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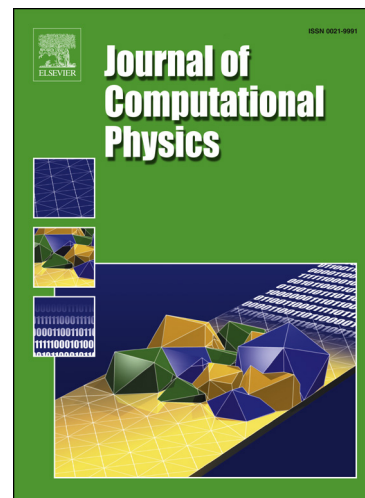
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SAMBA: Sparse Approximation of Moment-Based Arbitrary Polynomial Chaos

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Abstract

A new arbitrary Polynomial Chaos (aPC) method is presented for moderately high-dimensional problems characterised by limited input data availability. The proposed methodology improves the algorithm of aPC and extends the method, that was previously only introduced as tensor product expansion, to moderately high-dimensional stochastic problems. The fundamental idea of aPC is to use the statistical moments of the input random variables to develop the polynomial chaos expansion. This approach provides the possibility to propagate continuous or discrete probability density functions and also histograms (data sets) as long as their moments exist, are finite and the determinant of the moment matrix is strictly positive. For cases with limited data availability, this approach avoids bias and fitting errors caused by wrong assumptions. In this work, an alternative way to calculate the aPC is suggested, which provides the optimal polynomials, Gaussian quadrature collocation points and weights from the moments using only a handful of

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matrix operations on the Hankel matrix of moments. It can therefore be implemented without requiring prior knowledge about statistical data analysis or a detailed understanding of the mathematics of polynomial chaos expansions. The extension to more input variables suggested in this work, is an anisotropic and adaptive version of Smolyak's algorithm that is solely based on the moments of the input probability distributions. It is referred to as SAMBA (PC), which is short for Sparse Approximation of Moment-Based Arbitrary Polynomial Chaos. It is illustrated that for moderately high-dimensional problems (up to 20 different input variables or histograms) SAMBA can significantly simplify the calculation of sparse Gaussian quadrature rules. SAMBA's efficiency for multivariate functions with regard to data availability is further demonstrated by analysing higher order convergence and accuracy for a set of nonlinear test functions with 2, 5 and 10 different input distributions or histograms.

1. Introduction

Non-Intrusive Polynomial Chaos methods (NIPC) are popular uncertainty propagation techniques to determine the effect of aleatory input uncertainties on complex computational models [1, 2]. Their success is mostly due to the reduction in computational cost that can be achieved by expanding continuous input Probability Density Functions (PDF) into a basis of optimal orthogonal polynomials. The coefficients of the optimal polynomial

basis functions can be determined non-intrusively from response function evaluations, using either linear regression and sampling or quadrature based approaches on tensor-product or sparse grids. A comparison of these two NIPC approaches can be found in Eldred [3]. The list of parametric distributions, for which an optimal expansion exists, includes, among others, the Gaussian, Uniform, Beta and Gamma distribution and is referred to as 'generalised Polynomial Chaos' (gPC), based on the Askey scheme [4, 5, 6].

In recent years, however, engineering applications have created a growing demand for the extension of Polynomial Chaos techniques to more general input distributions [7]. The gPC was extended to arbitrary input distributions by splitting the random space into piecewise elements and propagating them locally using the Askey scheme [8, 9, 10, 11]. The splitting of the random space allows to treat discontinuous input distributions [12], but it comes at the cost of increased computational effort, especially for multiple input variables. Approaches to find global polynomial expansions for arbitrary distributions have been developed based on Gram-Schmidt orthogonalisation [13, 14]. Unfortunately, the convergence of gPC and Gram-Schmidt approaches both rely on the accurate availability of a parametric input PDF. More recently, it was therefore suggested to base the Polynomial Chaos Expansion (PCE) on the raw moments by Witteveen [14]. Oladyshkin and Nowak observed that as every set of random data, as well as a continuous or discrete PDF, can be described using the moments without making any assumptions about the shape or existence of a suitable probability distribution, the moments provided a very general approach to propagate data without requiring the determination of deterministic PDFs. Oladyshkin and

3

Nowak [7] promoted this concept in the geo-sciences by successfully applying it to identify uncertainties in carbon dioxide storage in geological formations [15, 16, 17] and also for robust design [18]. Moreover, Oladyshkin and Nowak presented a derivation of the optimal orthogonal polynomials from the moments. In the cases he reported, the convergence of the moment-based expansion was significantly better that for any other polynomial expansion [7] using fitted parametric PDFs.

The aPC formulation is especially useful for engineering Uncertainty Quantification (UQ). First of all, it offers a simple to apply method for real test data which are limited and bounded and can even be highly skewed or multi-modal [7]. Moreover, it offers an efficient method to account for rare events by propagating truncated heavy-tailed distributions. The main advantage of the aPC formulation is, however, a new answer to the question of how to deal with limited information for the input distributions. The construction of a parametric PDF in case the given data are limited always involves assumptions and subjectivity. Even the concept of maximum entropy, which was designed to deliver minimal subjectivity, imposes a specific shape on the distribution and still remains subject to debate [19]. The aPC, on the other hand, offers the possibility to propagate only the given information without making assumptions. This is advantageous, because basing the PCE on a wrong continuous PDF severely diminishes the convergence behaviour [7], whereas the aPC will converge to the correct solution as long as the moments are determinate in the Hamburger sense, which is only seldomly not the case as proven by Ernst [28]. He could show that the infinite lognormal distribution is an exception. Later in this work, it will be shown through

4

validation, that the truncated lognormal distribution is also determinate in the Hamburger sense. Moreover, Oladyshkin and Nowak showed that only moments are propagated in all Polynomial Chaos approaches. This is important because even a well-determined input PDF will at best have the same or similar first $2N$ moments as the aPC expansion of order N [15]. Hence, the aPC offers the most reliable evaluation of the effect that limited input data has on the model output. Despite the great benefits of aPC, the method has not been widely used so far. In addition, the work has mainly focused on mono-dimensional stochastic inputs [7]. This paper aims at resolving this issue by suggesting a new version of aPC whose main focus is on multiple arbitrary input distributions.

One important novelty of this work is a new algorithm which allows the calculation of the optimal collocation points and weights, needed for Gaussian quadrature, based on the moments only. All the quantities are calculated directly from the input data using only matrix operations performed on the Hankel matrix of moments. The matrix relations were derived by Mysovskih [20] for Gaussian quadrature with arbitrary weights and a summary was written by Gautschi, which can be found in Golub and Welsch [21]. A quadrature-based NIPC approach, that is, a non-intrusive evaluation of the Polynomial Chaos coefficients using Gaussian quadrature, is suggested for higher dimensions, because various sparse quadrature rules, like Smolyak's algorithm, exist to alleviate the curse of dimensionality while maintaining accuracy. In this work, Smolyak's algorithm was adapted to combine multiple univariate Gaussian quadrature rules to a single sparse multivariate quadrature rule. Conventionally, Smolyak's method is mostly used to sparsify a

5

single univariate rule to multiple dimensions. To the authors' knowledge, this is the first work that describes the complete procedure from moments to sparse multivariate PCE. In addition, the described methodology can be useful outside the field of UQ, because it simplifies the calculation of any anisotropic and adaptive Gaussian quadrature rule for multi-dimensional integrals (anisotropic meaning different weights in each direction and adaptive meaning individual polynomial expansion orders for the input variables), as it removes the need to refer to tabulated integration formulas. We also find that the described algorithm is generally more comprehensive than the previously suggested algorithm of aPC, because it provides the user directly with the optimal Gaussian quadrature points and weights, which are always needed to evaluate the statistics of the posterior distributions. Due to the fact that it is often difficult to differentiate between the various Polynomial Chaos methods and their different methodologies in the field of UQ, we refer to the described approach as SAMBA PC, which is an abbreviation of the main traits of the method, namely: the Sparse Approximation of Moment-Based Arbitrary Polynomial Chaos.

