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Fractional moment estimation from Polynomial Chaos Expansions

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Abstract

In the context of the estimation discrete moments of a response of interest, polynomial chaos expansions (PCE) have been shown to provide a highly efficient and accurate surrogate modelling strategy [1]. Let's assume a probability space $(\Omega, \mathcal{F}, \mathcal{P})$, where Ω is an event space, $\mathcal{F}$ a σ-algebra on Ω and $\mathcal{P}$ a probability measure defined on $\mathcal{F}$. If the input variable of a mathematical model, $Y = \mathcal{M}(X)$, is a random variable $X(\omega), \omega \in \Omega$, the model response $Y(\omega)$ is by definition also a random variable. Assuming that Y has a finite variance, a PCE represents the output variable Y as a function of another random variable ξ with given distribution:

$$Y = \mathcal{M}(X) \approx g^{PCE}(\xi) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^M} \beta_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

and as such represents the function $\mathcal{M}(X)$, which could be an expensive-to-evaluate numerical model, via polynomial expansion, where $\beta_{\boldsymbol{\alpha}}$ are deterministic coefficients and $\Psi_{\boldsymbol{\alpha}}$ are multivariate orthogonal polynomials according to the Askey scheme. The orthonormal nature of the basis, in combination with the specific form of the PCE allow for very efficient post-processing. Indeed, once a PCE approximation is calibrated (e.g., via Least-Angle regression), it is possible to analytically obtain statistical moments or global sensitivity indices of Y at almost no extra computational cost. Generally, a (discrete) statistical moment of the m^{th} order, $\langle Y^m \rangle$, with $m \in \mathbb{N}$ is defined as:

$$\langle Y^m \rangle = \int [g(\boldsymbol{X})]^m p_X(x) dx$$
$$= \sum_{\alpha_1 \in \mathbb{N}^M} \dots \sum_{\alpha_m \in \mathbb{N}^M} \beta_1 \dots \beta_m \int \boldsymbol{\Psi}_{\alpha_1}(\xi) \dots \boldsymbol{\Psi}_{\alpha_m}(\xi) p_\xi(\xi) d\xi.$$

As can be seen from the final part of the formula, in case of PCE, it is necessary to integrate over basis functions (which are orthonormal polynomials), which leads to a dramatic simplification in comparison to the integration of the original mathematical function. Moreover, it is well known that PCE allows for analytical solution of this equation. Besides well-known formulas for mean and variance, higher statistical central moments skewness (3rd moment) and kurtosis (4th moment) can be also obtained using analytical formulas for Legendre and Hermite polynomials [2]. While very powerful to estimate such discrete moments, the estimation of the full distribution of a response of interest, including its tails, is still an open challenge. This makes the method less applicable to for instance the analysis of medium to small failure probabilities in structural systems.

A potential route to estimate the full distribution of a response Y, including its tails, is through the PCE estimation of fractional moments $\langle Y^r \rangle$ of Y, with $r \in \mathbb{R}^+_{\setminus 0}$, as introduced in [3]. Indeed, it can be shown that a fractional moment $\langle Y^r \rangle$ in fact contains an infinite number of integer moments:

$$\langle Y^r \rangle = \sum_{i=1}^{\infty} \binom{r}{i} \mu_Y^{r-i} \left\langle (Y - \mu_Y)^i \right\rangle$$

with i any non-negative integer and $\binom{r}{i}$ a fractional integer operator. This illustrates that fractional moments indeed carry a wealth of information on the stochastic properties of the response variable Y. However, an estimation of these fractional statistical moments of costly mathematical models $\mathcal{M}$ by means of statistical sampling (e.g., following a Monte Carlo Simulation approach) is challenging since it is typically not possible or desirable to create a large experimental design. Therefore, this paper therefore presents a novel approach to allow for an analytical estimation of fractional moments directly from polynomial chaos expansions of a response of interest.

