

Appendix A

Essential Elements of Probability Theory and Random Processes

Probability theory is a mathematical construction to describe phenomena whose outcomes occur non-deterministically. Depending on the context, the probability of the outcome in a random phenomenon can be interpreted either as its long-run frequency of occurrence or as a measure of its subjective uncertainty. These two points of view correspond to the frequentist and Bayesian interpretations of probabilities. This distinction is not necessary here, and we restrict the presentation to materials used in this monograph. In particular, we only introduce notions of real-valued random variables. Further elements of the probability theory can be found in standard references; see for instance [78, 104, 137, 181].

This appendix follows the exposition in Chaps. 1 and 2 of the book *Stochastic calculus: applications in science and engineering* by M. Grigoriu [94]. The discussion below distills essential elements from this reference.

A.1 Probability Theory

A.1.1 Measurable Space

We consider a random phenomenon or experiment. We denote Θ the set of all possible outcomes of the experiment. The set Θ is called the **sample space**, while θ denotes an element of Θ . The sample space may have a finite or infinite (countable or uncountable) number of elements.

Let Σ be a non-empty collection of subsets of Θ . The collection Σ is called a **σ -field on Θ** if

- $\emptyset \in \Sigma$
- $A \in \Sigma \Rightarrow \bar{A} \in \Sigma$
- $A_i \in I \in \Sigma \Rightarrow \cup_{i \in I} A_i \in \Sigma$

where \bar{A} is the complement of A in Θ and I is a countable set. An element $A \in \Sigma$ is called an event or Σ -measurable subset of Θ ; it is a collection of outcomes. The pair

(Θ, Σ) is called a **measurable space**. A **Borel** σ -field is generated by the collection of all open sets of a topological set. The members of a Borel σ -field are called Borel sets. An important example of Borel σ -field is $\mathcal{B}(\mathbb{R})$, the collection of all open intervals of \mathbb{R} . The definition of $\mathcal{B}(\mathbb{R})$ extends to intervals; for instance $\mathcal{B}([a, b])$ denotes the Borel σ -field on the interval $[a, b]$. Denoting $\sigma(\mathcal{A})$ the smaller σ -field generated by a collection \mathcal{A} of subsets of Θ , we have

$$\mathcal{B}(\mathbb{R}) = \sigma((a, b), -\infty \leq a \leq b \leq +\infty).$$

A.1.2 Probability Measure

A set function $\mu : \Sigma \mapsto [0, \infty]$ is a **measure** on Σ if it is countably additive:

$$\mu\left(\bigcup_{i=1}^{\infty} A_i\right) = \sum_{i=1}^{\infty} \mu(A_i), \quad A_i \in \Sigma, A_i \cap A_{i \neq j} = \emptyset.$$

The triple (Θ, Σ, μ) is called a **measure space**. A **finite measure** is a measure such that $\mu(\Theta) < \infty$. A finite measure P such that

- $P : \Sigma \mapsto [0, 1]$
- $P(\Theta) = 1$

is called a **probability measure** or simply a probability.

A.1.3 Probability Space

The triple (Θ, Σ, P) is called a **probability space**. A probability space (Θ, Σ, P) such that for $A, B \in \Sigma$ with $A \subset B$ and $P(B) = 0 \Rightarrow P(A) = 0$ is said complete. A probability space can always be completed so we shall implicitly assume complete probability spaces. We then have the following properties of a probability space (Θ, Σ, P) for $A, B \in \Sigma$:

- $P(A) \leq P(B)$ for $A \subseteq B$,
- $P(\bar{A}) = 1 - P(A)$,
- $P(A \cup B) = P(A) + P(B) - P(A \cap B)$.

Consider the probability spaces $(\Theta_k, \Sigma_k, P_k)$ for $k = 1, \dots, n$. From this collection, we define the **product probability space** (Θ, Σ, P) as

$$\begin{aligned} \Theta &= \Theta_1 \times \dots \times \Theta_n, \\ \Sigma &= \Sigma_1 \times \dots \times \Sigma_n, \\ P &= P_1 \times \dots \times P_n. \end{aligned}$$

This definition also holds for $n = \infty$. Whenever, the spaces $(\Theta_k, \Sigma_k, P_k)$ are all identical, the product sample space, σ -field and probability measure will be denoted Θ^n, Σ^n and P^n respectively.

Let (Θ, Σ, P) be a probability space and let $B \in \Sigma$ be a given event such that $P(B) > 0$. We define a new probability measure, called the **probability conditional on B** as

$$P(A \in \Sigma | B) \equiv \frac{P(A \cap B)}{P(B)}.$$

From this definition, if the set of events $A_i \in \Sigma$ is a partition of the sample space (i.e. if $A_i \cap A_{j \neq i} = \emptyset$ and $\bigcup_i A_i = \Theta$), then

$$P(B) = \sum_i P(B \cap A_i) = \sum_i P(B|A_i)P(A_i),$$

(**law of total probability**) and

$$P(A_j|B) = \frac{P(A_j)P(B|A_j)}{P(B)} = \frac{P(A_j)P(B|A_j)}{\sum_i P(A_i)P(B|A_i)}, \quad P(B) > 0$$

(**Bayes formula**).

A.2 Measurable Functions

A.2.1 Induced Probability

Consider two measurable spaces (Θ, Σ_Θ) and $(\Theta', \Sigma_{\Theta'})$ and a function $h : \Theta \mapsto \Theta'$ with domain Θ and range Θ' . The function h is said **measurable from (Θ, Σ_Θ) to $(\Theta', \Sigma_{\Theta'})$** if for any event B in $\Sigma_{\Theta'}$

$$h^{-1}(B) \equiv \{\theta : h(\theta) \in B\} \in \Sigma_\Theta.$$

If h is measurable from (Θ, Σ_Θ) to $(\Theta', \Sigma_{\Theta'})$ and $(\Theta, \Sigma_\Theta, P)$ is a probability then $Q : \Sigma_{\Theta'} \mapsto [0, 1]$ defined by

$$Q(B \in \Sigma_{\Theta'}) \equiv P(h^{-1}(B))$$

is a probability measure on $(\Theta', \Sigma_{\Theta'})$ called the **probability induced** by h , or simply the distribution of h .

A.2.2 Random Variables

Consider a probability space (Θ, Σ, P) and a function $X : \Theta \mapsto \mathbb{R}$ measurable from (Θ, Σ) to $(\mathbb{R}, \mathcal{B})$. Then, X is a **\mathbb{R} -valued random variable**, sometimes denoted

$X(\theta)$. The **distribution** of X is the probability measure induced by the mapping $X : \Theta \mapsto \mathbb{R}$ on the measurable space $(\mathbb{R}, \mathcal{B})$, defined by

$$Q(B) = P(X^{-1}(B)), \quad B \in \mathcal{B}.$$

This definition implies that X is a random variable if and only if $X^{-1}((-\infty, x]) \in \Sigma, \forall x \in \mathbb{R}$. In other words, a \mathbb{R} -valued random variable is a function which maps the sample space Θ to \mathbb{R} .

The previous definition of a random variable can be extended to \mathbb{R}^d -valued functions \mathbf{X} measurable from (Θ, Σ) to $(\mathbb{R}^d, \mathcal{B}^d)$. If all the coordinates of \mathbf{X} are random variables, then \mathbf{X} is called a **random vector**.

A.2.3 Measurable Transformations

This monograph is concerned with numerical techniques for the characterization of the output of physical models involving random input. We are then dealing with transformations of random variables. Denoting \mathbf{X} the \mathbb{R}^d -valued random vector representing the model input, we are for instance interested in a model output $Y = g(\mathbf{X})$ where $g : \mathbb{R}^d \mapsto \mathbb{R}$. The model output is then defined by the mapping

$$(\Theta, \Sigma) \xrightarrow{\mathbf{X}} (\mathbb{R}^d, \mathcal{B}^d) \xrightarrow{g} (\mathbb{R}, \mathcal{B}).$$

It can be shown that if \mathbf{X} and g are measurable functions from (Θ, Σ) to $(\mathbb{R}^d, \mathcal{B}^d)$ and from $(\mathbb{R}^d, \mathcal{B}^d)$ to $(\mathbb{R}, \mathcal{B})$, respectively, then the composed mapping $g \circ \mathbf{X} : (\Theta, \Sigma) \mapsto (\mathbb{R}, \mathcal{B})$ is measurable. As a result, the model output is a \mathbb{R} -valued random variable.

A.3 Integration and Expectation Operators

A.3.1 Integrability

For $X : (\Theta, \Sigma) \mapsto (\mathbb{R}, \mathcal{B})$, the integral of X with respect to P over the event $A \in \Sigma$ is

$$\int_{\Theta} I_A(\theta)X(\theta)dP(\theta) = \int_A X(\theta)dP(\theta),$$

where I_A is the indicator function of A . If this integral exists and is finite, X is said to be **P -integrable over A** . A random vector \mathbf{X} is P -integrable over A , if all of its components are individually P -integrable over A .

Let X and Y be two random variables defined on a probability space (Θ, Σ, P) . We have the following properties:

- For $A \in \Sigma$,

$$\int_A |X| dP < \infty \Rightarrow \int_A X dP \text{ is finite.}$$

- If X, Y are P -integrable over $A \in \Sigma$, the random variable $aX + bY$ is P -integrable over A and (linearity):

$$\int_A (aX + bY) dP = a \int_A X dP + b \int_A Y dP.$$

- If X is P -integrable over Θ and $\{A_i \in \Sigma\}$ is a partition of Θ , then

$$\int_{\cup_i A_i} X dP = \sum_i \int_{A_i} X dP.$$

- If X is P -integrable on Θ , then X is finite a.s. (almost surely), i.e. $B = \{\theta : X(\theta) = \pm\infty\} \in \Sigma$ is such that $P(B) = 0$.
- If $X \geq 0$ a.s., then

$$\int_A X dP \geq 0.$$

- If $Y \leq X$ a.s. then

$$\int_A Y dP \leq \int_A X dP.$$

A.3.2 Expectation

The particular case of $A = \Theta$ for the integration domain corresponds to the expectation operator which will be denoted $E[\cdot]$:

$$E[X] \equiv \int_{\Theta} X(\theta) dP(\theta).$$

Provided it exists and is finite, the expectation has the following properties. Let X and Y be two \mathbb{R} -valued random variables defined on a probability space (Θ, Σ, P) and P -integrable over Θ . Then

- Linearity of the expectation:

$$E[aX + bY] = aE[X] + bE[Y].$$

- $X \geq 0$ a.s. $\Rightarrow E[X] \geq 0$.
- $Y \leq X$ a.s. $\Rightarrow E[Y] \leq E[X]$.
- $|E[X]| \leq E[|X|]$.

