Reliability Engineering and System Safety 254 (2025) 110594

Contents lists available at ScienceDirect

Reliability Engineering and System Safety

journal homepage: www.elsevier.com/locate/ress

On fractional moment estimation from polynomial chaos expansion

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ARTICLE INFO

Keywords:
Polynomial chaos expansion
Fractional moments
Statistical analysis
Hölder's inequality

ABSTRACT

Fractional statistical moments are utilized for various tasks of uncertainty quantification, including the estimation of probability distributions. However, an estimation of fractional statistical moments of costly mathematical models by statistical sampling is challenging since it is typically not possible to create a large experimental design due to limitations in computing capacity. This paper presents a novel approach for the analytical estimation of fractional moments, directly from polynomial chaos expansions. Specifically, the first four statistical moments obtained from the deterministic coefficients of polynomial chaos expansion are used for an estimation of arbitrary fractional moments via Hölder's inequality. The proposed approach is utilized for an estimation of statistical moments and probability distributions in four numerical examples of increasing complexity. Obtained results show that the proposed approach achieves a superior performance in estimating the distribution of the response, in comparison to a standard Latin hypercube sampling in the presented examples.

1. Introduction

Mathematical models of the response $\mathbf{Y}$ of physical systems can be generally represented by functions $\mathcal{M}$ of input vectors $\mathbf{X}$, which provide a mapping $\mathcal{M}\ :\ \mathbb{R}^{n_x} \mapsto \mathbb{R}^{n_y}$, $\mathbf{X} \rightarrow \mathbf{Y}$. Input variables $\mathbf{X}$ representing physical quantities (e.g. material parameters, geometrical properties, applied loads) may be affected by a certain level of uncertainty. Therefore, it is necessary to propagate the uncertainty associated with input variables described by specific probability distributions through the mathematical model in order to obtain realistic results predicting the model's response $\mathbf{Y}$ and its uncertainty. The task of the analyst is then in this case to perform uncertainty quantification (UQ) of the model response $\mathbf{Y}$, also called quantity of interest (QoI). In the simplest case, UQ can be based on pseudo-random sampling of the input random vector and performing corresponding repetitive evaluations of the deterministic model $\mathcal{M}(\mathbf{X})$. Obtained set of results can be further statistically processed to get statistical moments, and ultimately probability distribution of the QoI. The estimation of probability distribution function (PDF) or cumulative distribution function (CDF) from given set of statistical moments is not a trivial task and thus, there are various specialized methods for this purpose. On the one hand, it is possible to assume a known specific family of probability distributions and fit a PDF to given data. Although this is a simple approach requiring typically low number of statistical samples, an assumption of a probability distribution may significantly affects obtained results in further steps of UQ and/or reliability analysis. On top, it inherently introduces a measure of subjectivity into the analysis, which might not be warranted for critical applications. On the other hand, one can construct an arbitrary distribution function numerically, e.g. by kernel density estimation [1]. Numerically constructed distributions offer high versatility, though it is typically necessary to optimize hyper-parameters associated with them. Usually, an optimal balance between numerical efficiency and flexibility is offered by artificial distribution models parameterized by statistical moments. Classic representatives of parameterized distributions are Gram–Charlier expansion or Edgeworth series expansion based on perturbation of a Gaussian probability distribution. Unfortunately, it is well-known that both distributions have severe limitations in their flexibility and their convergence is not guaranteed for general distributions [2]. More recent developments offer for example three-parameter lognormal distribution [3], Hermite model [4], cubic normal distribution [5], generalized lambda distribution [6] or distribution functions that are parameterized by a higher number of moments or even fractional moments [7]. In this paper, we adopt the M-EIGD-LESND function, which is in essence a mixture of an extended inverse Gaussian distribution and a log extended skew-normal distribution (note that underlined letters explain the acronym M-EIGD-LESND). It is fully characterized by a set of eight parameters, making it highly flexible, and hence, powerful to fit any type of distribution on $\mathbf{Y}$.

Despite the flexibility of the approaches described above, they require a significant number of samples to allow them to represent

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https://doi.org/10.1016/j.ress.2024.110594
Received 9 April 2024; Received in revised form 11 October 2024; Accepted 16 October 2024
Available online 22 October 2024
0951-8320/

the *real* distribution of $\mathbf{Y}$ accurately. Unfortunately, a combination of sampling-based methods with costly mathematical models is highly time-consuming or even not feasible in industrial applications and surrogate models are often utilized as computationally efficient approximations of the original mathematical model. There are various types of surrogate models (e.g. artificial neural networks, Kriging, support vector machines), with polynomial chaos expansion (PCE) being a very popular method for UQ. PCE was originally proposed by Norbert Wiener [8] and further investigated in the context of engineering problems by many researchers, e.g. [9,10], and it provides an efficient tool for estimation of statistical moments and sensitivity indices. Especially the PCE in its non-intrusive form (spectral projection and regression) possesses significant potential for industrial applications, since it offers a convenient way to perform advanced probabilistic analysis of any black-box model without any modifications of existing numerical solvers. In practice, it becomes often necessary to employ sparse PCEs that yield efficient solutions for real-world physical systems. Regression-based non-intrusive PCE [11] offers large variety of solvers [12], sampling schemes [13–16] and adaptive algorithms [17–20] leading to a large variety of methods. Once a PCE is available for a given mathematical model, the constructed explicit function can be exploited to obtain additional information about that model. This information includes integer statistical moments [9], probability distribution of QoI or sensitivity indices [6,21], which can be calculated without additional evaluations of the underlying numerical model $\mathcal{M}$, which is especially beneficial in industrial applications [22,23]. Therefore PCE is especially suitable for its relative computational efficiency in training and usefulness for UQ tasks including moment estimation and sensitivity index computation, which derive from its orthogonality properties with respect to the probability measures of the input variables.

Despite many recent advances in the field of PCE, the challenge of estimating the distribution of $\mathbf{Y}$, especially in its tails, is still open. A particularly interesting route to estimate this distribution is through the estimation of fractional moments of $\mathbf{Y}$, since it can be shown that they carry information about an infinite number of integer moments [7]. This, in its turn, could potentially allow for a more accurate estimation of the distribution of $\mathbb{Y}$ following a moment matching procedure, see e.g. [24]. Although there are several methods for estimation of fractional moments by direct sampling of the mathematical model [25,26], they might be too costly in case of complex stochastic analysis including sensitivity and moment analysis. In this case, it is often preferred to create a surrogate model which can be efficiently analyzed in order to obtain various characteristics of quantity of interest. This paper is therefore focused on estimation of fractional moments directly from PCE, and their further utilization for an approximation of probability distribution of QoI by adopting a recently proposed distribution parameterized by fractional moments. The proposed approach thus further extends broad pallet of methods for post-processing of PCE surrogate models allowing for extensive analysis of the approximated quantity. Section 2 gives a brief introduction of the main mathematical concepts concerning PCE that are required to understand the developments later in the paper. Section 3 introduces the concept of fractional moments, and how they can be estimated analytically from a trained PCE. Section 4 illustrates the developments and their efficacy using three numerical examples, ranging from an analytical function, over a finite element model of a plate in bending, to a dynamically loaded mass–spring system and a confined seepage problem. Section 6 lists the conclusions of the work.

2. Polynomial chaos expansion

Assume a probability space $(\Omega, \mathcal{F}, \mathcal{P})$, where Ω is an event space, $\mathcal{F}$ is a σ-algebra on Ω and $\mathcal{P}$ is a probability measure on $\mathcal{F}$. If the input variable of a mathematical model, $\mathcal{M}$, is a random variable $X(\omega), \omega \in \Omega$, the model response $Y(\omega)$ is also a random variable. Assuming that Y has a finite variance, PCE represents the output variable Y as a function of an another random variable ξ called the *germ* with given distribution

$$Y = \mathcal{M}(X) = g^{PCE}(\xi), \tag{1}$$

and representing the function $\mathcal{M}(X)$ via polynomial expansion in a manner similar to the Fourier series of a periodic signal. A set of polynomials, orthogonal with respect to the distribution of the germ, are used as a basis of the Hilbert space $L^2\ (\Omega, \mathcal{F}, \mathcal{P})$ of all real-valued random variables of finite variance, where $\mathcal{P}$ takes over the meaning of the probability distribution. The orthogonality condition for all $j \neq k$ is given by the inner product of $L^2\ (\Omega, \mathcal{F}, \mathcal{P})$ defined for any two functions ψ_j and ψ_k with respect to the weight function p_ξ (probability density function of ξ) as:

$$\langle \psi_j, \psi_k \rangle = \int \psi_j(\xi)\psi_k(\xi)p_\xi(\xi)\, \mathrm{d}\xi = 0. \tag{2}$$

