mathcal{N}(0, I_d)$, we compare the minimal reconstruction error for $u_\sigma = u * \rho_\sigma$ with the one obtained by minimizing Poincaré error bound. We perform the comparison for $a_i = 1$, $i = 1, ..., d$ and for different values of σ. In this situation the reconstruction error is equal to $\frac{1}{2} \sum_{i \in -\tau} e^{-\omega_i^2 \sigma^2} (1 - e^{-2\omega_i^2})$ and the Poincaré error bound is equal to $\frac{1}{2} \sum_{i \in -\tau} \omega_i^2 e^{-\omega_i^2 \sigma^2} (1 + e^{-2\omega_i^2})$, where $-\tau$ is the complementary set of τ in $\{1, \dots, d\}$. We can compare the 2 functions $e_{\text{err}}(\omega) = \frac{1}{2} e^{-\omega^2 \sigma^2} (1 - e^{-2\omega^2})$ and $e_{\text{bound}}(\omega) = \frac{1}{2} \omega^2 e^{-\omega^2 \sigma^2} (1 + e^{-2\omega^2})$ to understand how the error and the bound behave for different values of the mollifying parameter σ. Figure 1 clearly shows that the reconstruction error and the error bound become closer together as the value of σ grows.



(a) $\sigma = 0$ (b) $\sigma = 0.5$ (c) $\sigma = 1$

Figure 1: Plots of e_{err} and e_{bound} according to ω for different values of σ

Short biography

I am a former student of ENSTA Paris where I studied mathematics and computer science. At the end of my engineering studies, to deepen my knowledge in general mathematics, I prepared for and passed mathematical aggregation. Finally, after a short experience as a teacher, I moved to Grenoble to work as PhD student with Clémentine Prieur and Olivier Zahm on nonlinear dimension reduction for function approximation. This thesis is funded by the French Research Agency (ANR).

References

[1] Daniele Bigoni, Youssef Marzouk, Clémentine Prieur, and Olivier Zahm. Nonlinear dimension reduction for surrogate modeling using gradient information. *Information and Inference: A Journal of the IMA*, 11(4):1597–1639, 2022.

[2] Paul G. Constantine, Eric Dow, and Qiqi Wang. Active subspace methods in theory and practice: Applications to kriging surfaces. *SIAM Journal on Scientific Computing*, 36(4):A1500–A1524, January 2014.

[3] Romain Verdière, Clémentine Prieur, and Olivier Zahm. Diffeomorphism-based feature learning using Poincaré inequalities on augmented input space. working paper or preprint, December 2023.

[4] Olivier Zahm, Paul Constantine, Clémentine Prieur, and Youssef Marzouk. Gradient-based dimension reduction of multivariate vector-valued functions. 2019.

[5] Guannan Zhang, Jiaxin Zhang, and Jacob Hinkle. Learning nonlinear level sets for dimensionality reduction in function approximation. *Advances in Neural Information Processing Systems*, 32, 2019.

Kernel-based uncertainty quantification of machine learning models: assessment and first advances

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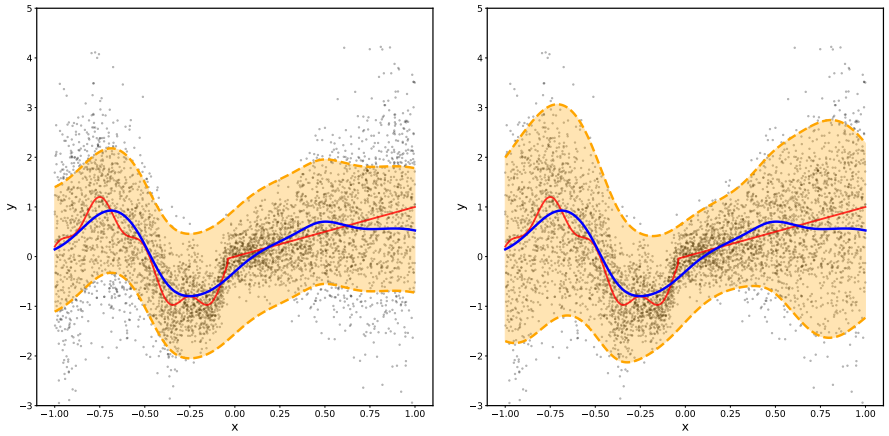
Abstract

In this work we focus on the construction of prediction intervals for machine learning models. Numerical simulation is widely used to predict the behavior of industrial pieces in order to identify designs that meet the desired performances. Finding the appropriate design (in terms of geometry and material, for instance) typically involves solving an optimization problem, requiring sometimes several hundreds calls to the simulation code that predicts the underlying physics. In most industrial applications, each call to the simulation code can take several hours to properly model the physics. For this reason, direct optimization is most of the time intractable. To overcome this issue, a common practice consists in building a surrogate model for the simulation code. Popular surrogate models include Gaussian processes, random forests, or more recently, neural networks for their high flexibility. While these machine learning models have been proven effective across several industries, there is a lack of rigorous uncertainty quantification for the predictions made by such models.

Recently, there has been a growing interest in conformal prediction methods which provide a systematic way to build prediction intervals with coverage guarantees, see [7, 1]. Conformal prediction is a distribution-free and model agnostic framework that provides prediction intervals with marginal coverage guarantees and also, for some variants, training-conditional coverage guarantees at the expense of additional assumptions. Nevertheless, it still suffers from a few shortcomings such as the incompatibility with deterministic design of experiments due to the exchangeability assumption, or its tendency to generate rather constant intervals. Although there has been much effort into developing adaptive conformal prediction bands [3, 6], it still remains an active research topic.

Here, we propose to investigate the kernel framework recently proposed by [4] and [2] that rely on semi-definite programming. The methodology consists in learning the conditional variance of the output given the input features. This function is learned in a complex and high dimensional space using a positive definite kernel and the representer theorem for non-negative functions [5]. The generated prediction intervals also enjoy marginal and training-conditional coverage guarantees without relying on the exchangeability assumption, which appears promising for handling deterministic design of experiments often used in numerical simulations. As an illustration, split conformal prediction is compared to the aforementioned kernel method in Figure 1.

Throughout this work, it has been found that the performance of the kernel methods [4, 2] is promising and outperforms conformal prediction variants on several synthetic regression prob-



(a) Split conformal. (b) Our kernel model.

Figure 1: Comparison between split conformal prediction and our kernel model. In red the true mean function, in blue the Gaussian process estimate and in orange the respective 90% prediction bands.

lems, especially in terms of adaptivity. We also show that the optimization problems defined in [4] and [2] can be casted into a single framework, and that the computational times can be greatly reduced by relying on the results presented in [5]. Finally, we also propose a completely novel methodology for tuning the lengthscales involved in the kernel methods, which was highly overlooked in [4, 2].

Short biography (PhD student)

Graduated from the statistics and data science engineering school ENSAI in 2024, the PhD thesis focuses on uncertainty quantification in the predictions of a machine learning model. The PhD is under the supervision of the CREST laboratory and Safran Tech research center.

References

[1] Rina Foygel Barber, Emmanuel J. Candes, Aaditya Ramdas, and Ryan J. Tibshirani. Predictive inference with the jackknife+, 2020.

[2] Jianqing Fan, Jiawei Ge, and Debarghya Mukherjee. Utopia: Universally trainable optimal prediction intervals aggregation, 2024.

[3] Jing Lei and Larry Wasserman. Distribution-free prediction bands for non-parametric regression. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 76, 01 2014.

[4] Tengyuan Liang. Universal prediction band via semi-definite programming. *Journal of the Royal Statistical Society Series B: Statistical Methodology*, 84(4):1558–1580, August 2022.

[5] Ulysse Marteau-Ferey, Francis Bach, and Alessandro Rudi. Non-parametric models for non-negative functions, 2020.

[6] Yaniv Romano, Evan Patterson, and Emmanuel J. Candès. Conformalized quantile regression, 2019.

[7] Vladimir Vovk, Alex Gammerman, and Glenn Shafer. *Algorithmic Learning in a Random World*. Springer, Berlin, Heidelberg, 01 2005.

Fast pick-freeze estimation of sensitivity maps using basis decomposition

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In the context of variance-based sensitivity analysis of functional outputs, a common goal is to compute *sensitivity maps* (SM), i.e Sobol' indices at each output dimension (e.g. time step for time series, or pixels for spatial outputs) [1, 2, 3]. In specific settings, some works have shown that the computation of Sobol' SM can be speeded up by using basis decomposition employed for dimension reduction (e.g. Principal Component Analysis, B-splines, wavelet, among others). However, how to efficiently compute such SM in a general setting has not received too much attention in the GSA literature.

In this work, we propose fast computations of Sobol' SM, with a focus on statistical estimation of these indices, using a general basis decomposition of output data $y_\ell(X)$, where $(\cdot)_\ell$ represents the index of each output dimension. The functional basis decomposition of dimension m is given by a linear combination of the basis coefficients vector c and the basis components vector v_ℓ:

$$y_\ell(X) = \sum_{i=1}^{m} c_i(X) v_{i,\ell}$$

We obtain closed-form expression of SM in function of the matrix-valued Sobol' index of the vector of basis coefficients, for all $I \subseteq \{1, \ldots, d\}$, where d is the number of input variables. Then, we write similar *basis-derived* formulas for the pick-freeze estimator of Sobol' SM $\widehat{S_I^{\mathrm{c}}}^{\mathrm{pf}}(y_\ell(X))$ in function of the normalized matrix-valued pick-freeze estimator of the vector of basis coefficients, as follows:

$$\widehat{S_I^{\mathrm{c}}}^{\mathrm{pf}}(y_\ell(X)) = \frac{v_{\cdot,\ell}^\top \, \widehat{D_I^{\mathrm{c}}}^{\mathrm{pf}}(c(X)) \, v_{\cdot,\ell}}{v_{\cdot,\ell}^\top \, \widehat{\mathbb{C}\mathrm{ov}}^{\mathrm{pf}}(c(X)) \, v_{\cdot,\ell}}$$

The relative cost in terms of mathematical operations between the *basis-derived* [2, 3] and *pixel-wise* [1] approaches scales as the ratio between the number of basis components m and the output dimensions L. When dimension reduction is possible, this ratio may be very small and the gain in computational time allows to calculate both SM and their associated bootstrap confidence bounds in a reasonable time.

As an application, we study the contribution of this work to a case in fluid mechanics: the idealized and gradual dam-break of a non-Newtonian fluid [4]. It consists of a known volume of material inside a reservoir delimited by the walls and a gate, which is lifted with a finite velocity and the material flows downstream a horizontal plane or channel (Fig. 1). By computing the SM, we aim to evaluate the influence of input variables over a chosen quantity of interest: the position of the wavefront over time $x_f(t)$.

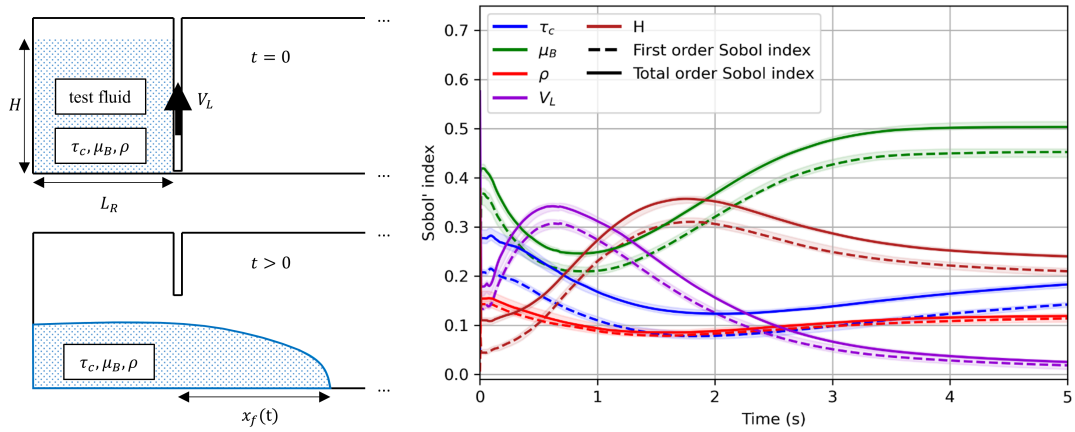

Figure 1: Schematics of the case study (left) and time series of Sobol' indices with associated confidence bounds in shaded colors (right).

The input variables of the model are the initial fluid height H, lifting velocity of the gate V_L, fluid's density ρ and rheological properties (yield stress τ_c and plastic viscosity μ_B). All input variables were considered as uniformly distributed. By using Latin-Hypercube Sampling (LHS), 226 scenarios were generated and simulated by the finite-volume fluid dynamics solver ANSYS Fluent. Then, Principal Component Analysis was applied as functional basis to reduce dimension ($m = 10$, accounting for 99.9% of the variance) and the basis coefficients were metamodelled using Gaussian Process Regression for fast prediction. To estimate the SM, 5000 pick-freeze samples were used with 20 bootstrap repetitions. The results in Fig. 1 show that the influence of input variables over the wavefront position vary significantly along time, except for ρ, highlighting the time-dependent characteristics of the flow. The small difference between 1st order and total indices indicates that interactions are small compared to the main effects. Overall, the basis-derived pick-freeze method showed to be capable of obtaining SMs with an acceptable accuracy, while performing less operations and allowing the bootstrapping technique in a reasonable computational time.

References:

[1] A. Marrel, B. Iooss, M. Jullien, B. Laurent, E. Volkova, "Global sensitivity analysis for models with spatially dependent outputs", *Environmetrics*, **22**:383–397, 2011.

[2] J.B. Nagel, J. Rieckermann, B. Sudret, "Principal component analysis and sparse polynomial chaos expansions for global sensitivity analysis and model calibration: Application to urban drainage simulation", *Reliab. Eng. Syst. Saf.*, **195**:106737, 2020.

[3] M. Li, R.Q. Wang, G. Jia, "Efficient dimension reduction and surrogate-based sensitivity analysis for expensive models with highdimensional outputs", *Reliab. Eng. Syst. Saf.*, **195**:106725, 2020.

[4] N.J. Balmforth, I.A. Frigaard, G. Ovarlez, "Yielding to stress: recent developments in viscoplastic fluid mechanics", *Annu. Rev. Fluid Mech.*, **46**:121–146, 2014.

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Knockoff'ed Total Indices

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Total indices are global sensitivity indicators subject of intensive investigation in the statistical, machine learning as well as simulation literature. They aim to capture the strength of dependence between a quantity of interest/target and covariates/features. In general, a total index is the fraction of the variance of Y that is left unexplained when all features are fixed but X_i.

Applying total indices in a dependent-input setting generally requires conditionally independent realizations. In [6], non-Cartesian input domains are studied using a rejection technique, in [2] the pick-and-freeze methodology is also applied in the dependent input case, with the introduction of an additional density quotient to adjust for the disparity between the product of marginal densities (where the pick-and-freeze sampling is formed) and the joint density (where the conditionally independent distributions are found).

In the machine learning context, it was noted by [5] that model-X knockoffs introduced by [3] may be used for assessing feature importance. We apply this reasoning to the sensitivity analysis context, and arrive at the surprising result that pick-and-freeze algorithms can be applied unmodified also in the dependent case when the alternative sample block is generated as knockoff.

This approach is extended to moment-invariant measures using kernel-based dissimilarity measures [4] and optimal-transport-based measures [1] which can be applied in case of stochastic output.

References:

[1] E. Borgonovo, A. Figalli, E. Plischke, and G. Savarè. Global sensitivity analysis via optimal transport. *Management Science*, 2024. Accepted.

[2] E. Borgonovo, E. Plischke, and C. Prieur. Total effects with constrained features. *Statistics and Computation*, 34(87):1–25, 2024.

[3] E. Candès, Y. Fan, L. Janson, and J. Lv. Panning for gold: 'model-X' knockoffs for high dimensional controlled variable selection. *Journal of the Royal Statistical Society, Series B*, 3(80):551–577, 2018.

[4] S. Da Veiga. Kernel-based ANOVA decomposition and Shapley effects – Application to global sensitivity analysis. preprint, Hyper articles en ligne, 2021. `https://hal.archives-ouvertes.fr/hal-03108628`.

[5] G. Hooker, L. Mentch, and S. Zhou. Unrestricted permutation forces extrapolation: variable importance requires at least one more model, or there is no free variable importance. *Statistics and Computing*, 31(6):82:1–16, 2021.

[6] S. Kucherenko, O. V. Klymenko, and N. Shah. Sobol´ indices for problems defined in non-rectangular domains. *Reliability Engineering&System Safety*, 167:218–231, 2017.

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Sensitivity analysis & implementation of a multi-fidelity approach for the biogeochemical model Eco3M-MED-CN in an 1DV configuration

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Abstract

The general aim of this work is to develop a design-of-experiments-type enrichment strategy, combined with a multi-fidelity approach, in order to improve knowledge of the same quantity of interest (e.g. a model output or an ecosystem indicator) from several versions of several models. While the long-term ambition is to adapt such a tool for climate models, we will initially develop it for the less complex context of marine biogeochemical models. These models compute the dynamics of the planktonic trophic network from a set of equations describing the main processes involved between the different functional groups of plankton, as well as the prey-predator relationships that exist between them.

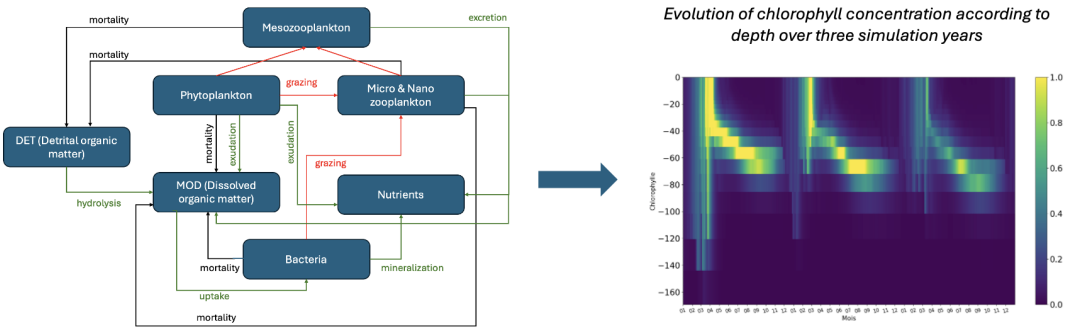

Figure 1: An example of a version of the Eco3M-MED-CN marine biogeochemical model. Left: conceptual diagram of the biogeochemical processes represented; right: an Eco3M-MED-CN output variable used in a 1DV configuration.

More specifically, we are working in a 1D Vertical (1DV) configuration with a simplified version of the Eco3M-MED model [Baklouti et al., 2021], identified as Eco3M-MED-CN. Like the model from which it is derived, this model has a flexible stoichiometry, and its main objective is to study biogeochemical cycles, particularly carbon, and plankton population dynamics in the Mediterranean. It is based on a system of 28 ordinary differential equations (one per state

variable), and a set of 93 parameters. We have chosen 9 scalar quantities of interest, which reflect different aspects of the trophic network, i.e. its state, structure or functioning.

We are developing two versions of the Eco3M-MED-CN model with the intention of integrating a multi-fidelity approach into our methodology. The first stage of the work consisted in conducting a sensitivity analysis on these models. In view of the large number of parameters involved, we opted for a screening-type sensitivity analysis. The Morris method was chosen for its conceptual simplicity and ease of implementation. It allows us to obtain a qualitative classification of parameters relative to each quantity of interest, while maintaining a reasonable use of computing resources for a model of this size. Sensitivity analyses were performed using 4900 simulations for each version of the model.

These analyses highlight particularly influential or non-influential parameters on our quantities of interest, enabling us to adjust the model's parameter space. This work will be presented in detail in the poster, and we will also discuss initial attempts and problems identified in connection with the multi-fidelity approach.

Short biography (PhD student)

After completing a master's degree in Statistics and Data Science at the University of Grenoble Alpes, I had the opportunity to start a thesis supervised by Eric Blayo and Elise Arnaud, within the AIRSEA team of the Jean Kuntzmann Laboratory in October 2023. This thesis is funded by the French numerical modeling project MEDIATION[1], selected as part of the "Ocean and Climate" Priority Research Program[2].

References

M. Baklouti, R. Pagès, E. Alekseenko, A. Guyennon, and G. Grégori. On the benefits of using cell quotas in addition to intracellular elemental ratios in flexible-stoichiometry plankton functional type models. application to the mediterranean sea. *Progress in Oceanography*, 197: 102634, 2021.

F. Campolongo, J. Cariboni, and A. Saltelli. An effective screening design for sensitivity analysis of large models. *Environmental modelling & software*, 22(10):1509–1518, 2007.

M. D. Morris. Factorial sampling plans for preliminary computational experiments. *Technometrics*, 33(2):161–174, 1991.

A. Saltelli, M. Ratto, T. Andres, F. Campolongo, J. Cariboni, D. Gatelli, and S. Tarantola. *Global sensitivity analysis: the primer*. John Wiley & Sons, 2008.

F. Zertuche, C. Helbert, and A. Antoniadis. Multi-fidelity regression using a non-parametric relationship. In *MASCOT 2014 - Méthodes d'Analyse Statistique pour les Codes et Traitements numériques*, April 2014.

[1] `https://www.ocean-climat.fr/Les-actions-et-projets/Les-projets-de-recherche/MEDIATION`
[2] `https://www.ocean-climat.fr`

Surrogate to Poincaré inequalities on manifolds for dimension reduction in nonlinear feature spaces

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Abstract

This work focuses on approximating a differentiable function $u : \mathbb{R}^d \to \mathbb{R}$ with $d \gg 1$ by a composition of functions $f \circ g$ where $g : \mathbb{R}^d \to \mathbb{R}^m$ and $f : \mathbb{R}^m \to \mathbb{R}$. The approximation error is assessed in the L^2_μ-norm where μ is some probability measure on $\mathbb{R}^d$. The approach considered is two-staged. Firstly the feature map g is selected among some prescribed functional class by minimizing some function $\mathcal{J}$ involved in the upper bound of the approximation error

$$\min_{f:\mathbb{R}^m\to\mathbb{R}} \mathbb{E}_\mu(|u - f \circ g|^2) \leq C_\mu \mathcal{J}(g), \tag{1}$$

which is based on Poincaré inequalities and requires evaluations of ∇u.

Secondly the function f is built using classical regression methods. Until recently, bounds of the form (1) were only available for linear feature maps g. This framework has been extensively studied under the name Active Subspace, see for example [2, 4], and the solution is given by the eigenvectors of the matrix $\mathbb{E}(\nabla u \nabla u^T) \in \mathbb{R}^d$. This approach is easy to implement, computationally efficient, has robust theoretical guarantees for some classical probability laws μ, and showed good performances in various numerical applications. However, there are many functions u for which such an approximation with $m < d$ is known to be not efficient.

Therefore, recent works consider non-linear feature maps in order to produce better dimension reduction. More especially, we will focus on the work from [1, 3] in which authors leverage Poincaré inequalities on smooth manifolds to obtain a bound of the form (1) for non-linear g. Although there are less theoretical guarantees, their numerical experiments showed improved performances compared with linear featuring. However, minimizing $\mathcal{J}$ is now much harder than finding eigenvectors of some matrix, and can only be done using iterative descent methods.

In this work we consider feature maps as in [1], of the form $g(x) = G^T\Phi(x)$ with $G \in \mathbb{R}^{K\times m}$ and where $\Phi : \mathbb{R}^d \to \mathbb{R}^K$, $K \geq d$, is fixed. We study a new quantity, denoted $\mathcal{L}(g)$, which can be expressed as the minimal singular value of some positive semi-definite matrix. We show that for a compact set of polynomial feature maps with $m = 1$, for some class of probability distributions, any minimizer g^* of $\mathcal{L}$ satisfies the sub-optimality result

$$\mathcal{J}(g^*) \lesssim \min_g \mathcal{J}(g)^\beta,$$

where $0 < \beta \leq 1$ is some constant which depends on the degree. We also extend this approach to the case $m > 1$ as well as for simultaneously learning a parametrized family of functions $u_y \in L^2_\mu$ by $y \in \mathcal{Y}$, although the theoretical results are weaker. Finally, we provide numerical examples to illustrate the performances of g^*, both as the feature map used in the regression step, or as the initializer for some iterative descent algorithm for minimizing $\mathcal{J}$.

Short biography (PhD student)

I graduated from Ecole Centrale de Nantes in 2022 as generalist engineer. It included 2 years focused on applied mathematics, from machine learning to numerical analysis. I continued at ECN by starting my PhD thesis on December 2022, funded by ANR COFNET, focusing on compositional function networks for nonlinear model reduction, for forward and inverse problems.

References

[1] Daniele Bigoni, Youssef Marzouk, Clémentine Prieur, and Olivier Zahm. Nonlinear dimension reduction for surrogate modeling using gradient information. *Information and Inference: A Journal of the IMA*, 11(4):1597–1639, December 2022.

[2] Paul G. Constantine, Eric Dow, and Qiqi Wang. Active Subspace Methods in Theory and Practice: Applications to Kriging Surfaces. *SIAM J. Sci. Comput.*, 36(4):A1500–A1524, January 2014.

[3] Romain Verdière, Clémentine Prieur, and Olivier Zahm. Diffeomorphism-based feature learning using Poincaré inequalities on augmented input space, December 2023.

[4] Olivier Zahm, Paul G. Constantine, Clémentine Prieur, and Youssef M. Marzouk. Gradient-Based Dimension Reduction of Multivariate Vector-Valued Functions. *SIAM J. Sci. Comput.*, 42(1):A534–A558, January 2020.

Sample Average Approximation for Portfolio Optimization under CVaR constraint in an (re)insurance context

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(Re)insurers are constantly looking for opportunities to develop their business, increase their incomes and improve their profitability. However, in every line of business, portfolio growth often leads to increased incomes and increased risk accumulation. The company's aim is to maximize profitability by achieving an optimal risk/reward ratio between exposure to losses and expected profits. Although, the assessment of individual risks is important, getting the right mix of risks is just as crucial.

In addition, on the European market, an insurer must meet the requirements of Solvency II regulations, in particular it must have an amount of own funds at least equal to the Solvency Capital Requirement (SCR). The SCR is the capital required to ensure that the (re)insurance company will be able to meet its obligations over the next 12 months with a probability greater than 99.5%. Formally, it is modeled with the Value-At-Risk (VaR) at the level $\alpha = 0.995$.

Other risk measures can be used to model the overall risk of a (re)insurance company, the most widely used alternative being the Conditional Value-At-Risk ($CVaR$), also called Tail Value-At-Risk (TVaR) or expected shortfall (ES) for continuous distributions. CVaR is usually preferred to VaR because it has better properties such as sub-additivity and its coherent in the sense of Artzner et al.[1]. It is in the company's interest to reduce risk through diversification, in order to achieve the best risk/return ratio.

The classic approach to portfolio optimization was introduced by Markowitz in 1952 [3]. It consists in the maximization of the expectation under the constraint of maximum variance or, equivalently, minimizing the variance of the portfolio, for a fixed return, this problem is called the mean-variance optimization. Its equivalent for the conditional value-at-risk (CVaR) is the mean-CVaR optimization.

We model the (re)insurance asset market with business lines represented by the random vector $\mathbf{X}$ of asset returns, taking values in a subset $\mathcal{R}_{\mathbf{X}}$ of $\mathbb{R}^d$. We assume that $\mathbb{E}(|\mathbf{X}|) < +\infty$. A (re)insurance portfolio is defined by a vector $\boldsymbol{\gamma} \in \mathbb{R}^d$ representing the quantity held in each business line by the (re)insurer.

Let us fix some notations, with $\alpha \in]0,1[$:

$$V_\alpha(\boldsymbol{\gamma}) = VaR_\alpha(-\boldsymbol{\gamma}^T\mathbf{X}) = \min\left\{M \in \mathbb{R} : \mathbb{P}\left(-\boldsymbol{\gamma}^T\mathbf{X} \le M\right) \ge \alpha\right\},$$
$$C_\alpha(\boldsymbol{\gamma}) = CVaR_\alpha(-\boldsymbol{\gamma}^T\mathbf{X}) = \mathbb{E}\left(-\boldsymbol{\gamma}^T\mathbf{X} \middle| -\boldsymbol{\gamma}^T\mathbf{X} \ge V_\alpha(\boldsymbol{\gamma})\right).$$

Our original goal is to solve the following equation with a fixed $\alpha \in]0,1[$ and constraints on the weights and a capital requirement limit $K > 0$. It is quite common that L_0 depends on $C_\alpha(\boldsymbol{\gamma})$.

$$\begin{aligned} v^* := \inf_{\boldsymbol{\gamma}\in\mathbb{R}^d_+} \quad & \mathbb{E}(L_0(\boldsymbol{\gamma}, C_\alpha(\boldsymbol{\gamma}), \mathbf{X})) \\ \text{s.t.} \quad & \gamma_i^{low} \le \gamma_i \le \gamma_i^{up} \qquad \forall i \in \{1,..,d\} \\ \text{s.t.} \quad & C_\alpha(\boldsymbol{\gamma}) \le K. \end{aligned} \tag{1}$$

A new approach was introduced by R.T. Rockafellar and S. Uryasev in 2000 [4] and was later extended by Krokhmal P., Jonas Palmquist J., Uryasev S. (2002) [2] who proposed an embedding technique to reformulate the CVaR.

We aim to maximize a return function or minimize a loss function of a portfolio under CVaR constraints, because this approach is well adapted to the needs of (re)insurance companies. In [2], it is solved using linear programming, but this resolution can be very time-consuming. In this work, we prefer to use *Sample Average Approximation* (SAA), see Rubinstein and Shapiro [5].

For this formulation with explicit constraints, no convergence or convergence speed results with the SAA method has been published as far as we know, the closest result to our work is [8]. In this last one, the function to be minimized does not depend on the data sample.

Under convexity, continuity, integrability assumptions, we prove a.s. the convergence and find a rate of convergence for the SAA version in the case where the function to be minimized depends on the data sample as do the constraint. Moreover, if the CVaR appears in the function to be minimized, we show that for the optimization, under monotonic assumption, it can be replaced by the auxiliary function introduced in [2] and [4]. We also propose a sufficient condition to obtain the uniqueness of the solution. These results give (re)insurers a practical solution to portfolio optimization under market regulatory constraints, i.e. a certain level of risk.

References:

[1] Philippe Artzner et al. "Coherent measures of risk". *Mathematical finance* 9.3 (1999), pp. 203–228.

[2] Pavlo Krokhmal, Jonas Palmquist, and Stanislav Uryasev. "Portfolio optimization with conditional value-at-risk objective and constraints". *Journal of risk* 4 (2002), pp. 43–68.

[3] Harry Markowitz. "Modern portfolio theory". *Journal of Finance* 7.11 (1952), pp. 77–91.

[4] R Tyrrell Rockafellar, Stanislav Uryasev, et al. "Optimization of conditional value-at-risk".

Journal of risk 2 (2000), pp. 21–42.

[5] Reuven Y Rubinstein and Alexander Shapiro. "Discrete event systems: sensitivity analysis and stochastic optimization by the score function method." Vol. 13. Wiley, 1993.

[6] Alexander Shapiro. "Monte Carlo sampling approach to stochastic programming". *ESAIM*: proceedings. Vol. 13. EDP Sciences. 2003, pp. 65–73.

[7] Alexander Shapiro, Darinka Dentcheva, and Andrzej Ruszczynski. "Lectures on Stochastic Programming: Modeling and Theory" (2009).

[8] Wei Wang and Shabbir Ahmed. "Sample average approximation of expected value constrained stochastic programs". *Operations Research Letters* 36.5 (2008), pp. 515–519.

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Global Sensitivity Analysis based on Multi-resolution Polynomial Chaos Expansion: Method and Example Application to Coupled Flow Problems

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For decades, global sensitivity analysis (GSA) has been the method of choice for identifying the most relevant or sensitive model parameters in nonlinear modeling [3]. This work focuses on the Sobol indices [9], which belong to the class of the variance-related sensitivity indices. However, despite their long successful history, the classical approach via the Sobol indices uses Monte-Carlo (MC) sampling, typically requiring a high number of model evaluations. Such high computational costs reduce the applicability of the classical MC-based Sobol approaches in applied scenarios, where even individual model evaluations may require substantial computational power.

Surrogate-based techniques, such as polynomial chaos expansions (PCE), can overcome this restriction. Notably, the Sobol coefficients can be computed directly from expansion coefficients, as proposed by Sudret in [10]. However, even PCE-based surrogates have some restrictions. In particular, the classical PCE tends to suffer from Gibbs' phenomenon, which leads to oscillations in the surrogate caused by discontinuities in the model response.

The arbitrary multi-resolution polynomial chaos (aMR-PC) combines two ideas: the data-driven Ansatz of the arbitrary PCE proposed in [8] and the multi-resolution/multi-element based localization initially introduced in the context of uncertainty quantification by Le Maître et al. in [6]. This localization inherently reduces Gibbs phenomena and can achieve higher accuracy without increasing the maximal polynomial degree.

In this work, we extend the concept of the surrogate-based GSA to aMR-PC-based surrogates as proposed in [5]. For demonstration, we apply the extended techniques to a problem taken from the context of porous media. Specifically, we consider fluid flow through a coupled system consisting of a free-flow region and a porous-medium domain. Here, the Stokes equation describes fluid flow in the free-flow domain, and Darcy's law holds in the porous-medium region e.g. [2, 7]. The coupling conditions, ensure the conservation of mass across the interface, the balance of normal forces and use the Beavers–Joseph condition [1] for tangential velocity. The latter contain the parameter characterising pore-space morphology near the fluid-porous interface. Developing and extending such complex models, particularly in the context of model calibration, requires powerful strategies for assessing the relevance of model parameters, for which GSA is an established tool.

