Emulation of stochastic simulators using latent polynomial chaos expansions

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Abstract:

Computational models, a.k.a. simulators, are nowadays widely used in engineering to assess the reliability, control the risk and optimize the behavior of complex systems. Classical simulators are usually deterministic, in the sense that repeated model evaluations with the same input parameters always produce the same value of the output quantity of interest (QoI). In contrast, running a *stochastic* simulator with the same input parameters can provide different values of the corresponding QoI. In other words, the QoI of a stochastic simulator is a random variable for a given vector of input parameters. Consequently, repeated model evaluations (called replications) with the same input parameters are necessary to obtain the associated output distribution.

For the purpose of uncertainty quantification, expensive numerical models are usually prohibitive, due to the high computational cost of model evaluations. To circumvent this limit, surrogate models can be constructed to emulate the original model. However, surrogate models that have been successfully developed for deterministic simulators, such as Gaussian processes [5] and polynomial chaos (PC) expansions [1], cannot represent complex stochastic simulators, due to the stochasticity in the output.

To account for the random nature, we extend classical PC expansions by including a latent variable [2, 6] and an additional noise term. More precisely, the surrogate model is expressed as

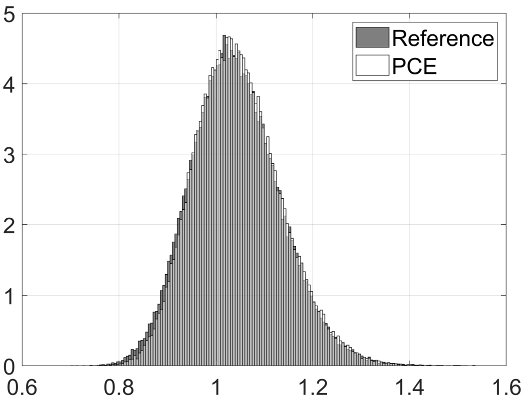
$$Y(\boldsymbol{X}) \overset{\mathrm{d}}{=} \sum_{\boldsymbol{\alpha}\in\mathcal{A}} c_\alpha \Psi_\alpha(\boldsymbol{X}, Z) + \epsilon, \quad \epsilon \sim \mathcal{N}(0,\sigma), \tag{1}$$

where $\boldsymbol{X}$ denotes the set of input variables, Z is the introduced latent variable, ϵ corresponds to the noise term with variance σ^2, $\boldsymbol{\alpha}$ denotes the multi-index defining the PC basis function $\psi_{\boldsymbol{\alpha}}(\boldsymbol{x}, z)$, and $c_{\boldsymbol{\alpha}}$ is the associated coefficient. In the proposed model, Z follows a simple distribution (*e.g.* standard normal or uniform) and is mainly used to mimic the intrinsic randomness of the simulator, whereas ϵ serves as a smoother to make the response PDF bounded and smooth. For $\boldsymbol{X} = \boldsymbol{x}$, the output of such a surrogate is a function of the latent variable with an additive noise. As a result, resampling from the surrogate model is straightforward.

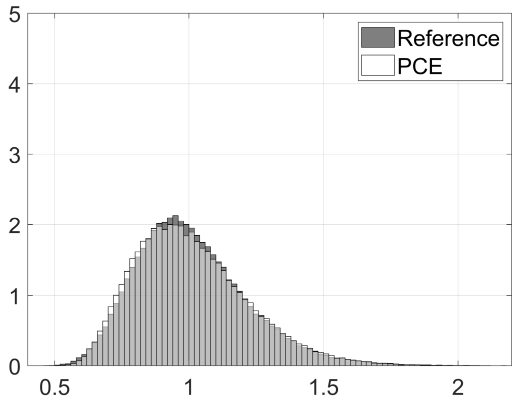
When fitting the model to data, maximum likelihood estimation (MLE) can be used to estimate the PC coefficients $\boldsymbol{c}$ and the noise variance σ^2. However, for $\sigma = 0$ and a certain choice of $\boldsymbol{c}$, the likelihood can attain $+\infty$. To avoid this numerical problem, we suggest treating σ as a hyperparameter. Therefore, we apply MLE to estimate $\boldsymbol{c}$ and cross-validation to select σ. In contrast to a replication-based approach [4], the suggested fitting procedure does not require any replications, *i.e.* any repeated runs of the simulator for the same input parameters.

In this communication, we illustrate the performance of the estimation method on various analytical examples, with a focus on the response PDF approximation accuracy. Moreover, we apply

the developed method to a case study in Asian option payoff [3]. In this application, the drift μ and volatility σ of an asset is considered as input variables. The average asset process at the maturity time is the QoI and represented by the surrogate. As shown in Figure 1, the proposed method demonstrates an accurate approximation of the underlying model.



(a) Response PDF for $\mu = 0.08$ and $\sigma = 0.15$



(b) Response PDF for $\mu = 0.02$ and $\sigma = 0.35$

Figure 1: 2-D Asian option case study–Surrogate built upon $N = 1\,000$ model evaluations.

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Short biography – Xujia Zhu received his engineer degree from Ecole Polytechnique (France) in 2015. He also holds a MSc in computational mechanics from the Technical University of Munich. Since October 2017, he is a Ph.D. student at the Chair of Risk, Safety and Uncertainty Quantification with the thesis entitled "*Surrogate modelling for stochastic simulators using statistical approaches*" funded by the Swiss National Science Foundation.