

# Gaussian Hilbert Spaces and Homogeneous Chaos: From theory to applications

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## Abstract

The goal of this brief note is to present the classical theory of homogeneous chaos decomposition of square integrable random variables and provide a clear connection to the practical applications of the theory.

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## 1 Introduction

Most books and papers dealing with homogeneous chaos either deal primarily with deeply theoretical aspects or focus exclusively on application. The goal of this brief note is to fill the gap by providing a survey of the classical theory and then a precise transition to the applications of the classical theory as it appears in numerous engineering articles. The presentation of the classical theory follows [4] mostly. The recent work

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in [2] was consulted also while writing this note. There is a large body of literature on the practical applications of polynomial chaos expansions. We mention here the recent book [5] and the references therein for recent advances in applications of polynomial chaos expansions and related topics.

## 2 Basic notation

In what follows we consider a probability space  $(\Omega, \mathcal{F}, P)$ , where  $\Omega$  is a sample space,  $\mathcal{F}$  is an appropriate  $\sigma$ -algebra on  $\Omega$  and  $P$  is a probability measure. A real valued random variable  $X$  on  $(\Omega, \mathcal{F}, P)$  is an  $\mathcal{F}/\mathcal{B}(\mathbb{R})$ -measurable mapping  $X : (\Omega, \mathcal{F}, P) \rightarrow (\mathbb{R}, \mathcal{B}(\mathbb{R}))$ . The expectation of a random variable  $X$  is denoted by,

$$E[X] := \int_{\Omega} X(\omega) dP(\omega).$$

$L^2(\Omega, \mathcal{F}, P)$  denotes the Hilbert space of (equivalence classes) of real valued square integrable random variables on  $\Omega$ :

$$L^2(\Omega, \mathcal{F}, P) = \{X : \Omega \rightarrow \mathbb{R} : \int_{\Omega} |X(\omega)|^2 dP(\omega) < \infty\}.$$

with inner product,  $\langle X, Y \rangle = E[XY] = \int_{\Omega} XY dP$  and norm  $\|X\|_2 = \langle X, X \rangle^{1/2}$ .

We denote by  $\xrightarrow{L^2}$  convergence in  $L^2$ , by  $\xrightarrow{P}$  convergence in probability, and by  $\xrightarrow{D}$  convergence in distribution. For more on different modes of convergence of random variables see for example [6] or [1].

## 3 Gaussian Hilbert Spaces

**Definition 3.1** (Gaussian linear space). *A linear subspace of  $L^2(\Omega, \mathcal{F}, P)$  consisting of zero-mean Gaussian random variables is called a Gaussian linear space.*

**Definition 3.2** (Gaussian Hilbert space). *A Gaussian Hilbert space is a complete Gaussian linear space. Equivalently, a Gaussian Hilbert space is a closed subspace of  $L^2(\Omega, \mathcal{F}, P)$  consisting of centered (zero mean) Gaussian random variables.*

The following result shows that we loose no generality if we restrict our attention to Gaussian Hilbert spaces[4].

**Lemma 3.3.** *Let  $\mathcal{H} \subset L^2(\Omega, \mathcal{F}, P)$  be a Gaussian linear space and let  $\overline{\mathcal{H}}$  denotes its closure in  $L^2(\Omega, \mathcal{F}, \mu)$ . Then,  $\overline{\mathcal{H}}$  is a Gaussian Hilbert space.*

*Proof.* Let  $\xi \in \overline{\mathcal{H}}$ . Then, there exists a sequence  $\{\xi_n\} \in \mathcal{H}$  such that,  $\xi_n \xrightarrow{L^2} \xi$ . First note that since  $E[\xi_n] = 0$  for all  $n$ , it follows that  $E[\xi] = 0$ , because

$$E[\xi_n - \xi] = \int_{\Omega} \xi_n - \xi dP \leq \int_{\Omega} |\xi_n - \xi| dP \leq \left( \int_{\Omega} |\xi_n - \xi|^2 \right)^{1/2} \rightarrow 0, \quad \text{as } n \rightarrow \infty.$$

Next, let  $\sigma^2 = \|\xi\|_2^2 = E[\xi^2] = \text{Var}[\xi]$ . We have,  $\sigma_n^2 = \|\xi_n\|_2^2 \rightarrow \|\xi\|_2^2 = \sigma^2$  as  $n \rightarrow \infty$ . Thus, we have  $\xi_n \sim N(0, \sigma_n^2) \xrightarrow{D} N(0, \sigma^2)$ . On the other hand, from  $\xi_n \xrightarrow{L^2} \xi$  it immediately follows that  $\xi_n \xrightarrow{D} \xi$  (convergence in  $L^2$  implies convergence in probability and convergence in probability implies convergence in distribution). Therefore,  $\xi \sim N(0, \sigma^2)$ .  $\square$

### 3.1 Examples of Gaussian Hilbert spaces

The following examples cover the cases that will be visited in this note. For a more complete set of examples see [4].