This means that there are specific orthogonal polynomials associated with the corresponding distribution of the germ via its weighting function. For example, Hermite polynomials orthogonal to the Gaussian measure are associated with normally distributed germs. Orthogonal polynomials corresponding to other distributions can be chosen according to Wiener-Askey scheme [27]. For further processing, it is beneficial to use normalized polynomials (orthonormal), where the inner product is equal to the Kronecker delta δ_{jk}, i.e. $\delta_{jk} = 1$ if and only if $j = k$, and $\delta_{jk} = 0$ otherwise:

$$\langle \psi_j, \psi_k \rangle = \delta_{jk}. \tag{3}$$

In the case of $\boldsymbol{X}$ and $\boldsymbol{\xi}$ being vectors containing M independent random variables, the polynomial $\Psi(\boldsymbol{\xi})$ is multivariate and it is built up as a tensor product of univariate orthogonal polynomials as

$$\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \prod_{i=1}^{M} \psi_{\alpha_i}(\xi_i), \tag{4}$$

where $\boldsymbol{\alpha} \in \mathbb{N}^M$ is a set of integers called the *multi-index*. The quantity of interest (QoI), i.e., the response of the mathematical model $Y = g(\boldsymbol{X})$, can then be represented, according to Ghanem and Spanos [10], as

$$Y = \mathcal{M}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^M} \beta_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}), \tag{5}$$

where $\beta_{\boldsymbol{\alpha}}$ are deterministic coefficients and $\Psi_{\boldsymbol{\alpha}}$ are multivariate orthogonal polynomials.

The main step in the solution procedure of determining the relation in Eq. (5) is to determine the deterministic coefficients $\beta_{\boldsymbol{\alpha}}$ to provide an accurate estimator. In a practical context, an analyst usually only has access to input–output pairs that are generated by $\mathcal{M}$, rather than the full internal solver machinery (such as, e.g., mass or stiffness matrices). Therefore, without losing generality, the rest of the text focuses on non-intrusive forms of PCE. Nonetheless, note that the ensuing developments are equally applicable to the intrusive PCE formulations.

For practical computation, PCE expressed in Eq. (5) must be truncated to a finite number of terms P. Although it is generally possible to create a basis set using a tensor product of 1D polynomials, it leads to an extremely high number of basis functions. This in its turn leads to a slow convergence of PCE construction. Therefore, the truncation is commonly achieved by retaining only terms whose total degree $|\boldsymbol{\alpha}|$ is less than, or equal to a given p.

Moreover, in engineering applications, it is beneficial to prefer only basis functions with lower-order interaction terms. This reduction of basis set is motivated by sparsity-of-effects principle, which states that a physical system is mostly affected only by main effects and low-order interactions. Therefore, it was proposed by Blatman and Sudret [11] to create a PCE basis by a *hyperbolic* truncation scheme:

$$\mathcal{A}^{M,p,q} = \left\{ \boldsymbol{\alpha} \in \mathbb{N}^M \,:\, \|\boldsymbol{\alpha}\|_q \equiv \left(\sum_{i=1}^{M} \alpha_i^q \right)^{1/q} \leq p \right\}. \tag{6}$$

Using this truncation scheme can be graphically represented by selection of terms under the hyperbola parameterized by $q < 1$. Such an approach leads to a dramatic reduction in the cardinality of the truncated set for high total polynomial orders p and high dimensions M.

Note that the number of terms P is highly dependent on the number of input random variables M and the maximum total degree of polynomials p. Estimation of $\boldsymbol{\beta}$ by regression then needs at least the number of samples $\mathcal{O}(P \ln(P))$ for stable solution [16,28]. Therefore, in case of a large stochastic model, the problem can become computationally highly demanding. However, one can utilize advanced model selection algorithms such as Least Angle Regression (LAR) [29] to find an optimal set of PCE terms and thus reduce the number of samples needed to compute the unknown coefficients if the true coefficient vector is sparse or compressible as proposed by Blatman and Sudret [11]. Note that beside LAR, there are other best model selection algorithms such as orthogonal matching pursuit [30] or Bayesian compressive sensing [31] with comparable numerical results.

2.1. Post-processing of PCE

The specific form of PCE together with the orthogonality of the polynomials allows for a powerful and efficient post-processing. Once a PCE approximation is created, it is possible to analytically obtain statistical moments or sensitivity indices of the QoI. Generally, a statistical moment of mth order is defined as:

$$\begin{aligned}\langle Y^m \rangle &= \int \left[g(\mathbf{X})\right]^m p_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} = \int \Big[\sum_{\alpha \in \mathbb{N}^M} \beta_\alpha \Psi_\alpha(\xi)\Big]^m p_\xi(\xi) d\xi \\ &= \int \sum_{\alpha_1 \in \mathbb{N}^M} \dots \sum_{\alpha_m \in \mathbb{N}^M} \beta_{\alpha_1} \dots \beta_{\alpha_m} \Psi_{\alpha_1}(\xi) \dots \Psi_{\alpha_m}(\xi) p_\xi(\xi) d\xi \\ &= \sum_{\alpha_1 \in \mathbb{N}^M} \dots \sum_{\alpha_m \in \mathbb{N}^M} \beta_{\alpha_1} \dots \beta_{\alpha_m} \int \Psi_{\alpha_1}(\xi) \dots \Psi_{\alpha_m}(\xi) p_\xi(\xi) d\xi.\end{aligned}$$

As can be seen from the final part of the formula, in case of PCE, it is necessary to integrate over basis functions (orthonormal polynomials), which leads to dramatic simplification in comparison to the integration of the original mathematical function. Moreover, it is well known that PCE allows for analytical solution of the associated integral. Besides well known formulas for mean ($\mu_Y = \beta_0$) and variance ($\sigma_Y^2 = \sum_{\alpha \in \mathcal{A}} \beta_\alpha^2 - \beta_0^2$), higher statistical central moments skewness γ_Y (3rd moment) and kurtosis κ_Y (4th moment) can be also obtained using analytical formulas for Legendre and Hermite polynomials [21]. Note that PCE is in the identical form as Hoeffding–Sobol decomposition of a function and thus it is possible to easily derive also conditional variances of any order and corresponding Sobol indices [9,32].

Finally, the PCE approximation can be also exploited for an estimation of a probability distribution of QoI. A first possible approach to build the PDF of QoI consists in directly evaluating a PCE for a large number of samples of input random vector and processing of the corresponding results by kernel density estimation (KDE) [33]. Although the combination of PCE and KDE is often utilized for UQ [34,35], it might be complicated to selected appropriate kernel function and band-width hyper-parameter leading to accurate identification of PDF.

A second general approach, further extended in this study, is based on approximations of PDF/CDF by analytical functions parameterized by statistical moments derived directly from PCE. Analytical forms of distribution functions offer significant benefit for UQ, e.g. sensitivity measures based on conditional distributions and thus it is often preferred over numerical solutions. A simple approximation can be in form of Gram–Charlier (G–C) expansion or similar Edgeworth series containing one more Hermite polynomial than G–C, both based on the first four statistical moments [2]. Similarly as in case of Sobol indices, conditional distributions can be easily obtained from PCE [36] as well as advanced distribution-based sensitivity indices [21,37]. The analytical approach has also three main drawbacks: flexibility of analytical approximations of PDF/CDF is typically limited, analytical formulas for direct estimation of statistical moments from PCE are known only for some polynomials. Moreover it is computationally efficient to estimate only the first four statistical moments, which significantly limits utilization of the advanced analytical PDF approximations typically based on higher number of statistical moments.

3. Fractional moments from polynomial chaos expansion

In this section, we introduce our proposed method to determine the probability density function $f_Y(y)$ of a random variable Y based on the post-processing of the PCE in the form of fractional moments. Recall in this context that the rth absolute fractional moment of the random variable Y is defined as [38]:

$$\mathbb{E}\left[|Y|^r\right] = \int_{-\infty}^{\infty} |y|^r \ f_Y(y) \ dy, \tag{7}$$

where r can be any real number. Clearly, when r in Eq. (7) takes an integer value, the equation reduces again to the description of a general moment, making Eq. (7) in essence a generalization of the well-known concept of statistical moments.

