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"Extraktion quantifizierbarer Information aus komplexen Systemen"

On the Convergence of Generalized Polynomial Chaos Expansions

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ON THE CONVERGENCE OF GENERALIZED POLYNOMIAL CHAOS EXPANSIONS*

OLIVER G. ERNST[†] ANTJE MUGLER[†] HANS-JÖRG STARKLOFF[†] AND ELISABETH ULLMANN[‡]

Abstract. A number of approaches for discretizing partial differential equations with random data are based on generalized polynomial chaos expansions of random variables. These constitute generalizations of the polynomial chaos expansions introduced by Norbert Wiener to expansions in polynomials orthogonal with respect to non-Gaussian probability measures. We present conditions on such measures which imply mean-square convergence of generalized polynomial chaos expansions to the correct limit and complement these with illustrative examples.

Key words. equations with random data, polynomial chaos, generalized polynomial chaos, Wiener-Hermite expansion, Wiener integral, determinate measure, moment problem.

1. Introduction. A fundamental task in computational stochastics is the accurate representation of random quantities such as random variables, stochastic processes and random fields using a manageable number of degrees of freedom. A popular approach, known by the names *polynomial chaos expansion*, *Wiener-Hermite expansion* or *Fourier-Hermite expansion*, represents a random variable by a series of Hermite polynomials in a countable sequence of independent standard Gaussian random variables—so-called *basic random variables*—, and employs truncations of such expansions as approximations. While the origins of this approach date back to the 1930s, renewed interest in Wiener-Hermite expansions has resulted from recent developments in computational techniques for solving stochastic partial differential equations (SPDEs), specifically partial differential equations with random data [13, 25, 1, 2, 40, 36]. The solutions of such equations are stochastic processes indexed by time and/or spatial coordinates, and in the latter case are referred to as *random fields*.

A fundamental result of Cameron and Martin [6] states that polynomials in a countable sequence of independent standard Gaussian random variables lie dense in the set of random variables with finite variance which are measurable with respect to these Gaussian random variables. However, the number of random variables and the polynomial degree required for a sufficient approximation depend on the functional dependence of this random variable on the Gaussian random variables. In a series of papers [42, 41, 44, 43, 46, 20], Xiu and Karniadakis discovered that in many cases better approximations of random variables can be achieved using polynomial expansions in non-Gaussian random variables, which they termed generalized polynomial chaos expansions. To retain the convenience of working with orthogonal polynomials in generalized polynomial chaos expansions, the Hermite polynomials are replaced by the sequence of polynomials orthogonal with respect to the probability measure associated with the basic random variables. The open question we address in this work is under what conditions the convergence of polynomial chaos expansions carries over to generalized polynomial chaos expansions. We show, based on classical results on the Hamburger moment problem, that an arbitrary random variable with finite variance

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can only be expanded in generalized polynomial chaos if the the underlying probability measure is uniquely determined by its moments.

The plan of the remainder of this paper is as follows: Section 2 recalls basic notation, definitions and convergence results of standard Wiener-Hermite polynomial chaos expansions, including the celebrated Cameron-Martin Theorem. Section 3 then treats generalized polynomial chaos expansions, with separate discussions of expansions in one, a finite number and a countably infinite number of basic random variables. A number of illustrative examples follow in Section 4.

2. Wiener-Hermite polynomial chaos expansions. In this section we recall the convergence theory of standard Wiener-Hermite polynomial chaos expansions. We begin with some remarks on the origins of the basic concepts, which date back to the beginnings of modern probability theory.

2.1. Origins. The term *polynomial chaos* was originally introduced by Norbert Wiener in his 1938 paper [39], in which he applies his generalized harmonic analysis (cf. [38, 26]) and what are now known as multiple Wiener integrals to a mathematical formulation of statistical mechanics. In that work, Wiener began with the concept of a continuous homogeneous chaos, which in modern terminology^{*} corresponds roughly to a homogeneous random field defined on \mathbb{R}^d which, when integrated over Borel sets, vields a stationary random measure. Essentially a mathematical description of multidimensional Brownian motion, Wiener's homogeneous chaos was a generalization to what Wiener called "pure one-dimensional chaos", the random measure given by, in modern terminology, the increments of the Wiener process. The term polynomial chaos was introduced in [39] as the set of all multiple integrals taken with respect to the Wiener process, and it was shown that these form a dense subset in the homogeneous chaos. Subsequently, Cameron and Martin [6] showed that any quadratically integrable functional (with respect to Wiener measure) on the set of continuous functions on the interval [0,1] vanishing at zero could be expanded in an L^2 -convergent series of Hermite polynomials in a countable sequence of Gaussian random variables. The connection between multiple Wiener integrals and Fourier-Hermite expansion is also given in [16]. A modern exposition of Hermite expansions of functionals of Brownian motion can be found e.g. in [15], [19] and [17]. The gestation of Wiener's work on polynomial chaos is described in [23] and additional articles in the same Wiener memorial issue of the Bulletin of the AMS, and more comprehensively in the biography [24].

In stochastic analysis there are three basic representations for square integrable functionals of Brownian motion:

- polynomial chaos expansions,
- mean-square convergent expansions with multiple Wiener integrals, and
- stochastic Itô integrals.

There exist deep connections between these representations and they can be converted to one other. *Polynomial chaos* is less frequently used in this area, as Itô integrals are often more convenient, e.g., in the study of differential equations driven by the Wiener process. Also, the term polynomial chaos is sometimes replaced by *Wiener-Hermite expansion* to avoid confusion with the more familiar concept of *chaos* as it arises in the context of dynamical systems.

^{*}One should note that a number of basic probabilistic concepts in Wiener's work, cf. also [37], were developed prior to the solid foundation of probability theory provided by Kolmogorov [21].

However, polynomial chaos has received renewed attention since the work of Ghanem and Spanos [13] on stochastic finite element methods, in which random variables as well as random fields representing inputs and solutions of partial differential equations with random data are represented as Fourier-Hermite series in Gaussian random variables.

2.2. Setting and Notation. Given a probability space $(\Omega, \mathfrak{A}, P)$, where Ω is the abstract set of elementary events, \mathfrak{A} a σ -algebra of subsets of Ω and P a probability measure on \mathfrak{A} , we assume this space to be sufficiently rich[†] that it admits the definition of nontrivial normally distributed random variables $\xi : \Omega \to \mathbb{R}$, and we denote such random variables with mean zero and variance $\sigma^2 > 0$ by $\xi \sim N(0, \sigma^2)$. The mean or expectation of a (not necessarily normally distributed) random variable ξ will be denoted by $\langle \xi \rangle$. The Hilbert space of (equivalence classes of) real-valued random variables defined on $(\Omega, \mathfrak{A}, P)$ with finite second moments is denoted by $L^2(\Omega, \mathfrak{A}, P)$, with inner product $(\cdot, \cdot)_{L^2}$ and norm $\|\cdot\|_{L^2}$. We refer to convergence with respect to $\|\cdot\|_{L^2}$ as mean-square convergence. We shall refer to a linear subspace of $L^2(\Omega, \mathfrak{A}, P)$ consisting of centered (i.e., with mean zero) Gaussian random variables as a Gaussian linear space and, when this space is complete, as a Gaussian Hilbert space. We emphasize that a Gaussian Hilbert space cannot contain all Gaussian random variables on the underlying probability space (see e.g. [33] for a counterexample).

