New results on Generalized Hoeffding decomposition of numerical models

Marouane Il Idrissi
Université du Québec à Montréal, Institut Intelligence et Données, Montréal, Canada

Nicolas Bousquet, Bertrand Iooss
EDF R&D, SINCLAIR AI Lab, Chatou, France

Fabrice Gamboa, Jean-Michel Loubes
Institut de Mathématiques de Toulouse, Toulouse, France

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

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

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

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

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

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

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

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

In addition, novel sensitivity indices based on this generalized decomposition can be proposed, along with theoretical arguments to justify their relevance. They first highlight that the popular SHAP method to decompose predictions is theoretically sound if and only if the inputs are mutually independent. Besides, they lead to four new indices for quantifying the importance of inputs, based on the variance decomposition of $G(X)$. They allow the disentanglement of effects due to interactions and the effects due to the dependence structure. Such indices will be discussed, and a first illustration of the generalized decomposition involving Bernoulli random inputs, typically used in failure tree modeling in the industrial world, will be presented.

References:

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

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

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

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

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

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

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

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

[Nicolas BOUSQUET; *]*

EDF R&D, SINCLAIR AI Lab, Chatou, France [`nicolas.bousquet@edf.fr` – `https://sinclair-lab.com/`]