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Abstract: ANOVA analysis is a very common numerical technique for computing a hierarchy of most important input parameters for a given output when variations are computed in terms of variance. This second central moment can not be retained as an universal criterion for ranking some variables, since a non-gaussian output could require higher order (more than second) statistics for a complete description and analysis.
In this work, we illustrate how third and fourth-order statistic moments, *i.e.* skewness and kurtosis, respectively, can be decomposed. It is shown that this decomposition is correlated to a polynomial chaos expansion, permitting to easily compute each term. Then, new sensitivity indices are proposed basing on the computation of the kurtosis. An analytical example is provided with the explicit computation of the variance and the skewness. Some test-cases are introduced showing the importance of ranking the kurtosis too.

Key-words: high-order statistics, skewness, kurtosis, Uncertainty Quantification.

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Décomposition des statistiques d'ordre élevé

Résumé : L'analyse ANOVA est une technique numérique pour calculer une hiérarchie des paramètres les plus importants pour une sortie spécifique quand les variations sont calculées en terme de variance. La variance ne peut pas être considérée comme un critère universel pour classifier les variables, vu qu'une sortie non-gaussienne pourrait demander des statistiques d'ordre plus élevé pour une description et une analyse complètes. Dans cette étude, nous illustrons comment les moments statistiques d'ordre trois et quatre peuvent être décomposés. De plus, on montre que cette décomposition est corrélée avec le développement du Chaos Polynomial, ce qui permet de calculer facilement chaque terme. Ensuite, des indices de sensibilité nouveaux sont proposés qui se basent sur le calcul du kurtosis. Un exemple analytique est fourni avec le calcul explicite de la variance et de la skewness. D'autres cas-tests sont introduits qui permettent de montrer l'importance du kurtosis.

Mots-clés : statistiques d'ordre élevé, skewness, kurtosis, quantification des incertitudes

1 Introduction

Optimization and design in the presence of uncertain operating conditions, material properties and manufacturing tolerances poses a tremendous challenge to the scientific computing community. In many industry-relevant situations the performance metrics depend in a complex, non-linear fashion on those factors and the construction of an accurate representation of this relationship is difficult. Probabilistic uncertainty quantification (UQ) approaches represent the inputs as random variables and seek to construct a statistical characterization of few quantities of interest. Several methodologies are proposed to tackle this issue, most of all focused on stochastic spectral methods [1, 2, 3, 4, 5], that can provide considerable speed-up in computational time when compared to Monte Carlo (MC) simulation. In realistic situations however, the presence of a large number of uncertain inputs leads to an exponential increase of the cost thus making these methodologies unfeasible [6]. This situation becomes even more challenging when robust design optimization is tackled [7, 8].

Several UQ methods have been developed with the objective of reducing the number of solution required to obtain a statistical characterization of the quantity of interest, such as Sparse grid techniques or adaptive mesh generation. These techniques can lead to a dramatical reduction of the quadrature points for moderate dimensional problem, provided that the function has some regularity. Classical sparse grids [9] are constructed from tensor products of one-dimensional quadrature formulas. Some Galerkin-based methods deals with multi-resolution wavelet expansions [10, 11], domain decomposition in the random space [12], adaptive h-refinement [3] for dealing with arbitrary probability distributions.

Among the collocation-based stochastic spectral methods, in [13] they proposed the use of sparse grid quadrature for stochastic collocation. Older studies show the errors and efficiency of sparse grid integration and interpolation [14, 15], Smolyak constructions based on one-dimensional nested Clenshaw-Curtis rules [14, 16] and the integration error of sparse grids based on one-dimensional Kronrod-Patterson rules [17].

An alternative solution for reducing the cost of the UQ method is based on approaches attempting to identify the relative importance of the input uncertainties on the output. If some dimensions could be identified as negligible, they could be discarded in a reduced stochastic problem. If the number of uncertainties could be reduced, a better statistic estimation could be achieved with a lower computational cost.

Concerning the computation of the most influent parameters, it is important to determine the uncertain inputs which have the largest impact on the variability of the model output. In literature, Global sensitivity analysis (GSA) aims at quantifying how uncertainties in the input parameters of a model contribute to the uncertainties in its output (see for example [18]), where global sensitivity analysis techniques are applied to probabilistic safety assessment models). Sometimes, GSA classifies the inputs according to their importance on the output variations and it gives a hierarchy of most important ones.

Traditionally, GSA is performed using methods based on the decomposition of the output variance [19], *i.e.* ANOVA. The ANOVA approach involves splitting a multi-dimensional function into its contributions from different groups of subdimensions. In 2001, Sobol used this formulation to define global sensitivity indices [19], displaying the relative variance contributions of different ANOVA terms. In [20], they introduced two High-Dimensional Model Reduction (HDMR) techniques to capture input-output relationships of physical systems with many input variables. These techniques are based on ANOVA-type decompositions.

Since it requires a large number of function evaluations, several techniques have been developed to compute the different so-called sensitivity indices at low cost [21]. In [22, 23, 24], generalized Polynomial Chaos Expansions (gPC) are used to build surrogate models for computing the Sobol's indices analytically as a post-processing of the PC coefficients. In [6], they combine multi-element polynomial chaos with analysis of variance (ANOVA) functional decomposition to enhance the convergence rate of polynomial chaos in high dimensions and in problems with low stochastic regularity. In [25], the use of adaptive ANOVA decomposition is investigated as an effective dimension-reduction technique in modeling incompressible and compressible flows with high-dimension of random space. In Sudret [26], sparse Polynomial Chaos (PC) expansions are introduced in order to compute sensitivity indices. An adaptive algorithm allows to build a PC-based metamodel that only contains the significant terms whereas the PC coefficients are computed by least-square regression.

Other approaches are developed if the assumption of independence of the input parameters is not valid. New indices have been proposed to address the dependence [27, 28], but this attempts are limited to a linear correlation. In [29], they introduce a global sensitivity indicator which looks at the influence of input uncertainty on the entire output distribution without reference to a specific moment of the output (moment independence) and which can be defined also in the presence of correlations among the parameters. In [30], a gPC methodology to address global sensitivity analysis for this kind of problems is introduced. A moment-independent sensitivity index that suits problems with dependent parameters is reviewed. Recently, in [31], a numerical procedure is set-up for moment-independent sensitivity methods.

The ANOVA-based analysis create a hierarchy of most important input parameters for a given output when variations are computed in terms of variance. A strong limitation of this approach is the fact that it is based on the variance since the second central moment can not be considered like a general indicator for a complete description of output variations. For example, any Gaussian signal is completely characterized by its mean and variance. Consequently the 3rd order moment of a Gaussian signal is zero. Unfortunately, many signals encountered in practice have non-zero high-order statistics, but second-order statistics contain no phase information. As a consequence of this, phase signals cannot be correctly identified by a 2nd-order technique. Remark also that many measurement noises are Gaussian, and so in principle the high-order statistics are less affected by Gaussian background noise than the 2nd order measures. For well describing the complexity of engineering systems, computation of Higher-Order (HO) statistics are of primary importance, for example the third order, the *skewness* (measure of the non-symmetry of the distribution, *i.e.* any symmetric distribution will have a third central moment of zero), and the fourth order, the *kurtosis* (measure of whether the distribution is tall or short, compared to the normal distribution of the same variance). Now, let us imagine to compute the more influential parameters for a given output. The hierarchy of important parameters based on 2nd-order statistical moment (like in ANOVA analysis) is not the same if a different statistic order is considered. Depending on the problem, a n-order decomposition could be of interest. It seems of primary importance to collect the set of hierarchies obtained from n-order statistical moment decomposition, for a correct ranking of all the uncertainties.

For computing HO statistics, the most diffused methods are related to Monte Carlo and quasi-Monte Carlo approaches. Very few papers exist showing the application of polynomial-chaos techniques to the computation of HO statistics [32, 33].

First objective of this paper is to provide a general method in order to compute the decomposition of high-order statistics, then to formulate an approach similar to ANOVA but for *skewness and kurtosis*. The idea is to compute the most influential parameters not only for the variance but also for higher orders permitting to improve the sensitivity analysis. This is a fundamental step in order to formulate also innovative optimization methods for obtaining very robust designs by taking into account a complete description of the output statistics. Second objective is to illustrate the correlation between the high-order functional decomposition and the PC-based techniques, thus displaying how to compute each term from a numerical point of view.

The paper is organized as follows. Section §2 illustrates some definitions for high-order statistics. In section §3, functional decompositions for variance, skewness and kurtosis are presented. In section §4, the correlation between the functional decomposition and a Polynomial Chaos framework is depicted. Section §5 extend some sensitivity indices to high-order decomposition. Then, Section §6 presents several results showing the importance of considering skewness in robust design problems and of computing kurtosis sensitivity indices when ranking a set of uncertainties. In section §7, conclusions and perspectives are drawn.

2 High-order statistics definition

Let us consider a real function $f = f(\boldsymbol{\xi})$ with $\boldsymbol{\xi}$ a vector of random inputs $\boldsymbol{\xi} \in \Xi^d = \Xi_1 \times \cdots \times \Xi_n$ ($\Xi \subset \mathbb{R}^d$) and $\boldsymbol{\xi} \in \Xi^d \longmapsto f(\boldsymbol{\xi}) \in L^2(\Xi^d, p(\boldsymbol{\xi}))$, where $p(\boldsymbol{\xi}) = \prod_{i=1}^d p(\xi_i)$ is the probability density function of $\boldsymbol{\xi}$.

We can define the central statistical moment of f of order n as

$$\mu^n(f) = \int_{\Xi^d} (f(\boldsymbol{\xi}) - E(f))^n p(\boldsymbol{\xi}) \mathrm{d}\xi, \tag{1}$$

where $E(f)$ indicates the expected value of f

$$E(f) = \int_{\Xi^d} f(\boldsymbol{\xi}) p(\boldsymbol{\xi}) \mathrm{d}\xi. \tag{2}$$

In the following, we indicate with σ^2, the variance (second-order moment), with s the skewness (third-order), and with k the kurtosis (fourth-order). We recall here some convenient formulas for skewness s and kurtosis k (see A for more details). They can be computed as follows

$$\begin{aligned} s &= E(f^3) - 3E(f^2)E(f) + 2E(f)^3 \\ s &= E(f^3) - 3\sigma^2 E(f) - E(f)^3, \end{aligned} \tag{3}$$

$$
\begin{aligned}
k &= E(f^4) - 4E(f^3)E(f) + 6E(f^2)E(f)^2 - 3E(f)^4 \\
k &= E(f^4) - 4sE(f) - 6\sigma^2 E(f)^2 - E(f)^4.
\end{aligned} \tag{4}
$$

These expressions are used for the functional decomposition shown in the following sections.

3 Functional decomposition

Let us apply the definition of the Sobol functional decomposition [19] to the function f as follows

$$
f(\boldsymbol{\xi}) = \sum_{i=0}^{N} f_{\boldsymbol{m_i}}(\boldsymbol{\xi} \cdot \boldsymbol{m_i}), \tag{5}
$$

where the multi-index $\boldsymbol{m}$, of cardinality $card(\boldsymbol{m}) = d$, can contain only elements equal to 0 or 1. Clearly, the total number of admissible multi-indices $\boldsymbol{m_i}$ is $N+1 = 2^d$; this number represent the total number of contributes up to the dth-order of the stochastic variables $\boldsymbol{\xi}$. The scalar product between the stochastic vector $\boldsymbol{\xi}$ and $\boldsymbol{m_i}$ is employed to identify the functional dependences of $f_{\boldsymbol{m_i}}$. In this framework, the multi-index $\boldsymbol{m}_0 = (0, \dots, 0)$, is associated to the mean term $f_{\boldsymbol{m}_0} = \int_{\Xi^d} f(\boldsymbol{\xi}) p(\boldsymbol{\xi}) \mathrm{d}\xi$. As a consequence, $f_{\boldsymbol{m}_0}$ is equal to the expectancy of f, *i.e.* $E(f)$. Let us assume, in the following, to order the N multi-indices $\boldsymbol{m_i}$ in the following way:

$$
\begin{array}{rcl}
\boldsymbol{m}_1 &=& (1, 0, \dots, 0) \\
\boldsymbol{m}_2 &=& (0, 1, \dots, 0) \\
\vdots && \\
\boldsymbol{m}_d &=& (0, \dots, 1) \\
\boldsymbol{m}_{d+1} &=& (1, 1, 0, \dots, 0) \\
\boldsymbol{m}_{d+2} &=& (1, 0, 1, 0, \dots, 0) \\
\vdots && \\
\boldsymbol{m}_N &=& (1, \dots, 1).
\end{array} \tag{6}
$$

Except the term $\boldsymbol{m}_0$, that should be the first in the series, the remaining N multi-indices $\boldsymbol{m_i}$ should be classified with respect to a prescribed criterion. However, this criterion does not affect in any way the successive ANOVA functional decomposition.

The decomposition (5) is of ANOVA-type in the sense of Sobol [19] if all the members in Eq. (5) are orthogonal, *i.e.* as follows

$$
\int_{\Xi^d} f_{\boldsymbol{m_i}}(\boldsymbol{\xi} \cdot \boldsymbol{m_i}) f_{\boldsymbol{m}_j}(\boldsymbol{\xi} \cdot \boldsymbol{m}_j) p(\boldsymbol{\xi}) \mathrm{d}\boldsymbol{\xi} = 0 \quad \text{with} \quad \boldsymbol{m_i} \neq \boldsymbol{m}_j, \tag{7}
$$

and for all the terms $f_{\boldsymbol{m_i}}$, except f_0, holds

$$
\int_{\Xi^d} f_{\boldsymbol{m_i}}(\boldsymbol{\xi} \cdot \boldsymbol{m_i}) p(\xi_j) \mathrm{d}\xi_j = 0 \quad \text{with} \quad \xi_j \in (\boldsymbol{\xi} \cdot \boldsymbol{m_i}) \,. \tag{8}
$$

Each term $f_{\boldsymbol{m_i}}$ of (5) can be expressed as

$$f_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) = \int_{\Xi^{d-\mathrm{card}(\hat{\boldsymbol{m}}_i)}} f_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})p(\bar{\boldsymbol{\xi}}_i)\bar{\boldsymbol{\xi}}_i \quad - \sum_{\substack{\boldsymbol{m}_j\neq\boldsymbol{m_i}\\ \mathrm{card}(\hat{\boldsymbol{m}}_j)<\mathrm{card}(\boldsymbol{m_i})}} f_{\boldsymbol{m}_j}(\boldsymbol{\xi}\cdot\boldsymbol{m}_j), \tag{9}$$

where the multi-indexes, $\hat{\boldsymbol{m}}_{\boldsymbol{i}}$, have cardinality equal to the number of non-null elements in $\boldsymbol{m_i}$ and $\bar{\boldsymbol{\xi}}_i$ contains all the variables not contained in $(\boldsymbol{\xi}\cdot\boldsymbol{m_i})$, *i.e.* $(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\cup\bar{\boldsymbol{\xi}}_i = \boldsymbol{\xi}$.

