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THE ALGEBRAIC METHOD IN QUADRATURE FOR UNCERTAINTY QUANTIFICATION

JORDAN KO AND HENRY P WYNN

Abstract. A general method of quadrature for uncertainty quantification (UQ) is introduced based on the algebraic method in experimental design. This is a method based on the theory of zero dimensional algebraic varieties. It allows quadrature of polynomials or polynomial approximands for quite general sets of quadrature points, here called 'designs'. The method goes some way to explaining when quadrature weights are non-negative and gives exact quadrature for monomials in the quotient ring defined by the algebraic method. The relationship to the classical methods based on zeros of orthogonal polynomials is discussed and numerical comparisons made with methods such as Gaussian quadrature and Smolyak grids. Application to UQ is examined in the context of polynomial chaos expansion and probabilistic collocation method where solution statistics are estimated.

Nomenclature

α	Multi–indices denoting the nominal polynomial orders of $\phi_\alpha(x)$
$\hat{f}(x)$	Metamodel or surrogate model of $f(x)$
$\mathcal{D}$	Input design
Ω	Support of the measures of random input X
$\phi_\alpha(x)$	Multivariate orthonormal polynomials
$\prec$	Monomial ordering
$\rho(x)$	Measures of random input X
A	Design matrix $A = \{x^\alpha\}$ with $\alpha \in L$ and $x \in \mathcal{D}$
a_α	PCE coefficient for the polynomial with multi–indice α
d	Number of random dimensions
$f(x)$	Deterministic function with a n–tuple random input vector
$g_i(x)$	Gröbner basis
$H_\alpha(x)$	Hermite polynomials.
I	Monomial ideal
L	Set of exponents of the quotient basis.
$L_\alpha(x)$	Legendre polynomials.
$LT(I)$	The leading term ideal of the monomial ideal
n	Size of input design $\mathcal{D}$
p	Polynomial order
$P_\alpha^{(a,b)}(x)$	Jacobi polynomials.
$Q(x)$	A polynomial function
$r(x)$	Remainder form of $f(x)$, identical to NF
u	n–tuple deterministic input vector
w_i	Quadrature weights

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x	n–tuple random input vector
Y	Random outputs of the function $f(X)$
z_i	Quadrature points
AQ	Algebraic quadrature
GQ	Gauss quadrature
LHS	Latin hypercube sampling
MC	Monte Carlo
NF	Normal form of $f(x)$ with respect to I and $\prec$, identical to $r(x)$
PCE	Polynomial chaos expansion
PCM	probabilistic collocation method
SQ	Sparse quadrature
SS	Sobol Sequence
SSS	Scrambled Sobol Sequence

Contents

1. Introduction

Uncertainty Quantification (UQ), as defined particularly in an engineering context, is a method in which input uncertainties are first identified and the uncertainties in the outputs are determined by the propagation of the uncertainty measure from input to output. This is also a framework for classical sensitivity analysis. Input uncertainty may arise from aleatoric environmental variables, when the boundary conditions or the model parameters are subject to variation or fluctuation in the physical conditions or as part of a subjective uncertainty analysis. Alternatively, the uncertainty may arise from the lack of knowledge on the system, a source that is also known as the epistemic uncertainty. Here we are interested in estimating output statistics with probabilistic collocation model (PCM) and polynomial chaos expansions (PCE).

PCE is a polynomial expansion of the output response as a function of random inputs. There are two main methodologies in solving for the PCE, that is to say in estimating the values of the coefficients. In the first approach, the input design is based on Gauss or sparse quadrature, appropriate for lower and higher input dimensionality, respectively [17]. The PCE coefficients are solved by numerically integrating the solution response and the orthogonal polynomial over the input measure. The main advantage of this method is that its polynomial exactness is known. However, the quadrature input design increases in a pre-determined manner and is not embedded in the case of the Gauss quadrature. In the second approach, the input design is a randomly generated set of points and the PCE coefficients are determined by minimizing the error between the value of the PCE and the model solutions at the input design points with a least–square method [7, 26]. While this method allows one to use an input design that is embedded, in the sense that the previous samples can be used in successive iterations, the accuracy of the method is not known in general. The accuracy of the PCE metamodel is then typically verified via cross–validation techniques. A similar quadrature based method is the PCM. As the statistical moments such as mean and variance are integral measures over the support of the random inputs, they can be approximated with PCM to improve the accuracy of estimators when only a few samples are available [28].

We first summarize briefly the main ideas of quadrature in the context of PCE and PCM. The main purpose of the paper is to introduce a new theory of quadrature based on the so-called *algebraic method* in experimental design. This method was introduced originally to study interpolation and aliasing in factorial design [6], but has the advantage of delivering a possible interpolator for any data over any experimental design with an *a priori* determination of the design's polynomial exactness. We refer to a set of quadrature points as a *design* to maintain the connection. The quotient-plus-remainder operation inherent in the algebraic method provides a suitable platform for the generalization of univariate quadrature based on arbitrary designs (quadrature points) over arbitrary multivariate regions.

2. Uncertainty quantification

We consider a system with multivariate inputs u and a single univariate output $y = f(u)$. Typically $f(.)$ may represent a solver for a system of differential equations. In the deterministic case a given set of deterministic input values $\{u_i\}$ will lead to a corresponding set of output values $y_i = f(u_i)$. However in a wide variety of cases we may consider that uncertainty or variability may lead to uncertainty in y. The simplest way to handle this is to capture the variability in distributional form, at each deterministic u_i. Review's suggestion: We model the variability by describing the system with a stochastic variable x rather than the deterministic input u. Our suggestion from first revision: For fixed input u, we model the variability with a stochastic variable x. This may represent uncertainty in u or may arise from noise parameters. We suppress u in what follows.

In the PCE method we model the output y as a function of x by a series whose coefficients, a_α, are deterministic but whose stochastic terms are functions of x:

$$\hat{f}(x) = \sum_{\alpha \in \mathbb{N}^d} a_\alpha \phi_\alpha(x),$$

where $\hat{f}(x)$ denotes a metamodel or a surrogate of $f(x)$ and the $\phi_\alpha(x)$ are multivariate orthonormal polynomials with respect to the measure ρ describing the random input x:

$$\mathbb{E}_\rho(\phi_\alpha(x)\phi_\beta(x)) = \delta_{\alpha,\beta}.$$

The multi–index α is an index for the polynomials in the expansion. The original Wiener polynomial chaos used the Hermite polynomials as the expansion basis for Gaussian random variables [29]. Such expansion form a complete basis in Hilbert space determined by their corresponding support and converges to any L^2 function in the L^2 sense when the number of terms approaches infinity according to the Cameron–Martin theorem [8]. The expansion was generalized by [31] to represent non–Gaussian random fields by the use of polynomials from the Wiener–Askey scheme [2]. For example, the Legendre and Laguerre polynomials' weighting functions reflect the pdf of the uniform and gamma distributions, respectively. Note, that, because we will be considering the multivariate case the α and β are a non-negative integer vector and we shall associate one orthonormal polynomial with every such vector. This notation will prove important in the algebraic development. Readers are referred to [30] for the application of spectral methods in uncertainty quantification, especially polynomial chaos expansion.

2.1. **Output statistics.** This paper is concerned primarily with quadrature, that is, numerical integration or equivalently taking expectations with respect to the measure ρ. There is one immediate reason for this, namely that integration is required to capture the PCE coefficients:

$$a_\alpha = \mathbb{E}_\rho\left[f(x)\phi_\alpha(x)\right] = \int_\Omega f(x)\phi_\alpha(x)\rho(dx), \tag{1}$$

where Ω is the support of ρ. We approximate (1) by choosing a set of quadrature points, here called a *design*, $\mathcal{D} = \{z_1, \ldots, z_n\} \subset \Omega$. We favour the word 'design,' rather than abscissae or other terms, to aid conceptual links to the design of experiments. The quadrature formula is written as

$$\int_\Omega f(x)\phi_\alpha(x)\rho(dx) \approx \sum_{z\in\mathcal{D}} f(z)\phi_\alpha(z)w_z$$

with suitable weights $\{w_z\}$. The quadrature approximation may be exact for polynomial integrands and converges very fast with increasing levels of quadrature for non–polynomial integrands. The convergence depends on the selection of the design as well as the generation of the corresponding weights which are the subject of this paper.

The accuracy of PCE could be established by cross validation methods such as leave-one-out or k-fold. However such validation requires one to divide $\mathcal{D}$ into a training set for the construction of PCE and a validation set for comparison against the metamodel. For numerical quadrature, the entire design $\mathcal{D}$ is needed in calculating the quadrature approximation and such cross validation is not feasible. The algebraic quadrature proposed can flexibly choose the training set and the application of leave–one–out cross validation in the context of algebraic quadrature will be investigated in Section 3.5.

From equation 1, PCE estimators of mean and variance are

$$\mathbb{E}[f(X)] = a_0, \tag{2}$$

$$\mathrm{Var}[f(X)] = \sum_{\alpha\geq 0} a_\alpha^2. \tag{3}$$

Means, variances, higher moments, sensitivity indices *etc.* can be approximated with PCM [28] using quadrature. For example, mean and variance are

$$\mathbb{E}[f(X)] \approx \sum_{z\in\mathcal{D}} f(z)w_z,$$

$$\mathrm{Var}[f(X)] \approx \sum_{z\in\mathcal{D}} \left(f(z) - \mathbb{E}[Y]\right)^2 w_z. \tag{4}$$

Since $\phi_0(x) = 1$ in equation 1 for all orthogonal polynomials, the PCM mean estimator is identical to the PCE estimator. Therefore, the main difference between the two methods is that the PCM variance relies only on the quadrature approximation and is not affected by the truncation error in PCE.

A sensitivity analysis of the system can also be carried out to identify which random dimensions dominate the solution. This is achieved by calculating the partial variances from the Sobol' sensitivity indices associated with each random variable X_n as follows [25]

$$S_n = \mathrm{Var}\left[\mathbb{E}\left\{f_\mathrm{r}(\boldsymbol{X})|X_n\right]\right\}/\mathrm{Var}[f(X)].$$

In the context of the gPC expansion, they can be computed as

$$S_n = \sum_{a\in I_n} a_m^2\mathbb{E}[\phi_m^2(\boldsymbol{X})]/\mathrm{Var}[f(X)] = \sum_{m\in I_n} a_m^2/\mathrm{Var}[f(X)], \tag{5}$$

where I_n is the set of indices to the polynomials containing only x_n and $\mathrm{Var}[f(X)]$ is estimated in equation 3. In practice, those indices are numerically very easy to compute due to the hierarchical nature of the orthogonal polynomial basis and its tensor–like form. Note that the Sobol' indices can also be calculated directly from collocation methods [27].

The response surfaces of $f(\boldsymbol{x})$ can be easily constructed from equation (1) which allows one to predict the system solution at arbitrary points in the support. We can also compute an empirical estimator of the cdf of $f(\boldsymbol{x})$ from

$$\hat{F}(y) = \frac{1}{n_\mathrm{MC}}\sum_{k=1}^{n_\mathrm{MC}} \mathbf{1}_{(-\infty,y]}(Y_k),$$

where $Y_k = f(\zeta_k)$ and n_{MC} is the number of independent random samples ζ_k generated according to the pdf $\rho(\boldsymbol{x})$. The α–quantile y_α of $f(\boldsymbol{X})$ can be approximated from the ordered set $Y_{(1)} \leq Y_{(2)} \leq \cdots \leq Y_{(k)}$

$$\hat{Y}_\alpha = Y_{(\lceil \alpha Z \rceil)}, \tag{6}$$

where a large number of MC samples can be used. A multi–element refinement method for high values of α is described in [18].

