Chapter 2
Random Field Representation

Nonlinear conservation laws subject to uncertainty are expected to develop solutions that are discontinuous in spatial as well as in stochastic dimensions. In order to allow piecewise continuous solutions to the problems of interest, we follow [7] and broaden the concept of solutions to the class of functions equivalent to a function f, denoted $\mathscr{C}_f$, and define a normed space that does not require its elements to be smooth functions. Let $(\Omega, \mathscr{F}, \mathscr{P})$ be a probability space with event space Ω, and probability measure $\mathscr{P}$ defined on the σ-field $\mathscr{F}$ of subsets of Ω. Let $\boldsymbol{\xi} = \{\xi_j(\omega)\}_{j=1}^N$ be a set of N independent and identically distributed random variables for $\omega \in \Omega$. We consider *second-order random fields*, i.e., we consider f belonging to the space

$$L^2(\Omega, \mathscr{P}) = \left\{ C_f \,|\, f \text{ measurable w.r.t.} \mathscr{P};\ \int_\Omega f^2 d\mathscr{P}(\xi) < \infty \right\}. \tag{2.1}$$

The inner product between two functionals $a(\xi)$ and $b(\xi)$ belonging to $L^2(\Omega, \mathscr{P})$ is defined by

$$\langle a(\xi) b(\xi) \rangle = \int_\Omega a(\xi) b(\xi) d\mathscr{P}(\xi). \tag{2.2}$$

This inner product induces the norm $\|f\|^2_{L_2(\Omega,\mathscr{P})} = \langle f^2 \rangle$.

Spectral representations of random functionals aim at finding a series expansion in the form

$$f(\xi) = \sum_{k=0}^{\infty} f_k \psi_k(\xi(\omega)),$$

where $\{\psi_k(\xi)\}_{k=0}^\infty$ is the set of basis functions and $\{f_k\}_{k=0}^\infty$ is the set of coefficients to be determined.

M.P. Pettersson et al., *Polynomial Chaos Methods for Hyperbolic Partial Differential Equations*, Mathematical Engineering,
DOI 10.1007/978-3-319-10714-1_2

The coefficients are defined by the *projections*

$$f_k = \langle \psi_k f \rangle, \quad k = 0, 1, \ldots$$

2.1 Karhunen-Loève Expansion

The Karhunen-Loève expansion [10, 14] provides a series representation of a random field in terms of its spatial correlation (covariance kernel). Any second-order random field $f(\boldsymbol{x}, \omega)$ on a spatial domain $\boldsymbol{\Omega}_{\boldsymbol{x}}$ can be represented as the Karhunen-Loève expansion

$$\boldsymbol{f}(\boldsymbol{x}, \omega) = \bar{\boldsymbol{f}}(\boldsymbol{x}) + \sum_{k=1}^{\infty} \eta_k(\omega) \sqrt{\lambda_k} \boldsymbol{\phi}_k^{KL}(\boldsymbol{x}),$$

where $\bar{\boldsymbol{f}}(\boldsymbol{x})$ is the mean of $\boldsymbol{f}(\boldsymbol{x}, \omega)$, the random variables η_k are uncorrelated with mean zero, and λ_k and $\boldsymbol{\phi}_k^{KL}$ are the eigenvalues and eigenfunctions of the covariance kernel, respectively.

The generalized eigenpairs $(\lambda_k, \boldsymbol{\phi}_k^{KL})$ can be determined from the solution of the generalized eigenvalue problem

$$\int_{\Omega_{\boldsymbol{x}}} \boldsymbol{C}_f(\boldsymbol{x}, \boldsymbol{x}') \boldsymbol{\phi}_k^{KL}(\boldsymbol{x}') d\boldsymbol{x}' = \lambda_k \boldsymbol{\phi}_k^{KL}(\boldsymbol{x}), \quad k \in \mathbb{N}^+, \tag{2.3}$$

where the *covariance function* $\boldsymbol{C}_f$ defines the two-point spatial statistics. The covariance function $\boldsymbol{C}_f$ does not contain information sufficient to determine the joint probability distribution of the random variables $\{\eta_k\}$. Instead, the joint probability of these random variables must be determined by data.