The main advantage of working with fractional moments, is that $\mathbb{E}\left[|Y|^r\right]$ carries information about an infinite number of discrete moments. This can be understood by first performing a Taylor series expansion of $|Y|^r$ around its mean value $\mu_Y = E[|Y|]$:

$$|Y|^r = \sum_{i=0}^{\infty} \binom{r}{i} \mu_y^{(r-i)} \left(y - \mu_Y\right)^i, \tag{8}$$

with i any non-negative integer, $\mu_y^{(r-i)}$ the expected value of $|Y|^{(r-i)}$ and the fractional binomial $\binom{r}{i}$ given by:

$$\binom{r}{i} = \frac{r(r-1)(r-2)\dots(r-i+1)}{i(i-1)(i-2)\dots 1}. \tag{9}$$

Taking the expectation of both sides of Eq. (8) yields:

$$\mathbb{E}\left[|Y|^r\right] = \sum_{i=0}^{\infty} \binom{r}{i} \mu_y^{(r-i)} \mathbb{E}\left[\left(y - \mu_Y\right)^i\right], \tag{10}$$

from which can be seen that the right-hand side indeed contains an infinite number $i = 1, \dots, \infty$ of integer moments while the left-hand side of the equation is the rth fractional moment of Y. In this equation, the term $\binom{r}{i}\mu_y^{(r-i)}$ can be thought of as a sort of weight that is assigned to the integer moment in the series expansion that describes the fractional moment. In this context, observe that when i is fixed, $\binom{r}{i}\mu_y^{(r-i)}$ increases as r increases, whereas when r is fixed, the value of $\binom{r}{i}\mu_y^{(r-i)}$ decreases when i increases. This indicates that the higher the fractional order r, the greater the contribution of higher-order integer moments to the rth fractional moment value. To effectively estimate $f_Y(y)$ from the PCE, it is as such important to estimate higher-order fractional moments. At the same time, it is important to keep in mind that these higher-order fractional moments are much more difficult to obtain than lower-order fractional moments. This trade-off needs to be addressed case-by-case when applying the proposed technique.

3.1. Estimation of the fractional moments via Hölder's inequality

Direct numerical estimation of fractional moments by Monte Carlo approach could be computationally expensive, especially in engineering applications. However, the estimation can be significantly accelerated by approximation in form of Hölder's inequality:

$$\mathbb{E}\left[|Y|^r\right] \leqslant \left(\mathbb{E}\left[|Y|^s\right]\right)^{\frac{r}{s}}. \tag{11}$$

Hölder's inequality is often utilized for estimation of error bounds in various applications of theory of probability, however it can be also utilized for an efficient estimation of fractional moments from standard integer statistical moments.

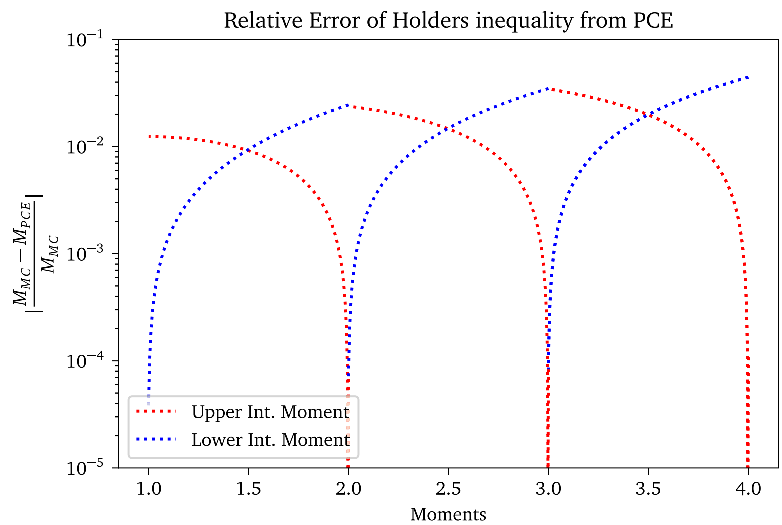

Fig. 1. Error analysis of the moments derived from PCE using Hölder's inequality.

However, it might be still computationally expensive to estimate higher integer moments by crude Monte Carlo methods. Therefore we propose to combine Hölder's inequality with PCE surrogate model, as the latter is well-known for an accurate and an efficient statistical analysis of QoI. Such approach should be significantly more stable in comparison to sampling methods, since the first four statistical moments can be obtained analytically from PCE coefficients, i.e. $s \in [1, 2, 3, 4]$. It is clear that the error of the approximation grows with the difference $|s - r|$. Therefore, an integer moment $\mathbb{E}\left[|Y|^s\right]$ utilized for the estimation of a fractional moment should be selected as close as possible to the selected r. Note that Hölder's inequality according to Eq. (11) is valid only for $1 < r < s < \infty$ and thus, for the sake of clarity, it is necessary to use Eq. (12), if the nearest integer moment $s > r$:

$$\mathbb{E}\left[|Y|^s\right] \geqslant \left(\mathbb{E}\left[|Y|^r\right]\right)^{\frac{s}{r}}. \tag{12}$$

Naturally it is possible to reliably estimate fractional moments only in the interval between integer moments obtained from PCE, i.e. $r \in (1, 4)$. The error caused by Hölder's inequality can be seen in Fig. 1 presenting a typical behavior of the algorithm (M_{PCE} and M_{MC} are moments estimated from PCE and by Monte Carlo sampling respectively). It can be seen, that the relative error is growing with a distance from integer moments. From the figure, it is also clear it is beneficial to use the closest integer moment for the derivation of a fractional moment. The red and blue lines represent estimations based on upper and lower integer moments. The numerical results were obtained from the first example presented in the next section.

The proposed framework has several benefits in comparison to standard approach based on statistical sampling. First of all, fractional moments are obtained from PCE without additional sampling as a part of analytical post-processing (including statistical and sensitivity analysis). The computational cost of the whole process is thus associated to construction of a surrogate model which can be further used for additional tasks in contrary to a standard approach. Moreover, the analytical post-processing could be more stable as will be investigated in the first numerical example. Naturally, the proposed approach is highly sensitive to an accuracy of the surrogate model affected by various sources, and thus one could use various advanced algorithms for construction of PCE, e.g. sparse solvers [12], domain decompositions [39,40], active learning [18,20] or recently proposed physics-informed PCE [41,42]. Moreover, one can easily use the proposed approach to derive also conditional fractional moments similarly as in the commonly used approach for integer-moments based sensitivity analysis [9,21]. Comparison to standard numerical methods will be presented also in Discussion section.

3.2. Description of the PDF based on the fractional moments

Fractional moments are especially important for estimation of the most suitable probability distribution of the QoI. Although it might be sufficient to fit a selected well-known distribution in simple applications, artificial distributions parameterized by statistical moments are more flexible and can capture more complicated shapes of probability distributions. Some of the simplest parameterized distributions are the Gram–Charlier expansion or Edgeworth series based on perturbation of Gaussian distribution exploiting information from the first four statistical moments [2]. It was shown, that Gram–Charlier expansion is efficient especially in combination with PCE, since we can obtain necessary statistical moments analytically [21]. However, once the fractional moments are estimated directly from PCE, it is possible to use more advanced and flexible distribution models such as recently proposed mixture of extended inverse Gaussian and log extended skew-normal distributions (M-EIGD-LESND) [7], which is described as:

$$\begin{aligned} &f_{M-EIGD-LESND}(x;\vartheta) = \\ &\quad w\eta\sqrt{\frac{b}{2\pi}}x^{-\eta/2-1}\exp\left[-\frac{b(x^\eta-a)^2}{2x^\eta a^2}\right] \\ &\quad +(1-w)\frac{1}{dx}\phi\left(\frac{log(x)-c}{d}\right)\frac{\Phi(\tau\sqrt{1+\theta^2}+\theta\frac{log(x)-c}{d})}{\Phi(\tau)}, \\ &\qquad \text{with } x>0, \end{aligned} \tag{13}$$

where $\phi(\cdot)$ and $\Phi(\cdot)$ are the probability density and cumulative density functions associated with a standard Gaussian distribution, respectively, and $log(\cdot)$ denotes natural logarithm. The M-EIGD-LESND contains a set of 8 free parameters, $\{w, \eta, a, b, c, d, \theta, \tau\}$, which are obtained by a matching of estimated fractional moments and fractional moments of M-EIGD-LESND. This task requires to solve system of nonlinear equations by any numerical solver (see [7] for more details). It is noteworthy that the rth fractional moment of the M-EIGD-LESND function, $M^r_{X_{M-EIGD-LESND}}$ can be analytically determined as [7]:

$$\begin{aligned} M^r_{X_{M-EIGD-LESND}} &= w\exp\left[\frac{b}{a}\right]\sqrt{\frac{2b}{\pi}}a^{r/\eta-0.5}K_{0.5-r/\eta}\left(\frac{b}{a}\right) \\ &\quad +(1-w)\exp\left(cr+0.5d^2r^2\right)\frac{\Phi\left(\tau+\frac{\theta dr}{\sqrt{1+\theta^2}}\right)}{\Phi(\tau)}, \end{aligned} \tag{14}$$

with $K_\alpha(\beta)$ the modified Bessel function of the second kind. The thus approximated distribution function can then be used further for reliability analysis or distribution-based sensitivity analysis. The M-EIGD-LESND is adopted in numerical examples to measure the error of the proposed method in comparison to a traditional Monte Carlo-type approach. However, note that this model was adopted just for the sake of illustration of the whole framework and it is generally possible to adopt any artificial distributions parameterized by fractional moments, which should be selected with respect to the analyzed problem at hand.

