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SAMO: oral presentation

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.

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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 $y = f(\mathbf{w}, z)$, where \mathbf{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 $\mathbf{w}_1, \dots, \mathbf{w}_L$, we now study $y = g(l, z) = f(\mathbf{w}_l, z)$. The Sobol' decomposition on g writes simply: $S_l + S_z + S_{lz} = 1$.

We introduce a general clustering function \mathcal{C} such that $\mathcal{C}(l) = c \in 1, \dots, K$ 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 $(l_1^c, \dots, l_{N_c}^c)$ 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: $h(c, z, u) = g(l_{\lfloor u \cdot N_c \rfloor + 1}^c, z)$, 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, \dots, c_K and probabilities p_1, \dots, 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: $\max_{\mathcal{C}(\cdot)} S_c$

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 $S_c = S_l - \frac{1}{V} \sum_{c=1}^K p_c \tilde{V}_c$, where

$\tilde{V}_c = \mathbb{V}_{l \in c} \mathbb{E}_z[g(l, z)]$. 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: $\min_{\mathcal{C}(\cdot)} S_u^T$

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.

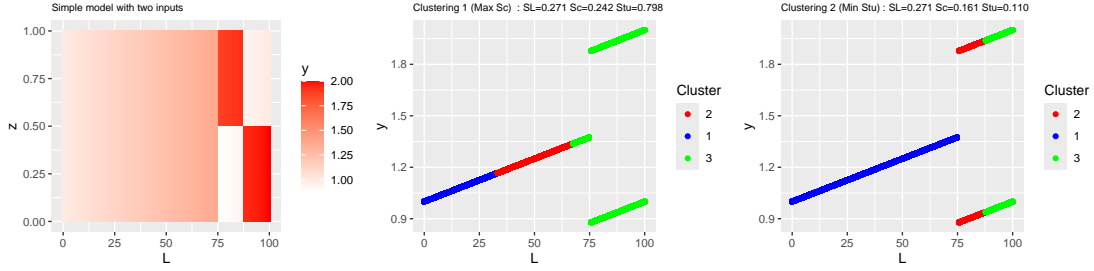


Figure 1: Clustering result of a simple model for the two criteria. Left: model definition; Middle: clustering based on S_c ; Right: clustering based on S_u^T .

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.

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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 θ of a downstream model conditionally on the uncertainty affecting the parameters λ of an upstream model. Consequently, the main challenge for the GSA is to incorporate the residual uncertainty of λ into the definition and estimation of HSIC indices. To deal with this specific bi-level uncertainty framework, addressing the uncertainties conveyed by both θ and λ , 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 θ of a downstream fission gas behavior model while taking into account the uncertainty of the conductivity λ of an upstream thermal model [3].

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

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Adequate representation of hydrological processes is crucial for effective water resource management, particularly in regions where socio-environmental pressures require robust decision making. Hydrological models are key to simulating complex processes such as rainfall-runoff dynamics, groundwater flow and water quality. However, their computational complexity often leads to high costs, especially when undertaking sensitivity and uncertainty analyses, limiting their applicability in large-scale or real-time contexts. To address these challenges, surrogate models offer a promising solution by approximating complex model behaviour and significantly reducing computational demands while maintaining sufficient accuracy.

Surrogate-based sensitivity analysis (SA), which combines surrogate modelling with sensitivity analysis techniques, helps to identify influential parameters for model calibration, validation and uncertainty quantification more efficiently. However, challenges persist in selecting the appropriate surrogate-based SA methods, particularly in balancing model complexity, computational efficiency, and performance.

This study investigates various combinations of surrogate models—such as Gaussian Process Regression (GPR), Random Forest (RF), Polynomial Chaos Expansions (PCE), and Sparse Grids — with sensitivity analysis techniques, including Sobol', Morris, PAWN, and Shapley effects, for general hydrological modelling. These surrogate-based SA methods are compared with direct SA approaches applied to the original hydrological models to evaluate their relative performance in terms of accuracy for screening and ranking and computational efficiency for a given convergence threshold. Model performance is assessed using metrics such as Root Mean Square Error (RMSE), Mean Absolute Error (MAE), R-squared (R^2), and Mean Absolute Percentage Error (MAPE), with various confidence interval techniques ensuring robustness. Training times are recorded to assess computational efficiency, and parameter sweeping is used to explore the smoothness of the response surface.

By comparing surrogate-based SA methods with direct SA, this study provides insights into the strengths and limitations of each approach in hydrological modelling. The findings contribute to the development of more efficient, scalable models for water resource management, with a focus on enhancing the integration of physical and emulation approaches to better manage uncertainties and improve predictive performance. Future research should focus on refining surrogate-based SA methods, improving model specificity, and enhancing the accuracy and efficiency of hydrological predictions.

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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 Lemaitre, 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.

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Global Sensitivity Analysis of Gamma-Ray Spectra in Uranium Logging

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Orano Mining is currently testing the CeBr_3 gamma-ray measuring device developed by ALT (Advanced Logic Technology) to estimate uranium content profile in boreholes. The CeBr_3 probe is a spectrometer that records the energy distribution of incoming gamma rays from naturally occurring radioactive materials. Due to the presence of decay chain disequilibrium in roll-fronts, the need has indeed arisen to go beyond the total gamma count rate to estimate uranium concentration. New approaches are increasingly moving towards the exploitation of the full shape of recorded spectra [1]. However, this shape is not solely determined by uranium content. Geological (apparent density) and drilling (borehole diameter, probe shift from the wall) parameters might also influence it. Moreover, training and testing prediction algorithms calls for the creation of a database of realistic well logs where variables are allowed to vary along the vertical axis. The vast number of potential configurations along with the high computational cost of simulations makes it necessary to reduce the input space through global sensitivity analysis.

This study relies on the simulations of natural gamma-ray spectra using the Monte Carlo Radiation Transport (MCNP) stochastic code. Due to the high number of particle histories to track, running accurate MCNP simulations is computationally expensive, which constrains the

size of the dataset. Given its reliable performance with limited sample sizes, we use the Hilbert-Schmidt Independence Criterion (HSIC) [2] to quantify input-output dependencies. Another one of its advantages, over Sobol indices for example, is that inputs are not assumed independent. Its recent extension to functional outputs based on the truncated functional Principal Component Analysis (fPCA) expansion [3] is particularly well suited for conducting sensitivity analysis on gamma-ray spectra, which are characterized by smooth curves with identifiable patterns. Findings indicate a significant global influence of uranium concentration, borehole parameter and probe position. Formation density has a negligible effect.

A key consideration in industrial applications is interpretability. One advantage of fPCA-based HSIC is to allow examining which input preferentially drives each component. Input influences can thus be interpreted by looking at the global patterns of variation identified by the leading eigenvectors. We observe that the most contributing eigenvector is related to the size of the low-energy bump. This clarifies how the uncovered dependencies are mediated. The influence of uranium content can be linked to the self-absorption effect, and the impact of borehole diameter and probe position to the magnitude of Compton scattering in the medium.