The Karhunen-Loève expansion is bi-orthogonal, i.e.,

$$\left\langle \boldsymbol{\phi}_j^{KL}(\boldsymbol{x}), \boldsymbol{\phi}_k^{KL}(\boldsymbol{x}) \right\rangle_{\Omega_{\boldsymbol{x}}} \equiv \int_{\Omega_{\boldsymbol{x}}} \left(\boldsymbol{\phi}_j^{KL}(\boldsymbol{x}) \right)^T \boldsymbol{\phi}_k^{KL}(\boldsymbol{x}) d\boldsymbol{x} = \delta_{jk}, \tag{2.4}$$

$$\left\langle \eta_j \eta_k \right\rangle_{\Omega} \equiv \int_{\Omega} \eta_j \eta_k d\mathscr{P} = \delta_{jk}. \tag{2.5}$$

For random fields with known covariance structure, the Karhunen-Loève expansion is optimal in the sense that it minimizes the mean-squared error. The covariance function of the output of a problem is in general not known a priori. However, Karhunen-Loève representations of the input data can often be combined with generalized chaos expansions, presented in the next section.

2.2 Generalized Chaos Expansions

Infinite series expansions in terms of functions that are orthogonal with respect to the probability measure of some random parametrization are used for representation of stochastic quantities of interest. The corresponding series expansions of these basis functions are referred to as generalized chaos expansions. Possible choices include polynomials and wavelets.

2.2.1 Generalized Polynomial Chaos Expansion

The polynomial chaos (PC) framework based on series expansions of Hermite polynomials of Gaussian random variables was introduced by Ghanem and Spanos [9] and builds on the theory of homogeneous chaos introduced by Wiener in 1938 [18]. Any second-order random field can be expanded as a generalized Fourier series in the set of orthogonal Hermite polynomials, which constitutes a complete basis in the Hilbert space $L^2(\Omega, \mathscr{P})$ defined by (2.1). The resulting polynomial chaos series converges in the $L^2(\Omega, \mathscr{P})$ sense as a consequence of the Cameron-Martin theorem [3]. Although not limited to represent functions with Gaussian distribution, the polynomial chaos expansion achieves the highest convergence rate for Gaussian functions. Xiu and Karniadakis [20] introduced the *generalized polynomial chaos* (gPC) expansion, where random functions are represented by any set of hypergeometric polynomials from the Askey scheme [2]. Hence, a function with uniform distribution is optimally represented by Legendre polynomials that are orthogonal with respect to the uniform measure, and a gamma-distributed input by Laguerre polynomials that are orthogonal with respect to the gamma measure, and so on. The optimality of the choice of stochastic expansion pertains to the representation of the input; the representation of the output of a nonlinear problem will likely be highly nonlinear as expressed in the basis of the input.

The Cameron-Martin theorem applies also to gPC with non-Gaussian random variables, but only when the probability measure $\mathscr{P}(\xi)$ of the stochastic expansion variable ξ is uniquely determined by the sequence of moments,

$$\langle \xi^k \rangle = \int_\Omega \xi^k \, d\,\mathscr{P}(\xi), \quad k \in \mathbb{N}_0.$$

This is not always the case in situations commonly encountered; for instance, the lognormal generalized chaos does not satisfy this property. Thus, there are cases when the gPC expansion does not converge to the true limit of the random variable under expansion [6]. However, lognormal random variables may be successfully represented by gPC satisfying the determinacy of moments (cf. [6] for a detailed exposition on this topic), e.g., Hermite polynomial chaos expansion. This motivates our choice to use Hermite polynomial chaos expansion to represent lognormal viscosity in Chap. 5.