3.3. Numerical algorithm

The proposed approach allows for significant extension of a statistical or sensitivity analysis of costly mathematical models. Specifically, estimated fractional moments can be used for an approximation of probability distribution of QoI as summarized in the following pseudo-algorithm employed in the numerical examples. In the algorithm, the vector $\mathbf{r}$ contains all fractional moments considered in the analysis (whose dimensionality is 8) and $\lceil\cdot\rfloor$ denotes rounding to the closest integer.

Algorithm 1 Estimation of fractional moments by PCE and construction of a probability distribution

Input: experimental design (ED) with samples of $\boldsymbol{X}$ and $\mathcal{Y} = \mathcal{M}(\boldsymbol{X})$, set of basis functions $\mathcal{A}$
1: get $\boldsymbol{\beta}$ by OLS
2: get μ_Y, σ_Y^2, γ_Y and κ_Y analytically from $\boldsymbol{\beta}$
3: **for** r in $\mathbf{r}$ **do**
4: find a nearest integer moment $s = \lceil r \rfloor$
5: get approximated rth fractional moment by Eq. (11) (or Eq. (12) if $r > s$)
6: **end for**
7: get parameters of M-EIGD-LESND from fractional moments [7]
Output: $\mathbb{E}\left[|Y|^{\mathbf{r}}\right]$ and corresponding PDF/CDF of M-EIGD-LESND

4. Numerical examples

The proposed approach (referenced as PCE in figures) is presented in four numerical examples of increasing complexity and which illustrated different aspects of the approach. The first toy example represents a proof of concept and convergence of the proposed method. The second example shows a typical application of the proposed method and its clear benefits over other existing techniques. In the third example, we investigate the impact of the bi-modal distribution on the convergence of the proposed technique. And finally, the last example shows the performance of the methodology in a finite element model of considerable dimension.

The proposed approach is utilized for estimation of the following fractional moments $\mathbb{E}\left[|Y|^r\right]$, $r \in \mathbf{r} = [1.1, 1.2, 1.8, 1.9, 2.1, 2.2, 2.9, 3]$. 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. Fractional moments are further used for identification of the most suitable probability distribution as described in the previous section. The PCE is constructed using the UQPy package [43]. The obtained results of the proposed approach are compared to approximation based on standard sampling approach represented by Latin Hypercube Sampling (LHS) [13,44]. Naturally, one can use various advanced or adaptive sampling schemes [20,45,46] instead of LHS for achieving higher accuracy, however this task is beyond the scope of this paper. Also note that, the sampling technique should be selected with respect to stability of PCE construction [12], and thus it might be problematic to use sampling techniques developed specifically for numerical integration or estimation of fractional moments. The reasoning is that the estimation of fractional moments is just a part of UQ and thus we need general statistical sample covering the whole design domain further used for statistical and sensitivity analysis or construction of various surrogates.

Additionally, results are also compared to classic G–C expansion derived from PCE [20] (PCE-GC) to show the benefits of advanced and flexible distribution models represented by M-EIGD-LESND in this paper. To compare the methods, we estimate error by non-negative Kullback–Leibler divergence $D_{\mathrm{KL}}\left(Y \parallel \tilde{Y}\right)$ of a reference CDF F_Y and an approximated CDF $F_{\tilde{Y}}$. The error is calculated on CDF for improved numerical stability [47] as implemented in SciPy [48]:

$$D_{\mathrm{KL}}\left(Y \parallel \tilde{Y}\right) = F_Y(\chi) \ln \frac{F_Y(\chi)}{F_{\tilde{Y}}(\chi)} + F_{\tilde{Y}}(\chi) - F_Y(\chi), \tag{15}$$

where $\chi \in \mathbb{R}$. The total error ϵ is than obtained by integration of D_{KL} simply as:

$$\epsilon = \int_{\mathbb{R}} D_{\mathrm{KL}}\left(Y \parallel \tilde{Y}\right) d\chi. \tag{16}$$

All approximations are constructed for increasing number of simulations. In order to get reliable statistical information on convergence, we run $n_{\mathrm{stat}} = 100$ repetitions of the algorithm and plot $\mathbb{E}[\epsilon] \pm \sigma$ interval of the obtained errors.

4.1. Academic example: Gaussian distribution

The very first example shows the convergence of the proposed method. This toy example is represented by a simple analytical function of input random vector containing three independent Gaussian variables $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu} = 10, \boldsymbol{\sigma^2} = 4)$ and thus the quantity of interest is also a Gaussian variable $Y \sim \mathcal{N}(\mu = 50, \sigma^2 = 12)$:

$$Y = 20 + X_1 + X_2 + X_3. \tag{17}$$

Typical realizations of identified probability distributions based on fractional moments estimated by LHS and the proposed approach for increasing size of ED can be seen in Fig. 2. Since it is possible to analytically obtain reference distribution, there is not any error caused by approximation of the probability distribution for a reference solution. Although the resulting distribution of QoI is very simple, the estimated distributions converge slower then expected due to over-parameterized approximating function taking 8 fractional moments into account. The convergence of LHS is further affected by sensitivity to outliers, while the proposed method via PCE is clearly more stable. General convergence of both methods can be seen in Fig. 7(a). Note that besides higher accuracy in mean values, the variance of the proposed method is significantly smaller in comparison to LHS for $n_{\mathrm{sim}} > 35$ samples. Utilized M-EIGD-LESND approximation is universal parameterized distribution suitable for various types of distribution, nonetheless it might be over sophisticated for approximation of a simple distribution and a simple models should be preferred, e.g. the well-known G–C expansion [2] as can be seen in this example. Since the resulting distribution of QoI is a Gaussian distribution, G–C leads very fast to the exact solution, though as can be seen for $n_{sim} = 10$ it could lead to unstable approximations of PDF/CDFs.

Although the main purpose of the proposed method lies in efficient post-processing of the existing surrogate model, it is also more stable and robust in comparison to standard sampling techniques. The stability of the proposed method can be seen in Fig. 3 showing obtained distributions for $n_{\mathrm{sim}} = 200$ simulations. Although PCE leads to a slight error near the mean value, it leads to almost perfect accuracy at both tails of the CDF. Although LHS is very efficient method for estimation of mean values, it has clearly worse performance in estimation of higher moments affected by tails and thus also fractional moments. Note that although PCE is based on identical samples, it is an approximation of QoI over the whole input space and thus its result is less affected by outliers. This fact is also supported by results obtained from 10^7 samples generated by LHS sampling using PCE surrogate model instead of the original mathematical model (PCE-LHS). The results of PCE-LHS are identical to LHS with 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 employ the proposed approach instead of numerical estimation if a PCE is

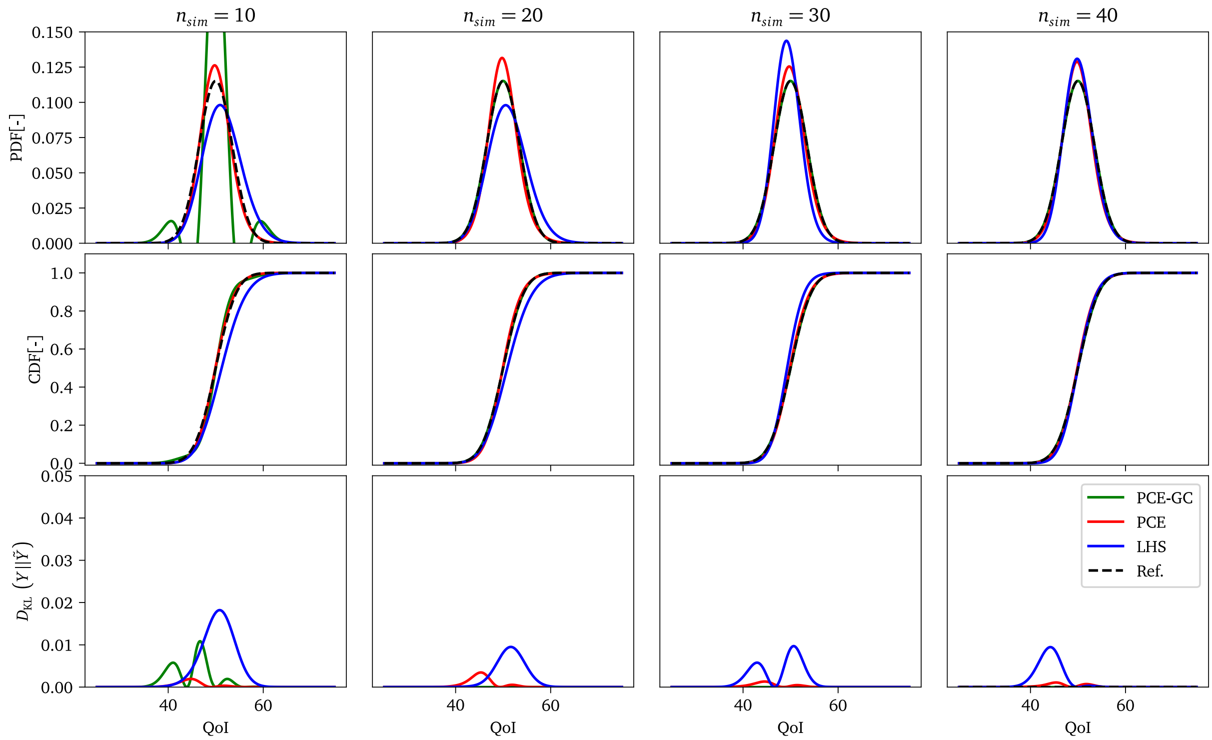

Fig. 2. Typical realization of results for the first example (Gaussian distribution). The rows show estimated PDFs, CDFs and errors in approximations respectively. Each column corresponds to increasing number of simulations used for estimation of fractional moments and probability distributions.