We assess the validity of this interpretation through a second analysis. For each spectrum, we decouple the Compton continuum from the photoelectric peaks. The HSIC is computed for each part separately to determine how each input affects the shape of the spectra. The significant dependencies found between the shape of the Compton continuum and the inputs (apart from density) support the original interpretation.

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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.

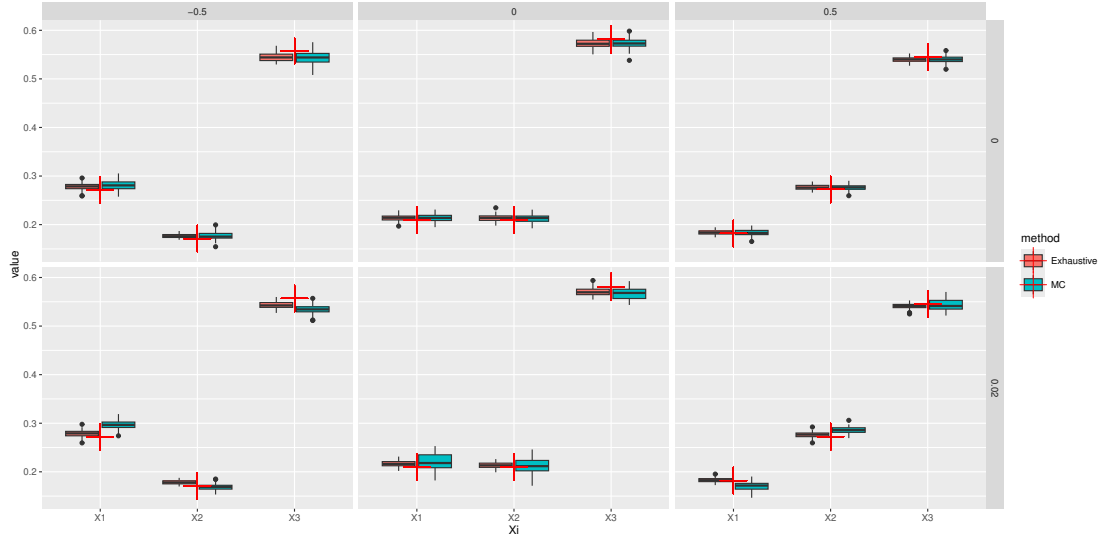


Figure 1: Box-plot on toy example with 100 repetitions. Red cross is ground truth. Red box is estimation from exhaustive search, blue box is our Monte-Carlo approximation result.

Model setting in Fig. 1:

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

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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 $P_f(\Theta_i)_{i=1,\dots,N}$. 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 $P_f(\Theta_i)$, obtaining a new sample density, new input samples and associated model outputs. These new data fit for this particular Θ_i allow us to improve the estimation of $P_f(\Theta_i)$, 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 $P_f(\Theta_i)_{i=1,\dots,N}$. Using multiple importance sampling (mIS) [3], we search for each $P_f(\Theta_i)$ the combination of available data that yields the best probability estimation. mIS does not require additional calls to \mathcal{M} and allow us to potentially improve on all the probability estimations. We repeat this process of selection of $P_f(\Theta_i)$, adapted resampling and mIS until all the $P_f(\Theta_i)_{i=1,\dots,N}$ 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.

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

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Abstract:

In about a decade, software and methodological development have made sensitivity studies viable which were impossible before or too demanding. In particular, in the field of variance-based estimators to carry out global sensitivity analysis (GSA) requiring a given sample design a few strategies such as the use of quasi-Monte Carlo sequences, groups of inputs, and the introduction of higher performing estimators enable to cut significantly the model runs needed to achieve a reasonable level of convergence. Nevertheless, the limit of a strict dependency of the analysis cost on the number of the investigated factors is not overcome and the respect of an input structure is still a major issue.

Very recently, the Authors have proposed a machine learning approach [4] that allows us to estimate Sobol' indices – first-order and total order indices - using an outstanding dynamic adaptive variances estimator starting from a set of Monte Carlo given data.

This estimator with dynamic adaptive variances [2] outperforms standard benchmark with a significant reduction of the model evaluation cost, its implementation is straightforward due to the fact that same formula can be applied for both first-order and total order indices, and it makes it possible to compute sensitivity indices for groups of inputs. However, a very specific sample structure has to be implemented to use it. In fact, the formula with adaptive variances requires four matrices, that is the independent A and B, and the derivative matrices Ab^i and Ba^i respectively resulting from A but the i -th column taken from B, and similarly from matrix B with the i -th column from A.

Therefore, a new machine learning approach has been proposed to create an adequate input to run variance-based sensitivity analysis using the Sobol' estimator with dynamic adaptive variances starting from a given data set. Two ensemble methods, bagging [5] and boosting [1, 7], have been implemented.

The framework implies three fundamental steps:

- Training&Learning: the training set is used to train the learning algorithm. Output of this step is a machine committee.
- A new structured sample is built to estimate sensitivity indices using the Sobol' estimator with dynamic adaptive variances.
- The sensitivity indices are estimated.

Results reported in [4], which were conducted with a set of functions with independent inputs, [3] appear very promising and encouraging.

In this work, the described framework is applied to perform the sensitivity study of the atmospheric dispersion module of the Accident Damage Analysis Module (ADAM) for consequence assessment, developed by the European Commission to support the EU competent authorities for the implementation of the Seveso Directive in their countries or other legislation associated with chemical safety and security. The analysis was conducted referring to three different cases characterised by the same input and a different model response.

The exercise positively confirmed the validity of the machine learning approach proposed by the Authors and the overcoming of the design-sample limitations while keeping all the advantages of the Sobol' radial estimation.

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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 good 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^* is a Nash equilibrium. That is, with payoff functions O_j and action set X_j , a Nash equilibrium is a vector $x^* = (x_1^*, \dots, x_J^*)$ such that for all $j = 1, \dots, J$, x_j^* solves the subproblem

$$\sup_{x_j \in X_j} O_j(x_j, x_{-j}^*),$$

where x_j and x_{-j} denote the action of player j and the other players' actions, respectively. The computation of equilibrium x^* 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^* but also measure how it is sensitive with respect to objective parameters O_j . For a three-player game with two levels of constraints, we count 18 parameters for which we want to understand the sensitivity. 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”.

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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 modified in a minimal manner to respect the external beliefs.

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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.

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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.

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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.

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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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Sensitivity analysis of multi-scale energy power system models

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This paper describes an application of global sensitivity analysis (GSA) in the context of energy power systems modelling. In this application, a multi-scale system is considered, where an overarching model describing the system integrates smaller models that represent various components of that system.

We refer to the overall model as the “macro-model”, and the individual component models as “micro-models”. Notably, macro-models can be significantly more computationally intensive to solve than their corresponding micro-models.

This study explores the relationship between the Sobol’ total sensitivity indices of the micro- and macro-models, specifically within the framework of fixing certain factors to potentially reduce the complexity of the macro-model through GSA on the micro-models [1].