Consider a generalized chaos basis $\{\psi_i(\xi)\}_{i=0}^{\infty}$ spanning the space of second-order (i.e., finite variance) random processes on this probability space. The basis functionals are assumed to be orthonormal, i.e., they satisfy

$$\langle \psi_i \psi_j \rangle = \delta_{ij}\,. \tag{2.6}$$

Any second-order random field $u(x,t,\xi)$ can be expressed as

$$u(x,t,\xi) = \sum_{i=0}^{\infty} u_i(x,t)\psi_i(\xi), \tag{2.7}$$

where the coefficients $u_i(x,t)$ are defined by the projections

$$u_i(x,t) = \langle u(x,t,\xi)\psi_i(\xi)\rangle, \quad i = 0, 1, \ldots. \tag{2.8}$$

For notational convenience, we will not distinguish between u and its generalized chaos expansion.

Independent of the choice of basis $\{\psi_i\}_{i=0}^{\infty}$, we can express the mean and variance of $u(x,t,\xi)$ as

$$E(u(x,t,\xi)) = u_0(x,t), \quad \mathrm{Var}(u(x,t,\xi)) = \sum_{i=1}^{\infty} u_i^2(x,t),$$

respectively. Similarly, higher-order statistics, e.g., skewness and kurtosis, can be derived as functions of the gPC coefficients. For practical purposes, (2.7) is truncated to a finite order M, and we set

$$u(x,t,\xi) \approx \sum_{i=0}^{M} u_i(x,t)\psi_i(\xi). \tag{2.9}$$

The number of basis functions $M + 1$ is dependent on the number of stochastic dimensions N and the order of truncation of the generalized chaos expansion.

In order to construct a multi-dimensional gPC basis, let $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_N)^T \in \mathbb{R}^N$ be a random vector of input uncertainties defined on the probability space $(\Omega, \mathscr{F}, \mathscr{P})$. Assume that the entries of $\boldsymbol{\xi}$ are independent and identically distributed (i.i.d.). For $l = 1, \ldots, d$, let $\{\psi_{k_l}(\xi_l)\}_{k=0}^{\infty}$ be a polynomial basis orthonormal with respect to the measure of the random variable ξ_l. The multi-dimensional gPC basis functions may then be obtained by tensorization of the univariate basis functions $\{\psi_{k_l}(\xi_l)\}_{k=0}^{\infty}$, i.e.,

$$\psi_{\boldsymbol{k}}(\boldsymbol{\xi}) = \prod_{l=1}^{N} \psi_{k_l}(\xi_l), \tag{2.10}$$

with the multi-index $\boldsymbol{k} \in \mathbb{N}_0^N := \{(k_1, \cdots, k_N) : k_l \in \mathbb{N} \cup \{0\}\}$. In practice, the multi-index $\boldsymbol{k}$ has to be truncated in order to generate a finite cardinality basis. This may be achieved by restricting $\boldsymbol{k}$ to the sets

$$\Lambda_{p,N} := \left\{\boldsymbol{k} \in \mathbb{N}_0^N : \|\boldsymbol{k}\|_1 \leq p\right\} \tag{2.11}$$

or

$$\Gamma_{p,N} := \left\{\boldsymbol{k} \in \mathbb{N}_0^N : k_l \leq p,\ l = 1, \ldots, N\right\} \tag{2.12}$$

to achieve the so-called *complete polynomial* or *tensor polynomial* basis, respectively. The bases defined by the index sets (2.11) and (2.12) are isotropic in the N stochastic dimensions. By replacing p with a dimension-dependent integer p_l, $l = 1, \ldots, N$, anisotropic bases tailored to accuracy requirements for each stochastic dimension may be obtained. For simplicity of notation, we subsequently consider a one-to-one relabeling of the form $\{\psi_k(\boldsymbol{\xi})\}_{k=0}^M$ for the gPC basis $\{\psi_{\boldsymbol{k}}(\boldsymbol{\xi})\}$, $\boldsymbol{k} \in \Lambda_{p,N}$ or $\Gamma_{p,N}$, where $M + 1$ is the cardinality of the gPC basis. In particular, for the complete polynomial basis, the cardinality is given by

$$M + 1 = \frac{(p + N)!}{p!N!},$$

while for the tensor polynomial basis, the cardinality is

$$M + 1 = (p + 1)^N.$$

As an example, consider the case of $p = 5$ and $N = 2$ stochastic dimensions. That means 21 and 36 basis functions for the complete polynomial basis and the tensor polynomial basis, respectively. If we keep $p = 5$ and include 5 stochastic dimensions, $N = 5$, the complete polynomial basis contains 252 basis functions. In contrast, the corresponding tensor polynomial basis contains as many as 7,776 basis functions.