2.2. **Product form methods and alternatives.** We suppose that the support of the measure $\rho(x)$ is R^d or a hypercube such as $[-1,1]^d$ (after centring and scaling). If $\phi_{\alpha_1}(x_1), \phi_{\alpha_2}(x_1)\dots$ is a sequence of orthogonal polynomial with respect a single variable x_i with $\rho(x_i)$ on R and $\mathcal{D}_i$ is a design (set of quadrature points) on R then for all integer multi-indices $\alpha = (\alpha_1, \dots, \alpha_d) \geq 0$, the products

$$\phi_\alpha(x) = \prod_{i=1}^{d} \phi_{\alpha_i}(x_i)$$

are multivariate orthogonal polynomials with respect to the product measure $\rho = \prod_{i=1}^{d} \rho(x_i)$. Moreover the product design $\mathcal{D} = \otimes^n \mathcal{D}_i$ is a natural design in R^d. We define the degree corresponding to α as $|\alpha| = \alpha_1 + \cdots + \alpha_d$.

In classical univariate Gauss quadrature (GQ), the n–point univariate design are the zeros of the orthogonal polynomial of degree $p = n$ with respect to ρ each having appropriate weights $\{w_i\}$ and we have exact quadrature:

$$\int_\Omega x^m \rho(dx) = \sum_z w_z x_z^m,$$

for $0 \leq m \leq 2n-1$. For the d-dimensional quadrature there is exact quadrature for any monomial $x^\alpha = x_1^{\alpha_1} \cdots x_1^{\alpha_d}; 0 \leq \alpha_i \leq 2n_i - 1; i = 1, \dots, d$ where n_i is the number of quadrature point in each nominal direction.

Figure 1 illustrates the accuracy from different quadrature schemes. This representation of quadrature accuracy was first proposed in [17] where each axis represents $\phi_\alpha(x)$ in its canonical order which is an one–to–one mapping of a sequence of polynomials $\phi_i(x)$ to $\phi_\alpha(x)$. For example, the first five canonical terms in $d = 3$ are $\phi_0(x) = \phi_{(0,0,0)}(x)$, $\phi_1(x) = \phi_{(1,0,0)}(x)$, $\phi_2(x) = \phi_{(0,1,0)}(x)$, $\phi_3(x) = \phi_{(0,0,1)}(x)$ and $\phi_4(x) = \phi_{(2,0,0)}(x)$. The intersection of the column i and row j represents the inner product $\langle \phi_i(x), \phi_j(x) \rangle$ and a dot at (i,j) denotes that the quadrature approximates of $\langle \phi_i(x), \phi_j(x) \rangle$ is exact. The thick line shown encloses all the terms satisfying $|\alpha| \leq 3$. This representation is a generalization of the corner cut diagram in algebraic methods proposed in [21] by compressing a d–dimensional representation onto two dimensions. A $(d-1)$ dimensional corner cut hyperplane separating the multi–indices with $|\alpha| \leq 3$ is now represented in two dimensions by the thick line.

For a three–dimensional full–tensor quadrature with $n_i = 2$, all the terms satisfying the full quadrature conditions, *i.e.* $\alpha_i \leq 2n_i - 1$, are shown in Figure 1(a). In response surface methods, the expansion is traditionally truncated at $|\alpha| = p$ even when higher order terms could be exactly approximated by the quadrature; we shall use the letter p for this case throughout the paper and sometimes use the term "polynomial exactness p".

A key problem in quadrature is to obtain good, and if possible exact, quadrature for monomials x^α up to a certain degree $|\alpha|$, without the expense of a full product design. A variety of quadrature grids have been suggested, such as Smolyak grids. The generic term *sparse grids* is often used and the zeros of orthogonal polynomials of different orders are useful building blocks. Thus, Smolyak sparse grids with polynomial exactness p approximate exactly terms whose α satisfies $\{\phi_\alpha : |\alpha| \leq p\}$. Figure 1 (b) shows the terms satisfying $|\alpha| \leq 3$. Using corner–cut staircase introduced by [21], these terms can also be represented as a hypertetrahedron satisfying $|\alpha| \leq p$ in $\alpha \in \mathbb{N}^d$. Indeed, Figure 1 (b) illustrate in two–dimensions the concept of a generic set which will be discussed in the following section.

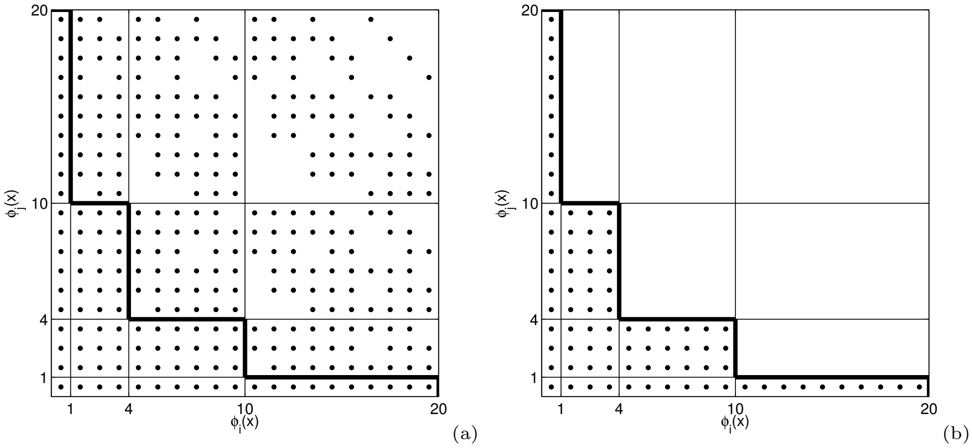

FIGURE 1. Each axis represents the canonical order of the orthonormal polynomials $\phi_i(x)$ & $\phi_j(x)$ and each element in the matrix represents $\langle \phi_i(x), \phi_j(x) \rangle$. The thin lines demarcate the increment of canonical increment in $\|p\|$ and the thick lines the canonical quadrature accuracy of $|p| = 3$. (a) the full quadrature approximation satisfying $\{\alpha : \alpha_i \leq 3\}$ and (b) the sparse quadrature approximation satisfying $\{\alpha : |\alpha| \leq 3\}$.

3. ALGEBRAIC METHOD

Following [19, 23, 24] the algebraic method in experimental design allows the construction of exact polynomial interpolators for data over an arbitrary design $\mathcal{D}$ in R^d. We give a brief introduction with the main steps. For background in basic algebraic geometry see [10]. The recent work in [11] employs also the algebraic quadrature method and concentrates particularly on the Hermite polynomial case where special formulae apply.

Elementary powers of a single variable have a natural ordering $1 \prec x \prec x^2 \prec x^3 \prec \ldots$ This is generalised to a special total ordering on monomials in n variables: $\{x^\alpha\} = x_1^{\alpha_1} \cdots x_n^{\alpha_n}$.

Definition 3.1. *A* monomial term ordering, *$\prec$, is a total ordering of monomials such that $1 \prec x^\alpha$ for all $\alpha \geq 0$ and, for all $\gamma \geq 0$, $x^\alpha \prec x^\beta$ implies $x^{\alpha+\gamma} \prec x^{\beta+\gamma}$*

We shall use the term *monomial ordering* for short and there are a number of standard monomial orderings. Given an monomial ordering any polynomial Q has a unique leading term and we write, suppressing $\prec$, $LT(Q)$.

Definition 3.2. *A monomial ideal I is an ideal for which there is a collection of monomials $p_1, \ldots, p_m$ such that any $g \in I$ can be expressed as a sum*

$$g = \sum_{i=1}^{m} g_i(x) p_i(x).$$

We can appeal to the representation of a monomial x^α by its exponent α. If $\beta \geq 0$ is another exponent then

$$x^\alpha x^\beta = x^{\alpha+\beta},$$

and $\alpha + \beta$ is in the positive (shorthand for non-negative) "orthant" with "corner" at α. The set of all monomials in a monomial ideal is the union of all positive orthants whose corners are given by the exponent vectors of the generating monomial $p_1, \ldots, p_m$.

There are, in general, many ways to express a given ideal I as being generated from a basis $I = \langle p_1, \ldots, p_m \rangle$. That is to say, there are many choices of basis.

Definition 3.3. *Given an ideal I, a set $\{g_1, \ldots g_m\}$ is called a Gröbner basis (G-basis) if:*

$$\langle LT(g_1), \ldots, LT(g_m) \rangle \;=\; \langle LT(I) \rangle,$$

where $\langle LT(I) \rangle$ is the ideal generated by all the monomials in I.

We sometimes refer to $\langle LT(I) \rangle$ as the *leading term ideal.*

Lemma 3.4. *Any ideal I has a Gröbner basis and any Gröbner basis in the ideal is a basis of the ideal.*

For any given monomial ordering, $\prec$, any ideal I has a unique "reduced" associated Gröbner basis (G-basis). The idea is that given a monomial ordering and an ideal expressed in terms of the G-basis, $I = \langle g_1, \ldots, g_m \rangle$, any polynomial Q has a unique remainder with respect the quotient operation $K[x_1, \ldots, x_k]/I$. That is

$$Q(x) = \sum_{i=1}^{m} s_i(x) g_i(x) + r(x).$$

We call the remainder $r(x)$ the *normal form* of Q with respect to I and write $NF(Q)$. Or, to stress the fact that it may depend on $\prec$, we write $NF(Q, \prec)$. Here are some formal definitions.

Definition 3.5. *Given a monomial ordering $\prec$, a polynomial $Q = \sum_{\alpha \in L} \theta_\alpha x^\alpha$, for a list L, is a normal form with respect to $\prec$ if $x^\alpha \notin \langle LT(f) \rangle$ for all $\alpha \in L$.*

The choice of monomial ordering is important but note that if a graded (total degree) ordering is used then all terms of a given degree appear in the ordering "first" before any terms of a given degree. The total number of terms of a given degree m is $\binom{d+d}{m}$. If the sample size is not enough to exactly fill up to degree m then the terms will depend on the initial order and will favour variable higher up the order. We find, in this case, that varying the initial order affects the weights, but not substantially. See [19] for more discussion of this issue and some examples will be given in Section 4.4.1.

A design is considered to be zero–dimensional variety, that is the solution of a set of algebraic equations. Thus the points $(\pm 1, \pm 1)$ are the solutions of $\{x_1^2 = 1, x_2^2 = 1\}$. There is a corresponding ideal, $I(D)$ which we call the design ideal. In this case, the set of monomial $\alpha \in L$ form a basis for the quotient ring and will drive whole construction, once the design $\mathcal{D}$ and monomial order $\prec$ have been selected. Note that L and D have the same $|L| = |\mathcal{D}| = n$ and L has natural order ideal, or hierarchical, property $\alpha \in L \Rightarrow \beta \in L$ for any $\beta \leq \alpha$ (componentwise). We can also define the $n \times n$ design matrix:

$$A = \{x^\alpha\}_{x \in \mathcal{D}, \alpha \in L}.$$

(Note that in the algebraic statistics literature A^T is often used.)