**Example 3.4.** Let  $\xi \sim N(0, 1)$ . Then,  $\text{Span}\{\xi\} = \{c\xi : c \in \mathbb{R}\}$  is a Gaussian Hilbert space.

**Example 3.5.** Let  $\xi_j \stackrel{iid}{\sim} N(0, 1)$  for  $j = 1, \dots, M$ . Then,  $\text{Span}\{\xi_1, \dots, \xi_M\}$  is a Gaussian Hilbert space.

**Example 3.6.** Let  $\{\xi_j\}_1^\infty$  be a countable set of independent  $N(0, 1)$  random variables. Then, the closed linear span,

$$\overline{\text{Span}\{\xi_j\}_1^\infty} = \left\{ \sum_k c_k \xi_k : \sum_j c_j^2 < \infty \right\}$$

is a Gaussian Hilbert space.

## 4 Polynomial spaces

Let  $\mathcal{H}$  be a Gaussian linear space. For  $n \geq 0$  define,

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

Since Gaussian random variables have moments of all orders and mixed moments of products of independent Gaussian random variables is the product of the individual moments, it follows that  $\mathcal{P}_n(\mathcal{H})$  is a linear subspace of  $L^2(\Omega, \mathcal{F}, P)$  for every  $n \geq 0$ . We denote by  $\overline{\mathcal{P}_n(\mathcal{H})}$  the closure of  $\mathcal{P}_n(\mathcal{H})$  with respect of the  $L^2(\Omega, \mathcal{F}, P)$  norm.

**Remark 4.1.** We note the following:

- $\mathcal{P}_0(\mathcal{H}) = \overline{\mathcal{P}_0(\mathcal{H})}$  consists of a.s. constant functions in  $L^2(\Omega, \mathcal{F}, P)$ .
- Elements of  $\mathcal{P}_1(\mathcal{H})$  and  $\overline{\mathcal{P}_1(\mathcal{H})}$  are Gaussian.
- $\{\overline{\mathcal{P}_n(\mathcal{H})}\}_0^\infty$  is a strictly increasing family of subspaces of  $L^2(\Omega, \mathcal{F}, P)$ .

Now, define the spaces  $\mathcal{H}_n$  as follows,

$$\mathcal{H}_0 = \overline{\mathcal{P}_0(\mathcal{H})} \\ \mathcal{H}_n = \overline{\mathcal{P}_n(\mathcal{H})} \cap \overline{\mathcal{P}_{n-1}(\mathcal{H})}^\perp, \quad n \geq 0.$$

Then, we have

$$\bigoplus_0^n \mathcal{H}_k = \overline{\mathcal{P}_n(\mathcal{H})},$$

and

$$\bigoplus_0^\infty \mathcal{H}_k = \overline{\bigcup_0^\infty \mathcal{P}_n(\mathcal{H})}.$$

**Theorem 4.2** (Cameron-Martin). Let  $\mathcal{H}$  be a Gaussian Hilbert space. The spaces  $\{\mathcal{H}_n\}_0^\infty$  form a sequence of closed and pairwise orthogonal subspaces of  $L^2(\Omega, \mathcal{F}, P)$  such that

$$\bigoplus_0^\infty \mathcal{H}_n = L^2(\Omega, \sigma(\mathcal{H}), P).$$

## 5 Chaos expansion

Let  $\mathcal{H}$  be a Gaussian Hilbert space and define

$$\Pi_k : L^2(\Omega, \mathcal{F}, P) \rightarrow \mathcal{H}_k$$

be the orthogonal projection of  $L^2(\Omega, \mathcal{F}, P)$  onto  $\mathcal{H}_k$ . Then, given a random variable  $\varphi \in L^2(\Omega, \sigma(\mathcal{H}), P)$  we have,

$$\varphi = \sum_{k=0}^{\infty} \Pi_k(\varphi),$$

where the sum converges in the  $L^2(\Omega, \sigma(\mathcal{H}), P)$  sense.