The paper is structured as follows: in Section 2, the mathematical foundation and notation that are the baseline of SAMBA are laid out. The theory of non-intrusive multi-dimensional PCEs is summarised and it is shown how stochastic collocation methods use Gaussian quadrature rules to obtain the expansion coefficients. In Section 3, SAMBA is explained in detail. Various possible inputs are illustrated and the sparse Smolyak extension based on only the moments to multiple dimensions is explained. In Section 4, the method is validated for several non-linear input functions for truncated con-

6

tinuous PDFs and histograms of increasing data size. The limitations which should be considered when applying SAMBA regarding integration errors, small data set error, convergence and higher levels are discussed in Section 5.

2. Theoretical Background

2.1. Multi-Dimensional Polynomial Chaos Expansions

Polynomial Chaos is an expansion approach which formulates a stochastic model output $f(\bar{\xi})$, dependent on a vector of N_U independent stochastic input random variables $\bar{\xi} = \xi_1, \xi_2, ..., \xi_{N_U}$ with space of events Ω, σ-algebra Λ and probability measure Γ (formally, a stochastic process in the probability space $(\Omega, \Lambda, \Gamma)$), as a linear combination of N_P stochastic multivariate orthogonal polynomials $\Psi_i(\bar{\xi})$ and deterministic coefficients α_i

$$f(\xi_1, \xi_2, ..., \xi_{N_U}) \approx \sum_{k=1}^{N_P} \alpha_k \cdot \Psi_k(\xi_1, \xi_2, ..., \xi_{N_U}). \tag{1}$$

In case a full tensor product is used, the number of linear combinations terms N_P for a polynomial expansion of order p is truncated to:

$$N_P = \frac{(N_U + p)!}{N_U! p!}. \tag{2}$$

The multivariate orthogonal polynomials Ψ_k are calculated as products of univariate orthogonal or orthonormal polynomials $\psi_j^{(i)}$

$$\Psi_k(\xi_1, \xi_2, ..., \xi_N) = \prod_{i=1}^{N_U} \psi_{I_k^{(i)}}^{(i)}(\xi_i), \ k \in \overline{1, N_P}. \tag{3}$$

such that $\sum_{i=1}^{N_U} I_k^{(i)} \leq N_P \ \forall i$. The superscript index in brackets $\psi^{(i)}$ refers to the input random variable, and the subscript index to the order ψ_j of

7

the orthogonal polynomial in the corresponding univariate basis. The rows of the index matrix $I_k^{(i)}$ contain the information, which order of each univariate input polynomial basis contributes to a particular global multivariate polynomial. For example, the 7th row of a three dimensional index matrix corresponds to the polynomial product:

$$\Psi_7 = \psi_0^{(1)} \cdot \psi_2^{(2)} \cdot \psi_0^{(3)} \quad \Leftrightarrow \quad I_7^{(1,..,3)} = \begin{bmatrix} 0 & 2 & 0 \end{bmatrix}. \tag{4}$$

The univariate orthogonal or orthonormal polynomials $\psi_j^{(i)}$ with $j \in 0, .., p$ and $\psi_0^{(i)} = 1$ need to be developed individually for each input random variable ξ_i for $i \in 1, .., N_U$ and have to fulfill the orthogonality condition

$$\int_{\xi \in \Omega} \psi_m^{(i)}(\xi) \psi_n^{(i)}(\xi) d\Gamma = \delta_{mn} \; \forall m, n \in \overline{0, p}. \tag{5}$$

The nth polynomial for the input distribution i can be defined through its $n + 1$ polynomial coefficients $p_{n,j}^{(i)}$ as

$$\psi_n^{(i)}(\xi) = \sum_{j=0}^{n} p_{n,j}^{(i)} \xi^j, \; n = \overline{0, p}. \tag{6}$$

The statistics of $Y(\bar{\xi})$ can be evaluated through the coefficients α_k. The mean and the variance of $Y(\bar{\xi})$ are

$$\mu_Y = \alpha_1 \quad \sigma_Y^2 = \sum_{k=2}^{N_P} \alpha_k^2 \langle \Psi_k^2 \rangle. \tag{7}$$

Similar formulas for skewness and kurtosis can be found in [22]. The coefficients α_k can be found through the integral

$$\alpha_k = \frac{1}{\langle \Psi_k^2 \rangle} \int_{\xi \in \Omega} Y(\bar{\xi}) \Psi_k(\bar{\xi}) d\Gamma(\bar{\xi}), \tag{8}$$

8

for $k = 1, .., N_p$, which can be solved using Galerkin projection, collocation or numerical integration. As the Ψ_k only consist of orthogonal polynomials, they can be accurately integrated by using a Gaussian quadrature rule as described in the next section. Although recent advances made by Navarro [23] have shown that a multivariate PCE of polynomials Ψ_k can be derived directly from dependent input variables using the Gram Schmidt method, the method described above is only valid in general, if the random variables are fully independent. Linear correlations between the input variables can be removed in advance, for instance with the Karhunen Loève expansion [6].

2.2. Gaussian Quadrature Rules

The concept of Gaussian quadrature is to find $p + 1$ optimal Gaussian collocation points ξ_i and weights ω_i, such that their sum yields an exact integral for polynomials of degree $2p + 1$ or less

$$\int_a^b f\left(\bar{\xi}\right) d\Gamma\left(\bar{\xi}\right) = \sum_{i=0}^p \omega_i f\left(\xi_i\right). \tag{9}$$

Multivariate quadrature formulas for multiple input random variables can be formed from one dimensional quadrature rules. Only tensor product quadrature and Smolyak's method are used in this work, but the combination of SAMBA with any other sparse quadrature is of course also possible. For a set of N_U random variables ξ_i with probability measure Γ the full tensor product quadrature formula is

$$\underbrace{\int_0^1 \cdots \int_0^1}_{N_U} f\left(\xi_1, ..., \xi_{N_U}\right) d\Gamma \approx \tag{10}$$

$$\approx \sum_{j_1=0}^{p_1} \cdots \sum_{j_{N_U}=0}^{p_{N_U}} f\left(\xi_{j_1}, ..., \xi_{j_{N_U}}\right) \left(\omega_{j_1} \otimes ... \otimes \omega_{j_{N_U}}\right).$$

9

In the literature, Gaussian-type quadrature formulas exist in many variations to cover all types of arbitrary parametric input distributions [24]. The approaches range from tabulated formulas [25] to moment matching equations [26] and the use of orthogonal polynomials [27]. For example, the Hermite polynomials can be derived for the normal distribution, the Legendre polynomials for the uniform distribution and the Laguerre polynomials for the exponential distribution [25] as summarised in Table 1.

Distribution	Interval	PDF	$w(x)$	Polynomial
Uniform	$[-1, 1]$	0.5	1	Legendre
Gaussian	$[-\infty, , \infty]$	$\frac{1}{\sqrt{2\pi}}e^{-\frac{x^2}{2}}$	$e^{-\frac{x^2}{2}}$	Hermite
Exponential	$[0, \infty)$	e^{-x}	e^{-x}	Laguerre

Table 1: Various orthogonal polynomials used for conventional Gaussian quadrature rules.

Another advantage of NIPC approaches using Gaussian quadrature is that the optimal polynomials derived for uncertainty propagation can be reused to obtain the expansion coefficients. Currently, however, such rules are only readily available and described in detail in the literature for parametric continuous probability distributions. In the following, it will be explained how optimal Gaussian quadrature rules can be found based on the moments using matrix relations derived by Mysovskih [20] and then be sparsified using Smolyak's rule.