The functional decomposition (5) is usually employed [19] to compute the contribution of each term to the overall variance, as shown in the next section.

3.1 Variance decomposition

ANOVA analysis is based on the variance decomposition in its conditional contributions. Variance can be written in terms of conditional expectancy of f and f^2 as (see A for more details):

$$\sigma^2 = E(f^2) - E(f)^2. \tag{10}$$

As a consequence, the problem is to compute $E(f^2)$, seeing that $E(f)$ is known and equal to $f_{\boldsymbol{m}_0}$. Starting from Eq. (5), it is easy to compute

$$f^2(\boldsymbol{\xi}) = \sum_{i=0}^{N} f^2_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) + 2\sum_{i=0}^{N}\sum_{j=i+1}^{N} f_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})f_{\boldsymbol{m}_j}(\boldsymbol{\xi}\cdot\boldsymbol{m}_j). \tag{11}$$

If the equation (11) is integrated in the stochastic space and the orthogonality property (7) is applied, variance can be decomposed as

$$\sigma^2 = \sum_{i=1}^{N}\int_{\Xi^d} f^2_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} = \sum_{i=1}^{N}\int_{\hat{\Xi}_i} f^2_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})p(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}), \tag{12}$$

where the symbol $\hat{\Xi}_i$ is employed to indicate $\Xi^{\mathrm{card}(\hat{\boldsymbol{m}}_i)}$ for brevity.

Variance can be expressed as the summation of all the conditional contributions

$$\sigma^2 = \sum_{i=1}^{N}\sigma^2_{\boldsymbol{m_i}}. \tag{13}$$

So, a comparison with the equation (12) shows that

$$\sigma^2_{\boldsymbol{m_i}} = \int_{\hat{\Xi}_i} f^2_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})p(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}). \tag{14}$$

Then, the same type of analysis is applied to skewness and kurtosis.

3.2 Skewness decomposition in conditional terms

Let us extend the same procedure already presented in the previous section to the computation of the skewness. As shown in §2 (see A for more details), skewness depends on $E(f)$, $E(f^2)$ and $E(f^3)$ (85). The skewness can be written in the following form

$$\begin{aligned} s = &\sum_{i=1}^{N} \int_{\hat{\Xi}_i} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})p(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \\ &+ 3\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} \int_{\hat{\Xi}_{ij}} f^2_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j})p(\boldsymbol{\xi}\cdot\boldsymbol{m}_{ij})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{ij}}) \\ &+ 6\sum_{i=1}^{N}\sum_{j=i+1}^{N}\sum_{k=j+1}^{N} \int_{\hat{\Xi}_{ijk}} f_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) f_{\boldsymbol{m}_k}(\boldsymbol{\xi}\cdot\boldsymbol{m}_k)p(\boldsymbol{\xi}\cdot\boldsymbol{m}_{ijk})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{ijk}}), \end{aligned} \tag{15}$$

where $\hat{\Xi}_{ij} = \Xi^{\mathrm{card}(\hat{\boldsymbol{m_{ij}}})}$ and $\hat{\Xi}_{ijk} = \Xi^{\mathrm{card}(\hat{\boldsymbol{m_{ijk}}})}$.

Here, a special notation is introduced to compute multi-indexes as $\boldsymbol{m}_{ab\cdots z}$,

$$\boldsymbol{m_{ab\cdots z}} = \boldsymbol{m_a}\boxplus\boldsymbol{m_b}\boxplus\cdots\boxplus\boldsymbol{m_z} = \left(\frac{m_{a_1}+m_{b_1}+\cdots m_{z_1}}{\Big|\Big|m_{a_1}+m_{b_1}+\cdots+m_{z_1}\Big|\Big|_{\neq 0}}, \ldots, \frac{m_{a_d}+m_{b_d}+\cdots+m_{z_d}}{\Big|\Big|m_{a_d}+m_{b_d}+\cdots+m_{z_d}\Big|\Big|_{\neq 0}} \right), \tag{16}$$

where the norm $\Big|\Big|\cdot\Big|\Big|_{\neq 0}$ is defined as

$$\Big|\Big|\alpha\Big|\Big|_{\neq 0} = \begin{cases} |\alpha| & \text{if} \quad \alpha \neq 0 \\ 1 & \text{if} \quad \alpha = 0. \end{cases} \tag{17}$$

Proof. Let us focus on the computation of $f^3(\boldsymbol{\xi})$. Starting from (5), $f^3(\boldsymbol{\xi})$ can be written as follows

$$\begin{aligned} f^3(\boldsymbol{\xi}) = &\sum_{i=0}^{N} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) + 3\sum_{i=0}^{N} f^2_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \sum_{\substack{j=0\\ j\neq i}}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) \\ &+ 6\sum_{i=0}^{N}\sum_{j=i+1}^{N}\sum_{k=j+1}^{N} f_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m}_j}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}). \end{aligned} \tag{18}$$

The first term is split in

$$\sum_{i=0}^{N} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) = \boxed{f^3_{\boldsymbol{m_0}}} + \sum_{i=1}^{N} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \tag{19}$$

and the second term in

$$
\begin{aligned}
3\sum_{i=0}^{N} f_{\boldsymbol{m_i}}^2(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\sum_{\substack{j=0\\ j\neq i}}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) = {} & \underline{3f_{\boldsymbol{m_0}}^2(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\sum_{j=1}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j})} \\
& + \boxed{3f_{\boldsymbol{m_0}}\sum_{i=1}^{N} f_{\boldsymbol{m_i}}^2(\boldsymbol{\xi}\cdot\boldsymbol{m_i})} \\
& + 3\sum_{i=1}^{N} f_{\boldsymbol{m_i}}^2(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\sum_{\substack{j=1\\ j\neq i}}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}).
\end{aligned}
\tag{20}
$$

For the third term, the mean contribution is put in evidence

$$
\begin{aligned}
& 6\sum_{i=0}^{N}\sum_{j=i+1}^{N}\sum_{k=j+1}^{N} f_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j})f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}) = \\
& \underline{6f_{\boldsymbol{m_0}}\sum_{j=1}^{N}\sum_{k=j+1}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j})f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k})} \\
& +6\sum_{i=1}^{N}\sum_{j=i+1}^{N}\sum_{k=j+1}^{N} f_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j})f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}).
\end{aligned}
\tag{21}
$$

Moving some terms to the left side and integrating on the whole stochastic space Ξ, we obtain

$$
\begin{aligned}
\int_{\Xi} f^3(\boldsymbol{\xi})p(\boldsymbol{\xi})\mathrm{d}\xi - \boxed{f_{\boldsymbol{m_0}}^3} - \boxed{3f_{\boldsymbol{m_0}}\sum_{i=1}^{N}\int_{\hat{\Xi}_i} f_{\boldsymbol{m_i}}^2(\boldsymbol{\xi}\cdot\boldsymbol{m_i})p(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})} = {} & \\
\sum_{i=1}^{N}\int_{\hat{\Xi}_i} f_{\boldsymbol{m_i}}^3(\boldsymbol{\xi}\cdot\boldsymbol{m_i})p(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) & \\
+ 3\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\int_{\hat{\Xi}_{ij}} f_{\boldsymbol{m_i}}^2(\boldsymbol{\xi}\cdot\boldsymbol{m_i})f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j})p(\boldsymbol{\xi}\cdot\boldsymbol{m_{ij}})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{ij}}) & \\
+ 6\sum_{i=1}^{N}\sum_{j=i+1}^{N}\sum_{k=j+1}^{N}\int_{\hat{\Xi}_{ijk}} f_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j})f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k})p(\boldsymbol{\xi}\cdot\boldsymbol{m_{ijk}})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{ijk}}), &
\end{aligned}
\tag{22}
$$

where the underlined terms of the equations (20) and (21) are equal to zero, because of the orthogonality, and because $f_{\boldsymbol{m_0}}$ does not depend on $\boldsymbol{\xi}$.

If we consider that the variance computed by the ANOVA functional decomposition

$$
\sigma^2 = \sum_{i=1}^{N}\int_{\hat{\Xi}_i} f_{\boldsymbol{m_i}}^2(\boldsymbol{\xi}\cdot\boldsymbol{m_i})p(\boldsymbol{\xi})\mathrm{d}\xi, \tag{23}
$$

that $\int_{\Xi^d} f^3(\boldsymbol{\xi})p(\boldsymbol{\xi})\mathrm{d}\xi = E(f^3(\boldsymbol{\xi}))$, and that $f_{\boldsymbol{m_0}}^3 = E(f)^3$, the left side of Eq. (22) is exactly equal to the skewness, s, as described in Equation (15). □

The number of terms that form the skewness can be estimated as $T_s = N + N(N-1) + \binom{N}{3}$. If we consider that $N+1 = 2^d$, we can compute the number of terms as a function of the stochastic dimension d

$$T_s = 2^d(2^d-2) + 1 + \binom{2^d-1}{3}, \quad \text{with} \quad d \geq 2. \tag{24}$$

In Table 1, the numbers of terms for an increasing dimension up to five are reported compared to the number of terms $(2^d - 1)$ allowing the computation of the variance.

Dimension	Variance	Skewness
2	3	10
3	7	84
4	15	680
5	31	5456

Table 1: Number of terms in the functional decomposition for the skewness

Concerning the skewness, identifying each conditional term becomes more difficult, with respect to the classical decomposition of variance, because of some terms depending from different multi-indexes. However, it is possible to use an additive form as follows

$$s = \sum_{i=1}^{N} s_{\boldsymbol{m_i}}, \tag{25}$$

where each of the conditional term can be expressed as

$$\begin{aligned} s_{\boldsymbol{m_i}} &= \int_{\hat{\Xi}_i} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \\ &+ 3\sum_{\boldsymbol{m_p}} \sum_{\substack{\boldsymbol{m_q}\neq\boldsymbol{m_p} \\ \boldsymbol{m_p}\boxplus\boldsymbol{m_q}=\boldsymbol{m_i}}}^{N} \int_{\hat{\Xi}_i} f^2_{\boldsymbol{m_p}}(\boldsymbol{\xi}\cdot\boldsymbol{m_p}) f_{\boldsymbol{m_q}}(\boldsymbol{\xi}\cdot\boldsymbol{m_q}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \\ &+ 6\sum_{\boldsymbol{m_p}} \sum_{\substack{\boldsymbol{m_p} \\ q\geq p+1}} \sum_{\substack{\boldsymbol{m_{pqr}}=\boldsymbol{m_i} \\ r\geq q+1}} \int_{\hat{\Xi}_i} f_{\boldsymbol{m_p}}(\boldsymbol{\xi}\cdot\boldsymbol{m_p}) f_{\boldsymbol{m_q}}(\boldsymbol{\xi}\cdot\boldsymbol{m_q}) f_{\boldsymbol{m_r}}(\boldsymbol{\xi}\cdot\boldsymbol{m_r}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}), \end{aligned} \tag{26}$$

with $\boldsymbol{m_{pqr}} = \boldsymbol{m_p} \boxplus \boldsymbol{m_q} \boxplus \boldsymbol{m_r}$.

3.2.1 Kurtosis decomposition in conditional term

In this section, we illustrate the decomposition of the kurtosis. The functional decomposition based on the functional Sobol form (Eq. (5)) is equal to

$$
\begin{aligned}
k = & \sum_{i=1}^{N} \int_{\hat{\Xi}_i} f^4_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) + 4 \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} \int_{\hat{\Xi}_{ij}} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_{ij}}) \mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{ij}}) \\
& + 6 \sum_{i=1}^{N} \sum_{j=i+1}^{N} \int_{\hat{\Xi}_{ij}} f^2_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f^2_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_{ij}}) \mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{ij}}) \\
& + 12 \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} \sum_{\substack{k=j+1 \\ k\neq i}}^{N} \int_{\hat{\Xi}_{ijk}} f^2_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_{ijk}}) \mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{ijk}}) \\
& + 24 \sum_{i=1}^{N} \sum_{j=i+1}^{N} \sum_{k=j+1}^{N} \sum_{h=k+1}^{N} \int_{\hat{\Xi}_{ijkh}} f_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}) f_{\boldsymbol{m_h}}(\boldsymbol{\xi}\cdot\boldsymbol{m_h}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_{ijkh}}) \mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{ijkh}})
\end{aligned}
\tag{27}
$$

Proof. The expectancy of f^4 (see §2) is needed. The term $f^4(\boldsymbol{\xi})$, based on the functional decomposition (Eq. (5)), can be computed as the summation of five terms:

$$
\begin{aligned}
f^4(\boldsymbol{\xi}) = & \sum_{i=0}^{N} f^4_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) + 4 \sum_{i=0}^{N} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \sum_{\substack{j=0 \\ j\neq i}}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) \\
& + 6 \sum_{i=0}^{N} f^2_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \sum_{j=i+1}^{N} f^2_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) \\
& + 12 \sum_{i=0}^{N} f^2_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \sum_{\substack{j=0 \\ j\neq i}}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) \sum_{\substack{k=j+1 \\ k\neq i}}^{N} f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}) \\
& + 24 \sum_{i=0}^{N} f_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \sum_{j=i+1}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) \sum_{k=j+1}^{N} f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}) \sum_{h=k+1}^{N} f_{\boldsymbol{m_h}}(\boldsymbol{\xi}\cdot\boldsymbol{m_h}).
\end{aligned}
\tag{28}
$$

In the following, each of the above terms is manipulated to isolate the kurtosis expression (see (88)).