An increase in the number of random parameters corresponds to an exponential increase in the cardinality of the series. This increase quickly leads to infeasible numerical problems and has spurred broad interest in alternative formulations not based on the tensorization introduced earlier. Sparse representations and adaptive techniques [8, 16, 17] are becoming increasingly popular, although their use remains fairly limited for hyperbolic problems. For this reason, and because the fundamental issues related to the numerical treatment of the stochastic Galerkin schemes are well expressed in one-dimensional uncertain problems, we will not discuss this issue further but rather focus on the $N = 1$ case.

The basis $\{\psi_i\}_{i=0}^{\infty}$ is often a set of orthogonal polynomials. Given the two lowest-order polynomials, higher-order polynomials can be generated by the recurrence relation

$$\psi_n(\xi) = (a_n \xi + b_n)\psi_{n-1}(\xi) + c_n \psi_{n-2}(\xi),$$

where the coefficients a_n, b_n, c_n are specific to the class of polynomials.

The truncated chaos series (2.9) may result in solutions that are unphysical. An extreme example is when a strictly positive quantity, say density, with uncertainty within a bounded range is represented by a polynomial expansion with infinite range, for instance Hermite polynomials of standard Gaussian variables. The Hermite series expansion converges to the true density with bounded range in the limit $M \to \infty$, but for a given order of expansion, say $M = 1$, the representation $\rho = \rho_0 + \rho_1 H_1(\xi)$ results in negative density with nonzero probability since the Hermite polynomial H_1 takes arbitrarily large negative values. Similar problems may be encountered also for polynomial representations with bounded support. Polynomial reconstruction of a discontinuity in stochastic space leads to Gibbs oscillations that may yield negative values of an approximation of a solution that is close to zero but strictly positive by definition. Whenever discontinuities are involved, care is needed with the use of global polynomial representations; this caveat underlies most of the development in Chap. 8.

Spectral convergence of the generalized polynomial chaos expansion is observed when the solutions are sufficiently regular and continuous [20], but for general non-linear conservation laws – such as in fluid dynamics problems – the convergence is usually less favorable. Spectral expansion representations are still of interest for these problems because of their potential efficiency with respect to brute force sampling methods and to gain insights from writing the governing equations for the stochastic problem. However, special attention must be devoted to the numerical methodology used. For some problems with steep gradients in the stochastic dimensions, polynomial chaos expansions completely fail to capture the solution [13]. Global methods can still give a superior overall performance, for instance Padé approximation methods based on rational function approximation [4], and hierarchical wavelet methods that are global methods with localized support of each resolution level [11]. These methods do not need input such as mesh refinement parameters, and they are not dependent on the initial discretization of the stochastic space. An alternative to polynomial expansions for non-smooth and oscillatory problems is generalized chaos based on a localization or discretization of the stochastic space [5,15]. Methods based on stochastic discretization such as adaptive stochastic multi-elements [17] and stochastic simplex collocation [19] will be described in some more detail in Sect. 3.2.3. The robust properties of discretized stochastic space can also be obtained by globally defined wavelets, see [11,12]. The next section outlines piecewise linear Haar wavelet chaos, followed by a description of piecewise polynomial multiwavelet generalized chaos. These classes of basis functions are robust to discontinuities.

2.2.2 *Haar Wavelet Expansion*

Haar wavelets are defined hierarchically on different resolution levels, representing successively finer features of the solution with increasing resolution. They have non-overlapping support within each resolution level, and in this sense they are localized. Still, the Haar basis is global due to the overlapping support of wavelets belonging to different resolution levels. Haar wavelets do not exhibit spectral convergence, but avoid the Gibbs phenomenon.