Lemma 3.6. *Given an ideal I and a monomial ordering $\prec$, for every $f \in K[x_1, \ldots, x_k]$ there is a unique normal form $NF(f)$ such that $f - NF(f) \in I$.*

We now summarize the main steps which provided the background for the algebraic quadrature of this paper:

(1) Choose a design $\mathcal{D}$ and a measure, ρ.
(2) Select a monomial term ordering, $\prec$.
(3) Compute Gröbner basis for $I(\mathcal{D})$ for given monomial ordering, $\prec$. By default, the graded lexicographical order should be used.
(4) The quotient ring $K[x_1, \ldots, x_k]/I(\mathcal{D})$ of the ring of polynomials $K[x_1, \ldots, x_k]$ in $x_1, \ldots, x_k$ forms is a vector space spanned by a special set of monomials: $x^\alpha, \alpha \in L$. These are all the monomials not divisible by the leading terms of the G-basis $G = \{g_i(x), i = 1, \ldots, m\}$ and $|L| = |\mathcal{D}|$. We shall refer to this as the quotient basis or *model basis.*
(5) The quotient operation implies that any polynomial $f(x)$ has a decomposition

$$f(x) = \sum_{i=1}^{m} s_i(x) g_i(x) + r(x),$$

where the remainder $r(x) = \sum_{\alpha \in L} c_\alpha x^\alpha$ is a member of the quotient ring, which we call the Normal Form of $r(x)$: $NF(r(x))$.
(6) The set of multi-indices L has the "order ideal", sometimes called "staircase" property: $\alpha \in L$ implies $\beta \in L$ for any $0 \leq \beta \leq \alpha$. For example, if $x_1^2 x_2$ in the model so is $1, x_1, x_2, x_1 x_2$.
(7) Any function $f(x)$ on $\mathcal{D}$ has a unique polynomial interpolator given by the list L:

$$p(x) = \sum_{\alpha \in L} \theta_\alpha x^\alpha,$$

such that $f(x) = p(x),\ x \in \mathcal{D}$.

(8) The cardinality of the design and the quotient basis is the same: $|L| = |\mathcal{D}|$.

(9) The design matrix

$$A = \{x^\alpha\}_{x\in\mathcal{D},\alpha\in L},$$

is $n \times n$, has full rank n and has rows indexed by the design points and columns indexed by the quotient basis.

3.1. **Multivariate quadrature using the algebraic approach.** Let ρ be a probability measure on R^d with finite moments: $\int_{R^d} x^p \,\rho(dx) < +\infty$ for all $p \in Z^d_{\geq 0}$. Also, let $\mathcal{D} = \{z_1, \dots, z_n\}$ be a finite set of distinct points in R^d, $G = \{g_1, \dots, g_m\}$ be a Gröbner basis of $I(\mathcal{D})$ with respect to the chosen monomial ordering and L the corresponding set of exponents for a basis of the quotient space. Following the algebraic theory, any polynomial p can be decomposed as

$$f(x) = \sum_{i=1}^{m} s_i(x) g_i(x) + r(x), \tag{7}$$

where $r(x)$ is a member of the quotient ring with basis elements $x^\alpha, \alpha \in L$, and recall that $|L| = |\mathcal{D}|$. The remainder $r(x)$ can be written as

$$r(x) = \sum_{z\in\mathcal{D}} p(z) l_z(x), \tag{8}$$

where the $l_z(x)$ are the polynomial indicator functions, in the model basis, for the design points:

$$l_z(x) = \delta_{x,z} = \begin{cases} 1, & \text{if } x = z, \\ 0, & \text{otherwise.} \end{cases}$$

Write $r(x) = NF(f(x))$, the Normal Form, so that

$$f(x) - r(x) = \sum_{i=1}^{m} s_i(x) g_i(x).$$

The condition for exact quadrature is, then,

$$\mathbb{E}_\rho \{f(X) - r(X)\} = \mathbb{E}_\rho \left\{ \sum_{i=1}^{m} s_i(X) g_i(X) \right\} = 0. \tag{9}$$

Equivalently, $(f(x) - r(x)) \perp_\rho 1$, where we use the scalar product: $\langle f, g\rangle = \int_{R^d} f(x)g(x)\,\rho(dx)$. If (9) holds we obtain the quadrature formula:

$$\begin{aligned} \mathbb{E}_\rho \{f(X)\} &= \mathbb{E}_\rho \{r(X)\}, \\ &= \textstyle\sum_{z\in\mathcal{D}} w(z) f(z). \end{aligned}$$

where

$$w(z) = \mathbb{E}_\rho \{l_z(X)\},\ z \in \mathcal{D}. \tag{10}$$

We can say that exact quadrature for the algebraic method is a special property of the 4-tuple $\{f(x), \mathcal{D}, \prec, \rho(x)\}$.

3.2. **Using orthogonal polynomials.** Let $\langle f, g\rangle$ be the induced scalar product and let $\{1, h_\alpha, \dots\}$ be the corresponding orthonormal polynomials with respect to ρ. A key point of the paper is that we recommend constructing the orthonormal polynomials ϕ_α according to a total monomial ordering $\prec$ in d-dimension, which is *the same* monomial order used in the algebraic theory. Using Gram-Schmidt or Cholesky facturization and proceeding in the $\prec$ order we can always generate orthonormal polynomials in this way. This idea of taking orthogonal polynomials in the same order as the monomial order appears in [22] where it was used for statistical analysis.

The art of quadrature is to choose the design in such a way that (9) holds, for selected polynomials, such as raw monomials. It can help to combine the algebraic method with the orthogonal expansion in the $h_i(x)$. Expand each of the $g_i(x)$ and $s_i(x)$ in (7):

$$g_i(x) = \sum_{\alpha\geq 0} a_{i,\alpha} \phi_\alpha(x),$$

$$s_i(x) = \sum_{\beta \geq 0} b_{i,\beta}\phi_\beta(x).$$

Then, integrating, using the orthogonality and collecting terms, we have the following.

Lemma 3.7. *Given the expansion $f(x) = \sum_{i=1}^m s_i(x)g_i(x) + r(x)$, the necessary and sufficient conditions for exact quadrature for $p(x)$ is*

$$\sum_{i=1}^m \sum_{\alpha \geq 0} a_{i,\alpha} b_{i,\alpha} = 0.$$

As an example consider $d = 2$ and (X_1, X_2) to be iid N(0,1). Then we have the product Hermite polynomial (we ignore normalisation):

$$H_{(\alpha_1,\alpha_2)} = H_{\alpha_1}(x_1)H_{\alpha_2}(x_2),$$

where the $H_i(x)$ are

$$1, x, x^2 - 2, x^3 - 3x, \ldots.$$

Take $\mathcal{D}$ to be the solution of $\{x_1(x_2^2 - 3) = 0, (x_1^2 - 3)x_2 = 0\}$ giving

$$\mathcal{D} = \left\{\left(\pm\frac{1}{\sqrt{3}}, \pm\frac{1}{\sqrt{3}}\right)\right\} \bigcup \{(0,0)\}.$$

With respect to the monomial ordering degree reverse lexicographic ordering a G-basis for $\mathcal{D}$ is $\{x_1x_2^2 - 3x_1x_2^2 - x_2^2, x_2^3 - 3x_2\}$. We can express these in terms of the $H_\alpha(x)$ and write out, in shorthand, for any polynomial $f(x_1, x_2) \in R[x_1, x_2]$

$$f(x_1, x_2) = s_1(H_{11} - 2H_{10}) + s_2(H_{20} - H_{02}) + s_3H_{03}.$$

The condition for exact quadrature is

$$a_{1,11} - 2a_{1,10} + a_{2,20} - a_{2,02} + a_{3,03} = 0.$$

The algebraic quadrature in the context of Hermite polynomial has recently been examined in [11] where a two–equation formula was proposed to generate the quadrature weights and points. While Hermite polynomial with a Gaussian $\rho(x)$ are used in the above example, the method proposed in this paper is general with respect to $\rho(x)$ and their corresponding supports as well as orthonormal polynomials. This interplay between the theory of orthogonal polynomials for general measures, exposed by Lemma 3.7 and the algebraic theory of discrete designs (ideals of points) requires considerably more research.

3.3. **Moments.** In most work on quadrature there is interest in determining how many, or indeed which, moments can be evaluated directly. For a given probability measure ρ and multi-index $\beta = (\beta_1, \ldots, \beta_d)$, the β-moment is

$$\mu_\beta = \mathbb{E}(X^\beta).$$

Then, for a given monomial ordering, the exact quadrature condition (9) is

$$\mu_\beta = \mathbb{E}\left\{r(X^\beta)\right\},$$

where $r(x) = NF(x^\beta)$. This gives a linear relationship between the μ_β and the moments μ_α, for $\alpha \in L$. We now give a matrix expression which will need the design matrix, A, for the algebraic method. Let $[x^\beta]$ is the vector of values of x^β, over the design, let $[x^\alpha]$ be the basis vector with entries $\{x^\alpha,\ \alpha \in L\}$ and μ the corresponding vector of moments. Then interpolate x^β over the design $\mathcal{D}$ $[x^\beta] = A\theta$, where A is the design matrix. Then

$$x^\beta = [x^\alpha]^T\theta = [x^\alpha]^T A^{-1}[x^\beta],$$

where $[x^\beta]$ is the vector of values of x^β, over the design and $[x^\alpha]$ is the basis vector with entries $\{x^\alpha,\ \alpha \in L\}$ where μ is the vector of moments corresponding to $\alpha \in L$. Replacing x by random X, according to ρ, and taking expectations, we have a matrix version of the exact the quadrature condition 9:

$$\mu_\beta = [\mu_\alpha]A^{-1}[x^\beta].$$

The following result is almost immediate.

Lemma 3.8. *Given a design $\mathcal{D}$, monomial order $\prec$ and corresponding list L, a moment μ_α for any $\alpha \in L$ has exact quadrature for any measure ρ.*

Proof. This follows since $\sum_{i=1}^{m} s_i(x)g_i(x)$ is identically zero for any polynomial in the quotient ring.

Thus, a quadrature formula with n distinct quadrature points that gives exact quadrature with n moments for any measure (for which the moments exist) always exists. In fact we can go a little further. Given any set of n moments whose index set has the order ideal staircase property we can construct a design with n points for which those moments have exact quadrature. We do this by taking a design having the same staircase pattern as L (we omit the proof). It is for μ_β, for $\beta \notin L$, that the relationship between β, $\mathcal{D}$, $\prec$, and ρ, for exact quadrature, becomes more complex.

The conditions for exact quadrature for a polynomial defined via a set of of monomials $x^\alpha, \alpha \in M$:

$$f(x) = \sum_{\alpha \in M} c_\alpha x^\alpha,$$

is, as we have seen, always a single linear restriction on the $c_\alpha, \alpha \in M$. The condition becomes

$$\sum_{\alpha \in M} c_\alpha \mu_\alpha - \sum_{z \in \mathcal{D}} w_z \sum_{\alpha \in M} c_\alpha z^\alpha = 0.$$

We write this as

$$\sum_{\alpha \in M} k_\alpha c_\alpha = 0,$$

where

$$k_\alpha = \mu_\alpha - \sum_{z \in \mathcal{D}} w_z z^\alpha, \ \alpha \geq 0.$$

Thus we have $k_\alpha = 0$ wherever we have exact interpolation for a monomial x^α. We note, also, that we can bound the error:

$$|\mathbb{E}_\rho p(X) - \sum_{z \in \mathcal{D}} w_z p(z)| = |\sum_{\alpha \geq 0} k_\alpha c_\alpha| \leq \|k\| \|c\|,$$

where $\|k\| = \sqrt{\sum_\alpha k_\alpha^2}, \ \|c\| = \sqrt{\sum_\alpha c_\alpha^2}$.

3.4. **Non-negative weights.** The difficult problem of when the weights in quadrature are non-negative is resolved in the algebraic method, discussed here. We have seen that given a design, $\mathcal{D}$, and monomial term order, $\prec$ we obtain a basis $x^\alpha, \alpha \in L$. Let ρ be a measure and let w be the vector of weights in our quadrature and let μ be the vector of moments corresponding to the model basis: $\{\mu_\alpha, \alpha \in L\}$. Let A be the design matrix. The weights in our quadrature are given by

$$w = {A^T}^{-1} \mu. \tag{11}$$

Thus the weights are non-negative if and only if

$$\mu = A^T w, \tag{12}$$

with $w \geq 0$. In the algebraic approach the constant term is always in the model basis so that the first column of A is a vector on ones and $\sum w_j = 1$ always holds. We can summarize:

Lemma 3.9. *The weights in the algebraic version of quadrature based on a design $\mathcal{D}$, a monomial order $\prec$ and a measure ρ are non-negative if and only if the moment vector μ lies in the convex hull of rows of the design matrix A (transposed).*

It should be emphasized that the moment space of A is independent of the measure ρ. The link is that both μ and the columns of A are predicated on the model basis $\{x^\alpha, \alpha \in L\}$.