In this talk, we demonstrate the application of the aMR-PC-based GSA for the Stokes–Darcy problem, analyzing the sensitivity of four uncertain parameters: the exact location of the interface, the permeability, the Beavers–Joseph slip coefficient, and an geometric uncertainty in the outflow boundary. Furthermore, we use this modeling example to compare aMR-PC and classical PCE-based GSA.

References:

[1] G.S. Beavers and D.D. Joseph, "Boundary conditions at a naturally permeable wall", *J. Fluid Mech.* **30**:197-–207, 1967.

[2] M. Discacciati, E. Miglio, A. Quarteroni, "Mathematical and numerical models for coupling surface and groundwater flows", *Appl. Num. Math.*, **43**:57–74, 2002.

[3] T. Homma and A. Saltelli, "Importance measures in global sensitivity analysis of nonlinear models", *Reliab. Eng. Syst. Saf.* **52**(1):1–17, 1996.

[4] I. Kröker and S. Oladyshkin, "Arbitrary multi-resolution multi-wavelet-based polynomial chaos

expansion for data-driven uncertainty quantification", *Reliab. Eng. Syst. Saf.*, **222**:108376, 2022.

[5] I. Kröker, S. Oladyshkin, I. Rybak, "Global sensitivity analysis using multi-resolution polynomial chaos expansion for coupled Stokes–Darcy flow problems", *Comput. Geosci.* **27**:805–827, 2023.

[6] O.P. Le Maître, H.N. Najm, R.G. Ghanem, O.M. Knio, "Multi-resolution analysis of Wiener-type uncertainty propagation schemes", *J. Comput. Phys.*, **197**(2):502—531, 2004.

[7] K. Mostaf, K. Baber, B. Flemisch, R. Helmig, A. Leijnse, I. Rybak, B. Wohlmuth, "A coupling concept for two-phase compositional porous-medium and single-phase compositional free flow", *Water Resour. Res.*, **47**:W10522, 2011.

[8] S. Oladyshkin and W. Nowak, "Data-driven uncertainty quantification using the arbitrary polynomial chaos expansion", *Reliab. Eng. Syst. Saf.*, **106**:179—190, 2012.

[9] I. M. Sobol, "Estimation of the sensitivity of nonlinear mathematical models", *Mat. Model.*, **2**(1):112—118, 1990.

[10] B. Sudret, "Global sensitivity analysis using polynomial chaos expansions", *Reliab. Eng. Syst. Saf.*, **93**(7):964—979, 2008.

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Sensitivity analysis using multilevel Monte Carlo and surrogate-based control variates

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Sensitivity analysis (SA) has become an essential part of the engineer's toolbox to analyze the variability of the output of a model and explain it from the different sources of uncertainty. However, the cost of simulators can be an obstacle to their use as SA techniques often implies to estimate statistics, *e.g.*, expectation, variance or sensitivity indices, using Monte Carlo (MC) sampling. An alternative consists of replacing the simulator by a surrogate model but when the input dimension increases, the curse of dimensionality degrades its quality and challenges its use. The same concern arises when using a lower fidelity model. Given these limitations, we propose to combine the best of both worlds: MC techniques to guarantee unbiasedness and multifidelity models and/or surrogate models to reduce the variance of the estimators.

Given a collection of numerical simulators with increasing accuracy and computational cost, [1] proposed the multilevel Monte Carlo (MLMC) technique to estimate the expectation unbiasedly. Then, MLMC methods have been extended to other statistics with algorithms designed to achieve a given precision. In [2], we proposed a unified MLMC framework where the unbiased MC estimator of the quantity of interest based on the finest level can be written as the telescoping sum of unbiased MC estimators. We applied this framework to the estimation of the covariance term of the pick-and-freeze estimator of a Sobol' index [3] and proposed an algorithm to allocate the sampling cost to the different fidelity models. The allocation rule is driven by the target computational cost, which may be more appropriate for engineering studies where one looks to reach the best accuracy under the constraint that the total simulation time is lower than a given requirement.

In [4], we proposed to combine MLMC techniques with control variates (CV) based on surrogate models to reduce the variance of the estimator. The CV method corrects the MC estimator with a term derived from auxiliary random variables that are highly correlated with the original random variable and we proved that using several control variates could not increase the variance. Based on this, we proposed to use the outputs of surrogate models as control variates, *e.g.*, Taylor polynomials (TP), Gaussian process (GP) regressors or polynomial chaos expansions (PCE) and illustrated this approach on an academic use case for which the simple use of a first-order TP can already improve the quality of the MC estimator of the expectation. We also proposed three extensions of this surrogate-based CV strategy to the multilevel framework. MLCV is presented as an extension of CV where the correction terms devised from surrogate models for simulators of different levels add up. MLMC-CV improves the MLMC estimator by using a CV based on a surrogate of the correction term at each level. Further variance reduction is achieved by using the surrogate-based CVs of all the levels in the MLMC-MLCV strategy. Although these techniques can be applied to an arbitrary statistic, we provided specific expressions for the expectation and the variance. In the case of the expectation, we also compared them in terms of accuracy and computational cost, depending on whether the construction of the surrogates, and the associated computational cost, precede the evaluation of the estimator.

Building on [4], we extend such estimators to sensitivity indices, *e.g.*, input-output correlation coefficients, Sobol' indices, derivative global sensitivity measures (DGSM) [5] and Hilbert-Schmidt Independence Criterion (HSIC) [6], as well as a generic framework for a wide family of estimators of sensitivity indices and a technique for the joint estimation of several sensitivity indices [7]. Finally, a Nastran-based mechanical use case with 50 uncertain parameters is used to assess these surrogate-based CV estimators of sensitivity indices and demonstrate the value of these variance reduction methods in engineering.

References:

[1] M.B. Giles. Multilevel Monte Carlo path simulation, Operations Research, **3**, pp. 607–617, 2008.

[2] P. Mycek and M. De Lozzo, "Multilevel Monte Carlo Covariance Estimation for the Computation of Sobol' Indices", *SIAM/ASA JUQ*, **7**(4):1323–1348, 2019.

[3] A. Janon, T. Klein, A. Lagnoux, M. Nodet, and C. Prieur, "Asymptotic normality and efficiency of two Sobol index estimators", ESAIM: PS, **18**, pp. 342–364, 2014.

[4] E.M. El Amri, P. Mycek, S. Ricci and M. De Lozzo, "Multilevel Surrogate-based Control Variates", *https://doi.org/10.48550/arXiv.2306.10800*, 2024.

[5] S. Kucherenko and B. Iooss. "Derivative-Based Global Sensitivity Measures". In: Ghanem, R., Higdon, D., Owhadi, H. (eds) Handbook of Uncertainty Quantification. Springer, Cham., 2015.

[6] S. Da Veiga. "Global sensitivity analysis with dependence measures", Journal of Statistical Computation and Simulation, **85**(7), 1283–1305, 2015.

[7] R. Y. Rubinstein and R. Marcus, "Efficiency of Multivariate Control Variates in Monte Carlo Simulation", Operations Research, **33**(3), 661–677, 1985.

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Surrogate-Based Sensitivity Analysis in Hydrological Modelling: A Comparative Evaluation with Direct Methods

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Keywords: Hydrological Modelling, Sensitivity Analysis, Surrogate Models

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Bayesian Adaptive Spline Surfaces: An Emulator Made For Sensitivity Analysis

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For models that are even slightly expensive to evaluate, many global sensitivity methods can be difficult to use. Accurate estimation of Sobol indices or delta indices can require many thousands to millions of model evaluations. While methods like derivative-based global sensitivity metrics allow the user to bound Sobol indices with very limited model runs, these bounds are not always small enough to be practical. Further, the practitioner is often faced with the "given data" scenario, where they have been given a set of model evaluations and they cannot further design more evaluations. Various approximations to sensitivity indices exist for the "given data" scenario, but accuracy can be a challenge.

Emulator-based sensitivity analysis is a frequent solution to these problems. The practitioner uses a reasonable number of model evaluations (or "given data") to train a statistical surrogate, or emulator, of the more expensive model of interest. Assuming sufficient emulator accuracy, the practitioner can then perform sensitivity analysis of the emulator (which is cheap to evaluate) to approximate sensitivity analysis of the model of interest. For example, Figure 1 shows accuracy of emulator-based delta sensitivity compared to the standard approach. Many classes of emulators exist, including Gaussian processes, basis function approaches, polynomial chaos, tree-based models, and neural networks, and some of these are nicely suited for use for sensitivity analysis problems. In this talk, I will describe in detail one emulator that I have found especially useful: Bayesian adaptive spline surfaces (BASS).

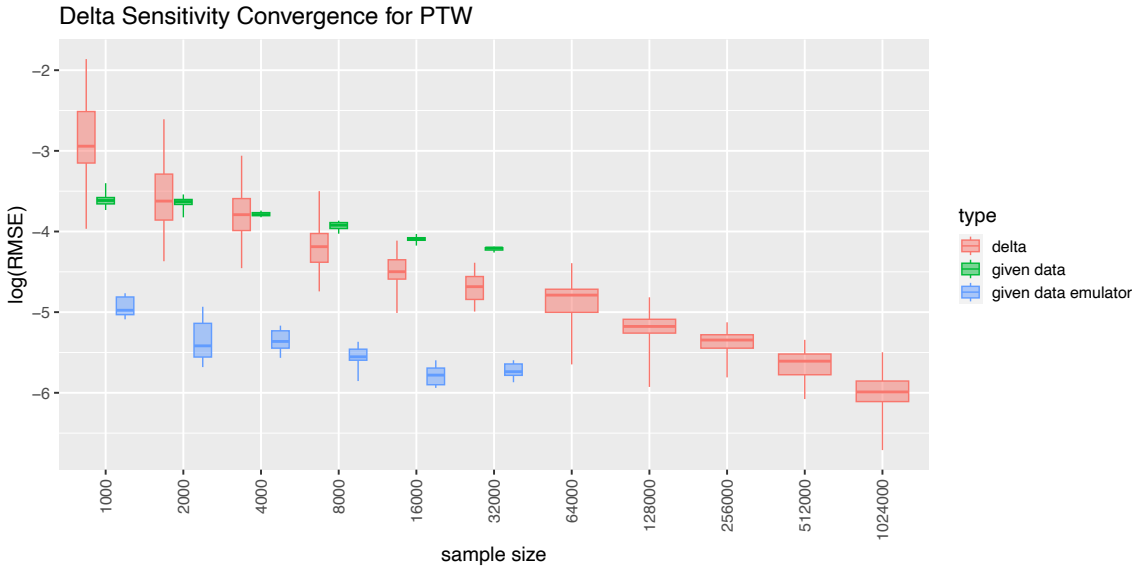

Figure 1: Convergence of three different approaches to calculating delta sensitivity indices for a material strength model called PTW. The emulator approach with given data achieves greater accuracy than the given data approach of python's SALib (with the same given data).

BASS [1-3] is a Bayesian version of Friedman's multivariate adaptive regression splines (MARS). Given training data, the response is modeled as a linear combination of tensor product spline basis functions. The variables and interactions involved in the basis functions, as well as the spline knots and the number of basis functions, are learned in a fully Bayesian framework. This emulator works well in practice: it is relatively fast, accurate, and scalable [4]. In addition, the form of the basis functions simplifies many sensitivity analysis tasks. For example, the Sobol indices can be calculated analytically for main effects, total effects, and all interactions under many input distribution assumptions, including truncated Gaussian mixtures. Tools in R (BASS package [1]) and python (pyBASS) allow for this kind of analysis to be performed routinely.

Recent work has also demonstrated that the active subspace is also available in closed form for BASS [5], and that, with a particular input dependence structure, Shapley effects are also analytical. Of course, all of these sensitivity metrics could be approximated using sampling for any number of emulators, but sampling-free formulations simplify many aspects of their use. Additionally, the error distribution of BASS can be generalized for use for robust regression, quantile regression, and other forms of flexible-likelihood regression, and the sensitivity metrics mentioned above can still be calculated analytically [6]. Figure 2 demonstrates how sensitivity changes with quantile for a stochastic epidemiology model [6].

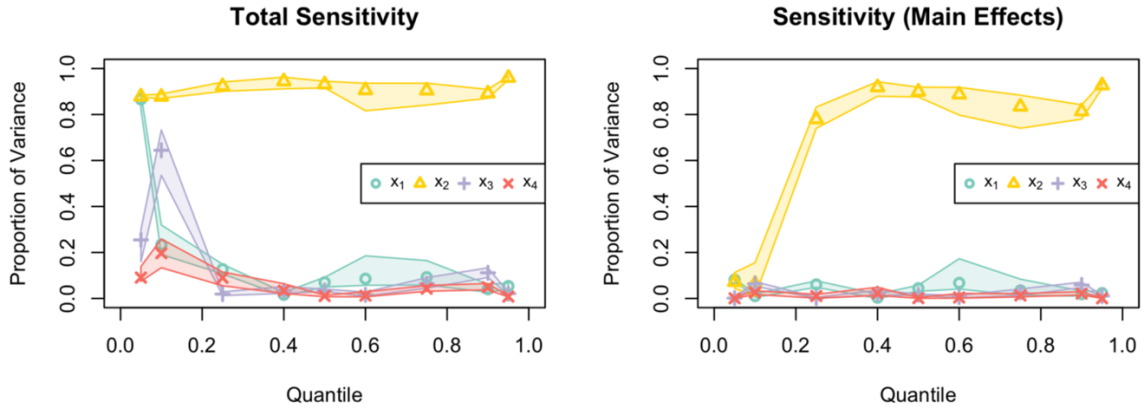

Figure 2: 80% posterior intervals for the Sobol indices of a stochastic SIR model as a function of response quantile. Low quantiles are sensitive to all inputs and their two-way interactions (not shown), but sensitivity in the large quantiles is dominated by x2.

References :

[1] Francom, D., & Sansó, B. (2020). BASS: An R package for fitting and performing sensitivity analysis of Bayesian adaptive spline surfaces. *Journal of Statistical Software*, *94*(LA-UR-20-23587).

[2] Francom, D., Sansó, B., Kupresanin, A., & Johannesson, G. (2018). Sensitivity analysis and emulation for functional data using Bayesian adaptive splines. *Statistica Sinica*, 791-816.

[3] Francom, D., Sansó, B., Bulaevskaya, V., Lucas, D., & Simpson, M. (2019). Inferring atmospheric release characteristics in a large computer experiment using Bayesian adaptive splines. *Journal of the American Statistical Association*.

[4] Hutchings, G., Sansó, B., Gattiker, J., Francom, D., & Pasqualini, D. (2023). Comparing emulation methods for a high-resolution storm surge model. *Environmetrics*, *34*(3), e2796.

[5] Rumsey, K., Francom, D., & Vander Wiel, S. (2024). Discovering active subspaces for high-dimensional computer models. *Journal of Computational and Graphical Statistics*, *33*(3), 896-908.

[6] Rumsey, K., Francom, D., & Shen, A. (2024). Generalized Bayesian MARS: Tools for Stochastic Computer Model Emulation. *SIAM/ASA Journal on Uncertainty Quantification*, *12*(2), 646-666.

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A new variance-based sensitivity analysis for models with non-independent variables.

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Functional ANOVA ([1-3]) and derivative-based FANOVA ([4]) are widely used in statistical modeling, uncertainty quantification and sensitivity analysis (e.g., [4-10]). Such decompositions of functions $f : \mathbb{R}^d \to \mathbb{R}$ have interesting properties when the input variables are independent, such as i) the uniqueness of the decomposition, ii) Sobol' main indices (i.e., S_js) and interaction indices sum up to one, iii) the Shapley effects of inputs (i.e., Sh_js from [11]) satisfy ([12])

$$0 \leq S_j \leq Sh_j \leq S_{T_j} \leq 1\,,$$

with S_{T_j} the total index of the input $X_j,\ j = 1, \ldots, d$.

For functions with non-independent input variables (i.e., $\mathbf{X} := (X_1, \ldots, X_d)$), dependency models (DMs) allow for extracting the dependency structures of such variables under the statistical and probabilistic framework ([13-14]). Using $(\sim j) := \{1, \ldots, d\} \setminus \{j\}$ and $\mathbf{Z}_{\sim j}$ for a random vector of $d-1$ independent variables, a DM of $\mathbf{X}$ is given by

$$(X_j, \mathbf{X}_{\sim j}) \overset{d}{=} (X_j, r_j\,(X_j, \mathbf{Z}_{\sim j}))\ ,$$

where X_j is at the first position, and $\mathbf{Z}_{\sim j}$ represents $\mathbf{X}_{\sim j}$ in that DM. Composing the function of interest by DMs is used for defining the dependent sensitivity indices (DSIs) of X_js and their upper-bounds (i.e., dS_j, dS_{T_j}, UB_j) in [13]. Such indices verify

$$dS_j = \frac{\mathbb{V}\left[\mathbb{E}\left[f(\mathbf{X})|X_j\right]\right]}{\mathbb{V}\left[f(\mathbf{X})\right]}; \qquad 0 < dS_j \leq dS_{T_j} \leq UB_j, \quad \forall\, j \in \{1, \ldots, d\}\,.$$

Despite the main DSIs are always less than the total ones, note that main indices and interactions do not sum up to one in general, leading to some interpretability issues. It is also the case in [15].

In this abstract, we propose new DSIs that improve the above approach by accounting for the effects of innovation variables Z_js, which represent X_js in some DMs. Basically, our approach consists in collecting necessary and sufficient equivalent representations of $f(\mathbf{X})$ in one multivariate outputs, and then applying the first-type generalized sensitivity indices ([7,8,10]) to assess the effects of X_js. The new main, interaction and total DSIs (i.e., DS_j, DS_u, DS_{T_j}) share the following properties:

$$0 \leq DS_j \leq DS_{T_j} \leq 1; \qquad \sum_{\substack{u \subseteq \{1,\ldots,d\} \\ |u|>0}} DS_u = 1\,.$$

Note that dS_js are DS_js when neglecting the effects of innovation variables. Also, when all the inputs are independent, we have $DS_j = dS_j = S_j$ and $DS_{T_j} = dS_{T_j} = S_{T_j}$. Our new approach can cope with every model and every distribution of the inputs. For linear models evaluated at the Gaussian random vector, Theorem 1 gives the (new) main and total DSIs of X_j.

Theorem 1 *Let $f(\mathbf{X}) = \boldsymbol{\beta}^T\mathbf{X}$ with $\mathbf{X} \sim \mathcal{N}(\mathbf{0}, \Sigma)$. If $\Sigma \in \mathbb{R}^{d\times d}$ has full rank, then*

$$DS_j = DS_{T_j} = \frac{1}{d\,\mathbb{V}[Y]} \sum_{u\subseteq(\sim j)} \binom{d-1}{|u|}^{-1} \frac{\mathbb{C}_{ov}\left[X_j, \mathbf{X}_{\sim u}^T\boldsymbol{\beta}_{\sim u} \middle| \mathbf{X}_u\right]^2}{\mathbb{V}\left[X_j \middle| \mathbf{X}_u\right]}.$$

Proof. *Given a matrix $\mathcal{L}_{\sim\{u,j\},\sim\{u,j\}}$, such results rely on a DM of $(\mathbf{X}_u, X_j, \mathbf{X}_{\sim\{u,j\}})$, that is,*

$$\begin{array}{c} X_j \overset{d}{=} \Sigma_{j,u}\left(\Sigma_{u,u}\right)^{-1}\mathbf{X}_u + \Sigma_{j|u}^{1/2}Z_j \\ \mathbf{X}_{\sim\{u,j\}} \overset{d}{=} \Sigma_{\sim\{u,j\},u}\left(\Sigma_{u,u}\right)^{-1}\mathbf{X}_u + \Sigma_{\sim\{u,j\},j|u}\Sigma_{j|u}^{-1/2}Z_j + \mathcal{L}_{\sim\{u,j\},\sim\{u,j\}}\mathbf{Z}_{\sim\{u,j\}} \end{array}. \qquad \square$$

In view of Theorem 1, the proposed DSIs are exactly the Shapley effects of Gaussian inputs using linear models (see [11]).

References:

[1] W. Hoeffding, A class of statistics with asymptotically normal distribution, Annals of Mathematical Statistics 19, 293–325, 1948.

[2] B. Efron, C. Stein, The jacknife estimate of variance, The Annals of Statistics 9 586–596, 1981.

[3] F. Kuo, I. Sloan, G. Wasilkowski, H. Woźniakowski, On decompositions of multivariate functions, Mathematics of computation 79 (270), 953–966, 2010.

[4] M. Lamboni, Weak derivative-based expansion of functions: ANOVA and some inequalities, Mathematics and Computers in Simulation 194, 691–718, 2022.

[5] I. M. Sobol, Sensitivity analysis for non-linear mathematical models, Mathematical Modelling and Computational Experiments 1, 407–414, 1993.

[6] A. Saltelli, K. Chan, E. Scott, Sensitivity Analysis, John Wiley and Sons, 2000.

[7] M. Lamboni, H. Monod, D. Makowski, Multivariate sensitivity analysis to measure global contribution of input factors in dynamic models, Reliability Engineering and System Safety 96, 450–459, 2011.

[8] F. Gamboa, A. Janon, T. Klein, A. Lagnoux, Sensitivity indices for multivariate outputs, Comptes Rendus Mathematique 351 (7), 307–310, 2013.

[9] R. Ghanem, D. Higdon, H. Owhadi, Handbook of Uncertainty Quantification, Springer, 2017.

[10] M. Lamboni, Multivariate sensitivity analysis: Minimum variance unbiased estimators of the first-order and total-effect covariance matrices, Reliability Engineering & System Safety 187, 67 – 92, 2019.

[11] A. B. Owen, C. Prieur, On shapley value for measuring importance of dependent inputs, SIAM/ASA Journal on Uncertainty Quantification 5 (1), 986–1002, 2017.

[12] B. Iooss, C. Prieur, Shapley effects for sensitivity analysis with correlated inputs: Comparisons with Sobol' indices, numerical estimation and applications, IJUQ 9 (5), 493–514, 2019.

[13] M. Lamboni, S. Kucherenko, Multivariate sensitivity analysis and derivative-based global sensitivity measures with dependent variables, Reliability Engineering & System Safety 212, 107519, 2021.

[14] M. Lamboni, Efficient dependency models: Simulating dependent random variables, MCS, 2022.

[15] T. Mara, S. Tarantola, P. Annoni, Non-parametric methods for global sensitivity analysis of model output with dependent inputs, EMS 72, 173-183, 2015.

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Generalized Hoeffding Decomposition for Models with Bernoulli Inputs

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Abstract

This study builds upon the recent doctoral work [3] on model decomposition theory aims to enhance interpretability in Machine Learning (ML) and sensitivity analysis [4]. A key result is the generalization of the Hoeffding decomposition [1] to cases with dependent input variables, offering new tools for fine-grained analysis of numerical and ML models. This understanding is essential for EDF, both in improving algorithms and ensuring their regulatory compliance.

The goal of the present study is to pursue the work in [3] by specifying this generalized Hoeffding decomposition in cases where input variables are Bernoulli-distributed. Although simplistic, this situation is motivated by various industrial applications, coming from the analysis of fault trees to the interpretability of control systems for hydraulic valleys or other industrial assets. These three industrial examples follow the typical scheme : *Input - Model - Output*, where we observe the actions or parameters as inputs to the system (switches in *on/off* position, whether a component has failed or not, etc, ...) and a quantity of interest as the output (a failure risk, the amount of electricity produced, etc, ...).

More formally, we consider an observed random input vector $X := (X_1, \dots, X_d)$ and the regression model $Y := G(X)$ is also observed through the model (algorithm, function, black-box, etc, ...) G. We assume that this output Y belongs to a $\mathbb{L}^2$ space, and we denote by σ_X the sigma-algebra generated by X, and more generally by σ_A the sigma-algebra generated by $X_A := (X_t)_{t\in A}$. With these notations, we then have: $Y \in \mathbb{L}^2(\sigma_X)$, which makes $\mathbb{L}^2(\sigma_X)$ be the main functionnal space for our study. Finally, as established in [3] we make the following two assumptions on X:

1. Non-perfect functional dependence between the components of X;
2. Non-degenerate stochastic dependence ; this assumption can be understood as a mild constraint on a generalized covariance matrix between subspaces of $\mathbb{L}^2$.

Under these assumptions in [2] it has be proved that:

$$\mathbb{L}^2(\sigma_X) = \bigoplus_{A \in \mathcal{P}_D} V_A$$

where:

1. $\forall A \in \mathcal{P}_D, V_A \subset \mathbb{L}^2(\sigma_A)$;
2. $\forall A, B \in \mathcal{P}_D, B \subset A \implies V_B \perp V_A$.

In our contribution, we explicitly construct a basis $(e_A)_{A \in \mathcal{P}_D}$ for the vector spaces V_A when the components of X are Bernoulli random variables is direct generalization of the Hoeffding decomposition for Bernoulli inputs can be handled easily whatever the dimension. This novel results allows us to directly access the generating elements of the V_A spaces, which depend only on the distribution of the input vector X, and ultimately to compute indicators on the behavior of the model.

Future work will extend these results to cases where input variables can take three or more discrete values, and might be considered as a first step towards the study of empirical and regular input measures.

Short biography (PhD student)

I completed a research internship at EDF R&D, where I developed a strong interest in model decomposition for sensitivity analysis and interpretability in machine learning. My passion for mathematics, particularly statistics, linear and quadratic algebra, drives my research interests and future ambitions. I am also preparing to begin a PhD at the end of 2024. This PhD will focus on developing practical applications of the decomposition properties, motivated by numerous industrial challenges.

References

[1] W. Hoeffding. A Class of Statistics with Asymptotically Normal Distribution. *The Annals of Mathematical Statistics*, 19(3):293–325, 1948.

[2] M. Il Idrissi, N. Bousquet, F. Gamboa, B. Iooss, and J.-M. Loubes. Hoeffding decomposition of black-box models with dependent inputs. *arXiv:2310.06567*, 2023.

[3] M. Il Idrissi. *Développement de méthodes d'interprétabilité en apprentissage automatique pour la certification des intelligences artificielles reliées aux systèmes critiques.* PhD thesis, Université de Toulouse (2023-....), 2024.

[4] S. Da Veiga, F. Gamboa, B. Iooss, and C. Prieur. *Basics and trends in sensitivity analysis: Theory and practice in R.* SIAM, 2021.

Combining Counterfactuals and Sensitivity Analysis: A New Approach to Explaining Black-Box Models

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Data-driven models increasingly support decision-making. However, their complexity poses challenges for human comprehension and troubleshooting and their lack of transparency can lead to unfair and biased decisions [2, 10]. To counteract the black box effect, explainable artificial intelligence (XAI) techniques are studied. One of the most commonly studied explanations is model key drivers, which can focus managerial attention on the most important factors during implementation [3]. Popular post-hoc explanation methods include SHapley Additive exPlanations (SHAP) [5] or Local Interpretable Model-agnostic Explanations (LIME) [9]. These methods focus on individual predictions and identify the features' contributions to a specific model decision. Recent works by [8] and [11] highlight the strong connection between post-hoc explanations and sensitivity analysis.

In the context of XAI, counterfactual analysis provides insights into how changes to one or more features of a given instance affect the model's prediction [12]. The application becomes even more important when the instance of interest is an individual looking for an explanation as to why the decision of an algorithm was positive or negative on their behalf. Consider the following situation. An individual, say Ms. X, is requesting a loan (or a certificate of admission) to a financial (educational) entity but gets denied. Then, Ms. X wishes to understand what she should change/improve about her characteristics to get admitted. Ms. X can look at a counterfactual, as the closest individual such that if she changed one or more of her features she would also get the loan/admission. One question that naturally emerges is which feature, if changed, would be most effective for Ms. X to achieve the desired outcome. However, [1, 6] argue that SHAP does not provide insight into what is important for the change in the above situation.

Alternatively, in a counterfactual framework, a commonly used index is the frequency of changes in a given feature when moving from Ms. X to her counterfactuals. A feature is deemed important if it is frequently modified [7]. However, counting provides a summary indication of importance. First, we cannot appreciate the magnitude of the impact. A feature may be frequently modified, but its impact on the change could be small. Second, we cannot appreciate the direction of impact and whether the feature is involved in interactions with the remaining variables. Also, when moving from Ms. X to her counterfactual, one needs to pay attention that no impossible points are attained, to avoid model predictions affected by extrapolation errors [4]. Without considering those aspects, explanations remain partial, leave the algorithmic decision opaque, and do not shed light on the actions to be taken.

In this work, we propose a novel approach combining counterfactual analysis and sensitivity analysis to explain the transition from the baseline to the counterfactual state. We apportion the change in model predictions moving from Ms. X to her counterfactual considering each feature's individual and interaction contributions. A data-driven algorithm is then introduced to study the transition, combining the search for the counterfactual and identification of the impossible point involved in the sensitivity measure calculation. The proposed method has been applied to a synthetic example and a series of datasets. Several novel insights were obtained from the two well-known datasets in the machine learning literature.

References:

[1] E. Albini, J. Long, D. Dervovic, and D. Magazzeni. Counterfactual shapley additive explanations. In *Proceedings of the 2022 ACM Conference on Fairness, Accountability, and Transparency*, pages 1054–1070, 2022.

[2] J. Dressel and H. Farid. The accuracy, fairness, and limits of predicting recidivism. *Science Advances*, 4(1):5, Jan. 2018.

[3] T. G. Eschenbach. Spiderplots versus tornado diagrams for sensitivity analysis. *Interfaces*, 22:40–46, 1992.

[4] G. Hooker, L. Mentch, and S. Zhou. Unrestricted permutation forces extrapolation: variable importance requires at least one more model, or there is no free variable importance. *Statistics and Computing*, 31, 2021.

[5] S. M. Lundberg, P. G. Allen, and S.-I. Lee. A unified approach to interpreting model predictions. *Advances in Neural Information Processing Systems*, 30:4765–4774, 2017.

[6] J. Marques-Silva and X. Huang. Explainability Is *Not* a Game. *Communications of the ACM*, 67(7):66–75, July 2024.

[7] R. K. Mothilal, D. Mahajan, C. Tan, and A. Sharma. Towards Unifying Feature Attribution and Counterfactual Explanations: Different Means to the Same End. In *Proceedings of the 2021 AAAI/ACM Conference on AI, Ethics, and Society*, pages 652–663, July 2021. arXiv:2011.04917 [cs].

[8] S. Razavi, A. Jakeman, A. Saltelli, C. Prieur, B. Iooss, E. Borgonovo, E. Plischke, S. L. Piano, T. Iwanaga, W. Becker, S. Tarantola, J. H. A. Guillaume, J. Jakeman, H. Gupta, N. Melillo, G. Rabitti, V. Chabridon, Q. Duan, X. Sun, S. Smith, R. Sheikholeslami, N. Hosseini, M. Asadzadeh, A. Puy, S. Kucherenko, and H. R. Maier. The future of sensitivity analysis: An essential discipline for systems modeling and policy support. *Environmental Modelling and Software*, 137:1–22, 2021.

[9] M. T. Ribeiro, S. Singh, and C. Guestrin. "why should i trust you?" explaining the predictions of any classifier. 2016.

[10] C. Rudin. Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead. *Nature Machine Intelligence*, 1(5):206–215, May 2019.

[11] C. A. Scholbeck, J. Moosbauer, G. Casalicchio, H. Gupta, B. Bischl, and C. Heumann. Bridging the gap between machine learning and sensitivity analysis. *ArXiv*, :2312.:1–14, 2023.

[12] S. Verma, J. Dickerson, and K. Hines. Counterfactual Explanations for Machine Learning: A Review, Oct. 2020. arXiv:2010.10596 [cs, stat].

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Global Sensitivity Analysis with Optimal Transport: Wasserstein Shapley and the Wasserstein Gap

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In this work, we first review the theory of global sensitivity analysis with optimal transport [1,2,5]. We also review recent applications [3,4]. We show that the associated global sensitivity measures possess several relevant properties, such as zero-independence and max-functionality. The former implies that the global sensitivity measure is zero if and only if the quantity of interest and the input(feature/parameter) of concern are statistically independent. The latter implies that the global sensitivity measure is maximal if and only if the quantity of interest is a deterministic function of the feature of concern. We also show that if the squared Euclidean distance is used in the cost function of the optimal transport, one obtains a decomposition which brings together moment-independent and variance-based indices. In fact, it holds that the distance between the distributions can be decomposed in three terms. The first term equals the individual variance-based contribution. The second term equals the contribution to the output second order moment and the third term accounts for contributions to any higher order moment. We call this third term the Wasserstein Gap.

We then discuss the connection between optimal transport sensitivity and design of experiments, introducing the notion of Wasserstein-Shapley value and discussing the properties of this notion.

References:

[1]E. Borgonovo, A. Figalli, E. Plischke, and G. Savaré. Global sensitivity analysis via optimal transport. *Management Science*, 2024. Accepted.

[2]E. Borgonovo, G. Savaré, A. Figalli, P. Ghosal, and E. Plischke. Convexity and measures of statistical association. 2024. In preparation.

[3]G. Cataldo, E. Borgonovo, A. Siddens, K. Carpenter, M. Nado, and E. Plischke. Global sensitivity analyses for test planning with black-box models in the mars sample return program. 2024. Under review.

[4]L. Chiani, E. Borgonovo, E. Plischke, and M. Tavoni. Global sensitivity analysis of integrated assessment models with multivariate outputs. 2024. In preparation.