Consider the following set-up, where two micro-models g and h are functions of subsets of input factors \vec{x} and \vec{y} , respectively:

$$z_1 = g(\vec{x}), \quad \vec{x} \in R^n, \quad (1a)$$

$$z_2 = h(\vec{y}), \quad \vec{y} \in R^m \quad (1b)$$

The combined macro-model is expressed as:

$$w = f(z_1, z_2). \quad (2)$$

This macro-model can also be represented as a function of the input vectors \vec{x} and \vec{y} :

$$w = f(g(\vec{x}), h(\vec{y})) = f(\vec{x}, \vec{y}). \quad (3)$$

We assume that \vec{x} and \vec{y} are two uncorrelated random vectors with known probability density functions. The authors in [1] demonstrate that a relationship exists between the Sobol’ total sensitivity indices $T_{x_i}^g$ and $T_{y_i}^h$ of the micro-models (1a) and (1b), and the indices $T_{x_i}^f$ and $T_{y_i}^f$ of the macro-model (3). For certain classes of functions, it can be proven that:

$$T_{x_i}^f \leq T_{x_i}^g \text{ and } T_{y_i}^f \leq T_{y_i}^h \quad (4)$$

If the estimated total sensitivity indices for g and h are found to be small, then, according to (4), the indices of f will be even smaller. Consequently, by performing GSA only on the micro-models, it is possible to reduce the dimensionality of the macro-model by fixing the input(s) with small total

sensitivity indices at a specific value x_i^0 (equivalently, y_i^0). This would lead to an approximation error $\delta(x_i^0)$ such that $\mathbb{E}\delta(x_i^0) = 2T_{x_i}^f$ (see [2]), where:

$$\delta(x_i^0) = \frac{\int [f(x,y) - f(x_{-i}, x_i^0, y)]^2 dx dy}{Var(w)} \quad (5)$$

The approach proposed in [1] is successfully tested on a case study in the domain of power energy systems. The case study aims at evaluating the performance of a protection relay designed to interrupt the flow of current along the circuit when a fault occurs in a 54-km high-voltage submarine transmission line (see Figure 1). The relay is supposed to determine the fault location with satisfactory accuracy so to put in place the necessary countermeasures for quickly clearing the fault and restoring the power supply. If the relay performs well, then the fault location is determined with small uncertainty. It is evident that accurately estimating the location of the fault is crucial, as the time to find and repair the fault becomes critical.

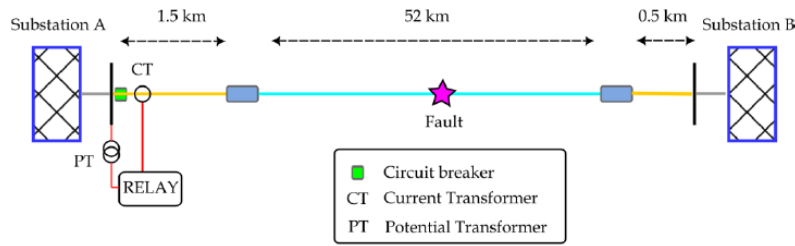


Figure 1: Schematic representation of the transmission power system under study

The metric used for assessing the relay performance, specifically the output of the macro-model, is the fault location error ε , defined as the difference between the actual fault location m and the location \hat{m} recorded by the relay:

$$\varepsilon = m - \hat{m} \quad (6)$$

The input factors are uncertain parameters related to the cross-section and the geometry of the cables.

GSA conducted solely on the micro-models reliably indicates that the output of the macro-model (i.e., the fault location error) is not sensitive to 23 out of the 34 inputs; these can be fixed at any value within their range of variation with the aim of model simplification. Furthermore, GSA reveals additional features of the model.

Applying this comprehensive methodology to the exemplary case study offers practical insights and general guidance on how to adapt the methodology for exploring alternative system models.

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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.

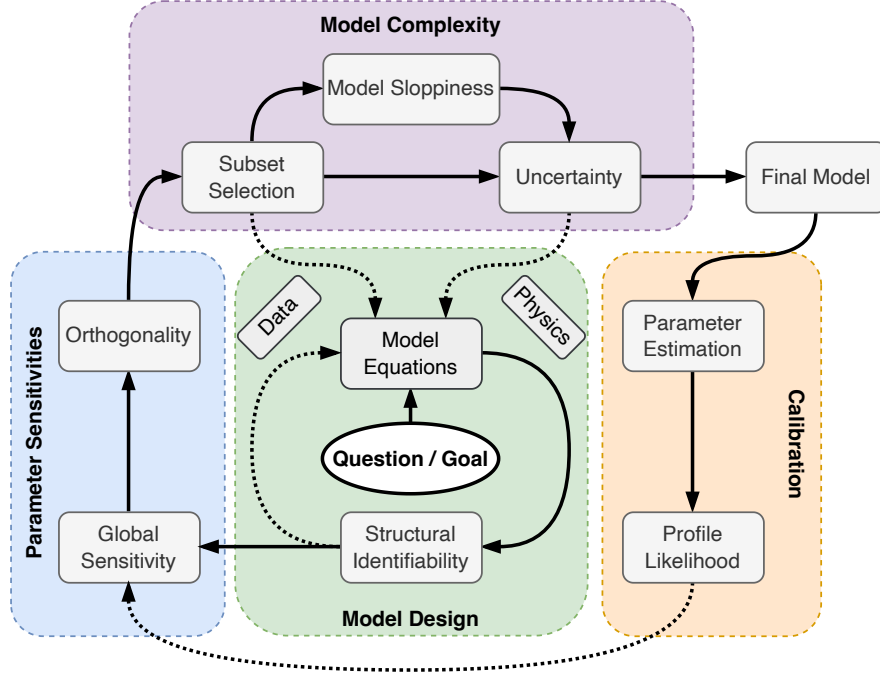


Figure 1: **The Personalisation Process:** Schematic highlighting the vital uncertainty quantification and sensitivity analysis stages involved in the personalisation of a systems biological model.

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.

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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.

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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.

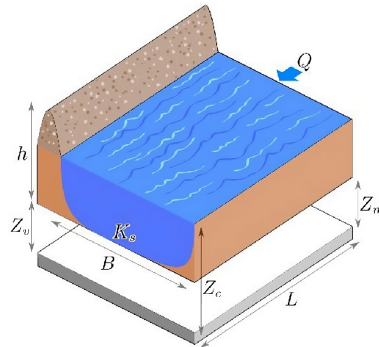


Figure 1: A dyke, a river and variables for flood modeling.

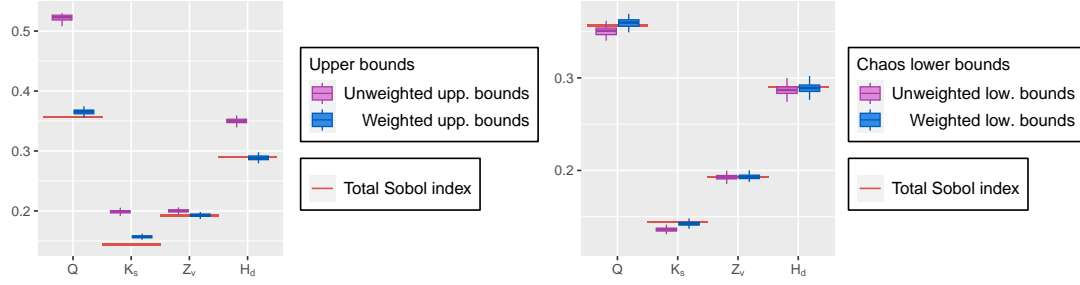


Figure 2: Total Sobol indices and several estimations of their: **(left)** upper bounds with/without a weight, **(right)** lower bounds with/without a weight, associated with variables Q , K_s , Z_v and H_d in the maximal overflow of a river.