The first term of Eq. (28) can be written as

$$
\sum_{i=0}^{N} f^4_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) = f^4_{\boldsymbol{m_0}}(\boldsymbol{\xi}\cdot\boldsymbol{m_0}) + \sum_{i=1}^{N} f^4_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}). \tag{29}
$$

If it is integrated on the domain Ξ^d with a probability density function $p(\boldsymbol{\xi})$, we obtain

$$
\sum_{i=0}^{N} \int_{\Xi^d} f^4_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) p(\boldsymbol{\xi}) \mathrm{d}\boldsymbol{\xi} = \boxed{f^4_{\boldsymbol{m_0}}} + \sum_{i=1}^{N} \int_{\hat{\Xi}_i} f^4_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}). \tag{30}
$$

The second term of Eq. (28) can be expressed as follows

$$
\begin{aligned}
4\sum_{i=0}^{N} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\sum_{\substack{j=0\\ j\neq i}} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) &= 4f^3_{\boldsymbol{m_0}}\sum_{j=1}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) + 4\sum_{i=1}^{N} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\sum_{\substack{j=0\\ j\neq i}} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j})\\
&= 4f^3_{\boldsymbol{m_0}}\sum_{j=1}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) + 4\sum_{i=1}^{N} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m_0}}\\
&+ 4\sum_{i=1}^{N} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\sum_{\substack{j=1\\ j\neq i}}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}).
\end{aligned}
\tag{31}
$$

Integrating the above expression, it follows that

$$
\begin{aligned}
4\sum_{i=0}^{N}\sum_{\substack{j=0\\ j\neq i}}\int_{\Xi^d} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} &= \cancel{4f^3_{\boldsymbol{m_0}}\sum_{j=1}^{N}\int_{\hat{\Xi}_j} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_j})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_j})}\\
&+ \underline{4f_{\boldsymbol{m_0}}\sum_{i=1}^{N}\int_{\hat{\Xi}_i} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})}\\
&+ 4\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\int_{\hat{\Xi}_{ij}} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_{ij}})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{ij}})\\
&= \underline{4f_{\boldsymbol{m_0}}\sum_{i=1}^{N}\int_{\hat{\Xi}_i} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})}\\
&+ 4\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\int_{\hat{\Xi}_{ij}} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_{ij}})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{ij}}),
\end{aligned}
\tag{32}
$$

where the barred term is equal to zero.

The third term of Eq. (28) could be decomposed as

$$
6\sum_{i=0}^{N} f^2_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\sum_{j=i+1}^{N} f^2_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) = 6f^2_{\boldsymbol{m_0}}\sum_{j=1}^{N} f^2_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) + 6\sum_{i=1}^{N} f^2_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\sum_{j=i+1}^{N} f^2_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}).
\tag{33}
$$

When integrated on Ξ, we obtain

$$
\begin{aligned}
6\sum_{i=0}^{N}\sum_{j=i+1}^{N}\int_{\Xi^d} f^2_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f^2_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} &= \underline{\underline{6f^2_{\boldsymbol{m_0}}\sum_{j=1}^{N}\int_{\hat{\Xi}_j} f^2_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_j})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_j})}}\\
&+ 6\sum_{i=1}^{N}\sum_{j=i+1}^{N}\int_{\hat{\Xi}_{ij}} f^2_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f^2_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_{ij}})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{ij}}).
\end{aligned}
\tag{34}
$$

The double underlined term of Eq. (34) can be expressed as follows using Eq. (23)

$$6 f_{\boldsymbol{m_0}}^2 \sum_{j=1}^{N} \int_{\hat{\Xi}_j} f_{\boldsymbol{m_j}}^2(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) \mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) = 6E(f)^2\sigma^2. \tag{35}$$

The fourth term of Eq. (28) requires more manipulations

$$\begin{aligned}
&12\sum_{i=0}^{N} f_{\boldsymbol{m_i}}^2(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \sum_{\substack{j=0\\ j\neq i}}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) \sum_{\substack{k=j+1\\ k\neq i}}^{N} f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k})\\
&= 12 f_{\boldsymbol{m_0}}^2 \sum_{j=1}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) \sum_{k=j+1}^{N} f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k})\\
&+12\sum_{i=1}^{N} f_{\boldsymbol{m_i}}^2(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \sum_{\substack{j=0\\ j\neq i}}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) \sum_{\substack{k=j+1\\ k\neq i}}^{N} f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k})\\
&= 12 f_{\boldsymbol{m_0}}^2 \sum_{j=1}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) \sum_{k=j+1}^{N} f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}) + 12 f_{\boldsymbol{m_0}} \sum_{i=1}^{N} f_{\boldsymbol{m_i}}^2(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \sum_{\substack{k=1\\ k\neq i}}^{N} f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k})\\
&+12\sum_{i=1}^{N} f_{\boldsymbol{m_i}}^2(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \sum_{\substack{j=1\\ j\neq i}}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) \sum_{\substack{k=j+1\\ k\neq i}}^{N} f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}).
\end{aligned} \tag{36}$$

When integrated, it can be written as follows

$$\begin{aligned}
&12\sum_{i=0}^{N}\sum_{\substack{j=0\\ j\neq i}}^{N}\sum_{\substack{k=j+1\\ k\neq i}}^{N} \int_{\Xi^d} f_{\boldsymbol{m_i}}^2(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}) p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi}\\
&= \cancel{12 f_{\boldsymbol{m_0}}^2 \sum_{j=1}^{N}\sum_{k=j+1}^{N} \int_{\hat{\Xi}_{jk}} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_{jk}}) \mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{jk}})}\\
&\underline{+12 f_{\boldsymbol{m_0}} \sum_{i=1}^{N}\sum_{\substack{k=1\\ k\neq i}}^{N} \int_{\hat{\Xi}_{ik}} f_{\boldsymbol{m_i}}^2(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_{ik}}) \mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{ik}})}\\
&+12\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\sum_{\substack{k=j+1\\ k\neq i}}^{N} \int_{\hat{\Xi}_{ijk}} f_{\boldsymbol{m_i}}^2(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_{ijk}}) \mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{ijk}}),
\end{aligned} \tag{37}$$

where the first term is zero due to the orthogonality.

The last term of Eq. (28), first, is split into

$$
\begin{aligned}
&24\sum_{i=0}^{N} f_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \sum_{j=i+1}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) \sum_{k=j+1}^{N} f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}) \sum_{h=k+1}^{N} f_{\boldsymbol{m_h}}(\boldsymbol{\xi}\cdot\boldsymbol{m_h})\\
&\qquad = 24 f_{\boldsymbol{m_0}} \sum_{j=1}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) \sum_{k=j+1}^{N} f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}) \sum_{h=k+1}^{N} f_{\boldsymbol{m_h}}(\boldsymbol{\xi}\cdot\boldsymbol{m_h})\\
&+24\sum_{i=1}^{N} f_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \sum_{j=i+1}^{N} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) \sum_{k=j+1}^{N} f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}) \sum_{h=k+1}^{N} f_{\boldsymbol{m_h}}(\boldsymbol{\xi}\cdot\boldsymbol{m_h}).
\end{aligned}
\tag{38}
$$

When integrated on Ξ, we obtain

$$
\begin{aligned}
&24\sum_{i=0}^{N}\sum_{j=i+1}^{N}\sum_{k=j+1}^{N}\sum_{h=k+1}^{N}\int_{\hat{\Xi}_{ijkh}} f_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}) f_{\boldsymbol{m_h}}(\boldsymbol{\xi}\cdot\boldsymbol{m_h}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_{ijkh}})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{ijkh}})\\
&\qquad = \underline{24 f_{\boldsymbol{m_0}}\sum_{j=1}^{N}\sum_{k=j+1}^{N}\sum_{h=k+1}^{N}\int_{\hat{\Xi}_{jkh}} f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}) f_{\boldsymbol{m_h}}(\boldsymbol{\xi}\cdot\boldsymbol{m_h}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_{jkh}})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{jkh}})}\\
&+24\sum_{i=1}^{N}\sum_{j=i+1}^{N}\sum_{k=j+1}^{N}\sum_{h=k+1}^{N}\int_{\hat{\Xi}_{ijkh}} f_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k}) f_{\boldsymbol{m_h}}(\boldsymbol{\xi}\cdot\boldsymbol{m_h}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_{ijkh}})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_{ijkh}}).
\end{aligned}
\tag{39}
$$

The underlined term of the previous equations, (32), (37) and (39), can be summed up and collected into the term

$$
\begin{aligned}
&4 f_{\boldsymbol{m_0}}\Big(\sum_{i=1}^{N}\int_{\hat{\Xi}_i} f^3_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) p(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) + 3\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\int_{\hat{\Xi}_{ij}} f^2_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j})\\
&\quad +6\sum_{i=1}^{N}\sum_{j=i+1}^{N}\sum_{k=j+1}^{N}\int_{\hat{\Xi}_{ijk}} f_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) f_{\boldsymbol{m_j}}(\boldsymbol{\xi}\cdot\boldsymbol{m_j}) f_{\boldsymbol{m_k}}(\boldsymbol{\xi}\cdot\boldsymbol{m_k})\Big) = 4E(f)s,
\end{aligned}
\tag{40}
$$

where $f_{\boldsymbol{m_0}} = E(f)$ and the equation (95) is employed.

Now, if Eq. (28) is integrated on the stochastic domain Ξ, if some terms are moved to the left side and Eqs. (30), (32), (34), (37) and (39) are used, the final form of the kurtosis expressed in term of its functional decomposition (27) is obtained. $\square$

The number of terms in the case of the kurtosis decomposition in its conditional terms is equal to

$$
T_k = N + N(N-1) + \binom{N}{2} + N\binom{N-1}{2} + \binom{N}{4}. \tag{41}
$$

The number of terms can be expressed as a function of the stochastic dimension

d of the problem, employing $N+1=2^d$ as follows

$$T_k = \begin{cases} 1+(2^d-2)\left(2^d+2^{d-1}-\dfrac{1}{2}+\dfrac{1}{2}(2^d-1)(2^d-3)\right), & \text{with} \quad d=2 \\ 1+(2^d-2)\left(2^d+2^{d-1}-\dfrac{1}{2}+\dfrac{1}{2}(2^d-1)(2^d-3)\right)+\dbinom{2^d-1}{4}, & \text{with} \quad d\geq 3. \end{cases} \tag{42}$$

Table 2 is obtained from Table 1 by adding the values for the kurtosis.

Dimension	Variance	Skewness	Kurtosis
2	3	10	15
3	7	84	210
4	15	680	3060
5	31	5456	46376

Table 2: Number of terms in the functional decomposition for variance, skewness and kurtosis

Also in this case, kurtosis (27) can be written using an additive form as follows

$$k=\sum_{i=1}^{N} k_{\boldsymbol{m_i}}, \tag{43}$$

where each term $k_{\boldsymbol{m_i}}$ can be computed as

$$\begin{aligned} k_{\boldsymbol{m_i}} = & \int_{\hat{\Xi}_i} f^4_{\boldsymbol{m_i}}(\boldsymbol{\xi}\cdot\boldsymbol{m_i})p(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) + 4\sum_{\boldsymbol{m_p}}\sum_{\substack{q\neq p\\ \boldsymbol{m_p}\boxplus\boldsymbol{m_q}=\boldsymbol{m_i}}}\int_{\hat{\Xi}_i} f^3_{\boldsymbol{m_p}}(\boldsymbol{\xi}\cdot\boldsymbol{m_p})f_{\boldsymbol{m_q}}(\boldsymbol{\xi}\cdot\boldsymbol{m_q})p(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \\ & + 6\sum_{\boldsymbol{m_p}}\sum_{\substack{q\neq p\\ \boldsymbol{m_p}\boxplus\boldsymbol{m_q}=\boldsymbol{m_i}}}\int_{\hat{\Xi}_i} f^2_{\boldsymbol{m_p}}(\boldsymbol{\xi}\cdot\boldsymbol{m_p})f^2_{\boldsymbol{m_q}}(\boldsymbol{\xi}\cdot\boldsymbol{m_q})p(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \\ & + 12\sum_{\boldsymbol{m_p}}\sum_{\boldsymbol{m_q}\neq\boldsymbol{m_p}}\sum_{\substack{\boldsymbol{m_{pqr}}=\boldsymbol{m_i}\\ r\geq q+1}}\int_{\hat{\Xi}_i} f^2_{\boldsymbol{m_p}}(\boldsymbol{\xi}\cdot\boldsymbol{m_p})f_{\boldsymbol{m_q}}(\boldsymbol{\xi}\cdot\boldsymbol{m_q})f_{\boldsymbol{m_r}}(\boldsymbol{\xi}\cdot\boldsymbol{m_r})p(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}) \\ & + 24\sum_{\boldsymbol{m_p}}\sum_{\substack{\boldsymbol{m_q}\\ q\geq p+1}}\sum_{\substack{\boldsymbol{m_r}\\ r\geq q+1}}\sum_{\substack{\boldsymbol{m_{pqrt}}=\boldsymbol{m_i}\\ t\geq r+1}}\int_{\hat{\Xi}_i} f_{\boldsymbol{m_p}}(\boldsymbol{\xi}\cdot\boldsymbol{m_p})f_{\boldsymbol{m_q}}(\boldsymbol{\xi}\cdot\boldsymbol{m_q})f_{\boldsymbol{m_r}}(\boldsymbol{\xi}\cdot\boldsymbol{m_r})f_{\boldsymbol{m_t}}(\boldsymbol{\xi}\cdot\boldsymbol{m_t})p(\boldsymbol{\xi}\cdot\boldsymbol{m_i})\mathrm{d}(\boldsymbol{\xi}\cdot\boldsymbol{m_i}), \end{aligned} \tag{44}$$

where obviously $\boldsymbol{m_{pqr}}=\boldsymbol{m_p}\boxplus\boldsymbol{m_q}\boxplus\boldsymbol{m_r}$ and $\boldsymbol{m_{pqrt}}=\boldsymbol{m_p}\boxplus\boldsymbol{m_q}\boxplus\boldsymbol{m_r}\boxplus\boldsymbol{m_t}$.

4 Correlation with Polynomial Chaos Framework

This section is devoted to show how formulas of variance, skewness and kurtosis from the functional decomposition are correlated with the polynomial chaos framework. If a polynomial chaos formulation is used, an approximation $\tilde{f}$ of the function f is provided

$$f(\boldsymbol{\xi})\approx\tilde{f}(\boldsymbol{\xi})=\sum_{k=0}^{P}\beta_k\Psi_k(\boldsymbol{\xi}), \tag{45}$$

where P is computed according to the order of the polynomial expansion n_0 and the stochastic dimension of the problem d

$$P + 1 = \frac{(n_0 + d)!}{n_0! d!}. \tag{46}$$

Each polynomial $\Psi_k(\boldsymbol{\xi})$ of total degree n_o is a multivariate polynomial form which involve tensorization of 1D polynomial form by using a multi-index $\boldsymbol{\alpha}^k \in \mathbb{R}^d$, with $\sum_{i=1}^d \boldsymbol{\alpha}_i^k \le n_0$:

$$\Psi_k(\boldsymbol{\xi} \cdot \boldsymbol{m}^{\star,k}) = \prod_{\substack{i=1 \\ m_i^{\star,k} \neq 0}}^{d} \psi_{\alpha_i^k}(\xi_i) \tag{47}$$

where the multi index $\boldsymbol{m}^{\star,k} = \boldsymbol{m}^{\star,k}(\boldsymbol{\alpha}^k) \in \mathbb{R}^d$ is a function of $\boldsymbol{\alpha}^k$: $\boldsymbol{m}^{\star,k} = (m_1^{\star,k}, \ldots, m_d^{\star,k})$, with $m_i^{\star,k} = \alpha_i^k / \left|\left|\alpha_i^k\right|\right|_{\neq 0}$.