A.3.3 L_2 Space

Consider a probability space (Θ, Σ, P) . For $q \geq 1$, we denote $L_q(\Theta, \Sigma, P)$ the collection of \mathbb{R} -valued random variables X defined on (Θ, Σ, P) such that

$$E[|X|^q] < \infty.$$

The case $q = 2$, corresponding to the L_2 -space is of particular importance in this book as it possesses some essential properties.

First, L_2 is a **vector space**. Indeed, for $X \in L_2, \lambda \in \mathbb{R} \Rightarrow \lambda X \in L_2$, since $E[(\lambda X)^2] = \lambda^2 E[X^2] < \infty$. It remains to show that for $X, Y \in L_2, X + Y \in L_2$, so $E[(X + Y)^2] = E[X^2] + E[Y^2] + 2E[XY] < \infty$. To prove the last inequality, we have to show that $E[XY]$ is finite; to this end consider $X \neq Y$ such that

$$p(\lambda) = E[(X + \lambda Y)^2] = E[X^2] + \lambda^2 E[Y^2] + \lambda 2E[XY],$$

has no real root; this leads to $E[XY]^2 - E[X^2]E[Y^2] \leq 0$ or equivalently

$$|E[XY]| \leq E[X^2]^{1/2} E[Y^2]^{1/2} \quad \text{for } X, Y \in L_2,$$

which is known as the **Cauchy-Schwarz** inequality.

Second, the expectation $E[XY]$ defines an **inner product** on L_2 , denoted $\langle X, Y \rangle$ with the associated L_2 **norm** $\|X\|_{L_2} = E[X^2]^{1/2}$. Indeed, $\langle \cdot, \cdot \rangle$ is an inner product since

$$\begin{aligned} \langle 0, X \rangle &= 0, & X \in L_2, \\ \langle X, X \rangle &> 0, & X \in L_2, X \neq 0, \\ \langle X, Y \rangle &= \langle Y, X \rangle, & X, Y \in L_2, \\ \langle X + Y, Z \rangle &= \langle X, Z \rangle + \langle Y, Z \rangle, & X, Y, Z \in L_2, \\ \langle \lambda X, Y \rangle &= \lambda \langle X, Y \rangle, & X, Y \in L_2, \lambda \in \mathbb{R}, \end{aligned}$$

and $d : L_2 \times L_2 \mapsto [0, +\infty)$ defined by $d(X, Y) = \|X - Y\|_{L_2}$ is a metric on L_2 since

$$\begin{aligned} d(X, Y) &= 0 \quad \text{iif } X = Y \text{ a.s.}, \\ d(X, Y) &= d(Y, X), \quad X, Y \in L_2, \\ d(X, Y) &\leq d(X, Z) + d(Z, Y), \quad \forall X, Y, Z \in L_2. \end{aligned}$$

Finally, L_2 equipped with the inner product $\langle \cdot, \cdot \rangle$ and the L_2 -norm is a **Hilbert space**. As a result, if $X \in L_2(\Theta, \Sigma, P)$ and Σ' is a sub- σ -field of Σ , then there is a unique random variable $X' \in L_2(\Theta, \Sigma', P)$ such that

$$\|X - X'\|_{L_2} = \min \{ \|X - Z\|_{L_2} : Z \in L_2(\Theta, \Sigma', P) \},$$

and

$$\langle X - X', Z \rangle = 0, \quad \forall Z \in L_2(\Theta, \Sigma', P).$$

The random variable X' is the **orthogonal projection** of X on $L_2(\Theta, \Sigma', P)$, or best mean square estimator of X , and has the smallest mean square error of all members of $L_2(\Theta, \Sigma', P)$.

A.4 Random Variables

We recall (see A.2.2) that a \mathbb{R} -valued random variable defined on a probability space (Θ, Σ, P) is a measurable function from (Θ, Σ) to $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$.

A.4.1 Distribution Function of a Random Variable

The **cumulative distribution function**, or simply distribution function, of a random variable X defined on a probability space (Θ, Σ, P) is defined by

$$F_X(x) = P\left(X^{-1}((-\infty, x])\right) = P(\{\theta : X(\theta) \leq x\}) = P(X \leq x).$$

The distribution function is right-continuous, increasing, with range $[0, 1]$. In addition,

$$\begin{aligned} \lim_{x \rightarrow +\infty} F_X(x) &= 1, & \lim_{x \rightarrow -\infty} F_X(x) &= 0, \\ P(a < x \leq b) &= F_X(b) - F_X(a) \geq 0, \\ P(a \leq x < b) &= F_X(b) - F_X(a) + P(x = a) - P(x = b). \end{aligned}$$

The distribution F_X of a random variable X has only a countable number of jump discontinuities and is continuous at $x \in \mathbb{R}$ if and only if $P(X = x) = 0$.

A.4.2 Density Function of a Random Variable

If F_X is absolutely continuous in \mathbb{R} , there is an integrable function f called the probability density function, or density function, such that

$$F_X(b) - F_X(a) = \int_a^b f_X(x) \, dx, \quad a \leq b.$$

A density function has the essential properties:

$$f_X(x) = F'_X(x) \quad \text{so} \quad \int_{-\infty}^x f_X(y) \, dy = F_X(x),$$

$$f_X(x) \geq 0,$$

$$\int_{-\infty}^{+\infty} f_X(x) \, dx = 1.$$

Let X be a random variable defined on a probability space (Θ, Σ, P) , and consider a measurable function $g : (\mathbb{R}, \mathcal{B}) \mapsto (\mathbb{R}, \mathcal{B})$. Then, $Y = g \circ X$ is a random variable defined on (Θ, Σ, P) and

$$\begin{aligned} E[Y] &= \int_{\Theta} Y(\theta) \, dP(\theta) = \int_{\Theta} g(X(\theta)) \, dP(\theta) \\ &= \int_{\mathbb{R}} g(x) \, dQ(x) = \int_{\mathbb{R}} g(x) \, dF_X(x) = \int_{\mathbb{R}} g(x) f_X(x) \, dx. \end{aligned}$$

This relation provides an expression of the expectation of Y involving the probability density function of X . In this book, we heavily rely on such expression of expectation operator in terms of density functions.

A.4.3 Moments of a Random Variable

Let X be a \mathbb{R} -valued random variable defined on a probability space (Θ, Σ, P) , and $Y = g(X) = X^r$ for $r \geq 1$. Since $g(x)$ is continuous, it is Borel-measurable and therefore $Y = X^r$ is a random variable. The expectation of Y is called the **moment of order** r of X , and is denoted $m_r(X)$:

$$m_r(X) = E[X^r] = \int_{-\infty}^{+\infty} x^r \, dF_X(x) = \int_{-\infty}^{+\infty} x^r f_X(x) \, dx.$$

If $X \in L_r(\Theta, \Sigma, P)$, then $m_r(X)$ exists and is finite. If instead we consider $Y = g(X) = (X - m_1(X))^r$, then the expectation of Y is the **central moment of order** r .

A.4.4 Convergence of Random Variables

Let X be a \mathbb{R} -valued random variable and $X_{n \geq 1}$ be a sequence of random variables defined on a probability space (Θ, Σ, P) . The convergence of the sequence X_n to X depends on the way we measure $X - X_n$. Alternatives are:

- **Almost sure** convergence,

$$X_n \xrightarrow{\text{a.s.}} X \quad \text{if} \quad \lim_{n \rightarrow \infty} X_n(\theta) = X(\theta), \quad \forall \theta \in \Theta \setminus N, \quad P(N) = 0.$$

- Convergence in **probability**,

$$X_n \xrightarrow{\text{pr}} X \quad \text{if} \quad \lim_{n \rightarrow \infty} P(|X_n(\theta) - X(\theta)| > \epsilon) = 0, \quad \forall \epsilon > 0.$$

- Convergence in **distribution**,

$$X_n \xrightarrow{\text{d}} X \quad \text{if} \quad \lim_{n \rightarrow \infty} F_{X_n}(x) = F_X(x), \quad \forall x \in \mathbb{R}.$$

- Convergence in L_p ,

$$X_n \xrightarrow{\text{m.p.}} X \quad \text{if} \quad \lim_{n \rightarrow \infty} E[|X_n - X|^p] = 0.$$

We will mostly use the mean square convergence, *i.e.* convergence in L_2 , and denote it as $X_n \xrightarrow{\text{m.s.}} X$.

A.5 Random Vectors

Consider a probability space (Θ, Σ, P) ; the measurable function

$$\mathbf{X}: (\Theta, \Sigma) \mapsto (\mathbb{R}^d, \mathcal{B}^d), \quad d > 1,$$

defines a random vector in \mathbb{R}^d or \mathbb{R}^d -valued random variable, with the induced probability measure

$$Q(B) = P(\mathbf{X} \in B) = P(\mathbf{X}^{-1}(B)).$$

A.5.1 Joint Distribution and Density Functions

The **joint distribution function** of \mathbf{X} is the direct extension of the definition of the random variable distribution function:

$$F_{\mathbf{X}}(\mathbf{x}) = P\left(\bigcap_{i=1}^d \{X_i \leq x_i\}\right), \quad \mathbf{x} = (x_1, \dots, x_d) \in \mathbb{R}^d.$$

The joint distribution function of a random vector \mathbf{X} has the following properties:

$$\lim_{x_k \rightarrow -\infty} F_{\mathbf{X}}(\mathbf{x}) = 0, \quad k = 1, \dots, d,$$

$x_k \mapsto F_{\mathbf{X}}(\mathbf{x})$ is increasing, $k = 1, \dots, d$,

$x_k \mapsto F_{\mathbf{X}}(\mathbf{x})$ is right-continuous, $k = 1, \dots, d$.