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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.

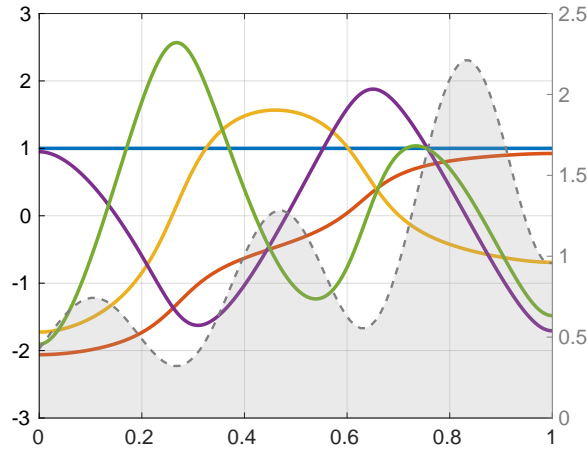


Figure 1: Illustration of the first five eigenfunctions of a one-dimensional Poincaré basis for a distribution with three modes (visualized by the gray area with y-scale on the right-hand side of the plot)

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.

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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 $\text{Mod}_i(\Theta)$ for modes, where $i \in 1, \dots, p$, 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 $\text{Mod}_i(\Theta)$ computed by the simulator are sufficiently close, within predefined thresholds, to the observed frequencies λ_i^* and modes Mod_i^* , derived from experimental data based on Operational Modal Analysis (OMA) (e.g., [3]).

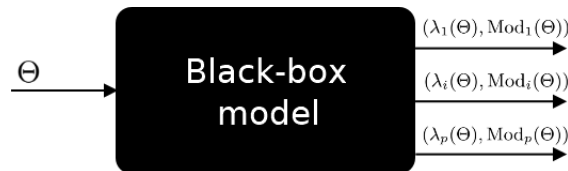


Figure 1: Schematic diagram of the wind turbine simulator.

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

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

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.

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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.

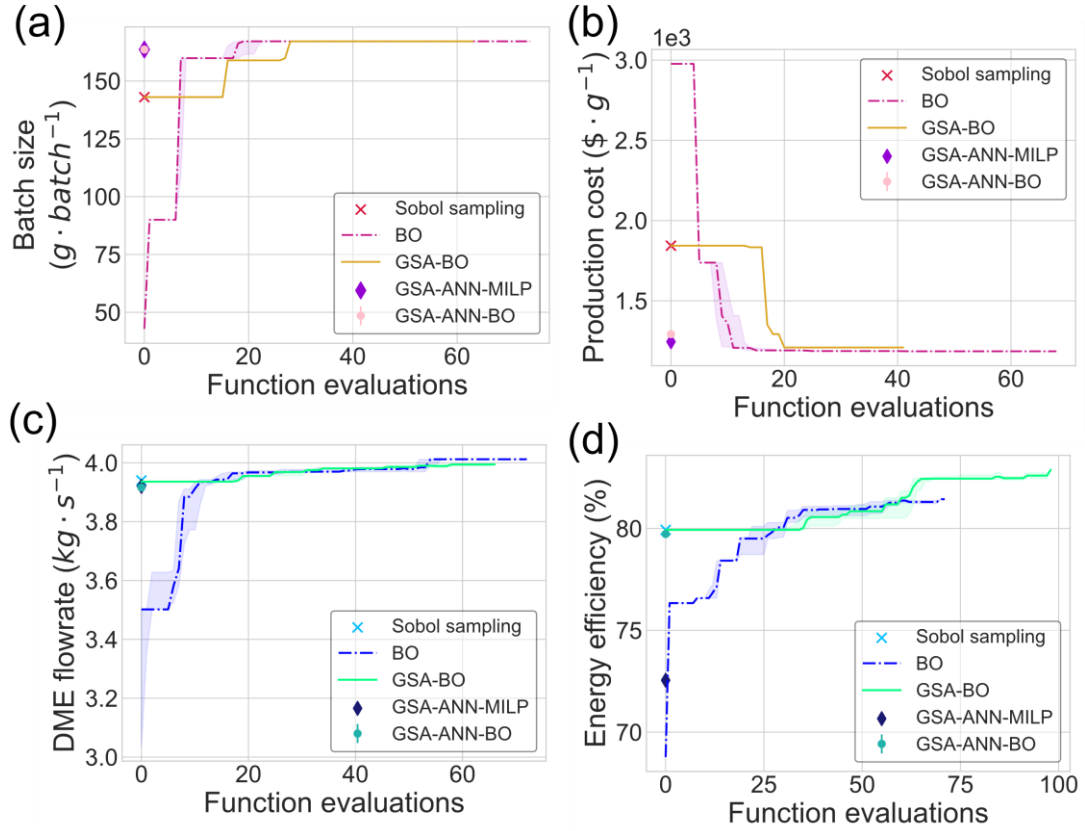


Figure 1. Overview of the optimization methods applied to manufacturing process optimization across the SuperPro Designer (a, b) and Aspen HYSYS (c, d) case studies (adapted from Triantafyllou et al., 2024). The simulation-based approaches include pure Bayesian optimization (BO) and Bayesian optimization 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.

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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 $\gamma \in \mathbb{R}^d$ representing the quantity held in each business line by the (re)insurer.

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

$$\begin{aligned} V_{\alpha}(\gamma) &= \text{VaR}_{\alpha}(-\gamma^T \mathbf{X}) = \min \{ M \in \mathbb{R} : \mathbb{P}(-\gamma^T \mathbf{X} \leq M) \geq \alpha \}, \\ C_{\alpha}(\gamma) &= \text{CVaR}_{\alpha}(-\gamma^T \mathbf{X}) = \mathbb{E}(-\gamma^T \mathbf{X} | -\gamma^T \mathbf{X} \geq V_{\alpha}(\gamma)). \end{aligned}$$

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 $C_{\alpha}(\gamma)$.

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

A new approach was introduced by R.T. Rockafellar and S. Uryasev in 2000 [4] and was later extended by Krokmal 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.

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SAMO: oral presentation

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).

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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.

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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. MLMCV 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.