Specifically, the first four statistical moments obtained from deterministic coefficients are used for an estimation of arbitrary fractional moments of Y via Hölder's inequality:

$$\mathbb{E}[|Y|^r] \leq (\mathbb{E}[|Y|^s])^{\frac{r}{s}},$$

where $s \in [1,2,3,4]$ are obtained using a standard PCE. Then, based on the fitting of a highly flexible probability density function (PDF) (as presented in [3]), the full PDF of the response of interest can be determined. It is clear that the error of the approximation grows with the difference $|s - r|$. Therefore, an integer moment $E[|Y|^s]$ that are utilized for the estimation of a fractional moment should be selected as close as possible

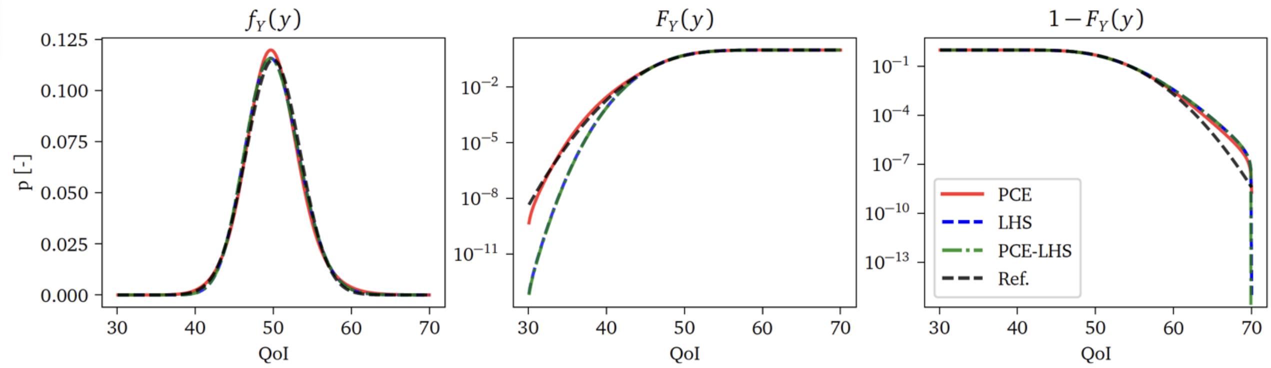

Figure 1. Comparison of the fitted distribution using PCE and LHS

to the selected r. Naturally it is possible to reliably estimate fractional moments only in the interval between integer moments obtained from PCE, i.e., $r \in (1,4)$. Based on the thus estimated fractional moments, further statistical analysis can be performed. For instance, the distribution of Y can be determined in a similar fashion as was proposed in [3].

A toy model is included to illustrate the efficacy of the developed approach. Specifically, a simple analytical function of an input random vector containing three independent Gaussian variables $\boldsymbol{X} \sim \mathcal{N}(\boldsymbol{\mu} = 10, \boldsymbol{\sigma}^2 = 4)$m, namely:

$$Y = 20 + X_1 + X_2 + X_3.$$

Therefore, the quantity of interest is also a Gaussian variable $Y \sim \mathcal{N}(\mu = 50, \sigma^2 = 12)$. The proposed approach is utilized for estimation of the following fractional moments $\langle |Y|^r \rangle$, with $r \in \boldsymbol{r} = [1.1, 1.2, 1.8, 1.9, 2.1, 2.2, 2.9, 3]$. Note that the fractional moments are close to the integer moments obtained analytically from PCE in order to reduce the error of approximation by Hölder's inequality. These obtained fractional moments are then further used for identification of the most suitable probability distribution to represent the stochastic nature of Y, assuming the M-EIGD-LESND that was presented in [3]. The obtained results of the proposed approach are compared to approximation based on standard sampling approach represented by Latin Hypercube Sampling (LHS) containing 200 samples.

Figure 1 illustrates the result obtained with the proposed approach. Although the PCE approach leads to a slight error near the mean value, it leads to almost perfect accuracy at both tails of the CDF. Opposed, LHS is a very efficient method for estimation of mean values, but it has clearly a worse performance in estimation of higher moments affected by tails and thus also fractional moments. Note that although the PCE approach is based on identical samples, it is an approximation of QoI over whole input space and thus its result is less affected by outliers. This fact is also supported by results obtained from LHS sampling using a PCE surrogate model instead of the original mathematical model (PCE-LHS). The results of PCE-LHS are identical to LHS with the original model, which clearly shows that although the surrogate model is accurate, LHS sampling adds additional error to estimated fractional moments and thus it is beneficial to the proposed approach instead of numerical estimation if a trained PCE is available.

Key words: polynomial chaos expansions; fractional moment estimation; statistical analysis, Hölder's inequality

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