2.3. The Cameron-Martin Theorem. Since Gaussian random variables possess moments of all orders and mixed moments of independent Gaussian random variables are simply the products of the corresponding individual moments, it is easily seen that, for any Gaussian linear space \mathcal{H} and $n \in \mathbb{N}_0$, the set

$$\mathcal{P}_n(\mathcal{H}) := \{ p(\xi_1, \dots, \xi_M) : p \text{ is an } M \text{-variate polynomial of degree} \le n, \\ \xi_j \in \mathcal{H}, \, j = 1, \dots, M, M \in \mathbb{N} \}$$

is a linear subspace of $L^2(\Omega, \mathfrak{A}, P)$, as is its closure $\overline{\mathscr{P}}_n(\mathscr{H})$. Note that $\mathscr{P}_n(\mathscr{H})$ consists of polynomials in an arbitrary number of random variables, which can be chosen arbitrarily from \mathscr{H} . The space $\mathscr{P}_0(\mathscr{H}) = \overline{\mathscr{P}}_0(\mathscr{H})$ consists of almost surely (a.s.) constant, i.e., degenerate, random variables. Furthermore, all elements of $\mathscr{P}_1(\mathscr{H})$ and $\overline{\mathscr{P}}_1(\mathscr{H})$ are normally distributed, whereas for n > 1 the spaces $\mathscr{P}_n(\mathscr{H})$ and $\overline{\mathscr{P}}_n(\mathscr{H})$ also contain random variables with non-Gaussian distributions. Moreover, one can show that the spaces $\mathscr{P}_n(\mathscr{H})$ as well as $\overline{\mathscr{P}}_n(\mathscr{H})$ are distinct for different values of n, so that in particular $\{\overline{\mathscr{P}}_n(\mathscr{H})\}_{n\in\mathbb{N}_0}$ forms a strictly increasing sequence of subspaces of $L^2(\Omega, \mathfrak{A}, P)$. Taking orthogonal complements, we define the spaces

$$\mathscr{H}_n := \overline{\mathscr{P}}_n(\mathscr{H}) \cap \mathscr{P}_{n-1}(\mathscr{H})^{\perp}, \qquad n \in \mathbb{N}$$

so that, setting also $\mathscr{H}_0 := \mathscr{P}_0(\mathscr{H}) = \overline{\mathscr{P}}_0(\mathscr{H})$, we have the orthogonal decomposition

$$\overline{\mathscr{P}}_n(\mathscr{H}) = \bigoplus_{k=0}^n \mathscr{H}_k$$

where we have used \oplus to denote the orthogonal sum of linear spaces. We also consider the full space

$$\bigoplus_{n=0}^{\infty} \mathscr{H}_n := \overline{\bigcup_{n=0}^{\infty} \mathscr{P}_n(\mathscr{H})}.$$

 $^{^{\}dagger}$ Otherwise there exist only trivial random variables taking the value zero with probability one, allowing only the modeling of deterministic phenomena.

Finally, we denote by $\sigma(S)$ the σ -algebra generated by a set S of random variables. Note that for a Gaussian linear space \mathscr{H} defined on $(\Omega, \mathfrak{A}, P)$ we always have $\sigma(\mathscr{H}) \subset \mathfrak{A}$.

The simplest nontrivial case of a one-dimensional Gaussian Hilbert space is that spanned by one random variable $\xi \sim N(0, 1)$. In this case each linear space \mathscr{H}_n is also one-dimensional and is spanned by the Hermite polynomial of exact degree n in ξ .

With this notation we can state the basic density theorem for polynomials of Gaussian random variables due originally to Cameron and Martin in 1947 [6]. We state the result in a somewhat more general^{\ddagger} form than the original, essentially following [17], where also a proof is given.

THEOREM 2.1 (Cameron-Martin Theorem). In terms of the notation introduced above, the spaces $\{\mathscr{H}_n\}_{n\in\mathbb{N}_0}$ form a sequence of closed, pairwise orthogonal linear subspaces of $L^2(\Omega, \mathfrak{A}, P)$ such that

$$\bigoplus_{n=0}^{\infty} \mathscr{H}_n = L^2(\Omega, \sigma(\mathscr{H}), P).$$

In particular, if $\sigma(\mathscr{H}) = \mathfrak{A}$, then $L^2(\Omega, \mathfrak{A}, P)$ admits the orthogonal decomposition

$$L^2(\Omega, \mathfrak{A}, P) = \bigoplus_{n=0}^{\infty} \mathscr{H}_n$$

Before proceeding to chaos expansions, we wish to point out a number of subtleties associated with the Cameron-Martin Theorem. First, the elements of the spaces L^2 , and hence also those of \mathscr{H} , are equivalence classes of random variables. Therefore the notation $\sigma(\mathscr{H})$ implies that all such equivalent functions must be measurable, i.e., this σ -algebra is generated by one representative from each equivalence class and the events with probability zero. This remark applies also to similar situations below. In particular, all statements and equalities are understood to hold almost surely, i.e., except for possibly sets of measure zero.

Second, we emphasize that the condition $\mathfrak{A} = \sigma(\mathscr{H})$ is necessary. This follows from basic measurability properties, a relevant result is the Doob-Dynkin lemma (see e.g. [18, Lemma 1.13]). A simple example where this condition is violated and the conclusion of the theorem is false can be given as follows: Consider a probability space on which two independent, non-degenerate, centered random variables ξ and η are defined, where $\xi \sim N(0, 1)$ and η has an arbitrary distribution with finite second moment. If $\mathscr{H} = \{c\xi : c \in \mathbb{R}\}$ denotes the one-dimensional Gaussian Hilbert space generated by ξ , then all projections of η on the spaces \mathscr{H}_n are almost surely constant with value zero, and the approximation error equals the variance of the random variable η . Another simple example where the probability space is too coarse can be given as follows. Take as probability space $\Omega = \mathbb{R}$ with σ -algebra $\mathfrak{A} = \sigma(\{0\}, \{1\}),$ $P(\{0\}) = p, P(\{1\}) = 1 - p, 0 . Then the only possible nonempty Gaussian$ Hilbert space for this probability space is trivial, i.e., it consists only of the equivalenceclass of random variables which are a.s. constant with value zero. For any random

[‡]Cameron and Martin considered the specific probability space $\Omega = \{x \in C[0, 1], x(0) = 0\}$, together with its Borel σ -algebra and P the Wiener measure. The associated Gaussian Hilbert space \mathscr{H} is then generated by Gaussian random variables corresponding to the evaluation of a function xat some $t \in [0, 1]$.

variable ξ_0 of this equivalence class it holds that $\xi_0(0) = \xi_0(1) = 0$, $\xi_0(\omega) = x_0 \in \mathbb{R}$ for $\omega \notin \{0, 1\}$. The corresponding generated σ -algebra $\sigma(\mathscr{H}) = \sigma(\xi_0)$ consists only of events with probability 0 or 1, hence it holds $\sigma(\mathscr{H}) = \{\emptyset, \{0, 1\}, \mathbb{R} \setminus \{0, 1\}, \mathbb{R}\}$ and only degenerate random variables can be approximated by polynomials in "Gaussian" random variables. Nevertheless on the probability space $(\Omega, \mathfrak{A}, P)$ there exist non-degenerate random variables with finite second order moments, e.g. the random variable ξ with $\xi(0) = 0$, $\xi(1) = 1$ and $\xi(\omega) = 2$ otherwise, which follows a Bernoulli distribution with parameter p. Completion of this probability space does not change the situation.

2.4. Chaos Expansions. For a Gaussian linear space \mathscr{H} , we denote by $P_k : L^2(\Omega, \mathfrak{A}, P) \to \mathscr{H}_k$ the orthogonal projection onto \mathscr{H}_k . The Wiener-Hermite polynomial chaos expansion of a random variable $\eta \in L^2(\Omega, \sigma(\mathscr{H}), P)$

$$\eta = \sum_{k=0}^{\infty} P_k \eta \tag{2.1}$$

thus converges in the mean-square sense and may be approximated by the partial sums

$$\eta \approx \eta_n := \sum_{k=0}^n P_k \eta.$$

We note that the expansion (2.1) is mean-square convergent also when $\mathfrak{A} \supseteq \sigma(\mathscr{H})$, in which case the limit is the orthogonal projection of η onto the closed subspace $L^2(\Omega, \sigma(\mathscr{H}), P)$.

In applications of Wiener-Hermite polynomial chaos expansions the underlying Gaussian Hilbert space is often taken to be the space spanned by a given fixed sequence $\{\xi_j\}_{j\in\mathbb{N}}$ of independent Gaussian random variables $\xi_j \sim N(0,1)$, which we shall refer to as the *basic random variables*. For computational purposes the countable sequence $\{\xi_j\}_{j\in\mathbb{N}}$ ist restricted to a finite number $M \in \mathbb{N}$ of random variables. Denoting by $\mathscr{P}_n^M = \mathscr{P}_n^M(\xi_1, \ldots, \xi_M)$ the space of *M*-variate polynomials of (total) degree *n* in the random variables ξ_1, \ldots, ξ_M , there holds that, for any random variable $\eta \in L^2(\Omega, \sigma(\{\xi_j\}_{j\in\mathbb{N}}), P)$, the approximations

$$\eta^M_n:=P^M_n\eta\xrightarrow{n,M\to\infty}\eta$$

where P_n^M denotes the orthogonal projection onto \mathscr{P}_n^M , converge in the mean-square sense. This follows, e.g., from the proof of Theorem 1 in [17].