As a simple example consider three quadrature points $\mathcal{D} = \{-1, 0, 1\}$ on one dimension and let ρ be a $N(\mu_1, \sigma^2)$, normal distribution. The basis is $\{1, x, x^2\}$ and $\mu = (1, \mu_1, \mu_2)$, where $\mu_2 = \mu_1^2 + \sigma^2$ and

$$A = \begin{pmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \end{pmatrix}.$$

From (11) condition of $w \geq 0$ become

$$-\mu_1 + \mu_2 \geq 0,$$
$$1 - \mu_2 \geq 0,$$
$$\mu_1 + \mu_2 \geq 0.$$

This is equivalent to (μ_1, μ_2) lying in the triangle with corners $\{(0,0), (-1,1), (1,1)\}$.

The following provides a quick test for non-negativity of the weights.

Lemma 3.10. *The weights $\{w_z, z \in \mathcal{D}\}$ in quadrature for the algebraic method are non-negative if and only if $\sum_{z\in\mathcal{D}} |w_z| - 1 = 0$*

Proof. If $w_z \geq 0$ for all $z \in \mathcal{D}$ then $\sum_{z\in\mathcal{D}} |w_z| - 1 = \sum_{z\in\mathcal{D}} w_z - 1 = 0$. On the other hand if some $w_z < 0$ then $\sum_{z\in\mathcal{D}} |w_z| - 1 > \sum_{z\in\mathcal{D}} w_z - 1 = 0$.

As it is desirable to have quadrature weights that are positive with small dispersion for reason of integration stability, we introduce the following measures to quantify these two effects:

$$\phi_1 = \left(\sum_{z\in\mathcal{D}} |w_z| - 1 \right) / n, \tag{13}$$

$$\phi_2 = \left(\sum_{z\in\mathcal{D}} (w_z - \bar{w})^2 / (n-1) \right)^{1/2}. \tag{14}$$

Where $\bar{w} = \frac{1}{n} \sum_{z\in\mathcal{D}} w_z$. Thus, ϕ_1 is small if most of the weights are positive and ϕ_2 is our measure of weight variance.

3.5. **Leave–one–out cross validation.** In order to estimate the accuracy of the metamodel, the leave–one–out cross validation is used. In this validation, the input design $\mathcal{D}$ is divided into a training set for the construction of the metamodel $\mathcal{D} \setminus x_j$ and the validation set which consists of one single point x_j. The accuracy of the metamodel $\hat{f}_{\mathcal{D}\setminus x_j}(x)$ is then estimated at the validation point x_j with $\epsilon_j = \hat{f}_{\mathcal{D}\setminus x_j}(x_j) - f(x_j)$. The leave–one–out (LOO) error is defined as the sum of the squares of errors $\mathcal{E}_{LOO} = \sum_{j=1}^{n} \epsilon_j^2 / n$ and a coefficient of determination can be estimated with $R^2 = \mathcal{E}_{LOO} / \mathrm{Var}[f(X)]$.

As the algebraic quadrature rule can be constructed from any arbitrary input design, such cross–validation could be performed even on a Gauss–quadrature input design and can be used to estimate the accuracy of the metamodels constructed with algebraic quadrature.

4. Examples

Using the methodology outlined in Section 3, the algebraic quadrature (AQ) is examined for univariate and multivariate cases in the following Section. The key steps in generating the algebraic quadrature points and weights are as follow:

(1) Choose a measure ρ and a design $\mathcal{D}$ consisting of points Z_1, Z_2, ..., Z_n,
(2) Select a monomial term ordering, $\prec$, and initial order if $d > 1$,
(3) Compute Gröbner basis $G = \{g_i(x), i = 1, \ldots, m\}$ for the ideal of $\mathcal{D}$, $I(\mathcal{D})$, and its quotient ring or quotient basis, $x^\alpha, \alpha \in L$,
(4) Define for each point, Z, in $\mathcal{D}$, the indicator function over the quotient basis such that

$$l_z(x) = \sum_{\alpha\in L} C_{Z,\alpha} x^\alpha = \delta_{x,Z}, \text{ for all } x \in \mathcal{D},$$

(5) For the indicator function of each design point $l_Z(X)$, find $C_{Z,\alpha}$ and compute the quadrature weights from $w_z = \mathbb{E}_\rho\{l_z(x)\}, \ x \in \mathcal{D}$,
(6) Or the weights can be determined by the design matrix with rows indexed by the design points and columns indexed by the quotient basis, where

$$A = \{x^\alpha\}_{x\in\mathcal{D}, \alpha\in L}$$

is $n \times n$ and has full rank n. The quadrature weights $w(z)$ for $z \in \mathcal{D}$ is $w = {A^T}^{-1}\mu$, where μ are the vector of moments corresponding to the model basis: $\{\mu_\alpha, \alpha \in L\}$. Note also that A can also be found by a rank–checking procedure: enter columns in the $\prec$ order skipping any column which leaves the current matrix non-full rank. This method is based on matroid theory and is described in [3, 19].

The software packages used in the current study are CoCoA 4.7 for algebraic quadrature [1, 9], Maxima 12.04.0 for the symbolic quadrature [20] DiceDesign for design discrepancy and coverage calculations [12] and Matlab R2008b with statistics toolbox. We invite readers to contact us to obtain the algebraic quadrature software package to help us test and improve the methodologies developed. From this package, the readers can examine the set-up of an algebraic quadrature from a general example and compute the algebraic quadrature of their own design.

4.1. **Univariate quadrature rules.** In this section, univariate algebraic quadrature (AQ) rules will be examined with some test functions.

4.1.1. *Classical quadrature designs.* The following classical rules are tested:

(1) Gauss–Hermite (normal measure) [13],
(2) Gauss–Laguerre (semi-infinite gamma measure),
(3) Gauss–Legendre (uniform measure),
(4) Gauss–Chebyshev (uniform measure),
(5) Clenshaw-Curtis-Chebyshev (uniform measure & nested),
(6) Fejer (uniform measure & nested),
(7) Gauss–Legendre Lobatto (uniform measure),
(8) Gauss–Legendre Radau (uniform measure),
(9) Kronrod–Patterson (normal measure & nested) [14].

The algebraic quadrature method reproduced the known weights for all of the above classical rules. Since the method proposed is similar to the derivation of the quadrature weights with Lagrange interpolating polynomial, it is expected that the quadrature weights are exactly reproduced for all univariate designs.

In the Gauss–Legendre quadrature cases, $n-$ and $n+1$–point designs, denoted as $\mathcal{D}_n$ and $\mathcal{D}_{n+1}$, are two unique sets. The algebraic quadrature weights of the union $\mathcal{D}_{n\cup(n+1)} = \mathcal{D}_n \cup \mathcal{D}_{n+1}$ are computed for the same ρ. Compared to the Gauss quadrature accuracies of $\mathcal{D}_n$ and $\mathcal{D}_{n+1}$, which are $p = 2n-1$ and $2n+1$ respectively, $\mathcal{D}_{n\cup(n+1)}$ has a theoretical algebraic quadrature accuracy of $p = 2n$ which is lower than that of $\mathcal{D}_{n+1}$. However, the AQ weights computed for $\mathcal{D}_{n+(n+1)}$ are 0 for points from $\mathcal{D}_n$ and the remaining weights are identical to the original Gauss–Legendre quadrature weights for points from $\mathcal{D}_{n+1}$, giving a quadrature accuracy of $2n+1$. In addition to being a general rule of quadrature weight generation, the AQ method also maximizes the polynomial exactness of the set of quadrature weights generated.

4.1.2. *Random input designs.* Univariate bounded and unbounded random design are tested. For the unbounded case, a Monte Carlo design from a normal distribution is tested. For the bounded case, Monte Carlo (MC), Latin hypercube sampling (LHS), Sobol sequence (SS) and scrambled Sobol sequence (SSS) input designs are tested. Given the same $\mathcal{D}$ and $\prec$, the weights can be determined for different measures ρ. Figure 2 shows the quadrature weights for two different input designs determined from three different measures on the same support. Uniform and beta are two well known measures with corresponding Gauss-quadrature rules. In contrast, the triangle measure is defined by a peak value at c with linear functions of $\rho(x)$ in $[0, c]$ and $[c, 1]$. There is no known classical quadrature rule for such measure. While there are are negative weights for all $\rho(x)$ examined, the sum of the weights are always 1 in all the measures tested, as required in Section 3.4.

Univariate input design with n points give a quotient basis that includes $\{\alpha : \alpha = 0, 1, \cdots n-1\}$ so that a n–point design will approximate exactly a polynomial function up to degree $p = n-1$. In the context of PCE numerical integration, the integrand is a product of $f(x)$ and $\phi_\alpha(x)$ in equation 1 and the expansion order that can be exactly estimated is limited up to $p^* = \lfloor \frac{n-1}{2} \rfloor$.

The qualities of the weights are checked with measures ϕ_1 and ϕ_2. As mentioned, it is desirable to have quadrature weights that are positive and with small dispersion for reason of integration stability. We show the evolution of ϕ_1 and ϕ_2 for different designs with increasing n in Figure 3. For the random designs, sample averages from 100 realizations of the input designs are used. Negative weights, as measured by ϕ_1, exist in all random designs tested but there are no negative weights for Gauss–Legendre and Gauss–Chebyshev designs. The absence of negative weights means that the

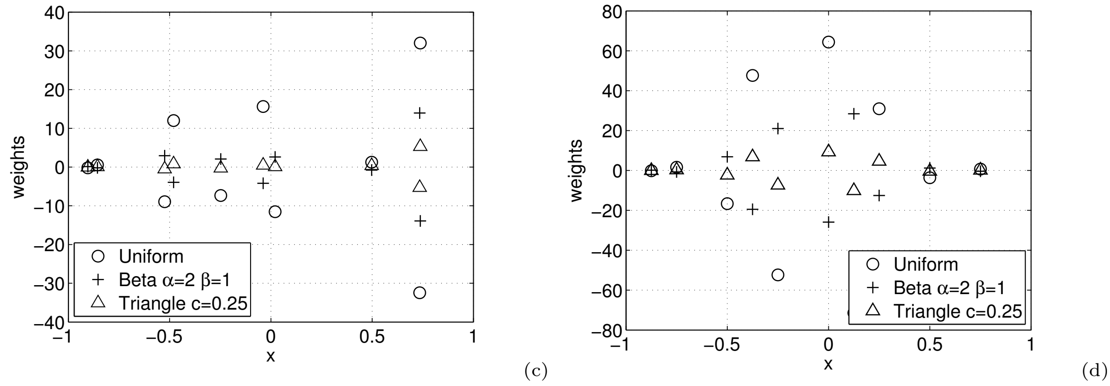

FIGURE 2. Algebraic quadrature weights at shown at the quadrature points for a 10–point (c) MC and (d) Sobol sequence with different $\rho(x)$.

weight variance, ϕ_2, decreases with increasing design size, cf. Figure 3.b. For other random input designs, MC inputs give AQ weights that are more negative with larger variance. In contrast, the values of ϕ_1 and ϕ_2 for LHS, SS and SSS input designs are comparable. The accuracy of the AQ rules will be discussed in Section 4.2.