Remark that, for each polynomial basis, $\psi_0(\xi_i) = 1$ and then $\Psi_0(\boldsymbol{\xi}) = 1$. Then, the first coefficient β_0 is equal to the expected value of the function, *i.e.* $E(f)$. The polynomial basis is chosen accordingly to the Wiener-Askey scheme in order to select orthogonal polynomials with respect to the probability density function $p(\boldsymbol{\xi})$ of the input. Thanks to the orthogonality, the following relation holds

$$\int_\Xi \Psi_i(\boldsymbol{\xi})\Psi_k(\boldsymbol{\xi})p(\boldsymbol{\xi})\mathrm{d}\xi = \delta_{ij}\langle \Psi_i(\boldsymbol{\xi}), \Psi_i(\boldsymbol{\xi})\rangle \tag{48}$$

where $\langle \cdot, \cdot \rangle$ indicates the inner product and δ_{ij} is the Kronecker delta function.

The orthogonality can be advantageously used to compute the coefficients of the expansion in a non-intrusive PC framework

$$\beta_k = \frac{\langle f(\boldsymbol{\xi}), \Psi_k(\boldsymbol{\xi})\rangle}{\langle \Psi_k(\boldsymbol{\xi}), \Psi_k(\boldsymbol{\xi})\rangle}, \quad \forall k. \tag{49}$$

4.1 Variance decomposition

First, we compute the term $E(f^2)$ as follows

$$\int_{\Xi^d} f(\boldsymbol{\xi})^2 p(\boldsymbol{\xi})\mathrm{d}\xi = \int_{\Xi^d} \left(\sum_{k=0}^{P} \beta_k \Psi_k(\boldsymbol{\xi})\right)^2 p(\boldsymbol{\xi})\mathrm{d}\xi. \tag{50}$$

This term can be computed easily due to the orthogonality :

$$\int_{\Xi^d} \left(\sum_{k=0}^{P} \beta_k \Psi_k(\boldsymbol{\xi})\right)^2 p(\boldsymbol{\xi})\mathrm{d}\xi = \sum_{k=0}^{P} \beta_k^2 \langle \Psi_k^2(\boldsymbol{\xi})\rangle. \tag{51}$$

As a consequence, variance can be easily computed as

$$\sigma^2 = E(f^2) - E(f)^2 = \sum_{k=1}^{P} \beta_k^2 \langle \Psi_k^2(\boldsymbol{\xi})\rangle. \tag{52}$$

Finally, an explicit correlation between the last expression and the Eq. (12) is found. As done for the the functional decomposition of the variance (see

§3.1), let us compute each conditional term of the variance. Remembering the equation (13), each conditional term can be computed as

$$\sigma^2_{\boldsymbol{m_i}} = \sum_{k \in K_{\boldsymbol{m_i}}} \beta_k^2 \langle \Psi_k^2(\boldsymbol{\xi}) \rangle, \tag{53}$$

where $K_{\boldsymbol{m_i}}$ represent the set of indexes in associated to the variable contained in the vector $(\boldsymbol{\xi} \cdot \boldsymbol{m_i})$:

$$K_{\boldsymbol{m_i}} = \left\{ k \in \{1, \ldots, P\} \,|\, \boldsymbol{m}^{\star,k} = \boldsymbol{m}^{\star,k}(\boldsymbol{\alpha}^k) = \boldsymbol{m_i} \right\} \tag{54}$$

4.2 Skewness decomposition

In this section, the conditional terms associated to the skewness are computed starting from the polynomial chaos formulation. This procedure is the same usually followed for the variance.

After many manipulations (reported in B.1), the final expression for the skewness is given by

$$\begin{aligned} s = &\sum_{k=1}^{P} \beta_k^3 \langle \Psi_k^3(\boldsymbol{\xi}) \rangle \\ &+ 3 \sum_{i=1}^{P} \beta_i^2 \sum_{\substack{j=1 \\ j \neq i}}^{P} \beta_j \langle \Psi_i^2(\boldsymbol{\xi}), \Psi_j(\boldsymbol{\xi}) \rangle \\ &+ 6 \sum_{i=1}^{P} \sum_{j=i+1}^{P} \sum_{k=j+1}^{P} \beta_i \beta_j \beta_k \langle \Psi_i(\boldsymbol{\xi}), \Psi_j(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi}) \rangle, \end{aligned} \tag{55}$$

that is constituted by the summation of *monadic*, *dyadic* and *triadic* interactions between the terms of the polynomial chaos approximation. Remark that this expression has the same structure than that one obtained by means of the functional decomposition (see Eq. (15)).

The number of terms composing the skewness can be estimated by using $T = P + P(P-1) + \binom{P}{3}$. Then, considering that $P + 1 = \frac{(n_0+d)!}{n_0! d!}$, the total number of terms depends on both the total degree of the polynomial expansion n_0 and the stochastic dimension d. In Table 3, the numbers of terms for an increasing dimension up to five and an increasing polynomial order n_0 up to five, are reported compared to the number of terms (P) allowing the computation of the variance.

$d \setminus n_0$	2	3	4	5
2	(5;35)	(9;165)	(14;560)	(20;1540)
3	(9;165)	(19;1330)	(34;7140)	(55;29260)
4	(14;560)	(34;7140)	(69;57155)	(125;333375)
5	(20;1540)	(55;29260)	(125;333375)	(251;2667126)

Table 3: Couple of terms $(\sigma^2; s)$ for several combinations of stochastic dimension d and total degree of approximation n_0.

In this case, the identification of each conditional term becomes more difficult due to high-order interactions between the polynomial terms of the basis.

Remembering the equation (25), we can express each conditional term as

$$
\begin{aligned}
s_{\boldsymbol{m_i}} = & \sum_{k \in K_{\boldsymbol{m_i}}} \beta_k^3 \langle \Psi_k^3(\boldsymbol{\xi}) \rangle + 3 \sum_{p \in K_{\boldsymbol{m_p}}} \beta_p^2 \sum_{\substack{q \in K_{\boldsymbol{m_q}} - \{p\} \\ \boldsymbol{m_p} \boxplus \boldsymbol{m_q} = \boldsymbol{m_i}}} \beta_q \langle \Psi_p^2(\boldsymbol{\xi}), \Psi_q(\boldsymbol{\xi}) \rangle \\
& + 6 \sum_{p \in K_{\boldsymbol{m_p}}} \sum_{\substack{q \in K_{\boldsymbol{m_q}} \\ q \geq p+1}} \sum_{\substack{r \in K_{\boldsymbol{m_r}} \\ \boldsymbol{m_{pqr}} = \boldsymbol{m_i}}} \beta_p \beta_q \beta_r \langle \Psi_p(\boldsymbol{\xi}), \Psi_q(\boldsymbol{\xi}) \Psi_r(\boldsymbol{\xi}) \rangle,
\end{aligned}
\tag{56}
$$

where, as usual, $\boldsymbol{m_{pqr}} = \boldsymbol{m_p} \boxplus \boldsymbol{m_q} \boxplus \boldsymbol{m_r}$.

4.3 Kurtosis decomposition

The conditional terms for the kurtosis are presented in this section.

Employing several manipulations (detailed in B.2), the equation (98) can be recast to recover the kurtosis, as it is written in Eq. (87)

$$
\begin{aligned}
k = & \int f^4(\boldsymbol{\xi}) p(\boldsymbol{\xi}) \mathrm{d}\xi - 4E(f)s - 6\sigma^2 E(f)^2 - E(f)^4 \\
= & \sum_{k=1}^{P} \beta_k^4 \langle \Psi_k^4(\boldsymbol{\xi}) \rangle + 4 \sum_{i=1}^{P} \beta_i^3 \sum_{\substack{j=1 \\ j \neq i}}^{P} \beta_j \langle \Psi_i^3, \Psi_j \rangle + 6 \sum_{i=1}^{P} \beta_i^2 \sum_{j=i+1}^{P} \beta_j^2 \langle \Psi_i^2, \Psi_j^2 \rangle \\
& + 12 \sum_{i=1}^{P} \beta_i^2 \sum_{\substack{j=1 \\ j \neq i}}^{P} \beta_j \sum_{\substack{k=j+1 \\ k \neq i}}^{P} \beta_k \langle \Psi_i^2, \Psi_j \Psi_k \rangle + 24 \sum_{i=1}^{P} \sum_{j=i+1}^{P} \sum_{k=j+1}^{P} \sum_{h=k+1}^{P} \beta_i \beta_j \beta_k \beta_h \langle \Psi_i \Psi_j, \Psi_k \Psi_h \rangle.
\end{aligned}
\tag{57}
$$

The total number of terms to compute is equal to

$$
T_k = P + P(P-1) + \binom{P}{2} + P\binom{P-1}{2} + \binom{P}{4}, \tag{58}
$$

where the number of terms P depends from both the total degree of the approximation n_0 and the stochastic dimension of the system d: $P + 1 = \frac{(n_0+d)!}{n_0! d!}$.

The single conditional terms associated to the multi-index $\boldsymbol{m_i}$ can be computed as

$$
\begin{aligned}
k_{\boldsymbol{m_i}} = & \sum_{k \in K_{\boldsymbol{m_i}}} \beta_k^4 \langle \Psi_k^4(\boldsymbol{\xi}) \rangle + 4 \sum_{p \in K_{\boldsymbol{m_p}}} \beta_p^3 \sum_{\substack{q \in K_{\boldsymbol{m_q}} - \{p\} \\ \boldsymbol{m_p} \boxplus \boldsymbol{m_q} = \boldsymbol{m_i}}} \beta_q \langle \Psi_p^3, \Psi_q \rangle \\
& + 6 \sum_{p \in K_{\boldsymbol{m_p}}} \beta_p^2 \sum_{\substack{q \in K_{\boldsymbol{m_q}} - \{p\} \\ \boldsymbol{m_p} \boxplus \boldsymbol{m_q} = \boldsymbol{m_i}}} \beta_q^2 \langle \Psi_p^2, \Psi_q^2 \rangle \\
& + 12 \sum_{p \in K_{\boldsymbol{m_p}}} \beta_p^2 \sum_{q \in K_{\boldsymbol{m_q}} - \{p\}} \beta_q \sum_{\substack{r \in K_{\boldsymbol{m_r}} \\ r \geq q+1 \\ \boldsymbol{m_{pqr}} = \boldsymbol{m_i}}} \beta_r \langle \Psi_p^2, \Psi_q \Psi_r \rangle \\
& + 24 \sum_{p \in K_{\boldsymbol{m_p}}} \sum_{\substack{q \in K_{\boldsymbol{m_q}} \\ q \geq p+1}} \sum_{\substack{r \in K_{\boldsymbol{m_r}} \\ r \geq q+1}} \sum_{\substack{t \in K_{\boldsymbol{m_t}} \\ t \geq r+1 \\ \boldsymbol{m_{pqrt}} = \boldsymbol{m_i}}} \beta_p \beta_q \beta_r \beta_t \langle \Psi_p \Psi_q, \Psi_r \Psi_t \rangle.
\end{aligned}
\tag{59}
$$

In the next section the sensitivity indexes are defined extending the classical framework [19] based on the variance.

4.4 Numerical example on a toy-function: computation and decomposition of high-order statistics

In this section, an analytical example is provided with the exact computation of the variance, skewness and kurtosis, showing the correlation between the PC framework and the functional decomposition.

Let us consider a function of total degree equal to two

$$f(\boldsymbol{\xi}) = \xi_1^2 + \xi_1\xi_2 + \xi_2^2, \tag{60}$$

with $\xi_i \sim \mathcal{U}(0,1)$. The exact solution for the expected value $E(f)$, the variance σ^2, the skewness s and kurtosis k are equal to

$$\begin{aligned} E(f) &= \frac{11}{12} \\ \sigma^2 &= \frac{283}{720} \\ s &= \frac{5203}{30240} \\ k &= \frac{543521}{1209600}. \end{aligned}$$

Moreover, the ANOVA functional expansion is computed as follows

$$f(\boldsymbol{\xi}) = f_0 + f_{\xi_1} + f_{\xi_2} + f_{\xi_1\xi_2}, \tag{61}$$

where

$$\begin{aligned} f_0 &= \int_{\Xi^2} f(\boldsymbol{\xi})p(\boldsymbol{\xi})\mathrm{d}\xi = \frac{11}{12} \\ f_{\xi_1} &= \int_{\Xi} f(\boldsymbol{\xi})p(\xi_2)\mathrm{d}\xi_2 - f_0 = \xi_1^2 - \frac{1}{2}\xi_1 - \frac{7}{12} \\ f_{\xi_2} &= \int_{\Xi} f(\boldsymbol{\xi})p(\xi_1)\mathrm{d}\xi_1 - f_0 = \xi_2^2 - \frac{1}{2}\xi_2 - \frac{7}{12} \\ f_{\xi_1\xi_2} &= f(\boldsymbol{\xi}) - f_{\xi_1} - f_{\xi_2} - f_0 = \xi_1\xi_2 - \frac{1}{2}\xi_1 - \frac{1}{2}\xi_2 + \frac{1}{4}. \end{aligned} \tag{62}$$

The overall variance σ^2 can be computed by means of the ANOVA expansion as

$$\sigma^2 = \sigma^2_{\xi_1} + \sigma^2_{\xi_2} + \sigma^2_{\xi_1\xi_2}, \tag{63}$$

where

$$\begin{aligned} \sigma^2_{\xi_1} &= \int_{\Xi} f^2_{\xi_1} p(\xi_1)\mathrm{d}\xi_1 = \frac{139}{720} \\ \sigma^2_{\xi_2} &= \int_{\Xi} f^2_{\xi_2} p(\xi_2)\mathrm{d}\xi_2 = \frac{139}{720} \\ \sigma^2_{\xi_1\xi_2} &= \int_{\Xi^2} f^2_{\xi_1\xi_2} p(\boldsymbol{\xi})\mathrm{d}\xi = \frac{1}{144} \end{aligned} \tag{64}$$