Consider the mother wavelet function defined by

$$\psi^W(y) = \begin{cases} 1 & \text{for } 0 \le y < \frac{1}{2} \\ -1 & \text{for } \frac{1}{2} \le y < 1 \\ 0 & \text{otherwise} \end{cases}. \tag{2.13}$$

Based on (2.13), we get the wavelet family

$$\psi^W_{j,k}(y) = 2^{j/2}\psi^W(2^j y - k), \qquad j = 0, 1, \ldots; \quad k = 0, \ldots, 2^{j-1}.$$

Given the probability measure of the stochastic variable ξ with cumulative distribution function $F_\xi(\xi_0) = \mathscr{P}(\omega : \xi(\omega) \le \xi_0)$, define the basis functions

$$W_{j,k}(\xi) = \psi^W_{j,k}(F_\xi(\xi)).$$

Adding the basis function $W_0(y) = 1$ in $y \in [0, 1]$ and concatenating the indices j and k into $i = 2^j + k$ so that $W_i(\xi) \equiv \psi^W_{n,k}(F_\xi(\xi))$, we can represent any random variable $u(x, t, \xi)$ with finite variance as

$$u(x, t, \xi) = \sum_{i=0}^{\infty} u_i(x, t) W_i(\xi),$$

which is of the form (2.7). Figure 2.1 depicts the first eight basis functions of the generalized Haar wavelet chaos.

2.2.3 Multiwavelet Expansion

The main idea of multiwavelets (MW) is to combine the localized and hierarchical structure of Haar wavelets with the convergence properties of orthogonal polynomials. The procedure of constructing these multiwavelets using Legendre polynomials follows the algorithm in [1] and is outlined in [12]; additional details are included in Appendix A.

Starting with the space $\mathbf{V}_{N_p}$ of polynomials of degree at most N_p defined on the interval $[-1, 1]$, the construction of multiwavelets aims at finding a basis of piecewise polynomials for the orthogonal complement of $\mathbf{V}_{N_p}$ in the space $\mathbf{V}_{N_p+1}$ of polynomials of degree at most $N_p + 1$. Merging the bases of $\mathbf{V}_{N_p}$ and that of the orthogonal complement of $\mathbf{V}_{N_p}$ in $\mathbf{V}_{N_p+1}$, we obtain a piecewise polynomial basis for $\mathbf{V}_{N_p+1}$. Continuing the process of finding orthogonal complements in spaces of increasing degree of piecewise polynomials leads to a basis for $L_2([-1, 1])$.

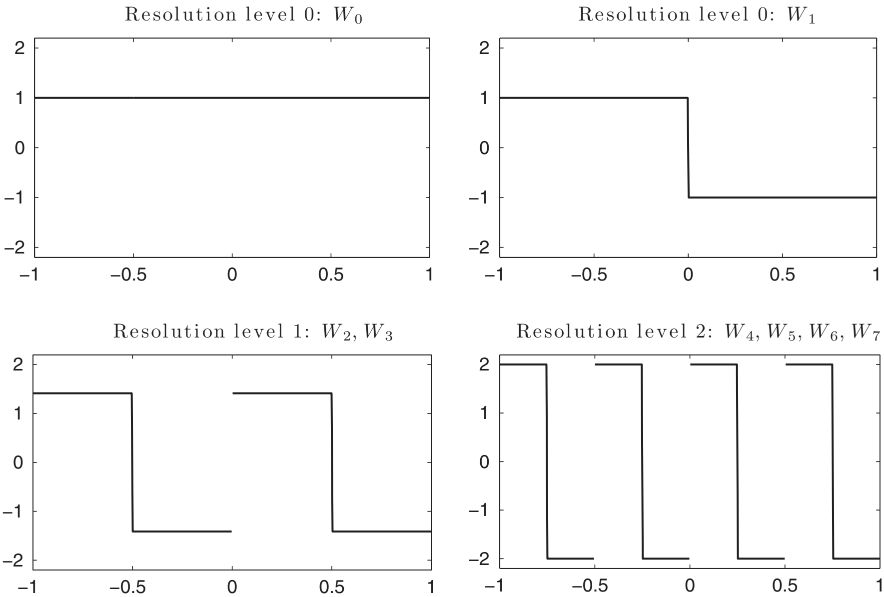

Fig. 2.1 Haar wavelets, resolution levels 0,1,2

We first introduce a smooth polynomial basis on $[-1, 1]$. Let $\{Le_i(\xi)\}_{i=0}^{\infty}$ be the set of Legendre polynomials that are defined on $[-1, 1]$ and orthogonal with respect to the uniform measure. The normalized Legendre polynomials are defined recursively by