We note that successive LHS samples are generated incrementally. When a n–point input design is to be enriched by an additional point, the support is divided into $(n+1)$ equally probable intervals and a point is randomly assigned in the interval missing a point. It may occur that more than one interval is missing a point and in this case sufficiently many points are added to ensure that all intervals are populated. Such irregular increment is more frequent for higher d and n.

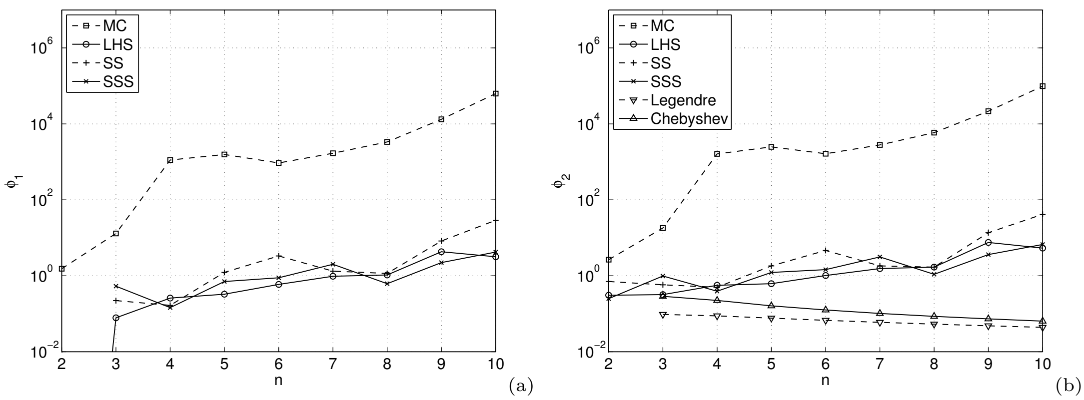

FIGURE 3. (a) ϕ_1 and (b) ϕ_2 for MC, LHS, SS, SSS, Chebyshev and Legendre with increasing n.

4.2. **Univariate integration.** The polynomial accuracy of the n–point AQ at $p = n-1$ is verified with the following moments of uniform distribution, which have the exact solutions

$$\int_{-1}^{1} \frac{x^k}{2} dx = \begin{cases} \frac{1}{k+1}, & \text{if } k \text{ even,} \\ 0, & \text{if } k \text{ is odd.} \end{cases} \tag{15}$$

The moments are first computed using classical n-point Gauss–Legendre and Gauss–Chebyshev rules, which have theoretical accuracies of $p = 2n-1$ and $p = n$, respectively. The error in the numerical quadrature is shown with increasing n in Figure 4 and it demonstrates that when 5-point quadrature rules are used, accuracies up to $p = 9$ and $p = 5$ were indeed obtained for these two quadratures. Using the AQ method, the quadrature weights for 5–point MC, LHS, SS and SSS designs are derived. Their approximations of the moments were accurate up to $p = 4$ and this confirms the theoretical AQ polynomial accuracy. In contrast, the Monte Carlo approximation with equally weighted input points is only able to approximate the constant term since the weights sum up to unity.

The effect of the non–linearity in the integrand is examined here by comparing the AQ with Gauss-Legendre quadrature for $f(x) = cos(x)$ with increasing size of input design, *cf.* Figure 4(b). The numerical quadrature approximates an integral over $[-1, 1]$ with a uniform support. As expected, the Gauss–Legendre quadrature is more accurate than results from random input desings with the same n. When the results from the random input designs are compared, their AQ estimators converge towards the true integral faster than the unbiased MC sum. When compared to the coefficients of Taylor expansion of the function shown for increasing n in Figure 4(b), the AQ results have the same rate of convergence with increasing n.

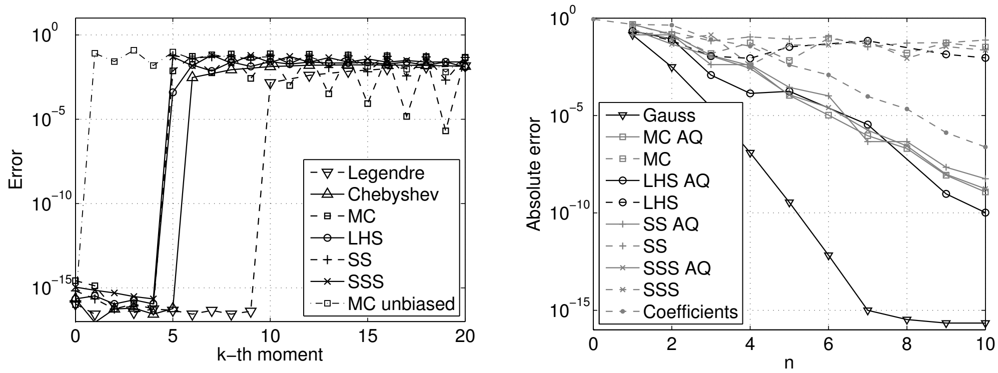

FIGURE 4. (a) The logarithmic values of absolute errors of different quadrature approximation of uniform distribution moments with different 5–point input designs. (b) Comparison of the errors with Monte Carlo (triangles), algebraic quadrature (circles) and Gauss Legendre quadrature (squares) for two different functions.

100 independent realizations of 10–point MC and LHS input designs are generated and the relationship the measures ϕ_1 and ϕ_2 and the quadrature accuracies of each design is examined. The goal is to predict the quadrature accuracy by judgment of the quality measures of the design. In addition to the ϕ_1 and ϕ_2 measures proposed in Section 3.4, the L2-discrepancy, the centered L2-discrepancy and the coverage measures from [12] are also computed for each realization of the input design. All the measures are compared against the AQ accuracy in integrating $f_{\cos}(x) = \cos\left(x + \frac{1}{2}\right)$ over the uniform support. The results are sorted according to the magnitude of ϕ_1 and are shown in Figure 5 for MC and LHS input designs. For the design discrepancy and coverage measures, no correlation is observed with the quadrature errors for either MC or LHS. In contrast, a clear correlation is observed between the magnitudes of the ϕ_1 and ϕ_2 of a design and its quadrature approximation accuracy. For the MC design, large variations exist in the values of ϕ_1 and ϕ_2 amongst the 100 realizations of $\mathcal{D}$ and these $\mathcal{D}$ with small values of ϕ_1 and ϕ_2 provide quadrature approximation with small error. In comparison, the LHS $\mathcal{D}$ have smaller and more uniform ϕ_1 and ϕ_2 measures and the variations in the quadrature errors are smaller. It can be concluded that the measures ϕ_1 and ϕ_2 are more accurate in predicting the quadrature approximation accuracy than conventional design discrepancy and coverage measures.

4.3. **Univariate uncertainty quantification.**

4.3.1. *Quadrature design.* In this section, one–dimensional Gauss quadratures are used as the input design for the algebraic quadrature method. Gauss quadrature construction of a PCE metamodel rely on the entire set of n quadrature inputs. Alternatively, AQ PCE metamodels can be constructed on n $\{D \setminus x_i\}$ training sets with which LOO cross–validation can be perform at each point x_i.

The function $f(x) = \exp(-(\frac{x-\mu_x}{\sigma_x})^2)$ over the bounded uniform support is used as a test function. In the first test case, $\mu_x = 1/4$ and $\sigma_x = 1/2$ are used and its exact response is shown in Figure 6(a). A 10-point Gauss quadrature design, shown in circles, is used to construct the GQ PCE metamodel with $p = 9$, shown in blue. In addition, 10 AQ PCE metamodels are constructed from a training

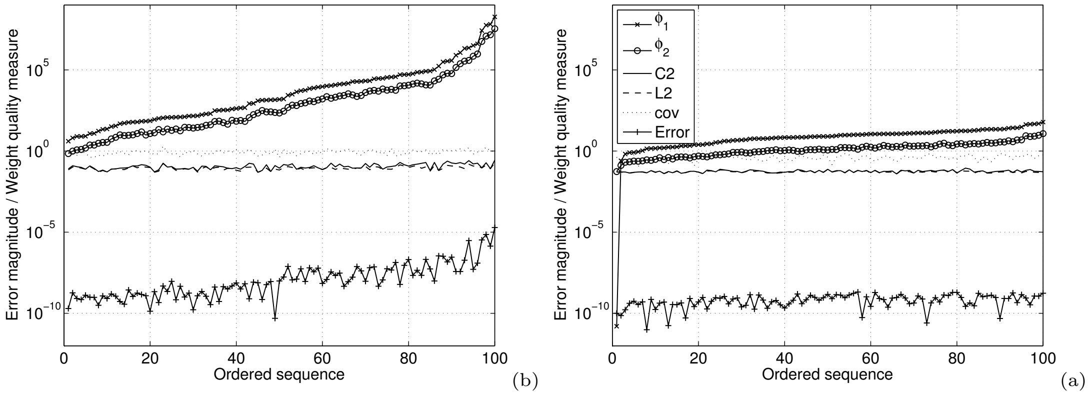

FIGURE 5. Comparison of the quality measures of 100 realizations of 10–point (a) MC and (b) LHS input designs and their respective algebraic quadrature approximation error magnitudes. The results are ordered in increasing magnitudes of ϕ_1.

set $D \setminus x_i$ and the 10 AQ PCE metamodel with $p = 4$ are traced with the red-lines. While the theoretical limit of the AQ PCE is $p = 4$, a range of polynomial orders is tested.

The LOO AQ PCE coefficients are determined by taking the average of all 10 AQ results and they were identical to the GQ PCE values at all p tested. Consequently, errors of the GQ PCE and LOO AQ PCE variance estimators with respect to the exact value are identical, *cf.* Figure 6(b). As the order of expansion exceeds the theoretical AQ order of $p = 4$, the metamodels become increasingly oscillatory. While the mean of all metamodels approaches the exact function response due to the symmetry in the quadrature points and in the LOO AG PCE metamodels, the LOO error grows when p exceeds the AQ theoretical exactness due to the increasingly oscillatory response in the PCE metamodels. If the LOO error is estimated from the absolute value of the arithmetic mean instead of the sum of squares, a continuous decrease in LOO error is observed up to $p = 4$ but increase after this point. The convergence of the errors are shown in dashed lines in Figure 6.(b) and similar error convergence with increasing p is observed. LOO error is thus a very conservative estimate of the AQ metamodel accuracy.

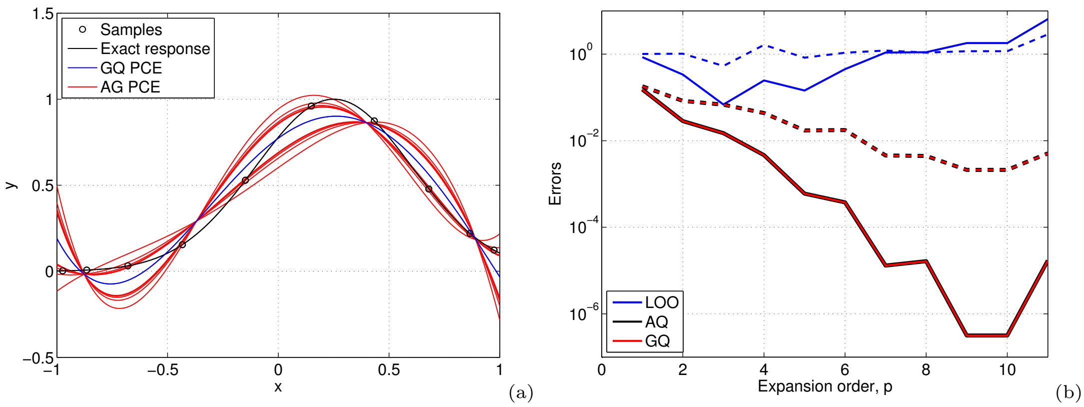

FIGURE 6. (a) The exact function response is approximated by the $p = 9$ GQ PCE metamodel in blue and the $p = 4$ LOO AQ PCE metamodels in red. The 10 Gauss–quadrature points used to construct the metamodels are shown in circles. (b) The errors in the GQ and LOO AQ PCE variance estimators with respect to the exact value for $\sigma_x = 1/2$ (in solid lines) and $\sigma_x = 1/4$ (in dashed lines).