**Remark 5.1.** *If  $X \in L^2(\Omega, \mathcal{F}, P)$  then, the sum*

$$\sum_{k=0}^{\infty} \Pi_k(X),$$

*converges in  $L^2(\Omega, \mathcal{F}, P)$  and its limit is the orthogonal projection of  $X$  onto  $L^2(\Omega, \sigma(\mathcal{H}), P)$ .*

**Remark 5.2.** *In view of the previous remark, we can consider the expansion*

$$\sum_{k=0}^{\infty} \Pi_k(X) \tag{5.1}$$

*of a random variable  $X \in L^2(\Omega, \mathcal{F}, P)$  as conditional expectation  $E[X|\mathcal{V}]$ , where  $\mathcal{V} = \sigma(\mathcal{H})$ . Intuitively, this says that the expansion (5.1) is our best approximation of  $X$  based on information available in  $\sigma(\mathcal{H})$ . For more on the notion of conditional expectation which is a fundamental concept in theory of stochastic processes, see for example [6].*

## 6 Applications

Here we consider the application of polynomial chaos expansions in models involving a physical system with finitely many random parameters. The physical response of the system at a given time is then a random variable in  $(\Omega, \sigma(\mathcal{H}), P)$ , where  $\mathcal{H} = \text{Span}\{\xi_1, \dots, \xi_M\}$  as in Example 3.5. In what follows, we will use the notation,  $\boldsymbol{\xi}(\omega) = (\xi_1(\omega), \dots, \xi_M(\omega))$ .

### 6.1 Cameron-Martin Theorem for the case of finite stochastic dimension

Here we proceed systematically and apply Theorem 4.2 to the case where  $\mathcal{H} = \text{Span}\{\xi_1, \dots, \xi_M\}$ . Note that the spaces  $\mathcal{P}_n(\mathcal{H})$  are finite-dimensional and hence closed in this case. In fact,

$$\mathcal{P}_n(\mathcal{H}) = \{p(\boldsymbol{\xi}) : p \text{ is a polynomial of degree at most } n \text{ in } \boldsymbol{\xi}\}.$$

The spaces  $\mathcal{H}_n = \mathcal{P}_n(\mathcal{H}) \cap \mathcal{P}_{n-1}(\mathcal{H})^\perp$  are defined as before except since we are working with closed subspaces here denoting closure of the spaces would be superfluous. Then, by Theorem 4.2,

$$L^2(\Omega, \sigma(\{\xi_j\}_1^M), P) = \bigoplus_0^{\infty} \mathcal{H}_k.$$

An orthonormal basis of  $\mathcal{H}_k$  is given by [5]:

$$\{\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) : |\boldsymbol{\alpha}| = k\},$$

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where  $\alpha = (\alpha_1, \dots, \alpha_M) \in \mathbb{Z}_{\geq 0}^M$  is a multi-index (here  $\mathbb{Z}_{\geq 0}$  denotes the set of nonnegative integers),  $|\alpha| = \sum_j \alpha_j$ , and

$$\Psi_{\alpha}(\xi) = \prod_{j=1}^M \psi_{\alpha_j}(\xi_j),$$

with  $\psi_i$  the one-dimensional normalized Hermite polynomial of order  $i$ .

Then, given a random variable  $\varphi \in L^2(\Omega, \sigma(\mathcal{H}), P)$ , we have

$$\varphi = \sum_0^{\infty} \Pi_k(\varphi) \tag{6.1}$$

with  $\Pi_k$  the orthogonal projection of  $L^2(\Omega, \sigma(\mathcal{H}), P)$  onto  $\mathcal{H}_k$ . For  $p \geq 0$ , let  $\varphi_p$  be given by,

$$\varphi_p = \sum_{|\alpha| \leq p} c_{\alpha} \Psi_{\alpha}(\xi) \tag{6.2}$$

$$= c_0 + \sum_{|\alpha|=1} c_{\alpha} \Psi_{\alpha}(\xi) + \sum_{|\alpha|=2} c_{\alpha} \Psi_{\alpha}(\xi) + \dots + \sum_{|\alpha|=p} c_{\alpha} \Psi_{\alpha}(\xi). \tag{6.3}$$

Then (6.1) says that

$$\varphi = \lim_{p \rightarrow \infty} \varphi_p.$$

Of course in practice  $p$  does not go to infinity and we will work with a truncated chaos expansion  $\varphi_p$ , which we call an expansion of order  $p$ . The number of terms in a truncated expansion is given by,

$$\sum_{s=0}^p \#\{\alpha \in \mathbb{Z}_{\geq 0}^M : |\alpha| = s\},$$

where we use  $\#$  to denote the number of elements in a finite set.