In this case ($d = 2$), the number of terms to compute for the skewness is 10. Considering the following nomenclature

$$\begin{aligned} f_{\xi_1} &= f_{\boldsymbol{m}_1} \\ f_{\xi_2} &= f_{\boldsymbol{m}_2} \\ f_{\xi_1\xi_2} &= f_{\boldsymbol{m}_3}, \end{aligned} \tag{65}$$

the equation (15) can be written as follows

$$
\begin{aligned}
s = & \int_{\Xi} f_{\xi_1}^3 p(\xi_1)\mathrm{d}\xi_1 + \int_{\Xi} f_{\xi_2}^3 p(\xi_2)\mathrm{d}\xi_2 + \int_{\Xi^2} f_{\xi_1\xi_2}^3 p(\boldsymbol{\xi})\mathrm{d}\xi \\
& + 3\Bigg(\int_{\Xi^2} f_{\xi_1}^2 f_{\xi_2} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_1}^2 f_{\xi_1\xi_2} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_2}^2 f_{\xi_1} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \\
& + \int_{\Xi^2} f_{\xi_2}^2 f_{\xi_1\xi_2} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_1\xi_2}^2 f_{\xi_1} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \int_{\Xi^2} f_{\xi_1\xi_2}^2 f_{\xi_2} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \Bigg) \\
& + 6 \int_{\Xi^2} f_{\xi_1} f_{\xi_2} f_{\xi_1\xi_2} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi}.
\end{aligned} \tag{66}
$$

Looking for an additive form for the skewness, *i.e.*

$$
s = s_{\xi_1} + s_{\xi_2} + s_{\xi_1\xi_2},
$$

the conditional skewness can be computed as follows

$$
\begin{aligned}
s_{\xi_1} &= \int_{\Xi} f_{\xi_1}^3 p(\xi_1)\mathrm{d}\xi_1 = \frac{571}{15120} \\
s_{\xi_2} &= \int_{\Xi} f_{\xi_2}^3 p(\xi_2)\mathrm{d}\xi_2 = \frac{571}{15120} \\
s_{\xi_1\xi_2} &= \int_{\Xi^2} f_{\xi_1\xi_2}^3 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \\
& \quad + 3\Bigg(\int_{\Xi^2} f_{\xi_1}^2 f_{\xi_2} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_1}^2 f_{\xi_1\xi_2} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_2}^2 f_{\xi_1} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \\
& \quad + \int_{\Xi^2} f_{\xi_2}^2 f_{\xi_1\xi_2} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_1\xi_2}^2 f_{\xi_1} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \int_{\Xi^2} f_{\xi_1\xi_2}^2 f_{\xi_2} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \Bigg) \\
& \quad + 6 \int_{\Xi^2} f_{\xi_1} f_{\xi_2} f_{\xi_1\xi_2} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} = \frac{139}{1440}.
\end{aligned} \tag{67}
$$

The kurtosis can be computed as

$$
\begin{aligned}
k = & \int_{\Xi} f_{\xi_1}^4 p(\xi_1)\mathrm{d}\xi_1 + \int_{\Xi} f_{\xi_2}^4 p(\xi_2)\mathrm{d}\xi_2 + \int_{\Xi^2} f_{\xi_1\xi_2}^4 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \\
& + 4\Bigg(\int_{\Xi^2} f_{\xi_1}^3 f_{\xi_2}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_1}^3 f_{\xi_1\xi_2}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_2}^3 f_{\xi_1}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \\
& + \int_{\Xi^2} f_{\xi_2}^3 f_{\xi_1\xi_2}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_1\xi_2}^3 f_{\xi_1}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_1\xi_2}^3 f_{\xi_2}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \Bigg) \\
& + 6\Bigg(\int_{\Xi^2} f_{\xi_1}^2 f_{\xi_2}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_1}^2 f_{\xi_1\xi_2}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_2}^2 f_{\xi_1\xi_2}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \Bigg) \\
& + 12\Bigg(\int_{\Xi^2} f_{\xi_1}^2 f_{\xi_2} f_{\xi_1\xi_2} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_2}^2 f_{\xi_1} f_{\xi_1\xi_2} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_1\xi_2}^2 f_{\xi_1} f_{\xi_2} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \Bigg),
\end{aligned} \tag{68}
$$

where the conditional indexes are equal to

$$
\begin{aligned}
k_{\xi_1} &= \int_{\Xi} f_{\xi_1}^4 p(\xi_1)\mathrm{d}\xi_1 = \frac{17701}{241920} \\
k_{\xi_2} &= \int_{\Xi} f_{\xi_2}^4 p(\xi_2)\mathrm{d}\xi_2 = \frac{17701}{241920} \\
k_{\xi_1\xi_2} &= \int_{\Xi^2} f_{\xi_1\xi_2}^4 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \\
&\quad + 4\Bigg(\int_{\Xi^2} f_{\xi_1}^3 f_{\xi_2}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_1}^3 f_{\xi_1\xi_2}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_2}^3 f_{\xi_1}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \\
&\quad + \int_{\Xi^2} f_{\xi_2}^3 f_{\xi_1\xi_2}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_1\xi_2}^3 f_{\xi_1}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_1\xi_2}^3 f_{\xi_2}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \Bigg) \\
&\quad + 6\Bigg(\int_{\Xi^2} f_{\xi_1}^2 f_{\xi_2}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_1}^2 f_{\xi_1\xi_2}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_2}^2 f_{\xi_1\xi_2}^2 p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \Bigg) \\
&\quad + 12\Bigg(\int_{\Xi^2} f_{\xi_1}^2 f_{\xi_2} f_{\xi_1\xi_2} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_2}^2 f_{\xi_1} f_{\xi_1\xi_2} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} + \int_{\Xi^2} f_{\xi_1\xi_2}^2 f_{\xi_1} f_{\xi_2} p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \Bigg) = \frac{366511}{1209600}.
\end{aligned}
\tag{69}
$$

The use of the polynomial chaos expansion permits to obtain the same results. In this case, we need to compute all the coefficients appearing in the Legendre polynomial basis. The number of terms of the polynomial chaos expansion is equal to $P+1=6$ for a total order of 2 and for two dimensions in the stochastic space. Then, in this case, a tensorization of the first three monodimensional Legendre basis is demanded, *i.e.*

$$
\begin{aligned}
P_0(\xi) &= 1 \\
P_1(\xi) &= 2\xi - 1 \\
P_2(\xi) &= 6\xi^2 - 6\xi + 1.
\end{aligned}
$$

The six terms of the PC basis are

$$
\begin{array}{lll}
\boldsymbol{\alpha}^0 = (0,0), & \boldsymbol{m}^{\star,0} = (0,0) & \rightarrow \quad \Psi_0(\boldsymbol{\xi}\cdot\boldsymbol{m}^{\star,0}) = 1 \\
\boldsymbol{\alpha}^1 = (1,0), & \boldsymbol{m}^{\star,1} = (1,0) & \rightarrow \quad \Psi_1(\boldsymbol{\xi}\cdot\boldsymbol{m}^{\star,1}) = 2\xi_1 - 1 \\
\boldsymbol{\alpha}^2 = (0,1), & \boldsymbol{m}^{\star,2} = (0,1) & \rightarrow \quad \Psi_2(\boldsymbol{\xi}\cdot\boldsymbol{m}^{\star,2}) = 2\xi_2 - 1 \\
\boldsymbol{\alpha}^3 = (1,1), & \boldsymbol{m}^{\star,3} = (1,1) & \rightarrow \quad \Psi_3(\boldsymbol{\xi}\cdot\boldsymbol{m}^{\star,3}) = (2\xi_1 - 1)(2\xi_1 - 1) \\
\boldsymbol{\alpha}^4 = (2,0), & \boldsymbol{m}^{\star,4} = (1,0) & \rightarrow \quad \Psi_4(\boldsymbol{\xi}\cdot\boldsymbol{m}^{\star,4}) = 6\xi_1^2 - 6\xi + 1 \\
\boldsymbol{\alpha}^5 = (0,2), & \boldsymbol{m}^{\star,5} = (0,1) & \rightarrow \quad \Psi_5(\boldsymbol{\xi}\cdot\boldsymbol{m}^{\star,5}) = 6\xi_2^2 - 6\xi + 1.
\end{array}
\tag{70}
$$

Each coefficient of the series can be computed using the orthogonality property (Eq. (49) is reported here for convenience)

$$
\beta_k = \frac{\int_{\Xi} f(\boldsymbol{\xi})\Psi_k(\boldsymbol{\xi})\, p(\boldsymbol{\xi})\mathrm{d}\xi}{\int_{\Xi} \Psi_k^2(\boldsymbol{\xi})\, p(\boldsymbol{\xi})\mathrm{d}\xi}, \quad \forall k
$$

obtaining

$$
\beta_0 = \frac{11}{12},\ \beta_1 = \beta_2 = \frac{3}{4},\ \beta_3 = \frac{1}{4},\ \text{and } \beta_4 = \beta_5 = \frac{1}{6}. \tag{71}
$$

Remark that the coefficient β_0 is the mean and the variance can be computed as shown in the equation (96)

$$\sigma^2 = \sum_{i=1}^{P} \beta_k^2 \Psi_k^2(\boldsymbol{\xi}) = \frac{283}{720}.$$

In order to compute the skewness, 35 terms should be computed for $d = 2$ and $n_0 = 2$. We can split Eq. (55) to obtain all the conditional terms

$$\begin{aligned}
s_{\xi_1} &= \beta_1^3 \langle \Psi_1^3 \rangle + \beta_4^3 \langle \Psi_4^3 \rangle + 3\beta_1^2 \beta_4 \langle \Psi_1^2, \Psi_4 \rangle + 3\beta_4^2 \beta_1 \langle \Psi_4^2, \Psi_1 \rangle = \frac{571}{15120} \\
s_{\xi_2} &= \beta_2^3 \langle \Psi_2^3 \rangle + \beta_5^3 \langle \Psi_5^3 \rangle + 3\beta_2^2 \beta_5 \langle \Psi_2^2, \Psi_5 \rangle + 3\beta_5^2 \beta_2 \langle \Psi_5^2, \Psi_2 \rangle = \frac{571}{15120} \\
s_{\xi_1 \xi_2} &= \beta_3^3 \langle \Psi_3^3 \rangle + 3\beta_1^2 \Bigg(\beta_2 \langle \Psi_1^2, \Psi_2 \rangle + \beta_3 \langle \Psi_1^2, \Psi_3 \rangle + \beta_5 \langle \Psi_1^2, \Psi_5 \rangle \Bigg) \\
&+ 3\beta_2^2 \Bigg(\beta_1 \langle \Psi_2^2, \Psi_1 \rangle + \beta_3 \langle \Psi_2^2, \Psi_3 \rangle + \beta_4 \langle \Psi_2^2, \Psi_4 \rangle \Bigg) \\
&+ 3\beta_3^2 \Bigg(\beta_1 \langle \Psi_3^2, \Psi_1 \rangle + \beta_2 \langle \Psi_3^2, \Psi_2 \rangle + \beta_4 \langle \Psi_2^2, \Psi_4 \rangle + \beta_5 \langle \Psi_2^2, \Psi_5 \rangle \Bigg) \\
&+ 3\beta_4^2 \Bigg(\beta_1 \langle \Psi_4^2, \Psi_1 \rangle + \beta_2 \langle \Psi_4^2, \Psi_2 \rangle + \beta_3 \langle \Psi_4^2, \Psi_3 \rangle + \beta_5 \langle \Psi_4^2, \Psi_5 \rangle \Bigg) \\
&+ 3\beta_5^2 \Bigg(\beta_1 \langle \Psi_5^2, \Psi_1 \rangle + \beta_3 \langle \Psi_5^2, \Psi_3 \rangle + \beta_4 \langle \Psi_5^2, \Psi_4 \rangle \Bigg) \\
&+ 6\beta_1 \beta_2 \Bigg(\beta_3 \langle \Psi_1 \Psi_2, \Psi_3 \rangle + \beta_4 \langle \Psi_1 \Psi_2, \Psi_4 \rangle + \beta_5 \langle \Psi_1 \Psi_2, \Psi_5 \rangle \Bigg) \\
&+ 6\beta_1 \beta_3 \Bigg(\beta_4 \langle \Psi_1 \Psi_3, \Psi_4 \rangle + \beta_5 \langle \Psi_1 \Psi_3, \Psi_5 \rangle \Bigg) + 6\beta_1 \beta_4 \beta_5 \langle \Psi_1, \Psi_4 \Psi_5 \rangle \\
&+ 6\beta_2 \beta_3 \Bigg(\beta_4 \langle \Psi_2 \Psi_3, \Psi_4 \rangle + \beta_5 \langle \Psi_2 \Psi_3, \Psi_5 \rangle \Bigg) + 6\beta_2 \beta_4 \beta_5 \langle \Psi_2, \Psi_4 \Psi_5 \rangle \\
&+ 6\beta_3 \beta_4 \beta_5 \langle \Psi_3, \Psi_4 \Psi_5 \rangle = \frac{139}{1440}.
\end{aligned}$$