4.3.2. *Random design.* The LOO cross validation is repeated in this section with one–dimensional random designs. In the first example, a 10–point LHS was used to construct a PCE metamodel of the test function $f(x) = \exp(-(\frac{x-\mu_x}{\sigma_x})^2)$ with $\mu_x = 1/4$ and $\sigma_x = 1/2$. The PCE estimators of mean and variance were compared to the exact values at different orders of PCE expansion p. In addition, an integral error of the PCE metamodel is defined as

$$\epsilon_{int} = \int_\Omega (\hat{f}_\mathcal{D}(x) - f(x))^2 \rho(x) dx,$$

whose value is approximated using 1×10^4 MC samples on $f(x)$. Since the metamodel accuracy depends on the input design, the sampling statistics of the LOO error, the integral error and the variance estimator error were estimated from 1000 realizations of 10–point LHS input design. In Figure 7.(a), the convergences of the mean of the sampling error means as well as the respective upper one standard–deviation envelopes are shown.

As repeated previously, the theoretical accuracy of a LOO AG PCE metamodel with a 10–point LHS input design is $p = 4$. From the errors in Figure 7(a), the variance estimator is the most accurate at $p = 4$ and the LOO error increase before the theoretical AQ accuracy level is reached, which is caused by the increasing oscillatory metamodel at higher p and the sum of square definition of the LOO error. Similarly, the integral error has similar convergence to the variance suggesting that the variance error is representative of the global metamodel accuracy in this example. In contrast to the variance estimator, the value of the mean estimator is independent of the expansion order and has a normalized error of of $0.59\% \pm 1.91\%$. The analysis is repeated for a 20–point LHS input design in Figure 7(b) and the errors are slightly worse than the theoretical estimates as error increases are observed already at $p = 7$. If 20–point MC input designs are used, the means of the sampling errors become much larger, as shown in Figure 7(b).

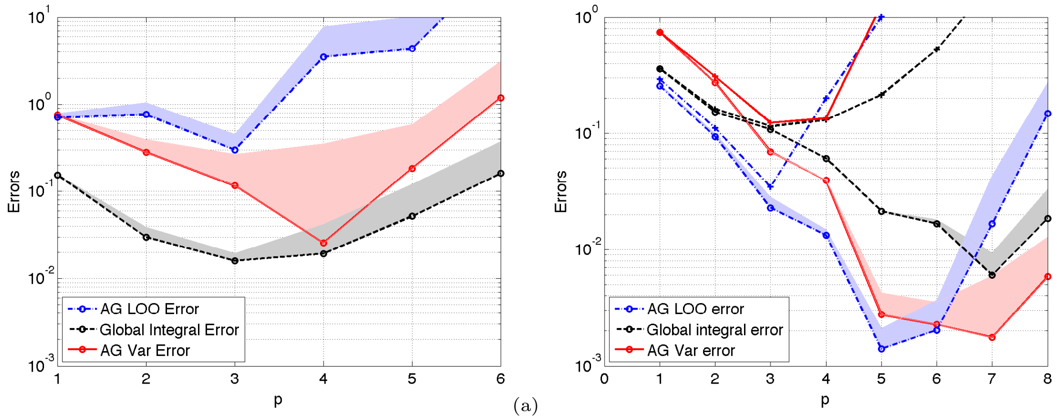

FIGURE 7. The sampling mean and one standard deviation envelope of LOO, integral and variance estimator errors estimated from (a) 10– and (b) 20–point LHS random input designs for increasing order of PCE expansion p. The same sampling statistics from 20–point MC random input designs are shown with '+' in (b).

Similar to results from previous sections, the weight quality measures of the LHS input designs as well as its quadrature approximation accuracies are better than these of the MC input designs. The global integral and the variance errors are consistent and give the same estimate of the maximum p allowed. In contrast, the LOO errors give a more conservative estimation of maximum p allowed.

4.4. **Multivariate quadrature rules.** Application of the algebraic quadrature rules for multivariate cases are discussed in the following sections.

4.4.1. *Monomial and initial ordering.* The AQ accuracy can be estimated from the quotient basis, which is dependent on the monomial ordering chosen in determining the Gröbner basis. While the monomial order does not have any effect in the univariate case (the G-basis is 'universal' or 'generic'), its definition plays an important role in the multivariate case. For example, a 7–point three–dimensional input design (MC, LHS or Sobol) yields the following quotient basis for different lexicographical orders implemented in CoCoA for the initial order $\{x_1 \prec x_2 \prec x_3\}$:

$$\{1, x_3, x_3^2, x_3^3, x_3^4, x_3^5, x_3^6\} : \text{degree lexicographical order,}$$
$$\{1, x_3, x_3^2, x_2, x_2x_3, x_2^2, x_1\} : \text{graded lexicographical order,}$$
$$\{1, x_3, x_3^2, x_2, x_2x_3, x_1, x_1x_3\} : \text{graded reverse lexicographical order.}$$

The degree lexicographical order fills only terms of the highest initial order. In contrast, graded reverse lexicographical order fills the interaction terms while the graded lexicographical order fills the higher terms before the interaction terms are considered [19]. The graded lexicographical monomial ordering will be used in the subsequent analyses to prioritize higher order terms.

The initial order is the sequence by which the input variables are ordered in the computation of the Gröbner basis. For example, a 7–point input design with graded lexicographical ordering gives the following quotient bases for the different initial orders:

$$\{1, x_1, x_2, x_3, x_2^2, x_2x_3, x_3^2\} : \text{for initial orders } \{x_1 \prec x_2 \prec x_3\} \;\&\; \{x_1 \prec x_3 \prec x_2\},$$
$$\{1, x_1, x_2, x_3, x_1^2, x_1x_3, x_3^2\} : \text{for initial orders } \{x_2 \prec x_1 \prec x_3\} \;\&\; \{x_2 \prec x_3 \prec x_1\},$$
$$\{1, x_1, x_2, x_3, x_1^2, x_2x_1, x_2^2\} : \text{for initial orders } \{x_3 \prec x_2 \prec x_1\} \;\&\; \{x_3 \prec x_1 \prec x_2\}.$$

As there is no *a priori* preference for the initial order, algebraic quadrature weights can be generated based on the Gröbner basis calculated using the $d!$ permutations of the initial orders. In the above example, a 7–point design gives three distinct sets of quadrature weights from each set of quotient bases. The union of these three sets of quotient bases gives all 10 terms in a polynomial expansion $\sum a_\alpha \phi_\alpha(x)$ up to $|\alpha| = 2$. When a set of algebraic weights is used to estimate a_α, the coefficient corresponding to each term in the quotient basis is exact if the expansion does not exceed $|\alpha| = 2$. If this condition is not satisfied, the quadrature accuracy will be affected aberration.

For a given initial order, the quotient basis incrementally adds sequentially higher terms in the canonical multivariate basis as n increases. For a complete set of quotient basis with polynomial order no greater than p, eg. $\{x^\alpha = x_1^{\alpha_1} \cdots x_1^{\alpha_d} : |\alpha| \leq p\}$, its cardinality is $n = \binom{d+p}{p}$ for all positive $p \in \mathbb{Z}$. When n is $\binom{d+p}{p}$, all initial orders will give the same quotient basis and thus the identical AQ weights. We denote this generic size as n^* and the quotient basis is said to be generic. Indeed, it was previously observed that a generic set of quotient basis exists at certain increments of n where the least aberration is observed [6]. If n is not generic, the quotient basis can be used to identify the polynomial accuracy of the algebraic quadrature but the confounding or aberration effects may have stronger influence on the accuracy of the algebraic quadrature.

The term "aberration" has been used in classical factorial design to evaluate the complexity of terms in a basis (factorial model) [16]. This complexity is close to looking at the maximum total degree of terms in the terms in the basis. In [5] [6], the authors study a type of aberration which looks at the profile of the upper boundary of the terms in the model, a kind of Nyquist sampling theory for polynomials. A particular type of design (i.e. generic) allows, in a well-defined sense, the maximum number of identifiable models. The accuracy of the AQ approximation will be discussed in the following Sections.

4.4.2. *Gauss quadrature.* To recall, an n–point univariate GQ rule approximates exactly a polynomial of degree up to $p = 2n - 1$ and these n points are the roots of the n–th order orthogonal polynomial. The corresponding multi–variate GQ's are constructed from full–tensor products of univariate GQ rules and the quadrature weights are products of the corresponding univariate weights. The AQ method is used to evaluate the weights of several multivariate GQ design, including Gauss–Hermite, Gauss–Legendre and Gauss–Laguerre quadratures. In all the cases tested, the corresponding GQ weights were recovered exactly. The initial order also did not have any effect on the Gauss quadrature weights. The GQ design is thus generic with respect to different initial orders even if n is not generic.

4.4.3. *Smolyak quadrature.* To alleviate the exponential increase in the number of quadrature points in the full–tensor GQ approach, the Smolyak sparse quadrature can be used. The Smolyak grids are the union of the tensor products of the difference sets between incremental univariate quadrature rules. Several sparse quadrature based on the Smolyak design was tested. The univariate quadrature rules used include Clenshaw–Curtis Chebyshev, Hermite Kronrod–Patterson [14] and Gauss–Legendre. In all cases, the algebraic method recovers the corresponding sparse quadrature weights. While all full–tensor quadrature weights are positive, Smolyak sparse quadrature may contains negative weights and the AQ method is able to correctly reproduce all positive and negative weights. The current method should also be able to reproduce the weights of quadratures with an anisotropic structure, c.f. [15]. As in the case of Gauss quadrature, the initial order has no effect on the quadrature weights.

4.4.4. *Random and deterministic input designs.* The qualities of the AQ weights of different input designs including MC, LHS and SS are examined at $d = 3$ on the $[-1, +1]$ support for a uniform measure for generic design sizes. For MC and LHS, a new input design is generated at each n tested while SS designs are generated by complementing existing designs. The means of the measures (13) and (14) are estimated from 100 realizations of the design and shown with solid lines in Figure 8. In addition, the minimum values of the measures found are shown with dashed lines. As the SS design is not random, only the deterministic measures is shown. In comparison to univariate cases in Figure 3, the measures increase more slowly with n for the multivariate case due to the slower increase in the nonlinearity of the quotient basis for the multivariate case. Both measures show that the Sobol' sequence does not always optimal with respect to measures (13) and (14), especially for high n, while LHS design is slightly better than MC on average. In addition, the measures for Smolyak sparse quadrature are also shown and they are perhaps the lower bound of measures for non–full tensor product designs. The accuracy of the multivariate AQ rules for different designs will be discussed in Section 4.5.