In addition,

$$\lim_{x_k \rightarrow +\infty} F_{\mathbf{X}}(\mathbf{x}) = F_{\mathbf{X}_{|k}}(\mathbf{x}_{|k}), \quad 1 \leq k \leq d,$$

is the joint distribution of the \mathbb{R}^{d-1} -valued random vector

$$\mathbf{X}_{|k} = (X_1, \dots, X_{k-1}, X_{k+1}, \dots, X_d).$$

The **joint density function** of the random vector \mathbf{X} , if it exists, is given by:

$$f_{\mathbf{X}}(\mathbf{x}) = \frac{\partial^d F_{\mathbf{X}}(\mathbf{x})}{\partial x_1 \cdots \partial x_d}.$$

The probability that the random vector takes values within the domain $(x_1, x_1 + dx_1] \times (x_d, x_d + dx_d]$, for given infinitesimal vector $\mathbf{dx} = (dx_1, \dots, dx_d)$ is related to the joint density by

$$P\left(\bigcap_{i=1}^d \{X_i \in (x_i, x_i + dx_i]\}\right) \approx f_{\mathbf{X}}(\mathbf{x}) \|\mathbf{dx}\|.$$

From the joint distribution and density, one can derive expressions for the joint density or distribution of a subset of coordinates of \mathbf{X} . Such reduction is known as **marginalization**. For instance, the joint distribution of $\mathbf{X}_{|k}$ is

$$F_{\mathbf{X}_{|k}}(\mathbf{x}_{|k}) = F_{\mathbf{X}}(x_1, \dots, x_{k-1}, \infty, x_{k+1}, \dots, x_d),$$

whereas

$$f_{\mathbf{X}_{|k}}(\mathbf{x}_{|k}) = \int_{-\infty}^{+\infty} f_{\mathbf{X}}(x_1, \dots, x_d) dx_k.$$

In particular, $F_{X_i}(x_i) = F_{\mathbf{X}}(\infty, \dots, \infty, x_i, \infty, \dots, \infty)$ is the **marginal distribution** of X_i and

$$f_{X_i}(x_i) = \int_{\mathbb{R}^{d-1}} f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x}_{|i}$$

is the **marginal density** of X_i .

Another useful expression concerns the **conditional density** of a subset of coordinates of \mathbf{X} . Consider for instance that the coordinates of \mathbf{X} have been split into

two subsets corresponding to two vectors $\mathbf{X}_1 \in \mathbb{R}^{0 < d_1 < d}$ and $\mathbf{X}_2 \in \mathbb{R}^{d-d_1}$. Then the joint density of \mathbf{X}_1 conditioned by $\mathbf{X}_2 = \mathbf{x}_2$ is

$$f_{\mathbf{X}_1|\mathbf{X}_2}(\mathbf{x}_1, \mathbf{x}_2) = \frac{f_{\mathbf{X}}(\mathbf{x}_1, \mathbf{x}_2)}{f_{\mathbf{X}_2}(\mathbf{x}_2)}.$$

The joint density of transformed random vectors can also be derived. Consider a one to one mapping $\mathbf{h} : \mathbf{x} \in \mathbb{R}^d \mapsto \mathbf{y} = \mathbf{h}(\mathbf{x}) \in \mathbb{R}^d$, and define the random vector $\mathbf{Y} = \mathbf{h}(\mathbf{X})$. The joint densities $f_{\mathbf{Y}}$ and $f_{\mathbf{X}}$ are related by

$$f_{\mathbf{Y}}(\mathbf{y}) = f_{\mathbf{X}}(\mathbf{h}^{-1}(\mathbf{y})) \left| \nabla_{\mathbf{y}} \mathbf{h}^{-1} \right|,$$

where \mathbf{h}^{-1} is the inverse mapping and $\nabla_{\mathbf{y}} \mathbf{h}^{-1}$ its Jacobian matrix. This relation can be intuitively derived from the principle of probability conservation. Indeed, denoting $D_{\mathbf{y}}$ a neighborhood of \mathbf{y} and $D_{\mathbf{x}}$ its image by the inverse transformation \mathbf{h}^{-1} , the equality $P(\mathbf{Y} \in D_{\mathbf{y}}) = P(\mathbf{X} \in D_{\mathbf{x}})$ leads to

$$\begin{aligned} P(\mathbf{X} \in D_{\mathbf{x}}) &= \int_{D_{\mathbf{x}}} f_{\mathbf{X}}(\boldsymbol{\eta}) \, d\boldsymbol{\eta} = \int_{D_{\mathbf{y}}} f_{\mathbf{X}}(\mathbf{h}^{-1}(\boldsymbol{\xi})) \left| \nabla_{\boldsymbol{\xi}} \mathbf{h}^{-1} \right| \, d\boldsymbol{\xi} \\ &= \int_{D_{\mathbf{y}}} f_{\mathbf{Y}}(\boldsymbol{\xi}) \, d\boldsymbol{\xi} = P(\mathbf{Y} \in D_{\mathbf{y}}). \end{aligned}$$

A.5.2 Independence of Random Variables

Consider a set of random variables X_i , $i \in I$, defined on a probability space (Θ, Σ, P) . These random variables are **independent** if and only if

$$P(X_i \leq x_i, i \in J) = \prod_{i \in J} P(X_i \leq x_i), \quad \forall J \subset I, x_i \in \mathbb{R}.$$

For finite index set $I = \{1, \dots, d\}$, the collection of random variables can be seen as a random vector \mathbf{X} of \mathbb{R}^d , and the independence implies a factorized structure for the joint distribution $F_{\mathbf{X}}$,

$$F_{\mathbf{X}}(x_1, \dots, x_d) = \prod_{i=1}^d F_{X_i}(x_i),$$

and joint density $f_{\mathbf{X}}$,

$$f_{\mathbf{X}}(x_1, \dots, x_d) = \prod_{i=1}^d f_{X_i}(x_i).$$

A.5.3 Moments of a Random Vector

Consider a random vector \mathbf{X}^d and an integer multi-index $\mathbf{l} = (l_1, \dots, l_d) \in \mathbb{N}^d$. We define $|\mathbf{l}| = \sum_i l_i$, and the function

$$g_{\mathbf{l}} : \mathbf{x} \in \mathbb{R}^d \mapsto g(\mathbf{x}) = \prod_{i=1}^{i=d} x_i^{l_i}. \quad (\text{A.1})$$

The function $g_{\mathbf{l}}(\mathbf{X})$ is a \mathbb{R} -valued random variable. If $\mathbf{X} \in L_{|\mathbf{l}|}$, *i.e.* for each of the vector coordinate $X_i \in L_{l_i}$, then the moments of order $|\mathbf{l}|$ of \mathbf{X} are given by

$$m_{\mathbf{l}}(\mathbf{X}) = \mathbb{E}[g_{\mathbf{l}}(\mathbf{X})]. \quad (\text{A.2})$$

If the coordinates of \mathbf{X} are mutually independent, the moments $m_{\mathbf{l}}$ can be expressed as:

$$m_{\mathbf{l}}(\mathbf{X}) = \mathbb{E}\left[\prod_{i=1}^{i=d} X_i^{l_i}\right] = \prod_{i=1}^{i=d} \mathbb{E}\left[X_i^{l_i}\right] = \prod_{i=1}^{i=d} m_{l_i}(X_i). \quad (\text{A.3})$$

Of particular importance are the mean μ_i of X_i which corresponds to the first-order moment with $l_j = \delta_{ij}$, and the correlation r_{ij} of (X_i, X_j) which is the second-order moment with all $l_k = 0$ except $l_i = l_j = 1$. Combining these first and second moments, we obtain the covariance c_{ij} of (X_i, X_j) ,

$$c_{ij} = \mathbb{E}[(X_i - \mu_i)(X_j - \mu_j)] = r_{ij} - \mu_i \mu_j, \quad (\text{A.4})$$

and the variance σ_i^2 of X_i :

$$\sigma_i^2 = \mathbb{E}[(X_i - \mu_i)^2] = r_{ii} - \mu_i^2 \geq 0. \quad (\text{A.5})$$

If $c_{ij} = 0$ for $i \neq j$, then X_i and X_j are said to be **uncorrelated**. If $r_{ij} = 0$ for $i \neq j$, X_i and X_j are said to be **orthogonal**. The first and second-order moments of a random vector can be summarized using the mean vector \mathbf{m} and correlation \mathbf{r} or covariance \mathbf{c} matrices:

$$\begin{aligned} \mathbf{m} &= \mathbb{E}[\mathbf{X}], \\ \mathbf{r} &= [r_{ij}] = \mathbb{E}[\mathbf{X}\mathbf{X}^t], \\ \mathbf{c} &= [c_{ij}] = \mathbb{E}[(\mathbf{X} - \mathbf{m})(\mathbf{X} - \mathbf{m})^t]. \end{aligned} \quad (\text{A.6})$$

Note that if X_i and X_j are independent, we have

$$c_{ij} = \mathbb{E}[(X_i - \mu_i)(X_j - \mu_j)] = \mathbb{E}[X_i - \mu_i]\mathbb{E}[X_j - \mu_j] = 0. \quad (\text{A.7})$$

In other words, independent random variables are uncorrelated. However, the converse is usually not true: uncorrelated random variables are not independent in general. Also, random vectors with mutually uncorrelated coordinates have diagonal correlation matrices.