For the kurtosis, employing the relation (59), the conditional terms can be obtained by PC as follows

$$k_{\xi_1} = \beta_1^4\langle\Psi_1^4\rangle + \beta_4^4\langle\Psi_4^4\rangle + 4\beta_1^3\beta_4\langle\Psi_1^3,\Psi_4\rangle + 4\beta_1\beta_4^3\langle\Psi_1,\Psi_4^3\rangle + 6\beta_1^2\beta_4^2\langle\Psi_1^2,\Psi_4^2\rangle = \frac{17701}{241920}$$

$$k_{\xi_2} = \beta_2^4\langle\Psi_2^4\rangle + \beta_5^4\langle\Psi_5^4\rangle + 4\beta_2^3\beta_5\langle\Psi_2^3,\Psi_5\rangle + 4\beta_2\beta_5^3\langle\Psi_2,\Psi_5^3\rangle + 6\beta_2^2\beta_5^2\langle\Psi_2^2,\Psi_5^2\rangle = \frac{17701}{241920}$$

$$\begin{aligned}
k_{\xi_1\xi_2} &= \beta_3^4\langle\Psi_3^4\rangle \\
&+ 4\beta_1^3\left(\beta_2\langle\Psi_1^3,\Psi_2\rangle + \beta_3\langle\Psi_1^3,\Psi_3\rangle + \beta_5\langle\Psi_1^3,\Psi_5\rangle\right) + 4\beta_2^3\left(\beta_1\langle\Psi_2^3,\Psi_1\rangle + \beta_3\langle\Psi_2^3,\Psi_3\rangle + \beta_4\langle\Psi_2^3,\Psi_4\rangle\right) \\
&+ 4\beta_3^3\left(\beta_1\langle\Psi_3^3,\Psi_1\rangle + \beta_2\langle\Psi_3^3,\Psi_2\rangle + \beta_4\langle\Psi_3^3,\Psi_4\rangle + \beta_5\langle\Psi_3^3,\Psi_5\rangle\right) \\
&+ 4\beta_4^3\left(\beta_2\langle\Psi_4^3,\Psi_2\rangle + \beta_3\langle\Psi_4^3,\Psi_3\rangle + \beta_5\langle\Psi_4^3,\Psi_5\rangle\right) + 4\beta_5^3\left(\beta_1\langle\Psi_5^3,\Psi_1\rangle + \beta_3\langle\Psi_5^3,\Psi_3\rangle + \beta_4\langle\Psi_5^3,\Psi_4\rangle\right) \\
&+ 6\beta_1^2\beta_2^2\langle\Psi_1^2,\Psi_2^2\rangle + 6\beta_1^2\beta_3^2\langle\Psi_1^2,\Psi_3^2\rangle + 6\beta_1^2\beta_5^2\langle\Psi_1^2,\Psi_5^2\rangle + 6\beta_2^2\beta_3^2\langle\Psi_2^2,\Psi_3^2\rangle \\
&+ 6\beta_2^2\beta_4^2\langle\Psi_2^2,\Psi_4^2\rangle + 6\beta_3^2\beta_4^2\langle\Psi_3^2,\Psi_4^2\rangle + 6\beta_3^2\beta_5^2\langle\Psi_3^2,\Psi_5^2\rangle + 6\beta_4^2\beta_5^2\langle\Psi_4^2,\Psi_5^2\rangle \\
&+ 12\beta_1^2\Big(\beta_2\beta_3\langle\Psi_1^2,\Psi_2\Psi_3\rangle + \beta_2\beta_4\langle\Psi_1^2,\Psi_2\Psi_4\rangle + \beta_2\beta_5\langle\Psi_1^2,\Psi_2\Psi_5\rangle \\
&\qquad + \beta_3\beta_4\langle\Psi_1^2,\Psi_3\Psi_4\rangle + \beta_3\beta_5\langle\Psi_1^2,\Psi_3\Psi_5\rangle + \beta_4\beta_5\langle\Psi_1^2,\Psi_4\Psi_5\rangle\Big) \\
&+ 12\beta_2^2\Big(\beta_1\beta_3\langle\Psi_2^2,\Psi_1\Psi_3\rangle + \beta_1\beta_4\langle\Psi_2^2,\Psi_1\Psi_4\rangle + \beta_1\beta_5\langle\Psi_2^2,\Psi_1\Psi_5\rangle \\
&\qquad + \beta_3\beta_4\langle\Psi_2^2,\Psi_3\Psi_4\rangle + \beta_3\beta_5\langle\Psi_2^2,\Psi_3\Psi_5\rangle + \beta_4\beta_5\langle\Psi_2^2,\Psi_4\Psi_5\rangle\Big) \\
&+ 12\beta_3^2\Big(\beta_1\beta_2\langle\Psi_3^2,\Psi_1\Psi_2\rangle + \beta_1\beta_4\langle\Psi_3^2,\Psi_1\Psi_4\rangle + \beta_1\beta_5\langle\Psi_3^2,\Psi_1\Psi_5\rangle \\
&\qquad + \beta_2\beta_4\langle\Psi_3^2,\Psi_2\Psi_4\rangle + \beta_2\beta_5\langle\Psi_3^2,\Psi_2\Psi_5\rangle + \beta_4\beta_5\langle\Psi_3^2,\Psi_4\Psi_5\rangle\Big) \\
&+ 12\beta_4^2\Big(\beta_1\beta_2\langle\Psi_4^2,\Psi_1\Psi_2\rangle + \beta_1\beta_3\langle\Psi_4^2,\Psi_1\Psi_3\rangle + \beta_1\beta_5\langle\Psi_4^2,\Psi_1\Psi_5\rangle \\
&\qquad + \beta_2\beta_3\langle\Psi_4^2,\Psi_2\Psi_3\rangle + \beta_2\beta_5\langle\Psi_4^2,\Psi_2\Psi_5\rangle + \beta_3\beta_5\langle\Psi_4^2,\Psi_3\Psi_5\rangle\Big) \\
&+ 12\beta_5^2\Big(\beta_1\beta_2\langle\Psi_5^2,\Psi_1\Psi_2\rangle + \beta_1\beta_3\langle\Psi_5^2,\Psi_1\Psi_3\rangle + \beta_1\beta_4\langle\Psi_5^2,\Psi_1\Psi_4\rangle \\
&\qquad + \beta_2\beta_3\langle\Psi_5^2,\Psi_2\Psi_3\rangle + \beta_2\beta_4\langle\Psi_5^2,\Psi_2\Psi_4\rangle + \beta_3\beta_4\langle\Psi_5^2,\Psi_3\Psi_4\rangle\Big) \\
&+ 24\beta_1\beta_2\beta_3\beta_4\langle\Psi_1\Psi_2,\Psi_3\Psi_4\rangle + 24\beta_1\beta_2\beta_3\beta_5\langle\Psi_1\Psi_2,\Psi_3\Psi_5\rangle + 24\beta_1\beta_2\beta_4\beta_5\langle\Psi_1\Psi_2,\Psi_4\Psi_5\rangle \\
&+ 24\beta_1\beta_3\beta_4\beta_5\langle\Psi_1\Psi_3,\Psi_4\Psi_5\rangle + 24\beta_2\beta_3\beta_4\beta_5\langle\Psi_2\Psi_3,\Psi_4\Psi_5\rangle = \frac{366511}{1209600}.
\end{aligned}$$

Remark that PC and ANOVA are analytically equivalent, but the PC provides more flexibility from a numerical point of view with respect to Monte Carlo methods, as it is shown in the section §6.

5 Introducing more sensitivity indices

As introduced by Sobol [19], sensitivity indexes for variance can be computed for each conditional contribution following Eq. (13):

$$\sigma^{2,\mathrm{SI}}_{\boldsymbol{m_i}} = \frac{\sigma^2_{\boldsymbol{m_i}}}{\sigma^2}. \tag{72}$$

Here, we introduce new sensitivity indexes, basing on the decomposition of kurtosis and using the definition of the conditional term in (43), as follows

$$k^{\mathrm{SI}}_{\boldsymbol{m_i}} = \frac{k_{\boldsymbol{m_i}}}{k}. \tag{73}$$

If a total sensitivity index is needed, *i.e.* it is necessary to compute the overall influence of a variable, it can be computed summing up all the contributions in which the variable is present

$$\begin{aligned} \mathrm{TSI}_j &= \sum_{\xi_j \in (\boldsymbol{\xi} \cdot \boldsymbol{m_i})} \sigma^{2,\mathrm{SI}}_{\boldsymbol{m_i}} \\ \mathrm{TSI}^k_j &= \sum_{\xi_j \in (\boldsymbol{\xi} \cdot \boldsymbol{m_i})} k^{\mathrm{SI}}_{\boldsymbol{m_i}}. \end{aligned} \tag{74}$$

Remark that some indexes could be introduced also for the skewness, but in this case the positivity of each term is not guaranteed.

6 Some numerical results

6.1 Importance of Skewness in decomposition

This paragraph is devoted to show how important is to control the skewness during an optimization process. Let us consider the following polynomial function :

$$f = a\left(xz + xy\right) + b\left(x^2 + z^2\right) + \left(cba\right) y^2 \tag{75}$$

where x, y and z vary between 0 and 1 with an uniform pdf. Parameters a, b and c are design parameters that vary between -5 and 5. For this function, it is possible to compute analytically high-order statistics, as functions of the design parameters. Basing on Eqs. (2), (84) and (86), formulas for mean, variance and skewness can be computed exactly

$$\mu = \frac{1}{3}cba + \frac{1}{2}a + \frac{2}{3}b, \tag{76}$$

$$\sigma^2 = \frac{8}{45}b^2 + \frac{1}{4}ab + \frac{5}{36}a^2 + \frac{1}{12}cba^2 + \frac{4}{45}c^2b^2a^2, \tag{77}$$

$$
\begin{aligned}
s = {} & \frac{11}{120}ab^2 + \frac{13}{120}a^2b + \frac{32}{945}b^3 + \frac{1}{24}a^3 + \frac{1}{24}cb^2a^2 \\
& + \frac{17}{360}a^3cb + \frac{1}{60}c^2b^2a^3 + \frac{16}{945}c^3b^3a^3.
\end{aligned} \tag{78}
$$

The skewness can be decomposed (see Eq. (15)), in conditional contributions, as follows

$$
\begin{aligned}
s_x &= \frac{1}{15}\left(\frac{1}{2}+\frac{1}{2}b\right)^2 b + \frac{1}{3780}b^3 \\
s_y &= \frac{1}{15}\left(\frac{1}{2}cba+\frac{1}{4}a\right)^2 cba + \frac{1}{3780}c^3b^3a^3 \\
s_z &= \frac{1}{15}\left(\frac{1}{4}a+\frac{1}{2}b\right)^2 b + \frac{1}{3780}b^3 \\
s_{xy} &= \frac{1}{45}a^2b + \frac{31}{720}a^3cb + \frac{1}{48}a^3 + \frac{1}{24}cb^2a^2 \\
s_{xz} &= \frac{1}{360}a^2b + \left(\frac{1}{6}\left(\frac{1}{2}a+\frac{1}{2}b\right)\right)\left(\frac{1}{4}a+\frac{1}{2}b\right)a \\
s_{yz} &= 0 \\
s_{xyz} &= 0
\end{aligned} \tag{79}
$$

In order to show the importance to take into account also the high-order statistics in the robust optimization, different types of optimization are performed using several objective functions.

First, a classical bi-objective optimization is performed, where the mean of the function (Eq. (76)) is maximized and its variance (Eq. (77)) minimized. The Pareto front is reported in Figure 1. No measures of skewness have been used during the optimization process, then the Pareto front is constituted by various designs displaying a very large variation of skewness.

Now, let us consider a three-objectives optimization, *i.e.* consisting in the maximization of the mean (Eq. (76)), the minimization of the variance (Eq. (77)) and the minimization of the absolute value of the conditional skewness s_{xy} (Eq. (79)). In this case, the Pareto front is no more constituted by a curve, but by a surface in a 3D plan. The Pareto front is represented by means of 2D representation in the Figures 1 and 2 with projections on the plans μ-σ^2, μ-s_{xy} and σ^2-s_{xy}, respectively. As shown in Figure 2, designs belonging to the Pareto front display a large variation of the conditional skewness.

Now, let us compare the results obtained with both optimizations. In Figure 1, we show Pareto fronts in the plan $\mu - \sigma^2$. Designs obtained with the three-objectives optimization are dominated (with respect to only μ and σ^2) by the designs coming from the bi-objectives optimization. This is reasonable seeing that designs from bi-objective optimization are not influenced by the skewness s_{xy} during the optimization.

In Figure 3, curves associated to the three-objectives optimization are obtained by the 3D Pareto front regarding only the designs having a skewness lower than 0.0001. Remark that individuals of this Pareto front take values of μ lower than 3.2 and values of σ^2 lower than 4.4. Moreover, they could be dominated

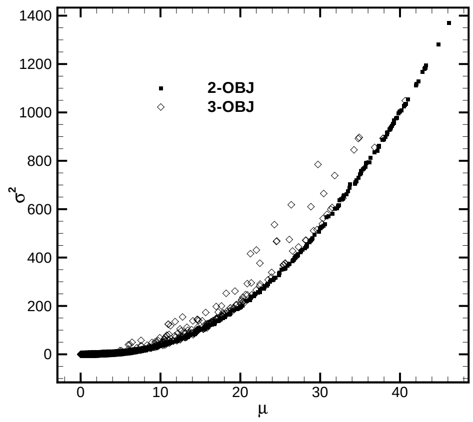

Figure 1: Pareto front in the plan $\mu - \sigma^2$ for the bi-objectives and three-objectives problem.

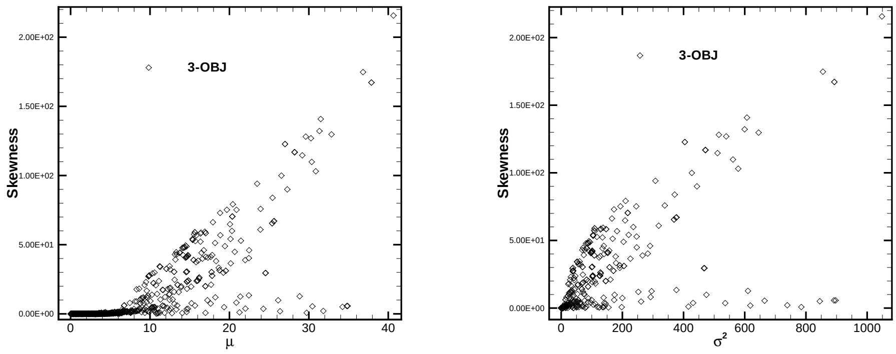

Figure 2: Pareto front in the plan $\mu - s_{xy}$ (on the left) and $\sigma^2 - s_{xy}$ (on the right) for the three-objectives optimization.

in terms of μ and σ^2 by some individuals of the Pareto front obtained from the bi-objectives optimization. Here, the interest is to get a Pareto front that is not sensitive to large variation in the skewness, since designs obtained from bi-objective optimization could present large skewness values. This displays the great interest to estimate high-order statistics during optimization.

6.2 Ranking uncertainties with respect to high-order statistical moments

Ranking uncertainties play a prominent role for managing large set of uncertainties problem. Here, we present a very simple test-case, for showing how

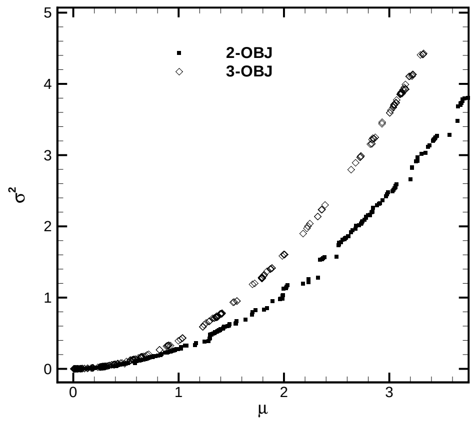

Figure 3: Pareto front in the plan $\mu - \sigma^2$ for the three-objectives optimization (extracted by the complete one considering only skewness inferior to 0.0001) and the bi-objective optimization.

variance-based decomposition (such as Anova) could lead to wrong analysis and decisions. As a consequence, high-order decompositions are needed for an accurate and complete ranking analysis. Let us consider the following polynomial function:

$$f = acx^2 + bxy + cby^2 + ay, \tag{80}$$

where x and y are two random variables with an uniform distribution between 0 and 1 and a, b and c are real design parameters.