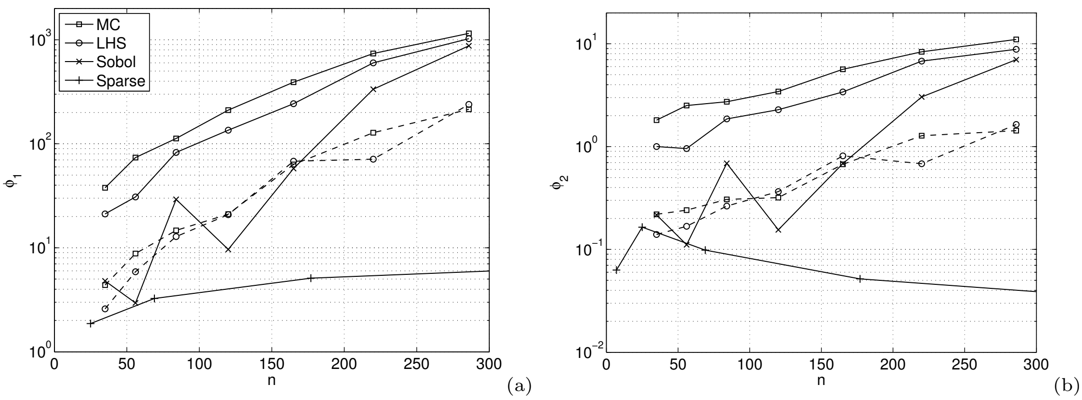

FIGURE 8. ϕ_1 and ϕ_2 for MC, LHS and SS with increasing values of generic n. The values for Smolyak sparse quadrature with Chebyshev Clenshaw–Curtis weights at some n are also plotted for comparison.

4.5. **Multivariate integration.** The AQ accuracy is estimated for several multivariate designs. It is first examined by comparing the moments of orthogonal polynomials against their exact values. Validation with the orthogonal conditions of the classical polynomial is useful because PCE relies on families of orthogonal polynomials. Given a quadrature rule of a certain dimension d and a desired PCE polynomial exactness p, it is important to know the size of input design, n, needed to exactly approximate the PCE. The AQ accuracy is then examined with respect to non–polynomial functions.

4.5.1. *Polynomial exactness.* The accuracy of multivariate AQ is established by checking its approximation of the orthogonal conditions of classical polynomials. The Legendre polynomial inner–product over the uniform support can be expressed analytically as

$$\langle L_i(x), L_j(x)\rangle = \int_{-1}^{+1} L_i(x)L_j(x)\rho(x)dx = \frac{2}{2i+1}\delta_{ij}.$$

A 7–point MC design and the corresponding AQ weights for different initial orders gives different accuracy in estimating the inner–product with symmetric integrands as predicted by the quotient basis as shown in Figure 9. However, the inner product approximation is exact for symmetric designs and the following Jacobi polynomial inner products with asymmetric shape parameters are tested in addition:

$$\langle P_i^{(a,b)}(x), P_j^{(a,b)}(x)\rangle = \frac{2^{a+b+1}}{2i+a+b+1}\frac{\Gamma(i+a+1)\Gamma(i+b+1)}{\Gamma(i+a+b+1)i!}\delta_{ij}.$$

The same 7–point MC input design is used to generate the AQ weights over the same support but with $\rho(x,a,b) = (1-x)^a(1+x)^b$ where $a = 2$ and $b = 1$. The resulting AQ approximation of the Jacobi polynomial inner products have an accuracy identical to those in Figure 9. The results of all permutations can be used to estimate all the terms satisfying $|p| \leq 2$. By changing $\rho(x)$ in the computation of the AQ weights in equation 10, the same input design could be used for quadrature approximate with a different weight on the same support. This gives the flexibility of altering the input measures without regenerating the input design and the corresponding outputs, as described in Section 4.1.2.

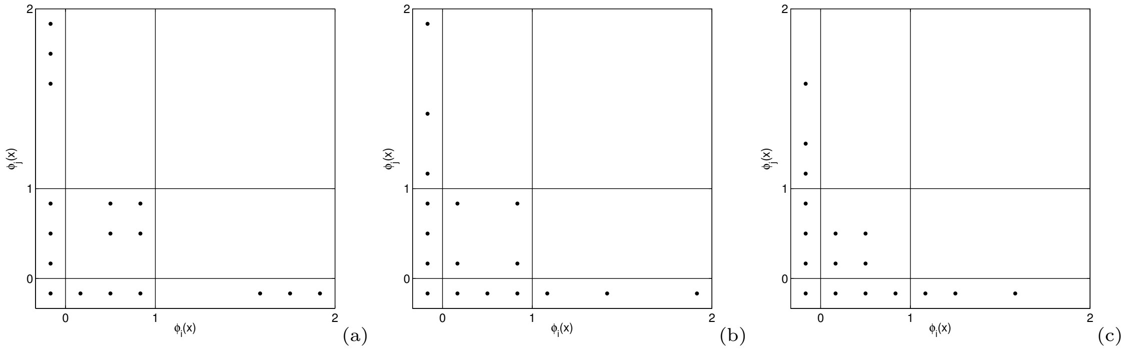

Figure 9. AQ polynomial accuracy of a 7–point Monte Carlo design in approximating the orthogonality condition of Legendre and Jacobi ($a = 2$ & $b = 1$) polynomials with initial orders (a) $\{x_1 \prec x_2 \prec x_3\}$ & $\{x_1 \prec x_3 \prec x_2\}$, (b) $\{x_2 \prec x_1 \prec x_3\}$ & $\{x_2 \prec x_3 \prec x_1\}$ and (c) $\{x_3 \prec x_1 \prec x_2\}$ & $\{x_3 \prec x_2 \prec x_1\}$.

For a given multivariate polynomial, it was found that a total of $n = \binom{d+2p}{2p}$ design points are needed to approximate a function of order $|\alpha| \leq p$ exactly. At these n values, the quotient bases are generic and the design has the least aberration [6].

4.5.2. *Non–polynomial functions.* The quadrature approximation of the following simple multivariate cosine function is examined where a parameter λ controls the nonlinearity of the integrand over a uniform support:

$$f(x) = \prod_{i=1}^{d} \cos\left(\frac{x_i}{\lambda}\right).$$

The effect of design quality measures on the accuracy of quadrature approximation is first examined. 100 independent realizations of generic MC and LHS input designs are generated and their quadrature approximation of the above function is compared against their design quality measures. Similar to the one–dimensional results in Section 4.2, design discrepancies and coverage, as well as ϕ_1 and ϕ_2 are computed for each realization $\mathcal{D}$. The results shown in Figure 10 are ordered in the increasing values of ϕ_1. In contrast to the one–dimensional results, the difference in the measures for the MC and the LHS designs are much smaller. However, a strong correlation between ϕ_1 and ϕ_2 and the quadrature error can still be observed; in contrast, the design discrepancies and coverage cannot predict the quadrature errors at all. The results from the test case $d = 3$ and $\lambda = 0.5$ in Figure 10 clearly underline the importance to use an input design with the smallest ϕ_1 and ϕ_2 values in order to reduce quadrature error.

The accuracies of GQ, SQ and AQ are compared below for increasing n and the input design tested for AQ include MC, LHS, SS and SSS for $d = 3$. The sizes of the algebraic design n are

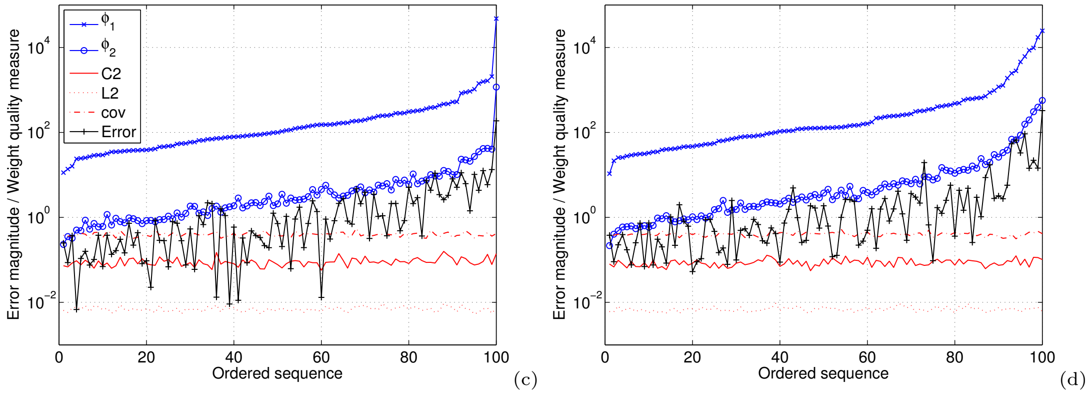

FIGURE 10. Comparison of the quality measures of 100 realizations of 84–point (a) MC and (b) LHS input designs and their respective algebraic quadrature approximation error magnitudes for $d = 3$ and $\lambda = 0.5$. The results are ordered in increasing magnitudes of ϕ_1.

generic such that $n^* = \binom{d+2p}{2p}$ for $p = 1$ to $p = 7$, with corresponding $n = 10$ to $n = 680$. AQ results with MC, LHS and SSS are not deterministic and only one realization of the input designs is tested. The LHS designs are generated independently of previous designs and not incrementally. GQ and SQ with increasing quadrature levels are used and equally–weighted MC results are shown for comparison.

As the quadrature approximation depends strongly on the non–linearity of the function, results from $\lambda = 1$ and $\lambda = 2$ are shown in Figure 11. In all cases tested, the GQ approximations of the integrals are more accurate than AQ or MC at all n. The accuracies are comparable for the different AQ designs tested but the Sobol' sequence based designs have slightly lower error magnitudes in comparison. Initially at high λ, AQ is more accurate than the MC. As λ approaches π (a complete period in $\Omega \in [-1, 1]$), the AQ approximation becomes poorer than MC. Due to the presence of negative weights in both AQ and SQ, the convergence of the integral approximation and the accuracy of the quadrature with increasing n are strongly influence by the function response with in the input support.

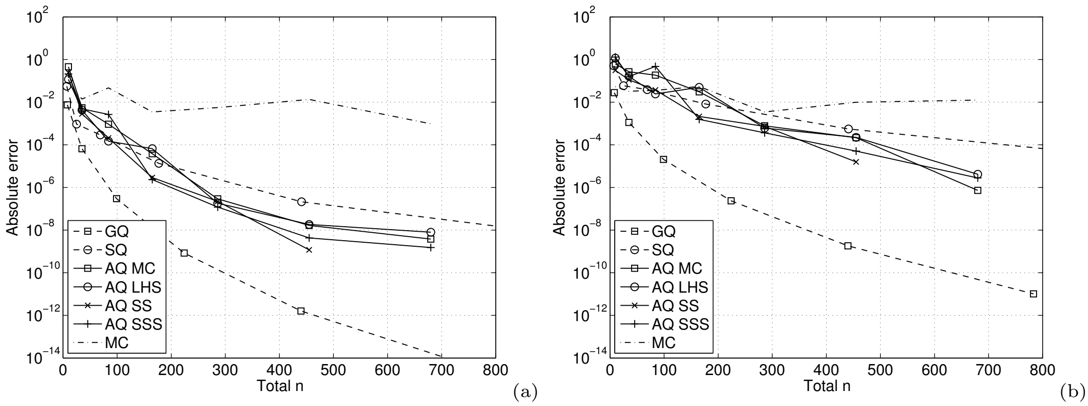

FIGURE 11. Change in the absolute error of a three–dimensional numerical integral with increasing n for the equation (4.6) with (a) $\lambda = 1$ (b) $\lambda = 2$.

4.6. **Multivariate uncertainty quantification.** The LOO cross–validation is used to provide a metamodel error estimate and the LOO errors found are consistent with the theoretical AQ accurate estimate in the univariate cases investigated. In order for the training sets of the LOO AQ PCE metamodel to be generic, the design for LOO AQ PCE needs to have a size $n = n^* + 1$. While one can optimize a design of size $n^* + 1$ for ϕ_1 and ϕ_2, the optimality is not necessarily preserved for the training set when one single design point is removed for LOO cross validation. Indeed, large values of ϕ_1 and ϕ_2 may be observed amongst the n^*+1 training sets. Therefore, the accuracies of the LOO AQ PCE metamodel based on an optimal design of size n^*+1 and the AQ PCE metamodel based on a least–aberration and optimal design of size n^* need to be compared.