10

3. The SAMBA PC: Sparse Approximation of Moment-Based Arbitrary Polynomial Chaos

3.1. Determing Gauss Quadrature Rules from Statistical Moments

Statistical moments are a quantitative measure to describe the shape of a set of random samples or a probability distribution. The zeroth moment represents the integral of the PDF, which is always one by definition, the first moment the mean, the second the variance, the third the skewness, the fourth the kurtosis and so on. For a continuous random variable $\xi \in \Omega$ with PDF $w(\xi)$, the kth raw moment μ_k can be determined by integrating

$$\mu_k = \int_{\xi \in \Omega} \xi^k w(\xi) d\xi. \tag{11}$$

For a discrete random variable $\xi \in \Omega^h$ with discrete PDF $w(\xi)$, the kth raw moment μ_k is

$$\mu_k = \sum_{\xi \in \Omega^h} \xi^k w(\xi) \tag{12}$$

and for set of N samples (random draws or random measurement data) $\zeta_1, ..., \zeta_N$, the kth raw moment μ_k can be calculated with

$$\mu_k = \frac{1}{N} \sum_{i=1}^{N} \zeta_i^k. \tag{13}$$

In general, a convergent PCE can be found for any arbitrary probability distribution or set of random data if its Hankel matrix of moments (defined in Eq. 15) is determinate in the Hamburger sense [28]. A given set of N samples is determinate in the Hamburger sense, if and only if all corresponding

11

quadratic forms are strictly positive, that is if

$$\det\left(M\right) = \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_p \\ \mu_1 & \mu_2 & & \mu_{p+1} \\ \vdots & & \ddots & \\ \mu_p & \mu_{p+1} & & \mu_{2p} \end{vmatrix} > 0, \tag{14}$$

where the entries μ_k for k from 0 to $2p$ are the statistical moments.

Due to the generality with regard to the input that is achieved by basing PCEs on the moments, one can consider continuous, discrete PDFs or even data sets for which no probability distribution is defined, without requiring a change of methodology. The idea to base PCEs on the moments has been mentioned in several previous works [14, 7, 28, 29], but was most prominently elaborated for UQ by Oladyshkin and Nowak [7]. The methodology described by Oladyshkin and Nowak is tailored to a small number (less than five) of uncertain input random variables. The algorithm described in the following dates back to matrix relations derived by Mysovskih [20] described in Golub and Welsch [21] and is more suitable for problems with more input uncertainties. The algorithm can be divided into two steps:

1. the three-term recurrence for the optimal orthogonal polynomials is found from the Hankel matrix of moments
2. the corresponding optimal Gaussian quadrature points and weights are calculated from the three-term recurrence.

These two steps have to be performed individually for each input variable. In this way the method allows a direct calculation of the optimal collocation points and weights needed for Gaussian quadrature rules from a given set of

12

moments. The Hankel matrix of the moments, required to perform the first step, is defined as

$$
M = \begin{bmatrix} \mu_0 & \mu_1 & \cdots & \mu_p \\ \mu_1 & \mu_2 & & \mu_{p+1} \\ \vdots & & \ddots & \\ \mu_p & \mu_{p+1} & & \mu_{2p} \end{bmatrix}. \tag{15}
$$

Because the Hankel matrix is positive definite its Cholesky decomposition of $M = R^T R$ can be computed, so that

$$
R = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1,p+1} \\ & r_{22} & \cdots & r_{2,p+1} \\ & & \ddots & \vdots \\ & & & r_{p+1,p+1} \end{bmatrix}. \tag{16}
$$

Mysovskih Theorem states that the entries of the inverse matrix R^{-1} of R

$$
R^{-1} = \begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1,p+1} \\ & s_{22} & \cdots & s_{2,p+1} \\ & & \ddots & \vdots \\ & & & s_{p+1,p+1} \end{bmatrix} \tag{17}
$$

form an orthogonal system of polynomials ψ_j according to the relation

$$
\psi_j = s_{0j}\xi^0 + s_{1j}\xi^1 + \ldots + s_{jj}\xi^j \quad for \quad j = 0, \ldots, p. \tag{18}
$$

To avoid the inversion of the matrix, Rutishauser [30] derived explicit analytic formulas to obtain the polynomial coefficients of the orthogonal polynomials s_{ij} from the Cholesky matrix entries r_{ij}. These relationships can be used to determine the coefficients a_j and b_j of the three-term recurrence, according

13

to which each orthogonal polynomial $\psi_j(\xi)$ for $j = 1, ..., p$ satisfies

$$\xi\psi_{j-1}(\xi) = b_{j-1}\psi_{j-2}(\xi) + a_j\psi_{j-1}(\xi) + b_j\psi_j(\xi). \qquad (19)$$

The coefficients a_j and b_j in terms of r_{ij} are

$$a_j = \frac{r_{j,j+1}}{r_{j,j}} - \frac{r_{j-1,j}}{r_{j-1,j-1}} \quad b_j = \frac{r_{j+1,j+1}}{r_{j,j}} \qquad (20)$$

with $r_{0,0} = 1$ and $r_{0,1} = 0$. The knowledge of the three term recurrence relation allows the calculation of the optimal collocation points and weights for any orthogonal polynomial [21]. They can be calculated by describing the three-term recurrence relation through a symmetric tri-diagonal Jacobi matrix J, which is again positive definite:

$$J = \begin{bmatrix} a_1 & b_1 & & & & \\ b_1 & a_2 & b_2 & & \emptyset & \\ & b_2 & a_3 & b_3 & & \\ & & \ddots & \ddots & \ddots & \\ & \emptyset & & b_{p-2} & a_{p-1} & b_{p-1} \\ & & & & b_{p-1} & a_p \end{bmatrix}. \qquad (21)$$

The eigenvalues of J are the roots of the polynomial of order p and the weights are found by

$$\omega_i = v_{1,i}^2, \qquad (22)$$

where $v_{1,i}$ is the first component of the normalized eigenvector corresponding to the ith eigenvalue.

3.2. Illustration of the Method for Continuous Distributions and Histograms

Using the method described above, the optimal collocation points for arbitrary continuous distributions can be calculated easily. Several examples for

14

various distributions, both contained and not contained in the Askey scheme, are displayed in Figure 1. It can be seen by comparing the graphs in Figure
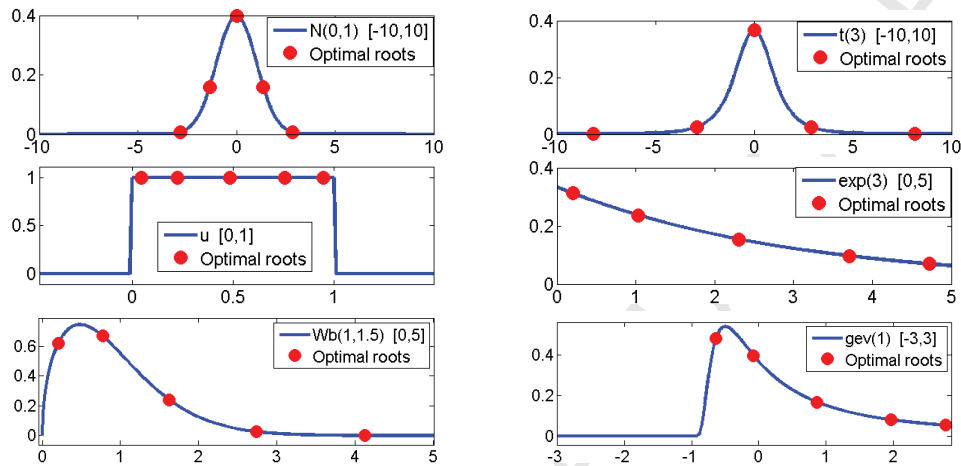

Figure 1: Optimal Gaussian collocation points for a standard Normal, fat-tailed Student-t, Uniform, Exponential (all three Askey scheme), Weibull and generalised Extreme Value Distribution (both not Askey scheme).