A.5.4 Gaussian Vector

The case of Gaussian vector is of particular importance in probability theory and in Polynomial Chaos expansions on Hermite bases. A Gaussian vector of \mathbb{R}^d with mean \mathbf{m} and covariance matrix \mathbf{c} has for joint density function:

$$f_{\mathbf{X}}(\mathbf{x}) = \frac{1}{(2\pi)^{d/2} \sqrt{|\mathbf{c}|}} \exp \left[-\frac{1}{2} (\mathbf{x} - \mathbf{m})^t \mathbf{c}^{-1} (\mathbf{x} - \mathbf{m}) \right], \tag{A.8}$$

where $|\mathbf{c}|$ is the determinant of the correlation matrix. A Gaussian vector is then completely specified by its second-order properties and we shall write

$$\mathbf{X} \sim \mathbf{N}(\mathbf{m}, \mathbf{c}). \tag{A.9}$$

An important property of Gaussian vector is that if \mathbf{c} is diagonal (its coordinate are uncorrelated) then the X_i are mutually independent. Indeed,

$$\begin{aligned} f_{\mathbf{X}}(\mathbf{x}) &= \frac{1}{(2\pi)^{d/2} \sqrt{|\mathbf{c}|}} \exp \left[-\frac{1}{2} \sum_{i=1}^d \sigma_i^{-1} (x_i - \mu_i)^2 \right] \\ &= \prod_{i=1}^d \frac{1}{\sqrt{2\pi \sigma_i^2}} \exp \left[-\frac{1}{2\sigma_i^2} (x_i - \mu_i)^2 \right], \end{aligned} \tag{A.10}$$

because $c_{ii} = \sigma_i^2$ and $|\mathbf{c}| = \prod c_{ii}$ for diagonal matrices. Also, if \mathbf{X} and \mathbf{Y} are two \mathbb{R}^d -valued Gaussian vectors, then $(\alpha\mathbf{X} + \beta\mathbf{Y})$ is a Gaussian random vector.

A.6 Stochastic Processes

A.6.1 Motivation and Basic Definitions

In this monograph, we are interested in the computation of the stochastic solutions of equations, essentially ODEs or PDEs. Therefore these solutions are functions of time and/or space. Then, the notion of random variable and random vector need be extended to incorporate a dependence on time or/and space coordinates.

Consider a function $\mathbf{X} : T \times \Theta \mapsto \mathbb{R}^d$ with arguments –time– $t \in T$ (a real interval) and –event– $\theta \in \Theta$. If $\mathbf{X}(t)$ is a \mathbb{R}^d -valued random vector on the probability space (Θ, Σ, P) for all $t \in T$, then \mathbf{X} is called a \mathbb{R}^d -valued **stochastic process** or vector stochastic process. The function $\mathbf{X}(\cdot, \theta) : t \in T \mapsto \mathbb{R}^d$ for given $\theta \in \Theta$ is called a **sample path** or simply a **realization** of \mathbf{X} . Conversely, the definition shows that $\mathbf{X}(t, \cdot) : \theta \in \Theta \mapsto \mathbb{R}^d$ is a random vector on (Θ, Σ, P) .

The definition can be extended to random vectors indexed by a spatial coordinate. For instance, consider $\mathbf{y} \in \mathcal{D} \subset \mathbb{R}^n$, then $\mathbf{X} : \mathcal{D} \times \Theta \mapsto \mathbf{X} \in \mathbb{R}^d$ is called a \mathbb{R}^d -valued

stochastic field if $\mathbf{X}(\mathbf{y}, \cdot)$ is a random vector for each $\mathbf{y} \in \mathcal{D}$. The function $\mathbf{X}(\cdot, \theta)$ is called a realization of the stochastic field.

The two definitions can be combined and results in **space-time stochastic processes**:

$$\mathbf{X} : T \times \mathcal{D} \times \Theta \mapsto \mathbb{R}^d, \quad \mathbf{X}(t, \mathbf{y}, \cdot) \in (\Theta, \Sigma, P) \quad \forall t \in T, \mathbf{y} \in \mathcal{D}. \quad (\text{A.11})$$

There are noticeable differences between stochastic processes and stochastic fields, arising from oriented nature of time. However, these differences will not appear in the present monograph, and we shall call stochastic processes, or random process, any type of random variable or vector indexed by a deterministic set of coordinates in \mathcal{D} . We shall often rely on the loose terminology of random process. Consequently, we shall denote \mathcal{D} the domain of indexation of the stochastic process, making no distinction between space and time coordinates in $\mathbf{y} \in \mathbb{R}^s$.

In the following, we restrict ourself to stochastic processes $\mathbf{X} : \mathcal{D} \times \Theta \mapsto \mathbb{R}^d$ defined on a probability space (Θ, Σ, P) , with $\mathcal{D} \subset \mathbb{R}$, *i.e.* $n = 1$. The definitions and concepts can be extended to stochastic fields $n \geq 1$, subject to appropriate resolution of some technical difficulties and notation issues.

A.6.2 Properties of Stochastic Processes

If \mathbf{X} is such that

$$\lim_{s \rightarrow t} P(\|\mathbf{X}(s) - \mathbf{X}(t)\| \geq \epsilon) = 0 \quad \forall \epsilon > 0, \quad (\text{A.12})$$

and any $t \in \mathcal{D}$, the process is said **continuous in probability**. If for given integer $p \geq 1$,

$$\lim_{s \rightarrow t} E[\|\mathbf{X}(s) - \mathbf{X}(t)\|^p] = 0, \quad \forall t \in \mathcal{D}, \quad (\text{A.13})$$

the process is said **continuous in the p -th mean**, and **continuous in the mean square sense** in the case of $p = 2$. If

$$P\left(\left\{\theta : \lim_{s \rightarrow t} \|\mathbf{X}(s, \theta) - \mathbf{X}(t, \theta)\| \neq 0\right\}\right) = 0, \quad \forall t \in \mathcal{D}, \quad (\text{A.14})$$

the process is said **almost surely continuous**.

In the previous definitions of continuity, the norm $\|\cdot\|$ is the classical Euclidean norm for vectors. The continuity can also be restricted to particular $t \in \mathcal{D}$ or subintervals.

A.6.2.1 Finite Dimensional Distributions and Densities

Let $m \geq 1$ be an integer, and a set of m distinct points t_i in \mathcal{D} . The **finite dimensional distribution (fdd) of order m** of X is defined by:

$$F_m \left(\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}; t_1, \dots, t_m \right) = P \left(\bigcap_{i=1}^m \{ \mathbf{X}(t_i) \in \times_{k=1}^d (-\infty, x_k^{(i)}] \} \right), \quad (\text{A.15})$$

where $\mathbf{x}^{(i)} = (x_1^{(i)}, \dots, x_d^{(i)}) \in \mathbb{R}^d$. Thus, the finite dimensional distributions, F_m , are probability measures induced by \mathbf{X} on the measurable space $(\mathbb{R}^{m \times d}, \mathcal{B}^{m \times d})$. The first-order fdd of \mathbf{X} at t is called the marginal distribution. It is in fact the distribution of the random vector $\mathbf{X}(t, \cdot)$. For $d = 1$, the m -th order fdd's are

$$F_m(x^{(1)}, \dots, x^{(m)}; t_1, \dots, t_m) = P \left(X(t_1) \leq x^{(1)}, \dots, X(t_m) \leq x^{(m)} \right), \quad (\text{A.16})$$

from which the **finite dimensional densities** of X can be obtained by differentiation:

$$\begin{aligned} f_m \left(x^{(1)}, \dots, x^{(m)}, t_1, \dots, t_m \right) \\ = \frac{\partial^m}{\partial x^{(1)} \dots \partial x^{(m)}} F_m(x^{(1)}, \dots, x^{(m)}; t_1, \dots, t_m). \end{aligned} \quad (\text{A.17})$$

The marginal density of X at time t corresponds to the first-order fdd $f_1(x; t)$.

The \mathbb{R}^d -valued stochastic process is said **stationary in the strict sense** if all its fdd's are invariant under arbitrary shift τ of all the $t_i \rightarrow t_i + \tau$. If \mathbf{X} is stationary, the marginal distribution of \mathbf{X} is t -invariant.

A stochastic process \mathbf{X} is a **Gaussian process** if all its fdd's are Gaussian.

A.6.3 Second Moment Properties

A **second-order stochastic process** \mathbf{X} has all its components $X_i \in L_2(\Theta, \Sigma, P)$ for all $t \in \mathcal{D}$. For a second-order random process, we define

- the mean function: $\bar{\mathbf{x}}(t) = E[\mathbf{X}]$
- the correlation function $\mathbf{r}(t, s) = E[\mathbf{X}(t, \cdot)\mathbf{X}(s, \cdot)^t]$
- the covariance function $\mathbf{c}(t, s) = E[(\mathbf{X}(t, \cdot) - \bar{\mathbf{x}}(t))(\mathbf{X}(s, \cdot) - \bar{\mathbf{x}}(s))^t]$

The **second moment properties** of a stochastic process are given by the couple $(\bar{\mathbf{x}}, \mathbf{r})$ or $(\bar{\mathbf{x}}, \mathbf{c})$. For a stationary process, the mean function $\bar{\mathbf{x}}$ is constant and the correlation and covariance functions depend only on the lag $\tau = t - s$. Conversely, a process with constant mean function and correlation and covariance functions of the form $\mathbf{r}(t, s) = \mathbf{r}(t - s)$ and $\mathbf{c}(t, s) = \mathbf{c}(t - s)$, is said **weakly stationary**. A weakly stationary process is non-necessarily strictly stationary.

The correlation function has the following remarkable properties:

- $r_{ii}(t, s) = r_{ii}(s, t)$. If the process is weakly stationary $r_{ii}(\tau) = r_{ii}(-\tau)$ where $\tau = t - s$.

- $\|r_{ii}(t, s)\|^2 \leq r_{ii}(t, t)r_{ii}(s, s)$. If the process is weakly stationary, $|r_{ii}(\tau)| \leq r_{ii}(0)$.
- $r_{ii}(t, s)$ is positive definite.
- \mathbf{X} is mean square continuous at t' if and only if $r_{ii}(t, s)$ is continuous at $t = s = t'$ for $1 \leq i \leq d$.
- For $i \neq j$, $r_{ij}(t, s) = r_{ji}(s, t)$. If the process is weakly stationary, $r_{ij}(\tau) = r_{ji}(-\tau)$.
- $|r_{ij}(s, t)|^2 \leq r_{ii}(t, t)r_{jj}(s, s)$. If the process is weakly stationary, $|r_{ij}(\tau)|^2 \leq r_{ii}(0)r_{jj}(0)$.