It should be emphasized that the Wiener-Hermite polynomial chaos expansion converges for quite general random variables, provided their second moment is finite. In particular, their distributions can be discrete, singularly continuous, absolutely continuous as well as of mixed type. Moreover, it can be shown that for a nontrivial Gaussian linear space \mathscr{H} and a distribution function with finite second moments there exist random variables in $L^2(\Omega, \sigma(\mathscr{H}), P)$ possessing this distribution function (cf. e.g. [33]). In particular, Wiener-Hermite polynomial chaos expansions are possible also for random variables which are not absolutely continuous. By contrast, note that all partial sums of a Wiener-Hermite expansion are either absolutely continuous or a.s. constant.

The following theorem collects further known and practically useful results on Wiener-Hermite polynomial chaos expansions. The statements are formulated for the approximations η_n , but they also hold for the approximations η_n^M .

THEOREM 2.2. Under the assumptions of the Cameron-Martin Theorem (Theorem 2.1), the following statements hold for the Wiener-Hermite polynomial chaos approximations

$$\eta_n = \sum_{k=0}^n P_k \eta, \qquad n \in \mathbb{N}_0$$

of a random variable $\eta \in L^2(\Omega, \sigma(\mathscr{H}), P)$ with respect to a Gaussian Hilbert space \mathscr{H} :

- (i) $\eta_n \xrightarrow{n \to \infty} \eta$ in $L^p(\Omega, \sigma(\mathscr{H}), P)$ for all 0 .
- (ii) Relative moments converge, when they exist, i.e., for 0 there holds

$$\lim_{n \to \infty} \frac{\langle |\eta_n - \eta|^p | \rangle}{\langle \eta^p \rangle} = \lim_{n \to \infty} \frac{\langle |\eta_n - \eta|^p | \rangle}{\langle |\eta|^p \rangle} = 0$$

if $\langle \eta^p \rangle \neq 0$ and $\langle |\eta|^p \rangle \neq 0$, respectively.

- (iii) $\eta_n \to \eta$ in probability.
- (iv) There is a subsequence $\{n_k\}_{k\in\mathbb{N}}$ with $\lim_{k\to\infty} n_k = \infty$ such that $\eta_{n_k} \to \eta$ almost surely.
- (v) $\eta_n \to \eta$ in distribution. This implies that the associated distribution functions converge, i.e., that

$$P(\eta_n \le x) =: F_{\eta_n}(x) \xrightarrow{n \to \infty} F_{\eta}(x) := P(\eta \le x)$$

at all points $x \in \mathbb{R}$ where F_{η} is continuous. If the distribution function F_{η} is continuous on \mathbb{R} then the distribution functions converge uniformly.

(vi) The previous property implies that the quantiles of the random variables η_n converge for $n \to \infty$ to the corresponding quantiles of η . (These can be set-valued.)

We remark that it may also be of interest to approximate statistical quantities other than distribution functions and moments, such as probability densities (see e.g. [9, 10]). In addition, other types of convergence may be relevant.

3. Generalized polynomial chaos expansions. Many stochastic problems involve non-Gaussian random variables. When these are approximated with Wiener-Hermite polynomial chaos expansions it is often observed that these expansions converge very slowly. The reason for this is that, when expressed as functions of a collection of Gaussian basic random variables, these functions are often highly nonlinear and can only be well approximated by truncated Wiener-Hermite expansions of very high order. A possible remedy is to base the expansion on non-Gaussian basic random variables whose distribution is closer to the random variables under expansion, thus permitting good approximations of lower order. As a consequence, such expansions involve polynomials orthogonal with respect to non-Gaussian measures replacing the Hermite polynomials. In principle a sequence of orthonormal polynomials exists for any probability distribution on \mathbb{R} with finite moments of all orders. In a series of papers [42, 41, 45, 44, 43] Karniadakis and Xiu proposed using polynomials from the Askey scheme of hypergeometric orthogonal polynomials and introduced the term generalized polynomial chaos expansions. In the following we restrict ourselves to continuous distributions, which suffices for most applications and avoids certain technical difficulties.

We thus consider chaos expansions with respect to a countable sequence $\{\xi_m\}_{m\in\mathbb{N}}$ of (not necessarily identically distributed) basic random variables which satisfy the following assumptions:

Assumption 1.

- (i) Each basic random variable ξ_m possesses finite moments of all orders, i.e., $\langle |\xi_m|^k \rangle < \infty$ for all $k, m \in \mathbb{N}$.
- (ii) The distribution functions $F_{\xi_m}(x) := P(\xi_m \leq x)$ of the basic random variables are continuous.

The linear subspaces of $L^2(\Omega, \mathfrak{A}, P)$ spanned by polynomials of arbitrary order in such families of basic random variables are always infinite dimensional. Furthermore, each random variable which can be represented by a (multivariate) polynomial in the basic random variables possesses both properties in Assumption 1 or reduces to a constant.

3.1. One basic random variable. As a first step we consider expansions in a single basic random variable ξ with distribution function F_{ξ} which satisfies Assumption 1. For any random variable $\eta \in L^2(\Omega, \sigma(\xi), P)$ which is measurable with respect to ξ there exists by the Doob-Dynkin Lemma (see e.g. [18, Lemma 1.13]) a measurable function $f : \mathbb{R} \to \mathbb{R}$ such that $\eta = f(\xi)$.

The distribution of the random variable ξ defines a measure on the real line resulting in the probability space $(\mathbb{R}, \mathfrak{B}(\mathbb{R}), F_{\xi}(dx))$ on the range of ξ , where $\mathfrak{B}(\mathbb{R})$ denotes the Borel σ -algebra on \mathbb{R} . Since all moments of this measure are finite by assumption this defines a sequence of orthonormal polynomials $\{p_n\}_{n \in \mathbb{N}_0}$ associated with this measure, which can be made unique e.g. by requiring that the leading coefficient be positive. These polynomials may be generated by orthonormalizing the monomials via the Gram-Schmidt procedure or directly by the usually more stable Stieltjes procedure.

The sequence of random variables $\{p_n(\xi)\}_{n\in\mathbb{N}_0}$ then constitutes an orthonormal system in the Hilbert space $L^2(\Omega, \sigma(\xi), P)$, as does the sequence $\{p_n\}_{n\in\mathbb{N}_0}$ in the Hilbert space $L^2(\mathbb{R}, \mathfrak{B}(\mathbb{R}), F_{\xi}(dx))$, and the question of approximability by generalized polynomial chaos expansions in a single random variable ξ is equivalent with the completeness of these two sequences, i.e., whether they lie dense in their respective Hilbert spaces.

The completeness of these systems is characterized by a classical theorem due to M. Riesz [29], which reduces the question of density of polynomials in an L^2 -space to the unique solvability of a moment problem.

DEFINITION 3.1. One says that the moment problem is uniquely solvable for a probability distribution on $(\mathbb{R}, \mathfrak{B}(\mathbb{R}))$ or that the distribution is determinate (in the Hamburger sense), if the distribution function is uniquely defined by the sequence of its moments

$$\mu_k := \left\langle \xi^k \right\rangle = \int_{\mathbb{R}} x^k F_{\xi}(dx), \qquad k \in \mathbb{N}_0.$$

In other words, if the moment problem is uniquely solvable then no other probability distribution can have the same sequence of moments. Riesz showed in [29] that the polynomials are dense in $L^2_{\alpha}(\mathbb{R})$ for a positive Radon measure α if and only if the measure $d\alpha(x)/(1+x^2)$ is determinate. For random variables ξ with continuous distribution function F_{ξ} (cf. Assumption 1) it can be shown that the polynomials are dense in $L^2(\Omega, \sigma(\xi), P)$, and thus also in $L^2(\mathbb{R}, \mathfrak{B}(\mathbb{R}), F_{\xi}(dx))$, if and only if F_{ξ} is determinate. A proof of this equivalence can be found, e.g., in the monograph of Freud [11, Theorem 4.3, Section II.4]. Additional results and background material on the moment problem and polynomial density can be found in [3] and [4] as well as the references included therein. We summarize these facts in the following theorem. THEOREM 3.2. The sequence of orthogonal polynomials associated with a real random variable ξ satisfying Assumption 1 is dense in $L^2(\mathbb{R}, \mathfrak{B}(\mathbb{R}), F_{\xi}(dx))$ if and only if the moment problem is uniquely solvable for its distribution.