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

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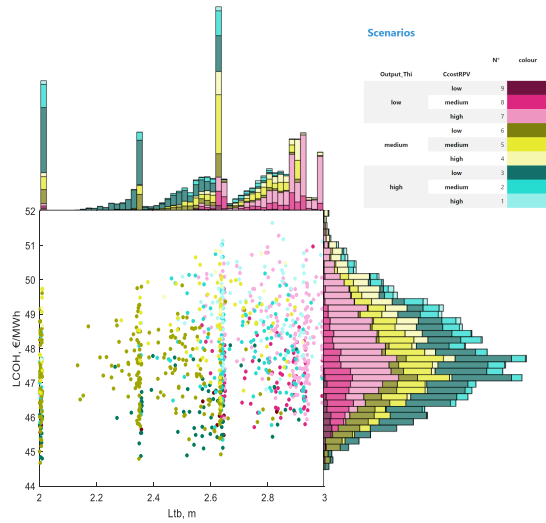
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Global sensitivity analysis (GSA) is undoubtedly a valuable exercise to understand the behavior of a computational model and to devise an effective intervention. Moreover, policies and decisions that were based on a limited comprehension of uncertainty 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 scatter-plot 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.

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

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Abstract:

Variance-based methods to conduct global sensitivity analysis based on sampling design are very popular techniques with a widely consolidated tradition, in particular for their versatility, straightforward interpretation, and easiness of coding.

However, major challenges of these techniques are the number of runs required to achieve an appropriate convergence, which strictly depends on the number of investigated inputs, and the needed independence of the input sample.

In literature, the issue of computing sensitivity indices for models with dependent variables still is not broadly examined. A valid proposal to estimate sensitivity indices for models with dependent variables is introduced in [3] for both first-order and total order indices as a generalization of the Sobol' measures without correlations. Moreover, in [4,5] a set of variance-based sensitivity indices for carrying out a comprehensive study of models with dependent inputs is defined which distinguishes between the mutual dependent contribution and the independent contribution of a variable to the output uncertainty.

A recent comparison among Monte Carlo estimators based on a radial design [1,2], proved some outstanding properties of a new formula where indices are computed over a dynamic adaptive variance specifically estimated for each factor index. Therefore, the estimation involves two independent matrices A and B , and two derived matrices that is the matrix Ab^i , that is equal to A but i -th column which is taken from the i -th column of B , and the matrix Ba^i , which is equal to B but the i -th column from A . In particular, due to its peculiar structure the same formula can be applied for both first-order and total order indices with very similar ranges of convergence. Tested on a broad set of test functions, in most cases, the new algorithm outperforms standard benchmark with a significant reduction of the model evaluation cost.

In this work, following [5], the Authors perform an estimation of the sensitivity indices of correlated input without requiring the knowledge of their conditional probability densities and referring to different sampling-based strategies. The applied method allows an easy non-parametric computation of the sensitivity measures compared to [3] however its computational cost is quite expensive.

Therefore, in order to increase the rate of convergence of the method, a comparative study has been undertaken using different design-based formulas, and in particular the algorithm with dynamic adaptive variance for both first-order and total order indices. The advantages identified/verified and the results referring to a broad set of test functions are reported.

Finally, the approach (method/best formula) has been extended to the computation of the sensitivity indices of groups of inputs. An example is given.

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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 al., 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: $P(Y=1|X) = 1 / (1 + e^{-(\beta_0 + \beta_1 X_1 + \dots + \beta_n X_n)})$ 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: $Y = \beta_0 + \beta_1 X_1 + \dots + \beta_n X_n + \epsilon$ 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: $\phi_i(v) = \sum_{S \subseteq N \setminus \{i\}} (|S|!(n-|S|-1)! / n!) [v(S \cup \{i\}) - v(S)]$ 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.

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General Sensitivity Indices for Hilbert Space-Valued Random Variables

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This paper introduces a family 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.

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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

$$U = (U_1, \dots, U_p) \longrightarrow \Gamma = \{x \in \mathcal{X}, f(x, U) \leq q \text{ and } g(x, U) \leq 0\}.$$

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.

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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 $\rho = (\rho_1, \dots, \rho_d) \in \mathbb{R}^{+d}$ 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 $f : \mathbb{R}^d \rightarrow \mathbb{R}$, for which there exists function of k inputs, $g : \mathbb{R}^k \rightarrow \mathbb{R}$, such that:

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

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 ρ_1, \dots, ρ_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 lengthscale 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_{HSIC}^2 indices [2] demonstrate promising results (see, e.g., Figure 1).

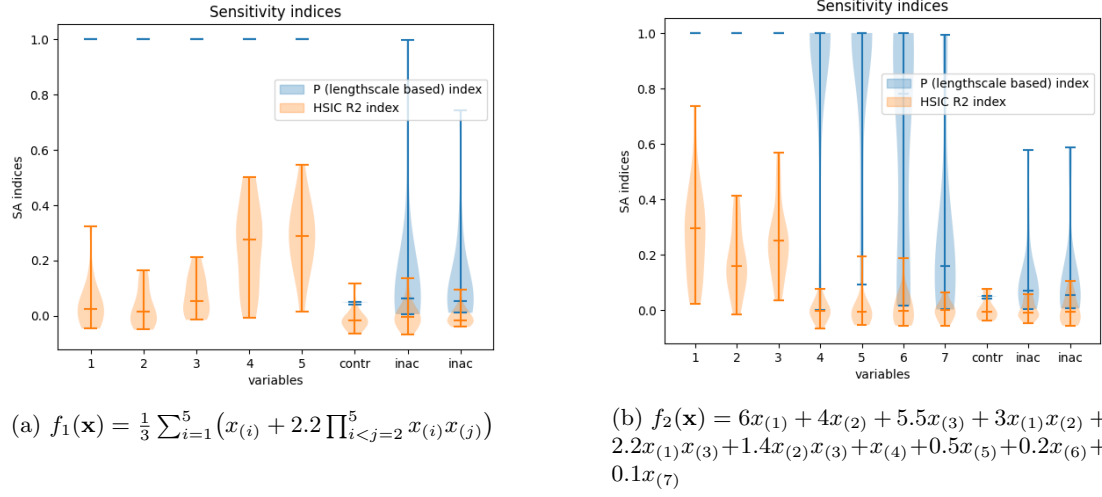


Figure 1: Distributions of the lengthscale-based indices P_i (blue, $\alpha = 5\%$) and the R_{HSIC}^2 indices [2] (orange), providing a comparison of variable importance, with a focus on distinguishing between active $(1, \dots, k)$, control (contr), and inactive (inac) variables, for 20 repetitions 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.

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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 $f : \mathbb{R}^d \rightarrow \mathbb{R}$ have interesting properties when the input variables are independent, such as i) the uniqueness of the decomposition, ii) Sobol' main indices (i.e., S_j s) and interaction indices sum up to one, iii) the Shapley effects of inputs (i.e., Sh_j s 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 , $j = 1, \dots, d$.