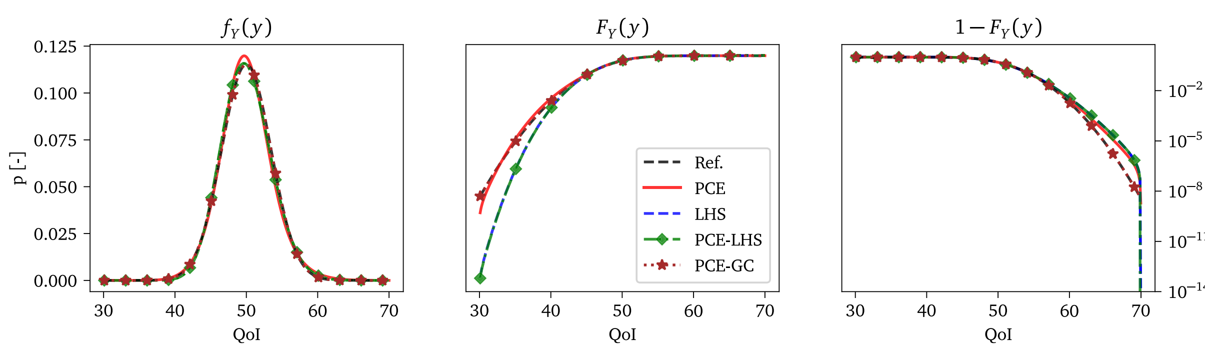

Fig. 3. Convergence study for $n_{sim} = 200$.

available. The PCE-LHS with 10^7 samples will be used for comparison of estimated fractional moments also in the following examples.

This result further supports our intention to derive probability distribution directly from PCE instead of utilization of standard sampling techniques in combination with existing surrogate model. Naturally, G–C expansion identified the exact solution of the QoI's distribution as can be expected, since the G–C expansion is based on perturbation of Gaussian distribution and thus very suitable for this example. Nevertheless, it shows very high accuracy of the integer statistical moments estimated directly from PCE coefficients.

4.2. Finite element model of a plate

The second case study deals with a model of a thin steel plate of 1 [m] by 1 [m] that is fully clamped at one side. The plate is subjected to a distributed load over the top surface, and its displacement $\boldsymbol{u}$ is computed using a finite element model consisting of 100 evenly distributed linear shell elements, resulting in 121 nodes. As such, there are 110 active nodes in the model. In the analysis, the degrees of freedom per node correspond to one translation and two rotations. The QoI for this problem is the vertical displacement of one of the corner nodes of the plate. Fig. 4 illustrates schematically the problem under consideration

The corresponding equilibrium equation associated with the finite element model of the plate is represented as:

$$\boldsymbol{K}(\boldsymbol{\theta})\boldsymbol{u} = \boldsymbol{f}, \tag{18}$$

with $\boldsymbol{K} \in \mathbb{R}^{330\times330}$ the stiffness matrix of the plate; $\boldsymbol{\theta} = [E, t, \nu]$, with E representing Young's modulus and t the thickness of the plate; ν Poisson's ratio, $\boldsymbol{f} \in \mathbb{R}^{330}$ is a vector collecting the forces acting on the nodes of the FE model; and $\boldsymbol{u} \in \mathbb{R}^{330}$ the resulting displacement vector. We assume E, t, ν to be (truncated) Gaussian variables with vector of mean values $\boldsymbol{\mu}^T = [2.1\times10^{11}, 5\times10^{-3}, 0.3]$ with vector of coefficients of variation $\mathbf{v} = [0.15, 0.1, 0.1]$. It is assumed that the degrees-of-freedom of the finite element model have been ordered such that the first 110 components of $\boldsymbol{u}$ correspond to vertical displacements.

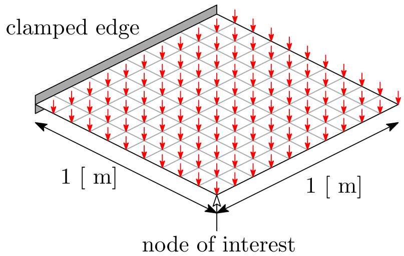

Fig. 4. Schematic representation of clamped plate.

Table 1
Relative errors of fractional moments estimated by PCE, LHS and PCE-LHS methods in the second example for $n_{sim} = 40$.

r	1.1	1.2	1.8	1.9	2.1	2.2	2.9	3
PCE	0.011	0.019	0.006	0.006	0.034	0.050	0.038	0.060
LHS	0.008	0.011	0.035	0.042	0.057	0.066	0.159	0.178
PCE-LHS	0.020	0.024	0.056	0.063	0.078	0.086	0.156	0.167

The selected realizations of approximations are compared in Fig. 5. In contrast to the previous example, a reference solution cannot be obtained analytically and thus we use empirical CDF obtained by LHS with $n_{\text{sim}} = 10^6$ simulations. The proposed approach leads to accurate approximation of the target distribution already for $n_{\text{sim}} = 20$ samples in contrast to standard LHS. Moreover the convergence of the accuracy for increasing n_{sim} is stable, while standard LHS approach achieves lower accuracy for $n_{\text{sim}} = 60$ in comparison to $n_{\text{sim}} = 40$. Identical behavior of both methods can be seen also in statistical results compared in Fig. 7(b). The proposed approach achieves both lower mean and variance of the estimated total error. Note that both methods converge to the identical mean accuracy, though the convergence of PCE is significantly faster. The obtained results clearly show the main benefits of PCE: numerical efficiency, consistency in the estimated moments even for low n_{sim} and analytical post-processing accelerating UQ of QoI. For more detailed comparison of a typical simulation, the relative errors of numerical values of estimated fractional moments for $n_{sim} = 40$ can be found in Table 1.

Interestingly, G–C expansion does not converge to the reference distribution and its solutions also do not represent valid PDFs/CDFs. This fact is clearly caused by the fact that the QoI's distribution is significantly different from Gaussian distribution (non-negative, high skewness etc.). The divergence of the G–C expansion can be seen also in Fig. 7(b) for increasing n_{sim}. From the numerical results, it can be concluded that G–C expansion is not suitable for general distributions of QoI. Note that, the well-known limitations of G–C expansions [2] are mitigated by the proposed approach based on the identical training data and the identical surrogate model in form of PCE. The proposed methodology can be further combined with various field-dependent distribution models parameterized by fractional moments, which will be investigated in further research.

4.3. Dynamic car model

The third case study in this paper considers a so-called quarter-car model. This is a 2 degree of freedom idealization of the dynamics of the suspension of a moving car. Specifically, this case study is concerned with assessing the distribution of the comfort of the vehicle suspension, given the uncertainty in some of the properties of the system. The quarter-car dynamics can be represented as a set of two ordinary differential equations:

$$m_s \ddot{x}_s + c_s(\dot{x}_s - \dot{x}_{us}) + k_s(x_s - x_{us}) = 0, \tag{19}$$

$$m_{us}\ddot{x}_{us} - c_s(\dot{x}_s - \dot{x}_{us}) - k_s(x_s - x_{us}) + c_t(\dot{x}_{us} - \dot{x}_0) + k_t(x_{us} - x_0) = 0, \tag{20}$$

with $\dot{\bullet}$ denoting the time derivative of $\bullet$, x_{us} the displacement of the unsprung mass (i.e., the suspension components, wheel and other components directly connected to them); x_s the displacement of the sprung mass (i.e., all components resting on the suspension); m_{us} and m_s the unsprung and sprung mass of a quarter of the car; c_s and c_t respectively the damping coefficients of the suspension and tire; k_s and k_t respectively the stiffness coefficients of the suspension and tire. We assume c_s, k_s, k_t to be (truncated) Gaussian variables with vector of mean values $\boldsymbol{\mu}^T = [1\times10^4, 4.8\times10^4, 2\times10^5]$ with identical coefficient of variation $v = 10\%$. Finally, x_0 and $\dot{x}_0$ are the displacement and velocity in vertical direction that excite the bottom of the wheel (i.e., the road profile). The complete road profile is denoted by $x_0(t)$, with t denoting the simulation time.