Thus, if this condition is satisfied the sequence of random variables $\{p_n(\xi)\}_{n\in\mathbb{N}_0}$ constitutes an orthonormal basis of the Hilbert space $L^2(\Omega, \sigma(\xi), P)$ and each element (i.e., each random variable or, more precisely, each equivalence class of random variables) of this space can be expanded with respect to this basis. The basis expansions are abstract Fourier series and can be written as

$$\eta = f(\xi) = \lim_{n \to \infty} \sum_{k=0}^{n} a_k p_k(\xi) = \sum_{k=0}^{\infty} a_k p_k(\xi)$$
(3.1)

where the limit is in quadratic mean and the coefficients can be calculated as

$$a_k = \langle \eta p_k(\xi) \rangle = \langle f(\xi) p_n(\xi) \rangle = \int_{\mathbb{R}} f(x) p_n(x) F_{\xi}(dx), \qquad k \in \mathbb{N}_0.$$
(3.2)

The additional properties of Wiener-Hermite expansions listed in Theorem 2.2 remain valid also in this situation.

The following theorem collects several known sufficient conditions ensuring the unique solvability of the moment problem in the Hamburger sense, i.e., probability distributions with support on the entire space $(\mathbb{R}, \mathfrak{B}(\mathbb{R}))$ are allowed. (see e.g. [11, Section II.5.], [14], [22], [34]). Basic properties of the moment generating function can be found e.g. in [8].

THEOREM 3.3. If one of the following conditions for the distribution F_{ξ} of a random variable ξ satisfying Assumption 1 is valid, then the moment problem is uniquely solvable and therefore the set of polynomials in the random variable ξ is dense in the space $L^2(\Omega, \sigma(\xi), P)$.

- (a) The distribution F_{ξ} has compact support, i.e., there exists a compact interval $[a,b], a, b \in \mathbb{R}$, such that $P(\xi \in [a,b]) = 1$.
- (b) The moment sequence $\{\mu_n\}_{n\in\mathbb{N}_0}$ of the distribution satisfies

$$\liminf_{n \to \infty} \frac{\sqrt[2n]{\mu_{2n}}}{2n} < \infty.$$

(c) The random variable is exponentially integrable, i.e., there holds

$$\langle \exp(a|\xi|) \rangle = \int_{\mathbb{R}} \exp(a|x|) F_{\xi}(dx) < \infty$$

for a strictly positive number a. An equivalent condition is the existence of a finite moment-generating function in a neighbourhood of the origin.

(d) (Carleman's condition) The moment sequence $\{\mu_n\}_{n\in\mathbb{N}_0}$ of the distribution satisfies

$$\sum_{n=0}^{\infty} \frac{1}{\sqrt[2n]{\mu_{2n}}} = \infty.$$

(e) (Lin's condition) If the distribution has a symmetric, differentiable and strictly positive density f_{ξ} and for a real number $x_0 > 0$ there holds

$$\int_{-\infty}^{\infty} \frac{-\log f_{\xi}(x)}{1+x^2} \, dx = \infty \quad and \quad \frac{-xf'_{\xi}(x)}{f_{\xi}(x)} \nearrow \infty \ (x \to \infty, x \ge x_0).$$

If in Lin's condition the integral for a probability distribution with strictly positive density is finite, then the distribution is indeterminate (Krein's condition).

Examples of probability distributions, for which the moment problem is uniquely solvable are the uniform, beta, gamma and the normal distributions.

By contrast, the moment problem is *not* uniquely solvable for the lognormal distribution, so that the sequence of random variables $\{p_n(\xi)\}_{n\in\mathbb{N}_0}$ for a lognormal random variable ξ does not constitute a basis of the Hilbert space $L^2(\Omega, \sigma(\xi), P)$, and there will be some elements (random variables) in this space which are not the limit of their generalized polynomial chaos expansion.

Further examples of random variables with indeterminate distribution are certain powers of random variables with normal or gamma distribution (see e.g. [31, 34]). Note that the expansion (3.1) still converges in quadratic mean, but its limit may be a second-order random variable different from η . In this case the convergence of the generalized polynomial chaos expansions to the desired limit must be shown in another way.

3.2. Finitely many basic random variables. We now turn to the case in which the stochasticity of the underlying problem is characterized by a finite number of independent random variables $\xi_1, \xi_2, \ldots, \xi_M$, which we collect in the random vector $\boldsymbol{\xi} = \boldsymbol{\xi}(\omega) \in \mathbb{R}^M$. This situation is often referred to as *finite-dimensional noise* in the stochastic finite element literature, and typically arises when a random field is approximated by a truncated Karhunen-Loève expansion. Denoting by $\{p_j^{(m)}\}_{j \in \mathbb{N}_0}, m = 1, \ldots, M$, the sequence of polynomials orthonormal with respect to the distribution of ξ_m , we note that the set of multivariate (tensor product) polynomials given by

$$p_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \prod_{m=1}^{M} p_{\alpha_m}^{(m)}(\xi_m), \qquad \boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_M) \in \mathbb{N}_0^M, \tag{3.3}$$

constitutes an orthonormal system of random variables in the space $L^2(\Omega, \sigma(\boldsymbol{\xi}), P)$. By consequence, the polynomials

$$p_{\boldsymbol{\alpha}}: \boldsymbol{x} \mapsto p_{\boldsymbol{\alpha}}(\boldsymbol{x}), \qquad \boldsymbol{\alpha} \in \mathbb{N}_0^M$$

form an orthonormal system in the image space $L^2(\mathbb{R}^M, \mathfrak{B}(\mathbb{R}^M))$ endowed with the product probability measure $F_{\xi_1}(dx_1) \times \cdots \times F_{\xi_M}(dx_M)$. As is well known, tensor products of systems of orthonormal bases of separable Hilbert spaces form an orthonormal basis of the tensor product Hilbert space (see e.g. [28], Section II.4, or [27]), which implies the following result:

THEOREM 3.4. Let $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_M)$ be a vector of $M \in \mathbb{N}$ independent random variables satisfying Assumption 1 and $\{p_j^{(m)}\}_{j \in \mathbb{N}_0}, m = 1, \ldots, M$, the associated orthonormal polynomial sequences. Then the orthonormal system of random variables

$$p_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \prod_{m=1}^{M} p_{\alpha_m}^{(m)}(\xi_m), \qquad \boldsymbol{\alpha} \in \mathbb{N}_0^M,$$

is an orthonormal basis of the space $L^2(\Omega, \sigma(\boldsymbol{\xi}), P)$ if and only if the moment problem is uniquely solvable for each random variable ξ_m , $m = 1, \ldots, M$. In this case any random variable $\eta \in L^2(\Omega, \sigma(\boldsymbol{\xi}), P)$ can be expanded in an abstract Fourier series of multivariate orthonormal polynomials in the basic random variables, the so called generalized polynomial chaos expansion,

$$\eta = \sum_{\boldsymbol{lpha} \in \mathbb{N}_0^M} a_{\boldsymbol{lpha}} p_{\boldsymbol{lpha}}(\boldsymbol{\xi}) \quad \text{ with coefficients } a_{\boldsymbol{lpha}} = \langle \eta \, p_{\boldsymbol{lpha}}(\boldsymbol{\xi}) \rangle$$

In other words, the set of multivariate tensor product polynomials (3.3) in a finite number of independent random variables ξ_1, \ldots, ξ_M is dense in $L^2(\Omega, \sigma(\boldsymbol{\xi}), P)$, as are the *M*-variate polynomials in the space $L^2(\mathbb{R}^M, \mathfrak{B}(\mathbb{R}^M), F_{\xi_1}(dx_1) \times \cdots \times F_{\xi_M}(dx_M))$, if and only if each sequence $\{p_j^{(m)}(\boldsymbol{\xi})\}_{j \in \mathbb{N}_0}$ is dense in $L^2(\Omega, \sigma(\xi_m), P)$ for m = $1, 2, \ldots, M$.

If the basic random variables are not independent, then the construction of a sequence of orthonormal polynomials is still always possible. In this case, however, the tensor product structure of the polynomial space is lost and additional difficulties arise. In particular, the sequence of orthonormal polynomials is no longer uniquely defined, but depends on the ordering of the monomials. Furthermore, the link between the determinacy of the distribution and the density of polynomials in the associated L^2 spaces becomes more intricate, and conditions on the determinacy of such distributions are more complicated (see more about these and related issues e.g. in [3, 27, 30, 47]). We therefore restrict ourselves here only to simple sufficient conditions for the density of multivariate polynomials in the corresponding L^2 spaces. These will generally suffice in practical applications.