$$Le_{j+1}(\xi) = \sqrt{2j+3}\left(\frac{\sqrt{2j+1}}{j+1}\xi Le_j(\xi) - \frac{j}{(j+1)\sqrt{2j-1}}Le_{j-1}(\xi)\right),$$
$$Le_0(\xi) = 1, \quad Le_1(\xi) = \sqrt{3}\xi.$$

The set $\{Le_i(\xi)\}_{i=0}^{N_p}$ is an orthonormal basis for $\mathbf{V}_{N_p}$. Double products are readily computed from (2.6), and higher-order products are precomputed using numerical integration.

Following the algorithm by Alpert [1] (see Appendix A), we construct a set of *mother wavelets* $\{\psi_i^W(\xi)\}_{i=0}^{N_p}$ defined on the domain $\xi \in [-1, 1]$, where

$$\psi_i^W(\xi) = \begin{cases} \pi_i(\xi) & -1 \le \xi < 0 \\ (-1)^{N_p+i+1}\pi_i(\xi) & 0 \le \xi < 1 \\ 0 & \text{otherwise,} \end{cases} \tag{2.14}$$

where $\pi_i(\xi)$ is an ith-order polynomial. By construction, the set of wavelets $\{\psi_i^W(\xi)\}_{i=0}^{N_p}$ are orthogonal to all polynomials of order at most N_p, hence the wavelets are orthogonal to the set $\{Le_i(\xi)\}_{i=0}^{N_p}$ of Legendre polynomials of order at most N_p. Based on translations and dilations of (2.14), we get the wavelet family

$$\psi^W_{i,j,k}(\xi) = 2^{j/2}\psi^W_i(2^j\xi - k), \qquad i = 0,\dots,N_p, \quad j = 0,1,\dots, \quad k = 0,\dots,2^{j-1}.$$

Let $\psi_m(\xi)$ for $m = 0,\dots,N_p$ be the set of Legendre polynomials up to order N_p, and concatenate the indices i, j, k into $m = (N_p + 1)(2^j + k - 1) + i$ so that $\psi_m(\xi) \equiv \psi^W_{i,j,k}(\xi)$ for $m > N_p$. With the MW basis $\{\psi_m(\xi)\}_{m=0}^{\infty}$, we can represent any random variable $u(x,t,\xi)$ with finite variance as

$$u(x,t,\xi) = \sum_{m=0}^{\infty} u_m(x,t)\psi_m(\xi),$$

which is again of the form (2.7). In the computations, we truncate the MW series both in terms of the piecewise polynomial order N_p and the *resolution level* N_r. With the index $j = 0,\dots,N_r$, we retain $P = (N_p + 1)2^{N_r}$ terms of the MW expansion.

The truncated MW basis is characterized by the piecewise polynomial order N_p and the number of resolution levels N_r, illustrated in Fig. 2.2 for $N_p = 2$ and $N_r = 3$. As special cases of the MW basis, we obtain the Legendre polynomial basis for $N_r = 0$ ($i = j = 0$), and the Haar wavelet basis of piecewise constant functions for $N_p = 0$.