Appendix B

Orthogonal Polynomials

By a system of orthogonal polynomials, we denote a set $\{P_n(x)\}_{n=1}^\infty$, where $P_n(x)$ is a polynomial of degree n . The polynomials are deemed orthogonal in the sense that the inner product

$$\langle P_n P_m \rangle$$

vanishes whenever $n \neq m$.

The variable x may be either continuous or discrete. In the former case, the inner product is defined as:

$$\langle P_n P_m \rangle = \int_a^b P_n(x) P_m(x) w(x) dx \tag{B.1}$$

whereas in the latter it is given by:

$$\langle P_n P_m \rangle = \sum_{i=1}^M P_n(x_i) P_m(x_i) w(x_i). \tag{B.2}$$

In both cases, $w(x)$ is a positive weight function. Note that the limits of integration a and b in (B.1), and the limit M in (B.2) may be either finite or infinite.

We are specifically interested in orthogonal families of polynomials that form a basis of the function space $L_w^2 = \{f : \langle ff \rangle < \infty\}$. Within this general setting, we further focus our attention on families for which expansions of the form:

$$f(x) = \sum_{n=1}^N a_n P_n(x)$$

result, for suitable functions f , in spectra that decay exponentially as $N \rightarrow \infty$.

In this appendix, we provide a brief outline of families of orthogonal polynomials that are frequently used in PC expansions.

B.1 Classical Families of Continuous Orthogonal Polynomials

In this section, we shall focus on the case of “continuous” polynomials defined for on the interval $a \leq x \leq b$. We shall denote by h_n the square of the L^2 norm of P_n , i.e.

$$h_n = \langle P_n P_n \rangle = \alpha \int_a^b P_n^2(x) w(x) dx. \quad (\text{B.3})$$

Note that for applications to PC expansions, it is convenient to adopt the convention that the space L_w^2 has measure one, or alternatively that the norm of the indicator function of the entire space is equal to one, i.e.

$$\int_a^b w(x) dx = 1. \quad (\text{B.4})$$

This amounts to a constant scaling of weights functions that are normally utilized in the definition of orthogonal polynomials.

We also recall [1] that orthogonal polynomials: (a) satisfy the differential equation:

$$g_2(x)P_n'' + g_1(x)P_n' + a_n P_n = 0 \quad (\text{B.5})$$

where g_1 and g_2 are independent of n and the a_n 's are constants that depend on n only; and (b) can be generated using Rodrigues' formula:

$$P_n(x) = \frac{1}{e_n w(x)} \frac{d^n}{dx^n} \{w(x) [g(x)]^n\} \quad (\text{B.6})$$

where g is a polynomial in x that is independent of n and the e_n 's are arbitrary normalization factors that depend on n only. Note that Rodrigues' formula immediately shows that a constant multiplicative scaling of w has no impact on the corresponding representation or normalization.

B.1.1 Legendre Polynomials

The Legendre polynomials, $\{L_n(x), n = 0, 1, \dots\}$, are an orthogonal basis of $L_w^2[-1, 1]$ with respect to the weight function $w(x) = 1/2$ for all $x \in [-1, 1]$. The are typically normalized so that $L_n(1) = 1$, in which case they are given by [26]:

$$L_n(x) = \frac{1}{2^n} \sum_{l=0}^{[n/2]} (-1)^l \binom{n}{l} \binom{2n-2l}{n} x^{n-2l}. \quad (\text{B.7})$$

Here $[n/2]$ denotes the integral part of $n/2$. The polynomials are even when n is even and odd when n is odd.

The Legendre polynomials satisfy the recurrence relation:

$$Le_{n+1}(x) = \frac{2n+1}{n+1}xLe_n(x) - \frac{n}{n+1}Le_{n-1}(x) \quad (\text{B.8})$$

with $Le_0(x) = 1$ and $Le_1(x) = x$. The first seven Legendre polynomials are given by [1, 26]:

$$Le_0(x) = 1,$$

$$Le_1(x) = x,$$

$$Le_2(x) = \frac{1}{2}(3x^2 - 1),$$

$$Le_3(x) = \frac{1}{2}(5x^3 - 3x),$$

$$Le_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3),$$

$$Le_5(x) = \frac{1}{8}(63x^5 - 70x^3 + 15x),$$

$$Le_6(x) = \frac{1}{16}(2313x^6 - 315x^4 + 105x^2 - 5).$$

With the definition of w and the normalization convention specified above, the square norms of the Legendre polynomials are given by [1]:

$$h_n = \langle Le_n, Le_n \rangle = \int_{-1}^1 Le_n^2(x)w(x) dx = \frac{1}{2n+1}. \quad (\text{B.9})$$

They satisfy (B.5) with [1]:

$$g_2(x) = 1 - x^2, \quad g_1(x) = -2x, \quad \text{and} \quad a_n = n(n+1), \quad (\text{B.10})$$

and (B.6) with:

$$g(x) = 1 - x^2, \quad \text{and} \quad e_n = (-1)^n 2^n n!. \quad (\text{B.11})$$

B.1.2 Hermite Polynomials

There are two widespread definitions of the Hermite polynomials, according to whether the weight functions are given by:

$$w(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) \quad (\text{B.12})$$

or

$$w(x) = \frac{1}{\sqrt{\pi}} \exp(-x^2). \quad (\text{B.13})$$

In both cases, x is defined over the real line, i.e. $a = -\infty$ and $b = \infty$.

To distinguish between the two families, we shall use the conventional notation $He_n(x)$ to indicate that (B.12) is used, and $H_n(x)$ to indicate that (B.13) is adopted. Note that in PC expansions, we rely exclusively on He_n , but for completeness and computational convenience (see Appendix C) we address both cases.

For both definitions of w , the Hermite polynomials are conventionally normalized so that the factors appearing in Rodrigues' formula (B.6) are given by [1]:

$$e_n = (-1)^n. \quad (\text{B.14})$$

The functions $g(x)$ appearing in (B.6) are also identical, $g(x) = 1$. It follows that the Hermite families are defined according to [111]:

$$He_n(x) = \frac{1}{(-1)^n \exp(-x^2/2)} \frac{d^n}{dx^n} \left[\exp(-x^2/2) \right], \quad (\text{B.15})$$

$$H_n(x) = \frac{1}{(-1)^n \exp(-x^2)} \frac{d^n}{dx^n} \left[\exp(-x^2) \right]. \quad (\text{B.16})$$

They have the following explicit representations:

$$He_n(x) = n! \sum_{m=0}^{[n/2]} (-1)^m \frac{1}{m! 2^m (n-2m)!} x^{n-2m}, \quad (\text{B.17})$$

$$H_n(x) = n! \sum_{m=0}^{[n/2]} (-1)^m \frac{1}{m!(n-2m)!} (2x)^{n-2m}. \quad (\text{B.18})$$

The polynomials $He_n(x)$ obey (B.5) with:

$$g_2(x) = 1, \quad g_1(x) = -x, \quad \text{and} \quad a_n = n, \quad (\text{B.19})$$

and the recursion relation:

$$He_{n+1}(x) = xHe_n(x) - nHe_{n-1}(x). \quad (\text{B.20})$$

With the standardization above, the square norms of the Hermite polynomials He_n are given by:

$$h_n = \langle He_n, He_n \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} [He_n(x)]^2 \exp(-x^2/2) dx = n!. \quad (\text{B.21})$$

The first seven polynomials $He_n(x)$ are given by:

$$He_0(x) = 1, \quad (\text{B.22})$$

$$He_1(x) = x, \quad (\text{B.23})$$

$$He_2(x) = x^2 - 1, \quad (\text{B.24})$$

$$He_3(x) = x^3 - 3x, \quad (\text{B.25})$$

$$He_4(x) = x^4 - 6x^2 + 3, \quad (\text{B.26})$$

$$He_5(x) = x^5 - 10x^3 + 15x, \quad (\text{B.27})$$

$$He_6(x) = x^6 - 15x^4 + 45x^2 - 15. \quad (\text{B.28})$$

The polynomials $H_n(x)$ obey (B.5) with:

$$g_2(x) = 1, \quad g_1(x) = -2x, \quad \text{and} \quad a_n = 2n, \quad (\text{B.29})$$

and the recursion relation:

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x). \quad (\text{B.30})$$

With the standardization above, the square norms of the Hermite polynomials H_n are given by:

$$h_n = \langle H_n, H_n \rangle = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} [H_n(x)]^2 \exp(-x^2) dx = 2^n n!. \quad (\text{B.31})$$

The first seven polynomials $He_n(x)$ are given by:

$$H_0(x) = 1, \quad (\text{B.32})$$

$$H_1(x) = 2x, \quad (\text{B.33})$$

$$H_2(x) = 4x^2 - 2, \quad (\text{B.34})$$

$$H_3(x) = 8x^3 - 12x, \quad (\text{B.35})$$

$$H_4(x) = 16x^4 - 48x^2 + 12, \quad (\text{B.36})$$

$$H_5(x) = 32x^5 - 160x^3 + 120x, \quad (\text{B.37})$$

$$H_6(x) = 64x^6 - 480x^4 + 720x^2 - 120. \quad (\text{B.38})$$

B.1.3 Laguerre Polynomials

The Laguerre polynomials, $\{L_n(x), n = 0, 1, \dots\}$, are an orthogonal basis of $L_w^2[0, \infty]$ with respect to the weight function $w(x) = \exp(-x)$. They are conventionally normalized so that the factors appearing in Rodrigues' formula (B.6) are given by [1]:

$$e_n = n!. \quad (\text{B.39})$$

The function g appearing in (B.6) is $g(x) = x$. Accordingly, the polynomials La are defined by:

$$La(x) = \frac{1}{n! \exp(-x)} \frac{d^n}{dx^n} (\exp(-x)x^n), \quad (\text{B.40})$$

and admit the following explicit representation:

$$La(x) = \sum_{m=0}^n (-1)^m \frac{n!}{(n-m)!(m!)^2} x^m. \quad (\text{B.41})$$

The polynomials $La_n(x)$ obey (B.5) with:

$$g_2(x) = x, \quad g_1(x) = 1 - x, \quad \text{and} \quad a_n = n, \quad (\text{B.42})$$

and the recursion relation:

$$La_{n+1}(x) = \frac{1}{n+1} [(2n+1-x)La_n(x) - nLa_{n-1}(x)]. \quad (\text{B.43})$$