[5]J. C. W. Wiesel. Measuring association with Wasserstein distances. *Bernoulli*, 28(4):2816–2832, 2022.

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Enabling Time Series Sensitivity Analysis with Iterative Variance Orthogonal Decomposition

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In many critical areas, large amounts of historical data are collected to monitor complex dynamic systems, such as in nuclear industry, finance, manufacturing, etc. To ensure that these systems function properly, a response variable (output) is observed along with environment variables (inputs) that may have an influence on its outcome. Explaining the latter with respect to the input variables has then become a crucial need. Answering this question is non-trivial due to the functional nature of the variables and the response [4], the temporal correlation of the inputs (for example, the presence of a daily periodicity in the data), or memory effects (ie. the fact that the impact of an event at a time t is observed at a time $t + \tau$ for a non-negligible response time τ).

To this end, Sensitivity Analysis (SA) provides powerful tools to engineers and practitioners. In particular, the framework of variance-based SA allows to link the output's variance to the individual (or combined) inputs variances and interpret them as contributions to the total variance. Generalizations to functional and temporal outputs have been the subjects of many works (see, for example, [4, 1]).

In this work, we propose a decomposition procedure for time series to enable a quantitative variance-based SA that clarifies the role of memory effects. The methodology is a two-stage approach. First, a linear model taking into account only the instantaneous input variables and their polynomial transforms is fitted to approach the output. Then, iteratively, for each input variable, a distributed-lag model [5] is fitted to take into account its memory effects while ensuring, by construction, the orthogonality to the already fitted models. This allows to decompose the total variance of the output as the sum of the variances of the resulting components.

The proposed framework is illustrated on multiple toy examples, and, then, applied to a real-world application case of wind power production [3, 2].

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References:

[1] Alen Alexanderian, Pierre A. Gremaud, and Ralph C. Smith. Variance-based sensitivity analysis for time-dependent processes. *Reliability Engineering System Safety*, 196:106722, 2020.

[2] Dimitri Bouche, Rémi Flamary, Florence d'Alché Buc, Riwal Plougonven, Marianne Clausel, Jordi Badosa, and Philippe Drobinski. Wind power predictions from nowcasts to 4-hour forecasts: A learning approach with variable selection. *Renewable Energy*, 211:938–947, 2023.

[3] Aurore Dupré, Philippe Drobinski, Jordi Badosa, Christian Briard, and Peter Tankov. The economic value of wind energy nowcasting. *Energies*, 13(20), 2020.

[4] Fabrice Gamboa, Alexandre Janon, Thierry Klein, and Agnès Lagnoux. Sensitivity analysis for multidimensional and functional outputs. *Electronic Journal of Statistics*, 8(1):575 – 603, 2014.

[5] A. Gasparrini, B. Armstrong, and M. G. Kenward. Distributed lag non-linear models. *Statistics in Medicine*, 29(21):2224–2234, 2010.

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Global Sensitivity Analysis of Gamma-Ray Spectra in Uranium Logging

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Novel Sensitivity Analysis Using SHAPLEY for PROMETHEUS Resilience Modelling

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Abstract:

In the context of increasing global uncertainties, understanding the sensitivity of complex systems is paramount for effective resilience modelling. This study addresses the sensitivity analysis based on the Shapley value, a concept derived from cooperative game theory (Shapley, 1953), which provides a robust framework for evaluating the contribution of individual variables to overall model outcomes.

This study presents the evolution of a resilience modelling approach within the PROMETHEUS project, from its inception using classical statistical methods to the current application of advanced sensitivity analysis techniques. Initially, our model leveraged t-statistics to determine the significance of indicators in predicting resilience outcomes, drawing from a comprehensive set of metrics compiled by institutions such as the European Commission's Joint Research Centre (JRC) and other international bodies (Benczur et ali., 2023 and European Commission, 2020).

The PROMETHEUS model's development progressed from logistic regression to linear regression, allowing for a more nuanced understanding of the relationships between various resilience indicators and system outcomes resilience. This transition enabled a more precise quantification of each indicator's impact on overall resilience measures. The following considerations apply:

1. Logistic Regression (LogRes): A simple, well-established "expert decision modelling" approach, represented by the formula: $P(Y=1|X) = 1 / (1 + e^{-(\beta_0 + \beta_1X_1 + ... + \beta_nX_n)})$ where $P(Y=1|X)$ is the probability of the outcome given the input variables, and β_i are the regression coefficients.
   LogRes has limited modulation of the outcomes and assumes independence among independent variables.
2. Linear Regression (LinRes=: Allowing for a more nuanced understanding of relationships between various resilience indicators and system outcomes, quantified by: $Y = \beta_0 + \beta_1X_1 + ... + \beta_nX_n + \varepsilon$ where Y is the outcome variable, X_i are the predictor variables, β_i are the coefficients, and ε is the error term.
   LinRes assumes independence among independent variables while our testing has shown strong multicollinearity.
3. SHAPLEY Method: An advanced approach that accounts for interactions between variables and provides a fair distribution of contributions among predictors. The Shapley value for variable i is calculated as: $\varphi_i(v) = \Sigma[S \subseteq N\{i\}] (|S|!(n-|S|-1)! / n!) [v(S \cup \{i\}) - v(S)]$ where N is the set of all variables, S is a subset of variables, v is the characteristic function, and n is the total number of variables.
   Shapley's advantage is to account for interactions and fair distribution across different independent variables while being computationally intensive ((Iooss, B., & Prieur, C. 2019 and Linkov, I., Trump, B. D., & Keisler, J. 2018).

With this abstract, we aim to introduce the application of the Shapley value method, a concept derived from cooperative game theory, to further enhance our sensitivity analysis. This novel approach allows for a fair distribution of contributions among predictors, enabling researchers to identify key factors influencing resilience in socio-economic systems with predicted higher accuracy.

The Shapley method addresses limitations of traditional sensitivity analysis techniques by accounting for complex interactions between variables. This advancement not only quantifies individual contributions but also captures the intricate interdependencies among variables, leading to more nuanced insights into system behaviour.
The Shapley value allows for a fair distribution of contributions among predictors, enabling researchers to identify key factors influencing resilience in socio-economic systems. By applying this method, we analyse various resilience indicators compiled by institutions such as the European Commission's Joint Research Centre (JRC) and other international bodies. These indicators serve as critical inputs for our model, which aims to predict system responses under different scenarios of external shocks.
The Shapley approach not only quantifies individual contributions but also accounts for interactions between variables and provides complementary insights into model (system) behaviour as compared with traditional variance-based sensitivity analysis (a.k.a Sobol' indices).
Through case studies involving resilience metrics from sectors such as health, environment, and security, we demonstrate how the Shapley method enhances predictive accuracy and informs policy-making.
This research contributes to ongoing efforts to bolster societal resilience against multifaceted challenges by providing a comprehensive analytical tool that integrates empirical data with theoretical foundations (European Commission, 2020). In conclusion, leveraging the Shapley value in sensitivity analysis represents a significant advancement in modelling resilience. This approach not only enriches our understanding of variable interactions but also supports decision-makers in developing strategies that enhance system robustness in an increasingly volatile world.

References:

L. S. Shapley, A value for n-person games, in Contributions to the Theory of Games. Volume II, H. W. Kuhn and A. W.Tucker, eds., vol. 28 of Annals of Mathematics Studies, Princeton University Press, Princeton, NJ, 1953, pp. 307–317
Benczur et al., "Resilience dashboards: Spring 2023 update", Dashboard database, European Commission, Joint Research Centre (JRC).
European Commission (2020), "2020 Strategic Foresight Report", p. 2
Iooss, B., & Prieur, C. (2019). Shapley effects for sensitivity analysis with correlated inputs: comparisons with Sobol' indices, numerical estimation and applications. International Journal for Uncertainty Quantification, 9(5).
Linkov, I., Trump, B. D., & Keisler, J. (2018). Risk and resilience must be independently managed. Nature, 555(7694), 30.

Variance-Informed Subspace: a Gradient-free Dimension Reduction for Adaptive Bayesian Inference

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Abstract

Inverse problems are encountered in many applications whenever one search for information about a physical system based on measurements [7]. In this work, we are interested in estimating a physical field thanks to a set of indirect observations $\boldsymbol{d}$. The Bayesian inference is an attractive approach for adressing such problems, as it provides a full estimation of the unknown parameters distributions. In that framework, the aim is to estimate the posterior probability of the field parameters $\boldsymbol{x}$ based on the observations

$$\pi_{\text{post}}(\boldsymbol{x}|\boldsymbol{d}) \propto \mathcal{L}(\boldsymbol{d}|\boldsymbol{x})\pi_{\text{prior}}(\boldsymbol{x}), \tag{1}$$

where $\mathcal{L}$ is the likelihood of the observations given a field and π_{prior} the prior probability of the field. The posterior distribution is then sampled with Markov Chain Monte–Carlo (MCMC) [4]. In order to accelerate the MCMC sampling, the forward model predictions are replaced with surrogate models based on polynomial chaos (PC) expansions [8, 5]. In order to reduce the input dimension of the surrogate model, a parsimonious representation of the field is introduced by means of the Karhunen-Loève (KL) decomposition, on the assumption that the field of interest is a particular realization of a Gaussian random field. Despite this parametrization, several hundred inputs could be required to represent accurately a two-dimensional field. This is expensive with regard to both the forward model surrogate training and the MCMC convergence.

Linear dimension reduction techniques have been developed to decrease the number of parameters to infer. These techniques assume that most of the information provided by the likelihood can be captured by a low-dimensional linear subspace. The input parameter space is decomposed into two subsets

$$\boldsymbol{x} = Ax_a + A_\perp x_i, \tag{2}$$

where x_a is informed by the likelihood, while x_i is constrained by the prior. The posterior distribution (1) rewrites

$$\pi_{\text{post}}(\boldsymbol{x}|\boldsymbol{d}) \propto \mathcal{L}(\boldsymbol{d}|x_a)\pi_{\text{prior}}(x_a)\pi_{\text{prior}}(x_i|x_a), \tag{3}$$

such that only x_a is sampled during the MCMC procedure. Several methods to define the linear transformation operator A have been developed. Cui et al. [3] build a Likelihood-Informed Subspace (LIS) which relies on the Hessian of the log-likelihood. The optimality of such construction

has been proven in [6] for the linear case. Constantine et al. [2] adapt the Active Subspace (AS) approach [1] to the Bayesian framework by using the misfit gradient. In both methods, the curvature of the log-posterior density is more constrained by the log-likelihood than by the prior along the subspace directions.

This study presents a new construction for the linear transformation operator A. The general idea is inspired from the work of [6] which states that, in the linear case, approximating the posterior covariance is equivalent to approximating its inverse. Instead of relying on the Hessian of the log-likelihood, the approximation of the inverse posterior covariance involves the ratio of the posterior and the prior variances.

For nonlinear inverse problems, we propose to generalize this variance ratio. The low-dimensional subspace is defined as the directions in which the posterior variance is drastically reduced in comparison to the prior variance. This method is gradient-free. We show on state-of-the-art examples that it is sufficient for unimodal posteriors, while some adjustments are required in the case of multimodal results. An application on a two-dimensional field inference case illustrates the interest of the method for high-dimensional problems.

Short biography (PhD student)

Nadège Polette studied applied mathematics at ENPC as well as at Sorbonne Université. Her PhD is funded by CEA. The supervision is ensured by Dr. A. Gesret (Geosciences center, École des Mines de Paris), Dr. P. Sochala (CEA), and Dr. O. Le Maître (CNRS, CMAP). Her PhD falls within the aim of the CTBTO to detect and analyse seismic events. The goal is to develop numerical methods for solving inverse problems applied to geophysical events analysis.

References

[1] P. G. Constantine. *Active Subspaces: Emerging Ideas for Dimension Reduction in Parameter Studies*. SIAM Spotlights. SIAM, 2015.

[2] P. G. Constantine, C. Kent, and T. Bui-Thanh. Accelerating MCMC with Active Subspaces. *SIAM Journal on Scientific Computing*, 38(5):A2779–A2805, January 2016.

[3] T. Cui, J. Martin, Y. M. Marzouk, A. Solonen, and A. Spantini. Likelihood-informed Dimension Reduction for Nonlinear Inverse Problems. *Inverse Problems*, 30(11):114015, November 2014.

[4] A. Doucet, A. Smith, N. de Freitas, and N. Gordon. *Sequential Monte Carlo Methods in Practice*. Information Science and Statistics. Springer New York, 2013.

[5] R. G. Ghanem and P. D. Spanos. Stochastic Finite Element Method: Response Statistics. In *Stochastic Finite Elements: A Spectral Approach*, pages 101–119. Springer New York, New York, NY, 1991.

[6] A. Spantini, A. Solonen, T. Cui, J. Martin, L. Tenorio, and Y. M. Marzouk. Optimal Low-Rank Approximations of Bayesian Linear Inverse Problems, July 2015.

[7] A. Tarantola. *Inverse Problem Theory and Methods for Model Parameter Estimation*, volume xii. SIAM, January 2005.

[8] N. Wiener. The Homogeneous Chaos. *American Journal of Mathematics*, 60(4):897–936, 1938.

A Machine Learning Approach to compute Sobol' sensitivity indices with Given Data – ADAM model study

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Keywords: Machine learning, Sobol' sensitivity indices, Given data, Learning algorithm, ADAM model.

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Derivative-based upper bound for entropic total effect sensitivity with high dimensional and dependent inputs

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This research is motivated by applications of global sensitivity analysis (GSA) towards mathematical models of engineering problems. Such problems are common in computer experiments, where a physical phenomenon is studied with a complex numerical code, and GSA is employed to increase understanding of how the system works, reduce the problem's dimensionality, and help with calibration and verification. In this context, an important question for GSA is: 'Which model inputs can be fixed anywhere over its range of variability without affecting the output?'.

The most common GSA approach examines variability using the output variance. The variance-based total sensitivity indices provide the proportion of variance explained by the input variables. Such tools are limited to second-moment information, which presents a challenge if the underlying distribution is highly skewed or multi-modal. Entropy-based measures overcome this limitation, as they are applicable independent of the shape of the distribution. However, entropy-based indices have limited application in practice, mainly due to the heavy computational burden, as knowledge of conditional probability distributions is required.

In contrast, for a differentiable function, derivative-based methods can be more efficient. An inequality linking variance-based GSA and derivative-based measures has been established [1, 2] to detect un-influential input variables. A recent study [3] has proposed a derivative-based upper bound for entropy-based sensitivity indices, which is computationally cheap to estimate.

In this paper, we present a tighter entropic upper bound by including a differential mutual information correction that accounts for the impact of interactions between dependent input variables. We provide proof that for a differentiable deterministic function $y = g(\mathbf{x}) : R^d \to R$ with continuous random inputs, there exists an upper bound for the conditional entropy-based SA indices:

$$E[H(Y|\mathbf{X}_{\sim i})] \leq H(X_i) + l_i - I(X_i; \mathbf{X}_{\sim i}) \tag{1}$$

where $\sim i$ indicates the index ranges from 1 to d excluding i. $H(X_i)$ is the differential entropy of the input variable X_i and l_i is the expected log-derivatives $l_i = E\left[\ln |\partial g(\mathbf{x})/\partial x_i|\right]$. The mutual information $I(\cdot\,;\cdot)$ is a moment-independent quantification of the statistical dependence between variables reflecting their amount of shared information. As the mutual information is nonnegative, the new upper bound is tight when dependencies among input variables are known or suspected. This greatly improves the screening power, as the effectiveness of the screening improves with the tightness of the upper bound.

Another issue for the derivative-based upper bound is the lack of verification for high-dimensional problems. The simulation of differential entropy, mutual information, and related information theoretic quantities typically proceeds using 'plug-in' Monte Carlo estimators where the densities required are approximated using nonparametric kernel density estimation techniques. However, it is well-known that even in dimensions as low as 10, kernel density estimation is prohibitively data-inefficient [4].

To overcome this issue, we utilize neural density estimation techniques, including recent algorithmic advancements such as MINE [5], KNIFE [6], and REMEDI [7], for efficient approximation of information-theoretic quantities in high dimensions. These estimators are differentiable with respect to the data, enabling the global sensitivity measures to be optimized for outer-loop tasks in engineering design.

Simulation-based prototyping for engineering design problems often involves high-dimensional

spaces of possibly correlated and dependent control variables. This paper extends the derivative-based entropic upper bound to high-dimensional and dependent inputs, thus providing a versatile and efficient tool for general engineering applications.

Reference

[1] I.M. Sobol' and S. Kucherenko. Derivative based global sensitivity measures and their link with global sensitivity indices. *Mathematics and Computers in Simulation*, 79(10):3009–3017, 2009.

[2] M. Lamboni, B. Iooss, A.-L. Popelin, and F. Gamboa. Derivative-based global sensitivity measures: General links with sobol' indices and numerical tests. *Mathematics and Computers in Simulation*, 87:45–54, 2013.

[3] Jiannan Yang. Derivative based global sensitivity analysis and its entropic link. *arXiv preprint arXiv:2310.00551*, 2023.

[4] Larry Wasserman. *All of Statistics*. Springer-Verlag, New York, 2004.

[5] Mohamed Ishmael Belghazi, Aristide Baratin, Sai Rajeshwar, Sherjil Ozair, Yoshua Bengio, Aaron Courville, and Devon Hjelm. Mutual information neural estimation. In *Proceedings of the 35th International Conference on Machine Learning*, volume 80 of *Proceedings of Machine Learning Research*, pages 531–540. PMLR, 10–15 Jul 2018.

[6] Georg Pichler, Pierre Jean A. Colombo, Malik Boudiaf, Günther Koliander, and Pablo Piantanida. A differential entropy estimator for training neural networks. In *Proceedings of the 39th International Conference on Machine Learning*, volume 162 of *Proceedings of Machine Learning Research*, pages 17691–17715. PMLR, 17–23 Jul 2022.

[7] Viktor Nilsson, Anirban Samaddar, Sandeep Madireddy, and Pierre Nyquist. REMEDI: Corrective transformations for improved neural entropy estimation. In *Proceedings of the 41st International Conference on Machine Learning*, volume 235 of *Proceedings of Machine Learning Research*, pages 38207–38236. PMLR, 21–27 Jul 2024.

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Addressing the Rashomon Effect through ranking aggregation

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Abstract

When dealing with prediction problems, analysts rely on variable importance measures and global sensitivity measures to understand the predictive power of variables and uncover the relationships in the data [10]. When the data generating process (DGP) is unknown, analysts typically train machine learning models to use as surrogates, and derive explanations for the patterns in the data computing the variable importance of the best performing model. The validity of this approach is threatened by the Rashomon Effect [2], whereby multiple models achieve similar predictive accuracy but offer different and sometimes conflicting explanations for the underlying patterns. Indeed, the Rashomon Set [5] – the collection of all almost-optimal prediction models – can be seen both as a challenge and an opportunity for analysts: while this adds uncertainty to inference, it also allows for broader exploration of potential explanations.

A number of studies have succeeded in framing a procedure to compute or approximate the Rashomon Set for some specific model classes [11, 12, 4, 9]. Few attempts, however, have been made to explain the relationships in the data by exploiting the whole Rashomon Set [5, 4]. In this work, we propose a novel methodological framework that leverages all the models in the Rashomon Set to produce more reliable and consistent insights into variable importance. Our idea is to view the Rashomon Set for a dataset as a collection of agents, each expressing its own possibly different preference for the features, much like how different experts may offer varying interpretations of the same data. The strength of this preference corresponds to the importance of each variable for the prediction, quantified through an importance measure. By transforming the importance vectors for all the models into rankings and then aggregating them, our method allows analysts to generate a consensus ranking which reflects the preferences of the entire Rashomon Set, offering a comprehensive view on the mechanisms in the data. We draw upon the established literature on ranking aggregation techniques [3, 6, 8] to combine the individual importance rankings into a unified ranking that is robust to model variability.

The proposed framework complements existing variable importance measures and provides analysts with a powerful tool to handle model multiplicity in practical applications. We validate our methodology using both simulated data from known DGPs and real-world datasets, to demonstrate how the framework reconciles conflicting signals from multiple models and produces an

importance ranking of variables that is more aligned with the true DGP. We test different aggregation techniques to show how the choice of the technique impacts the consensus ranking. Furthermore, we provide theoretical results on the structure of the Rashomon Set for the specific class of linear regression models. In particular, we clarify the connection between the coefficients of linear models in the Rashomon Set and the permutation importance measure [1], a widely used measure in machine learning, exploring its relation to total indices [7].

Short biography (PhD student)

Claudia Sessa is a PhD Candidate at LIUC Business University in Castellanza, Italy. Previously, she obtained a MSc in Data Science and Business Analytics (cum laude) and a BSc in Economics, Management and Computer Science, both from Bocconi University in Milan. Her research lies at the intersection of operations research and machine learning.

References

[1] Leo Breiman. Random forests. *Machine Learning*, 45(1):5–32, 2001.

[2] Leo Breiman. Statistical modeling: The two cultures. *Statistical Science*, 16(3), August 2001.

[3] Wade D. Cook. Distance-based and ad hoc consensus models in ordinal preference ranking. *European Journal of Operational Research*, 172(2):369–385, July 2006.

[4] Jiayun Dong and Cynthia Rudin. Exploring the cloud of variable importance for the set of all good models. *Nature Machine Intelligence*, 2(12):810–824, 2020.

[5] Aaron Fisher, Cynthia Rudin, and Francesca Dominici. All models are wrong, but many are useful: Learning a variable's importance by studying an entire class of prediction models simultaneously. *Journal of Machine Learning Research*, 20(177):1–81, 2019.

[6] Dorit S. Hochbaum and Asaf Levin. Methodologies and algorithms for group-rankings decision. *Management Science*, 52(9):1394–1408, September 2006.

[7] Toshimitsu Homma and Andrea Saltelli. Importance measures in global sensitivity analysis of nonlinear models. *Reliability Engineering & System Safety*, 52(1):1–17, April 1996.

[8] Xue Li, Xinlei Wang, and Guanghua Xiao. A comparative study of rank aggregation methods for partial and top ranked lists in genomic applications. *Briefings in Bioinformatics*, 20(1):178–189, August 2017.

[9] Kota Mata, Kentaro Kanamori, and Hiroki Arimura. Computing the collection of good models for rule lists. In *Proc. the 18th International Conference on Machine Learning and Data Mining (MLDM 2022)*, 2022.

[10] Brian D. Williamson, Peter B. Gilbert, Noah R. Simon, and Marco Carone. A general framework for inference on algorithm-agnostic variable importance. *Journal of the American Statistical Association*, 118(543):1645–1658, January 2022.

[11] Rui Xin, Chudi Zhong, Zhi Chen, Takuya Takagi, Margo Seltzer, and Cynthia Rudin. Exploring the whole rashomon set of sparse decision trees. *Advances in Neural Information Processing Systems*, 35:14071–14084, 2022.

[12] Chudi Zhong, Zhi Chen, Jiachang Liu, Margo Seltzer, and Cynthia Rudin. Exploring and interacting with the set of good sparse generalized additive models. *Advances in Neural Information Processing Systems*, 36, 2024.

Barycentre of Models

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When models are trained on data alone, they may not accurately reflect a modeller's view, an expert's judgement, or user inputs. Moreover, on many occasions the experts disagree and thus their models, potentially trained on different datasets, need to be combined. To amalgamate the conflicting nature of expert's views, we propose a modified Barycentre approach. Specifically, each expert proposes an n-dimensional stochastic process driven by different Brownian motions. The combined meta model is created by penalising each experts' model using a weighted relative entropy, where the weights may be proportional to an expert's historical performance. We prove existence and uniqueness of the meta model, derive its dynamics, and develop deep learning algorithms to estimate the barycentre of models. Furthermore, we allow the meta model to satisfy agreed upon external views, in which case the meta model is modify in a minimal manner to respect the external beliefs.

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Global sensitivity analysis for imputation of missing data as an instance of the modelling of the modelling process

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Imputation of missing data is a pivotal step in statistical analysis, ensuring that the integrity of analyses is maintained, data usage is maximized, and bias is mitigated. Missing data, if not handled properly, can lead to biased conclusions, incomplete analyses, and reduced statistical power. A common but suboptimal method of dealing with missing data is listwise deletion, where cases with missing values are discarded, reducing the sample size and potentially introducing bias if the data is not Missing Completely at Random (MCAR) [1]. This method not only wastes valuable information but also compromises the generalizability of the results, particularly when the missingness mechanism is more complex, such as Missing at Random (MAR) or Missing Not at Random (MNAR). To avoid these pitfalls, imputation offers a more robust approach by estimating and filling in the missing values, thereby preserving the sample size and minimizing bias [2, 3].

Imputation is especially important in fields like machine learning, predictive modeling, and real-world applications where missing data is almost unavoidable. Reasons for missingness range from human errors and non-responses to technical failures, all of which can hinder the performance of analytical models if not addressed properly. Most machine learning algorithms do not handle missing data natively, and failure to impute missing values can result in poorer model accuracy, weaker generalization, and skewed insights. By imputing missing values, all available data can be leveraged, which strengthens the statistical power and ensures that model training and evaluation are performed with a complete dataset [4]. In these contexts, effective imputation not only improves model performance but also enables robust, data-driven decisions, even when data is far from ideal [5].

Beyond individual datasets, imputing missing data also facilitates cross-dataset comparisons and integrations. In many real-world analytical applications, integrating or comparing multiple datasets is crucial, especially when trying to synthesize findings across studies or domains. However, missing values can impede such efforts by introducing inconsistencies. Imputation helps standardize the data across these datasets, ensuring the analysis is valid and reducing discrepancies caused by incomplete information [3].

In this study, we advance the field of missing data imputation by applying global sensitivity analysis (GSA) to develop a comprehensive protocol for imputing missing values. The guiding principle behind our approach is to model the modeling process itself—applying GSA to evaluate not only the input parameters but also the assumptions and relationships embedded within the imputation model. By doing so, we assess how uncertainties in input variables affect the imputation outcomes, ultimately aiming to maximize imputation accuracy. This innovative approach represents a step forward in enhancing the robustness of imputation algorithms by systematically optimizing the conditions under which they perform best [6].

Our test case involves the Harmonised European Time Use Survey (HETUS), where participants provide detailed information on how they allocate their daily activities and the locations where these activities occur. In this survey, missing data often affects the location information for certain activities. Our goal is to determine whether socioeconomic input variables can be used to impute the missing location data associated with these activities. We approach this problem using a two-stage imputation process. In the first stage, missing socioeconomic features are imputed, and in the second stage, we estimate activity-location probabilities based on the imputed socioeconomic data. To assess the performance of our method, we use artificially generated datasets with varying percentages of missing data, allowing us to measure the accuracy of the imputation under different conditions.

The results of our analysis highlight the usefulness of global sensitivity analysis in identifying the conditions under which the imputation algorithm performs most effectively. Through GSA, we are able to systematically explore how variations in model parameters and assumptions influence the

output, ultimately leading to more accurate and reliable imputations. This contribution sits at the intersection of machine learning and global sensitivity analysis, an emerging nexus that emphasizes the need for transparent, robust, and well-informed use of algorithms in statistical and predictive modeling contexts. Our work builds on previous research that advocates for the integration of fairness and interpretability in machine learning models, ensuring that imputation processes are not only accurate but also contextually appropriate and equitable [7].

References

[1] R. J. Little and D. B. Rubin. *Statistical Analysis with Missing Data*. John Wiley & Sons, 2002.

[2] J. L. Schafer. *Analysis of Incomplete Multivariate Data*. CRC Press, 1997.

[3] C. K. Enders. *Applied Missing Data Analysis*. Guilford Press, 2010.

[4] K. J. Janssen et al. "Missing Covariate Data in Medical Research: To Impute is Better than to Ignore". *Journal of Clinical Epidemiology* 63.7 (2010), 721–727.

[5] J. A. Sterne et al. "Multiple Imputation for Missing Data in Epidemiological and Clinical Research: Potential and Pitfalls". *BMJ* 338 (2009), b2393.

[6] G. Vannucci, R. Siciliano, and A. Saltelli. *Enhancing Variable Importance in Random Forests: A Novel Application of Global Sensitivity Analysis*. arXiv:2407.14194 [cs, stat]. July 2024. DOI: 10.48550/arXiv.2407.14194. URL: http://arxiv.org/abs/2407.14194 (visited on 09/30/2024).

[7] C. Bénesse et al. "Fairness seen as global sensitivity analysis". En. *Machine Learning* 113.5 (June 2022). Number: 5 Publisher: Springer, 3205–3232. ISSN: 1573-0565. DOI: 10.1007/s10994-022-06202-y. URL: https://link.springer.com/article/10.1007/s10994-022-06202-y (visited on 09/30/2024).

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Analysis and improvement of the convergence of physics-informed neural networks

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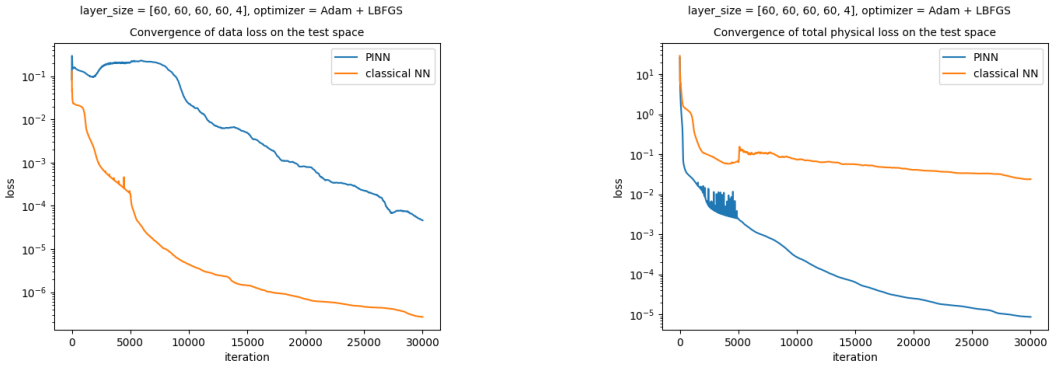
Abstract

Partial Differential Equations (PDEs) can be efficiently solved by well-established numerical methods, such as Finite-Elements (FE) or Finite-Volumes (FV). However, these methods suffer from the necessity to construct grids and discretization schemes specific to the equations considered. Moreover, the account for possible existing data is tedious and multi-query problems, like design optimization or uncertainty quantification, require several resolutions.

Recently, Physics Informed Neural Networks (PINNs) [1] have emerged as an alternate approach, whose objective is to approximate the solution by the output of a feed-forward neural network. The inputs are the space-time coordinates of the problem and the network parameters (weights and biases) are calibrated by minimizimg a loss function that combines the PDE residuals and the boundary conditions, evaluated on a set of sampling points. PINNs have many advantages [2]: they can solve forward, inverse or parametric problems, they allow to add data measurements in the training loss, if available, and they only require a sampling of the space-time domain. Nevertheless, several studies reported convergence difficulties in the training [3], plus a long and painful selection of hyper-parameters (network architecture, optimizer, activation function, sampling, etc.) is often necessary to make the approach successful. Therefore, the goal of this work is to analyse and improve PINNs convergence, with novel dedicated optimization methods.

Firstly, we analyse the convergence of PINNs on a benchmark problem involving the steady flow in a differentially heated cavity, based on the incompressible Navier-Stokes equations with boyancy and heat transport. Specifically, we compared the convergence of the training with two different loss functions: a first one based on the PDE residuals, according to the PINNs paradigm, and a second one based on a classical data fitting, using a FE solution as data. We observed that PINNs converge slower in terms of solution values (estimated for an independent set of points) but outclass the data-fitting formulation in terms of respect of the physics (via the PDE residuals), as illustrated in figure (1). We also reported that the PINNs formulation yields an ill-conditioned Hessian matrix, which necessitates the use of second-order optimizers (quasi-Newton), contrary to the data fitting formulation for which the standard first-order Adam algorithm performs well. Finally, we characterized the antagonism between the loss terms related to the PDE residuals and the one related to the boundary conditions, which could be a cause of the ill-conditioning. Some approaches have been proposed to mitigate this difficulty using adaptive weights [4] or gradient projections [5], but poor results are reported in practice, one criterion dominating often the other one.

Therefore, we propose to adopt a multi-criteria viewpoint for the training, to determine a balanced compromise between the minimisation of the PDE residuals and the satisfaction of the



(a) Error related to solution value

(b) Error related to physical residuals

Figure 1: Comparison between a PINN and a data-fitting NN

boundary conditions. In particular, a Nash game is defined by subdividing the network parameters in different sets, each of them being calibrated to minimize specific loss term. Promising results are obtained for a simple 1D problem. The extension to more complex problems is in progress.

Short biography (PhD student)

After obtaining my master's degree in mathematical engineering with a digital engineering option at Polytech Nice Sophia, during which I did a work-study placement at Thales Alenia Space for anomaly detection, I started a thesis in applied mathematics at the Inria Center at Université Côte d'Azur in November 2023. The subject of this is Physics-Informed Neural Networks for multidisciplinary design.

References

[1] Maziar Raissi, Paris Perdikaris, and George E Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational physics*, 378:686–707, 2019.

[2] Edward Small. An analysis of physics-informed neural networks. *arXiv preprint arXiv:2303.02890*, 2023.

[3] Aditi Krishnapriyan, Amir Gholami, Shandian Zhe, Robert Kirby, and Michael W Mahoney. Characterizing possible failure modes in physics-informed neural networks. *Advances in neural information processing systems*, 34:26548–26560, 2021.

[4] Aviv Navon, Aviv Shamsian, Idan Achituve, Haggai Maron, Kenji Kawaguchi, Gal Chechik, and Ethan Fetaya. Multi-task learning as a bargaining game. *arXiv preprint arXiv:2202.01017*, 2022.