THEOREM 3.5. If the distribution function $F_{\boldsymbol{\xi}}$ of a random vector $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_M)$ with continuous distribution and finite moments of all orders satisfies one of the following conditions, then the multivariate polynomials in ξ_1, \ldots, ξ_M are dense in $L^2(\Omega, \sigma(\boldsymbol{\xi}), P)$. In this case any random variable $\eta \in L^2(\Omega, \sigma(\boldsymbol{\xi}), P)$ is the limit of its generalized polynomial chaos expansion which converges in quadratic mean.

- (a) The distribution function $F_{\boldsymbol{\xi}}$ has compact support, i.e., there exists a compact set $K \subset \mathbb{R}^M$ such that $P(\boldsymbol{\xi} \in K) = 1$.
- (b) The random vector is exponentially integrable, i.e., there exists a > 0 such that

$$\langle \exp(a \| \boldsymbol{\xi} \|) \rangle = \int_{\mathbb{R}^M} \exp(a \| \boldsymbol{x} \|) F_{\boldsymbol{\xi}}(d\boldsymbol{x}) < \infty,$$

where $\|\cdot\|$ denotes any norm on \mathbb{R}^M .

Proof. By a result of Petersen (see [27, Theorem 3]) the distribution of the random vector $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_M)$ is determinate if the distribution of each random variable $\xi_m, m = 1, \ldots, M$, is determinate. Moreover, the set of multivariate polynomials is dense in $L^q(\mathbb{R}^M, \mathfrak{B}(\mathbb{R}^M), F_{\boldsymbol{\xi}}(dx))$ for any $1 \leq q < p$ if the polynomials are dense in $L^p(\mathbb{R}, \mathfrak{B}(\mathbb{R}), F_{\boldsymbol{\xi}_m}(dx_m))$ for each $m = 1, \ldots, M$ (the proposition following Theorem 3 in [27]). But if the exponential integrability condition is satisfied, then it is satisfied for each random variable $\xi_m, m = 1, \ldots, M$. Now by Theorem 6 in [4], the polynomials are dense in the space $L^p(\mathbb{R}, \mathfrak{B}(\mathbb{R}), F_{\boldsymbol{\xi}_m}(dx_m))$ for each $p \geq 1$. \Box

3.3. Infinitely many basic random variables. We now consider the situation where the stochasticity of the underlying problem is characterized by a countable sequence $\{\xi_m\}_{m\in\mathbb{N}}$ of random variables of which each satisfies Assumption 1, all defined on a fixed, sufficiently rich probability space $(\Omega, \mathfrak{A}, P)$.

As in the case of Gaussian polynomial chaos, we define the following subspaces

of $L^2(\Omega, \mathfrak{A}, P)$ for $M \in \mathbb{N}$ and $n \in \mathbb{N}_0$:

$$\begin{split} \mathscr{P}_{n}^{M} &:= \{p(\xi_{1}, \dots, \xi_{M}) : p \text{ a polynomial of degree} \leq n\}, \\ \widetilde{\mathscr{P}}^{M} &:= \overline{\bigcup_{n=0}^{\infty}} \mathscr{P}_{n}^{M}, \\ \mathscr{P}_{n} &:= \overline{\bigcup_{n=0}^{\infty}} \mathscr{P}_{n}^{M}, \\ \widetilde{\mathscr{P}} &:= \overline{\bigcup_{n=0}^{\infty}} \mathscr{P}_{n}^{n}. \end{split}$$

Furthermore we denote the relevant σ -algebras

 $\mathfrak{A}_M := \sigma(\{\xi_m\}_{m=1}^M), \ M \in \mathbb{N}, \quad \text{and} \quad \mathfrak{A}_\infty := \sigma(\{\xi_m\}_{m \in \mathbb{N}}).$

We then have the inclusions

$$\begin{split} \mathscr{P}_n^M \subset \widetilde{\mathscr{P}}^M \subset L^2(\Omega, \mathfrak{A}_M, P), & n \in \mathbb{N}_0, \ M \in \mathbb{N}, \\ \mathscr{P}_n \subset \overline{\mathscr{P}_n} \subset \widetilde{\mathscr{P}} \subset L^2(\Omega, \mathfrak{A}_\infty, P), & n \in \mathbb{N}_0. \end{split}$$

For $M \in \mathbb{N}$ the set $\widetilde{\mathscr{P}}^M$ is the closed linear subspace of $L^2(\Omega, \mathfrak{A}_M, P)$ containing all L^2 -limits of polynomials in the basic random variables (ξ_1, \ldots, ξ_M) , and the set $\widetilde{\mathscr{P}}$ is the closed linear subspace of $L^2(\Omega, \mathfrak{A}_{\infty}, P)$ containing all L^2 -limits of polynomials in all basic random variables $\{\xi_m\}_{m\in\mathbb{N}}$. Theorem 3.6 below asserts that a sufficient condition for the polynomials in all basic random variables $\{\xi_m\}_{m\in\mathbb{N}}$ to be dense in $L^2(\Omega, \mathfrak{A}_{\infty}, P)$ is that the polynomials in each finite subset $\{\xi_m\}_{m=1}^M$ of the basic random variables be dense in $L^2(\Omega, \mathfrak{A}_M, P)$.

THEOREM 3.6. If

$$\widetilde{\mathscr{P}}^M = L^2(\Omega, \mathfrak{A}_M, P) \quad \text{for all } M \in \mathbb{N},$$
(3.4)

then $\widetilde{\mathscr{P}} = L^2(\Omega, \mathfrak{A}_{\infty}, P).$

Proof. We show that under the assumption (3.4) any random variable η in the orthogonal complement of $\widetilde{\mathscr{P}}$ in $L^2(\Omega, \mathfrak{A}_{\infty}, P)$ must vanish. Otherwise any such random variable η can be normalized such that $\langle \eta^2 \rangle = 1$. The union $\cup_{M=1}^{\infty} L^2(\Omega, \mathfrak{A}_M, P)$ of the nested sequence of L^2 -spaces lies dense in $L^2(\Omega, \mathfrak{A}_{\infty}, P)$ (see e.g. [5, p. 109, Corollary 3.6.8]). Therefore, given $\epsilon > 0$, there exists $\eta_0 \in L^2(\Omega, \mathfrak{A}_{M_0}, P)$ with M_0 sufficiently large such that

$$\|\eta - \eta_0\|_{L^2} < \epsilon. \tag{3.5}$$

By the reverse triangle inequality this implies

$$\|\eta_0\|_{L^2} \ge \|\eta\|_{L^2} - \|\eta - \eta_0\|_{L^2} \ge 1 - \epsilon.$$

On the other hand, since $\eta_0 \in L^2(\Omega, \mathfrak{A}_{M_0}, P) = \widetilde{\mathscr{P}}^{M_0} \subset \widetilde{\mathscr{P}} \perp \eta$, we also have

$$\|\eta - \eta_0\|_{L^2}^2 = \|\eta\|_{L^2}^2 + \|\eta_0\|_{L^2}^2 \ge 1 + (1-\epsilon)^2,$$

which contradicts (3.5) for sufficiently small ϵ . \Box

COROLLARY 3.7. Let $\{\xi_m\}_{m\in\mathbb{N}}$ be a sequence of basic random variables satisfying Assumption 1 and $\eta \in L^2(\Omega, \mathfrak{A}_{\infty}, P)$. If for each $M \in \mathbb{N}$ the polynomials in $\{\xi_m\}_{m=1}^M$ are dense in $L^2(\Omega, \mathfrak{A}_M, P)$, then the generalized polynomial chaos expansion of η converges to η in quadratic mean.

Polynomial chaos expansions and generalized polynomial chaos expansions generally work with basic random variables which are, in addition, *independent*. In this case the sufficient condition given in Theorem 3.6 is also necessary. Moreover, the density result is then equivalent to the density of each univariate family of polynomials.

COROLLARY 3.8. Let $\{\xi_m\}_{m\in\mathbb{N}}$ be a sequence of independent basic random variables satisfying Assumption 1 and $\eta \in L^2(\Omega, \mathfrak{A}_{\infty}, P)$. Then the generalized polynomial chaos expansion of η converges in quadratic mean to the random variable η if and only if the moment problem for the distribution of each random variable ξ_m is uniquely solvable (or, equivalently, the polynomials in the random variable ξ_m are dense in $L^2(\Omega, \sigma(\xi_m), P)$ for each $m \in \mathbb{N}$).