With the standardization above, the Laguerre polynomials La_n form an orthonormal basis of $L_w^2[0, \infty)$, i.e.

$$\langle La_n, La_m \rangle = \int_0^\infty La_n(x)La_m(x) \exp(-x) dx = \delta_{nm}. \quad (\text{B.44})$$

In particular, the square norm $h_n = 1$. The first six Laguerre polynomials are:

$$La_0(x) = 1, \quad (\text{B.45})$$

$$La_1(x) = -x + 1, \quad (\text{B.46})$$

$$La_2(x) = \frac{1}{2}(x^2 - 4x + 2), \quad (\text{B.47})$$

$$La_3(x) = \frac{1}{6}(-x^3 + 9x^2 - 18x + 6), \quad (\text{B.48})$$

$$La_4(x) = \frac{1}{24}(x^4 - 16x^3 + 72x^2 - 96x + 24), \quad (\text{B.49})$$

$$La_5(x) = \frac{1}{120}(-x^5 + 25x^4 - 200x^3 + 600x^2 - 600x + 120). \quad (\text{B.50})$$

B.2 Gauss Quadrature

In the application of PC methods, one needs in particular to evaluate moments of PC expansions. As further discussed in Appendix C, this task can be generally boiled down to evaluating inner products of one-dimensional polynomials. This section discusses evaluation of these inner products by means of Gauss quadratures which,

due to their high order accuracy, provide efficient means of computing the corresponding integrals.

We focus our attention to the Legendre, Hermite and Laguerre families discussed in the previous section. Accordingly, we are interested in evaluating integrals of polynomial functions defined over the intervals $[-1, 1]$, $(-\infty, \infty)$, and $[0, \infty)$.

B.2.1 Gauss-Legendre Quadrature

The Gauss-Legendre quadrature is based on the following formula:

$$\int_{-1}^1 f(x) dx = \sum_{i=1}^{nq} w_i f(x_i) + R_{nq}, \tag{B.51}$$

where

$$R_{nq} = \frac{2^{2nq+1}(nq!)^4}{(2nq+1)[(2nq)!]^3} f^{(2nq)}(\xi), \quad -1 < \xi < 1. \tag{B.52}$$

Here, nq is the number of collocation points, x_i denote the coordinate of the i -th collocation point, and w_i the corresponding weight. R_n denotes the remainder of the quadrature; it indicates that the formula is exact if the order of the polynomials $No < 2nq$.

The coordinates x_i are the zeros of $Le_{nq}(x)$, and the weights are given by:

$$w_i = \frac{2}{(1-x_i^2)[Le'_{nq}(x_i)]^2}. \tag{B.53}$$

Explicit formulas for the Gauss-Legendre quadrature nodes are not known, and so they must be evaluated numerically.

The GAUSSQ routine available from netlib (<http://netlib.org>) can be used to determine the weights and abscissas appearing in (B.51). Table B.1 provides results using this routine for selected values of nq .

B.2.2 Gauss-Hermite Quadratures

Gauss-Hermite quadratures can be based on the following formula (see [1] p. 890):

$$\int_{-\infty}^{\infty} f(x) \exp(-x^2) dx = \sum_{i=1}^{nq} w_i f(x_i) + R_{nq} \tag{B.54}$$

where nq is the number of collocation points, x_i denote the quadrature nodes and w_i are the corresponding weights. x_i is the i -th zero of the polynomial H_{nq} , and the

Table B.1 Nodes and weights for Gauss-Legendre quadrature for different values of nq

$nq = 5$		$nq = 10$		$nq = 15$	
x_i	w_i	x_i	w_i	x_i	w_i
-0.906180	0.236927E+00	-0.973907	0.666713E-01	-0.987993	0.307532E-01
-0.538469	0.478629E+00	-0.865063	0.149451E+00	-0.937273	0.703660E-01
0.000000	0.568889E+00	-0.679410	0.219086E+00	-0.848207	0.107159E+00
0.538469	0.478629E+00	-0.433395	0.269267E+00	-0.724418	0.139571E+00
0.906180	0.236927E+00	-0.148874	0.295524E+00	-0.570972	0.166269E+00
-	-	0.148874	0.295524E+00	-0.394151	0.186161E+00
-	-	0.433395	0.269267E+00	-0.201194	0.198431E+00
-	-	0.679410	0.219086E+00	0.000000	0.202578E+00
-	-	0.865063	0.149451E+00	0.201194	0.198431E+00
-	-	0.973907	0.666713E-01	0.394151	0.186161E+00
-	-	-	-	0.570972	0.166269E+00
-	-	-	-	0.724418	0.139571E+00
-	-	-	-	0.848207	0.107159E+00
-	-	-	-	0.937273	0.703660E-01
-	-	-	-	0.987993	0.307532E-01

weight w_i is given by:

$$w_i = \frac{2^{nq-1} nq! \sqrt{\pi}}{nq^2 [H_{nq-1}(x_i)]^2}. \tag{B.55}$$

The remainder in the quadrature (B.54) is given by:

$$R_{nq} = \frac{nq! \sqrt{\pi}}{2^n q (2nq)!} f^{(2nq)}(\zeta) \tag{B.56}$$

for some finite ζ . Thus, the formula (B.54) is exact if the polynomial $f(x)$ has degree smaller than $2nq$.

The GAUSSQ routine available from netlib (<http://netlib.org>) can be used to determine the weights and nodes appearing in (B.54). Table B.2 provides results using this routine for selected values of nq .

Note, however, the application of PC methods typically rely on the Hermite family He_n , and so the quadrature in (B.54) does not coincide with to the measure in the corresponding Hilbert space, which can be expressed as:

$$\langle f \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \exp(-x^2/2) dx. \tag{B.57}$$

Table B.2 Gauss nodes and weights for the quadrature in (B.54) for different values of nq

$nq = 5$		$nq = 10$		$nq = 15$	
x_i	w_i	x_i	w_i	x_i	w_i
-2.020183	0.199532E-01	-3.436159	0.764043E-05	-4.499991	0.152248E-08
-0.958572	0.393619E+00	-2.532732	0.134365E-02	-3.669950	0.105912E-05
0.000000	0.945309E+00	-1.756684	0.338744E-01	-2.967167	0.100004E-03
0.958572	0.393619E+00	-1.036611	0.240139E+00	-2.325732	0.277807E-02
2.020183	0.199532E-01	-0.342901	0.610863E+00	-1.719993	0.307800E-01
-	-	0.342901	0.610863E+00	-1.136116	0.158489E+00
-	-	1.036611	0.240139E+00	-0.565070	0.412029E+00
-	-	1.756684	0.338744E-01	0.000000	0.564100E+00
-	-	2.532732	0.134365E-02	0.565070	0.412029E+00
-	-	3.436159	0.764043E-05	1.136116	0.158489E+00
-	-	-	-	1.719993	0.307800E-01
-	-	-	-	2.325732	0.277807E-02
-	-	-	-	2.967167	0.100004E-03
-	-	-	-	3.669950	0.105912E-05
-	-	-	-	4.499991	0.152248E-08

In order to make use of the results above, one can apply the following change of variables:

$$\langle f \rangle = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} g(x) \exp(-x^2) dx \tag{B.58}$$

where $g(x) = f(\sqrt{2}x)$. Consequently, application of the previous quadrature to the above integral immediately results in:

$$\langle f \rangle \simeq \frac{1}{\sqrt{\pi}} \sum_{i=1}^{nq} w_i g(x_i) \tag{B.59}$$

or alternatively,

$$\langle f \rangle \simeq \sum_{i=1}^{nq} w'_i f(x'_i) \tag{B.60}$$

where $w'_i \equiv w_i/\sqrt{\pi}$ and $x'_i \equiv \sqrt{2}x_i$. Equation (B.60) can now be readily used to evaluate moments and products of Hermite polynomials, He_n .

Table B.3 provides values of x'_i and w'_i for selected values of nq .

Note that our earlier observation that the quadrature in (B.54) is exact for polynomials of degree less than $2nq$ still applies to the quadrature in (B.60). In particular,

Table B.3 Gauss nodes and weights for the quadrature in (B.60) for different values of nq

$nq = 5$		$nq = 10$		$nq = 15$	
x'_i	w'_i	x'_i	w'_i	x'_i	w'_i
-2.856970	0.112574E-01	-4.859463	0.431065E-05	-6.363948	0.858965E-09
-1.355626	0.222076E+00	-3.581823	0.758071E-03	-5.190094	0.597542E-06
0.000000	0.533333E+00	-2.484326	0.191116E-01	-4.196208	0.564215E-04
1.355626	0.222076E+00	-1.465989	0.135484E+00	-3.289082	0.156736E-02
2.856970	0.112574E-01	-0.484936	0.344642E+00	-2.432437	0.173658E-01
-	-	0.484936	0.344642E+00	-1.606710	0.894178E-01
-	-	1.465989	0.135484E+00	-0.799129	0.232462E+00
-	-	2.484326	0.191116E-01	0.000000	0.318260E+00
-	-	3.581823	0.758071E-03	0.799129	0.232462E+00
-	-	4.859463	0.431065E-05	1.606710	0.894178E-01
-	-	-	-	2.432437	0.173658E-01
-	-	-	-	3.289082	0.156736E-02
-	-	-	-	4.196208	0.564215E-04
-	-	-	-	5.190094	0.597542E-06
-	-	-	-	6.363948	0.858965E-09

when sufficient quadrature points are provided, (B.60) reproduces the correct norm:

$$\langle He_m^2 \rangle = m!. \tag{B.61}$$

B.2.3 Gauss-Laguerre Quadrature

The Gauss-Laguerre quadrature is based on the following formula:

$$\int_0^\infty f(x) \exp(-x) dx = \sum_{i=1}^{nq} w_i f(x_i) + R_{nq}, \tag{B.62}$$

where

$$R_{nq} = \frac{(nq!)^2}{(2nq)!} f^{(2nq)}(\xi), \quad 0 < \xi < \infty. \tag{B.63}$$

As before, nq is the number of collocation points, while x_i and w_i respectively denote the nodes and weights. From (B.63), it follows immediately that the quadrature (B.62) is exact when the order of the polynomial, f , is smaller than $2nq$.