Basing on Eqs. (2), (84) and (88), mean, variance and kurtosis are

$$\begin{aligned}
\mu &= \frac{1}{3}cb + \frac{1}{4}b + \frac{1}{2}a + \frac{1}{3}ac \\
\sigma^2 &= \frac{1}{4}cba + \frac{4}{45}c^2b^2 + \frac{1}{12}cb^2 + \frac{1}{12}ab + \frac{4}{45}a^2c^2 + \frac{7}{144}b^2 + \frac{1}{12}a^2 \\
k &= \frac{37}{1440}cb^4 + \frac{11}{480}b^3a + \frac{17}{480}b^2a^2 + \frac{1}{40}ba^3 + \frac{16}{945}c^4b^4 + \frac{16}{945}a^4c^4 + \frac{2}{45}a^4c^2 \\
&+ \frac{163}{3780}c^2b^4 + \frac{37}{1260}c^3b^4 + \frac{11}{90}cb^2a^2 + \frac{1}{18}a^3bc^2 + \frac{1}{18}c^3b^2a^2 + \frac{11}{120}cba^3 + \frac{32}{675}c^4b^2a^2 \\
&+ \frac{149}{1260}c^3ba^3 + \frac{49}{480}b^3ca + \frac{5009}{37800}b^3c^2a + \frac{4}{35}b^3c^3a + \frac{41}{189}c^2b^2a^2 + \frac{143}{19200}b^4 + \frac{1}{80}a^4
\end{aligned} \tag{81}$$

Considering different sets for (a, b, c), appreciable variations of $\sigma^{2,\mathrm{SI}}_{\boldsymbol{m}_i}$ and $k^{\mathrm{SI}}_{\boldsymbol{m}_i}$ can be observed. In C, formulas for these indices are reported. In Figure 4, each contribution $\sigma^{2,\mathrm{SI}}_{\boldsymbol{m}_i}$ and $k^{\mathrm{SI}}_{\boldsymbol{m}_i}$ are reported for $a = -42.204$, $b = -66.655$, $c = 2.9687$. The first-order effects on x and y explain more than 99.0% of the variance. The function stochastic model is of *additive* form with negligible interaction effects concerning the variance. Concerning the kurtosis decomposition, the interaction term is more predominant than the first-order terms. Remark also that the variance sensitivity index for the variable x, *i.e.* $\sigma_x^{2,\mathrm{SI}}$, is nearly five times higher than kurtosis sensitivity index, *i.e.* k_x^{SI}. As a consequence, $\sigma_x^{2,\mathrm{SI}} > \sigma_{xy}^{2,\mathrm{SI}}$ while $k_x^{\mathrm{SI}} < k_{xy}^{\mathrm{SI}}$, then the ranking based on sensitivity indexes changes if variance or kurtosis are considered.

Let us recall the total sensitivity indexes, defined in (74). For the function described in (80), these indexes are equal to

$$\begin{aligned}
\mathrm{TSI}_x &= \sigma_x^{2,\mathrm{SI}} + \sigma_{xy}^{2,\mathrm{SI}} \\
\mathrm{TSI}_y &= \sigma_y^{2,\mathrm{SI}} + \sigma_{xy}^{2,\mathrm{SI}} \\
\mathrm{TSI}_x^k &= k_x^{\mathrm{SI}} + k_{xy}^{\mathrm{SI}} \\
\mathrm{TSI}_y^k &= k_y^{\mathrm{SI}} + k_{xy}^{\mathrm{SI}}.
\end{aligned} \tag{82}$$

Referring to Figure 4, TSI_j and TSI_j^k are obviously different for each j, but the ranking is not influenced, *i.e.* $\mathrm{TSI}_x < \mathrm{TSI}_y$ and $\mathrm{TSI}_x^k < \mathrm{TSI}_y^k$.

In Figure 5, a different set of coefficients is considered ($a = 15.611$, $b = 92.919$, $c = 5.4995$). As seen earlier, first-order effects are predominant for the variance also in this case(explaining more than 99.5%). On the contrary, total sensitivity index for the variance changes consistently for x with respect to the kurtosis one (3 times more), *i.e.* $\mathrm{TSI}_x^k \approx 3\mathrm{TSI}_x$. This means that the variable x could be considered potentially negligible for the variance, but this hypothesis could be false when looking at the kurtosis.

This shows how much it can be dangerous to rank the variables with respect to the variance only.

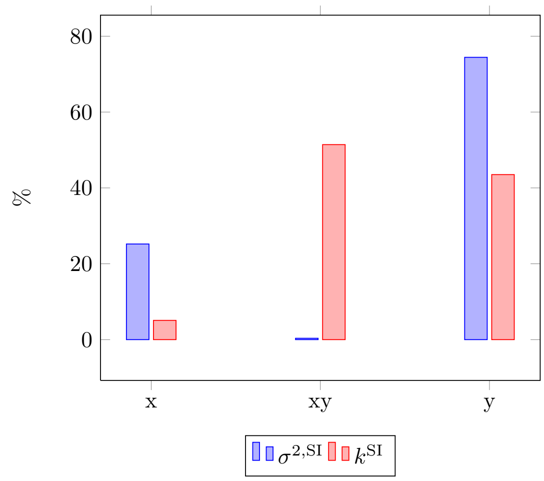

Figure 4: Sensitivity indices for variance (S_i) and kurtosis (Sk_i) obtained with $a = -42.204$, $b = -66.655$, $c = 2.9687$.

7 Conclusions

This paper deals with the decomposition of high-order statistics, *i.e.* such as skewness and kurtosis. The main contributions are the following:

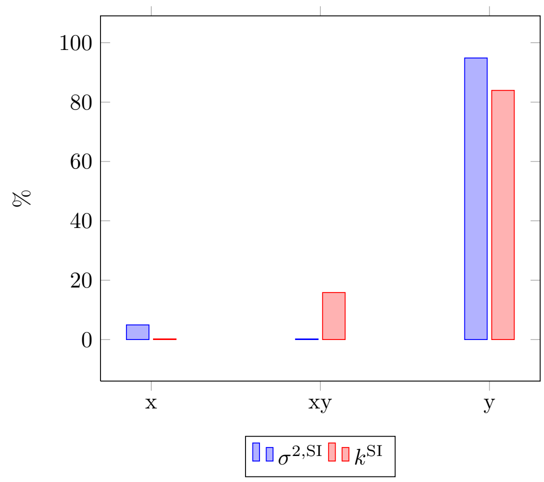

Figure 5: Sensitivity indices for variance (S_i) and kurtosis (Sk_i) obtained with $a = 15.611$, $b = 92.919$, $c = 5.4995$.

- A correlation was found between the functional decomposition, as depicted by Sobol, and the polynomial chaos development. This permitted to identify clearly each term of the decomposition, drawing also a practical way to compute all these terms.
- Computing skewness was shown to be of great importance for an exhaustive and complete stochastic analysis.
- Sensitivity indices bases on kurtosis decomposition were introduced. The importance of ranking the predominant uncertainties in terms not only of the variance but also of higher order moments (then extending the ANOVA analysis also to higher order statistic moments), was demonstrated with an algebraic function, where all the decomposition terms can be calculated analytically.

Future works will be oriented towards adaptive strategies for the reduction of the global computational cost.

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A Definition of High-order statistics

Here, let us demonstrate that the statistics (of order n) of f can be computed from the conditional expectancy of n-powers of f. First, let us consider the definition of the variance

$$\sigma^2 = \int_{\Xi^d} (f(\boldsymbol{\xi}) - E(f))^2 p(\boldsymbol{\xi}) \mathrm{d}\xi. \tag{83}$$

As a consequence, it can be easily computed as

$$\sigma^2 = E(f^2) - E(f)^2. \tag{84}$$

Starting from the definition of the skewness, we can obtain the following formula

$$\begin{aligned} s &= \int_{\Xi^d} (f(\boldsymbol{\xi}) - E(f))^3 p(\boldsymbol{\xi}) \mathrm{d}\xi \\ &= \int_{\Xi^d} \left(f^3(\boldsymbol{\xi}) - 3f^2(\boldsymbol{\xi})E(f) + 3f(\boldsymbol{\xi})E(f)^2 - E(f)^3\right) p(\boldsymbol{\xi}) \mathrm{d}\xi \\ &= E(f^3) - 3E(f^2)E(f) + 3E(f)E(f)^2 - E(f)^3 \\ &= E(f^3) - 3E(f^2)E(f) + 2E(f)^3. \end{aligned} \tag{85}$$

Then, skewness, as defined in Eq. 85, depend only from the expected values of the function f, f^2 and f^3. Using the formula for $E(f^2)$ obtained from Eq. 84, equation 85 becomes

$$\begin{aligned} s &= E(f^3) - 3E(f^2)E(f) + 2E(f)^3 \\ &= E(f^3) - 3\sigma^2 E(f) - 3E(f)^3 + 2E(f)^3 \\ &= E(f^3) - 3\sigma^2 E(f) - E(f)^3. \end{aligned} \tag{86}$$

Following the same procedure, kurtosis can assume the following form

$$\begin{aligned} k &= \int_{\Xi^d} (f(\boldsymbol{\xi}) - E(f))^4 p(\boldsymbol{\xi}) \mathrm{d}\xi \\ &= \int_{\Xi^d} \left(f^4(\boldsymbol{\xi}) - 4f^3(\boldsymbol{\xi})E(f) + 6f(\boldsymbol{\xi})^2 E(f)^2 - 4E(f)^3 f(\boldsymbol{\xi}) + E(f)^4\right) p(\boldsymbol{\xi}) \mathrm{d}\xi \\ &= E(f^4) - 4E(f^3)E(f) + 6E(f^2)E(f)^2 - 4E(f)^4 + E(f)^4 \\ &= E(f^4) - 4E(f^3)E(f) + 6E(f^2)E(f)^2 - 3E(f)^4. \end{aligned} \tag{87}$$

Using the value of $E(f)^3$ from Eq. 86 and the value of $E(f^2)$ from Eq. 84 the formula of the kurtosis becomes

$$k = E(f^4) - 4E(f)s - 6\sigma^2 E(f)^2 - E(f)^4. \tag{88}$$

B Computation of skewness and kurtosis decomposition in a PC framework

B.1 Skewness

First of all, the following term should be computed

$$\int_{\Xi^d} f(\boldsymbol{\xi})^3 p(\boldsymbol{\xi}) \mathrm{d}\xi = \int_{\Xi^d} \left(\sum_{k=0}^{P} \beta_k \Psi_k(\boldsymbol{\xi}) \right)^3 p(\boldsymbol{\xi}) \mathrm{d}\xi \tag{89}$$

This expression is equal to the sum of three terms:

$$\begin{aligned} \int_{\Xi^d} \left(\sum_{k=0}^{P} \beta_k \Psi_k(\boldsymbol{\xi}) \right)^3 p(\boldsymbol{\xi}) \mathrm{d}\xi = {} & \sum_{k=0}^{P} \beta_k^3 \langle \Psi_k^3(\boldsymbol{\xi}) \rangle + 3 \sum_{i=0}^{P} \beta_i^2 \sum_{\substack{j=0 \\ j \neq i}}^{P} \beta_j \langle \Psi_i^2(\boldsymbol{\xi}), \Psi_j(\boldsymbol{\xi}) \rangle \\ & + 6 \sum_{i=0}^{P} \sum_{j=i+1}^{P} \sum_{k=j+1}^{P} \beta_i \beta_j \beta_k \langle \Psi_i(\boldsymbol{\xi}), \Psi_j(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi}) \rangle. \end{aligned} \tag{90}$$

Let us analyze more in detail the three terms. The first summation can be split as follows

$$\sum_{k=0}^{P} \beta_k^3 \langle \Psi_k^3(\boldsymbol{\xi}) \rangle = \boxed{\beta_0^3} + \sum_{k=1}^{P} \beta_k^3 \langle \Psi_k^3(\boldsymbol{\xi}) \rangle. \tag{91}$$

The second summation of equation 90 requires some further manipulations

$$\begin{aligned} 3 \sum_{i=0}^{P} \beta_i^2 \sum_{\substack{j=0 \\ j \neq i}}^{P} \beta_j \langle \Psi_i^2(\boldsymbol{\xi}), \Psi_j(\boldsymbol{\xi}) \rangle = {} & 3\beta_0^2 \sum_{j=1}^{P} \beta_j \langle \Psi_0^2(\boldsymbol{\xi}), \Psi_j(\boldsymbol{\xi}) \rangle \\ & + 3 \sum_{i=1}^{P} \beta_i^2 \sum_{\substack{j=0 \\ j \neq i}}^{P} \beta_j \langle \Psi_i^2(\boldsymbol{\xi}), \Psi_j(\boldsymbol{\xi}) \rangle. \end{aligned} \tag{92}$$

Remark that the first term on the right side of the equation 92 is equal to zero because of the orthogonality, i.e. $\langle \Psi_0^2, \Psi_j \rangle = \langle \Psi_0, \Psi_j \rangle = 0$.

The second term on the right side of the equation 92 can be split in the following way

$$\begin{aligned} 3 \sum_{i=1}^{P} \beta_i^2 \sum_{\substack{j=0 \\ j \neq i}}^{P} \beta_j \langle \Psi_i^2(\boldsymbol{\xi}), \Psi_j(\boldsymbol{\xi}) \rangle & = 3 \sum_{i=1}^{P} \beta_i^2 \beta_0 \langle \Psi_i^2(\boldsymbol{\xi}), \Psi_0(\boldsymbol{\xi}) \rangle + 3 \sum_{i=1}^{P} \beta_i^2 \sum_{\substack{j=1 \\ j \neq i}}^{P} \beta_j \langle \Psi_i^2(\boldsymbol{\xi}), \Psi_j(\boldsymbol{\xi}) \rangle \\ & = \boxed{3\beta_0 \sum_{i=1}^{P} \beta_i^2 \langle \Psi_i^2(\boldsymbol{\xi}) \rangle} + 3 \sum_{i=1}^{P} \beta_i^2 \sum_{\substack{j=1 \\ j \neq i}}^{P} \beta_j \langle \Psi_i^2(\boldsymbol{\xi}), \Psi_j(\boldsymbol{\xi}) \rangle. \end{aligned} \tag{93}$$

The last term of the 90 can be written in the following way

$$6\sum_{i=0}^{P}\sum_{j=i+1}^{P}\sum_{k=j+1}^{P}\beta_i\beta_j\beta_k\langle\Psi_i(\boldsymbol{\xi}),\Psi_j(\boldsymbol{\xi})\Psi_k(\boldsymbol{\xi})\rangle =$$
$$6\beta_0\sum_{j=i+1}^{P}\sum_{k=j+1}^{P}\beta_j\beta_k\langle\Psi_j(\boldsymbol{\xi}),\Psi_k(\boldsymbol{\xi})\rangle + 6\sum_{i=1}^{P}\sum_{j=i+1}^{P}\sum_{k=j+1}^{P}\beta_i\beta_j\beta_k\langle\Psi_i(\boldsymbol{\xi}),\Psi_j(\boldsymbol{\xi})\Psi_k(\boldsymbol{\xi})\rangle, \tag{94}$$

where the first term on the right side is equal to zero because of the orthogonality property of the polynomial basis.