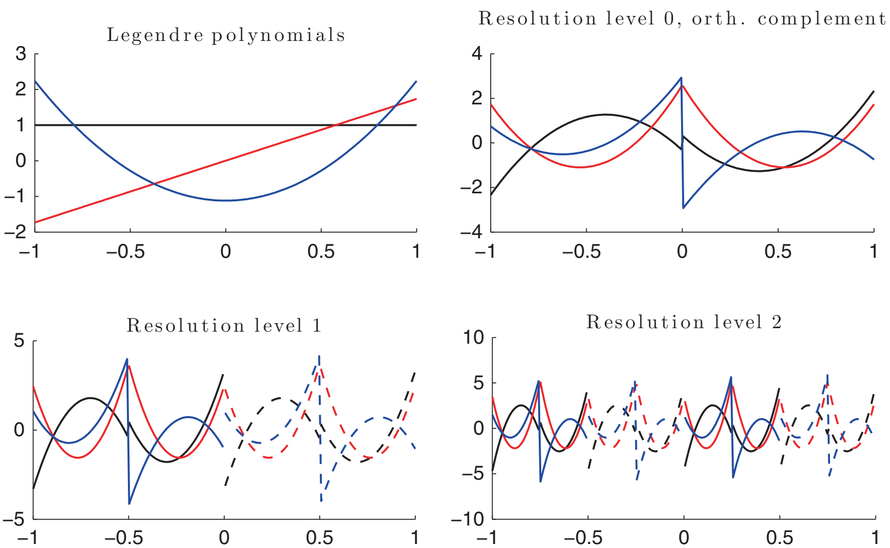

Fig. 2.2 Multiwavelets for $N_p = 2$, $N_r = 3$. Resolution level 0 consists of the first $N_p + 1$ Legendre polynomials and their orthogonal complement. Resolution level $j > 0$ contains $(N_p + 1)2^j$ wavelets each. Each basis function is a piecewise polynomial of order N_p

2.2.4 Choice of Basis Functions for Generalized Chaos

The choice of basis functions for the generalized chaos expansion of a given problem of interest is in general non-trivial. An optimal set of basis functions for the input parameters may be highly inappropriate for the propagation of uncertainty to the output. In particular, this is the case for the nonlinear hyperbolic problems that will be encountered in subsequent chapters. These problems develop discontinuities in finite time, and a polynomial reconstruction will lead to oscillations. The consequence is lack of accuracy or even breakdown of the numerical method.

For smooth problems, the situation is not that severe. Transformations between probability measures allow the use of non-optimal basis functions, e.g., Legendre polynomials to represent normal distributions. The exponential convergence rate of PC expansions is in general not maintained when a non-optimal basis is chosen [21].

2.3 Exercises

2.1. PC formulations of UQ problems typically start from infinite series expansions, ending up with a formulation involving a finite number of PC terms. This truncation introduces a stochastic truncation error that propagates in subsequent operations on the PC series. Verify that the finite order expansion of the product of $F * G$ is different from the product of the expansions of F and G.

2.2. Orthogonal polynomial representations are often used with the hope that a small number of terms are sufficient to accurately represent a given function. Study the truncation error of Hermite expansions of the non-linear functions $\sin(\xi)$, $x^3(\xi)$, $\log(\xi)$, $x^2(\xi)/(3-\xi)$, assuming that ξ is a standard normal random variable. Plot the L_2 error as a function of the order M of the expansion (you need to find functions that can be integrated analytically for the coefficients – or ensure that sufficient accuracy is achieved by the numerical integration).

2.3. Orthogonal polynomials are frequently used to represent PDE solutions in UQ. Depending on the PDE, we may have an idea of the kind of solution we can expect. To accurately represent the PDE solution, it is necessary to know how to accurately represent a function similar to the solution, i.e., how many gPC terms to be retained, and whether the chosen gPC basis is suitable. Consider Legendre polynomial expansion of the sine and Heaviside functions. Consider expansions of different order and compare the resulting approximations with the true function.

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http://www.springer.com/978-3-319-10713-4

Polynomial Chaos Methods for Hyperbolic Partial Differential Equations
Numerical Techniques for Fluid Dynamics Problems in the Presence of Uncertainties
Pettersson, M.P.; Iaccarino, G.; Nordström, J.
2015, XI, 214 p. 60 illus., 54 illus. in color., Hardcover
ISBN: 978-3-319-10713-4