1 that the Gaussian collocation points change their position according to the input distributions. Unfortunately, they also change their position according to the polynomial expansion order p, which is why Gaussian quadrature rules are generally not nested. This means that lower order expansions cannot be reused for higher orders. On the upside, optimal Gaussian quadrature rules are more accurate than other quadratures using weights and collocation points. They are most commonly used based on tabulated formulas. However, the use of tabulated formulas restricts Gaussian quadrature methods to a limited set of continuous probability distributions. Moreover, it becomes tedious to combine individual rules to obtain integrals for multi-dimensional integrals with several different input distributions. Therefore, the examples

15

in Figure 1 show that all Polynomial Chaos approaches already in existence can be calculated using the SAMBA algorithm.
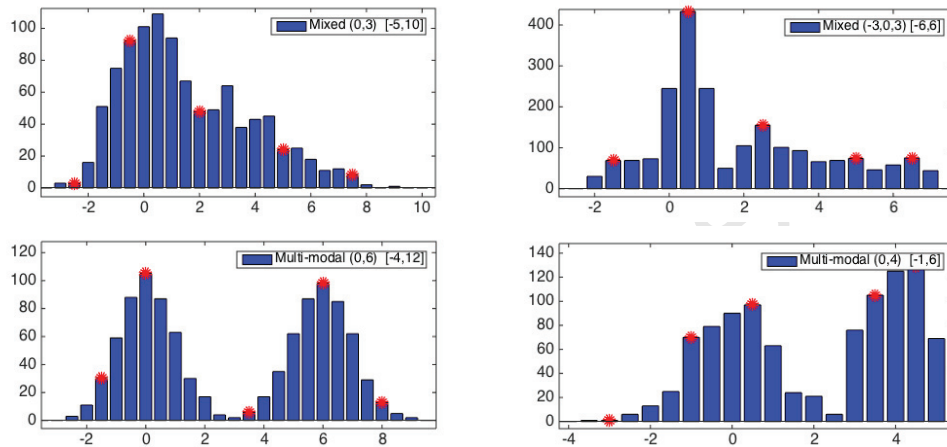

Figure 2: Optimal Gaussian collocation points for various mixed and multi-modal histograms, numerically generated from overlapping distributions.

Not only parametric distributions, but also histograms can be propagated using the moments without change in methodology. Figure 2 shows that a moment-based arbitrary PCE can even be calculated for multi-modal, or mixed probability distributions, as shown by the collocation points (dots) in Figure 2. It is visible how the moment-based approach favours regions in the input histograms of high probability. The input data can then be propagated through the computational model with exponential convergence, if the input-output mapping is analytic. In general, the rate of convergence improves with increasing smoothness of the input-output mapping. Finally, the moments of the posterior distribution can be trivially evaluated using quadrature, since the SAMBA algorithm provides the optimal quadrature

weights. If, however, the shape of the posterior PDF is desired, it can only be obtained by sampling the PCE. A rough estimate of its shape can be obtained using the input samples, but for more accurate illustrations of the posterior PDF a refined random number generator based on the samples is required.

3.3. Anisotropic Sparse Smolyak Grids Based on Moments

As the dimension of the problem increases, the computational cost grows exponentially and the rate of convergence becomes slower. This is referred to as the 'curse of dimensionality' [3]. To remedy this, sparse grids corresponding to a nodal set with a significantly smaller number of nodes can be used instead of the full tensor grids generated by the Gaussian quadrature rules. In this way, the accuracy of the problem can be mostly preserved, but with a lower number of evaluations required, so that the method can be applied to complex and computationally expensive models. Sparse tensor product spaces were first proposed by Smolyak [31]. The central principle of Smolyak's algorithm is to select a small number of the most important elements of a full tensor quadrature to represent the multi-dimensional function. The idea behind this is that most often the low-order interactions between the input variables are the most important ones. Similar to the full tensor Gaussian quadrature being improved with higher polynomial levels, the Smolyak quadrature can be improved by increasing a parameter called the level [32].

Most works, see for instance example [3, 33], cite the Smolyak formulas based on polynomial interpolation at the extrema of the Chebyshev polynomials (Clenshaw-Curtis nodes). Similarly, Smolyak formulas based on

17

Gaussian nodes in the literature are often only explained based on a single univariate rule. The following Smolyak is adapted for multiple univariate optimal Gaussian quadrature rules all based on moments. The N_u sequences of one-dimensional quadrature rules $\{U^{i_j}\}_{j=1,...,N_u}$ are denoted as

$$U^{i_j} = \sum_{k=1}^{m_{i_j}} f(\xi_k^{i_j})\omega_k^{i_j}, \qquad (23)$$

where m_{i_j} $j \in \{1,...,N_u\}$ is the maximum order, individually chosen for a quadrature, in case an adaptive quadrature is wanted (adaptive meaning that individual orders for the input distributions can be realised). For the Smolyak quadrature based on moments, the set of nodes corresponds to the eigenvalues of the matrices J. The Smolyak quadrature based on different input distributions is calculated with the formula

$$A\left(N_u + l, N_u\right) = \sum_{\substack{l+1 \\ \leq |i| \leq \\ l+N_u}} (l-1)^{l+N_u-|i|} \begin{pmatrix} N_u - 1 \\ l + N_u - |i| \end{pmatrix} \otimes_{k=1}^{N_U} U^{i_k} \qquad (24)$$

where l is the level. It is used to control the accuracy of the result, similar to the order in full Gaussian quadrature. For the same number of uncertain inputs, increasing the level l may make for a better accuracy, but it comes with an exponential growth of the number of points. The term $|i|$ is the norm of the vector $i = \{i_1,...,i_{N_u}\}$ which also stands for the sum of a row j of the index matrix $I_j^{(k)}$:

$$|i| = \sum_{k=1}^{N_u} i_k = \sum_{k=1}^{N_u} I_j^{(k)}. \qquad (25)$$

Equation (24) is a linear combination of the tensor products, where only a small number of nodes is used, but the interpolation properties for $N_u = 1$

18

are preserved for higher dimensions [34]. The array of sparse grid points $H(N_u + l, N_u)$ can be obtained through the following formula:

$$H\left(N_u + l, N_U\right) = \bigcup_{l+1 \leq |i| \leq l+N_u} \left(\bar{\xi}^{i_1} \times \cdots \times \bar{\xi}^{i_{N_u}}\right), \tag{26}$$

where the $\bar{\xi}^{i_j}$ are $m_{i_j} + 1$ points used by the quadrature U^{i_j} for $j \in \{1, ..., N_u\}$. The Fourier coefficients α_k can be calculated either by sparse integration of

$$\alpha_k = \int_\Omega f\left(\bar{\xi}_1, ..., \bar{\xi}_{N_u}\right) \Psi_k\left(\xi_1, ..., \xi_{N_u}\right) d\Gamma \tag{27}$$

or by linear regression

$$\hat{\alpha} = \arg\min\left[\bar{\alpha}^T \psi\left(\xi\right) - \bar{Y}\right]^2, \tag{28}$$

where $Y = \left[f\left(\bar{\xi}_0\right), ..., f\left(\bar{\xi}_{N_{sp}}\right)\right]$ and $\Psi\left(\xi\right) = \left[\psi_0\left(\xi\right), ..., \psi_{N_{sp}}\left(\xi\right)\right]$ with N_{sp} as the number of sparse points. The minimum of Equation (28) can be solved by defining

$$A = \begin{bmatrix} \psi_1\left(\xi_1\right) & \cdots & \psi_1\left(\xi_{N_u}\right) \\ \vdots & \ddots & \vdots \\ \psi_{N_{sp}}\left(\xi_1\right) & & \psi_{N_{sp}}\left(\xi_{N_u}\right) \end{bmatrix} \tag{29}$$

and solving

$$\left(A^T A\right) \hat{\alpha} = A^T Y. \tag{30}$$

The regression approach becomes increasingly useful for higher levels. The coefficients are useful in case the shape of the posterior distribution is of interest. If only the moments of the posterior distribution $E\left[f^k\right]$ are required, they can be obtained more easily by using the sparse quadrature formulas directly on the formula for the kth moment. For a model f they can be

19

calculated by sparsely integrating

$$E\left[f^k\right] = \underbrace{\int_0^1 \cdots \int_0^1}_{N_U} \left(f\left(\xi_1, ..., \xi_{N_U}\right) - E\left[f^{k-1}\right]\right)^k d\Gamma. \tag{31}$$

A comparison of the increasing computational effort of the lowest level Smolyak quadrature with full tensor Gaussian quadrature of third order is shown in Figure 3.
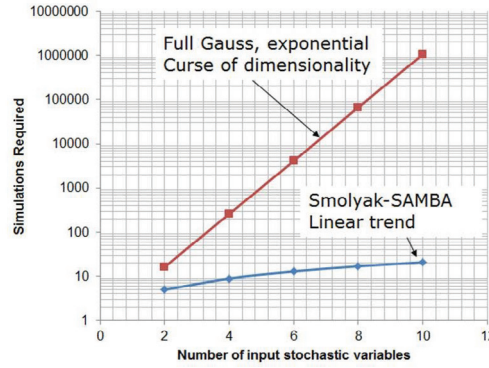

Figure 3: Number of collocation points for level 1 Smolyak and 3rd order full tensor.