Proof. If for each $m \in \mathbb{N}$ the moment problem for the distribution of the random variable ξ_m is uniquely solvable and, equivalently the set of polynomials in the random variable ξ_m is dense in $L^2(\Omega, \sigma(\xi_m), P)$, then this holds by Theorem 3.4 for any finite subfamily and hence, from Theorem 3.6 the conclusion follows.

In order to prove the converse statement we assume that for an index $m_0 \in \mathbb{N}$ the polynomials in the random variable ξ_{m_0} are not dense in $L^2(\Omega, \sigma(\xi_{m_0}), P)$. Then there exists a second-order random variable $\eta_0 \in L^2(\Omega, \sigma(\xi_{m_0}), P)$ with norm 1, which cannot be approximated by polynomials in ξ_{m_0} . Due to the independence of the basic random variables, we have that polynomials in the remaining basic random variables, and therefore also their closure, are orthogonal to $L^2(\Omega, \sigma(\xi_{m_0}), P)$. Consequently, such polynomials have a distance to η_0 of at least one. We therefore conclude that $\eta_0 \in L^2(\Omega, \mathfrak{A}_{\infty}, P) \setminus \widetilde{\mathscr{P}}$. \Box

REMARK 3.9. If the basic random variables $\{\xi_m\}_{m\in\mathbb{N}}$ are not independent, it may happen that for a finite number $M_0 \in \mathbb{N}$, we have $\widetilde{\mathscr{P}}^{M_0} \subsetneq L^2(\Omega, \mathfrak{A}_{M_0}, P)$ but $\widetilde{\mathscr{P}} = L^2(\Omega, \mathfrak{A}_{\infty}, P).$

As an example, take an infinite sequence of independent and normalized basic variables $\{\xi_m\}_{m\in\mathbb{N}}$ satisfying Assumption 1, such that the distribution of ξ_1 is indeterminate while those of the remaining random variables are determinate. Furthermore choose a sequence $\{\zeta_m\}_{m\in\mathbb{N}}$ of random variables such that the set $\{\xi_1, \zeta_j; j \in \mathbb{N}\}$ is an orthonormal basis of the Hilbert space $L^2(\Omega, \sigma(\xi_1), P)$. This is possible because this space is separable. Then arrange a countable number of random variables, e.g. by the rule $\tilde{\xi}_{2k-1} := \xi_k, \tilde{\xi}_{2k} := \zeta_k, k \in \mathbb{N}$ and consider this sequence $\{\tilde{\xi}_i\}_{i\in\mathbb{N}}$ as a sequence of basic random variables. Then we have $\widetilde{\mathscr{P}}^1 \neq L^2(\Omega, \mathfrak{A}_1, P)$ but

$$\widetilde{\mathscr{P}} = L^2(\Omega, \mathfrak{A}_{\infty}, P) = \bigoplus_{m=1}^{\infty} L^2(\Omega, \sigma(\xi_m), P).$$

4. Examples. In this section we present several illustrative examples for the preceding results.

4.1. Periodic functions of a lognormal random variable. As noted in Section 3.1, the lognormal distribution is not determinate, i.e., its moment problem fails to possess a unique solution. By consequence, polynomials in a lognormal random variable η are not dense in $L^2(\Omega, \sigma(\eta), P)$. We give an example of a nontrivial class of functions in the orthogonal complement of the span of these polynomials.

Denote by $\xi \sim N(0, 1)$ a standard Gaussian random variable and recall that the density function of the lognormal random variable $\eta := e^{\xi}$ is given by

$$f_{\eta}(x) = \begin{cases} \frac{1}{x\sqrt{2\pi}} e^{-\frac{\log^2 x}{2}}, & x > 0, \\ 0, & \text{otherwise.} \end{cases}$$
(4.1)

PROPOSITION 4.1. Let η be a lognormal random variable with density (4.1). Then for any function $g : \mathbb{R} \to \mathbb{R}$ which is measurable, odd and 1-periodic, i.e., g(y+1) = g(y) and for which $\langle g(\log(\eta))^2 \rangle < \infty$, there holds

$$\langle \eta^k g(\log \eta) \rangle = \int_0^\infty x^k f_\eta(x) g(\log x) \, dx = 0 \qquad \forall k \in \mathbb{N}_0.$$
 (4.2)

Proof. The change of variables $y = \log x$ yields, for all $k \in \mathbb{N}_0$,

$$\begin{split} \int_0^\infty x^k \frac{1}{x\sqrt{2\pi}} e^{-\frac{\log^2 x}{2}} g(\log x) \, dx &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty e^{ky} e^{-\frac{y^2}{2}} g(y) \, dy \\ &= \frac{e^{\frac{k^2}{2}}}{\sqrt{2\pi}} \int_{-\infty}^\infty e^{-\frac{(y-k)^2}{2}} g(y) \, dy = \frac{e^{\frac{k^2}{2}}}{\sqrt{2\pi}} \int_{-\infty}^\infty e^{-\frac{z^2}{2}} g(z+k) \, dz \\ &= \frac{e^{\frac{k^2}{2}}}{\sqrt{2\pi}} \int_{-\infty}^\infty e^{-\frac{z^2}{2}} g(z) \, dz = 0, \end{split}$$

where we have substituted z = y - k in the third identity and subsequently used the periodicity and the oddness of g. \Box

Note that the set of all random variables of the form $g(\log \eta)$ with g as in Proposition 4.1 constitutes a (nontrivial) linear subspace of $L^2(\Omega, \sigma(\eta), P)$, and that (4.2) extends to the closure of this subspace. An immediate consequence of (4.2) is that the generalized polynomial chaos coefficients of the random variable $g(\log \eta)$ with respect to the lognormal random variable η must also all vanish. The limit of this expansion is therefore zero, which does not coincide with the random variable under expansion.

Specifically, the nonzero function $g(x) = \sin(2\pi x)$, a popular example for nondeterminacy cf. [31, 34], satisfies the requirements of Proposition 4.1. The generalized polynomial chaos expansion of $g(\log \eta)$ with respect to the lognormal random variable η therefore fails to converge in quadratic mean to the random variable $g(\log \eta)$. By contrast, the (classical) polynomial chaos expansion of $g(\log \eta)$ with respect to the Gaussian random variable $\xi = \log \eta$ is mean-square convergent to $g(\log(\eta)) = g(\xi)$. This expansion is given by

$$\sin(2\pi\log\eta) = \sum_{k=0}^{\infty} a_k h_k(\log\eta), \quad \text{where } a_k = \begin{cases} \frac{(-1)^{(k-1)/2}(2\pi)^k}{\sqrt{k!}} e^{-2\pi^2}, & k \text{ odd,} \\ 0, & k \text{ even,} \end{cases}$$

and $\{h_k\}_{k\in\mathbb{N}_0}$ denote the normalized ("probabilist's") Hermite polynomials

$$h_k(x) = \frac{(-1)^k}{\sqrt{k!}} e^{\frac{x^2}{2}} \frac{d^k}{dx^k} e^{-\frac{x^2}{2}},$$

which are orthonormal with respect to the standard Gaussian density function

$$f_{\xi}(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$$

4.2. The reciprocal of a lognormal random variable. Before proceeding with the next example we give an explicit representation of the orthonormal polynomials associated with the lognormal density (4.1). These can be constructed in terms of *Stieltjes-Wigert polynomials* (cf. [35, Section 2.7]), which are orthogonal with respect to the family of weight functions

$$w_{\nu}(x) = \frac{\nu}{\sqrt{\pi}} e^{-\nu^2 \log^2 x}, \qquad x > 0, \quad \nu > 0.$$