[5] Yuhao Liu, Xiaojian Li, and Zhengxian Liu. An improved physics-informed neural network based on a new adaptive gradient descent algorithm for solving partial differential equations of nonlinear systems. 2022.

Enhanced Metamodeling and Sensitivity Analysis for Complex Models Using Tree-PCE. Applications to Hydro-Morphodynamics Modeling.

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Hydro-morphodynamic modelling is affected from different sources of uncertainty, which occur in process-based models, such as inaccuracy in the model inputs, errors in model structure (e.g., poorly described or omitted physical processes), and from limited computing resources. This study is motivated by the analysis and the characterization of some of these uncertainties, elucidating the factors contributing most significantly to the variability of the model output by employing Sobol sensitivity analysis indices [1]. In practice, the computation of Sobol indices, which involves the stochastic estimation of statistical moments and sensitivity indices, is commonly performed using the Monte Carlo method. However, this approach can be computationally expensive, and the runtime can be significantly reduced by employing a surrogate model in place of the high-fidelity solver. One such surrogate modeling technique is the Polynomial Chaos Expansion (PCE) strategy [2], which approximates the model output $Y = f(X)$, where $X \in \mathcal{D}_X \subset \mathbb{R}^d$, by a polynomial $\hat{Y}$ of degree P, constructed from a set of polynomial basis functions $\{\Phi_\alpha\}_\alpha$ defined on $\mathcal{D}_X$, which are orthonormal with respect to the law of the input vector X. The PCE approximation is defined as:

$$\hat{Y} = \sum_{|\alpha| \leq P} y_\alpha \Phi_\alpha(X)$$

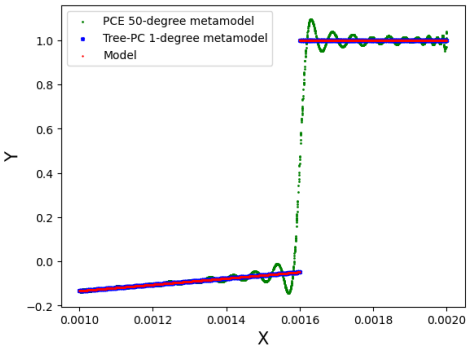
where $\{y_\alpha\}_\alpha$ are the coefficients of Y in the orthonormal basis $\{\Phi_\alpha\}_\alpha$.

The inherent non-linearity of processes in morphological models often causes model outputs to exhibit low sensitivity to input variations until a critical morphological threshold is reached. To accurately represent this variability using a global polynomial approximation, high-degree polynomials would be required, leading to increased numerical complexity. Drawing inspiration from regression trees in supervised learning, we propose an adaptation of the Polynomial Chaos Expansion (PCE) method, called Tree-PCE [3], to address this challenge in complex models. This approach decomposes the input domain into hyperrectangular subdomains, indexed by a binary tree, where local PCE is applied within each subdomain R. The Tree-PCE global metamodel obtained from local metamodels defined by

$$\hat{Y} = \sum_{R} \sum_{|\alpha| \leq P} y_\alpha^R \Phi_\alpha^R(X)$$

with $\{\Phi_\alpha^R\}_\alpha$ being a polynomial basis orthonormal with respect to the low of X on the subdomain R and $\{y_\alpha\}_\alpha^R$ are the coefficients of Y in the orthonormal basis $\{\Phi_\alpha\}_\alpha^R$.

By minimizing the influence of irregularities within these subdomains, the method enables the use of local low-degree polynomial approximations. The resulting local metamodels effectively capture the model's behavior in each region, significantly improving the representation of complex dynamics. In contrast, a global polynomial model would require a much higher degree to achieve comparable performance. Moreover, a by-product of this approach is an analytical formula allowing the computation of global Sobol indices from the coefficients of the local PCE with almost no additional cost.



Comparison of approximating a discontinuous function by standard PCE and Tree-PCE.

The idea of using local Polynomial Chaos Expansions (PCE) has already been explored in the literature. For instance, works such as El Garnoussi et al. (2020) [4] and Dréau et al. (2023) [5] have proposed techniques to decompose the input domain into subdomains and apply local PCE within each. Additionally, Poette and Lucor (2012) [6] introduced an iterative PCE method to enhance the accuracy of non-linear models. However, these approaches have not yet achieved the capability to directly compute Sobol indices from the obtained metamodel coefficients, which is a distinctive advantage of our method.

In conclusion, the proposed method provides a cost-effective solution for uncertainty quantification of complex model behaviors, particularly in hydro-morphodynamic modeling, by enhancing the precision of metamodeling and Sobol indices estimation. The results demonstrate its potential to significantly improve the accuracy and reliability of model predictions, especially when addressing complex dynamics.

References:

[1] A. Saltelli, "Making best use of model evaluations to compute sensitivity indices", *Computer Physics Communication.*, **145**: 280-297, 2002.

[2] B. Sudret, "Global sensitivity using polynomial chaos expansion", *Reliability engineering & system safety.*, **93***(7): 964-979, 2008.*

[3] F. Ben Said, A. Alfonsi, A. Dutfoy, K. El Kadi Abderrezzak, C. Goeury, J. Reygner, F. Zaoui, "Tree PCE for surrogate modelling and sensitivity analysis of complex numerical models", work in preparation.

[4] S. El Garroussi, S. Ricci, M. De Lozzo, N. Goutal, D. Lucor, "Assessing uncertainties in flood forecasts using a mixture of generalized polynomial chaos expansions". 2020 TELEMAC-MASCARET User Conference , 2020.

[5] J. Dréau, B. Magnain, A. Batailly, "Multi-element polynomial chaos expansion based on automatic discontinuity detection for nonlinear systems". Journal of Sound and Vibration, **567***: 117920. 2023.*

[6] G. Poëtte, D. Lucor, "Non intrusive iterative stochastic spectral representation with application to compressible gas dynamics". Journal of Computational Physics, **231***(9): 3587-3609, 2012.*

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Derivative-based Global Sensitivity Analysis for Energy System Optimization Models via Implicit Differentiation

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Energy system optimization models (ESOMs) have emerged as valuable tools for guiding present-day decisions for the energy transition based on assumptions about the future. These future assumptions hold much uncertainty, which propagates to the model outputs. If not considered, this uncertainty can lead to unintended future outcomes. One way to address this uncertainty is by identifying the most influential parameters on the model output variability. With this information, we can refine the corresponding assumptions, or make present-day decisions more resilient to them.

Global sensitivity analysis (GSA) is a powerful tool for determining the most influential parameters on a model's output variability [1]. However, GSA can be challenging for computationally intensive models with thousands of parameters. ESOMs usually fall into this classification due to the required spatial and temporal resolution and the energy sectors they consider. GSA via variance decomposition for Sobol indices requires $N \cdot (p+2)$ model evaluations, with p being the number of model parameters (on the order of 10^2-10^3) and N a number greater than 500 [2]. The model evaluations required for GSA can significantly decrease via the Morris method, requiring $r \cdot (p+1)$ model evaluations with r being the number of trajectories (often between 5 and 50). However, the Morris method mainly serves for screening without quantitative information on uncertainty contributions from parameter interactions [1]. Due to these limitations, performing GSAs on large-scale ESOMs with quantified uncertainty contributions is a current challenge.

In this work, we propose an efficient method for GSA of computationally intense ESOMs. For this purpose, we employ derivative-based global sensitivity measures (DGSMs), derived from the expected square of the model derivatives with respect to each parameter. DGSMs are a promising GSA alternative, as calculation of the DGSMs requires a sample size, N, of model evaluations, independent of the number of model parameters, while providing an upper bound on the total Sobol indices [3]. DGSMs combine the quantitative benefits of Sobol index-based methods with the computational efficiency of the Morris screening method.

Calculating the DGSMs, however, requires derivatives of the model outputs with respect to the input parameters. Optimization problems don't have an analytical form relating the decision variables to the model parameters. Therefore, there's no analytical expression for the derivatives. However, derivatives can be calculated at the optimal point by implicit differentiation of the set of Karush-Kuhn-Tucker (KKT) conditions [4]. The KKT conditions provide a set of necessary and sufficient conditions for optimality. The KKT conditions take the form $K(\theta, z^*) = 0$, where θ are the optimization problem parameters and z^* is a vector containing the optimal decision variables x^* and the problem dual variables (λ^*, μ^*). Implicit differentiation stems from the implicit function theorem, which states that given an implicit system of equations, $F(x, y)$, and a point (x_0, y_0) at which $F(x_0, y_0) = 0$ and $J_y F(x_0, y_0) \neq 0$, there exists an explicit system of equations $y(x)$ on an interval containing x_0 such that $J_y F(x_0) = -[J_y F(x_0, y_0)]^{-1} \cdot J_x F(x_0, y_0)$. As long as the partial Jacobian of the KKT conditions, $J_z K(\theta, z^*)$ is non-singular, one can apply the implicit function theorem to the KKT conditions to obtain the sensitivities of the model decision variables to the model parameters, $J_\theta z^*(\theta)$ (Equation 1).

$$J_\theta z^*(\theta) = -[J_z K(\theta, z^*)]^{-1} \cdot J_\theta K(\theta, z^*) \tag{1}$$

Implicit differentiation of an optimization problem's KKT conditions has been applied in several disciplines such as process controls for determining on-line parameter sensitivities, machine learning for gradient-based neural network training, and energy systems optimization for calculating emissions factors. In this work, we use this technique to enable DGSM-based GSA for computationally intensive ESOMs for which calculation of Sobol indices is not feasible.

We carry out our DGSM-based GSA via implicit differentiation on a small ESOM and compare the resulting DGSMs to the total Sobol indices, S_T, calculated via variance decomposition using the SALib library in Python [5]. Our model minimizes the cost of n operating electricity generation technologies, x_i, with costs, c_i, subject to maximum generation constraints, G_i, and a total load, L, which must be satisfied.

Our preliminary results show that for most model parameters, DGSM-based GSA provides upper bounds for the total Sobol indices for with 78% less computation time (Table 1). The piece-wise constant nature of the decision variables of linear optimization problems with respect to objective function coefficients leads to zero-valued derivatives, highlighting a limitation of our method. We address this limitation by adding a quadratic penalty term to the objective function. Overall, we propose a method that enables GSA of computationally intense ESOMs, allowing to better-consider uncertainty in present-day decision-making.

Table 1: Computation time and sensitivity measure comparisons for total Sobol indices, S_T, calculated via variance decomposition, and DGSMs calculated via implicit differentiation.

		sensitivity of model decision variable, x_i to model parameters:				
method	computation time	L	$G_{j\neq i}$	$G_{j=i}$	$c_{j\neq i}$	$c_{j=i}$
DGSM	16 min	1.4	0.006	0.02	0	0
DGSM (+ penalty term)	18 min	1.1	0.003	0.02	0.2	0.8
S_T	72 min	0.5	0.004	0.01	0.1	0.6

References:

[1] A. Saltelli, S. Tarantola, F. Campolongo and M. Ratto, "Sensitivity analysis in practice: a guide to assessing scientific models", *volume 1, Wiley Online Library*, 2004.

[2] A. Saltelli, P. Annoni, I. Azzini, F. Campolongo, M. Ratto and S. Tarantola, "Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index", *Computer physics communications*, **181**(2):259–270, 2010.

[3] I.M. Sobol and S. Kucherenko, "A new derivative based importance criterion for groups of variables and its link with the global sensitivity indices." *Computer Physics Communications* **181**(7):1212-1217, 2010.

[4] S. Barratt, "On the differentiability of the solution to convex optimization problems." *arXiv preprint* **arXiv:1804.05098**, 2018.

[5] J. Herman and W. Usher, "SALib: An open-source Python library for Sensitivity Analysis" *The Journal of Open Source Software* **9**(2), 2017.

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Reconstruction of fluid flow fields from data using Gaussian process regression with physics–informed kernels

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Abstract

The approximation of solutions of partial differential equations (PDE) using techniques issued from Gaussian process regression (GPR) has evolved significantly in recent years [2, 4]. The key element in GPR methods is the construction of a kernel function satisfying specific properties, such as continuous conditioning around a curve [3]. These properties are in turn transferred to the corresponding reproducing kernel Hilbert space (RKHS) and can be associated to specific PDE constraints. In fluid mechanics, there have been advances on using GPR techniques whether from a pure data approach in order to estimate target functionals of interest [1], or even for obtaining alternative numerical methods through the definition of a representer formula over a RKHS [6].

Given a scalar Gaussian process $f \sim GP(0, G)$ indexed over a domain $\Omega \subset \mathbb{R}^2$, consider the vector Gaussian process given by $\boldsymbol{Z} = \boldsymbol{\nabla} f^{\perp} = (-\partial_{x_2} f, \partial_{x_1} f)^{\intercal} \sim GP(0, \boldsymbol{K})$ where $\boldsymbol{K}$ is a matrix–valued kernel satisfying a divergence–free condition. A reconstruction formula $\boldsymbol{u}^{\star}$ for velocity $\boldsymbol{u}$, based on a Lagrangian simulation of a viscous flow over the periodic domain Ω during a time interval $[0, T]$, is proposed [6] :

$$\boldsymbol{u}^{\star}(\boldsymbol{x}, t) = \mathbb{E}\left(\boldsymbol{Z}(\boldsymbol{x}) \mid \mathbf{curl}\ \boldsymbol{Z}(\boldsymbol{Q}(t)) = \boldsymbol{W}(t)\ \right), \quad \boldsymbol{x} \in \Omega,\ t \in [0, T], \tag{1}$$

where $\boldsymbol{Q} = (\boldsymbol{q}_i)_{i=1}^{N}$ is a set of N collocation trajectories associated to the vorticity values $\boldsymbol{W} = (w_i)_{i=1}^{N}$. Thus, a vorticity reconstruction formula follows directly from $w^{\star} = \operatorname{curl} \boldsymbol{u}^{\star}$.

We propose a reconstruction approach to simulate 2D incompressible flows in a tunnel setting with an obstacle (*e.g.* cylinder or airfoil profile) through estimation from a physics–informed curve–constrained Gaussian process. Considering flow data obtained from high–precision external simulations, where $\boldsymbol{V} = (\boldsymbol{v}_j)_{j=1}^{N_{\mathrm{data}}}$ are the velocity values on the N_{data} trajectories $\boldsymbol{Y} = \left(\boldsymbol{y}_j\right)_{j=1}^{N_{\mathrm{data}}}$; inlet and exit boundary conditions on velocity $\widetilde{\boldsymbol{V}} = (\widetilde{\boldsymbol{v}}_k)_{k=1}^{N_{\mathrm{bd}}}$ over N_{bd} boundary points $\widetilde{\boldsymbol{X}} = (\widetilde{\boldsymbol{x}}_k)_{k=1}^{N_{\mathrm{bd}}}$, and physical constraints around an obstacle $\mathcal{D}$, we study a reconstruction approach that combines data and a numerical method on the vorticity system. For the centered Gaussian process $\boldsymbol{Z}_{\mathcal{D}}$ associated to a curve–constrained kernel $\boldsymbol{K}_{\mathcal{D}}$, an estimation formula for velocity will be of the form :

$$\boldsymbol{u}^{\star}(\boldsymbol{x}, t) = \mathbb{E}\left(\boldsymbol{Z}_{\mathcal{D}}(\boldsymbol{x}) \mid \boldsymbol{Z}_{\mathcal{D}}(\boldsymbol{Y}(t)) = \boldsymbol{V}(t),\ \boldsymbol{Z}_{\mathcal{D}}(\widetilde{\boldsymbol{X}}) = \widetilde{\boldsymbol{V}},\ \mathbf{curl}\ \boldsymbol{Z}_{\mathcal{D}}(\boldsymbol{Q}(t)) = \boldsymbol{W}(t)\ \right), \tag{2}$$

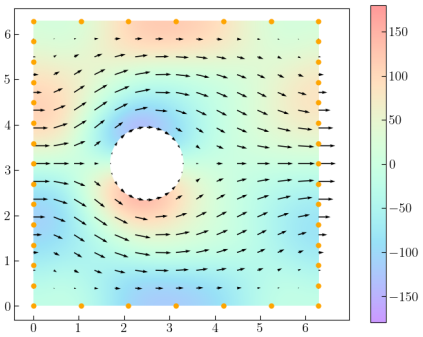

Figure 1: Velocity field and vorticity (colormap) reconstruction from GPR using an obstacle–constrained physics–informed kernel and $N_{\mathrm{bd}} = 40$ domain boundary condition points (orange). No discrete condition points are used in the obstacle boundary for the interpolation.

for $\boldsymbol{x} \in \Omega$ and $t \in [0, T]$. These approaches allows us to quantify uncertainty by means of the covariance versions of representation formulas (1) and (2).

Further data and collocation sub–sampling techniques are being studied to enhance the performance of the estimation at each time step, as well as kernel parameters identification by maximum likelihood estimation (MLE). We aim to adapt this reconstruction approach to integrate particle tracking velocimetry (PTV) data in a 2D and 3D Lagrangian setting [5].

Short biography (PhD student)

This research project is at the intersection of probabilities, data assimilation and numerical analysis of PDE. Adrian Padilla–Segarra holds a Master in Mathematics and Applications from University Paris–Saclay (track Analysis, Modelling, Simulation at Orsay and ENSTA, with a FMJH scholarship) and a Bachelor in Mathematics from Yachay Tech (Ecuador). The PhD contract is jointly financed by ONERA and INSA Toulouse and is attached to the IMT.

References

[1] Jean-Luc Akian, Luc Bonnet, Houman Owhadi, and Éric Savin. Learning “best” kernels from data in Gaussian process regression, with application to aerodynamics. *Journal of Computational Physics*, 470:111595, 2022.

[2] Yifan Chen, Bamdad Hosseini, Houman Owhadi, and Andrew M Stuart. Solving and learning nonlinear PDEs with Gaussian processes. *Journal of Computational Physics*, 447:110668, 2021.

[3] Bertrand Gauthier and Xavier Bay. Spectral approach for kernel-based interpolation. *Annales de la Faculté des sciences de Toulouse : Mathématiques*, Ser. 6, 21(3):439–479, 2012.

[4] Iain Henderson, Pascal Noble, and Olivier Roustant. Characterization of the second order random fields subject to linear distributional PDE constraints. *Bernoulli*, 29(4):3396–3422, 2023.

[5] Benjamin Leclaire, Philippe Cornic, Frédéric Champagnat, Eric Fabre, and Frédéric Calmels. A web portal for automatic performance evaluation of lagrangian particle tracking and data assimilation algorithms. In *20th International Symposium on the Application of Laser and Imaging Techniques to Fluid Mechanics, Lisbon, Portugal*, 2022.

[6] Houman Owhadi. Gaussian process hydrodynamics. *Applied Mathematics and Mechanics*, 44(7):1175–1198, 2023.

Bayesian approach to assessing the overal counter-performance of housing block fabric

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The building sector in France represents 25 % of its annual national carbon footprint. A future low-carbon economy must rely on effective energy conservation measures implemented today in the existing building stock. However, energy retrofits of building fabric face the issue of the so-called performance gap: actual energy use is significantly higher than initially designed [1]. The causes of the performance gap are manifold, bt primarily due to different and carbon-intensive usage patterns and/or poor workmanship. Addressing the performance gap by ensuring the quality of energy conservation measures in buildings is essential.

On-site measurement of a building's thermal performance is considered as a major tool to guarantee actual energy savings. The thermal performance can be characterized by measuring the overall Heat transfer Coefficient (HTC) of the building envelope [2], which indicates the amount of heat flowing through the fabric given a temperature difference between the indoor and outdoor environments. The measurement involves solving an inverse problem: (1) heat is uniformly delivered indoors through heating devices while indoor and outdoor temperatures are measured (2) these measurements feed an appropriate model, dynamic or steady-state, that predicts the indoor temperature from the outdoor air temperature and the heat delivered, depending on the HTC.

Today, HTC measurement methods for detached housing have been the focus of a decade of academic and industrial research, and a few can be considered as mature. However, no method has yet been developed for housing blocks. This is because direct measurement is rarely feasible. It is technically challenging to uniformly heat dozens of apartments simultaneously. Sampling the entire envelope by measuring a predetermined set of apartments is a viable alternative but raises several issues. The measurement of each apartment si more uncertain than for detached housing due to heat transfer to neighboring units [3]. Consequently, only the apartments with the largest exterior surface areas are included in the sample, typically limiting the number of measured apartments to four due to operational constraints. This sampling is likely sub-optimal and not representative of th overall building fabric. In addition, inferring the entire building heat transfer coefficient from the samples is intractable: its definition in Equation (1) is calculated from estimates of U_i (the areal heat loss coefficient of each wall type) and Ψ_j (the linear thermal bridge coefficients), which themselves are estimated from the measurement of the HTC_k for each apartment, as in Equation (2).

$$HTC = \sum_{i \geq 3} U_i \cdot S_i^{overal} + \sum_{j \geq 2} \Psi_j \cdot L_j^{overal} \tag{1}$$

$$\text{for } k \leq 4 \text{ apartments: } HTC_k = \sum_{i \geq 3} U_i \cdot S_i^k + \sum_{j \geq 2} \Psi_j \cdot L_j^k \tag{2}$$

However, from a Bayesian point of view, the problem becomes tractable as long as the prior distributions are proper [4]. This can be done by translating the prior degree of belief about the thermal performance of the building fabric into probability distribution. Accordingly, the issue addressed by this study is (1) to create an appropriate probabilistic model and (2) to identify the minimal set of apartment and local U_i measurements required to detect a counter-performance with sufficient certainty.

In this context, the probabilistic model aims at answering the following question: given the available information and data, what is the risk of a counter-performance relative to what was expected in the design phase? To address this, the model translates the set of equations in Equation (2), treating each parameter Ψ_j as a normal distribution and each U_i as a mixture of normal distributions of size $n + 1$ where n is the number of local U_i measurement performed. A mixture normal distribution

accounts for potential thermal heterogeneity in walls, as would happen with construction defects.

The priors are set based on design-phase expectations, with an expanded uncertainty of 20%. This has the advantage of assigning zero probability all non-significant thermal bridges, which considerably reduces the parameter space. However, neglecting thermal bridges might introduce a model error, preventing the posterior distribution of the HTC from being considered a reliable estimate of the actual HTC, as practical identifiability may be lost in the process.

Updating the parameter distributions is done by integrating the HTC_k measurements of each apartment and any local measurements of U_i. Although the predicted posterior HTC is no longer identifiable, it still reflects the probability of an overal counter-performance given the collected data. To evaluate the performance hypothesis, the highest density interval (HDI) of the HTC distribution is compared to a target zone called Region of Practical Equivalence (ROPE) [5, 6], defined as $]-\infty; HTC_{design} + 20\%]$. The performance hypothesis is accepted if the HDI falls entirely within the ROPE, rejected if it falls entirely outside of the ROPE, and undecided if its spans both sides.

At this point, solving the problem using a Bayesian approach becomes feasible. Nevertheless, there is no free lunch and uncertainty in the measurements could undermine the process. In other words, the approach would be ineffective if the hypothesis is always undecided or if there are false positives–i.e. accepting the hypothesis when the building is highly counter-performant. To test the process, a set of numerical experiments was conducted, showing that with the defined ROPE, and with at least three apartment measurements and two wall-types repeated U measurements, there are no false positives, and counter-performance is detected with 35% or greater HTC difference.

As a conclusion, the current approach to assessing counter-performance of a housing block provides a formal probabilistic understanding of the actual belief in the building fabric's performance. The approach has been proven reliable and can detect counter-performances of 35 % and higher with reasonable certainty.

References:

[1] S. Thébault and M. Humbert, "Programme Diane : Retour d'expérience sur les niveaux de déperditions thermiques mesurées en maison neuve avec la méthode ISABELE", *Conference of the Building Performance Simulation Association France*, 565–572, 2024.

[2] ISO ...

[3] S. Juricic, F. Lahlou, S. Thébault and A. Challansonnex, "Conditions de validité pour l'inférence d'une performance globale d'enveloppe de bâtiment à logements collectifs à partir d'une mesure par échantillonnage", *Conference of the Building Performance Simulation Association France*, 333–340, 2024.

[4] Y. Xie and B. P. Carlin "Measures of Bayesian learning and identifiability in hierarchical models", *Journal of Statistical Planning and Inference*, **136**(10):3458–3477, 2006.

[5]J. K. Kruschke "Rejecting or Accepting Parameter Values in Bayesian Estimation", *Advances in Methods and Practices in Psychological Science* **1**(2): 270–80, 2018.

[6] P. Schwaferts and T. Augustin "Bayesian Decisions Using Regions of Practical Equivalence (ROPE): Foundations", *Technical Report 235 University of Munich - Department of Statistics*, 2020.

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A comparison of variance-based estimations of sensitivity indices for models with dependent variables

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Keywords: Sobol' sensitivity index, dependent variables, design driven sensitivity analysis, variance based methods

*Speaker

A distributional perturbation method based on the Fisher-Rao distance for robustness analysis in uncertainty quantification

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Abstract

Robustness analysis is a subdomain of uncertainty quantification that deals with the uncertainty propagation through a computer code G (assumed costly) of its input probability distributions. More specifically, the inputs $(X_1, ..., X_d)$ of G take uncertain values which usually correspond to physical measurements. Therefore, the uncertainty on these inputs X_i is modeled by a probability distribution f_i that is determined through physical experiments, hence f_i is itself uncertain. The goal of a robustness analysis method is then to: (a) take into account the uncertainty on f_i, this is done by defining a distributional perturbation method; (b) assess the impact on a quantity of interest (QoI) of the output $Y = G(\mathbf{X})$ of a perturbation on the inputs through robustness indices.

In this talk, we will present these two aspects of a specific robustness analysis method initially proposed in [1].

In the first part of this presentation, we will focus on the distributional perturbation method that is based on the Fisher-Rao distance on parametric families of probability distributions $\mathcal{P} = \{g_\theta\}_{\theta\in\Theta}$. This particular distance, on $\mathcal{P}$, derived from the Fisher information metric, has a geometric origin: it is the length of the shortest path connecting two points in $\mathcal{P}$. The Fisher-Rao distance presents many interesting properties for the purpose of robustness analysis. One of these properties is the universality of a (small) distance value $\delta > 0$ in two different families: if $\mathcal{P} = \{g_\theta\}_{\theta\in\Theta}$ and $\mathcal{Q} = \{h_\xi\}_{\xi\in\Xi}$ are two parametric families of probability distributions with their respective Fisher-Rao distance $d_\mathcal{P}$ and $d_\mathcal{Q}$, then if $d_\mathcal{P}(g_\theta, g_{\theta'}) = d_\mathcal{Q}(h_\xi, h_{\xi'}) = \delta > 0$ we can conclude that g_θ and $g_{\theta'}$ are "as far apart as" h_ξ and $h_{\xi'}$. This is a consequence of the Cramér-Rao lower bound and holds even though these distributions belong to two different families each possessing its own Fisher-Rao distance.

In the second part of this presentation, we will explain how the impact of a distributional perturbation on the inputs is assessed through robustness indices. These indices are denoted $S_{i\delta}$ for each input X_i and a perturbation level δ. They quantify the relative variation of the QoI of the output before and after perturbation of the input distributions

$$S_{i\delta} = \frac{Q(Y^{i\delta}) - Q(Y)}{Q(Y)},$$

where $Q(Y)$ is a QoI of Y, usually a quantile, and Y and $Y^{i\delta}$ are respectively the initial and perturbed output of G. Since these statistical quantities are not explicitly known, a statistical estimation method is necessary which takes into account the computation cost of G. The estimation method that we use is importance sampling. A central limit theorem is available for the estimators of both $Q(Y)$ and $Q(Y^{i\delta})$ but the asymptotic variance depends respectively on the density function of Y and $Y^{i\delta}$ which is hard to estimate [1, 2]. For this reason, we decided to construct non-asymptotic confidence intervals for the output QoI based on well known concentration inequalities [3]. This will be illustrated on different analytical and industrial cases.

Short biography (PhD student)

I did my bachelor's and master's degree in mathematics at Paul Sabatier University. I then pursued a PhD career in mathematics at EDF R&D in collaboration with the Mathematics Institute of Toulouse (IMT). The main goal in my thesis is to perform robustness analysis of computer codes for uncertainty quantification using information geometry. I am currently a second year PhD student and I was funded by the Labex CIMI (Toulouse) for the first few months of my PhD and by EDF for the remaining duration.

References

[1] C. Gauchy, J. Stenger, R. Sueur, and B. Iooss. An information geometry approach to robustness analysis for the uncertainty quantification of computer codes. *Technometrics*, 64(1):80–91, 2022.

[2] P. W. Glynn. Importance sampling for Monte Carlo estimation of quantiles. In *Mathematical Methods in Stochastic Simulation and Experimental Design: Proceedings of the 2nd St. Petersburg Workshop on Simulation*, pages 180–185. Citeseer, 1996.

[3] B. B. Ketema, N. Bousquet, F. Costantino, F. Gamboa, B. Iooss, and R. Sueur. Non-asymptotic confidence intervals for importance sampling estimators of quantiles. In *55ème Journées de statistique de la SFdS*, Bordeaux, France, May 2024.

Bayesian approach for the detection of inactive variables in Gaussian process approximation

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Gaussian Processes (GPs) are recognized for their effectiveness as metamodels of numerical simulators [6]. They offer a Bayesian framework for supervised learning, allowing the incorporation of prior knowledge about a function through suitable kernel selection [7].

A widely used kernel in GP modeling is the anisotropic Matérn covariance function [7], which can be written as

$$k_{\nu,\sigma,\rho}(x,y) := \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu} h_\rho\right)^\nu K_\nu \left(\sqrt{2\nu} h_\rho\right), \quad \text{with } h_\rho = \left(\sum_i^d \frac{(x_i - y_i)^2}{\rho_i^2}\right)^{1/2},$$

and where Γ is the Gamma function, and K_ν is the modified Bessel function of the second kind. The parameters $\nu \in \mathbb{R}^+$, $\sigma \in \mathbb{R}^+$ and $\rho = (\rho_1, \ldots, \rho_d) \in \mathbb{R}^{+d}$ are usually selected using the maximum likelihood approach (see, e.g., [4]). This covariance function is known for its ability to model functions with different degrees of smoothness and variable correlations across different dimensions.

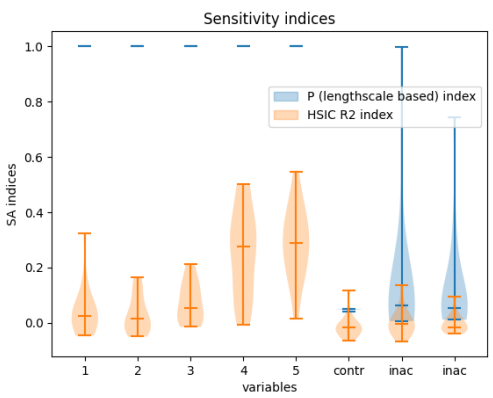
Building upon this framework, our work focuses on identifying inactive variables—those with no influence on the function output—in settings where the number of active variables is small (e.g., fewer than 20) but the overall dimensionality is large (e.g., greater than 50). Specifically, we consider functions $f : \mathbb{R}^d \to \mathbb{R}$, for which there exists function of k inputs, $g : \mathbb{R}^k \to \mathbb{R}$, such that:

$$f(\mathbf{x}) = g(x_{(1)}, x_{(2)}, \ldots, x_{(k)}), \quad \mathbf{x} = (x_1, \ldots, x_d) \in \mathbb{R}^d \text{ and } \{(1), ..., (k)\} \subset \{1, ..., d\}.$$

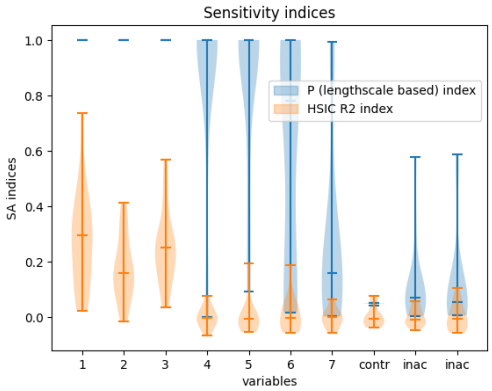
To sequentially identify inactive variables and reduce dimensionality using GPs, a common first idea is to use sensitivity analysis, such as in the work of Marrel et al. [3], where GPs are combined with HSIC (Hilbert-Schmidt Independence Criterion) indices to assess variable importance. Another approach, as demonstrated by Salem et al. [5], relies on the lengthscale parameters $\rho_1, \ldots, \rho_d$ of the GP covariance function $k_{\nu,\sigma,\rho}$. In this method, large values of a lengthscale parameter indicate slow variation of the output with respect to the corresponding variable, signifying that the variable is likely inactive.

Our method builds on the latter approach, relying on the lengthscale parameters and adopting a fully Bayesian framework (see, e.g., [1]). We generate samples from the posterior distribution of the lengthscale parameters using a Metropolis-Hastings algorithm. The main idea of the proposed approach is to introduce an inactive control variable x_{d+1}, which allows us to establish a reference posterior density for the lengthscale parameters of inactive variables. To determine whether a given variable is active, a significance level α is first fixed, and a threshold t_α is computed such that the posterior probability $\mathbb{P}_n(\rho_{d+1} > t_\alpha) \geq 1 - \alpha$, where ρ_{d+1} is the lenghscale parameter of the control variable x_{d+1}. Then, we introduce indices $P_i = \mathbb{P}_n(\rho_i \leq t_\alpha)$, which reflect the probability that the variable x_i is active.