3.4. Numerical Example and Implementation Advice

The following two dimensional example illustrates how SAMBA can be implemented in matrix format. To obtain simple numbers two continuous distributions, namely the standard normal and the uniform distribution, are chosen: $N(0,1)$ and $U(0,1)$ and the Smolyak quadrature is chosen at level 1. The resulting sparse Smolyak index matrix for $l = 1$ is:

$$I_{l+1 \leq |i| \leq l+N_u} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 2 & 1 \end{bmatrix}. \tag{32}$$

20

For more than 10 input variables, it is recommendable to calculate the index matrix recursively because the memory consumption of saving the full combination matrix becomes very high. Using the SAMBA algorithm from Section 3, first the collocation points corresponding to each input variable can be calculated

$$
X^{(i_1)} = \begin{bmatrix} 0 & -1 & -1.73 \\ 0 & 1 & 0 \\ 0 & 0 & 1.73 \end{bmatrix} \quad X^{(i_2)} = \begin{bmatrix} 0.5 & 0.21 & 0.11 \\ 0 & 0.79 & 0.5 \\ 0 & 0 & 0.88 \end{bmatrix} \tag{33}
$$

and then the corresponding weights

$$
W^{(i_1)} = \begin{bmatrix} 1 & 0.5 & 0.16 \\ 0 & 0.5 & 0.66 \\ 0 & 0 & 0.16 \end{bmatrix} \quad W^{(i_2)} = \begin{bmatrix} 1 & 0.5 & 0.28 \\ 0 & 0.5 & 0.44 \\ 0 & 0 & 0.28 \end{bmatrix}, \tag{34}
$$

where the superscript index in brackets refers to the random variable. Recall that i_1 represents the first column of the index matrix in Equation (32) while i_2 goes through the second one. The sparse collocation points can then obtained with

$$
\bar{\xi}_j = \bigcup_{2 \leq i_1 + i_2 \leq 3} \chi^{i_1} \times \chi^{i_2} \tag{35}
$$

which is in detail:

$$
[0] \times [0.5], \quad [0] \times \begin{bmatrix} 0.21 \\ 0.79 \end{bmatrix}, \quad \begin{bmatrix} -1 \\ 1 \end{bmatrix} \times [0.5], \tag{36}
$$

21

so that the array of sparse collocation points becomes

$$
\xi_j^{(i)} = \begin{bmatrix} 0 & 0.5 \\ 0 & 0.21 \\ 0 & 0.79 \\ -1 & 0.5 \\ 1 & 0.5 \end{bmatrix}.
\tag{37}
$$

For the conventional Smolyak algorithm, it can happen that in higher dimensions the same point is repeated several times. If that happens, the same points can be summarised to one position to decrease the number of necessary model runs, but the weights have to be added together. The corresponding sparse weights can be calculated through the tensor product

$$
\bar{\omega}_j = k_S \cdot \left(\otimes_{k=1}^{N_u} W^{i_k} \right) \quad j = \{1, 2, 3\}
\tag{38}
$$

where k_S is the Smolyak counting coefficient

$$
k_S = (-1)^{l + N_u - \sum\limits_{i=1}^{N_u} I_j^{(i)}} \begin{pmatrix} N_u - 1 \\ l + N_u - \sum\limits_{i=1}^{N_u} I_j^{(i)} \end{pmatrix}
\tag{39}
$$

which is in detail:

$$
-1 \cdot \prod_{i=1}^{N_u} [1] \otimes [1], \quad 1 \cdot \prod_{i=1}^{N_u} [1] \otimes \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}, \quad 1 \cdot \prod_{i=1}^{N_u} \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} \otimes [1],
\tag{40}
$$

so that the array of sparse integration weights becomes

$$
\omega_j^{(i)} = \begin{bmatrix} -1 \\ 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix}.
\tag{41}
$$

22

The mean and standard deviation of the posterior distribution of a model f can then be calculated through the scalar products

$$\mu = f\left(\bar{\xi}^{(1)}, \bar{\xi}^{(2)}\right) \circ \bar{\omega}, \quad \sigma = \left(f\left(\bar{\xi}^{(1)}, \bar{\xi}^{(2)}\right) - \mu\right)^2 \circ \bar{\omega}. \tag{42}$$

Several more examples of anisotropic grids, obtained from the moments of one Gaussian and one Weibull probability distribution, are shown in Figure 4.
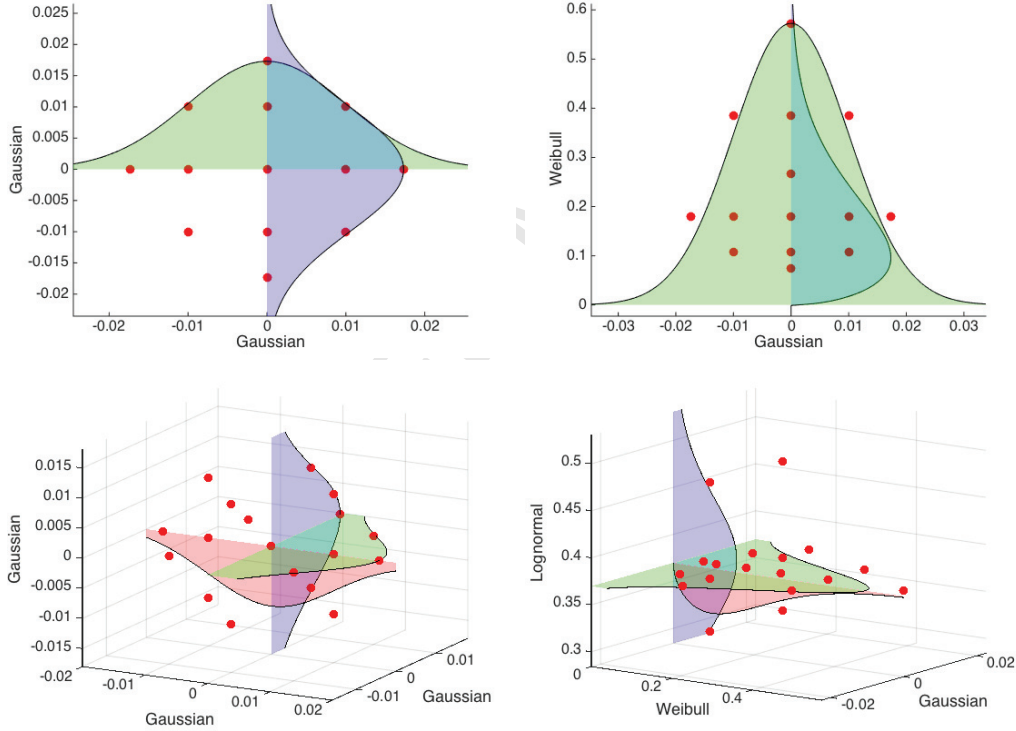

Figure 4: Symmetric and asymmetric moment-based Gaussian Smolyak grids at level 3 in 2D and 3D including PDFs used for the directions.