**Lemma 6.1.** *Let  $p$  be a positive integer. The following identity holds.*

$$\sum_{s=0}^p \#\{\alpha \in \mathbb{Z}_{\geq 0}^M : |\alpha| = s\} = \frac{(M+p)!}{M!p!}.$$

*Proof.* First note that for an integer  $a \geq 0$ , it is straightforward to show that

$$\sum_{s=0}^p \binom{a+s}{s} = \binom{a+p+1}{p}.$$

Thus, by the well known formula [3],

$$\#\{\alpha \in \mathbb{Z}_{\geq 0}^M : |\alpha| = s\} = \binom{M+s-1}{s},$$

we have,

$$\sum_{s=0}^p \#\{\alpha \in \mathbb{Z}_{\geq 0}^M : |\alpha| = s\} = \sum_{s=0}^p \binom{M+s-1}{s} = \binom{M+p}{p} = \frac{(M+p)!}{p!M!}. \quad \square$$

Thus, by the above result, we can rewrite (6.2) as follows,

$$\varphi_p = \sum_{k=0}^P a_k \Psi_k(\xi), \tag{6.4}$$

where  $P$  satisfies,

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

and there is a one-to-one correspondence between the coefficients  $a_k$  in (6.4) and  $c_\alpha$  in (6.2). A carefully constructed indexing scheme suitable for purposes of programming can be found in [5].

Moreover, we note that the zero order polynomial  $\Psi_0 \equiv 1$ , and thus one may write,

$$\varphi_p = a_0 + \sum_{k=1}^P a_k \Psi_k(\boldsymbol{\xi}).$$

Next, since  $\varphi_p$  is  $\sigma(\{\xi_1, \dots, \xi_M\})$ -measurable, there exists<sup>1</sup> a Borel function  $\phi$  such that  $\varphi_p(\omega) = \phi(\xi_1(\omega), \dots, \xi_M(\omega))$ , that is,

$$\varphi_p(\omega) = \phi(\boldsymbol{\xi}(\omega)) = a_0 + \sum_{k=1}^P a_k \Psi_k(\boldsymbol{\xi}(\omega)).$$

**Remark 6.2.** We note that since  $\xi_j \stackrel{iid}{\sim} N(0, 1)$  for  $j = 1, \dots, M$ , it follows that their joint probability density function,  $f_\xi$  is the product of the probability density for a standard normal random variable. We denote the joint distribution function of  $\boldsymbol{\xi}$  by  $F_\xi$ . In applications, instead of working in the abstract probability space  $(\Omega, \mathcal{F}, P)$  one often works in the image probability space  $(\mathbb{R}^M, \mathcal{B}(\mathbb{R}^M), F_\xi)$ .

This latter representation is the most common way of writing a chaos expansion in engineering literature.

Finally, we note that the solution of a dynamical system with  $M$  random parameters is a stochastic process  $X(t, \boldsymbol{\xi}(\omega))$ , which we will approximate by a truncated chaos expansion as follows:

$$X(t, \boldsymbol{\xi}) \doteq \sum_{k=0}^P a_k(t) \Psi_k(\boldsymbol{\xi}).$$

Using orthogonality of  $\Psi_k$ 's and  $E[\Psi_k(\boldsymbol{\xi})] = 0$ , it is immediate to note that the approximate mean and variance of  $X$  over time are given by

$$\widehat{\mu}_X(t) = E \left[ \sum_{k=0}^P a_k(t) \Psi_k(\boldsymbol{\xi}) \right] = \left\langle \sum_{k=0}^P a_k(t) \Psi_k(\boldsymbol{\xi}), 1 \right\rangle = a_0(t),$$

and

$$\begin{aligned} \widehat{\sigma}_X^2(t) &= E \left[ \left[ \sum_{k=0}^P a_k(t) \Psi_k(\boldsymbol{\xi}) \right]^2 \right] - E \left[ \sum_{k=0}^P a_k(t) \Psi_k(\boldsymbol{\xi}) \right]^2 \\ &= E \left[ \left[ \sum_{k=0}^P a_k(t) \Psi_k(\boldsymbol{\xi}) \right]^2 \right] - a_0(t)^2 \\ &= \sum_{k=1}^P a_k^2(t) E[\Psi_k^2]. \end{aligned}$$

Moreover, if we have chaos expansions for  $X(t, \boldsymbol{\xi})$  and  $Y(t, \boldsymbol{\xi})$ ,

$$X(t, \boldsymbol{\xi}) \doteq \sum_{k=0}^P x_k(t) \Psi_k(\boldsymbol{\xi}), \quad Y(t, \boldsymbol{\xi}) \doteq \sum_{k=0}^P y_k(t) \Psi_k(\boldsymbol{\xi}),$$

<sup>1</sup>This is due to a basic result from probability theory which sometimes is called the Doob's Dynkin Lemma.