Initial comparisons between our method and R^2_{HSIC} indices [2] demonstrate promising results (see, e.g., Figure 1).



(a) $f_1(\mathbf{x}) = \frac{1}{3}\sum_{i=1}^{5}\left(x_{(i)} + 2.2\prod_{i<j=2}^{5} x_{(i)}x_{(j)}\right)$



(b) $f_2(\mathbf{x}) = 6x_{(1)} + 4x_{(2)} + 5.5x_{(3)} + 3x_{(1)}x_{(2)} + 2.2x_{(1)}x_{(3)} + 1.4x_{(2)}x_{(3)} + x_{(4)} + 0.5x_{(5)} + 0.2x_{(6)} + 0.1x_{(7)}$

Figure 1: Distributions of the lengthscale-based indices P_i (blue, $\alpha = 5\%$) and the R^2_{HSIC} indices [2] (orange), providing a comparison of variable importance, with a focus on distinguishing between active $(1, \ldots, k)$, control (contr), and inactive (inac) variables, for 20 repetitions of random uniform designs of size $n = 30$. Functions f_1 and f_2 have $k = 5$ and $k = 7$ active variables, respectively, within an overall dimension of $d = 50$. Two randomly selected inactive variables from the set of $d - k$ are also represented.

References

[1] R. Benassi, J. Bect, and E. Vazquez. Robust gaussian process-based global optimization using a fully bayesian expected improvement criterion. In *Learning and Intelligent Optimization: 5th Int. Conf., LION 5, Rome, Italy*. Springer, 2011.

[2] S. Da Veiga. Global sensitivity analysis with dependence measures. *J. Statistical Computation and Simulation*, 85(7):1283–1305, 2015.

[3] A. Marrel, B. Iooss, and V. Chabridon. The ICSCREAM methodology: Identification of penalizing configurations in computer experiments using screening and metamodel—applications in thermal hydraulics. *Nuclear Science and Engineering*, 196(3):301–321, 2022.

[4] S. J. Petit, J. Bect, P. Feliot, and E. Vazquez. Parameter selection in gaussian process interpolation: an empirical study of selection criteria. *SIAM/ASA J. on Uncertainty Quantification*, 11(4):1308–1328, 2023.

[5] M. Ben Salem, F. Bachoc, O. Roustant, F. Gamboa, and L. Tomaso. Gaussian process-based dimension reduction for goal-oriented sequential design. *SIAM/ASA Journal on Uncertainty Quantification*, 7(4):1369–1397, 2019.

[6] T. J. Santner, B. J Williams, and W. I.r Notz. *The Design and Analysis of Computer Experiments*. Springer, 2018.

[7] M. L. Stein. *Interpolation of spatial data: some theory for kriging*. Springer, 1999.

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Optimized clustering of model input samples based on sensitivity indices

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The present work is motivated by the Sensitivity Analysis (SA) of models having multivariate (MV) inputs among their input factors. SA in this context is challenging because of dependency issues within the MV input components, which prevents to find and characterize easily the sensitive ones.

We investigate the use of clustering in order to provide more insights on the sensitive components of MV sensitive inputs. More precisely, we propose to use clustering to find groups of MV inputs samples such that group characteristics explains as best as possible the influence of the MV inputs. When successful, this strategy means that group characteristics are good summaries of the MV inputs influence on the model outputs.

In order to apply this strategy, two questions must be answered: i) how to define quantitatively the influence of groups on the output variability and ii) how to find clustering that maximize the associated criteria.

Notations:
We study $y = f(\boldsymbol{w}, z)$, where $\boldsymbol{w}$ is a complex input (typically a vector of weather variables in environmental models) and z an independent input (possibly a large vector grouping all other inputs of interest). Using a labeling approach [2] based on samples $\boldsymbol{w}_1, ..., \boldsymbol{w}_L$, we now study $y = g(l, z) = f(\boldsymbol{w}_l, z)$. The Sobol' decomposition on g writes simply: $S_l + S_z + S_{lz} = 1$.

We introduce a general clustering function $\mathcal{C}$ such that $\mathcal{C}(l) = c \in 1, .., K$ is the cluster label of the input with label l. We introduce also a 'within-cluster selection factor' $u \in [0, 1[$ that is used to choose elements within a cluster.
Let us note $(l_1^c, .., l_{N_c}^c)$ the N_c elements in cluster c. We denote as h the model having cluster labels and selection factors (along with the co-variable z) as inputs: $h(c, z, u) = g(l^c_{\lfloor u.N_c \rfloor + 1}, z)$, where $\lfloor x \rfloor$ is the integer part of x.

Sensitivity analysis with selection factor u:
Our central idea to define clustering criteria is to use the sensitivity indices associated to model h, where the cluster label c has a discrete distribution with values $c_1, .., c_K$ and probabilities $p_1, .., p_K$ (probabilities of clusters according to their size), where u has an uniform distribution within $[0, 1[$ and z its (unchanged) uncertainty distribution. Writing the Sobol' decomposition on h, we have: $S_c + S_z + S_{cz} + S_u^T = 1$,where S^T denotes a total Sobol' index.

First clustering problem: $\max_{\mathcal{C}(.)} S_c$
This optimization problem will allow to find clustering that maximize the main effect of the cluster type, which is at best equal to S_l. More precisely, we show that $S_c = S_l - \frac{1}{V}\sum_{c=1}^{K} p_c \widetilde{V}_c$, where $\widetilde{V}_c = \mathbb{V}_{l \in c}\mathbb{E}_z[g(l, z)]$. We show that solutions of this problem are defined using quantiles of the distributions $\mathbb{E}_z[g(l, z)]$, leading to an efficient numerical algorithm to find solutions of the global optimization problem. However a drawback of this criterion is that it does not take into account the variability of model responses along direction z.

Second clustering problem: $\min_{\mathcal{C}(.)} S_u^T$

Using this criterion, we try to minimize the effect of the within-cluster selection factor u, thus to minimize the effect (this time including interaction effects) of the within-cluster variability. We show that $S_u^T = \frac{1}{V}\mathbb{E}_z[\sum_{c=1}^{K} p_c V_c(z)]$, with $V_c(z) = \mathbb{V}_{l\in c}[g(l,z)]$. We show that numerical solutions of this problem can be found using a K-means like algorithm. Compared to a classical K-means problem, our algorithm uses distances in the space of outputs, i.e not in the space of the variable to be clustered.

Numerical examples

We implemented the algorithms for solving the two previous problems and tested them firstly on a simple function at the level of g_l (i.e. on functions having label l and co-variable z as inputs). The model output y has no variability along z for $l \leq 75$, where $y = 1 + 0.005\ l$. For $l > 75$, $\mathbb{E}_z[y]$ is also equal to $1 + 0.005\ l$, but y can take two values depending on z, which are inverted if $l > 87$. We can see in Figure 1 that the S_u^T-based criterion takes into account the variability along z and creates clusters in the region of variability in z, which was not the case of the S^c-based criterion.

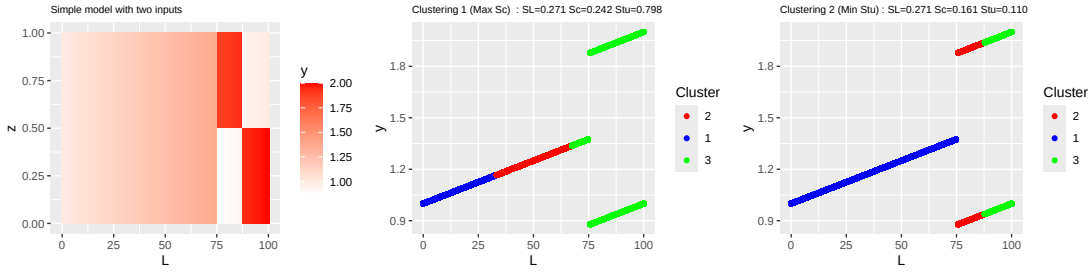

Figure 1: Clustering result of a simple model for the two criteria. Left: model definition; Middle: clustering based on S_c; Right: clustering based on S_u^T.

We will also present during the conference clustering on a crop model [1] having vector of weather variables among its inputs. We will be particularly interested in looking at the influence of the number of clusters and in showing how the produced clusters can help to better understand the influence of weather inputs.

References:

[1] Nadine Brisson et al. "An overview of the crop model STICS". In: *European Journal of agronomy* 18.3-4 (2003), pp. 309–332.

[2] Linda Lilburne and Stefano Tarantola. "Sensitivity analysis of spatial models". In: *International Journal of Geographical Information Science* 23.2 (2009), pp. 151–168.

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Global activity scores

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We present a generalization of the active subspace method called "global active subspace method", and its corresponding sensitivity measure called "global activity scores". The new methods are based on the expectation of finite-differences of the underlying function, as opposed to the gradient information in the active subspace method. We will present theoretical and numerical results showing the advantages of the new methods. In particular, we will present numerical examples where we compare the results of the global sensitivity analysis of some models using Sobol' sensitivity indices, derivative-based sensitivity measures, activity scores, and global activity scores. The numerical results reveal the scenarios when the global activity score has advantages over derivative-based sensitivity measures and activity scores, and when the three measures give similar results..

References:

[1] Ruilong Yue, Giray Ökten, "The Global Active Subspace Method", *arXiv:2304.14142*, 2023.

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Importance Sampling in high dimension

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Abstract

Rare event analysis often involves the estimation of the rare event probability $p = \mathbb{P}_f(X \in A)$, where $f = N(0, I)$ is the d-dimensional standard Gaussian distribution, which is a fairly general setting owing to isoprobabilistic transformations [8]. Whereas Adaptive Splitting [3] concerns the modification of the trajectories of the samples towards the region of interest A, Importance Sampling (IS) considers an auxiliary distribution g which allocates more probability mass in A than f. Given n_g samples $(Y_i)_{i=1\dots n}$ generated according to g to whom $\mathbb{1}(\cdot \in A)\, f$ is absolutely continuous, the IS estimator is written as

$$\hat{p}_g = \frac{1}{n_g} \sum_{i=1}^{n_g} \frac{f(Y_i)}{g(Y_i)} \mathbb{1}(Y_i \in A)$$

In low dimension, IS estimators are often employed due to the desired variance reduction property compared to Monte Carlo estimator. However, in high dimension, IS estimators suffer from convergence issues and become extremely sensitive to the choice of auxiliary distribution. This motivates a theoretical study on the convergence of IS estimators in the high-dimensional setting, $d \to +\infty$.

As $d \to +\infty$, two settings can arise: either the probability to be estimated is bounded away from zero: $\inf_d p > 0$, or the probability tends to zero with the dimension: $p \to 0$. The first setting $\inf_d p > 0$, considered by [1, 4], occurs when p involves a stochastic process which is approximated by a finite sum of random variables by principal component analysis. Then, the probability to estimate becomes p_d, which tends to $p > 0$ when $d \to \infty$. In this setting, We will discuss our work on the convergence of the Cross-Entropy scheme [2] as well as its projection and improved variants [5, 10, 9].

The second setting, $p \to 0$ as $d \to \infty$, considered by [7, 6], occurs in specific settings such as in Highly Reliable Markovian Systems or in static network reliability estimation. This setting is more complex since the properties of IS estimators are reliant on the rate of convergence of p to 0. To tackle this setting, we first establish necessary and sufficient conditions for general IS estimators to be consistent, and conditions to verify a Central Limit Theorem towards a normal distribution. We then translate these conditions into the necessary rate of growth of the sample size n_g for various auxiliary distributions in a classical large deviation setting, $A = \{x \in \mathbb{R}^d : \sum_{j=1}^d x(j) \geq d^\gamma\}$ with $\gamma > 1/2$. It will be observed that the 'optimal' Gaussian density for IS largely depends on the error metric considered.

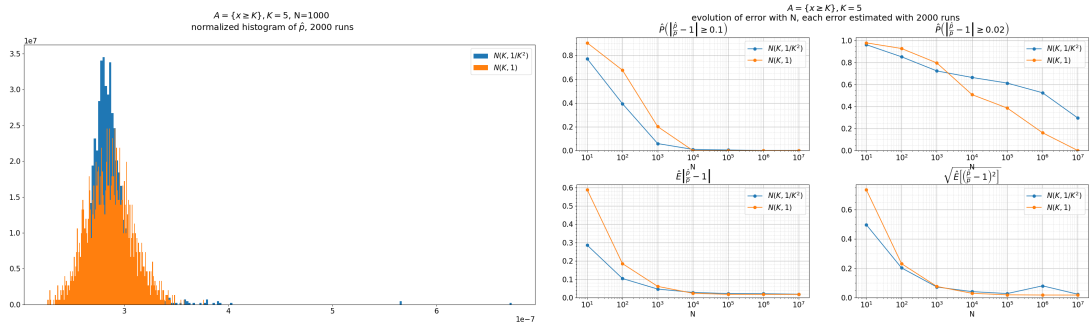

Figure 1: The histogram ($n_g = 1000$) and the evolution of usual error metrics with n_g of $\hat{p}_g$ for two choices of auxiliary density: which is better?

Short biography (PhD student)

I hold an M. Sc. in engineering from ISAE-SUPAERO in Toulouse. I completed my final-year internship at ISAE-SUPAERO which led to my current PhD thesis co-funded by EUR-MINT and ONERA, under the supervision of F. Simatos and J. Morio. The main goal of the thesis is to study the cause of the well-known curse-of-dimensionality for adaptive importance sampling, and to provide means to circumvent it based on this knowledge.

References

[1] S. Au and J. Beck. Important sampling in high dimensions. *Structural Safety* 25.2 (2003), pp. 139–163.

[2] J. Beh, Y. Shadmi, and F. Simatos. Insight from the Kullback–Leibler divergence into adaptive importance sampling schemes for rare event analysis in high dimension. *arXiv preprint* (2023). arXiv: `2309.16828 [math.ST]`.

[3] F. Cérou, A. Guyader, and M. Rousset. Adaptive multilevel splitting: Historical perspective and recent results. *Chaos: An Interdisciplinary Journal of Nonlinear Science* 29.4 (2019), p. 043108.

[4] S. Chatterjee and P. Diaconis. The sample size required in importance sampling. *The Annals of Applied Probability* 28.2 (2018).

[5] M. El Masri, J. Morio, and F. Simatos. Improvement of the cross-entropy method in high dimension for failure probability estimation through a one-dimensional projection without gradient estimation. *Reliability Engineering & System Safety* 216 (2021), p. 107991.

[6] A. Guyader and H. Touchette. Efficient Large Deviation Estimation Based on Importance Sampling. *Journal of Statistical Physics* 181.2 (2020), pp. 551–586.

[7] P. L'Ecuyer et al. Asymptotic robustness of estimators in rare-event simulation. *ACM Trans. Model. Comput. Simul.* 20.1 (2010).

[8] R. Lebrun and A. Dutfoy. Do Rosenblatt and Nataf isoprobabilistic transformations really differ? *Probabilistic Engineering Mechanics* 24.4 (2009), pp. 577–584.

[9] I. Papaioannou, S. Geyer, and D. Straub. Improved cross entropy-based importance sampling with a flexible mixture model. *Reliability Engineering & System Safety* 191 (2019), p. 106564.

[10] F. Uribe et al. Cross-Entropy-Based Importance Sampling with Failure-Informed Dimension Reduction for Rare Event Simulation. *SIAM/ASA Journal on Uncertainty Quantification* 9.2 (2021), pp. 818–847.

Variance-based selection of variables to improve prediction capability of innovative sensors in uncontrolled environment

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Air and water pollution are now a major public health issue, and developing efficient detection methods to better monitor this pollution is essential to reduce the risk of exposure. Innovative materials such as nanomaterial-based sensors [1] have been proposed for their high sensitivity to different chemical species in air and water and their ability to detect them even in very low concentrations. However, if in laboratory these sensors are able to show encouraging results, the passage in real conditions generally pose difficulties. This is often due to the fact that these sensors are not very selective, and that in addition to reacting to changes in the concentrations of the pollutants of interest, they may also depend on several other environmental variables, such as temperature or relative humidity.

As the calibration relationship between the sensor outputs, the pollutant concentrations and the other environmental variables is often unknown, two distinct phases are needed for these sensors to be used in uncontrolled environments. In the first step, this relationship is estimated using labelled data provided by reference sensors. In the second step, this relationship is used to predict the pollutant concentration from the sensor outputs only. Several factors make this estimation challenging: the potential existence of unmeasured but influential pollutants, the measurement noise on the input and output data, and the likely non-linearity of the calibration relationship (see [2,3] for more details).

A key point of the calibration process is the selection of the appropriate environmental variables in the prediction model. In fact, due to strong correlations between environmental variables, one often observes that the calibration model performance improves when including a variable not directly influencing the sensor. On the other hand, this improvement actually constitutes "overlearning", as it does not transfer to times or places where the correlations between environmental variables are different. Conversely, if one does not take into account an environmental variable that has a true influence on the sensor, one directly degrades its measurement performance. Identifying the optimal number of environmental variables to include in the calibration process for effective sensor deployment is therefore critical.

The present contribution focuses on this selection process. Based on experimental data, and simulated data (designed to be similar to the experimental one), we show that conventional sensitivity analysis techniques are confronted with considerable difficulties due to measurement noise and due to the high degree of correlation between variables. Similarly, we show that linear regressions and statistical tests allowing to identify the variables with very limited influence on the sensor responses are hindered by unobserved variables and do not fully answer the question.

As an alternative, we propose a new variance-based selection method. It allows a better compromise between significant influence on the sensor and noise levels for their measurement by auxiliary sensors.

References :

[1] Deepika Tyagi Huide Wang Weichun Huang Lanping Hu Yanfeng Tang Zhinan Guo Zheng-biao Ouyang Han Zhang. Recent advances in two-dimensional-material-based sensing techonology toward health and environmental monitoring applications. Nanoscale, 12:3535–3559, 2005.

[2] Bérengère Lebental Guillaume Perin. Uncertainty-based calibration method for environmental sensors - application to chlorine and ph monitoring with carbon nanotube sensor array. IEEE sensors journal, 2023.

[3] Marine Dumon, Bérengère Lebental, Guillaume Perrin, Optimizing Sensor Calibration in Open Environments: A Bayesian Approach for Non-Specific Multisensory Systems, accepted to SMAI-JCM.

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A multifidelity approach to dimension reduction of stochastic dynamical systems based on invariant statistics

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Many physical systems in nature are described by stochastic differential equations (SDEs) of the form $\mathrm{d}\mathbf{x}_t = b(\mathbf{x}_t, \theta)\mathrm{d}t + \sigma(\mathbf{x}_t, \theta)\mathrm{d}\xi_t$ with some initial state $\mathbf{x}_0 = \mathbf{x}$. For these systems, key quantities of interest (QoIs) often take the form of expectations of an observable function $f : \mathcal{X} \to \mathbb{R}$ over the invariant measure of the system p, parameterized by a set of input variables $\theta \in \Omega$ which relate to the drift function b and/or the diffusion function σ of the SDE:

$$Q(\theta) = \mathbb{E}_{\mathbf{x}\sim p}[f(\mathbf{x})] = \int_{\mathcal{X}} f(\mathbf{x})\, p(\mathbf{x}; \theta)\mathrm{d}\mathbf{x} \tag{1}$$

Here, the QoI $Q : \Omega \to \mathbb{R}$ is referred to as an *invariant statistic* of the stochastic process. In settings where the parameter space is high-dimensional, dimension reduction techniques may be employed to improve the efficiency of uncertainty quantification and sensitivity analysis of the QoI.

This work makes two primary contributions. First, we propose using *active subspaces* [1] as a goal-oriented dimension reduction scheme for QoIs which take the form of invariant statistics of the stochastic process. A low-dimensional subspace of the parameter space on which variation in the QoI is greatest is identified from the eigendecomposition of the uncentered covariance matrix $\mathbf{C}$ of the gradient of the QoI over a given parameter density ν:

$$\mathbf{C} = \mathbb{E}_\nu\big[(\nabla_\theta Q)(\nabla_\theta Q)^{\mathrm{T}}\big] = \int (\nabla_\theta Q)(\nabla_\theta Q)^{\mathrm{T}} \nu(\theta)\mathrm{d}\theta \tag{2}$$

Crucially, we show that the gradient of this class of QoIs can be derived analytically and that it also takes the form of an expectation over the invariant measure, which is computable with Monte Carlo using long-time simulation of the stochastic process [2] rather than by approximate finite difference schemes which suffer in high dimensions. On an illustrative example, we show that variation along the low-dimensional subspace illuminates key geometric features of the invariant distribution which have the greatest influence on the QoI, where the features identified are consistent across different choices of parameterization of the invariant measure.

Second, we develop a multifidelity approach based on a novel combination of importance sampling and control variates to address the challenge of computing a nested expectation for the gradient covariance matrix. In particular, we construct a log-Euclidean multifidelity (LEMF) estimator [3] of the gradient covariance matrix, $\hat{\mathbf{C}}_\beta^{\mathrm{LEMF}}$, where the "high-fidelity" estimate $\hat{\mathbf{C}}_{(\cdot,\cdot)}$ is based on direct evaluation of the nested expectation in Eq. (2), which calls on an expensive stochastic simulation routine for every parameter instance; and the cheaper, "low-fidelity" estimate $\hat{\mathbf{C}}^{\mathrm{IS}}_{(\cdot,\cdot)}$ is based on an importance sampling approximation of the gradient which requires no additional simulation or specification of an alternate model, as done in [4]. The LEMF estimator is constructed as:

$$\mathrm{Log}\ \hat{\mathbf{C}}_\beta^{\mathrm{LEMF}} = \mathrm{Log}\ \hat{\mathbf{C}}_{(n_0,l_0)} + \beta\big(\mathrm{Log}\ \hat{\mathbf{C}}^{\mathrm{IS}}_{(n_1,l_1)} - \mathrm{Log}\ \hat{\mathbf{C}}^{\mathrm{IS}}_{(n_0,l_1)}\big) \tag{3}$$

where $\beta \in \mathbb{R}$ is the regression parameter, subscript l denotes the number of samples $\mathbf{x} \sim p(\mathbf{x}, \theta)$ used to evaluate the inner expectation, and subscript n denotes the number of Monte Carlo samples of the parameters $\theta \sim \nu$ used to evaluate the outer expectation. We show that by adopting a control variate framework, the only requirement on the importance sampling-based estimator

is that it maintains non-zero correlation with the target covariance matrix, leading to reduced dependency on the fit of the biasing distribution and a flexible and cost-efficient scheme for variance reduction. We analyze properties of the multi-fidelity estimator, such as its Monte Carlo variance and error in the resulting active subspace, as measured by weighted subspace distances (WSD) [5]. We demonstrate our proposed methodology for sensitivity analysis of QoIs arising in molecular dynamics, parameterized according to a high-dimensional interatomic potential model [6].

References

[1] P. Constantine. *Active Subspaces: Emerging Ideas for Dimension Reduction in Parameter Studies*. Society for Industrial and Applied Mathematics, 2020.

[2] S. Mohamed et al. "Monte Carlo Gradient Estimation in Machine Learning". In: *Journal of Machine Learning Research* 21 (2020), pp. 1–62.

[3] Aimee Maurais et al. "Multi-Fidelity Covariance Estimation in the Log-Euclidean Geometry". In: Proceedings of Machine Learning Research 202 (2023), pp. 24214–24235.

[4] Rémi Lam et al. "Multifidelity Dimension Reduction via Active Subspaces". In: *SIAM Journal on Scientific Computing* 42 (2020).

[5] T Cui et al. "Likelihood-informed dimension reduction for nonlinear inverse problems". In: *Inverse Problems* 30.11 (2014), p. 114015.

[6] Ralf Drautz. "Atomic cluster expansion for accurate and transferable interatomic potentials". In: *Phys. Rev. B* 99 (1 Jan. 2019), p. 014104.

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Reliability-oriented sensitivity analysis with multiple importance sampling

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Critical systems demand strong guaranties of safety throughout their mission. According to the type of critical system considered, these guaranties are expressed as the fulfillment of quantitative and/or qualitative requirements. One of the common key quantitative requirement is to ensure that the probability of failure P_f of the system before the end of its mission is inferior to a target threshold (typically $P_f \leq 10^{-4}$ for the aerospace applications we consider). The critical system is here represented by a numerical input-output model with random inputs. The system failure is associated to an output threshold exceedance. Reliability-oriented sensitivity analysis [5] aims at evaluating the sensitivity of the inputs on the output failure. In this work, we are more precisely interested in estimating the influence of the input distribution parameters on the failure probability with a variance-based approach through the estimation of Sobol indices.

The input distribution parameters are usually fixed in numerical models, with the source of uncertainties in the models limited to the known input distributions. In reality the parameters values that best represent the system behavior may be unknown. This lack of knowledge about parameters values constitutes another level of uncertainty in the modelling of the system. Quantifying how much these uncertainties affect the probability of failure P_f can help us identify which input distribution parameters should be precisely estimated for a better estimation of P_f. With the introduction of these parameteric uncertainties, naive estimation of the Sobol indices becomes very expensive, needing many calls to the model to obtain input-output samples. We propose a method to estimate the Sobol indices with adaptive enrichment of the samples.

We consider a numerical model $\mathcal{M}$ as a deterministic black-box, function of a random vector $\mathbf{X}$ of d independent random inputs with a real output $\mathcal{M}(\mathbf{X})$. $\mathbf{X}$ is characterized by a probability distribution function $f_{\mathbf{X}|\boldsymbol{\theta}}$ where $\boldsymbol{\theta}$ is a distribution parameter vector. The failure event is represented by the variable $\mathbb{1}_{\mathcal{M}(\mathbf{X})\leq T}$ with T the threshold characterizing the failure event. The quantity of interest is $P_f(\boldsymbol{\theta}) = P(\mathcal{M}(\mathbf{X}) \leq T)$. When $\boldsymbol{\theta}$ is fixed, $P_f(\boldsymbol{\theta})$ is an unknown deterministic quantity. To represent epistemic uncertainty, the variability of $\boldsymbol{\theta}$ is modeled with a continuous random variable $\boldsymbol{\Theta}$. The failure probability $P_f(\boldsymbol{\Theta})$ becomes a random variable. The Sobol indices on $P_f(\boldsymbol{\Theta})$ associated to the independant components of $\boldsymbol{\Theta}$ can be estimated with the pick-freeze estimator [2], based on an iid N-sample $(\boldsymbol{\Theta}_i)_{i=1,\dots,N}$ from $\boldsymbol{\Theta}$. However two difficulties arise for the computation of this estimator. First, a high number of accurate probability estimations $P_f(\boldsymbol{\Theta}_i)_{i=1,\dots,N}$ have to be performed. Second, we are in the case of rare event estimations, meaning that classical Monte Carlo are not efficient to provide accurate probability estimation.

A possible solution is proposed in [1] for an estimation of all the Sobol indices with reverse importance sampling (RIS). For a given $\boldsymbol{\theta}_0$, the failure probability $P_f(\boldsymbol{\theta}_0)$ is estimated with Monte Carlo method or importance sampling with sampling density g. RIS enables then to estimate $P_f(\boldsymbol{\Theta}_i)_{i=1,\dots,N}$ without any calls to $\mathcal{M}$. The corresponding Sobol indices can then be derived at a limited cost. Nevertheless the accuracy of $P_f(\boldsymbol{\Theta}_i)$ with RIS estimates depends mainly on the Kullback–Leibler divergence between the optimal sampling density $\propto \mathbb{1}_{\mathcal{M}(\mathbf{X})\leq T} f_{\mathbf{X}|\boldsymbol{\theta}_i}$ and g. When the variability of $\boldsymbol{\Theta}$ around $\boldsymbol{\theta}_0$ is too high, the RIS approximation is not sufficiently accurate and can lead to a misestimation of the Sobol indices.

We propose an improvement of this solution with adaptive enrichment of the sample to improve

the estimation of the Sobol indices while limiting the additional calls to $\mathcal{M}$. We aim to improve the Sobol estimation by improving the estimation of the probabilities $P_f(\mathbf{\Theta}_i)_{i=1,\dots,N}$. We chose a criterion to estimate the accuracy of the estimations of these different probabilities (e.g. the estimated coefficient of variation of the estimator or the effective sample size [6]). After a first estimation of the Sobol with the method of [1], we perform an IS for the least well estimated $P_f(\mathbf{\Theta}_i)$, obtaining a new sample density, new input samples and associated model outputs. These new data fit for this particular $\mathbf{\Theta}_i$ allow us to improve the estimation of $P_f(\mathbf{\Theta}_i)$, but we also use these new data in combination with the previous available data to improve as much as possible the estimations of all the $P_f(\mathbf{\Theta}_i)_{i=1,\dots,N}$. Using multiple importance sampling (mIS) [3], we search for each $P_f(\mathbf{\Theta}_i)$ the combination of available data that yields the best probability estimation. mIS does not require additional calls to M and allow us to potentially improve on all the probability estimations. We repeat this process of selection of $P_f(\mathbf{\Theta}_i)$, adapted resampling and mIS until all the $P_f(\mathbf{\Theta}_i)_{i=1,\dots,N}$ are considered sufficiently well estimated.

As case study, we will consider a drone operation safety evaluation model test case. The numerical model considered is a timed automaton based on a functional modelling of a drone. This model is created using the safety modelling language AltaRica 3.0 [4], we consider the model as a black box for our study. The model takes as input vector of dimension 40 with one distribution parameter for each dimension, corresponding to the failure time of the various components, and outputs the time of failure of the drone after the start of operations. We are interested in studying the probability that the drone fails within one hour of operation, and how the uncertainties about the input distribution affect this probability.

References

[1] Jérôme Morio. "Influence of Input PDF Parameters of a Model on a Failure Probability Estimation". In: *Simulation Modelling Practice and Theory* 19.10 (Nov. 2011), pp. 2244–2255. ISSN: 1569190X. DOI: 10.1016/j.simpat.2011.08.003.

[2] Fabrice Gamboa et al. *Statistical Inference for Sobol Pick Freeze Monte Carlo Method*. Mar. 2013. DOI: 10.48550/arXiv.1303.6447. arXiv: 1303.6447 [math, stat].

[3] Art B. Owen. *Monte Carlo theory, methods and examples*. https://artowen.su.domains/mc/, 2013. Chap. 9.

[4] Tatiana Prosvirnova. "AltaRica 3.0: a Model-Based approach for Safety Analyses". Theses. Ecole Polytechnique, Nov. 2014. URL: https://pastel.hal.science/tel-01119730.

[5] Vincent Chabridon. "Reliability-oriented sensitivity analysis under probabilistic model uncertainty – Application to aerospace systems". Theses. Université Clermont Auvergne [2017-2020], Nov. 2018. URL: https://theses.hal.science/tel-02087860.

[6] Víctor Elvira, Luca Martino, and Christian P. Robert. "Rethinking the Effective Sample Size". In: *International Statistical Review* 90.3 (Apr. 2022), pp. 525–550. ISSN: 1751-5823. DOI: 10.1111/insr.12500. URL: http://dx.doi.org/10.1111/insr.12500.

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Surrogate GSA with categorical and continuous inputs.

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Many real-world problems combine qualitative and quantitative input features. To address these, we perform Global Sensitivity Analysis in the presence of categorical (i.e. discrete valued) inputs alongside continuous ones. The strategy employed is to treat each categorical combination or state as a separate output in a multi-output Gaussian process (MOGP), using an RBF kernel for continuous inputs. Sobol' indices are extended to assess the influence of continuous inputs on the correlation between categorical states. This in turn is related to the influence of the categorical state on the Sobol' indices of the output. In this way one may effectively consider cooperation between categorical and continuous inputs to influence the output. The possibility of multi-task learning, where different categorical states inform each other via the MOGP is investigated, and its effect on GSA is outlined.

Applications are presented to engineering problems, such as a synthesis where certain chemical analyses may fail under some conditions, or certain categorical combinations have only been sparsely investigated as they are considered unpromising. An important application is to syntheses where the categorical inputs are the choice of ingredients or conditions, recently explored using a related approach [1].

The ultimate benefit of GSA is often to reduce the number of inputs in order to aid experimental design and optimisation of the synthesised material. The appoach outlined here is particularly suited to situations where training data is sparse, and must be utilised to maximum effect, for example in pharamaceutical production where syntheses may be extremely expensive. This should also prove useful in wider applications, not related to synthesis.

[1] Y. Comlek, L. Wang, and W. Chen, "Mixed-Variable Global Sensitivity Analysis for Knowledge Discovery and Efficient Combinatorial Materials Design.", ASME. J. Mech. Des., **146**(5):1–10, 2024.

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Ensemble weather forecasting? Sensitivity analysis would help

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This paper explores the integration of Sensitivity Analysis (SA) with ensemble weather forecasting to improve uncertainty quantification (UQ) in Numerical Weather Prediction (NWP).

Ensemble weather forecasting plays a crucial role in meteorology by representing uncertainty through multiple model simulations, accounting for variability in initial conditions, model dynamics, and external influences. Widely used techniques, such as Stochastically Perturbed Parameterization Tendencies (SPPT) [Buizza et al., 1999, Leutbecher and Palmer, 2008], Stochastically Perturbed Parameterization (SPP) [Ollinaho et al., 2017], Ensemble Data Assimilation (EDA) [Houtekamer and Mitchell, 1998, Bonavita et al., 2012], Singular Vectors (SV) [Buizza and Palmer, 1995] have been fundamental in addressing uncertainties within ensemble forecasting frameworks. However, these methods often operate under assumptions of linearity and Gaussian error distributions, which limit their capacity to fully capture the non-linearities, interdependencies, and broader range of uncertainties inherent in complex atmospheric systems.