Table B.4 Nodes and weights for Gauss-Laguerre quadrature for different values of nq

$nq = 5$		$nq = 10$		$nq = 15$	
x_i	w_i	x_i	w_i	x_i	w_i
0.263560	0.521756E+00	0.137793	0.308441E+00	0.093308	0.218235E+00
1.413403	0.398667E+00	0.729455	0.401120E+00	0.492692	0.342210E+00
3.596426	0.759424E-01	1.808343	0.218068E+00	1.215595	0.263028E+00
7.085810	0.361176E-02	3.401434	0.620875E-01	2.269950	0.126426E+00
12.640801	0.233700E-04	5.552496	0.950152E-02	3.667623	0.402069E-01
-	-	8.330153	0.753008E-03	5.425337	0.856388E-02
-	-	11.843786	0.282592E-04	7.565916	0.121244E-02
-	-	16.279258	0.424931E-06	10.120229	0.111674E-03
-	-	21.996586	0.183956E-08	13.130282	0.645993E-05
-	-	29.920697	0.991183E-12	16.654408	0.222632E-06
-	-	-	-	20.776479	0.422743E-08
-	-	-	-	25.623894	0.392190E-10
-	-	-	-	31.407519	0.145652E-12
-	-	-	-	38.530683	0.148303E-15
-	-	-	-	48.026086	0.160059E-19

The coordinates x_i are the zeros of $La_{nq}(x)$, and the weights are given by:

$$w_i = \frac{(nq!)^2 x_i}{(nq + 1)^2 [La_{nq+1}(x_i)]^2}. \tag{B.64}$$

The GAUSSQ routine available from netlib (<http://netlib.org>) can be used to determine the weights and abscissas appearing in (B.62). Table B.4 provides results using this routine for selected values of nq .

B.3 Askey Scheme

As discussed by Xiu and Karniadakis [249], the above families of orthogonal polynomials are members of the so-called Askey scheme of polynomials [6]. The schemes classifies continuous and discrete hypergeometric orthogonal polynomials that obey certain difference and difference equations, and identifies limit relationship between them [117, 203]. The interesting aspect of the Askey family is that the weighting functions associated with some its members corresponds to frequently used probability distributions.

Specifically, in addition to the orthogonal polynomial systems discussed above, the Askey family includes the Jacobi polynomials, which in turn include the Legendre family, as well as the Charlier, Meixner, Krawtchouk and Hahn families of discrete orthogonal polynomials. The weighting functions associated with the Jacobi

polynomials correspond to the beta distribution, whereas the weighting functions of the Charlier, Meixner, Krawtchouk and Hahn families respectively correspond to the Poisson, negative binomial, binomial, and hypergeometric distributions.

For brevity, and since these additional families are not used in the examples provided in the present volume, we restrict ourselves to providing definitions of corresponding polynomials, and outlining the orthogonality relationships that they obey. Implementation of these families into the corresponding Wiener chaos can be readily performed once the orthogonality relationships are exploited to define a suitable inner product, specifically in a similar fashion to the development above.

B.3.1 Jacobi Polynomials

The Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$, $n = 0, 1, \dots$, are an orthogonal family of polynomials over $[-1, 1]$ with respect to the weight function

$$w(x) = (1 - x)^\alpha (1 + x)^\beta.$$

They are typically normalized so that

$$P_n^{(\alpha,\beta)}(1) = \binom{n + \alpha}{n}$$

in which case they are given by [1]:

$$P_n^{(\alpha,\beta)}(x) = \frac{1}{2^n} \sum_{m=0}^n \binom{n + \alpha}{m} \binom{n + \beta}{n - m} (x - 1)^{n-m} (x + 1)^m. \tag{B.65}$$

The Jacobi polynomials satisfy (B.5) with [1]:

$$g_2(x) = 1 - x^2, \quad g_1(x) = \beta - \alpha - (\alpha + \beta + 2)x, \quad \text{and} \quad a_n = n(n + \alpha + \beta + 1), \tag{B.66}$$

the Rodrigues formula (B.6) with:

$$g(x) = 1 - x^2, \quad \text{and} \quad e_n = (-1)^n 2^n n!, \tag{B.67}$$

the orthogonality condition:

$$\begin{aligned} & \int_{-1}^1 P_n^{(\alpha,\beta)}(x) P_m^{(\alpha,\beta)}(x) w(x) dx \\ &= \frac{2^\alpha + \beta + 1}{2n + \alpha + \beta + 1} \frac{\Gamma(n + \alpha + 1)\Gamma(n + \beta + 1)}{n! \Gamma(n + \alpha + \beta + 1)} \delta_{nm}, \end{aligned} \tag{B.68}$$

and the recurrence relation:

$$2(n + 1)(n + \alpha + \beta + 1)(2n + \alpha + \beta) P_{n+1}^{(\alpha,\beta)}(x)$$

$$\begin{aligned}
 &= \left[(2n + \alpha + \beta + 1)(\alpha^2 - \beta^2) + (2n + \alpha + \beta)3x \right] P_n^{(\alpha, \beta)}(x) \\
 &\quad - 2(n + \alpha)(n + \beta)(2n + \alpha + \beta + n) P_{n-1}^{(\alpha, \beta)}(x)
 \end{aligned} \tag{B.69}$$

where $(m)_n = m(m + 1) \cdots (m + n - 1)$ denotes the Pochhammer symbol.

Note that the orthogonality condition (B.68) may be readily used to rescale $w(x)$ so that the resulting space $L_w^2[-1, 1]$ has measure 1, and that the GAUSSQ routine also provides nodes and weights for Gauss-Jacobi quadratures.

B.3.2 Discrete Polynomials

The Charlier, Meixner, Krawtchouk, and Hahn polynomials are respectively denoted by $C_n(x, a)$, $M_n(x; \beta, c)$, $K_n(x; p, N)$, and $Q_n(x; \alpha, \beta, N)$. In all cases, x is discrete variable. For the Hahn and Krawtchouk polynomials, x is defined over the set $\{0, 1, \dots, N\}$, whereas for the Charlier and Meixner polynomials x is defined over the integers $0, 1, \dots$.

As discussed in [117], the Charlier, Meixner, Krawtchouk, and Hahn polynomials may be defined in terms of the hypergeometric series:

$${}_\tau F_s \left(\begin{matrix} a_1, \dots, a_\tau \\ b_1, \dots, b_s \end{matrix} \middle| z \right) \equiv \sum_{k=0}^{\infty} \frac{(a_1)_k \cdots (a_\tau)_k}{(b_1)_k \cdots (b_s)_k} \frac{z^k}{k!}. \tag{B.70}$$

Relevant definitions are summarized Table B.5

The first two polynomials are:

$$C_0(x, a) = 1, \tag{B.71}$$

$$C_1(x, a) = 1 - \frac{x}{a}, \tag{B.72}$$

$$M_0(x; \beta, c) = 1, \tag{B.73}$$

Table B.5 Definition of Charlier, Meixner, Krawtchouk, and Hahn polynomials in terms of hypergeometric series

Polynomial	Definition
Charlier	${}_2F_0 \left(\begin{matrix} -n, -x \\ - \end{matrix} \middle -\frac{1}{a} \right)$
Meixner	${}_2F_1 \left(\begin{matrix} -n, -x \\ \beta \end{matrix} \middle 1 - \frac{1}{c} \right)$
Krawtchouk	${}_2F_1 \left(\begin{matrix} -n, -x \\ -N \end{matrix} \middle \frac{1}{p} \right)$
Hahn	${}_3F_2 \left(\begin{matrix} -n, n + \alpha + \beta + 1, -x \\ \alpha + 1, -N \end{matrix} \middle 1 \right)$

Table B.6 Weights and square norms of the Charlier, Meixner, Krawtchouk, and Hahn polynomials

Polynomial	$w(x)$	h_n
Charlier	$\frac{a^x}{x!}$	$a^{-n} \exp(-a)n!$
Meixner	$\frac{(\beta)_x c^x}{x!}$	$\frac{c^{-n} n!}{(\beta)_n (1-c)^\beta}$
Krawtchouk	$\binom{N}{x} p^x (1-p)^{N-x}$	$\frac{(1)^{-n} n!}{(-N)_n} \left(\frac{1-p}{p}\right)^n$
Hahn	$\binom{\alpha+x}{x} \binom{\beta+N-x}{N-x}$	$\frac{(-1)^n (n+\alpha+\beta+1)_{N+1} (\beta+1)_n n!}{(2n+\alpha+\beta+1)(\alpha+1)_n (-N)_n N!}$

$$M_1(x; \beta, c) = 1 + \frac{x}{\beta} \left(1 - \frac{1}{c}\right), \tag{B.74}$$

$$K_0(x; p, N) = 1, \tag{B.75}$$

$$K_1(x; p, N) = 1 - \frac{x}{Np}, \tag{B.76}$$

$$Q_0(x; \alpha, \beta, N) = 1, \tag{B.77}$$

$$Q_1(x; \alpha, \beta, N) = 1 - \frac{(\alpha + \beta + 2)x}{(\alpha + 1)N}. \tag{B.78}$$

With the definitions above, these families of discrete polynomials satisfy the discrete orthogonality relation:

$$\sum_i f_n(x_i) f_m(x_i) w(x_i) = h_n \delta_{nm} \tag{B.79}$$

where the index i ranges over the entire domain of the discrete variable x . Relevant formulas for the weights, w , and square norms, h_n , are given in Table B.6.

The discrete polynomials satisfy the Rodrigues-type formula:

$$w(x) f_n(x) = r_n \nabla^n [g(x)] \tag{B.80}$$

where $w(x)$ is the weight function, r_n is a normalizing function independent of x , g is a polynomial in x , and ∇ denotes the backward difference operator $\nabla f(x) = f(x) - f(x - 1)$. Relevant formulas for the factors r and g are given in Table B.7.

