Fast pick-freeze estimation of sensitivity maps using basis decomposition

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

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

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

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

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

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

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

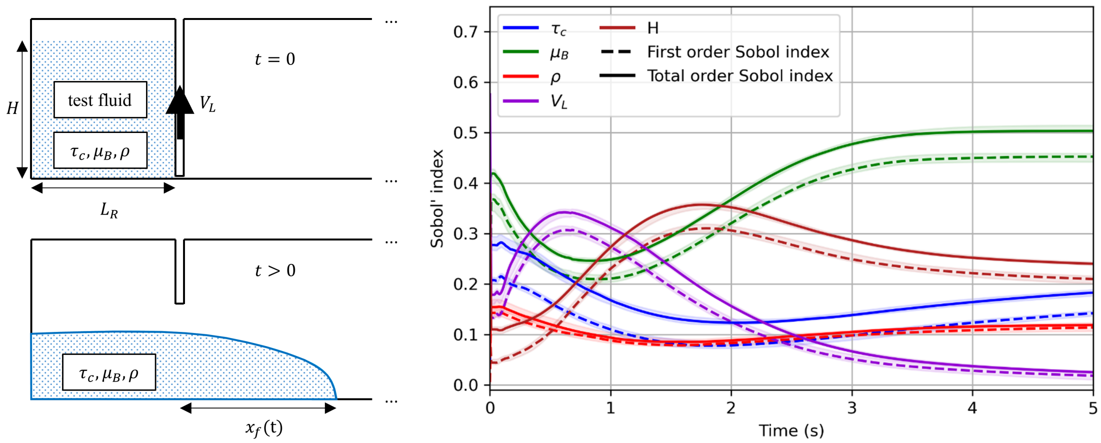

Figure 1: Schematics of the case study (left) and time series of Sobol' indices with associated confidence bounds in shaded colors (right).

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

References:

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

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

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

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

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