Sensitivity analysis [Saltelli, 2008, Saltelli et al., 2004, Iooss and Lemaître, 2015] offers a robust and complementary technique to overcome these limitations by systematically identifying, ranking, and quantifying the influence of input parameters on model outputs. Unlike traditional ensemble methods, SA provides a structured approach for understanding how variations in model parameters impact forecast outcomes, enabling a more comprehensive analysis of non-linear interactions and parameter dependencies. Sensitivity analysis has long been recommended and widely applied for UQ across various scientific domains, including hydrological modeling [Ratto et al., 2007] and environmental studies [Saltelli et al., 2004]. These applications demonstrate the effectiveness of global sensitivity analysis in exploring the multidimensional space of the input parameters and capturing the effects of non-linearity and of interactions among parameters in the model, thereby improving model evaluation and calibration. Its successful implementation in other fields emphasises the potential benefits of integrating SA into ensemble weather forecasting, enhancing the robustness and accuracy of uncertainty representation in meteorological models.

This paper explores the integration of SA into ensemble weather forecasting, demonstrating how this synthesis enhances UQ in NWP models. By integrating SA into ensemble forecasting, we discuss the representation of multivariate uncertainties, how to improve the accuracy of parameter perturbations, and refine probabilistic forecasts. We detail the current ensemble techniques, emphasising how SA can inform the adjustment of perturbation strategies and better capture non-Gaussian error structures. Additionally, SA enables a more accurate representation of joint distributions [Mara et al., 2015], leading to improved identification of critical thresholds and tipping points in model behaviour, particularly for extreme weather events [Bousquet and Bernardara, 2021, Allen et al., 2017]. The integration of SA has the potential to refine stochastic perturbation techniques, such as SPPT and SPP, by providing evidence-based parameter ranges and interdependencies. By incorporating SA, meteorologists can better capture the complexities of atmospheric systems, advancing the accuracy and reliability of probabilistic weather predictions. This work emphasises the need for adopting SA techniques in ensemble forecasting to achieve more comprehensive uncertainty quantification in NWP models while offering meteorologists a more nuanced understanding of model uncertainties, and improving the communication of forecast uncertainty to stakeholders.

Bibliography

[Allen et al., 2017] Allen, J. T., Tippett, M. K., Kaheil, Y., Sobel, A. H., Lepore, C., Nong, S., and Muehlbauer, A. (2017). An extreme value model for us hail size. *Monthly Weather Review*, 145(11):4501–4519.

[Bonavita et al., 2012] Bonavita, M., Isaksen, L., and Hólm, E. (2012). On the use of eda background error variances in the ecmwf 4d-var. *Quarterly journal of the royal meteorological society*, 138(667):1540–1559.

[Bousquet and Bernardara, 2021] Bousquet, N. and Bernardara, P. (2021). *Extreme value theory with applications to natural hazards*. Springer.

[Buizza et al., 1999] Buizza, R., Milleer, M., and Palmer, T. (1999). Stochastic representation of model uncertainties in the ecmwf ensemble prediction system. *Quarterly Journal of the Royal Meteorological Society*, 125(560):2887–2908.

[Buizza and Palmer, 1995] Buizza, R. and Palmer, T. (1995). The singular-vector structure of the atmospheric global circulation. *Journal of the Atmospheric Sciences*, 52(9):1434–1456.

[Houtekamer and Mitchell, 1998] Houtekamer, P. L. and Mitchell, H. L. (1998). Data assimilation using an ensemble kalman filter technique. *Monthly weather review*, 126(3):796–811.

[Iooss and Lemaître, 2015] Iooss, B. and Lemaître, P. (2015). A review on global sensitivity analysis methods. *Uncertainty management in simulation-optimization of complex systems: algorithms and applications*, pages 101–122.

[Leutbecher and Palmer, 2008] Leutbecher, M. and Palmer, T. N. (2008). Ensemble forecasting. *Journal of Computational Physics*, 227(7):3515–3539.

[Mara et al., 2015] Mara, T. A., Tarantola, S., and Annoni, P. (2015). Non-parametric methods for global sensitivity analysis of model output with dependent inputs. *Environmental Modelling Software*, 72:173–183.

[Ollinaho et al., 2017] Ollinaho, P., Lock, S.-J., Leutbecher, M., Bechtold, P., Beljaars, A., Bozzo, A., Forbes, R. M., Haiden, T., Hogan, R. J., and Sandu, I. (2017). Towards process-level representation of model uncertainties: stochastically perturbed parametrizations in the ecmwf ensemble. *Quarterly Journal of the Royal Meteorological Society*, 143(702):408–422.

[Ratto et al., 2007] Ratto, M., Young, P., Romanowicz, R., Pappenberger, F., Saltelli, A., and Pagano, A. (2007). Uncertainty, sensitivity analysis and the role of data based mechanistic modeling in hydrology. *Hydrology and Earth System Sciences*, 11(4):1249–1266.

[Saltelli, 2008] Saltelli, A. (2008). *Global Sensitivity Analysis: the Primer*. John Wiley & Sons.

[Saltelli et al., 2004] Saltelli, A., Tarantola, S., Campolongo, F., Ratto, M., et al. (2004). *Sensitivity analysis in practice: a guide to assessing scientific models*, volume 1. Wiley Online Library.

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Effect of forcing uncertainty in the sensitivity and calibration of a pesticide transfer model

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The use of pesticides poses major challenges to sustainable agriculture and water quality, necessitating the development of risk assessment tools to better understand and manage these impacts. One such tool is the PESHMELBA model [1] (Pesticides and Hydrology: modeling at the catchment scale), a distributed, physically based model that integrates water and pesticide transfer processes at the catchment level. This model enables the comparison of different landscape management scenarios and their effects on water quality.

Before employing it as a decision-making tool, it is essential to properly quantify its uncertainties, coming from various sources. While parameter uncertainty has been increasingly studied, forcing uncertainties (e.g., rainfall/evapotranspiration forcings, or pesticide application dates and quantities) are often overlooked. The uncertainty in hydrological data used for forcing input directly impacts model simulations and further decision-making [2], but it also has indirect impacts when used in the process of parameter calibration [3]. Ignoring forcing uncertainty can result in biased parameter values or sensitivity indices that are only valid in one forcing condition and cannot be extrapolated to different forcing conditions [4].

We investigate how the uncertainty in forcing data propagates to the model output, particularly how it affects the sensitivity of model outputs to their parameters. Additionally, we examine how forcing uncertainty influences parameter calibration.

First, we perform a global sensitivity analysis (GSA) to identify the main parameters contributing to output uncertainty and focus on their calibration [5]. An operational approach [6] to GSA is employed. This approach considers the different nature in the variability of the forcing inputs and the parameter values, i.e. it distinguishes the stochastic (and thus uncontrollable) variability of the forcings from the variability of the model parameters' possible design values, thus demonstrating how the forcing uncertainty impacts the model's sensitivity to parameter values.

We then assess the advantages of a robust approach to parameter calibration for the PESHMELBA model. As the uncertainty of forcing inputs highly depends on the specific problem and model, we opt for a methodology that does not assume a particular structure of the forcing inputs. Rather, the methodology relies on a sufficiently large set of realizations that represent the forcing uncertainty. To manage the high computational burden of robust calibration methods and ensure the non-intrusiveness in the forcing input space, we employ a polynomial chaos-based metamodel for stochastic simulators based on [7], which approximates the response surface across parameters while emulating the uncertainty of the forcing input.

Two case studies are considered, each with varying model outputs and sources of forcing uncertainty, representing increasing complexity in model processes and scale of application:

- the first case examines the soil moisture profile of a single catchment plot. Here, forcing uncertainty arises from measurement errors and the spatial heterogeneity of a rainfall event.
- the second case focuses on the daily pesticide concentration at the river outlet. In this scenario, forcing uncertainty stems from the lack of knowledge regarding the exact dates

of pesticide treatment. This case study is more complex due to the intricacies of pesticide transfer processes and spatial interactions between catchment plots.

Our GSA results demonstrate that the sensitivity of model outputs to parameters varies across the domain of forcing uncertainty. We find that rainfall uncertainty leads to varying sensitivities of soil moisture to hydrodynamical properties at different horizon depths. Meanwhile, varying pesticide application dates by just a few days impacts the dominant processes of pesticide transfer. This results in a greater influence of parameters governing surface runoff when pesticides are applied prior to heavy rainfall events.

Comparing robust parameter calibration with classical calibration, evaluated on an unseen set of new forcing data, reveals improvements in robustness criteria for moisture profile parameter calibration. However, in complex cases, the difficulty of fitting a stochastic emulator that accurately captures the original model behavior increases rapidly with the growing interactions between forcings and model parameters. This raises questions about the scalability of the presented approach in complex studies.

References:

[1] E. Rouzies, C. Lauvernet, C. Barachet, T. Morel, F. Branger, I. Braud and N. Carluer, "From agricultural catchment to management scenarios: A modular tool to assess effects of landscape features on water and pesticide behavior", *Science of The Total Environment*, **671**:1144–1160, 2019. doi: 10.1016/j.scitotenv.2019.03.060

[2] A. Devers, J.-P. Vidal, C. Lauvernet, O. Vannier, and L. Caillouet, "140-year daily ensemble streamflow reconstructions over 661 catchments in France", *Hydrology and Earth System Sciences*, **28**:3457–3474, 2024. doi: 10.5194/hess-28-3457-2024

[3] H. K. McMillans, I. K. Westerberg and T. Krueger, "Hydrological data uncertainty and its implications", *WIREs Water*, **5**:e1319, 2018. doi: 10.1002/wat2.1319

[4] V. Andréassian, N. Le Moine, C. Perrin, M.-H. Ramos, L. Oudin, T. Mathevet, J. Lerat, and L. Berthet, "All that glitters is not gold: the case of calibrating hydrological models", *Hydrological Processes*, **26**:2206–2210, 2012. doi: 10.1002/hyp.9264

[5] J. Mai, "Ten strategies towards successful calibration of environmental models", *Journal of hydrology*, **620**:129414, 2023. doi: 10.1016/j.jhydrol.2023.129414

[6] A. Dell'Oca, "Sensitivity Analysis: An Operational Picture",
Water Resources Research, **59**:e2022WR033780, 2023. doi: 10.1029/2022WR033780

[7] N. Lüthen, S. Marelli and B. Sudret, "A spectral surrogate model for stochastic simulators computed from trajectory samples", *Computer methods in applied mechanics and engineering*, **406**:115875, 2023. doi: 10.1016/j.cma.2022.115875

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Decision sensitivity for engineering applications with epistemic uncertainty

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Decision sensitivity measures, specifically *information values*, quantify the effect of input uncertainty on the optimality of a decision taken based on a predictive model. The information value of an input X is the expected value of partial perfect information associated with making a better decision when learning X. The information value has become popular mainly in the field of medical decision-making, but it is also a natural sensitivity measure in engineering, where models serve the purpose of making decisions about design, operation, retrofitting, upgrading or decommissioning of systems. In this contribution, we focus on decision sensitivity for engineering applications and discuss the modeling of decisions and the associated utility function (or scoring rule). We then focus on the separation of aleatory and epistemic uncertainty in engineering applications and investigate the implications of this separation on the interpretation of the sensitivity measures. We also discuss strategies for computationally efficient sampling-based estimation of the information values under aleatory and epistemic uncertainty. We illustrate the theory using two real-life applications concerned with the site selection for a nuclear waste deposit and the optimization of flood protection measures.

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Variance-based importance measures for high-dimensional linear model via Johnson indices: Insights and comparisons

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In regression analysis, importance measures are effective tools for feature selection and model interpretation, allowing for the ranking of the most influential regressors. In particular, *variance-based importance measures* (VIMs) are a prominent topic in both fields of statistics and global sensitivity analysis. This is due to their accessible interpretation as variance shares of the explained variable. As proposed in [1], this work focuses on a linear regression model between an explained real-valued output random variable Y and d explanatory input random variables $\boldsymbol{X} = (X_1, \ldots, X_d)$: $Y = \boldsymbol{X}\boldsymbol{\beta} + \varepsilon$ with $\boldsymbol{\beta} \in \mathbb{R}^d$ is an unknown vector of coefficients and ε is a centered Gaussian random error. It addresses some of the practical challenges that arise when the component of $\boldsymbol{X}$ are dependent inputs and the input dimensionality d is large. Specifically, the goal is to discuss the formulation and interpretation of Johnson indices [2, 3], which have empirically demonstrated their value both in high-dimensional contexts and their ability to approximate the not so well-known LMG indices [4].

We start by providing some theoretical elements and interpretations to define the context in which Johnson indices can be used in comparison to LMG and PMVD indices [5]. In the literature of linear regression analysis, VIMs are built from the decomposition of the *coefficient of determination* R^2 which quantifies the percentage of output variability explained by the model. A VIM associated with a regressor is thus defined as its proportional contribution to R^2, accounting for both its direct effect (correlation with Y) and combined effects with other variables [6]. Various R^2 decomposition strategies have thus been proposed, leading to different interpretations. The choice of the R^2 decomposition suitable for defining the VIM can then be established based on *desirability criteria*:

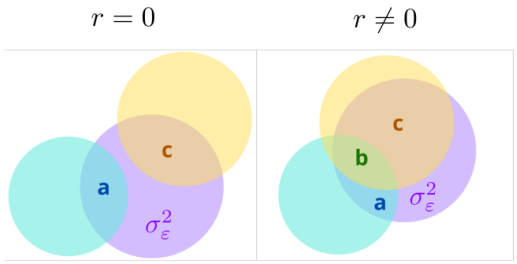
- (C_1) *Proper decomposition*: the sum of all shares should be equal to the R^2;
- (C_2) *Nonnegativity*: all shares should be nonnegative;
- (C_3) *Exclusion*: if $\beta_j = 0$, then the share of X_j should be zero;
- (C_4) *Inclusion*: if $\beta_j \neq 0$, then the share of X_j should be nonzero;
- (C_5) *Grouping*: all shares should tend to equate for highly correlated inputs.

The first four criteria were defined by Gromping [7], while the last one relates to regularization techniques [8]. Criteria (C_1) and (C_2) are essential for interpreting VIMs as a percentage of R^2. Criterion (C_4) is also fundamental to highlight inputs with direct influence. However, (C_5) contradicts the exclusion property (C_3). If the interpretation is focused on the direct influence of the inputs on the model output, then (C_3) is appropriate; if the correlations among data can carry necessary information for the interpretation, (C_5) is relevant instead. In this context, the LMG and Johnson indices favor the (C_5) criterion whereas the PMVD indices (C_3). In fact, both methods aim to decompose the R^2, but they differ in how they average the marginal contribution of each variable across all the permutations. LMG uses an arithmetic average while PMVD weights these contributions based on the proportion of variance attributable to each variable.

To better understand and illustrate the concept of *multicollinearity*, we also use Venn diagrams on a two-input regression model ($d = 2$), see Fig. 1. The Venn diagrams are formed by three circles associated with the variances of Y (in purple), X_1 (σ_1 in blue) and X_2 (σ_2 in yellow), by two overlapping area measuring the *additional explanatory power* of X_1 (a) and of X_2 (c), and by the area representing the *combined effect* of the inputs on the model $Y(\mathbf{X})$ (b). We prove, in particular, (with a different demonstration from the one of [9] which relies on geometrical arguments) that there is an equivalence between the LMG and the standardized Johnson indices in the case of a two-input model [1].

Finally, we apply these indices to the well-known dataset of the `R` package `AmesHousing`, which contains 79 features describing house sale prices in Ames, USA [1]. The computational cost of the LMG and PMVD indices is exponential with the number of input variables. It appears impossible to calculate them for the

entire set of input variables. This example shows that there are cases where it is impossible to determine the LMG and PMVD indices, and where it is necessary to use approximate methods to conduct sensitivity analyses. In this case, we calculate the Johnson and the well-known SRC^2 indices [1] for the set of 34 quantitative variables. We then determined the 10 most influential variables and we determine all the VIMs for these 10 variables (see Fig. 2).



$\mathbf{a} = \beta_1^2\sigma_1^2(1-r^2)$
$\mathbf{b} = \beta_1^2\sigma_1^2r^2 + 2\beta_1\beta_2\sigma_1\sigma_2 r + \beta_2^2\sigma_2^2r^2$
$\mathbf{c} = \beta_2^2\sigma_2^2(1-r^2)$

	$r=0$	$r\neq 0$	$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$
$\text{LMG}_1 = \text{Johnson}_1$	$\frac{a}{a+c+\sigma^2_\varepsilon}$	$\frac{a+b/2}{a+b+c+\sigma^2_\varepsilon}$	yes	yes	no if $r\neq 0$	yes	yes
PMVD_1	$\frac{a}{a+c+\sigma^2_\varepsilon}$	$\frac{a[1+b/(a+c)]}{a+b+c+\sigma^2_\varepsilon}$	yes	yes	yes	yes	no
R^2	$\frac{a+c}{a+c+\sigma^2_\varepsilon}$	$\frac{a+b+c}{a+b+c+\sigma^2_\varepsilon}$					

Figure 1: Interpretations of VIMs: Venn diagrams and desirability criteria.

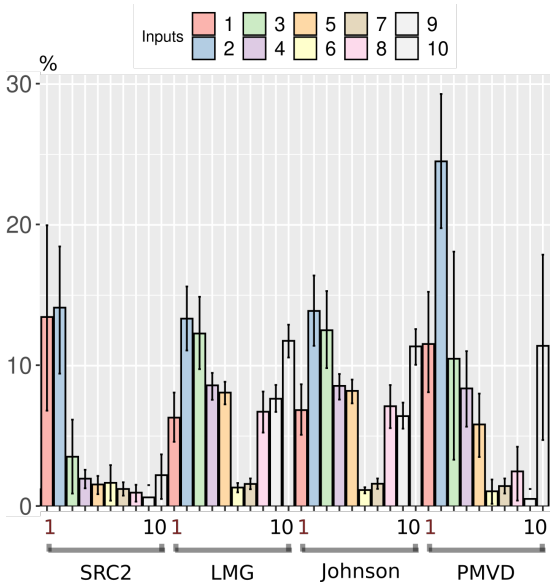


Figure 2: Results on the Ames housing dataset.

References:

[1] L. Clouvel et al. "An overview of variance-based importance measures in the linear regression context: comparative analyses and numerical tests". In: *Preprint* (2024). URL: https://hal.science/hal-04102053.

[2] J.W. Johnson. "A heuristic method for estimating the relative weight of predictor variables in multiple regression". In: *Multivariate Behavioral Research* 35 (2000), pp. 1–19.

[3] A. Genizi. "Decomposition of R^2 in multiple regression with correlated regressors". In: *Statistica Sinica* (1993), pp. 407–420.

[4] R. H. Lindeman, P. F. Merenda, and R. Z. Gold. *Introduction to bivariate and multivariate analysis*. Glenview, IL: Scott Foresman and Company, 1980.

[5] B. Feldman. "Relative Importance and Value". In: *SSRN Electronic Journal* (Mar. 2005). DOI: 10.2139/ssrn.2255827.

[6] J.W. Johnson and J.M. LeBreton. "History and use of relative importance indices in organizational research". In: *Organizational Research Methods* 7 (2004), pp. 238–257.

[7] U. Grömping. "Estimators of relative importance in linear regression based on variance decomposition". In: *The American Statistician* 61.2 (2007).

[8] H. Zou and T. Hastie. "Regularization and Variable Selection via the Elastic Net". In: *Journal of the Royal Statistical Society. Series B (Statistical Methodology)* 67.2 (2005), pp. 301–320.

[9] D.R. Thomas et al. "On Johnson's (2000) relative weigths method for assessing variable importance: A reanalysis". In: *Multivariate Behavioral Research* 49 (2014), pp. 329–338.

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Efficient estimation of Sobol' indices of any order from a single input/output sample.

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Despite the numerous advances and insightful proposals in the recent years, estimation of Sobol' indices at any order d (with particular case total indices) is still a challenge. When it comes to theoretical convergence guarantees, two classes of methods are of particular interest. On the one hand, the class of Pick Freeze estimators allows to estimate Sobol' indices at rate $\sqrt{n}$ for any d with minimal assumptions on the computer code, but requires a sample with highly specific structure. On the other hand, local-averaging estimators such as kernel or nearest neighbor estimators can handle any vanilla n-sample of the inputs/output pair (*given-data* context), but the $\sqrt{n}$-parametric rate of convergence was only proved for $d \leq 3$ for nearest neighbors. In addition, such estimators suffer in practice from large bias and variance.

In the present work, we introduce a new class of kernel estimators which enjoys a central limit theorem and asymptotic efficiency for estimating Sobol' indices at rate $\sqrt{n}$ for any d from a vanilla n-sample, unlike all previous works. From a broad perspective, our approach consists of three main ingredients. First, we build upon the explicit expression of the efficient influence function of Sobol' indices which depends on the unknown regression function, and propose a plug-in estimator where the regression function is estimated with a specific kernel estimator, in the same spirit as [1]. Second, for the latter and to ensure $\sqrt{n}$-consistency, we use high-order kernels as classically done in nonparametric regression. Finally, it is crucial to handle boundary effects inherent to kernel estimation procedures: we adapt here recent mirror-type transformations introduced in [2,3]. All in one, we introduce two different estimators that are proved to be asymptotically normal and efficient for Sobol' indices at any order. From a numerical perspective, we conduct extensive comparisons and discuss stability of high-order kernels, showing that one of our estimators performs remarkably well on standard sensitivity analysis examples.

References:

[1] K. Doksum and A. Samarov. Nonparametric estimation of global functionals and a measure of the explanatory power of covariates in regression. *The Annals of Statistics*, 1443–1473, 1995.

[2] K. Bertin, N. Klutchnikoff, J. R. Léon, and C. Prieur. Adaptive density estimation on bounded domains under mixing conditions. *Electronic Journal of Statistics*, **14**(1):2198–2237, 2020.

[3] L. Pujol. Nonparametric estimation of a multivariate density under Kullback-Leibler loss with ISDE. `arXiv preprint arXiv:2205.03199`, 2022.

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Global sensitivity analysis for time-variant reliability

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Time-variant reliability analysis involves the estimation of the reliability of a structural system accounting for the time-varying nature of structural parameters and applied loads. This contribution studies the application of global reliability sensitivity measures to time-variant reliability analysis and discusses the estimation of these sensitivity indices with the first order reliability method (FORM). We focus on time-deteriorating systems and in this context study two approaches for time-variant reliability analysis: one based on approximating the first passage probability with the probability of a series of time interval failure events and another that expresses the failure event through an auxiliary limit state in terms of the conditional failure probability given the structural parameters. Estimation of the reliability sensitivity indices for the two considered approaches can be performed through leveraging the FORM approximations introduced in [1, 2]. We demonstrate the behavior of these approximations through numerical examples involving deteriorating structural systems.

References :

[1] Papaioannou, I. and Straub, D., “Variance-based reliability sensitivity analysis and the FORM α-factors”. *Reliab. Eng. Syst. Saf.*, **210**, 107496, 2021.

[2] Papaioannou I. and Straub D., "FORM-based global reliability sensitivity analysis of systems with multiple failure modes", *arXiv preprint arXiv:2403.12822*, 2024.

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Sensitivity analysis for Bayesian optimization with uncertainties

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This work tackles the challenge of chance-constrained optimization under uncertainties, which entails significant computational burdens in practical applications (such as the robust design of an electrical machine). Such robust optimization problem can be defined as follows

$$x^* = \arg\min_{x \in \mathcal{K}} \mathbb{E}[f(x,U)] \text{ where } \mathcal{K} = \{x \in \mathcal{X} \subset \mathbb{R}^d \text{ s.t. } \mathbb{P}[g(x,U) \leq 0] \geq \alpha\}$$

with x the vector of design variables and U the vector of uncertain variables.

Since the underlying models of f and g usually are costly computer codes, classical methods are out of the table as they often require numerous evaluations of these codes.

Thus, we use instead Bayesian Optimization and, more specifically, rely on EFISUR [1], an adaptation for constrained Bayesian optimization in presence of uncertainties. First, f and g are modeled using Gaussian process regression in the joint design and uncertain variable space and an acquisition criterion that considers both the average improvement in the objective function and the reliability of the constraints is defined. However, high dimensionality in either the design space or the uncertain parameter space can pose challenges due to the complexity of the optimization steps and Gaussian Processes (GPs) fitting.

Among all the different strategies to deal with the limitations of EFISUR in high dimensions, we propose an adaptation through a dimension reduction of the search space by incorporating Sensitivity Analysis in the sequential approach. Sensitivity analysis approaches allow to understand how each input affect the outputs and to mitigate the effects of the curse of dimensionality by retaining only the influential variables. The first important aspect of this work is the development of new sensitivity indices in order to deal with uncertain variables. Indeed, instead of considering how the inputs affect a scalar-valued output, which is already widely addressed in the literature, we measure the influence of uncertain variables by their impact on a set-valued output characterized as

$$U = (U_1, \ldots, U_p) \longrightarrow \Gamma = \{x \in \mathcal{X}, f(x,U) \leq q \text{ and } g(x,U) \leq 0\}.$$

We derive kernel-based sensitivity indices using an appropriated kernel to compare sets with the necessary properties in [2]. Other approaches were also considered on an industrial test-case for comparison [3].

Using existing goal-oriented indices for deterministic variables and these new indices for uncertain variables, different methodological developments based on various strategies of incorporating sensitivity analysis into EFISUR have been proposed. They will be presented in this work, with applications on comprehensive toy functions and a real-life test case of the robust optimization of an electrical machine.

References:

[1] R. E. Amri, R. Le Riche, C. Helbert, C. Blanchet-Scalliet, & S. Da Veiga. "A sampling criterion for constrained Bayesian optimization with uncertainties." *arXiv preprint arXiv:2103.05706.*, 2021.

[2] N. Fellmann, C. Blanchet-Scalliet, C. Helbert, A. Spagnol, & D. Sinoquet. "Kernel-based sensitivity analysis for (excursion) sets." *Technometrics*, 1-13, 2024.

[3] N. Fellmann, M. Pasquier, C. Blanchet-Scalliet, C. Helbert, A. Spagnol, D. Sinoquet. "Sensitivity analysis for sets: Application to pollutant concentration maps." *Qual Reliab Eng Int*, 1-19 2024. https://doi.org/10.1002/qre.3638

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Recent advances in the understanding and implementation of the HSIC-ANOVA decomposition

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For anyone wishing to perfom GSA[1] on the output of a black-box model, the ANOVA[2] framework, relying on the estimation of the first-order and total-order Sobol' indices, appears to be the most enticing solution, since it combines both simplicity and explainability. Indeed, each subset of input variables is assigned a specific share of variance equal to the variance induced by the associated sub-function in the Sobol'-Hoeffding decomposition. Due to their nice mathematical properties, the total-order Sobol' allow to perform both the ranking and screening of input variables, making them appear as some of the most attractive sensitivity measures. Unfortunately, when the output variable is computed by a highly expensive computer code, the simulation budget required to achieve an accurate estimation of Sobol' indices is often prohibitive, unless constructing a surrogate model, which is a challenging task in high dimension. In the light of this problem, the sensitivity measures based on the HSIC[3] offer a great alternative, as they are particularly easy to estimate, even when the available data comes from a small Monte Carlo sample. However, while HSIC indices are well adapted to screening, they are not recommended for ranking purposes, as comparing them to one another is not mathematically rigorous.

In this context, the HSIC-ANOVA approach is a cutting-edge kernel method seeking to strike a harmonious balance between Sobol' and HSIC indices [1]. The key idea of this breakthrough is to handle the input variables with ANOVA kernels (instead of more usual kernels such as the Gaussian ones). This specific choice allows to derive a kernel-based ANOVA decomposition in which the output variance is replaced by the HSIC between the input vector set and the output variable. Unlike standard HSIC indices, for which there is no notion of order, the HSIC-ANOVA decomposition enables the definition of kernel-based sensitivity indices at all orders, particularly at the first and total orders, in the same spirit as Sobol' indices.

To obtain such an ANOVA decomposition, the kernel selected for each input variable must be ANOVA, meaning that is it must satisfy an orthogonality condition with respect to the input marginal distribution. Unfortunately, for most parametric families of distributions encountered in practice, it is pretty hard to find an ANOVA kernel which is also characteristic. The only exception is the standard uniform distribution, for which there are many possible candidates in the literature, including the so-called unanchored Sobolev kernels [1]. In almost all other cases, it is advisable to orthogonalize the Gaussian kernel, but this implies an extra step of numerical integration whose complexity will increase linearly with sample size.

When first introduced, the HSIC-ANOVA decomposition was praised for two main reasons:

(a) the fact that all HSIC-ANOVA terms can be accurately estimated from a single sample of input-output observations, regardless of the dimension of the input space ;

[1] **GSA:** Global Sensitivity Analysis
[2] **ANOVA:** ANalysis Of VAriance
[3] **HSIC:** Hilbert-Schmidt Independence Criterion

(b) the fact that the HSIC-ANOVA measure may be used as a cost function for Shapley values, thus leading to HSIC-Shapley effects, a collection of importance measures combining most expected properties in GSA.

However, a grey area persists around the HSIC-ANOVA framework, hindering its wider adoption as a reference methodology in GSA. In fact, there are two main areas for improvement.

(P1) An obvious limitation of HSIC-ANOVA indices is their lack of interpretability, which is partly due to the fact that the HSIC-ANOVA decomposition is not a direct consequence of the Sobol'-Hoeffding decomposition. In particular, it is not clear which kind of extra information is captured by the total-order indices (compared to their first-order counterparts). This lack of transparency is a serious issue, as engineers are unlikely to apply a methodology without having a thorough understanding of it.

(P2) The question of how to use HSIC-ANOVA indices for screening was not investigated in [1].

Our talk aims to provide some answers to these two problems. For the sake of simplicity, the discussion is limited to the case where the input variables are mutually independent and all follow the standard uniform distribution.

In response to (P1), the first part of the talk will reveal the inner workings of the HSIC-ANOVA methodology and will establish a connection between the kernel feature maps and the dependence patterns captured by the two types of HSIC-ANOVA indices. The key to greater interpretability is to express the HSIC as a sum of squared covariances over the entire collection of random features induced by the input and output kernels. In fact, adopting this viewpoint on the HSIC-ANOVA decomposition allows to clarify which random features are captured at each order. Among other benefits, this change of perspective will guide the construction of analytical test functions for which HSIC-ANOVA interactions are controllable, ranging from negligible to dominant contributions.

In response to (P2), the second part of the talk will promote HSIC-ANOVA indices as a promising solution for kernel-based independence testing. The starting point is to realize that the unanchored Sobolev kernels are characteristic [2]. This ensures both the first-order and total-order indices characterize independence. A straightforward strategy to test independence is to apply existing methods for HSIC indices to the numerators of the first-order HSIC-ANOVA indices, because they are simply HSIC indices computed with ANOVA kernels. Another possible strategy is to develop specific test procedures for the total-order HSIC-ANOVA indices. It will be shown that three different test procedures can be employed, each suited to a specific range of sample sizes. Finally, an extensive simulation study will reveal that testing independence with the total-order indices can be more powerful, especially when HSIC-ANOVA interactions come into play.

References:

[1] S. Da Veiga, "Kernel-based ANOVA decomposition and Shapley effects – Application to global sensitivity analysis", 2021. Preprint under review, available at `https://hal.science/hal-03108628v1`

[2] G. Sarazin, A. Marrel, S. Da Veiga and V. Chabridon, "New insights into the feature maps of Sobolev kernels: Application in global sensitivity analysis", 2023. Preprint under review, available at `https://cea.hal.science/cea-04320711`

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On the use of sensitivity analysis for a game-theoretic approach of environmental management problem

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Prioritizing environmental sustainability is a core strategy for securing the health and prosperity of modern societies. A goog practice for a company to identify, manage, monitor and control its environmental impact is to use an environmental management system (EMS), such as the internationally recognized standard ISO 14001, based on environmental management problems proposed and solved by researchers. In the present work, we study the environmental management problem proposed by Haurie & Krawczyk [1] where they consider the pollution by multiple economic agents located along a river. An administrative authority aims to induce competing industrial agents to some sort of cooperation which would result in the satisfaction of the common environmental constraints.

To answer this question, Haurie & Krawczyk propose a (static) non-cooperative game which allows to set a Pigouvian tax for industrial agents in practice. Regarding non-cooperative games, two types of models have been considered in competitive markets: a) the Cournot oligopoly where industrial strategies are based on the choice of business volume and b) the Bertrand oligopoly where agents set prices. Haurie & Krawczyk assume industrial agents behave like the Cournot oligopolists where they set economic level x_j for $j = 1, \dots, J$. The equilibrium level $x^\star$ is a Nash equilibrium. That is, with payoff functions O_j and action set X_j, a Nash equilibrium is a vector $x^\star = (x_1^\star, \dots, x_J^\star)$ such that for all $j = 1, \dots, J$, $x_j^\star$ solves the subproblem

$$\sup_{x_j \in X_j} O_j(x_j, x_{-j}^\star),$$

where x_j and x_{-j} denote the action of player j and the other players' actions, respectively. The computation of equilibrium $x^\star$ for the model proposed by Haurie & Krawczyk relies on numerical methods, see [1].

For practical use of approach proposed by Haurie & Krawczyk, one must not only compute the equilibrium $x^\star$ but also measure how it is sensitive with respect to objective parameters O_j. For a three-player game with two levels of contraints, we count 18 parameters for which we want to understand the sensivity. Using [2], we propose an in-depth analysis of the proposed game. We compare our approach with the current economics standard known as "comparative statics".

References:

[1] Alain Haurie & Jacek B. Krawczyk, "Optimal charges on river effluent from lumped and distributed sources", *Environmental Modeling and Assessment*, (2):177–189, 1997.