To solve this coupled system of ODEs, a state-space model is employed:

$$\frac{d}{dt}\begin{bmatrix} x_{us}-x_0 \\ \dot{x}_{us} \\ x_s - x_{us} \\ \dot{x}_s \end{bmatrix} = \boldsymbol{A}\begin{bmatrix} x_{us}-x_0 \\ \dot{x}_{us} \\ x_s - x_{us} \\ \dot{x}_s \end{bmatrix} + \begin{bmatrix} -1 \\ \frac{4c_t}{m_{us}} \\ 0 \\ 0 \end{bmatrix}\dot{x}_0, \tag{21}$$

with the matrix $\boldsymbol{A}$ equal to:

$$\boldsymbol{A} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ \frac{-4k_t}{m_{us}} & \frac{-4(c_s+c_t)}{m_{us}} & \frac{4k_s}{m_{us}} & \frac{4c_s}{m_{us}} \\ 0 & -1 & 0 & 1 \\ 0 & \frac{4c_s}{m_s} & \frac{-4k_s}{m_s} & \frac{-4c_s}{m_s} \end{bmatrix}. \tag{22}$$

Four state variables are considered, being respectively the tire deflection $(x_{us} - x_0)$; the unsprung mass velocity $\dot{x}_{us}$; the suspension stroke $x_s - x_{us}$, and sprung mass velocity $\dot{x}_s$. Typically, in the context of assessing the dynamical comfort of a car, two parameters are of interest: the suspension stroke (i.e., the relative displacement of the car body with respect to the unsprung mass) and the acceleration of the sprung mass. In the proceeding study, the damping effect of the tire, c_t is considered negligible. The limit state function in this example is based on the first excursion event of the suspension stroke, and explicitly defined as:

$$1 - \max_t \left(\frac{1}{x_c} \left| x_s(t) - x_{us}(t) \right| \right), \tag{23}$$

with $x_c = 30$ mm the threshold value for the stroke.

Similarly as in the previous examples, selected realizations of approximations for increasing n_{sim} can be seen in Fig. 6. Note that the distribution of QoI is bimodal (as can be clearly seen from empirical CDFs) and thus it cannot be accurately approximated by the adopted M-EIGD-LESND. However, the obtained results show very fast convergence of the proposed approach to the optimal solution with minimum possible error, while standard LHS converges to the optimum significantly slower as can be seen in the last column showing the obtained distributions for $n_{\text{sim}} = 200$. For more detailed comparison of a typical simulation, the relative errors of numerical values of estimated fractional moments for $n_{sim} = 100$ can be found in Table 2.

Statistical results compared in Fig. 7 show stable accuracy of the proposed method for $n_{\text{sim}} > 60$, while LHS has significantly larger variance and lower mean accuracy. Although this general behavior of standard LHS could be seen also in the previous example, it is amplified in the last example by the fact that fractional moments of the investigated bimodal distribution are even more affected by position of samples in the input random space. The convergence of G–C expansion has similar trend as in the previous example, though it still leads to valid distribution functions of QoI. However, the obtained accuracy has a very large variance and a diverging trend for increasing n_{sim}. The behavior of G–C expansion is clearly affected by the fact, that fractional moments play much higher role in this example and thus it is not possible to get accurate approximations only from the first four integer moments.

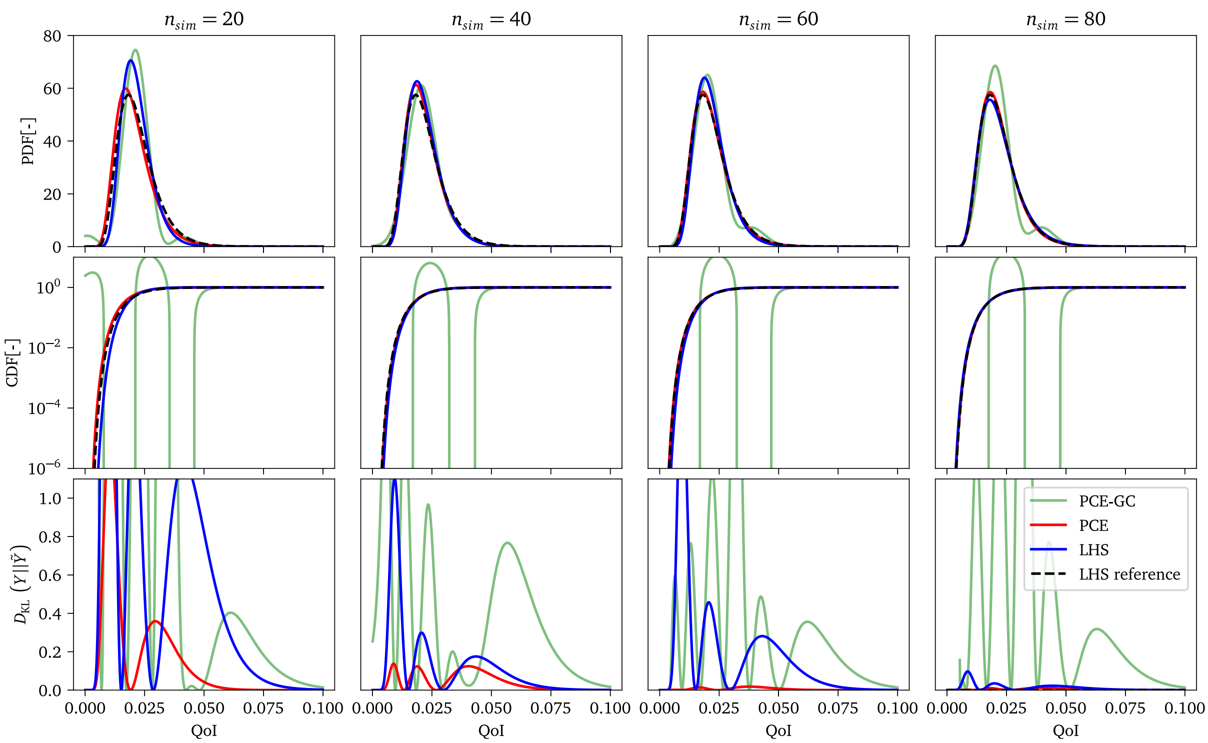

Fig. 5. Typical realization of results for the second example (FEM of a plate). The rows show estimated PDFs, CDFs and errors in approximations respectively. Each column corresponds to increasing number of simulations used for estimation of fractional moments and probability distributions.