4. Method Validation

4.1. Method Validation using Non-Linear Multivariate Functions

In this section the method is demonstrated using a set of different input distributions and the results are validated against Monte Carlo Simulations with 10^7 samples. The used multivariate test functions are listed in Table 2. As shown by the 2D cross sections in Figure 5, the test functions were chosen to cover a wide range of possible response surfaces exhibiting for instance sinusoidal behaviour or exponential growth. To demonstrate the high potential of Smolyak's quadrature the two lowest possible levels were used. For accuracy comparison, also full tensor Gaussian quadrature of 3rd order was performed.

#	$f\left(\xi_1, \xi_2, ..., \xi_N\right)$
1	$\sum_{i=1}^{N} \xi_i$
2	$\exp\left(\sum_{i=1}^{N} \xi_i\right)$
3	$\sum_{i=1}^{N} \sin\left(\xi_i - 0.5\right)$
4	$1 \Big/ \sum_{i=1}^{N} \left(\xi_i - 1\right)^2$

Table 2: Multivariate test functions f used for 5 and 10 input random variables.

The stochastic input random variables used for 5D and 10D testing are listed in Table 3. The ten distributions used for validation are the Normal (N), Uniform (U), Cauchy (t) or also called student-t with one degree of freedom, Lognormal (Nlog), Weibull (Wb), Exponential (exp), Gamma (Γ), Beta (β), generalised Pareto (gPD) and generalised Extreme Value distribution (gEVD). To include the effect of the fat tails of the Cauchy distribution,
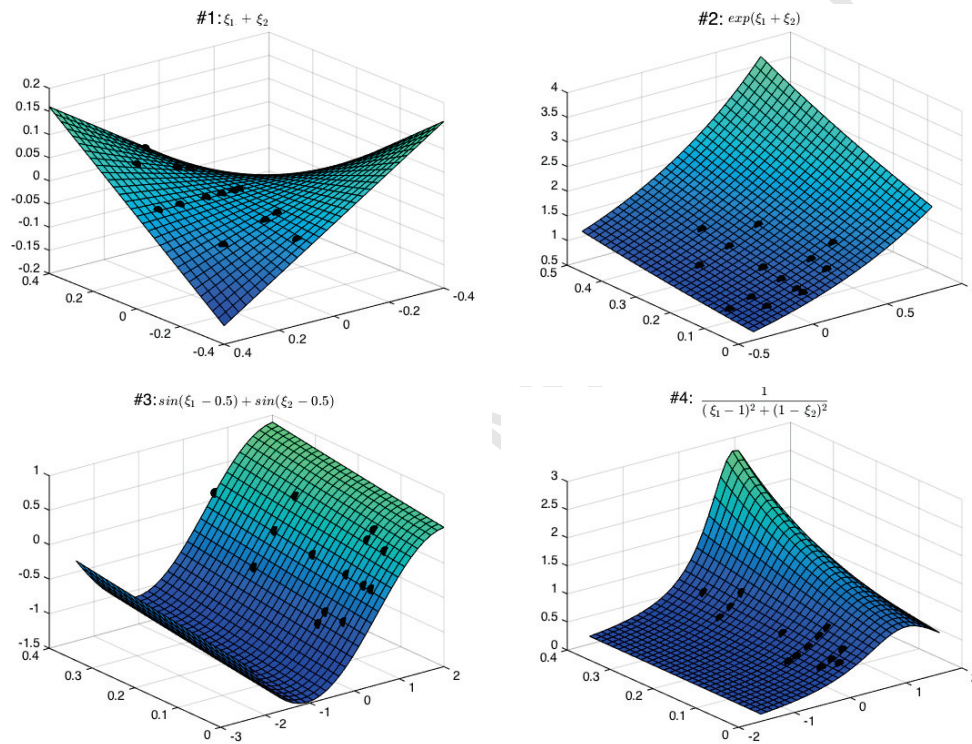
24

Figure 5: 2D response surfaces of the four multi-dimensional nonlinear test functions including level 2 moment-based Smolyak grids for one Gaussian and one Weibull input distribution.

it was not only truncated but also squeezed to a shorter x range by calculating $t(1000x)$ instead of $t(x)$. In this way a long part of the tails can be considered. The selected set of distributions does not only comprise Askey-scheme, but also more unusual distributions. From a conventional point of view, setting-up a sparse quadrature rule for this case would be difficult, but for SAMBA there is no difference to the use of a single univariate Gaussian rule. Similarly, also the truncation of the distributions can be performed without effort. For the continuous case, merely the integration boundaries need to be adapted.

Input	Parametric PDF
ξ_1	$N(\mu = 0, \sigma = 0.1)_{[-1,1]}$
ξ_2	$U(a = 0, b = 0.1)_{[0,0.1]}$
ξ_3	$Nlog(\mu = 0, \sigma = 4)_{[0,1]}$
ξ_4	$Wb(a = 0.12, b = 1.5)_{[0,1]}$
ξ_5	$t(\nu = 1, x_t = 1000x)_{[-0.5,0.5]}$
ξ_6	$exp(\mu = 0.1)_{[0,1]}$
ξ_7	$\Gamma(a = 2, b = 0.1)_{[0,2]}$
ξ_8	$\beta(a = 1, b = 10)_{[0,1]}$
ξ_9	$gPD(\theta = 0, \sigma = 0.1, k = 3)_{[0,2]}$
ξ_{10}	$gEVD(\mu = 0, \sigma = 0.1)_{[0,1]}$

Table 3: Probability distributions used for the input random variables ξ_i during testing with their parameters (e.g. μ, σ, a, b) and the used truncation interval $[l, r]$.

The relative errors compared to Monte Carlo for five input distributions are shown in Table 4 and for 10 distributions in Table 5. It can be seen that

despite the asymmetry, the sparse asymmetric Smolyak quadrature results in maximum relative errors of order 10^{-1} and minimum relative errors of order 10^{-3} for the standard deviation. The full tensor quadrature is more accurate, but it needs significantly more points. The results in Table 4 and 5 are based

$f(\xi_1, .., \xi_5)$	MCS σ_{ref} $N = 5 \cdot 10^7$	Tensor ε_{rel} $N = 1024$ $P = 3$	SAMBA ε_{rel} $N = 11$ $\mathbf{l = 1}$	SAMBA ε_{rel} $N = 65$ $\mathbf{l = 2}$
1	0.281289	0.000182	0.000182	0.000182
2	0.491630	0.000142	0.040644	0.001254
3	0.267742	0.000139	0.008996	0.000065
4	0.021974	0.000015	0.006559	0.000021

Table 4: Relative error of standard deviation for five different input distributions compared to MC reference solution.

on the moments calculated from continuous distributions.

The great advantage of SAMBA is that histograms can also be used. For this reason, sample sets were drawn from all input distributions $\xi_1, ..., \xi_{10}$. The obtained histograms were propagated directly through the test functions. To investigate the effect that the size of the input data set has on the accuracy of the solution, a Monte Carlo Simulation using SAMBA one thousand times for random draws with different seed numbers was performed. The accuracy was estimated with a comparison to a brute-force Monte Carlo solution with 10^7 samples. The propagated histogram bin sizes range from 10 to 10^6 random samples, which were drawn from the truncated input distributions characterised in Table 3. The obtained convergence plots are shown in

Figure 6. The plots show the minimum and maximum error occurring in the Monte Carlo Simulation as upper and lower bound of the occurring relative error. Thus, the upper and lower lines in Figure 6 represent 100% confidence interval. The results in Figure 6 show that a 10% maximum relative error

$f(\xi_1, .., \xi_{10})$	MCS σ_{ref} $N = 5 \cdot 10^7$	Tensor ε_{rel} $N \approx 1.05 \cdot 10^6$ $P = 3$	SAMBA ε_{rel} $N = 11$ $\mathbf{l = 1}$	SAMBA ε_{rel} $N = 231$ $\mathbf{l = 2}$
1	0.685013	0.000428	0.000428	0.000428
2	3.171731	0.000064	0.220369	0.035225
3	0.497968	0.000407	0.025444	0.000376
4	0.009219	0.000675	0.071664	0.005869

Table 5: Relative error of standard deviation for ten different input distributions compared to MC reference solution.