The LOO AQ and AQ methods are used to construct PCE metamdel for a Gaussian function with the following form

$$f(x) = \prod_{i=1}^{d} \exp\left(\frac{-(x_i-\mu_i)^2}{\sigma_i}\right),$$

where x_i are iid uniform random variables. The degree of non–linearity is controlled by σ_i. Generic input design size n^* is determined for different p and the errors of the PCE mean and variance estimators are compared against the analytical values. Values of $\sigma = 3$ and $\mu = 0.25$ are used in the current analysis.

At each n^*, 100 realizations of LHS input designs are generated and the design with the smallest weight measure ϕ_1 is retained. $\mathcal{D}_{n^*}$ is used to construct AQ PCE and $\mathcal{D}_{n^*+1}$ is used to construct AQ LOO PCE. For the variance estimator, the PCM approximation is also used and the mean from n^*+1 PCM variances are used as the final result. The error in the mean and variance estimators from the different methods are shown in Figure 12. In addition, the mean and the variance are also estimated from the unbiased sum of LHS samples. For comparison, the GQ mean and variance estimators are shown for reference.

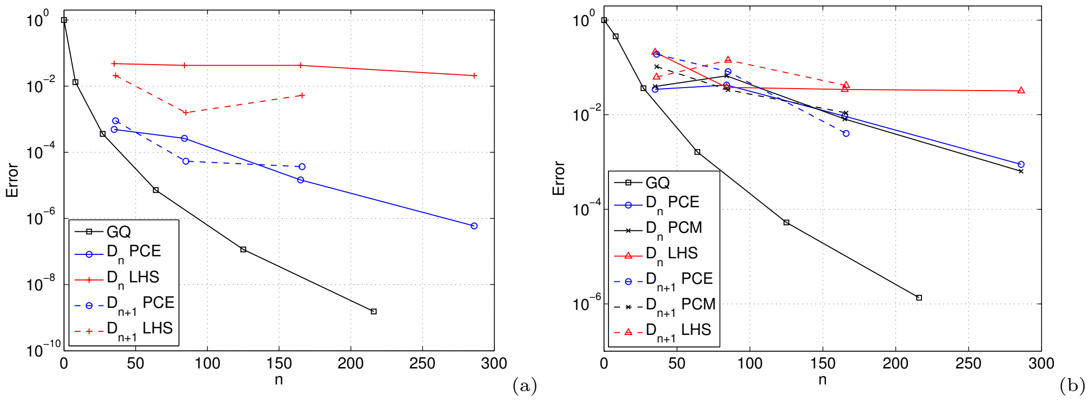

FIGURE 12. (a) Mean and (b) variance estimated from different quadrature methods for a $d = 3$ Gaussian test function with $\sigma = 3$ and $\mu = 0.25$.

For the solution mean, little difference is observed between the $\mathcal{D}_{n^*}$ PCE and the $\mathcal{D}_{n^*+1}$ LOO PCE. In contrast, the AQ results are more accurate than the unweighted LHS estimators when the same LHS designs are used. For the solution variance, little difference is observed between neither the $\mathcal{D}_{n^*}$ PCE and the $\mathcal{D}_{n^*+1}$ LOO PCE estimators nor the PCE and PCM estimators. While the LHS variances are comparable to the AQ values at small n, the AQ results are more accurate than LHS for higher n. As observed in the univariate case, the Gauss quadrature results are more accurate than the AQ or the LHS results. While n^*–point designs have smaller abberation, (n^*+1)–point design give an average of many solutions which improves the accuracy of the estimators.

One issue is how the quality of the interpolation, of the type covered here, affects the quality of the quadrature. Recent work [4] extends the polynomial basis beyond $n = |D|$ and uses the extra degrees of freedom to maximise the smoothness, counteracting the Runge phenomenon. This typically leads to improved integrated mean squared error. It would be interesting to extend the ideas to improve quadrature.

5. Conclusion

An alternative quadrature solution to polynomial chaos expansion (PCE) is explored where the algebraic method in experimental design is used to estimate the polynomial expansion accuracy of a random input design. This method is based on the theory of zero dimensional algebraic varieties and allows quadrature for quite general sets of input designs. Algebraic method in quadrature is used to generate the quadrature weights for an arbitrary input design $\mathcal{D}$ on a support Ω to create a numerical quadrature with a known polynomial order of accuracy. The definition of a measure $\rho(x)$ and monomial ordering $\prec$ completes the definition of the algebraic quadrature method. Indeed, the algebraic quadrature is a general method to determine the appropriate quadrature weights and it reproduces the quadrature weights for all classical univariate and multivariate Gauss and Smolyak sparse quadrature schemes. While the quadrature corresponding to random input designs such as Monte Carlo, Latin hypercube sampling or low–discrepancy sequences can be derived, their qualities in terms of non–negativity and variance in the quadrature weights demonstrate the difference in the quadrature solution. The algebraic quadrature results are not deterministic when design are not based on tensor products of polynomial roots. For different realizations of random input samples, the maximum quadrature accuracy is bounded by the quadrature's theoretical polynomial exactness given by the quotient ring defined by the algebraic method. Before its application to PCE, the algebraic method in quadrature is first validated against analytical solutions of univariate and multivariate integrals. For integrals of polynomial test functions, the algebraic quadrature polynomial exactness agrees with its theoretical estimate. In the multivariate case, testing all permutations of the initial orders in the algebraic quadrature generation of the quotient basis can be used to maximize the number of terms that one input design can accurately approximate. To minimize the aberration in the design, the generic size of the input design can be used and the weight quality measures are also used to select the random input design. For an integration test at $d = 3$, algebraic quadrature is observed to be comparable with the results of sparse quadrature. The PCE mean and variance estimators approach the analytical values much faster for increasingly linear functions; refinement methods to improve the method's accuracy should be examined. It is in this context that the algebraic method in quadrature allows different deterministic and random input designs to be compared and such comparison can be extended in the future to the least–square solution of PCE. More experience is needed in the implementation and application of AQ to UQ problems and we invite readers to contact us to obtain the AQ software tools to examine the methodologies developed.

References

[1] J. Abbott and A.M. Bigatti, *CoCoALib: a c++ library for doing Computations in Commutative Algebra*. Available at `http://cocoa.dima.unige.it/cocoalib`, 2013.

[2] R. Askey and J. Wilson, *Some basic hypergeometric orthogonal polynomials that generalize jacobi polynomials*, Memoirs of the American Mathematics Society Series, 54 (1985).

[3] E. Babson, S. Onn, and R. Thomas, *The hilbert zonotope and a polynomial time algorithm for universal grobner bases*, Advances in Applied Mathematics, 30 (2003), pp. 529–544.

[4] R. A. Bates, H. Maruri-Aguilar, and H. P. Wynn, *Smooth supersaturated models*, Journal of Statistical Computation and Simulation, 84 (2014), pp. 2453–2464.

[5] Yael Berstein, J. Lee, Hugo Maruri-Aguilar, Shmuel Onn, Eva Riccomagno, R. Weismantel, and Henry P Wynn, *Nonlinear matroid optimization and experimental design*, SIAM J. Discrete Math, 22 (2008), pp. 901–919.

[6] Yael Berstein, Hugo Maruri-Aguilar, Shmuel Onn, Eva Riccomagno, and Henry P Wynn, *Minimal average degree aberration and the state polytope for experimental designs*, Annals of the Institute of Statistical Mathematics, 62 (2010), pp. 673–698.

[7] M. Berveiller, B. Sudret, and M. Lemaire, *Stochastic finite elements : a non intrusive approach by regression*, Revue Européenne de Mécanique Numérique, 15 (2006), pp. 81–92.

[8] R.H. Cameron and W.T. Martin, *The orthogonal development of nonlinear functionals in series of Fourier–Hermite functionals*, Annals of Mathematics, 48 (1947), pp. 385–392.

[9] CoCoATeam, *CoCoA: a system for doing Computations in Commutative Algebra*. Available at `http://cocoa.dima.unige.it`, 2013.

[10] D. Cox, J. Little, and D. O'Shea, *Ideals, Varieties, and Algorithms*, Springer-Verlag, New York, 1997. Second Edition.

[11] C. Fassino, G. Pistone, and E. Riccomagno, *The algebra of quadrature formulæ for generic nodes*. arXiv, 2013.

[12] Jessica Franco, Delphine Dupuy, Olivier Roustant, Guillaume Damblin, and Bertrand Iooss., *DiceDesign: Designs of Computer Experiments*, http://CRAN.R-project.org/package=DiceDesign, 2013.

[13] W. Gautschi, *Construction of gauss-christoffel quadrature formulas*, Math. Comp., 22 (1968), pp. 251–270.

[14] A. Genz and B. D. Keister, *Fully symmetric interpolatory rules for multiple integrals over infinite regions with Gaussian weight*, Journal of Computational and Applied Mathematics, 71 (1996), pp. 299–309.

[15] T. Gerstner and M. Griebel, *Dimension-adaptive tensor-product quadrature*, Computing, 71 (2003), pp. 65–87.

[16] M. Hamada and C. F. J. Wu, *Analysis of designed experiments with complex aliasing*, Journal of Quality Technology, 24 (1992), pp. 130–137.

[17] J. Ko, *Applications of the generalized polynomial chaos to the numerical simulations of stochastic shear flow*, PhD thesis, Université Pierre et Marie Curie, 2009.

[18] J. Ko and J. Garnier, *Multi-element stochastic spectral projection for high quantile estimation*, in Journal of Computational Physics, vol. 243, 2013, pp. 87–108.

[19] H. Maruri-Aguilar and H.P. Wynn, *The algebraic method in experimental design*, in Handbook of design and analysis of experiments, A. Dean, M. Morris, J. Stufken, and D .Bingham, eds., Chapman & Hall/CRC, 2015, ch. 11.

[20] Maxima, *Maxima, a computer algebra system. version 5.25.1.* Available at `http://maxima.sourceforge.net/`, 2011.

[21] S. Onn and B. Sturmfels, *Cutting corners*, Advances in Applied Mathematics, 23 (1999), pp. 29–48.

[22] Giovanni Pistone, Eva Riccomagno, and Henry P Wynn, *Gröbner basis methods for structuring and analysing complex industrial experiments*, International Journal of Reliability, Quality and Safety Engineering, 7 (2000), pp. 285–300.

[23] ———, *Algebraic Statistics*, vol. 89 of Monographs on Statistics and Applied Probability, Chapman & Hall/CRC, Boca Raton, 2001.

[24] G. Pistone and H.P. Wynn, *Generalised confounding with Gröbner bases*, Biometrika, 83 (1996), pp. 653–666.

[25] I. M. Sobol', *Sensitivity estimate for non-linear mathematical models*, Mathematical modelling and computational experiments, 1 (1993), pp. 407–414.

[26] B. Sudret, *Global sensitivity analysis using polynomial chaos expansion*, Reliability Engineering & System Safety, 93 (2008), pp. 964–979.

[27] G. Tang, G. Iaccarino, and M. S. Eldred, *SDM 2010 student papers competition global sensitivity analysis for stochastic collocation*, in 51st AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, 2010.

[28] M. A. Tatang, *Direct incorporation of uncertainty in chemical and environmental engineering systems*, PhD thesis, Department of Chemical, Massachusetts Institute of Technology, Boston, USA, 1995.

[29] N. Wiener, *The homogeneous chaos*, American Journal of Mathematics, 60 (1938), pp. 897–936.

[30] D. Xiu, *Numerical Methods for Stochastic Computations: A Spectral Method Approach*, Princeton University Press, 2010.

[31] D. Xiu and G. E. Karniadakis, *The Wiener-Askey polynomial chaos for stochastic differential equations*, SIAM Journal of Scientific Computing, 24 (2002), pp. 691–644.

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