The last step in order to obtain the final form of the skewness is to move some terms to the left of the equation 89

$$\begin{aligned}\int_{\Xi^d} f(\boldsymbol{\xi})^3 p(\boldsymbol{\xi})\mathrm{d}\xi - \boxed{\beta_0^3} - \boxed{3\beta_0\sum_{i=1}^{P}\beta_i^2\langle\Psi_i^2(\boldsymbol{\xi})\rangle} &= \sum_{k=1}^{P}\beta_k^3\langle\Psi_k^3(\boldsymbol{\xi})\rangle \\ &+ 3\sum_{i=1}^{P}\beta_i^2\sum_{\substack{j=1\\ j\neq i}}^{P}\beta_j\langle\Psi_i^2(\boldsymbol{\xi}),\Psi_j(\boldsymbol{\xi})\rangle \\ &+ 6\sum_{i=1}^{P}\sum_{j=i+1}^{P}\sum_{k=j+1}^{P}\beta_i\beta_j\beta_k\langle\Psi_i(\boldsymbol{\xi}),\Psi_j(\boldsymbol{\xi})\Psi_k(\boldsymbol{\xi})\rangle\end{aligned} \tag{95}$$

and recognize that $\beta_0 = E(f)$ is the expected value of f and the term

$$\sum_{i=1}^{P}\beta_i^2\langle\Psi_i^2(\boldsymbol{\xi})\rangle = \sigma^2 \tag{96}$$

is the variance of f computed by the PC expansion.

The left hand side of the equation 95 can be re-written as

$$\int_{\Xi^d} f(\boldsymbol{\xi})^3 p(\boldsymbol{\xi})\mathrm{d}\xi - \beta_0^3 - 3\beta_0\sum_{i=1}^{P}\beta_i^2\langle\Psi_i^2(\boldsymbol{\xi})\rangle = E(f^3) - E(f)^3 - 3E(f)\sigma^2 \tag{97}$$

that is exactly the skewness as defined in the equation 86.

B.2 Kurtosis

First, the term $\int f^4(\boldsymbol{\xi})p(\boldsymbol{\xi})\mathrm{d}\xi$ should be computed as follows

$$\begin{aligned}
\int_{\Xi^d} f^4(\boldsymbol{\xi})p(\boldsymbol{\xi})\mathrm{d}\xi &= \int_{\Xi^d}\left(\sum_{k=0}^{P}\beta_k\Psi_k(\boldsymbol{\xi})\right)^4 \\
&= \sum_{k=0}^{P}\beta_k^4\langle\Psi_k^4(\boldsymbol{\xi})\rangle + 4\sum_{i=0}^{P}\beta_i^3\sum_{\substack{j=0\\ j\neq i}}\beta_j\langle\Psi_i^3,\Psi_j\rangle \\
&+ 3\sum_{i=0}^{P}\beta_i^2\sum_{\substack{j=0\\ j\neq i}}\beta_j^2\langle\Psi_i^2,\Psi_j^2\rangle + 12\sum_{i=0}^{P}\beta_i^2\sum_{\substack{j=0\\ j\neq i}}^{P}\beta_j\sum_{\substack{k=j+1\\ k\neq i}}\beta_k\langle\Psi_i^2,\Psi_j\Psi_k\rangle \\
&+ 24\sum_{i=0}^{P}\beta_i\sum_{j=i+1}^{P}\beta_j\sum_{k=j+1}^{P}\beta_k\sum_{h=k+1}^{P}\beta_h\langle\Psi_i\Psi_j,\Psi_k\Psi_h\rangle.
\end{aligned} \tag{98}$$

The five terms must be analyzed more in details. The first term can be written as

$$\sum_{k=0}^{P}\beta_k^4\langle\Psi_k^4(\boldsymbol{\xi})\rangle = \boxed{\beta_0^4} + \sum_{k=1}^{P}\beta_k^4\langle\Psi_k^4(\boldsymbol{\xi})\rangle. \tag{99}$$

The second term requires adding manipulations

$$4\sum_{i=0}^{P}\beta_i^3\sum_{\substack{j=0\\ j\neq i}}^{P}\beta_j\langle\Psi_i^3,\Psi_j\rangle = 4\beta_0^3\sum_{j=1}^{P}\beta_j\langle\Psi_0^3,\Psi_j\rangle + 4\sum_{i=1}^{P}\beta_i^3\sum_{\substack{j=0\\ j\neq i}}^{P}\beta_j\langle\Psi_i^3,\Psi_j\rangle. \tag{100}$$

The first term at the right hand side is zero due to the orthogonality while the second can be further decomposed as

$$\begin{aligned}
4\sum_{i=1}^{P}\beta_i^3\sum_{\substack{j=0\\ j\neq i}}^{P}\beta_j\langle\Psi_i^3,\Psi_j\rangle &= 4\sum_{i=1}^{P}\beta_i^3\beta_0\langle\Psi_i^3\rangle + 4\sum_{i=1}^{P}\beta_i^3\sum_{\substack{j=1\\ j\neq i}}^{P}\beta_j\langle\Psi_i^3,\Psi_j\rangle \\
&= \underline{4\beta_0\sum_{i=1}^{P}\beta_i^3\langle\Psi_i^3\rangle} + 4\sum_{i=1}^{P}\beta_i^3\sum_{\substack{j=1\\ j\neq 1}}^{P}\beta_j\langle\Psi_i^3,\Psi_j\rangle.
\end{aligned} \tag{101}$$

The third term of the equation (98) can be manipulated as

$$\begin{aligned}
3\sum_{i=0}^{P}\beta_i^2\sum_{\substack{j=0\\ j\neq i}}^{P}\beta_j^2\langle\Psi_i^2,\Psi_j^2\rangle &= 3\beta_0^2\sum_{j=1}^{P}\beta_j^2\langle\Psi_j^2\rangle + 3\beta_0^2\sum_{i=1}^{P}\beta_i^2\langle\Psi_i^2\rangle + 3\sum_{i=1}^{P}\beta_i^2\sum_{\substack{j=1\\ j\neq i}}^{P}\beta_j^2\langle\Psi_i^2,\Psi_j^2\rangle \\
&= \underline{\underline{6\beta_0^2\sum_{i=1}^{P}\beta_i^2\langle\Psi_i^2\rangle}} + 3\sum_{i=1}^{P}\beta_i^2\sum_{\substack{j=1\\ j\neq i}}^{P}\beta_j^2\langle\Psi_i^2,\Psi_j^2\rangle
\end{aligned} \tag{102}$$

Manipulating the fourth term of the equation (98), we obtain

$$12\sum_{i=0}^{P}\beta_i^2\sum_{\substack{j=0\\j\neq i}}^{P}\beta_j\sum_{\substack{k=j+1\\k\neq i}}\beta_k\langle\Psi_i^2,\Psi_j\Psi_k\rangle = 12\beta_0^2\sum_{j=1}^{P}\beta_j\sum_{k=j+1}\beta_k\langle\Psi_j,\Psi_k\rangle + 12\sum_{i=1}^{P}\beta_i^2\sum_{\substack{j=0\\j\neq i}}\beta_j\sum_{\substack{k=j+1\\k\neq i}}\beta_k\langle\Psi_i^2,\Psi_j\Psi_k\rangle. \quad (103)$$

The first term at the right side is zero due to the orthogonality and then the second one can be decomposed as

$$12\sum_{i=1}^{P}\beta_i^2\sum_{\substack{j=0\\j\neq i}}^{P}\beta_j\sum_{\substack{k=j+1\\k\neq i}}^{P}\beta_k\langle\Psi_i^2,\Psi_j\Psi_k\rangle = \underline{12\beta_0\sum_{i=1}^{P}\beta_i^2\sum_{\substack{k=1\\k\neq i}}^{P}\beta_k\langle\Psi_i^2,\Psi_k\rangle} + 12\sum_{i=1}^{P}\beta_i^2\sum_{\substack{j=1\\j\neq i}}^{P}\beta_j\sum_{\substack{k=j+1\\k\neq i}}^{P}\beta_k\langle\Psi_i^2,\Psi_j\Psi_k\rangle. \quad (104)$$

The fifth term of the equation (98) should be split as follows

$$24\sum_{i=0}^{P}\sum_{j=i+1}^{P}\sum_{k=j+1}^{P}\sum_{h=k+1}^{P}\beta_i\beta_j\beta_k\beta_h\langle\Psi_i\Psi_j,\Psi_k\Psi_h\rangle = \underline{24\beta_0\sum_{j=i+1}^{P}\sum_{k=j+1}^{P}\sum_{h=k+1}^{P}\beta_j\beta_k\beta_h\langle\Psi_j,\Psi_k\Psi_h\rangle} + 24\sum_{i=1}^{P}\sum_{j=i+1}^{P}\sum_{k=j+1}^{P}\sum_{h=k+1}^{P}\beta_i\beta_j\beta_k\beta_h\langle\Psi_i\Psi_j,\Psi_k\Psi_h\rangle. \quad (105)$$

The boxed term in the equation (99) is equal to $E(f)^4$, while the underlined terms in the equations (101), (104) and (105) can be summed

$$4\beta_0\sum_{i=1}^{P}\beta_i^3\langle\Psi_i^3\rangle + 12\beta_0\sum_{i=1}^{P}\beta_i^2\sum_{\substack{k=1\\k\neq i}}^{P}\beta_k\langle\Psi_i^2,\Psi_k\rangle + 24\beta_0\sum_{j=i+1}^{P}\sum_{k=j+1}^{P}\sum_{h=k+1}^{P}\beta_j\beta_k\beta_h\langle\Psi_j,\Psi_k\Psi_h\rangle = 4\beta_0\left(\sum_{i=1}^{P}\beta_i^3\langle\Psi_i^3\rangle + 3\sum_{i=1}^{P}\beta_i^2\sum_{\substack{k=1\\k\neq i}}^{P}\beta_k\langle\Psi_i^2,\Psi_k\rangle + 6\sum_{j=i+1}^{P}\sum_{k=j+1}^{P}\sum_{h=k+1}^{P}\beta_j\beta_k\beta_h\langle\Psi_j,\Psi_k\Psi_h\rangle\right). \quad (106)$$

Employing the equation (55), we can identify the skewness in the term between parenthesis so

$$4\beta_0\sum_{i=1}^{P}\beta_i^3\langle\Psi_i^3\rangle + 12\beta_0\sum_{i=1}^{P}\beta_i^2\sum_{\substack{k=1\\k\neq i}}^{P}\beta_k\langle\Psi_i^2,\Psi_k\rangle + 24\beta_0\sum_{j=i+1}^{P}\sum_{k=j+1}^{P}\sum_{h=k+1}^{P}\beta_j\beta_k\beta_h\langle\Psi_j,\Psi_k\Psi_h\rangle = 4\beta_0 s = 4E(f)s. \quad (107)$$

Moreover in the double underlined term of the equation (102) the expression for the expectancy and the variance (96) can be recognized

$$6\beta_0^2 \sum_{j=1}^{P} \beta_j^2 \langle \Psi_j^2 \rangle = 6E(f)^2\sigma^2. \tag{108}$$

Replacing every term in Eq. (98), Eq. (57) is obtained.

C Computation of sensitivity indices

Here, we provide the variance and kurtosis sensitivity indices for the function described in Eq. (80). Basing on formulas (12), (15) and (27), sensitivity indexes can be easily computed from Eqs. (72) and 73 as follows

$$
\begin{aligned}
\sigma_x^{2,\mathrm{SI}} &= [\frac{1}{5}a^2c^2 + \frac{1}{4}cba + \frac{2}{3}(-\frac{1}{4}b - \frac{1}{3}ac)ac + \frac{1}{12}b^2 + \frac{1}{2}(-\frac{1}{4}b - \frac{1}{3}ac)b + (-\frac{1}{4}b - \frac{1}{3}ac)^2]/\sigma^2 \\
\sigma_y^{2,\mathrm{SI}} &= [\frac{1}{5}c^2b^2 + \frac{1}{2}(\frac{1}{2}b + a)cb + \frac{2}{3}(-\frac{1}{4}b - \frac{1}{2}a - \frac{1}{3}cb)cb + \frac{1}{3}(\frac{1}{2}b + a)^2 \\
&\quad + (-\frac{1}{4}b - \frac{1}{2}a - \frac{1}{3}cb)(\frac{1}{2}b + a) + (-\frac{1}{4}b - \frac{1}{2}a - \frac{1}{3}cb)^2]/\sigma^2 \\
\sigma_{xy}^{2,\mathrm{SI}} &= (\frac{1}{144}b^2)/\sigma^2 \\
k_x^{\mathrm{SI}} &= \left(\frac{16}{945}a^4c^4 + \frac{37}{1260}c^3ba^3 + \frac{5}{252}c^2b^2a^2 + \frac{1}{160}b^3ca + \frac{1}{1280}b^4\right)/k \\
k_y^{\mathrm{SI}} &= (\frac{16}{945}c^4b^4 + \frac{37}{1260}c^3b^4 + \frac{5}{252}c^2b^4 + \frac{1}{160}cb^4 + \frac{1}{160}b^3a + \frac{3}{160}b^2a^2 + \frac{1}{40}ba^3 \\
&\quad + \frac{37}{630}b^3c^3a + \frac{5}{63}b^3c^2a + \frac{5}{63}c^2b^2a^2 + \frac{3}{80}b^3ca + \frac{3}{40}cb^2a^2 + \frac{1}{20}cba^3 + \frac{1}{1280}b^4 + \frac{1}{80}a^4)/k \\
k_{xy}^{\mathrm{SI}} &= (\frac{2}{45}a^4c^2 + \frac{22}{945}c^2b^4 + \frac{7}{360}cb^4 + \frac{1}{60}b^3a + \frac{1}{60}b^2a^2 + \frac{113}{19200}b^4 + \frac{89}{756}c^2b^2a^2 + \frac{32}{675}c^4b^2a^2 \\
&\quad + \frac{287}{5400}b^3c^2a + \frac{1}{18}c^3b^2a^2 + \frac{4}{45}c^3ba^3 + \frac{1}{18}a^3bc^2 + \frac{1}{18}b^3c^3a + \frac{7}{120}b^3ca + \frac{17}{360}cb^2a^2 + \frac{1}{24}cba^3)/k
\end{aligned}
\tag{109}
$$

where formulas for σ and k are given in Section 6.2.

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