can be obtained from as few as 100 input samples for the standard deviation. Moreover, it was found that the convergence of the solution's accuracy depends on the number of input distributions. For more input distributions the general accuracy decreases. All the same, one digit accuracy can still be obtained for 100 samples. However, the accuracy decreases to a mere 2 digits for 10^5 samples for 5 inputs, whereas it reaches 3 digits for 10^5 samples for 2 inputs. In conclusion, the results show that decent estimates of probabilistic output quantities can be obtained even if only small data sets are used as input distributions.
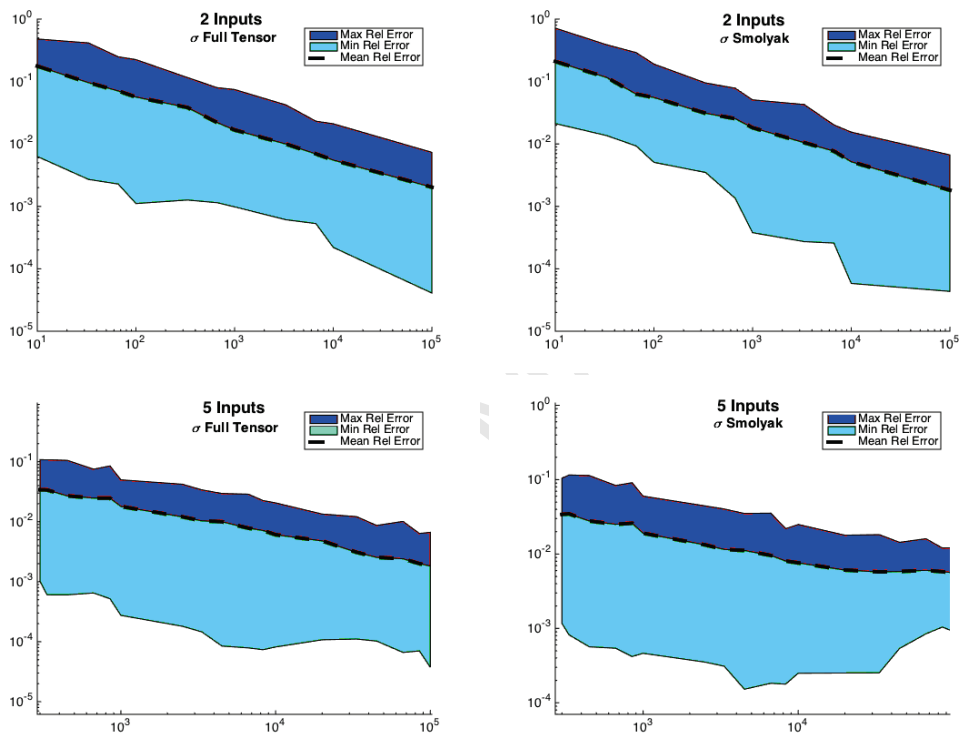
Figure 6: Relative error with 100% confidence intervals of standard deviation for full tensor Gaussian and Smolyak's method for increasing sample size for 2 and 5 different input distributions.

29

5. Applicability and Limitations

The mathematical simplifications offered by SAMBA come with certain limitations, which should be taken into account if the method is to be used accurately. First of all, it has to be noted that the use of the moments becomes less reliable for higher order polynomials. The results in the following section indicate that for a given number of inputs level 10 should not be exceeded. The origin of this effect can easily be seen, if the moments are obtained using numerical integration. As the calculated moments become higher, the integration error will cause an increasing deviation from the correct values. If the moments are obtained from data, smaller data size of the input data will also result in lower overall accuracy. Moreover, it should be taken into account that the response surface should be smooth in order to use Smolyak quadrature.

5.0.1. Integration Errors

If the moments are obtained from continuous distributions using numerical integration, integration errors have to be considered. In the author's experience, the use of state-of-the-art adaptive numerical integration techniques will allow an accurate calculation of the first 50 moments without exceeding error thresholds of 10^{-6}. For example, for two continuous Gaussian input distributions the polynomials up to order 28, that means at least the first 56 moments can be integrated accurately. Therefore, up to 25 different continuous input distributions at level 2 can be considered with SAMBA without large integration errors. Moreover, the accuracy of the numerical integration depends on the chosen probability distribution and the length of

the integration interval. For heavier tailed distributions, the moments grow significantly faster. In case the integration fails to converge to the required accuracy, it is possible to truncate the probability distributions. For example, by considering the normal distribution on the interval $[-10, 10]$ instead of on the interval $[-\infty, \infty]$ integration errors can be significantly reduced, whereas the the major part of the PDF remains unchanged.

5.0.2. Small Data Set Errors

No integration errors occur, if the moments are obtained from histograms. However, the calculated moments will deviate more from what could be assumed their true value, the higher the moment becomes and the smaller the given data set is. Nevertheless, the calculated moments are at least based on the actually available information. In case the wrong distribution is chosen for a set of samples, the higher moments up to infinity will deviate even more from what can be considered their accurate value. As was shown in the method validation section using a Monte Carlo Simulation on SAMBA for different sample sizes, even small sample sizes result in good estimates of the moments of the posterior distribution. More evidence of the superior convergence of the aPC and several examples demonstrating it can be found in Oladyshkin and Nowak [7].

5.0.3. Convergence

As mentioned before, PCEs based on moments converge if the input random variables are independent, have finite moments and are determinate in the Hamburger sense. The determination of the Hamburger sense is especially important if the aPC is applied for fat-tailed PDFs, because if very long

31

truncated fat tails are considered, the moment matrix can become indeterminate in the Hamburger sense. This may stop the method from converging to the correct solution as demonstrated in Ernst et al. [28]. The rate of convergence improves with increasing smoothness of the input-output mapping. In the cases reported by Oladyshkin and Nowak the convergence of data based aPC was superior to expansions based on incorrect parametric distributions. The crucial factor that decides whether the aPC will be more accurate than a fitted parametric PDF is the suitability of the fitted distribution. In case a given sample is small and not representative of the distribution, a fitted distribution will create a larger error than the direct use of the moments.

5.0.4. Higher Orders

SAMBA is a pseudospectral projection method using an adaptive and anisotropic Smolyak sparse grid rule. This means that the quantities of interest are formulated as a spectral expansion in multivariate orthonormal polynomials and the Fourier coefficients α are calculated with a sparse numerical quadrature rule. This formulation is known to lead to large errors in the higher order Fourier coefficients, due to internal aliasing [35] , if the expansion level is increased for the same number of input parameters.

To find the maximum order at which SAMBA as proposed in this work can be used for increasing expansion orders, the numerical integration examples as proposed in [36] were reproduced and tested for rising expansion level l. The two-dimensional test functions used in [36] are repeated in Table 6 .

Figure 7 shows the resulting relative error in the standard deviation for increasing level compared to 10^8 Monte Carlo simulation samples. To emphasize the fact that SAMBA can be used for continuous distributions and

#	$f\left(\xi_1, \xi_2\right)$
1	$\xi_1^{10}\xi_2^{10}$
2	$e^{\xi_1+\xi_2}$
3	$\sin\left(5\left(\xi_1 - 0.5\right)\right) + \cos\left(3\left(\xi_2 - 1\right)\right)$
4	$1/\left(2 + 16(\xi_1 - 0.1)^2 + 25(\xi_2 + 0.1)^2\right)$

Table 6: Test cases used in Constantine [36] to demonstrate errors in higher order Fourier coefficients.

discrete sample sets, the left side of Figure 7 shows the convergence assuming 2 independent continuous uniform distribution $U[-1, 1]$ as inputs. The right side shows the use of two different and independently created random sets of 50 samples drawn from $U[-1, 1]$ using a random number generator. Since the samples are not identical and the sample size is very small, the resulting expansion is not symmetric. In general the following behaviour can be observed:

- The ill conditioning of the mapping from moments to recurrence coefficients prevents expansion orders of higher levels than 21 for the continuous case and level 19 if only 50 samples are given. Consequently, the effect of the data set error on the ill-posedness of the problem is not too large. The main reason that the method fails for higher levels than 20 is that the Cholesky decomposition is no longer positive definite. At order 21 the first eigenvalue of the Hankel matrix of moments becomes negative, namely -4e-17.