[2] Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., Saisana, M. & Tarantola, S. (2008), "Global Sensitivity Analysis: the Primer", *Wiley Interscience*.

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Kernel-based parameter screening for conditional Bayesian calibration of chained computer models

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Computer models are commonly used in many areas of science and engineering to simulate, analyze, understand and predict complex physical systems, such as nuclear power plants. These models, which are designed to faithfully represent the underlying physical phenomena, often involve a large number of uncertain physical parameters. Traditionally, a distinction is made between two types of uncertain parameters (aleatoric or epistemic), depending on whether the uncertainty arises from irreducible natural variability or a potentially reducible lack of knowledge. Among epistemic uncertainties, some can be reduced and quantified by a model calibration process based on available observed data (experiments), such as deterministic calibration or Bayesian calibration [4]. The latter type of calibration is particularly useful for quantifying and reducing epistemic uncertainties, as it provides probability distributions for the parameters to be calibrated [5]. In support of the calibration process, it can be very useful to perform a preliminary global sensitivity analysis (GSA) in order to quantify how much each source of uncertainty contributes to the variability of the quantity of interest. As will be highlighted in the presentation, it turns out that the sensitivity indices based on the Hilbert-Schmidt Independence Criterion (HSIC), introduced by [2] and promoted by [7] for GSA purposes, are particularly suited to parameter screening in the context of Bayesian calibration. We will see that HSIC indices actually keep all their promises and clearly stand out from other competing sensitivity measures. However, beyond simply promoting HSIC indices, which are now widely used in many application fields, the main objective of this work is to develop a GSA methodology for the Bayesian calibration of chained computer models. More specifically, in the application under consideration, the goal in fine is to identify the calibration parameters $\boldsymbol{\theta}$ of a downstream model conditionally on the uncertainty affecting the parameters $\boldsymbol{\lambda}$ of an upstream model. Consequently, the main challenge for the GSA is to incorporate the residual uncertainty of $\boldsymbol{\lambda}$ into the definition and estimation of HSIC indices. To deal with this specific bi-level uncertainty framework, addressing the uncertainties conveyed by both $\boldsymbol{\theta}$ and $\boldsymbol{\lambda}$, purpose-built sensitivity measures are introduced and several estimators are derived for them. We will show that they are (asymptotically) unbiased, consistent and have Monte Carlo-like convergence rates. Importantly, their estimation does not require any extra computational load, since the estimates can be directly computed from the Monte Carlo samples built for the conditional model calibration task. Like HSIC indices, the key advantage of these indices is the ability to perform independence tests and make decisions based on p-values, rather than subjective criteria [1,6]. Finally, our approach is applied in nuclear fuel simulation. In this particular industrial context, the challenge is to find the most influential calibration parameters $\boldsymbol{\theta}$ of a downstream fission gas behavior model while taking into account the uncertainty of the conductivity $\boldsymbol{\lambda}$ of an upstream thermal model [3].

References:

[1] A. Gretton, K. Fukumizu, C. H. Teo, L. Song, B. Schölkopf and A. J. Smola,"A kernel statistical

test of independence", *Advanced in neural information processing systems*, **20**, 2007.

[2] A. Gretton, O. Bousquet, A. Smola and B. Schölkopf, "Measuring statistical dependence with Hilbert-Schmidt norm", *International conference on algorithmic learning theory*, pages 63-77, Springer, 2005.

[3] B. Michel, I. Ramière, I. Vaillard, C. Introini, M. Lainet, N. Chauvin,V. Marelle, A. Bouloré, T. Helfer, R. Masson, J. Sercombe, J. C. Dumas, L. Noirot and S. Bernaud, "Two fuel performance codes of the PLEIADES platform: ALCYONE and GERMINAL", *Nuclear Power Plant Design and Analysis Codes*, pages 207-233, Elsevier, 2021.

[4] K. Campbell, "Statistical calibration of computer simulations", *J. Reliability Engineering & System Safety*, **91**(10-11):1358-1363, 2006.

[5] M. C. Kennedy and A. O'Hagan, "Bayesian calibration of computer models", *J. Royal Stastistical Society*, **B63**(3):425-464, 2001.

[6] M. R. El Amri and A. Marrel, "More powerful HSIC-based independence tests, extension to space-filling designs and functional data", *J. International Journal for Uncertainty Quantification*, **14**(2):69-98, 2024.

[7] S. Da Veiga, "Global sensitivity analysis with dependence measures", *J. Statistical Computation and Simulation*, **85**(7):1283-1305, 2015.

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From the analysis of experimental shock dynamic films to Bayesian calibration of physical models

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Abstract

In this PhD thesis, we are interested in studying shock dynamic phenomenon (unstationnary). More particularly, we focus on experiments in which water drops are hit by a shock wave. After the shock has passed, the drops are subject to strong deformations and transformations. Several physical processes are taking place : the mother drop can break up into daughter drops (it is called the « break up » phenomenon) ; the drops can also go through surface alterations (it is called the « stripping » phenomenon) which produce a fog making the observation of the drops difficult. These experiments are meant to improve our knowledge on models, some of which relatively simple whereas some have to be implemented into CEA codes to be compared. In practice, a lot of experiments are done, for several sizes of drop and for several Mach numbers (several shock speeds).

The objective of the thesis is to exploit these experiments, to calibrate the parameters of the CEA models and to select the more appropriate one.

Figure 1.a presents images of a film at different times : at time $0\mu s$, the drop is on the left hand side, put on two threads. At the next time, the shock wave (vertical bar at the center of the image) has hit the drop and the fog (black mass) is moving and being distorted. At time $251\mu s$, only the fog is left, hiding the mother drop and potentially the daughter drops. The extraction of data from these films is not always easy. To give an idea, let's focus on the points of beginning $\left(t \to x_m(t)\right)$ and end $\left(t \to x_M(t)\right)$of the fog : if the beginning of the fog is easily identifiable, the end is subject to uncertainties (commonly accepted by the experts). The extraction must take into account those uncertainties.

A first part of the thesis consists in extracting the necessary quantities for calibration [1]. Only one film is presented here but we have to be able to process many more and so to automate the extraction. To do so, we exploit the strength of supervised neural networks. The figure 1.b shows the prediction of the network for one image and the result of the extraction. α is used as a kind of measure for uncertainties : it is a threshold to select the red pixels from which the more at the left is $x_m(t,\alpha)$, an extraction of $x_m(t)$ and the more at the right, $x_M(t,\alpha)$, an extraction of $x_M(t)$.The result is presented in figure 1.c : $t \to x_m(t,\alpha)$ for $\alpha \in \{0,\cdots,255\}$ is used to extract $t \to x_m(t)$. In the same manner, $t \to x_M(t,\alpha)$ is used to extract $t \to x_M(t)$.

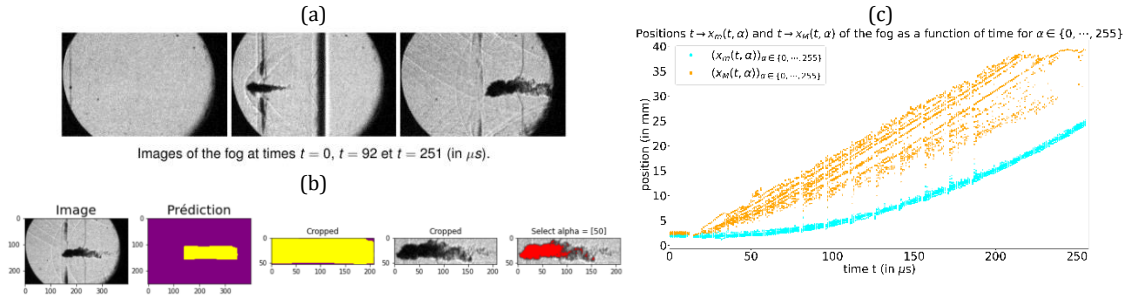

Figure 1: (a) Images of a film of a shocked droplet leading to a fog, at different times (b) Pre-processing of an image (c) Extraction with uncertainties of $t \to x_m(t)$ and $t \to x_M(t)$.

Amongst the different models to be calibrated and studied during this PhD thesis, the simplest one is a model of x_m. We focus on this model in three parts (constant, parabolic and linear in time) in the following paragraph:

$$x_m(t, x_0, t_d, t_g, a) = x_0 + a\left[\left(\frac{1}{2}(t^2 - t_d^2)\right)1_{t_d \le t \le t_g} + \left(t_g(t - t_g) + \frac{1}{2}(t_g^2 - t_d^2)\right)1_{t \ge t_g}\right]. \quad (1)$$

In the above expression, t_d is the time at which the shock wave goes through the drop, t_g the time at which the fog is moving at gaz speed, x_0 the position of beginning of the drop at time 0, before the shock wave has passed, a the acceleration, closely related to the shock strength, the mass of the drops, etc. We want to calibrate the parameter $\eta = (x_0, t_d, t_g, a)$.

To do so, the Bayesian framework [2,3,4] offers the possibility to consider both the knowledge brought by the experimental measures through the likelihood and the *a priori* knowledge brought by the experts on η through the *prior* density. From these, the *posterior* density can be expressed up to a positive factor. The best estimator for η, in the sense of the quadratic loss function is the *a posteriori* mean. As we cannot get it by classical means as optimization algorithms (contrary to other estimator as the *a posteriori* maximizer), we rely on MCMC sampling algorithms to sample the *posterior* density and then calculate an approximation of the *a posteriori* mean.

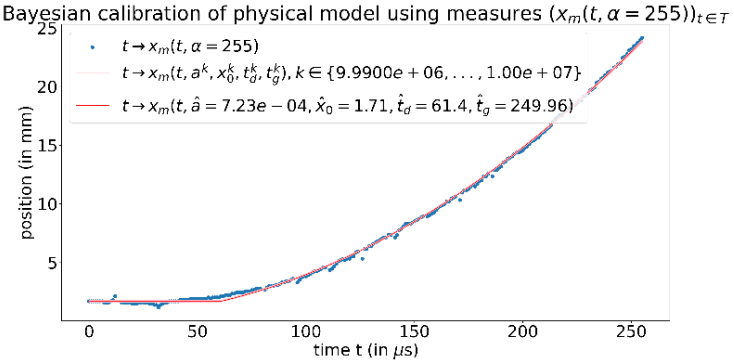

Figure 2: Bayesian calibration of $x_m$model by MCMC algorithm.

The figure 2 shows the experimental measures for a given α, the model taken at the empirical average of the MCMC samples and at some samples of the MCMC chain. We will show that our simple model for $x_m(t)$ is certainly accurate enough. These results are preliminary ones: they do not yet take into account all the information extracted from the film, especially in terms of uncertainties. It is not the only challenge, as we have other films which we can use to calibrate the parameters. Later on during the thesis, we will tackle the question of selecting the best model *via* model selection.

Short biography (PhD student)

I completed a Master's degree in Statistics and Computer Science Engineering, which is a five-year course focused on big data science, at the University of Bordeaux. I completed my Master's internship at CEA-CESTA, following which I accepted to continue with a thesis entitled *"Machine Learning for fast dynamic: analysis of experimental data, parameter calibration and comparison of physical models".*

References

[1] L. Garcia. Détection et suivi d'objets par apprentissage profond appliqué à des films d'essais en dynamique rapide. Master's thesis, 2023.

[2] C. P. Robert. The Bayesian Choice. From Decision-Theoretic Foundations to Computational Implementation. Springer-Verlag, 2007.

[3] A. Hazart, J.-F. Giovannelli, S. Dubost, L. Chatellier. Inverse transport problem of estimating point-like source using a Bayesian parametric method with MCMC. Signal Processing 96 (2014), pp. 346–361.

[4] E. Launay, V. Hergault, M. Bocquet and J. Dumont Le Brazidec, Y. Roustan. Bayesian inversion of emissions from large urban fire using *in situ* observations. Atmospheric Environment 323 (2024)

Sensitivity analysis of multi-scale energy power system models

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Keywords: Multi scale models, Total indices, Model Simplification, Energy, Power Systems Modelling

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Rethinking the Surrogate Model in Efficient Global Optimization

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Abstract

In today's data-driven world, decision-making increasingly relies on complex simulations that bridge theoretical models and real-world applications. These simulations are indispensable in fields ranging from scientific research to policy and management [1]. However, they present significant computational challenges, particularly due to intricate internal interactions and high-dimensional parameter spaces. Efficient Global Optimization (EGO) [2], also called simulation optimization, has emerged as a prominent solution to optimize these simulations within constrained budgets, with applications spanning machine learning [3], healthcare system [4], material science [5], and beyond. EGO's effectiveness lies in its integration of Kriging, a surrogate modelling technique, and Expected Improvement (EI), a criterion designed to balance exploration and exploitation during optimization. Despite its success, EGO faces challenges, particularly in managing the trade-off between exploration and exploitation and in the growing interest in replacing Kriging with alternative machine learning surrogate models.

This study focuses on two primary challenges of EGO: the infill criterion and the use of alternative surrogate models. We analyze classical infill criteria, such as EI and Expected Regret (ER) [6], under different assumptions, and visualize their performance using toy examples. Furthermore, we examine the literature on substituting Kriging with machine learning models, highlighting a common issue—underestimation of exploration, especially when assumptions are absent. We systematically categorize existing methods based on how they guide exploration, demonstrating that many rely on the distance between candidate points and training data. Our findings provide valuable insights into improving exploration in EGO frameworks, contributing to future research in simulation optimization.

Short biography (PhD student)

Zizhou Ouyang is currently pursuing a Ph.D. in Management Science and Business Economics at The University of Edinburgh. Her research focuses on Machine Learning, Explainable AI (XAI), and Bayesian Optimization, aiming to optimize decision-making processes. She has experience in data science, having interned at SPARKEPOS UK, where she contributed to workforce optimization. Additionally, she serves as a reviewer for some journals, including the International Journal of Computer Vision, IEEE Transactions on Automation Science and Engineering, and Neurocomputing Journal.

References

[1] Amaran, S., Sahinidis, N. V., Sharda, B., & Bury, S. J. (2016). Simulation optimization: a review of algorithms and applications. Annals of Operations Research, 240, 351-380.
[2] Jones, D. R., Schonlau, M., & Welch, W. J. (1998). Efficient global optimization of expensive black-box functions. Journal of Global optimization, 13, 455-492.
[3] Hernández-Lobato, J. M., Hoffman, M. W., & Ghahramani, Z. (2014). Predictive entropy search for efficient global optimization of black-box functions. Advances in neural information processing systems, 27.
[4] Coelho, G. F., & Pinto, L. R. (2018). Kriging-based simulation optimization: An emergency medical system application. Journal of the Operational Research Society, 69(12), 2006-2020.
[5] Lookman, T., Balachandran, P. V., Xue, D., & Yuan, R. (2019). Active learning in materials science with emphasis on adaptive sampling using uncertainties for targeted design. npj Computational Materials, 5(1), 21.
[6] Nguyen, V., & Osborne, M. A. (2020, November). Knowing the what but not the where in Bayesian optimization. In International Conference on Machine Learning (pp. 7317-7326). PMLR.

Bayesian calibration for hybrid prognostics of steam generators clogging

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Abstract

Clogging of steam generators (SGs) in pressurized water reactors is a complex phenomenon that develops over extended operational periods. This deposit may affect the SG in several ways: for instance, through a modification of the heat transfer between both primary and secondary circuits, or through vibrations induced by the flow redistribution. Therefore, the clogging rate τ_c is periodically measured during outages and, if necessary, expensive chemical cleaning can be performed. A good preventive maintenance planning is thus crucial for EDF, which explains the R&D effort to better understand this complex phenomenon and to estimate a robust Remaining Useful Life (RUL) [1].

To improve predictions for maintenance scheduling, a physical model and the computer code THYC-Puffer-DEPOTHYC [8, 2] have been developed, simulating clogging kinetics over long SG operational periods. Previous work [3] has identified several uncertain input variables of this code, and sensitivity analysis was conducted to evaluate their impact on τ_c over the simulated period of time. One such influent variable is the physical model calibration parameter. It has also been observed that the dispersion of the clogging trajectories with respect to the probabilistic modeling used proved that the RUL estimation for the SG using the simulation code is unreliable.

Field data on clogging for specific SGs are typically collected through televised camera inspections, though this data is often limited, or of low quality therefore often unreliable. To enhance the available dataset, EDF R&D has developed statistical regression strategies, based on operational data [7].

We propose a hybrid approach to improve the predictive accuracy of the computer model by applying Bayesian calibration [5, 4] to the calibration parameter across different operational scenarios, utilizing various types of clogging field data. This method enables a more precise estimation of the asset's RUL, aiding in prognostics and maintenance planning. We also explore an integration method [6] within the calibration process for taking into account the uncertainty of the other parameters.

Short biography (PhD student)

Edgar Jaber graduated from CentraleSupélec in 2022 with a degree in Applied Mathematics. He also got an MSc in partial differential equations from Université Paris-Saclay. After his final internship at EDF R&D, he began a PhD in Applied Mathematics in 2023, funded by a CIFRE grant between Centre Borelli at ENS Paris-Saclay and LISN. His work focuses on building robust hybrid approaches combining statistical and simulation models to address the industrial challenge of steam generator clogging prediction in nuclear power plants.

References

[1] Luca Biggio and Iason Kastanis. Prognostics and Health Management of Industrial Assets: Current Progress and Road Ahead. *Frontiers in Artificial Intelligence*, 3:578613, November 2020.

[2] Q. Feng, J. Nebes, M. Bachet, S. Pujet, D. You, and E. Deri. Tube support plates blockage of PWR steam generators: thermalhydraulics and chemical modeling, September 2023.

[3] E. Jaber, V. Chabridon, E. Remy, M. Baudin, D. Lucor, M. Mougeot, and B. Iooss. Sensitivity analyses of a multi-physics long-term clogging model for steam generators. *International Journal for Uncertainty Quantificaiton*, 2024.

[4] Merlin Keller, Guillaume Damblin, Alberto Pasanisi, Mathieu Schumann, Pierre Barbillon, Fabrizio Ruggeri, and Eric Parent. Validation of a computer code for the energy consumption of a building, with application to optimal electric bill pricing. *Econometrics*, 10(4), 2022.

[5] Marc C. Kennedy and Anthony O'Hagan. Bayesian calibration of computer models. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 63(3):425–464, 2001.

[6] Guillaume Perrin and Cédric Durantin. Taking into account input uncertainties in the Bayesian calibration of time-consuming simulators. *Journal de la Société Française de Statistique*, 160(2), 2019.

[7] Luca Pinciroli, Piero Baraldi, Ahmed Shokry, Enrico Zio, Redouane Seraoui, and Carole Mai. A semi-supervised method for the characterization of degradation of nuclear power plants steam generators. *Progress in Nuclear Energy*, 131:103580, 2021.

[8] T. Prusek. *Modélisation et simulation numérique du colmatage à l'échelle du sous-canal dans les générateurs de vapeur*. Thèse de l'Université Aix-Marseille, 2012.

Parametric Shape Optimization of Flagellated Micro-Swimmers Using Bayesian optimization techniques

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Abstract

Micro-swimming is emerging as a significant research area due to its potential applications, particularly in the medical field for tasks like cargo transport and drug delivery [1]. A key factor in the performance of micro-robots is the optimization of their shape, which directly influences their motion.

This poster investigates shape optimization of micro-swimmers with one or two helical flagella. The Boundary Element Method (BEM) is used to simulate the dynamic [5]. Due to the complexity of our model, we focus on parametric shape optimization by using Bayesian Optimization (BO), which overcomes the challenges of computing gradient, constraints treatment and reduce the number of costly function evaluations inherent in swimmer dynamics. Additionally, we employ the Free-Form Deformation (FFD) technique [4], which provides a sufficiently complex admissible shape space. This is integrated with the Scalable Constrained Bayesian Optimization (SCBO) method [3], ideal for high-dimensional constrained optimization problems.

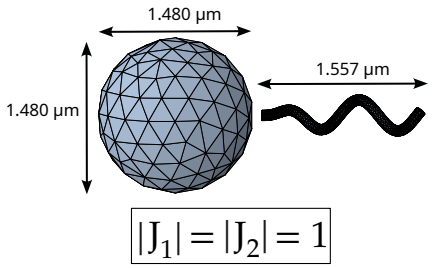

Figure 1: Reference swimmer with one helical flagellum.

The optimized designs are compared to biological swimmers, revealing a wide variety of efficient swimming strategies, including both *pushers* and *pullers* as can be observed in Figure 2.

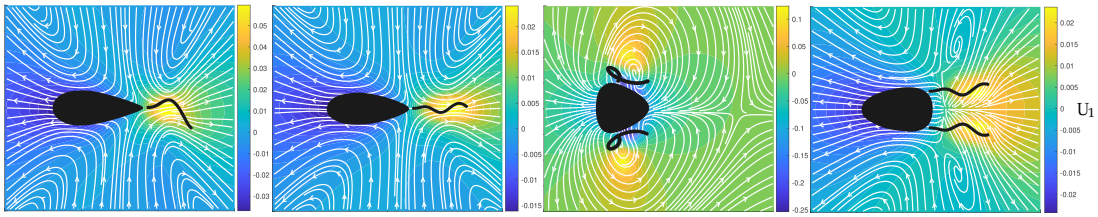

Figure 2: Time-averaged velocity field around optimized swimmers: (first) optimized monoflagellated swimmer for J_1, (second) optimized monoflagellated for J_2, (third) optimized biflagellate for J_1, and (fourth) optimized biflagellate for J_2. The fluid streamlines in the plane $y = 0$ are depicted in white. The colormap represents the fluid velocity along e_1.

Numerous results on the controllability of certain micro-swimmers, such as the Golestanian three-sphere swimmer or N-link models, have been achieved. However, accounting for walls and obstacles remains a significant challenge in both the development of micro-robots and the study of microscopic living organisms [2]. Hence current works focus on improving the control of micro-swimmer trajectories using novel Bayesian optimization techniques.

Short biography (PhD student)

I started my PhD in October 2023 under the supervision of Laetitia Giraldi and co-supervision of Mickaël Binois. My research focuses on applying Bayesian techniques to optimal control and optimal shape design for microswimmers. This work is supported by the French Agence Nationale de la Recherche (ANR) through the NEMO project (grant ANR-21-CE45-0013). The project has potential links with industry, particularly in biomedical engineering and robotics.

References

[1] Hakan Ceylan, Immihan C Yasa, Ugur Kilic, Wenqi Hu, and Metin Sitti. Translational prospects of untethered medical microrobots. *Progress in Biomedical Engineering*, 1(1):012002, jul 2019.

[2] Giancarlo Cicconofri and Antonio DeSimone. Modelling biological and bio-inspired swimming at microscopic scales: Recent results and perspectives. *Computers & Fluids*, 179:799–805, 2019.

[3] David Eriksson and Matthias Poloczek. Scalable Constrained Bayesian Optimization. In *International Conference on Artificial Intelligence and Statistics*, pages 730–738. PMLR, 2021.

[4] Thomas W Sederberg and Scott R Parry. Free-form deformation of solid geometric models. In *Proceedings of the 13th annual conference on Computer graphics and interactive techniques*, pages 151–160, 1986.

[5] Henry Shum. Microswimmer propulsion by two steadily rotating helical flagella. *Micromachines*, 10(1), 2019.

Forward Sweep Interval Sensitivity in Neural Network Functional Approximation

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Interval-based sensitivity is an efficient global sensitivity analysis method that is based on interval arithmetic [1]. It works by partitioning the input of interest into sub intervals, while the other inputs are intact intervals. The method is non-probabilistic and can be used to calculate the sensitivity of a function without relying on sampling, which might not capture the whole input space. For example, methods based on sampling need the definition of a probability distribution, which is often chosen arbitrarily. Interval sensitivity only need specification of the input space where the sensitivity is to be calculated [2].

Global sensitivity analysis can be an effective tool against over parametrization in neural networks. Over parametrization arises when a trained model has too many units or layers and can cause issues, including over-fitting, poor explainability, suboptimality, excessive memory usage, and more. Being able to determine sensitivities towards the output and knowing if there are parameters/units that have a negligible effect and as such can be discarded with no significant loss of performance can be consequential, leading to leaner layouts and more explainable models. Deep learning models are often deemed to be "black boxes" because of their nearly impenetrable mathematical layout. Interestingly however, neural network models always imply a clear, albeit intricate, mathematical function, whose expression is the composition of as many functions as there are layers. The model's mathematical expression can be obtained simply knowing the network's architecture and the trained weights and biases.

The network's forward sweep is a function of the network inputs t, the weights W and biases b. In this study, the inputs of the sensitivity analysis are W and b, so we can write the forward sweep as follows $y = f(t, x)$, where t is the network input and $x \in \mathrm{R}^d$ is the vector of sensitivity inputs (network parameters).

Let $f : \mathrm{R}^d \to \mathrm{R}$ be the forward sweep that is a function only of the network parameters, and let f be the its interval extension. Let $[\underline{y}, \overline{y}]_{i,n}$ be the output corresponding to the n-th subinterval when only the i-th input is partitioned and the other intervals are intact, in notation $[\underline{y}, \overline{y}]_{i,n} = \mathsf{f}([\underline{x_1}, \overline{x_1}], ..., [\underline{x_i}, \overline{x_i}]_n, ..., [\underline{x_d}, \overline{x_d}])$. The interval-based sensitivity index, for the i-th input, is

$$S_i = 1 - \frac{\sum_n^N [\underline{x_i}, \overline{x_i}]_n \cdot [\underline{y}, \overline{y}]_{i,n}}{[\underline{y}, \overline{y}] \cdot [\underline{x_i}, \overline{x_i}]}, \tag{1}$$

where N is the number of subintervals for the i-th partition, $\cdot$ is the interval multiplication used to calculate the area of the (sub) rectangles, $[\underline{x_i}, \overline{x_i}]_n$ is the n-th subinterval for the i-th partition, such that $\cup_n^N [\underline{x_i}, \overline{x_i}]_n = [\underline{x_i}, \overline{x_i}]$, and $[\underline{y}, \overline{y}] = \mathsf{f}([\underline{x}, \overline{x}])$ is the overall output range. The numerator in (1) is the sum of all subinterval areas and the denominator is the area of the box enclosing the xy graph. The sensitivity index $S_i,\ i = 1, ..., d$ ranges from 0 to 1. When $S_i = 0$, the partitioning has no effect, the numerator is equal to the denominator and so y has no functional dependence on x_i. When $S_i = 1$, the sub rectangular areas are zero and so y has full functional dependence on x_i. It is worth noticing that this sensitivity indices are immune to the curse of dimensionality because the partitioning takes place in one dimension

In the example, a neural network with two layers and five ReLU units is trained to approximate the cubic function $y = t^3 - 3t^2 + 2t + 5$. Sensitivity indices are computed for each parameter in the trained neural network, namely weights and biases $W^{(1)} \in \mathrm{R}^{1\times5}$, $b^{(1)} \in \mathrm{R}^5$, $W^{(2)} \in \mathrm{R}^{5\times1}$, $b^{(2)} \in \mathrm{R}$. The trained network settled on the following values: $W^{(1)} = ((-1, -1, 0, 1, 1))$, $b^{(1)} = (-1, 0, 0, -2, -3)$, $W^{(2)} = ((-13, -5, 0, 5, 13))$, and $b^{(2)} = 5$. The interval sensitivity is calculated by intervalizing the inputs with a radius of ±1 for each parameter and a partition of $N = 30$. The inputs are organized in the single vector $x = (W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)})$ of size $d = 16$.

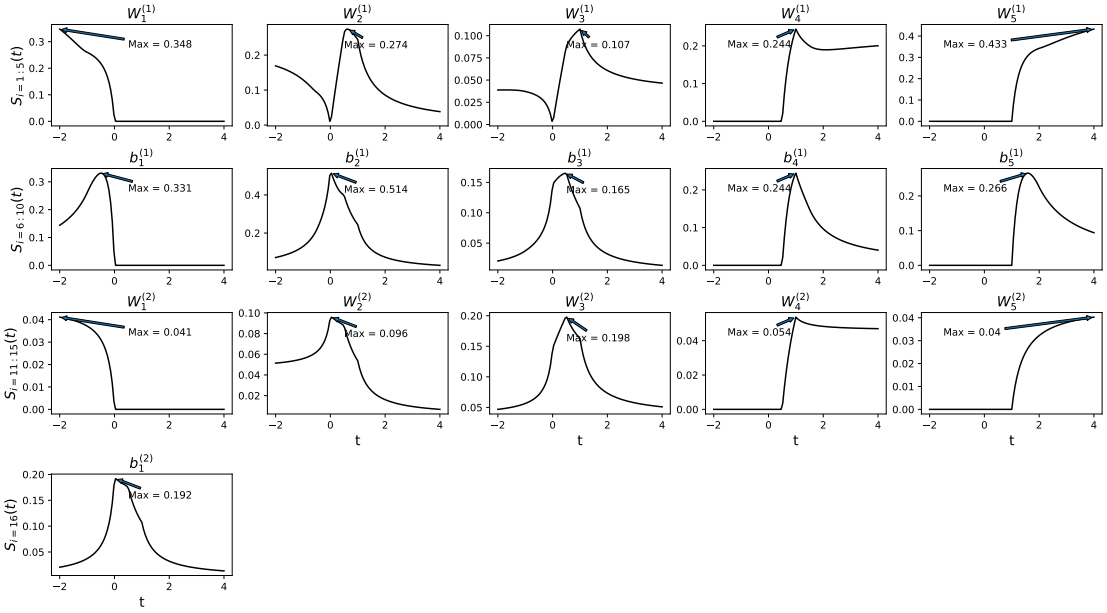

Figure 1: Sensitivity indices across network's input t for $x = (W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)})$.

The neural network is trained to approximate the above cubic function, whose graph changes sign at $t = 1$. All sensitivity indices reflect this displaying peaked values around it, as shown in Figure 1. We notice that the weights describing the negative values of the cubic function, namely $W_1^{(1)}$, $b_1^{(1)}$, $W_1^{(2)}$ display high sensitivities for the negative values and zero sensitivities for the positive values. Similarly, the weights describing the positive values $W_4^{(1)}$, $b_4^{(1)}$, $W_4^{(2)}$, $W_5^{(1)}$, $b_5^{(1)}$, $W_5^{(2)}$ show the same pattern for positive and negative values respectively. It is worth noticing that these network parameters display zero sensitivities for the region of the space that they do not describe, as expected. Other parameters have more complex dependencies on the output. This study has also shown that for this particular example, the network is not over parametrized so, none of the inputs can be ignored without affecting the network's accuracy in approximating the cubic function. The sensitivities can also be used to see what units are active in the regions of interest, providing a diagnostic tool to reason about the parameters role in the overall architecture.

References

[1] "IEEE Standard for Interval Arithmetic," in *IEEE Std 1788-2015*, pp.1-97, 30 June 2015

[2] Miralles-Dolz E., Gray A., de Angelis M., Patelli E. "Interval-Based Global Sensitivity Analysis for Epistemic Uncertainty", in: *Proceedings of the 32nd European Safety and Reliability Conference (ESREL 2022).* Research Publishing, IRL, pp. 2545-2552, 2022.

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Application of HSIC-Lasso for high-dimensional feature selection in shapelet-based decomposition

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In this work, we present a novel approach for selecting an optimal projection basis for time series objects when using shapelet decomposition in a classification framework, leveraging a Lasso-like high-dimensional non-linear feature selection method based on the Hilbert-Schmidt Independence Criterion (HSIC)[1].

Time series analysis frequently faces challenges such as high dimensionality, autocorrelation, and the difficulty of identifying key features that capture essential dynamics across different temporal scales and phase offsets. To address these issues, we employ shapelet decomposition[2], a technique designed to extract shape-based features from time series, preserving both temporal and frequency information. The core idea is to represent a time series dataset through minimal distances to specific representative patterns. Shapelet decomposition not only performs well compared to other state-of-the-art methods for time series learning but also provides enhanced interpretability by identifying patterns most relevant to the algorithm decisions, often offering insights into the physical meaning behind these decisions.

Given the large number of possible shapes that can be extracted from a dataset, selecting the most relevant shapes-i.e., the most informative projection basis-is crucial for numerical tractability. In most prior works, this selection is achieved by iteratively optimizing the information gain among a set of candidate patterns[3]. However, this approach has two main drawbacks: its high computational cost due to two nested optimization problems and the potential for selecting interdependent features, leading to redundant information.

As an alternative, we propose selecting the optimal shapelet decomposition basis using HSIC Lasso, a Lasso-like non-linear high-dimensional feature selection method that uses HSIC to identify a sparse subset of the most informative and mutually independent features[4]. This approach requires only a single optimization loop over the Lasso weights, making it a significantly more computationally efficient alternative to the standard method. Additionally, as already mentioned, the set of informative features selected by this approach is so that its components do not present strong interdependence.

We validate our approach on both synthetic and real-world datasets, demonstrating its potential to improve performance, scalability, and interpretability of time series classification models. Our method offers a powerful tool for a wide range of application domains.

References:

[1] Gretton, A., Bousquet, O., Smola, A., and Schölkopf, B. (2005, October). Measuring statistical dependence with Hilbert-Schmidt norms. In International conference on algorithmic learning theory (pp. 63-77). Berlin, Heidelberg: Springer Berlin Heidelberg.

[2] Ye, L., and Keogh, E. (2011). Time series shapelets: a novel technique that allows accurate, interpretable and fast classification. Data mining and knowledge discovery, 22, 149-182.

[3] Hills, J., Lines, J., Baranauskas, E., Mapp, J., and Bagnall, A. (2014). Classification of time series by shapelet transformation. Data mining and knowledge discovery, 28, 851-881.