For the details of this construction we refer to the appendix. The coefficients α_k and β_k of the associated three-term recurrence

$$p_{-1}(x) \equiv 0, \quad p_0(x) \equiv 1,$$
 (4.3a)

$$\sqrt{\beta_{k+1}} p_{k+1}(x) = (x - \alpha_k) p_k(x) - \sqrt{\beta_k} p_{k-1}(x), \quad k \ge 0$$
 (4.3b)

are found to be (cf. [32])

$$\alpha_k = (e^k(e+1) - 1)e^{(2k-1)/2}, \qquad \beta_k = (e^k - 1)e^{3k-2}.$$

We shall use these to derive the generalized polynomial chaos expansion of the random variable

$$\zeta := \frac{1}{\eta}.\tag{4.4}$$

PROPOSITION 4.2. The generalized polynomial chaos coefficients $\{a_k\}_{k\in\mathbb{N}_0}$ of the random variable ζ defined in (4.4) with respect to the polynomials $\{p_k\}_{k\in\mathbb{N}_0}$ in η are given by

$$a_0 = e^{1/2}, \qquad a_k = (-1)^k e^{-(k^2 + 3k - 2)/4} \sqrt{\prod_{i=1}^k (e^i - 1)}, \quad k \ge 1.$$
 (4.5)

Proof. The first coefficient a_0 of ζ is obtained as

$$a_0 = \langle \zeta p_0(\eta) \rangle = \int_0^\infty \frac{1}{x} \cdot 1 \cdot f_\eta(x) \, dx = \int_0^\infty \frac{e^{-\frac{1}{2}\log^2 x}}{x^2 \sqrt{2\pi}} \, dx$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty e^{-y} e^{-\frac{1}{2}y^2} \, dy = \sqrt{e}.$$

The remaining coefficients a_k are obtained by induction making use of the recurrence (4.3). For k = 1 this results in

$$a_1 = \langle \zeta p_1(\eta) \rangle = \left\langle \frac{1}{\eta} \frac{\eta - \alpha_0}{\sqrt{\beta_1}} \right\rangle = \frac{1}{\sqrt{\beta_1}} - \frac{\alpha_0}{\sqrt{\beta_1}} \left\langle \frac{1}{\eta} \right\rangle = -e^{-1/2}\sqrt{e-1},$$

in agreement with (4.5). Assuming (4.5) holds for all $0 \le j \le k$, we obtain from the recurrence relation (4.3)

$$a_{k+1} = \langle \zeta p_{k+1}(\eta) \rangle = \left\langle \frac{(\eta - \alpha_k)p_k(\eta) - \sqrt{\beta_k}p_{k-1}(\eta)}{\eta\sqrt{\beta_{k+1}}} \right\rangle = -\frac{\alpha_k a_k + \sqrt{\beta_k}a_{k-1}}{\sqrt{\beta_{k+1}}}$$
$$= -\frac{(e^{k/2} + e^{k/2 - 1} - e^{-k/2 - 1})a_k + \sqrt{e^k - 1}e^{-3/2}a_{k-1}}{\sqrt{e^{k+1} - 1}}$$
$$= (-1)^{k+1}e^{-(k^2 + 3k - 2)/4} \sqrt{\prod_{i=1}^k (e^i - 1)} \frac{e^{k/2} - e^{-k/2 - 1}}{\sqrt{e^{k+1} - 1}}$$
$$= (-1)^{k+1}e^{-(k^2 + 3k - 2)/4} \sqrt{\prod_{i=1}^k (e^i - 1)}e^{-k/2 - 1} \frac{e^{k+1} - 1}{\sqrt{e^{k+1} - 1}}$$
$$= (-1)^{k+1}e^{-((k+1)^2 + 3(k+1) - 2)/4} \sqrt{\prod_{i=1}^{k+1} (e^i - 1)}.$$

PROPOSITION 4.3. The generalized polynomial chaos expansion of the random variable ζ defined in (4.4) with respect to the orthonormal polynomials $\{p_k\}_{k \in \mathbb{N}_0}$ in η does not converge in mean-square to the random variable ζ .

Proof. The truncated chaos expansion of order n

$$\zeta_n := \sum_{k=0}^n a_k p_k(\eta) = e^{1/2} + \sum_{k=1}^n (-1)^k e^{-(k^2 + 3k - 2)/4} \sqrt{\prod_{i=1}^k (e^i - 1) p_k(\eta)}$$

can be bounded as follows:

$$\begin{aligned} \|\zeta_n\|_{L^2}^2 &= e + \sum_{k=1}^n e^{-(k^2 + 3k - 2)/2} \prod_{i=1}^k (e^i - 1) \le e + \sum_{k=1}^n e^{-(k^2 + 3k - 2)/2} \prod_{i=1}^k e^i \\ &\le e + \sum_{k=1}^\infty e^{-k+1} = \frac{e^2}{e - 1}. \end{aligned}$$

By consequence, and the fact that $\|\zeta\|_{L^2} = e$, the remainder of the truncated expansion is bounded below by

$$\|\zeta - \zeta_n\|_{L^2}^2 = \|\zeta\|_{L^2}^2 - \|\zeta_n\|_{L^2}^2 \ge e^2 - \frac{e^2}{e-1} > 0$$
.

4.3. Stochastic Galerkin approximation. We now turn to a common application of (generalized) polynomial chaos expansions, namely the approximation of the solutions of differential equations with random data. Consider the boundary-value problem for the one-dimensional diffusion equation posed on the unit interval (0, 1)

$$-(au')' = f,$$
 $u(0) = 0,$ $(au')(1) = F,$ (4.6)

where $a = a(x, \omega)$ is a given positive random field, f = f(x) a deterministic function, and F a given constant. The solution of (4.6) is

$$u(x,\omega) = \int_0^x \frac{1}{a(y,\omega)} \left(F + \int_y^1 f(z) \, dz\right) dy$$

Consider first the case that a is simply the fixed lognormal random variable $\eta(\omega)$ from the previous subsection. The solution then simplifies to

$$u(x,\omega) = \zeta(\omega) \int_0^x \left(F + \int_y^1 f(z) \, dz\right) dy,$$

i.e., it is the product of the random variable ζ with a purely deterministic function of x. An approximation of u based on generalized polynomial chaos, i.e., expansion in the orthogonal polynomials $\{p_k\}$ in η , cannot converge to the solution in view of Proposition 4.3. Therefore, if the solution of the boundary value problem with random data (4.6) is approximated with a stochastic Galerkin method employing lognormal chaos in the stochastic variables, the approximation thus obtained can be no better than the best approximation provided by a truncated chaos expansion. Since the latter has been shown not to converge to the solution, the Galerkin approximation cannot do so either.

Next, consider the same boundary value problem (4.6) with random field $a(x, \omega) = \exp(|\xi(\omega)|x)$ with a standard Gaussian random variable $\xi \sim N(0, 1)$. The distribution of the random variable $|\xi|$, sometimes called a *reflected Gaussian* distribution, is determinate in the sense of Definition 3.1 by Theorem 3.3 (c). Polynomials in $|\xi|$ are therefore dense in $L^2(\Omega, \sigma(|\xi|), P)$ and the associated generalized polynomial chaos expansion of u therefore converges to u in mean square.

In the following, we therefore compare two stochastic Galerkin approximations (see e.g. [1] for an introduction) to the solution of (4.6) based on two different types of polynomial chaos expansion. In the first case we use as trial space in the stochastic dimension the Hermite polynomials in ξ up to a fixed degree p. In the second, we use the orthonormal polynomials up to degree p with respect to $|\xi|$.

The load function was chosen as $f \equiv 1$ and the boundary data as F = 1. In the spatial dimension we have used a single Gauss-Lobatto-Legendre spectral finite element of degree 20.

Figure 4.1 shows the relative errors in the mean and second moment over the spatial domain of a Stochastic Galerkin approximation to the solution of (4.6) using standard Hermite chaos approximations in ξ of degrees 5, 10, 15 and 20 compared to generalized polynomial chaos with respect to the reflected Gaussian random variable $|\xi|$ of degrees 2 and 5. It is apparent that the latter show an approximation quality which is orders of magnitude better than the former.

This example clearly confirms the benefits of generalized polynomial chaos expansions in Stochastic Galerkin approximations compared to standard Wiener-Hermite chaos expansions. By using chaos polynomials taylored to the particular probabilistic setting/basic random variables a much faster convergence of the Galerkin approximation can be achieved. Considering lognormal random variables as an example, we have, however, demonstrated that a careful study of the basic random variables is necessary in order to ensure the convergence of generalized polynomial chaos expansions to the desired limit.



FIG. 4.1. Relative errors of mean (left) and second moment (right) of the Stochastic Galerkin approximation to the solution of (4.6) with $f \equiv 1$, F = 1 and random field $a(x, \omega) = \exp(|\xi(\omega)|x)$ using standard and generalized polynomial chaos expansions of various orders in the stochastic variables.