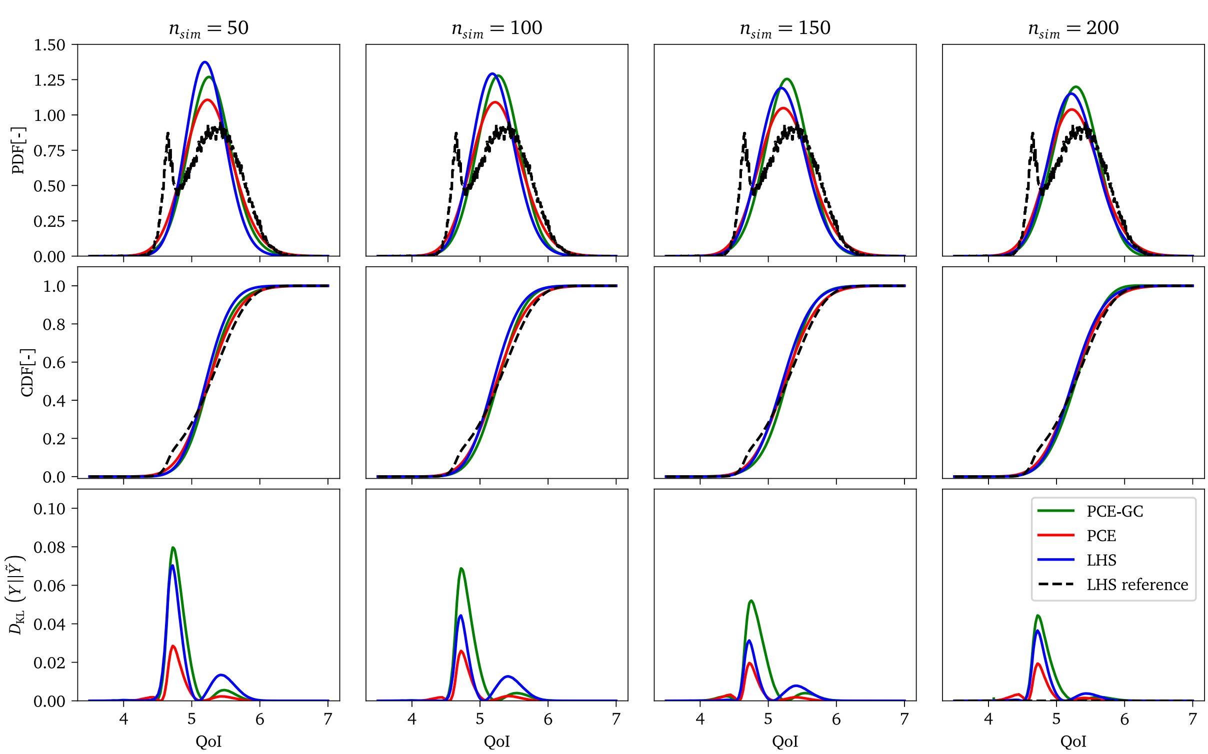

Fig. 6. Typical realization of results for the third example (dynamic car model). The rows show estimated PDFs, CDFs and errors in approximations respectively. Each column corresponds to increasing number of simulations used for estimation of fractional moments and probability distributions.

4.4. Case study: Seepage under a sheet pile

This case study involves characterizing the uncertainty associated with the seepage flow Y_{flow} under a sheet pile. The physical problem is represented schematically in Fig. 8.

The sheet pile retains a water column of 7 [m] and it is buried 8 [m] deep into a permeable silty sand soil layer. The permeability of the soil is modeled as an isotropic log-normal random field, with mean value 5×10^{-6} [m/s], a coefficient of variation of 100% and a correlation modeled considering a quadratic exponential function. The correlation

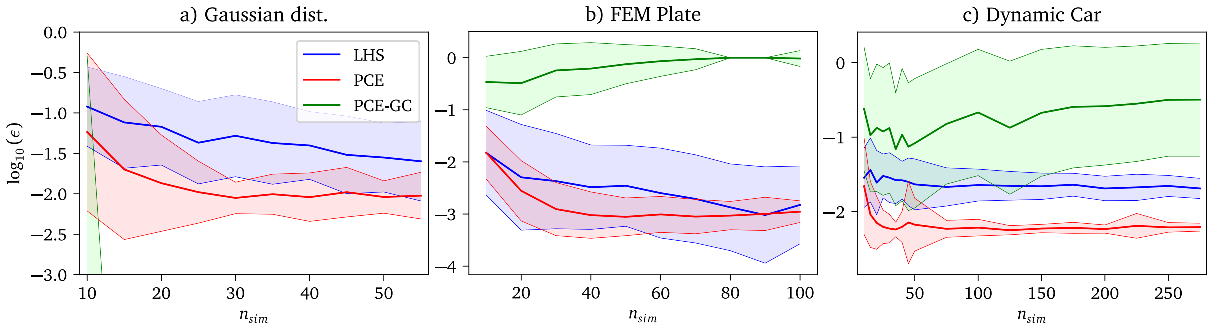

Fig. 7. Convergence plots showing mean values and $\pm\sigma$ interval of the total error ϵ obtained by the proposed method and standard LHS approach for (a) Gaussian model, (b) plate model and (c) Dynamic car model.

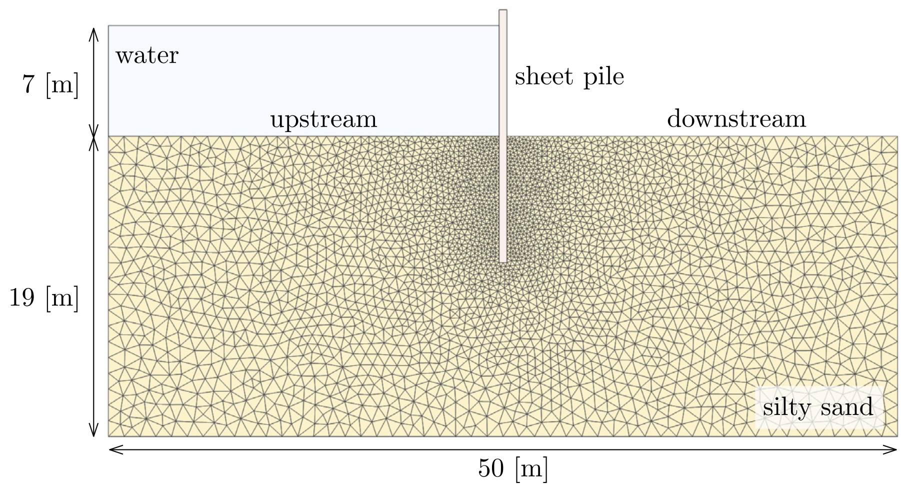

Fig. 8. Scheme of the investigated example: Seepage under sheet pile.

Table 2
Relative errors of fractional moments estimated by PCE, LHS and PCE-LHS methods in the third example for $n_{sim} = 100$.

r	1.1	1.2	1.8	1.9	2.1	2.2	2.9	3
PCE	0.001	0.001	0.000	0.000	0.001	0.002	0.001	0.002
LHS	0.004	0.004	0.007	0.007	0.008	0.008	0.012	0.013
PCE-LHS	0.016	0.017	0.025	0.026	0.029	0.030	0.038	0.039

is equal to e^{-d^2/L^2}, where d denotes Euclidean distance between locations in the soil layer and L is the correlation length, considered here as $L = 10$ [m]. The random field is discretized using the midpoint method and is described through the Karhunen–Loève expansion with 10 terms. This ensures that more than 95% of the variability of the underlying Gaussian random field is retained. The seepage flow is assumed to follow Darcy's law. The associated partial differential equation that allows quantifying the seepage flow corresponds to the Laplace type and it is solved using the finite element method. The finite element mesh involves 6090 quadratic triangular elements and 12 427 nodes, as represented schematically in 8. For the boundary conditions, it is assumed that all sides of the soil layer illustrated in Fig. 8 are impermeable, except for the sides marked as *upstream* (water inlet) and *downstream* (water outlet). The QoI is defined as the following safety margin with given deterministic threshold $Y = 20 \times 10^{-5} - Y_{\text{flow}}$.

This example represents very complicated task for the proposed approach, since the input random vector contains 10 random variables (weights from Karhunen–Loève expansion) and thus the PCE contains very large number of basis functions. Moreover, the resulting distribution of QoI is highly non-Gaussian as can be seen from the reference empirical distribution obtained from 1000 simulations depicted in Fig. 9 (right) together with the typical realization of the algorithm for $n_{\text{sim}} = 100$. It can be seen that the fractional moments estimated from the experimental design (LHS) are highly sensitive to outliers and thus the approximated distribution is significantly different in comparison to the reference solution. This trend can be seen also in the error plots measuring a difference between the approximated distribution and the empirical distribution for the increasing $n_{\text{sim}} \in [50, 100, 150, 200]$ shown in Fig. 9 (left).

5. Discussion

In the previous section, we presented thorough comparison of the proposed method to M-EIGD-LESND based on fractional moments estimated directly from the experimental design generated by LHS, and G–C expansion derived from the PCE. It was shown that although G–C expansion based on the first four statistical moments derived analytically from PCE is superior in the first example, it can become unstable for significantly non-Gaussian distributions and more suitable parametric distributions should be employed. Moreover, from the numerical results it can be concluded it is beneficial to derive fractional moments analytically from PCE as a part of the post-processing instead of the direct numerical estimation from training data. Moreover it was also shown in Tables 1 and 2, that analytical derivation of fractional moments directly from PCE is more accurate in comparison to numerical estimation from large set of realizations generated from PCE approximation.

Naturally, the total accuracy of the estimated probability distribution is highly dependent on a selected parametric distribution. Therefore, a comparison to general data-driven methods will be presented in

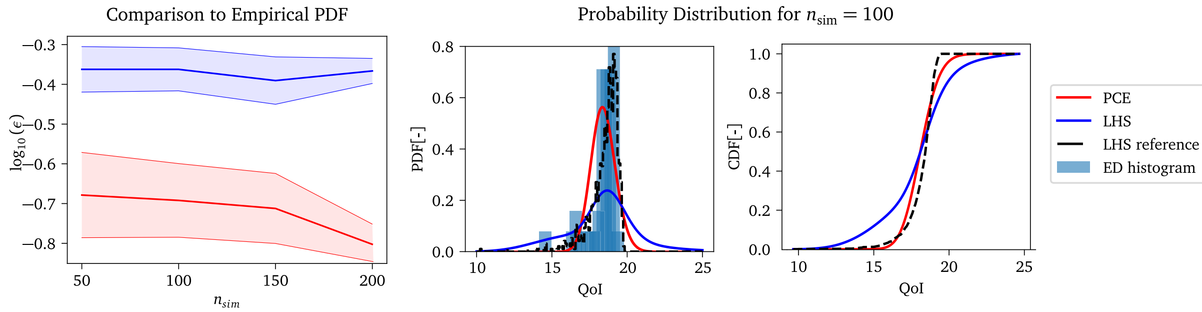

Fig. 9. Convergence plots showing mean values and $\pm\sigma$ interval of the total error ϵ obtained by the proposed method and standard LHS approach for the last example (left). A typical realization of the algorithm for $n_{\text{sim}} = 100$ (right).