[4] Yamada, M., Jitkrittum, W., Sigal, L., Xing, E. P., and Sugiyama, M. (2014). High-dimensional feature selection by feature-wise kernelized lasso. Neural computation, 26(1), 185-207.

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Epistemic uncertainty management in risk assessment: connections between robustness and sensitivity analysis tools

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Uncertainty quantification (UQ) in computer models has become increasingly important over recent decades, particularly in the context of risk assessment. Numerous techniques exist to propagate aleatory uncertainty, enabling the evaluation of risk-oriented quantities of interest, such as low failure probabilities or high-order quantiles. However, these evaluations often rely on subjective assumptions, including the choice of the input joint probability distribution, which may be based on limited information. Therefore, input densities are tainted with *epistemic uncertainties* which have to be taken into account, especially in risk or safety analyses. The core idea is to find a relevant framework to model such uncertainties and to evaluate the robustness of the estimated key risk measures (typically, failure probabilities, quantiles or any other risk measure) with respect to these assumptions on the input probabilistic modeling.

On the one hand, a first solution is to adopt a "sensitivity analysis" viewpoint. More specifically, *robustness analysis* (see, e.g., [1, Chap. 6]) offers a useful approach by quantifying how perturbations in the assumptions impact the key quantities of interest on which industrial decisions are based. Among several methods, the *Perturbed Law-based sensitivity Indices* (PLI) have been proposed by [2] as a way of measuring the impact of perturbations of input densities (in a parametric case) on a risk measure (e.g., a failure probability, a high-order quantile or a superquantile in [3]). More recently, a novel formulation of these indices has been proposed in [3] by revisiting the initial formulation through an information-geometric approach, leading to a more sound and rigorous framework for the input-perturbation statistical procedure.

On the other hand, the modeling, quantification and propagation is an old topic in the UQ community. Several mathematical frameworks have been proposed and studied. Among others, two are of specific interest here: the *Optimal UQ* framework [5] and the *Info-gap* framework [6]. In Optimal UQ, epistemic uncertainties are handled through solving an optimization problem leading to maximizing a risk measure (e.g., a quantile) over a class of bounded distributions satisfying moments constraints. As for Info-gap, it relies on maximizing the risk measure over increasingly large input uncertainty domains. By looking at those formulations closer, it appears that methodological links can be drawn from the two frameworks and the PLI-based robustess analysis described above. More specifically, connections and differences can be derived from several keypoints such as the a priori assumptions made, the way perturbations/optimization are solved as well as the final results available at the end of each analysis.

Thus, the goal of this work is to exhibit, discuss and analyze these links both theoretically and numerically, in the context of risk-oriented analyses. From a sensitivity analysis perspective, such a work aims at pointing out the fruitful connections that handling "epistemic" or "second-level" uncertainties impose between this field and the UQ practice in engineering. As a perspective, one can wonder whether designing "optimal" sensitivity measures would be possible in order to assess the robustess of any risk measure with respect to prior assumptions on the input probabilistic model.

References:

[1] Da Veiga S., F. Gamboa, B. Iooss and C. Prieur, "Basics and Trends in Sensitivity Analysis: Theory and Practice in R", *Society for Industrial and Applied Mathematics*, Philadelphia, PA, 2021.

[2] Lemaître P., E. Sergienko, A. Arnaud, N. Bousquet, F. Gamboa and B. Iooss, "Density modification-based reliability sensitivity analysis", *J. of Stat. Comp. and Simul.*, **85**(6):1200–1223,

2015.

[3] Gauchy C., J. Stenger, R. Sueur and B. Iooss, "An Information Geometry Approach to Robustness Analysis for the Uncertainty Quantification of Computer Codes", *Techno.*, **64**(1):80–91, 2021.

[4] Iooss B. and V. Vergès, "BEPU robustness analysis via perturbed law-based sensitivity indices", *Proc. of the Inst. of Mech. Eng (Part O).*, **236**(5):855–865, 2022.

[5] Stenger J., F. Gamboa, M. Keller and B. Iooss, "Optimal Uncertainty Quantification of a risk measurement from a thermal-hydraulic code using canonical moments", *Int. J. for Unc. Quant.*, **10**(1):35–53, 2020.

[6] Ben HaÏm Y., "Info-Gap Decision Theory: Decisions under Severe Uncertainty", *Elsevier*, Second Edition, 2006.

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Gradient-enhanced surrogate modelling and sensitivity analysis with chaos expansions

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To surrogate expensive computer simulations and calculate Sobol' sensitivity indices, sparse regression-based polynomial chaos expansions are a well-known tool. They represent the model in a basis of multivariate polynomials which are orthogonal with respect to the distribution of the input parameters. Recently, another type of chaos has been proposed, whose basis consists of the eigenfunctions of an associated Sturm-Liouville equation [1,2,3], see Fig. 1 for an illustration. The advantage of this basis is that by construction, the partial derivatives of the basis form again a basis which is orthogonal with respect to the same distribution as the original basis. This makes it possible to use model derivatives, if available, for the surrogate, while keeping advantageous orthogonality properties of the regression matrix.

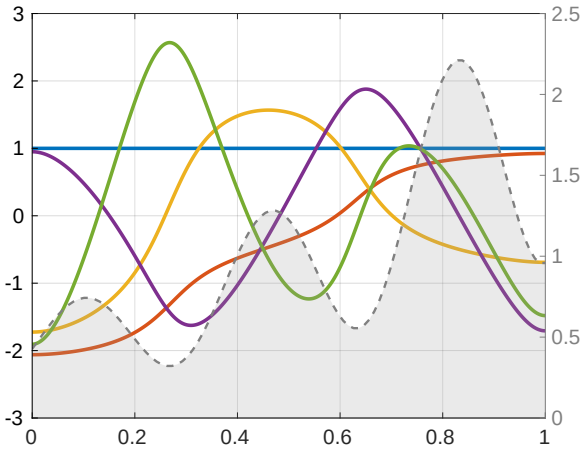

Figure 1: Illustration of the first five eigenfunctions of a one-dimensional Poincaré basis for a distribution with three modes (visualized by the gray area with y-scale on the right-hand side of the plot)

In our previous work [2], we used sparse regression-based Poincaré chaos expansions to compute surrogate models and sensitivity indices (Sobol' indices and DGSM) from model evaluations and derivatives separately. We found that while the Poincaré methodology did not outperform PCE as a surrogate model in our experiments, the Sobol' indices computed through derivative-based Poincaré expansions seem to be an efficient screening tool.

However, we did not yet built surrogates from both model evaluations and derivative values at once. This problem has been analyzed by Adcock and Sui (2019) [3]. They have shown that by applying weighted ℓ^1 regression to gradient-augmented data, the surrogate converges in a stronger norm than for model evaluations alone, with an equivalent number of model (resp. gradient) evaluations.

In this contribution, we provide an all-included methodology for gradient-augmented analysis which combines model evaluations and derivatives in the two main stages of surrogate modeling and global sensitivity analysis. First, we further examine the gradient-augmented regression problem by handling different orders of magnitude for model evaluations and partial derivatives. Second, we present a new estimator for Sobol' indices which uses both model evaluations and derivative values. It is built as a minimal-variance aggregation of estimators computed from chaos expansions and is particularly well suited for screening. We demonstrate the performance of the methodology on a hydrological problem where gradients are available via the adjoint method.

References:

[1] O. Roustant, F. Gamboa and B. Iooss, "Parseval inequalities and lower bounds for variance-based sensitivity indices", *Electronic Journal of Statistics*, **14**(1):386–412, 2020.

[2] N. Lüthen, O. Roustant, F. Gamboa, B. Iooss, S. Marelli and B. Sudret, "Global sensitivity analysis using derivative-based sparse Poincaré chaos expansions", *International Journal for Uncertainty Quantification*, **13**(6), 2023.

[3] B. Adcock and Y. Sui, "Compressive Hermite Interpolation: Sparse, high-dimensional approximation from gradient-augmented measurements", *Constructive Approximation*, **50**(1):167–207, 2019.

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Robustness analysis of gaussian process metamodels using Fisher density perturbations

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In recent years, a growing interest was taken in studying the robustness of a model output to a potential misspecification of input uncertainties [1, 2]. In a common uncertainty quantification (UQ) scheme, based on a numerical model G which uncertain inputs $X_1, \ldots, X_d$ are random variables, and a given QoI defined on the output $Y = G(X_1, \ldots, , X_d)$, this means considering a whole range of potential laws for the X_i. The idea initially proposed in [3] is to apply a perturbation to the density f_{i0} representing the baseline distribution of the i-th input X_i, and estimate the corresponding perturbed QoI.

This perturbation approach could be profitably extended to situations involving more advanced UQ tools such as sensitivity indices or metamodels. Here we propose a first exploration of how the perturbation method introduced in [4], which is based on the Fisher distance, could be applied in UQ studies involving gaussian process (GP) metamodels. To do so, we define $\mathcal{I}(\boldsymbol{\theta})$ the Fisher information Matrix (FIM) associated to the law of a GP $Z_{\boldsymbol{\theta}}$ with hyper-parameters $\boldsymbol{\theta} \in \Theta$:

$$\mathcal{I}(\boldsymbol{\theta}) = -\mathbb{E}\left[\frac{\partial^2 \ln f_Z(\boldsymbol{\theta}, \boldsymbol{z})}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^T}\right],$$

where $f_Z(\boldsymbol{\theta}, \cdot)$ is the (gaussian) density of the random process $Z_{\boldsymbol{\theta}}$, and $\boldsymbol{z} = [z^{(n)}]_{n=1,\ldots,N}$ the vector of observed outputs of the model at design points $\boldsymbol{x}^{(1)}, ..., \boldsymbol{x}^{(N)}$. This matrix induces a metric on Θ the parametric space in which the vector of hyper-parameters lies. The distance between two processes with parameters θ_0 and θ_1 is then given by:

$$d_F(\boldsymbol{\theta}_0, \boldsymbol{\theta}_1) = \inf_{\gamma \in \mathcal{P}(\boldsymbol{\theta}_0, \boldsymbol{\theta}_1)} \int_0^1 \sqrt{\dot{\gamma}(t)^T \mathcal{I}(t) \dot{\gamma}(t)} dt,$$

$\mathcal{P}(\boldsymbol{\theta}_0, \boldsymbol{\theta}_1)$ denoting the set of path joining $\boldsymbol{\theta}_0$ to $\boldsymbol{\theta}_1$.

In this setting, each law at distance δ from the baseline one $f_Z(\boldsymbol{\theta}_0, \cdot)$ can be seen as a perturbed law at level δ. The principle of robustness analysis is then to consider Fisher spheres centered in $\boldsymbol{\theta}_0$ with growing radius, and find, for each perturbation level, the most impactful model towards the used QoI. It can be noted that in the specific case of GP surrogate models with stationary covariance kernels, the latter can be characterized by a probability density function in the Fourier space thanks to Bochner's theorem. Hence the described perturbation method could be implemented using this spectral representation of the law of the process.

In the most simple case, one can examine the robustness of an output probability when estimated through a GP emulator of a costly numerical model. But GP are also used to sequentially select numerical experiments, using some uncertainty reduction criteria, in order to estimate efficiently the target QoI with a limited computational budget. It is then possible to evaluate the robustness of the QoI as well as the employed criterion as regards the law of the GP. We will illustrate this principle on very simple toy-models as well as on well-known examples of the UQ community.

References:

[1] G. Perrin, G. Defaux, "Efficient Evaluation of Reliability-Oriented Sensitivity Indices", *J. Sci. Comput.* **79**, 1433–1455, 2019.

[2] A. Ajenjo, E. Ardillon, V. Chabridon, B. Iooss, S. Cogan and E. Sadoulet-Reboul, "An info-gap framework for robustness assessment of epistemic uncertainty models in hybrid structural reliability analysis", *Structural Safety*, **96**, 102196, 2022.

[3] P. Lemaitre, E. Sergienko, A. Arnaud, N. Bousquet, F. Gamboa and B. Iooss, "Density modification based reliability sensitivity analysis", *Journal of Statistical Computation and Simulation*, **85**, 1200-1223, 2015.

[4] C. Gauchy, J. Stenger, R. Sueur and B. Iooss, "An Information Geometry Approach to Robustness Analysis for the Uncertainty Quantification of Computer Codes", *Technometrics* , **64**(1), 80–91, 2022.

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An adaptive method for nonlinear model order reduction using sparse polynomials

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Abstract

Model order reduction methods are used to approximate a manifold of functions from a high-dimensional space by a low-dimensional space or manifold. We here propose a new approach that aims at building a low-dimensional nonlinear manifold M_n, given a desired target precision. The description of the manifold is similar to [1] or [2], with $M_n = \{L(a) + N(a) : a \in \mathbb{R}^n\}$, where L is a linear map onto a n-dimensional space V_n and N is a nonlinear map onto a complementary space. Here, we propose an adaptive strategy for the construction of the maps L and N, the latter using compositions of sparse polynomials. The manifold M_n is estimated "offline" from a set of training samples and then used "online" to approximate the solution of parameter-dependent equations, using a Galerkin-type projection method.

We investigate through numerical experiments the performance of our method on several parameter-dependent problems. The results reveal the advantage of our approach compared to linear approximation, and also to state of the art nonlinear methods.

Short biography (PhD student)

I am a PhD student in applied mathematics at Airbus and Nantes Université/Centrale Nantes, Laboratoire de mathématiques Jean Leray. My background is mainly on statistics, machine learning and numerical analysis. My work focuses on developing new mathematical and numerical data-driven methods, for solving partial differential equations, especially the ones describing acoustic waves propagation. My PhD is funded by Airbus Central Research and Technology.

References

[1] Joshua L Barnett, Charbel Farhat, and Yvon Maday. Neural-network-augmented projection-based model order reduction for mitigating the kolmogorov barrier to reducibility of cfd models, 2022.

[2] Rudy Geelen, Laura Balzano, Stephen Wright, and Karen Willcox. Learning physics-based reduced-order models from data using nonlinear manifolds, 2024.

Uncertainty in Life Cycle Assessment: Sources, Types, Propagation, Evaluation, Mitigation and Reporting

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Life cycle assessment (LCA) has become a widely recognized methodology for evaluating the environmental impacts of products, technologies, and policies [1]. However, uncertainty remains a key challenge affecting its transparency and reliability, particularly due to the lack of a systematic framework for uncertainty analysis. To address this gap, we conducted a comprehensive review of new ISO standard [2], European Union standard [3], latest guidebook [4], and recent publications [5-6], and proposed a comprehensive framework that clearly presents the sources, types, propagation, evaluation, mitigation, and reporting of uncertainty in LCA, as illustrated in **Figure 1**.

Specifically, this framework provides direct answers to the following questions:
(1) What are the sources of uncertainty in LCA applications?
(2) What types of uncertainty exist in each phase?
(3) How does uncertainty propagate through to the results?
(4) How can the uncertainty of results be evaluated?
(5) At which stages should researchers conduct sensitivity analysis and sensitivity checks?
(6) How can uncertainty be reduced throughout the entire process?
(7) How should uncertainty in LCA be reported?

In conclusion, this framework integrates both the standard phases of LCA and systematic behaviors of uncertainty from a proper perspective. It has significant potential to help researchers better understand the intrinsic relationships between uncertainty and LCA, while also contributing to uncertainty reduction and improving the transparency and reliability of LCA studies.

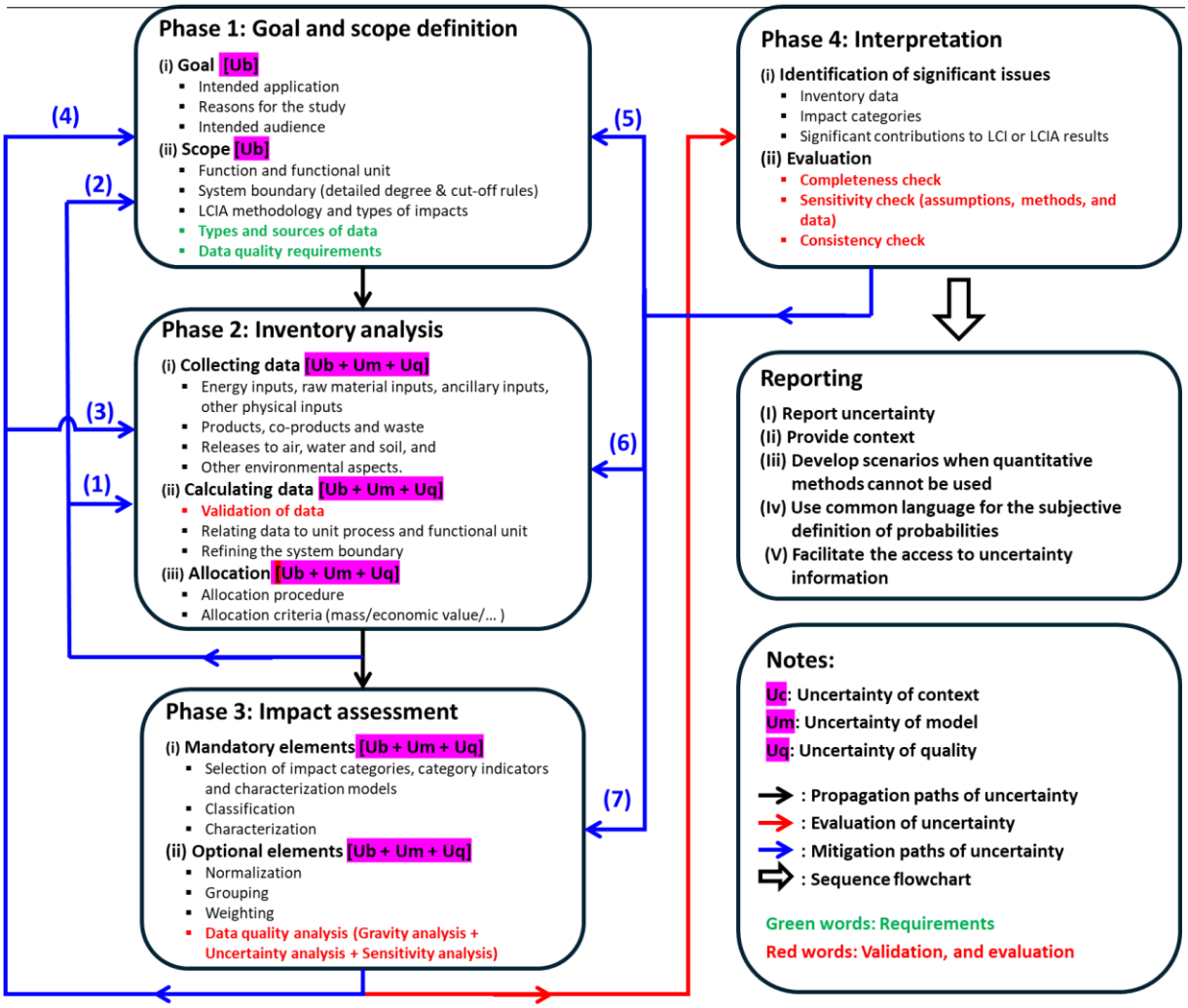

Figure 1. A Suggested Comprehensive Framework for Uncertainty analysis in Life Cycle Assessment: Sources, Types, Propagation, Evaluation, Mitigation and Reporting

References:

[1] E. Igos, E. Benetto, R. Meyer, P. Baustert, and B. Othoniel, "How to treat uncertainties in life cycle assessment studies?", *Int J Life Cycle Assess*. **24**(4): 794-807, 2019.
[2] Technical Committee, "Environmental management - Life cycle assessment - Principles and framework - amendment 1", *International Organization for Standardization*, 2020.
[3] European Commission, "LCA4CCU: guidelines for life cycle assessment of carbon capture and utilization", *Publications Office of the European Union*, 2022.
[4] European Commission, "Guide for interpreting life cycle assessment result", *Publications Office of the European Union*, 2016.
[5] A. Laurent et al., "Methodological review and detailed guidance for the life cycle interpretation phase", *J. Ind. Ecol*. **24**(5): 986-1003, 2020.
[6] A. Saltelli et al., "Why so many published sensitivity analyses are false: A systematic review of sensitivity analysis practices", *Environ. Model. Softw.*, **114**: 29-39, 2019.

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General reproducing properties in RKHS with application to derivative operator

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Abstract

Machine learning algorithms often involve penalized regression problems of the form

$$\min_{h\in\mathcal{H}} \sum_{i=1}^{n} (Lh(x_i) - y_i)^2 + \lambda \|h\|^2.$$

Here $(x_i, y_i)_{1\leq i\leq n}$ is a dataset where x_i belongs to some set $\mathbb{X}$ and $y_i \in \mathbb{R}$, $\lambda \in \mathbb{R}_+$ is a penalty coefficient, $\mathcal{H}$ is a Hilbert space of real-valued functions on $\mathbb{X}$, and L is a linear operator on $\mathcal{H}$. When $\mathcal{H}$ is a reproducing kernel Hilbert space (RKHS), it turns out that the solution lives in a finite-dimensional space, a famous result known as "representer theorem" [1, 3].

A key property to prove this result is the generalized "reproducing property"

$$\forall x \in \mathbb{X}, \forall h \in \mathcal{H} : \qquad Lh(x) = \langle h, \widetilde{L}(x) \rangle \tag{1}$$

where $\widetilde{L}(x)$ belongs to $\mathcal{H}$ and $\langle \cdot, \cdot \rangle$ denotes the inner product associated to $\mathcal{H}$. When L is the identity operator, we have $\widetilde{L}(x) = K(x, .)$ where K is the kernel associated to $\mathcal{H}$,

$$\forall x \in \mathbb{X}, \forall h \in \mathcal{H} : \qquad h(x) = \langle h, K(x, .) \rangle$$

which is the original reproducing property of RKHS [1]. This immediately extends to finite linear combinations, i.e. when L has the form

$$Lf(x) = \sum_{i=1}^{q} \alpha_i f(v_i(x))$$

where $\alpha_i \in \mathbb{R}$ and $v_i(x) \in \mathbb{X}$. In that case, $\widetilde{L}(x) = \sum_{i=1}^{q} \alpha_i K(v_i(x), .)$. However, the generalization to more complex operators such as derivative or integral operators is not straightforward as it involves a passage to the limit.

In this work, we consider a broad class of operators corresponding to limits of linear combinations and we give a necessary and sufficient condition on K for (1) to hold under the assumption that (1) remains true when passing to the limit. Then we focus on the derivative operator, and show that the generalized reproducing property holds if the cross derivative of the kernel exists and is continuous on the diagonal of $\mathbb{X} \times \mathbb{X}$. We prove that this condition is less restrictive than the known sufficient condition that K is of class C^2 [4, 2].

Short biography (PhD student)

I graduated from École Polytechnique (X20) and hold a Master's degree in Mathematics, Vision, and Learning (MVA) from the Institut Polytechnique de Paris. My PhD focuses on developing physics-informed methods for predicting water-related extreme events, aiming to improve accuracy and reduce computational costs. The research is funded by specific doctoral grants for École Polytechnique graduates and ANITI.

References

[1] Nachman Aronszajn. Theory of reproducing kernels. *Transactions of the American mathematical society*, 68(3):337–404, 1950.

[2] JC Ferreira and Valdir Antônio Menegatto. Positive definiteness, reproducing kernel hilbert spaces and beyond. *Annals of Functional Analysis*, 4(1), 2013.

[3] Bernhard Schölkopf, Ralf Herbrich, and Alex J Smola. A generalized representer theorem. In *International conference on computational learning theory*, pages 416–426. Springer, 2001.

[4] Ding-Xuan Zhou. Derivative reproducing properties for kernel methods in learning theory. *Journal of computational and Applied Mathematics*, 220(1-2):456–463, 2008.

Constructing Quasi-Monte Carlo Points With and Without Sensitivity Analysis

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Good point sets for quasi-Monte Carlo (QMC) integration are usually constructed by selecting parameters to minimize a figure of merit (FOM) that measures the discrepancy between the empirical distribution of the points and the uniform distribution [1, 2, 6]. These FOMs often give weights to the different subsets of coordinates, to account for their relative importance, as done by the software in [7, 8], for example. The weights should reflect the variance contributions (or sensitivity indices) of these subsets, which are typically unknown and costly to estimate.

A much simpler alternative is to bypass these FOMs and simply draw the parameters of the QMC rule at random from some distribution. It turns out that for the popular QMC constructions, the probability of drawing bad parameters (that give a large RQMC variance) is pretty small.

With randomized QMC (RQMC), we randomize the points r times independently to compute r independent replicates of the unbiased RQMC estimator, and we usually take the empirical mean and variance of these r replicates to estimate the true mean (the integral) and perhaps compute a confidence interval [9]. When the QMC parameters are selected at random, independently for the r replications, it may be better to replace the empirical mean by a more robust estimator such as the median or something more refined, so that the outliers that may come from the rare unlucky parameter choices have little impact on the final estimator. This idea was proposed and studied recently in [3, 4, 5, 10, 11].

In this talk, we review these recent studies and we report on experiments that compare the mean square error (MSE) of various estimators (the mean, the median, and others) in RQMC settings. We also look at how to compute confidence intervals for the mean in these settings.

References:

[1] J. Dick, P. Kritzer, and F. Pillichshammer. *Lattice Rules: Numerical Integration, Approximation, and Discrepancy*. Springer, 2022.

[2] J. Dick and F. Pillichshammer. *Digital Nets and Sequences: Discrepancy Theory and Quasi-Monte Carlo Integration*. Cambridge University Press, Cambridge, U.K., 2010.

[3] E. Gobet, M. Lerasle, and D. Métivier. Accelerated convergence of error quantiles using robust randomized quasi Monte Carlo methods. Preprint, `https://hal.science/hal-03631879`, 2024.

[4] T. Goda and P. L'Ecuyer. Construction-free median quasi-Monte Carlo rules for function spaces with unspecified smoothness and general weights. *SIAM Journal on Scientific Computing*, 44(4):A2765–A2788, 2022.

[5] T. Goda, K. Suzuki, and M. Matsumoto. A universal median quasi-Monte Carlo integration. *SIAM Journal on Numerical Analysis*, 62(1):533–566, 2024.

[6] P. L'Ecuyer, Y. Cherkanihassani, and M. El Amine Derkaoui. Pre-scrambled digital nets for randomized quasi-Monte Carlo. In *Proceedings of the 2024 Winter Simulation Conference*, pages 443–454. IEEE Press, 2024.

[7] P. L'Ecuyer, P. Marion, M. Godin, and F. Puchhammer. A tool for custom construction of QMC and RQMC point sets. In A. Keller, editor, *Monte Carlo and Quasi-Monte Carlo Methods: MCQMC 2020*, pages 51–70, Berlin, 2022. Springer.

[8] P. L'Ecuyer and D. Munger. Algorithm 958: Lattice builder: A general software tool for constructing rank-1 lattice rules. *ACM Transactions on Mathematical Software*, 42(2):Article 15, 2016.

[9] P. L'Ecuyer, M. Nakayama, A. B. Owen, and B. Tuffin. Confidence intervals for randomized

quasi-Monte Carlo estimators. In *Proceedings of the 2023 Winter Simulation Conference*, pages 445–456. IEEE Press, 2023.

[10] Z. Pan and A. B. Owen. Super-polynomial accuracy of one dimensional randomized nets using the median of means. *Mathematics of Computation*, 92(340):805–837, 2023.

[11] Z. Pan and A. B. Owen. Super-polynomial accuracy of multidimensional randomized nets using the median of means. *Mathematics of Computation*, 93(349):2265–2289, 2024.

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Sensitivity Analysis (SA) Comparisons on Geologic Case Studies: An International Collaboration

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Over the past six years, an informal working group under the auspices of the Organization for Economic Cooperation and Development (OECD)/NEA's Integration Group for the Safety Case (IGSC) has explored existing and new sensitivity analysis (SA) methods and provided recommendations for best practices. The focus is on the use of sensitivity analysis in case studies involving geological disposal of nuclear waste. To examine ideas and have applicable test cases for comparison purposes, we used multiple existing case studies. Four of these were presented in a first Volume [1].

Three additional case studies are investigated in the recently published Volume 2 [2]: the GRS LILW (low and intermediate level waste) case in a salt repository, the SNL generic crystalline case, and the UDC reactive transport case. The three case studies are more complicated than those in Volume 1, due to more nonlinear behavior, outputs which exhibit bifurcation, regime changes, and nested sampling.

The sensitivity methods used in the three case studies include: scatterplots, correlation and regression coefficients, Sobol' indices estimated by using a variety of surrogate approximations, distribution-based methods such as PAWN (a density-based method, acronym derived from the names of its proponents Pianosi and Wagener), graphical methods like CUSUNORO (Cumulative Sum of Normalized Reordered Output), various feature importance metrics, VARS (Variogram analysis of response surfaces), and quantile-based importance.

Here we present selected results and highlights from Volume 2 as well as recommendations gained from the results and experiences from both the case studies of Volumes 1 and 2. These recommendations head towards defining the goals of the SA study, then scoping the analysis and finally selecting appropriate SA methods with considerations for proper use of the methods. We learned from these cases with their inherent challenges that SA is an iterative process for such cases. Our guidelines are provided at a high level to allow for necessary flexibility and iteration for case-specific challenges.

These findings are provided in Volume 2 [2]. A very short summary of the takeaway recommendations is as follows:

Defining the goals: We recommend that the SA practitioners start by identifying all the potential goals of the sensitivity analysis. This will guide their decisions around scoping and methods.

Scoping the study: We suggest that the SA practitioners systematically address input identification and description, computational costs, potential sampling schemes, and known behavior of the physical model to scope their analysis. We advise that the SA practitioners account for the availability of resources, acceptability of methods, and prioritized goals in scoping a study so that it provides the level of analysis needed to support safety statements.

Selecting the methods: We recommend that the SA practitioners use several approaches and methods. The analysis of the differences should lead to exploring the reasons for discrepancies. We suggest the following high-level process: 1. Begin with graphical methods for uncertainty of the output (e.g., histograms, horsetail time series plots) and sensitivity analysis (e.g., scatterplots, CUSUNORO curves). 2. Estimate first-order sensitivities, including correlation coefficients (Pearson, Spearman), regression coefficients, and/or main effects Sobol' indices. Assess whether these indices accomplish the goals of the study. 3. Examine parameter interactions by analyzing higher-order and total effects and/or moment independent methods if needed to accomplish the goals of the study, especially if the main effects fail to capture a significant portion of the output variance. The above recommendations should be seen as an iterative guideline. At each step, the analyst should consider which of the analysis goals have not been accomplished and whether the results from the previous step can inform the most effective methods and models to apply in the next iteration.

Using metamodels: We advise that the SA practitioners consider employing metamodeling approaches for case studies with potentially important higher-order effects, which may be difficult to detect without the computational efficiency of a metamodel. We recommend that SA practitioners who employ metamodeling utilize best practices for goodness of-fit metrics, cross validation, reduction of overfitting, and regularization methods as well as use graphical sensitivity analysis to confirm and supplement results from metamodeling methods.

References:

[1] L.P. Swiler, D.-A. Becker, D. Brooks, J. Govaerts, L. Koskinen, P. Kupiainen, E. Plischke, K.-J. Röhlig, E. Saveleva, S.M. Spiessl, E. Stein and V. Svitelman, "Sensitivity Analysis Comparisons on Geologic Case Studies: An International Collaboration", *Technical Report SAND2021-11053, SANDIA National Laboratories, DOI: https://doi.org/10.2172/1822591*, 2021.

[2] L.P. Swiler, D.-A. Becker, D. Brooks, L. Koskinen, P. Kupiainen, E. Plischke, K.-J. Röhlig, J. Samper and S.M. Spiessl, "Sensitivity Analysis Comparisons on Geologic Case Studies: An International Collaboration, Volume 2", *Technical Report SAND2025-00230, SANDIA National Laboratories,* 2025.

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Overcoming challenges in sensitivity analysis for complex models in nuclear and renewable energy applications

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Our presentation will focus on the critical challenges and advancements in sensitivity analysis for complex models used in nuclear and renewable energy applications.

Firstly, we will discuss the intricacies of sensitivity analysis for models involving dependent variables, time series, and multiphysics couplings, each requiring the adaptation of standard methodologies. When dealing with dependent inputs, the challenge is to strike a balance between interpretability, effective screening performance and constrained inference. Current trends, such as Johnson's relative weights, Shapley values and dependence measures based on Hilbert-Schmidt independence criterion (HSIC), do not fully meet engineers' expectations. Moreover, the treatment of time series, where the data come from a single time series, raises theoretical questions about the probabilistic guarantees of the usual methods (confidence intervals for Sobol indices or p-values for HSIC indices). In addition, multiphysics simulation, where several sub-models sharing state variables are interconnected, presents the challenge of how to use sensitivity analyses of each sub-model to reconstruct an overall analysis of the system.

Secondly, we will address how sensitivity analysis integrates into the robust optimization under constraints framework, especially when dealing with a large number of inputs, including uncertain ones.

Thirdly, we will explore the role that sensitivity analysis can play in enhancing the explicability of machine learning (ML) models, thereby serving their intelligibility and auditability. The extensive use of ML models in data-driven AI systems, particularly those subject to new European regulations, requires a deep understanding of the decisions and results provided by these models. This notably involves comprehending the influence of input features on predicted variables and providing global interpretability diagnostics. Strong connections between Explainable AI (XAI) and global sensitivity analysis have been recently highlighted, and constitute an appealing research perspective.

Finally, some software developed by our companies will be presented, and the issues addressed will be illustrated by application cases from our respective sectors (reactor performance analysis, accident transient monitoring, fuel behavior simulation and seismic analysis).

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