5. Summary. We have reviewed the constructions of standard as well as generalized polynomial chaos expansions of random variables with finite second moments, and we have shown under what conditions the results of the Cameron Martin Theorem extend from standard to generalized polynomial chaos expansions with specific analysis of expansions in one, finitely many and countably many random variables. Finally, we have presented examples illustrating non-approximability by generalized polynomial chaos expansions as well as accelerated convergence compared to standard polynomial chaos expansion. The appendix gives a self-contained derivation of the orthonormal polynomials associated with the lognormal probability density function.

Appendix A. The Orthonormal Polynomials for a Lognormal Density. The Stieltjes-Wigert polynomials (cf. [35, Section 2.7] and [7, Chapter VI, Section 2]) are orthonormal with respect to the family of weight functions

$$w_{\nu}(x) = \begin{cases} \frac{\nu}{\sqrt{\pi}} e^{-\nu^{2} \log^{2} x}, & x > 0, \\ 0, & \text{otherwise,} \end{cases} \qquad \nu > 0,$$

and are given by

$$q_k(x) = (-1)^k a^{(2k+1)/4} [a]_k^{-1/2} \sum_{j=0}^k \begin{bmatrix} k \\ j \end{bmatrix}_a a^{j^2} (-a^{1/2}x)^j, \qquad k \ge 0,$$
(A.1)

where $a = \exp\left(-1/(2\nu^2)\right)$ and we have introduced the notation

$$[a]_0 = 1,$$
 $[a]_k = (1 - a^k)(1 - a^{k-1})\cdots(1 - a),$ $k \ge 1,$

as well as the generalized binomial coefficient or Gauss symbol

$$\begin{bmatrix} k \\ j \end{bmatrix}_a = \frac{[a]_k}{[a]_{k-j}[a]_j} = \frac{(1-a^k)(1-a^{k-1})\cdots(1-a^{k-j+1})}{(1-a^j)(1-a^{j-1})\cdots(1-a)}, \quad \begin{bmatrix} k \\ 0 \end{bmatrix}_a = \begin{bmatrix} k \\ k \end{bmatrix}_a = 1.$$

We proceed to construct from these the orthonormal polynomials associated with the lognormal probability density function

$$f(x) = \begin{cases} \frac{1}{x\sqrt{2\pi}} e^{-\frac{1}{2}\log^2 x}, & x > 0, \\ 0, & x \le 0. \end{cases}$$
(A.2)

PROPOSITION A.1. The polynomials $\{p_k\}_{k\in\mathbb{N}_0}$ orthonormal with respect to the lognormal density (A.2) are given by

$$p_0(x) \equiv 1, \qquad p_k(x) = \frac{(-1)^k e^{k(k-1)/4}}{\sqrt{\prod_{i=1}^k (e^i - 1)}} \sum_{j=0}^k (-1)^j \begin{bmatrix} k\\ j \end{bmatrix}_a e^{-j^2 + j/2} x^j, \quad k \ge 1, \quad (A.3)$$

with a = 1/e.

Proof. We denote by $\{\tilde{q}_k\}_{k\in\mathbb{N}_0}$ the particular sequence of Stieltjes-Wigert polynomials obtained for the parameter value $\nu = 1/\sqrt{2}$ with associated weight function

$$\widetilde{w}(x) = \begin{cases} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}\log^2 x}, & x > 0, \\ 0, & \text{otherwise.} \end{cases}$$

In view of

$$e^{1/4}\widetilde{q}_0(ex) = e^{1/4}e^{-1/4} = 1$$

as well as

$$\begin{split} e^{1/4} \widetilde{q}_k(ex) &= \frac{(-1)^k e^{-k/2}}{\sqrt{\prod_{i=1}^k (1-e^{-i})}} \sum_{j=0}^k \begin{bmatrix} k \\ j \end{bmatrix}_a e^{-j^2} (-e^{-1/2} ex)^j \\ &= \frac{(-1)^k e^{-k/2+k(k+1)/4}}{\sqrt{\prod_{i=1}^k (e^i-1)}} \sum_{j=0}^k \begin{bmatrix} k \\ j \end{bmatrix}_a (-1)^j e^{-j^2+j/2} x^j \\ &= \frac{(-1)^k e^{k(k-1)/4}}{\sqrt{\prod_{i=1}^k (e^i-1)}} \sum_{j=0}^k \begin{bmatrix} k \\ j \end{bmatrix}_a (-1)^j e^{-j^2+j/2} x^j, \qquad k \ge 1, \end{split}$$

we obtain the relation

$$p_k(x) = e^{1/4} \widetilde{q}_k(ex), \qquad k \in \mathbb{N}_0.$$

Orthonormality now follows after a succession of changes of variables from

$$\int_{0}^{\infty} p_{k}(x)p_{\ell}(x)f(x) dx = \int_{0}^{\infty} e^{1/4} \tilde{q}_{k}(ex)e^{1/4} \tilde{q}_{\ell}(ex)f(x) dx$$
$$= \sqrt{\frac{e}{2\pi}} \int_{-\infty}^{\infty} \tilde{q}_{k} \left(e^{y+1}\right) \tilde{q}_{\ell} \left(e^{y+1}\right) e^{-\frac{1}{2}y^{2}} dy = \int_{-\infty}^{\infty} \tilde{q}_{k} \left(e^{z}\right) \tilde{q}_{\ell} \left(e^{z}\right) \frac{e^{-\frac{1}{2}z^{2}}e^{z}}{\sqrt{2\pi}} dz$$
$$= \int_{0}^{\infty} \tilde{q}_{k}(t) \tilde{q}_{\ell}(t) \frac{e^{-\frac{1}{2}\log^{2}t}}{\sqrt{2\pi}} dt = \int_{0}^{\infty} \tilde{q}_{k}(t) \tilde{q}_{\ell}(t) \tilde{w}(t) dt = \delta_{k\ell}.$$

Like all orthogonal polynomials over the real numbers, the polynomials $\{p_k\}_{k\in\mathbb{N}}$ satisfy a three-term recurrence relation

$$\sqrt{\beta_{k+1}}p_{k+1}(x) = (x - \alpha_k)p_k(x) - \sqrt{\beta_k}p_{k-1}(x), \quad k \ge 0,$$
(A.4)

with $p_{-1} \equiv 0$ and $p_0 \equiv 1$, where we follow the common convention of denoting by $\{\alpha_k\}_{k\in\mathbb{N}_0}$ and $\{\beta_k\}_{k\in\mathbb{N}_0}$ the recurrence coefficients of the associated *monic* orthogonal polynomials (cf. [12, Section 1.3]). Since the weight function f of the $\{p_k\}$ is a probability density function we must have

$$\beta_0 = \int_0^\infty p_0(x)^2 f(x) \, dx = 1.$$

The remaining coefficients are obtained from the explicit representation (A.3). If we denote the *j*-th polynomial coefficient of p_k by $c_j^{(k)}$, i.e., such that

$$p_k(x) = \sum_{j=0}^k c_j^{(k)} x^j, \qquad k \in \mathbb{N}_0,$$

then by (A.3) we have

$$c_j^{(k)} = \frac{(-1)^{k+j} e^{k(k-1)/4}}{\sqrt{\prod_{i=1}^k (e^i - 1)}} \begin{bmatrix} k \\ j \end{bmatrix}_a e^{-j^2 + j/2}, \qquad j = 0, \dots, k, \quad k \in \mathbb{N}_0.$$
(A.5)

Comparing coefficients in (A.4) taking account of $p_{-1} \equiv 0$ and $p_0 \equiv 1$, we find

$$\beta_1 = \left(\frac{1}{c_1^{(1)}}\right)^2, \quad \alpha_0 = -\frac{c_0^{(1)}}{c_1^{(1)}}$$

and, in general,

$$\beta_{k+1} = \left(\frac{c_k^{(k)}}{c_{k+1}^{(k+1)}}\right)^2, \quad \alpha_k = \frac{c_{k-1}^{(k)}}{c_k^{(k)}} - \frac{c_k^{(k+1)}}{c_{k+1}^{(k+1)}}, \qquad k \in \mathbb{N}.$$

Together with (A.5), a straightforward calculation yields

$$\alpha_k = e^{k-1/2} \left(e^k (e+1) - 1 \right), \quad \beta_{k+1} = (e^{k+1} - 1)e^{3k+1}, \qquad k \in \mathbb{N}_0.$$
 (A.6)

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