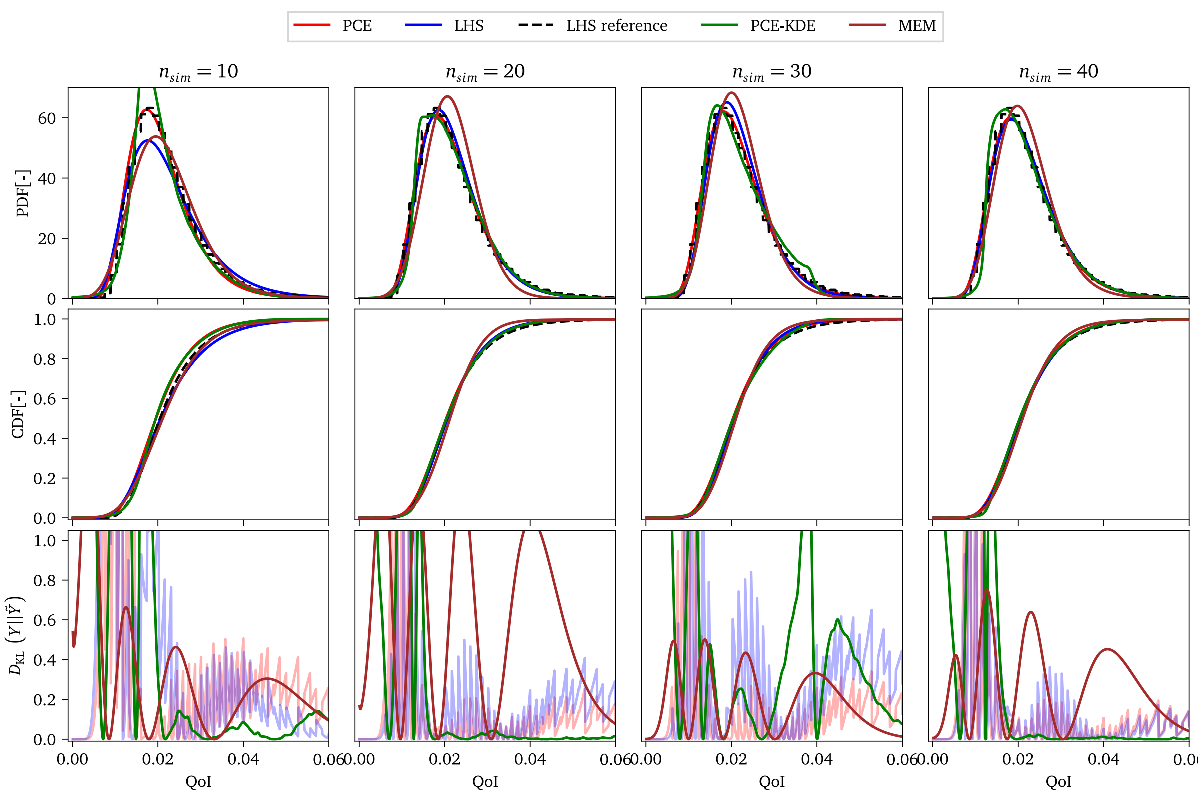

Fig. 10. Typical realization of results for the second example (FEM of a plate). The rows show estimated PDFs, CDFs and errors in approximations respectively. Each column corresponds to increasing number of simulations used for estimation of fractional moments and probability distributions.

this section. The first standard data-driven method is based on well-known Kernel Density Estimation (KDE) using the Gaussian kernel with the bandwidth given by the most common Silverman's rule of thumb based on 10^7 samples generated from PCE (PCE-KDE). The second approach for general comparison is Maximum Entropy Method using fractional moments (MEM) [49] based on training data. The MEM is popular technique for approximation of the target probability distribution, which could be further used for general UQ of physical systems [50], sensitivity analysis [51] or combined with dimensional reduction method to perform reliability analysis [52]. Note that for the sake of a fair comparison, training data were generated by LHS although more advanced sampling methods could be used specifically for improvement of KDE and MEM [53,54], or one can use more advanced sampling techniques for construction of PCE [55].

The selected methods were compared in the second example — FEM of a plate. The obtained numerical results of a typical realization can be seen in Fig. 10. Note that the errors are calculated with respect to the reference empirical PDF based on 10^7 simulations of the original mathematical model. It can be seen that the proposed approach is very accurate and stable also for very low number of simulations, while PCE-KDE is highly sensitive to the accuracy of PCE predictions (including outliers) and its stability is improving with the size of ED. Moreover, it can lead to unrealistic approximations due to the selected bandwidth as can be seen in the third column. Although the MEM is generally very accurate and efficient method, its results are significantly worse for very low number of samples as shown in this example. The statistical convergence graphs presented in Fig. 11 confirms the previous results. While KDE-PCE starts with a very high variance of the error, it converges rapidly to accurate results with increasing n_{sim} and thus increasing accuracy of the PCE. On the other hand, MEM does not converge for such low sizes of ED due to the fact that it is purely data-driven approach, though it achieves very high accuracy for large EDs.

6. Conclusions & further work

A novel approach for estimation of fractional moments directly from polynomial chaos expansion was proposed in this paper. The proposed

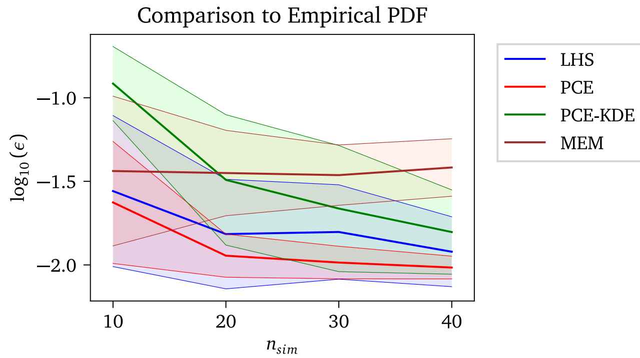

Fig. 11. Convergence plots showing mean values and $\pm\sigma$ interval of the total error ϵ obtained by the proposed method, LHS, PCE-KDE and MEM for the second example (FEM of a plate).

method combines well-known formulas for estimation of integer statistical moments from PCE coefficients together with Hölder's inequality in order to analytically obtain arbitrary fractional moments. The fractional moments were further used for a construction of probability distribution based on adopted M-EIGD-LESND algorithm. Obtained results from the presented numerical examples clearly show that the proposed method leads to stable and accurate estimations. Moreover, it achieves also a superior computational efficiency in comparison to a standard method based on Latin hypercube sampling and higher flexibility in comparison to classic Gram–Charlier expansion derived directly from PCE. Therefore, it can be concluded that an error caused by an Hölder's inequality approximation is typically lower than error caused by discrete sampling methods, at least for low-size ED. Naturally, the benefits of the proposed method will be crucial for distribution-based sensitivity measures typically based on differences between conditional probability distributions, which can be accessed from a single PCE [21]. On the other hand, it is well-known that PCE suffers from *curse of dimensionality* and thus the proposed approach is not suitable for high-dimensional applications. There are also still some important topics for further research. First of all, the accuracy of PCE is highly dependent on the type of sampling scheme [12] and thus it will be necessary to investigate the most suitable sampling schemes and/or active learning algorithms with respect to an estimation of statistical moments [20].

CRediT authorship contribution statement

Lukáš Novák: Writing – original draft, Visualization, Software, Methodology, Investigation, Funding acquisition, Formal analysis, Conceptualization. **Marcos Valdebenito:** Writing – review & editing, Validation, Methodology. **Matthias Faes:** Writing – review & editing, Writing – original draft, Validation, Methodology, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

The first author acknowledges financial support provided by the Czech Science Foundation under project number 23-04712S. The international collaboration was supported by the Ministry of Education, Youth and Sports of the Czech Republic under project No. LUAUS24260. The help of Dr. Chao Dang (Chair for Reliability Engineering, TU Dortmund University, Germany) for preparing some numerical implementations pertinent to this work is deeply appreciated.

Data availability

Data will be made available on request.

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