- The accuracy of the solution is reduced by the sample size. Since the

33

continuous expansion uses the same distributions as the Monte Carlo solution, the accuracy achieved using only 50 samples is smaller. The use of the moments provides better results, if the accurate underlying parametric distribution cannot be determined.

- The method converges to the correct solution for increasing level, even if only 50 data points are used.

- The maximum accuracy is reached for lower levels than 10 in case only limited information is available about the input distribution.

- The use of sparse methods can be preferable, if data is very limited. The reason is that the additional effort spent on the tensor product is no use, if the overall possible accuracy is bounded by the limitation in input information. If this is the case, the maximum possible accuracy can be reached significantly faster and with lower computational effort using SAMBA.

An illustration of how the error for the individual coefficients grows for increasing order is given by Figure 8. The figure shows the magnitude of the relative error in the Fourier coefficients for function 3 from Table 6. It can be seen that the Fourier coefficients are highly accurate for lower levels. The maximum error is only of magnitude e^{-4} for polynomial orders lower than 11, i.e. level 10 in Smolyak. For higher levels the error in the coefficient increases to around 100%. Comparing these results with the convergence behaviour from Figure 7 leads to the conclusion that the increasing error in the coefficients does not result in an additional error, because no increase in relative error can be seen for higher orders. The error remains constant. For
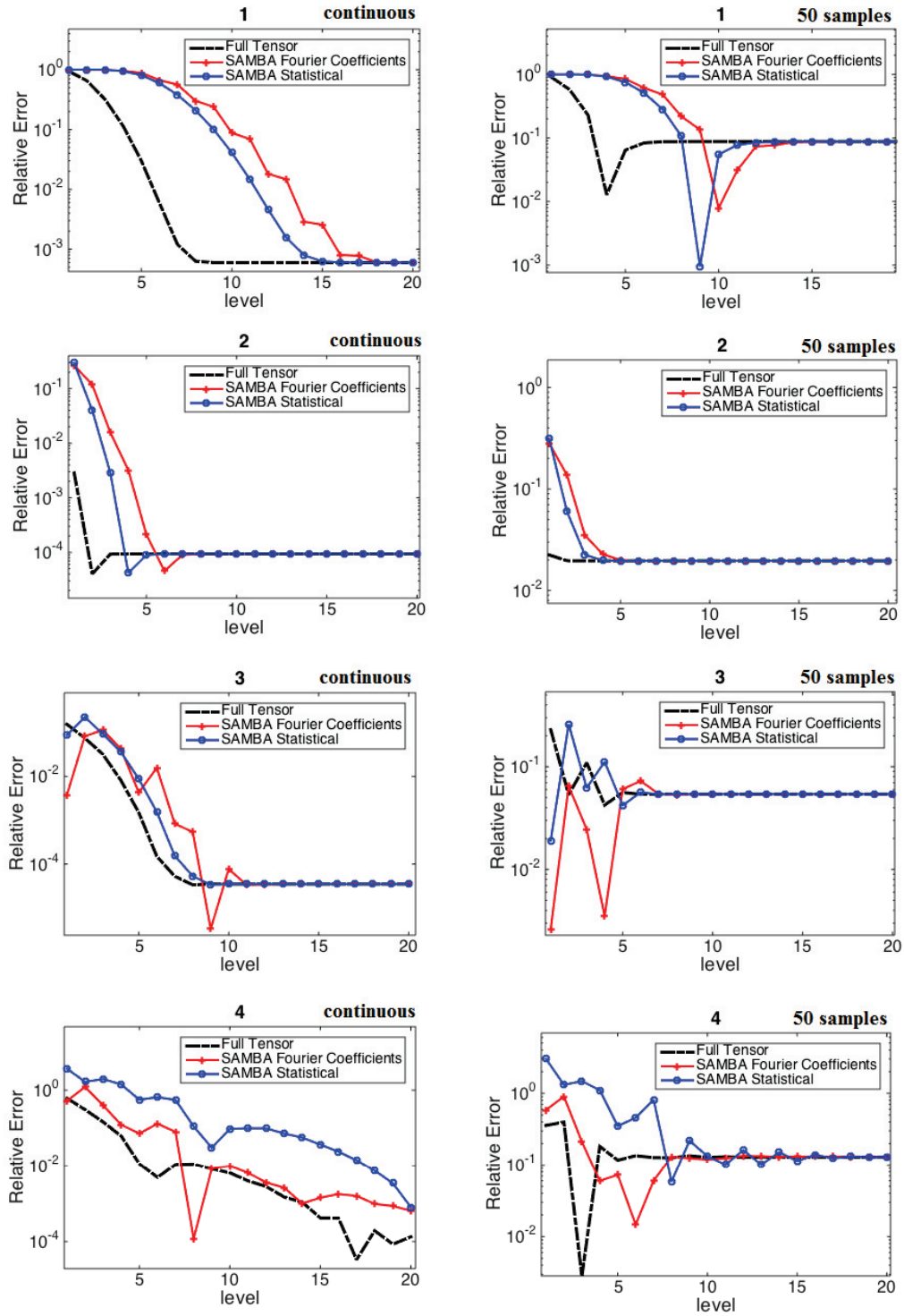
35

Figure 7: Relative error of standard deviation for increasing order compared to 10^8 Monte Carlo samples.

all cases the error in the standard deviation stagnates for higher levels. This means that the additional computational effort for higher levels will most likely not result in improved accuracy.
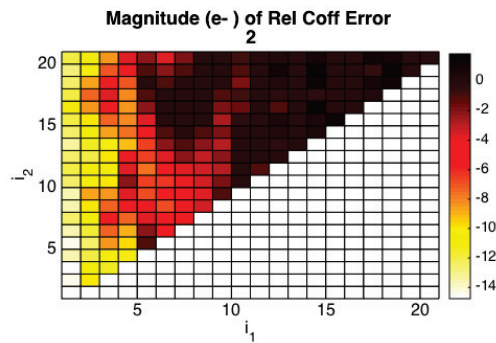

Figure 8: Magnitude of the relative error in sparse Fourier coefficients based on moments compared to tensor product coefficients .

In summary, the use of Smolyak's quadrature in SAMBA is justified and preferable to full tensor product methods, if the method is applied to a case where only scarce information is available for 10-20 input random variables. The coefficients up to level 10 can be determined accurately. Higher levels are not likely to result in improved accuracy. In case accurate parametric distributions can be determined, the use of the SPAM [36] is therefore recommended.

36

6. Conclusion

The contribution of this work is a new algorithm called SAMBA that simplifies the calculation of sparse multivariate Gaussian quadrature rules, based on multi-dimensional aPC expansions for any combination of continuous, discrete or histogram input random variables if input data is scarce. The algorithm's main advantage with respect to the previous aPC method is that it provides all values required to solve NIPC expansions using Gaussian quadrature, that is, the collocation points, weights and coefficients of the optimal orthogonal polynomials, in a fully comprehensive and easy-to-implement form. This is achieved by providing all quantities required using matrix operations on the Hankel matrix of moments. In order to alleviate the curse of dimensionality, the optimal Gaussian grids were sparsified using Smolyak's method. A sparse anisotropic and adaptive Smolyak quadrature was developed for multiple Gaussian quadrature rules based on only the moments for different input variables. It allows the sparse integration of functions of independent and arbitrarily distributed continuous, discrete and or histogram random variables and not only independent and identically distributed continuous random variables for smooth response surfaces. The given rule is not-nested, but, as it is Gaussian, it provides the highest possible accuracy among all quadrature based multi-dimensional integration methods. The method's efficiency, accuracy, higher order convergence and dependence on data availability were demonstrated for moderately high-dimensional stochastic test cases using a set of multivariate and non-linear test functions.

37

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