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

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

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_j s and their upper-bounds (i.e., dS_j, dS_{T_j}, UB_j) in [13]. Such indices verify

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

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_j s, which represent X_j s 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_j s. The new main, interaction and total DSIs (i.e., DS_j, DS_u, DS_{T_j}) share the following properties:

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

Note that dS_j s are DS_j s 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 $f(\mathbf{X}) = \beta^T \mathbf{X}$ with $\mathbf{X} \sim \mathcal{N}(\mathbf{0}, \Sigma)$. If $\Sigma \in \mathbb{R}^{d \times d}$ has full rank, then

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

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,

$$\begin{aligned} X_j &\stackrel{d}{=} \Sigma_{j,u} (\Sigma_{u,u})^{-1} \mathbf{X}_u + \Sigma_{j|u}^{1/2} Z_j \\ \mathbf{X}_{\sim\{u,j\}} &\stackrel{d}{=} \Sigma_{\sim\{u,j\},u} (\Sigma_{u,u})^{-1} \mathbf{X}_u + \Sigma_{\sim\{u,j\},j|u} \Sigma_{j|u}^{-1/2} Z_j + \mathcal{L}_{\sim\{u,j\}, \sim\{u,j\}} \mathbf{Z}_{\sim\{u,j\}} \end{aligned} \quad \square$$

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

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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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Hoeffding HDMR, Sobol' HDMR and the Shapley Value

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Let $y = f(\mathbf{x})$ be the quantity of interest, function of some predictors $\mathbf{x} = (x_1, \dots, x_d)$, also called features or inputs. We denote $\mathcal{D} = (1, \dots, d)$, \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,

$$f(\mathbf{x}) = f_0^H + \sum_{i_1=1}^d f_{i_1}^H(x_{i_1}) + \sum_{i_2>i_1}^d f_{i_1,i_2}^H(x_{i_1}, x_{i_2}) + \dots + f_{1\dots d}^H(x_1, \dots, x_d) \quad (1)$$

where, $f_0^H = \mathbb{E}[f(\mathbf{x})]$ and $f_{\alpha}^H = \sum_{\beta \subseteq \alpha} (-1)^{|\alpha|-|\beta|} \mathbb{E}[f(\mathbf{x}) | \mathbf{x}_{\beta}]$, $\alpha \subseteq \mathcal{D}$. 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 $f(\mathbf{x})$ or to its variance $\mathbb{V}[f(\mathbf{x})]$ given that they can contribute alone or mutually (due to correlations and interactions). L. Shapley [5] derived some statistic $\phi_i(\mathbf{x})$ 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,

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

and it can be shown that $\phi_i(\mathbf{x}) = \sum_{\alpha \subseteq \mathcal{D}_{+i}} \frac{f_{\alpha}^H(\mathbf{x}_{\alpha})}{|\alpha|}$. Besides, by denoting $\boldsymbol{\phi} = (\phi_1, \dots, \phi_d)$ and $C = \text{Cov}(\boldsymbol{\phi})$ 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 $\mathbf{u} \sim \mathcal{U}(0, 1)^d$, we can write,

$$g(\mathbf{u}) = g_0 + \sum_{i_1=1}^d g_{i_1}(u_{i_1}) + \sum_{i_2>i_1}^d g_{i_1,i_2}(u_{i_1}, u_{i_2}) + \dots + g_{1\dots d}(u_1, \dots, u_d) \quad (3)$$

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

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

where (i_1, \dots, i_d) is an arbitrary ordering of the set $(1, \dots, d)$, F_{i_1} is the marginal cumulative density function (cdf) of x_{i_1} , $F_{\alpha|\beta}$ is the conditional cdf of \mathbf{x}_{α} on \mathbf{x}_{β} with $\alpha \cap \beta = \emptyset$. Obviously, $y = f(\mathbf{x}) = g(\mathbf{u})$, 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],

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

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

$$S_{x_{i_d}}^{ind} = \frac{\mathbb{V}[\mathbb{E}[y|u_{i_d}]]}{\mathbb{V}[y]} = \frac{\mathbb{V}[g_{1\dots d}(u_1, \dots, u_d)]}{\mathbb{V}[y]}, \quad (7)$$

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

$S_{x_{i_1}}$ is the amount of variance explained by x_{i_1} alone including its cooperative contribution due to its dependence on $\mathbf{x}_{\sim i_1}$ while $S_{x_{i_d}}^{ind}$ 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 $\mathbf{x}_{\sim i_1}$ while $ST_{x_{i_d}}^{ind}$ does not take into account contributions due to the dependences of x_{i_d} on $\mathbf{x}_{\sim i_d}$.

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.

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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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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 approach outlined here is particularly suited to situations where training data is sparse, and must be utilised to maximum effect, for example in pharmaceutical production where syntheses may be extremely expensive. This should also prove useful in wider applications, not related to synthesis.

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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.

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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).

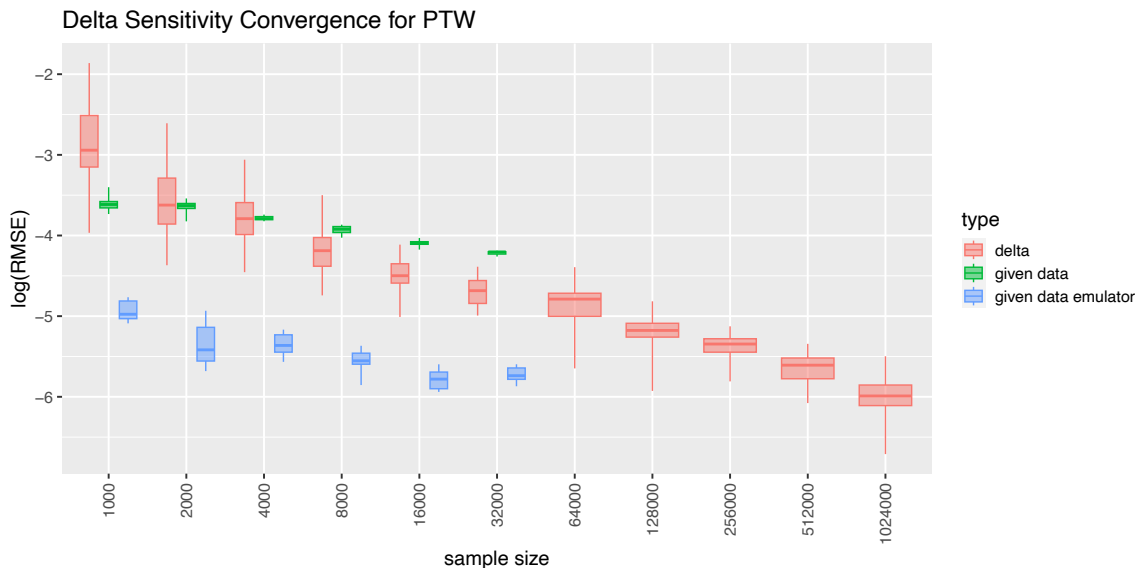


Figure 1: Convergence of three different approaches to calculating delta sensitivity indices for a material strength model called PTW. The emulator approach with given data achieves greater accuracy than the given data approach of python’s SALib (with the same given data).

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].