For computational purposes, polynomial evaluations may be conveniently performed on the basis of recursion relations. Relevant formulas for the Charlier, Meixner, Krawtchouk and Hahn polynomials are given by:

$$aC_{n+1} = (n + a - x)C_n - nC_{n-1}, \tag{B.81}$$

$$c(n + \beta)M_{n+1} = [n + (n + \beta)_c - (c - 1)x] M_n - nM_{n-1}, \tag{B.82}$$

Table B.7 Factors r and g in (B.80) for the Charlier, Meixner, Krawtchouk, and Hahn polynomials

Polynomial	r_n	$g(x)$
Charlier	1	$\frac{a^x}{x!}$
Meixner	1	$\frac{(\beta + n)_x c^x}{x!}$
Krawtchouk	$(1 - p)^{-N}$	$\binom{N - n}{x} \left(\frac{p}{1 - p}\right)^x$
Hahn	$\frac{(-1)^n (\beta + 1)_n}{(-N)_n}$	$\binom{\alpha + n + x}{x} \binom{\beta + N - x}{N - n - x}$

$$p(N - n)K_{n+1} = [p(N - n) + n(1 - p) - x]K_n - n(1 - p)K_{n-1}, \tag{B.83}$$

$$A_n Q_{n+1}(x) = (A_n + D_n - x)Q_n(x) - D_n Q_{n-1}(x) \tag{B.84}$$

where $C_n \equiv C_n(x; a)$, $M_n \equiv M_n(x; \beta, c)$, $K_n \equiv K_n(x; p, N)$, $Q_n(x) \equiv Q_n(x; \alpha, \beta, N)$, and

$$A_n = \frac{(n + \alpha + \beta + 1)(n + \alpha + 1)(N - n)}{(2n + \alpha + \beta + 1)(2n + \alpha + \beta + 2)},$$

$$D_n = \frac{n(n + \alpha + \beta + N + 1)(n + \beta)}{(2n + \alpha + \beta)(2n + \alpha + \beta + 1)}.$$

We finally note that, with the standardizations above, the weighting functions of Charlier, Meixner, Krawtchouk, and Hahn polynomials correspond, up to a scaling factor independent of x , to the probability density functions of the Poisson, negative binomial, binomial, and hypergeometric distributions. The scaling factors can be readily obtained from the orthogonality expressions, and can be used to rescale the standard forms of w to define a suitable inner product, namely one for which the measure of the corresponding ℓ_2 space is unity.

Appendix C

Implementation of Product and Moment Formulas

In the development of computer codes implementing PC expansions, one is faced with the problem of evaluating moments of classical orthogonal polynomials, or more often of multidimensional generalizations of these polynomials. This Appendix outlines the main ingredient of a general approach that has proven to be quite useful in the construction of utility libraries that are capable of performing fundamental operations and nonlinear transformations of PC representations of random variables.

C.1 One-Dimensional Polynomials

For most situations, it is quite advantageous for users to compute and store polynomials appearing in PC expansions. As mentioned in Chapter 2, these expansions involve orthogonal polynomials that are typically defined in terms of series expansions. For computational purposes, however, it is more convenient to evaluate the polynomials recursion relations. As discussed in Appendix B, in the Hermite case, one has

$$\begin{aligned}\psi_0(x) &= 1, \\ \psi_1(x) &= x, \\ \psi_n(x) &= x\psi_{n-1}(x) - (n-1)\psi_{n-2}(x), \quad n = 2, 3, \dots\end{aligned}\tag{C.1}$$

and similar recursion relations exist for orthogonal polynomials that are member of the Askey family. The exploitation of these relationships is recommended whenever possible.

C.1.1 Moments of One-Dimensional Polynomials

We are interested in evaluating second-order moments of the form

$$\langle f \rangle \quad \text{where } f(x) \equiv \psi_i(x)\psi_j(x), \quad (\text{C.2})$$

and more generally in higher-order moments which may be expressed as:

$$\langle f \rangle \quad \text{where } f(x) \equiv \prod_{m=1}^M \psi_{i_m}(x). \quad (\text{C.3})$$

Such moments may be evaluated on the basis of analytical expressions. Alternatively as discussed in Appendix B, Gauss quadratures may be readily applied, and these yield exact values so long as a sufficient number of collocation points is provided, namely to ensure a vanishing remainder.

C.2 Multidimensional PC Basis

As discussed in Chap. 2, in the multidimensional case the PC basis functions are defined from an incomplete tensorization of the corresponding 1D basis functions. As a result, each member of the multidimensional PC basis can be written as a product of 1D polynomials in the appropriate random variable. In order to specify (and hence immediately evaluate) the elements of the multidimensional basis, it is advantageous to associate with each basis function, Ψ_i a multi-index $\alpha^i = (\alpha_1^i, \alpha_2^i, \dots, \alpha_N^i)$, where α_k^i denotes the order of the 1D polynomial in ξ_k . Once these multi-indices are available, evaluation of the multidimensional basis function is straightforward. We illustrate this for the case of the N-dimensional Hermite polynomials. We denote the latter by Ψ_k , in order to distinguish them from, ψ_j , their 1D counterparts.

By definition of the multi-indices, the N-dimensional polynomial chaos can be obtained from:

$$\Psi_k(\xi_1, \xi_2, \dots, \xi_N) = \prod_{i=1}^N \psi_{\alpha_i^k}(\xi_i). \quad (\text{C.4})$$

Thus, knowledge of the multi-indices, together with the 1D basis functions, provides a very efficient and convenient means of evaluating the N-dimensional PCs.

C.2.1 Multi-Index Construction

To complete this construction, one needs to define the multi-indices α^i , $i = 0, \dots, P$. While multiple definitions are possible, we have adopted the same indexing scheme used in [90]. Using this indexing scheme, the multi-indices are defined recursively for arbitrary order, No, and dimension, N, as described in the following pseudo-code:

1. For the 0-th order polynomial, set:

$$\alpha_i^0 = 0, \quad i = 1, \dots, N.$$

Note that if $No = 0$, then we set $P = 0$ and the process is interrupted.

2. For the N first-order polynomials, set:

$$\alpha_j^i = \delta_{ij} \quad \text{for } 1 \leq i, j \leq N.$$

Note that if $No = 1$, then we set $P = N$ and the process is interrupted.

3. Set $P = N$
4. Set $p_i(1) = 1, i = 1, \dots, N$
5. For $k = 2, \dots, No$:
 - Set $L = P$
 - Set $p_i(k) = \sum_{m=i}^N p_m(k-1), i = 1, \dots, N$
 - For $j = 1, \dots, N$:
 - + For $m = L - p_j(k) + 1, \dots, L$:
 - Set $P = P + 1$
 - Set $\alpha_i^P = \alpha_i^m, i = 1, \dots, N$
 - Set $\alpha_j^P = \alpha_j^m + 1$

In this algorithm, for a specific k , L denotes the number of terms that have been constructed so far with order less than k . The terms of order k are then constructed from the terms of order $(k - 1)$ by increasing the order of the factors in those terms belonging to a specific dimension, one at the time. For example, for the three-dimensional stochastic case, there are 6 terms of order 2. The first 6 terms of order 3 are constructed by taking all 6 terms of order 2, and increasing the multi-index corresponding to the order of the first stochastic dimension by 1. The next 3 terms of order 3 are constructed by taking the last 3 terms of order 2, and increasing the order of the contribution of the second stochastic dimension. The last term is obtained by increasing the multi-index corresponding to the third dimension with 1 in the last term of order 2. Investigation of the process shows that the terms at the current order, in which the order of the contribution of dimension j will be increased to get terms at the next order, are the terms that were generated at the current order from the previous order by increasing the order of dimension j . This bookkeeping is done by the $p_i(k)$.

Note that the procedure above also provides the number, P , of N -dimensional Polynomial Chaos of order $\leq No$.

C.2.2 Moments of Multidimensional Polynomials

We are now interested in generalizing the results of the previous section to the N -dimensional case. To this end, we exploit the tensor product construction of

the multidimensional inner product, and again rely on the multi-indices α^i to express the moments of N-dimensional Polynomial Chaos in terms of products of 1-dimensional moments. For instance, the second-order moment $\langle \Psi_i \Psi_j \rangle$ can be expressed as:

$$\langle \Psi_i \Psi_j \rangle_N = \prod_{k=1}^N \langle \psi_{\alpha_k^i} \psi_{\alpha_k^j} \rangle_1 \quad (\text{C.5})$$

where we have used subscripts to distinguish between the inner products in 1D and N-dimensional space. Similarly, for a moment of order M we have

$$\left\langle \prod_{m=1}^M \Psi_{i_m} \right\rangle_N = \prod_{k=1}^N \left\langle \prod_{m=1}^M \psi_{\alpha_k^{i_m}} \right\rangle_1. \quad (\text{C.6})$$

The advantage of this product factorization is that in practice only a few one-dimensional moments need to be actually computed, and this results in order-of-magnitude reduction in the effort required to form the required N-dimensional moments. It also greatly facilitates the computation of moments involving mixed bases, namely those involving tensor products of different families of orthogonal polynomials.

C.2.3 Implementation Details

We conclude with a brief outline of an attractive approach for the implementation of PC computations, especially in the multidimensional case. This approach is based on the establishment of a code infrastructure in which the multi-indices defined in Sect. C.2.1 are computed in a pre-processing step, together with the necessary multidimensional moments, namely those appearing in the definition of multiplication tensors used to evaluate products and other nonlinear transformations (see Sect. 4.5). As can be anticipated, it is generally advantageous to compute and store these tensors in a pre-processing step. One should particularly seek to take advantage of the sparse nature of these tensors, namely by storing (and using) only the non-vanishing entries of these tensors. Once properly defined in this compact format, these “transformation” tensors can be used as a basis for the construction of utility libraries that implement various transformations of PC representations.

The approach outlined above in fact forms the basis of the UQ toolkit,¹ which constitutes one incarnation of a PC-utility-library software infrastructure.

¹B.J. Debusschere *et al.*, <http://www.sandia.gov/UQToolkit/>.

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