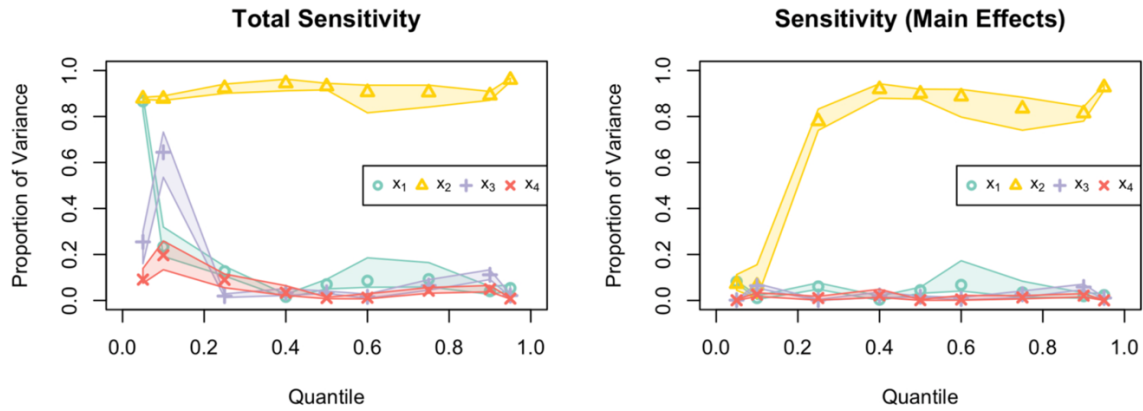


Figure 2: 80% posterior intervals for the Sobol indices of a stochastic SIR model as a function of response quantile. Low quantiles are sensitive to all inputs and their two-way interactions (not shown), but sensitivity in the large quantiles is dominated by x_2 .

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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 $\mathbf{X} = (X_1, \dots, X_d)$: $Y = \mathbf{X}\beta + \varepsilon$ with $\beta \in \mathbb{R}^d$ 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 \mathbf{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*:

- (C₁) *Proper decomposition*: the sum of all shares should be equal to the R^2 ;
- (C₂) *Nonnegativity*: all shares should be nonnegative;
- (C₃) *Exclusion*: if $\beta_j = 0$, then the share of X_j should be zero;
- (C₄) *Inclusion*: if $\beta_j \neq 0$, then the share of X_j should be nonzero;
- (C₅) *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 (C₁) and (C₂) are essential for interpreting VIMs as a percentage of R^2 . Criterion (C₄) is also fundamental to highlight inputs with direct influence. However, (C₅) contradicts the exclusion property (C₃). If the interpretation is focused on the direct influence of the inputs on the model output, then (C₃) is appropriate; if the correlations among data can carry necessary information for the interpretation, (C₅) is relevant instead. In this context, the LMG and Johnson indices favor the (C₅) criterion whereas the PMVD indices (C₃). 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 SRC² 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).

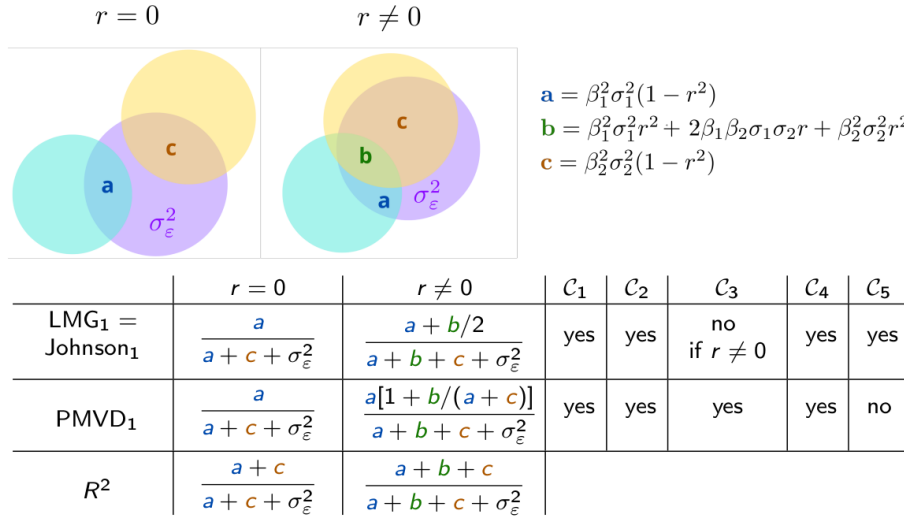


Figure 1: Interpretations of VIMs: Venn diagrams and desirability criteria.

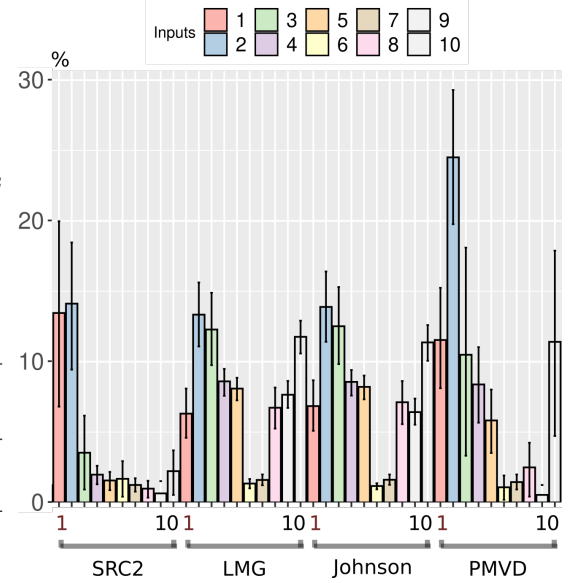


Figure 2: Results on the Ames housing dataset.

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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

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

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] highlights 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-multicollinearity, 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 formal 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.

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SAMO: oral presentation

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.

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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 $I \subseteq \{1, \dots, d\}$, where d is the number of input variables. Then, we write similar *basis-derived* formulas for the pick-freeze estimator of Sobol’ SM $\widehat{S}_I^{\text{c, pf}}(y_\ell(X))$ in function of the normalized matrix-valued pick-freeze estimator of the vector of basis coefficients, as follows:

$$\widehat{S}_I^{\text{c, pf}}(y_\ell(X)) = \frac{v_{\cdot,\ell}^\top \widehat{D}_I^{\text{c, pf}}(c(X)) v_{\cdot,\ell}}{v_{\cdot,\ell}^\top \widehat{\text{Cov}}^{\text{c, pf}}(c(X)) v_{\cdot,\ell}}$$

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 $x_f(t)$.

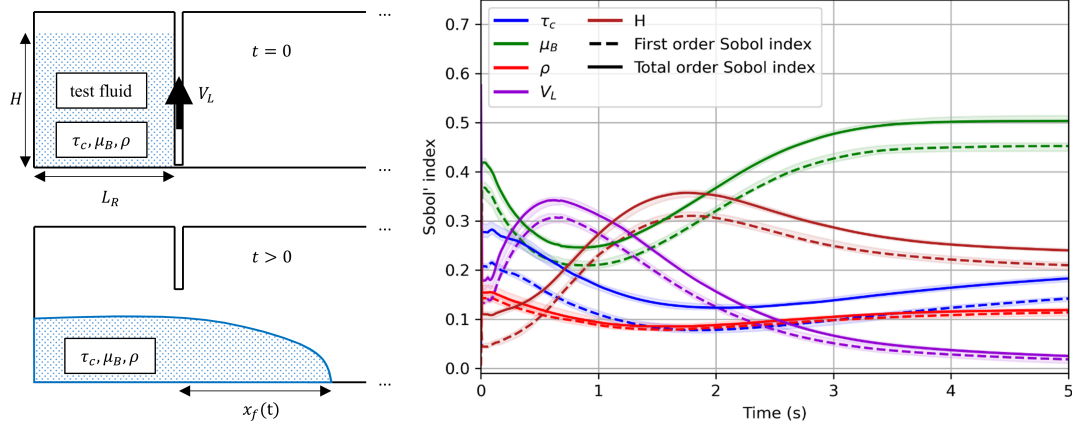


Figure 1: Schematics of the case study (left) and time series of Sobol' indices with associated confidence bounds in shaded colors (right).

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 modelled 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.

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Recent advances in the understanding and implementation of the HSIC-ANOVA decomposition

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For anyone wishing to perform GSA¹ on the output of a black-box model, the ANOVA² 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 HSIC³ 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 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.

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⁴Simulation Analytics and Meta-model-based solutions for Optimization, Uncertainty and Reliability Analysis.

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.

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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.

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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, \dots, X_d are random variables, and a given QoI defined on the output $Y = G(X_1, \dots, X_d)$, 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 $\mathcal{I}(\theta)$ the Fisher information Matrix (FIM) associated to the law of a GP Z_θ with hyper-parameters $\theta \in \Theta$:

$$\mathcal{I}(\theta) = -\mathbb{E} \left[\frac{\partial^2 \ln f_Z(\theta, \mathbf{z})}{\partial \theta \partial \theta^T} \right],$$

where $f_Z(\theta, \cdot)$ is the (gaussian) density of the random process Z_θ , and $\mathbf{z} = [z^{(n)}]_{n=1, \dots, N}$ the vector of observed outputs of the model at design points $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)}$. 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:

$$d_F(\theta_0, \theta_1) = \inf_{\gamma \in \mathcal{P}(\theta_0, \theta_1)} \int_0^1 \sqrt{\dot{\gamma}(t)^T \mathcal{I}(t) \dot{\gamma}(t)} dt,$$

$\mathcal{P}(\theta_0, \theta_1)$ denoting the set of path joining θ_0 to θ_1 .

In this setting, each law at distance δ from the baseline one $f_Z(\theta_0, \cdot)$ can be seen as a perturbed law at level δ . The principle of robustness analysis is then to consider Fisher spheres centered in θ_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.

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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).

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

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.

method	computation time	sensitivity of model decision variable, x_i to model parameters:				
		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

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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 $y = g(\mathbf{x}) : R^d \rightarrow R$ with continuous random inputs, there exists an upper bound for the conditional entropy-based SA indices:

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

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 $l_i = E[\ln |\partial g(\mathbf{x})/\partial x_i|]$. 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.

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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.

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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:

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

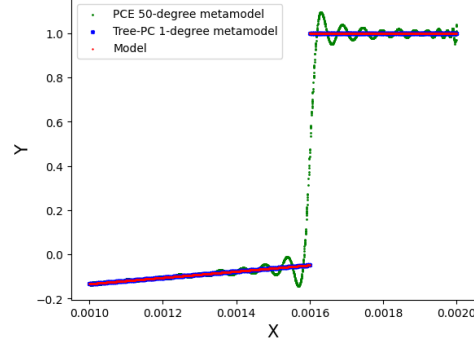
where $\{y_\alpha\}_\alpha$ are the coefficients of Y in the orthonormal basis $\{\Phi_\alpha\}_\alpha$.

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 law 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, Poëtte 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.

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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 robustness 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 robustness of any risk measure with respect to prior assumptions on the input probabilistic model.

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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 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 – to 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.

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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..

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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.

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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 out 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.

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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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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 $x \in \mathbb{R}^d$ is the vector of sensitivity inputs (network parameters).

Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ be the forward sweep that is a function only of the network parameters, and let \mathbf{f} be the its interval extension. Let $[y, \bar{y}]_{i,n}$ 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 $[y, \bar{y}]_{i,n} = \mathbf{f}([x_1, \bar{x}_1], \dots, [x_i, \bar{x}_i]_n, \dots, [x_d, \bar{x}_d])$. The interval-based sensitivity index, for the i -th input, is

$$S_i = 1 - \frac{\sum_n^N [x_i, \bar{x}_i]_n \cdot [y, \bar{y}]_{i,n}}{[y, \bar{y}] \cdot [x_i, \bar{x}_i]}, \quad (1)$$

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, $[x_i, \bar{x}_i]_n$ is the n -th subinterval for the i -th partition, such that $\cup_n^N [x_i, \bar{x}_i]_n = [x_i, \bar{x}_i]$, and $[y, \bar{y}] = \mathbf{f}([x, \bar{x}])$ 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 , $i = 1, \dots, d$ 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 $W^{(1)} \in \mathbb{R}^{1 \times 5}$, $b^{(1)} \in \mathbb{R}^5$, $W^{(2)} \in \mathbb{R}^{5 \times 1}$, $b^{(2)} \in \mathbb{R}$. 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 $d = 16$.

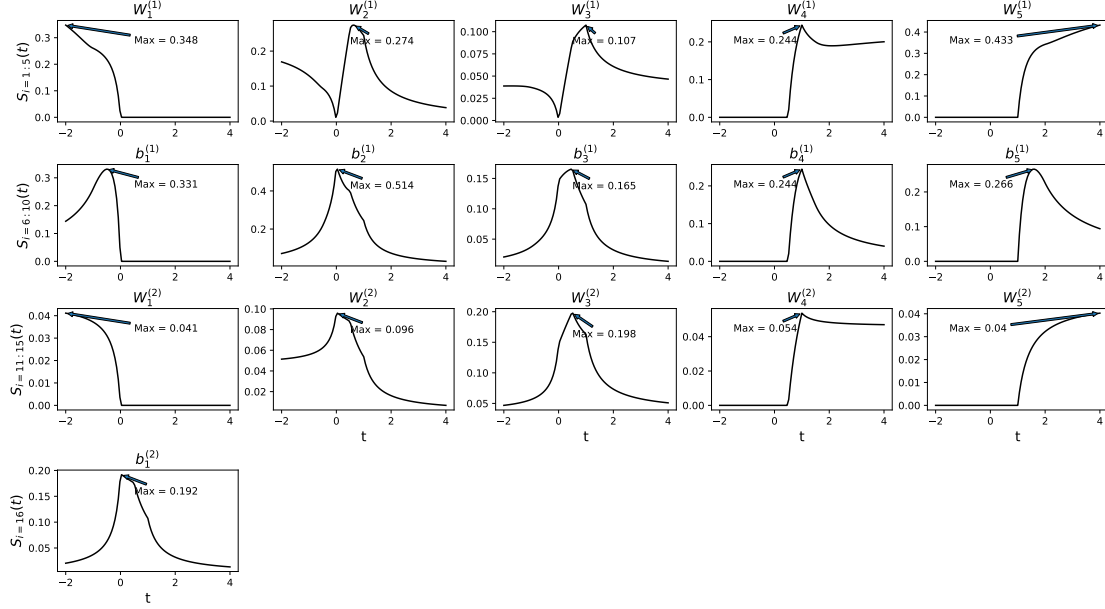


Figure 1: Sensitivity indices across network's input t for $x = (W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)})$.

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.

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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.

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