then an approximation to covariance of  $X$  and  $Y$  over time is given by

$$\begin{aligned} \text{cov}(X, Y)(t) &= \mathbb{E} \left( (X(t, \cdot) - \mathbb{E}[X(t, \cdot)]) (Y(t, \cdot) - \mathbb{E}[Y(t, \cdot)]) \right) \\ &\doteq \sum_{k=1}^P x_k(t) y_k(t) \mathbb{E}[\Psi_k^2]. \end{aligned}$$

## 6.2 Random dynamical systems

Consider the autonomous ODE system,

$$\begin{cases} \dot{\mathbf{X}} = F(\mathbf{X}), \\ \mathbf{X}(0) = \mathbf{X}_0, \end{cases} \quad (6.5)$$

where the solution  $\mathbf{X}$  of the system is a function  $\mathbf{X} : [0, T_{fin}] \rightarrow \mathbb{R}^n$ :

$$\mathbf{X}(t) = [X^1(t), \dots, X^n(t)]^T.$$

Assuming the right-hand-side function  $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$  is Lipschitz continuous,  $\mathbf{X}$  exists and is unique. We consider the case, where we have parametric uncertainty in the right-hand-side function  $F$ , that is  $F = F(\mathbf{X}, \boldsymbol{\xi})$ , where  $\boldsymbol{\xi} = (\xi_1, \dots, \xi_M)$  with  $\xi_j \stackrel{iid}{\sim} N(0, 1)$ . Hence, the solution to (6.5) is a stochastic process,

$$\mathbf{X} : [0, T_{fin}] \times (\Omega, \sigma(\{\xi_j\}_1^M), P) \rightarrow \mathbb{R}^n.$$

We can rewrite (6.5) more precisely as below,

$$\begin{cases} \dot{\mathbf{X}}(t, \boldsymbol{\xi}) = F(\mathbf{X}(t, \boldsymbol{\xi}), \boldsymbol{\xi}) \\ \mathbf{X}(0, \boldsymbol{\xi}) = \mathbf{X}_0, \quad a.s. \end{cases} \quad (6.6)$$

To capture the distribution of  $X^i(t, \boldsymbol{\xi})$  at a given time, we will rely on the truncated polynomial chaos PC expansion,

$$X^i(t, \boldsymbol{\xi}) \doteq \sum_{k=0}^P c_k^i(t) \Psi_k(\boldsymbol{\xi}).$$

## 6.3 Two major paradigms in applications of polynomial chaos expansion

Here we describe two general strategies in using PC expansions when dealing with dynamical systems with random parameters. The first method, which is known as the *intrusive method* involves inserting the PC expansion in the dynamical system and solving for the PC coefficients using a reformulated (and larger) dynamical system. The reformulated system is obtained via process of Galerkin projection into the PC basis.

The second method, which is known as the *non-intrusive method* or *non-intrusive spectral projection* (NISP) does not require a reformulation of the original problem; instead, we solve the dynamical system for a relatively small (especially in low stochastic dimension) number of realizations of the random parameters and use the realizations of the solution to project the solution into a PC basis. We illustrate and discuss these two methods in the context of a simple predator prey model as described below.

#### 6.4 A model problem

Consider a classic predator prey model:

$$\begin{cases} \dot{X} = \alpha X - \beta XY \\ \dot{Y} = -\gamma Y + \delta XY \end{cases} \quad (6.7)$$

Here  $X$  and  $Y$  denote the populations of the prey and the predator over time. We let randomness enter the system through the parameters  $\alpha$  and  $\gamma$ . The stochastic parameters space is then a two dimensional space parameterized by the random vector  $\boldsymbol{\xi} = (\xi_1, \xi_2)$  with  $\xi_1$  and  $\xi_2$  standard normal random variables. We let,

$$\alpha(\boldsymbol{\xi}) = a_1 + b_1 \xi_1, \quad \text{and} \quad \gamma(\boldsymbol{\xi}) = a_2 + b_2 \xi_2.$$

The initial conditions are assumed to be deterministic in this problem:

$$X(0) = X_0, \quad Y(0) = Y_0.$$

#### 6.5 The intrusive method

We use the approximation to  $X$  and  $Y$  through truncated PC expansions:

$$X(t, \boldsymbol{\xi}) = \sum_{k=0}^P X_k(t) \Psi_k(\boldsymbol{\xi}), \quad (6.8)$$

$$Y(t, \boldsymbol{\xi}) = \sum_{k=0}^P Y_k(t) \Psi_k(\boldsymbol{\xi}), \quad (6.9)$$

The goal is to solve for the modes  $X_k$  and  $Y_k$  in the above expansions.

We insert (6.8) into the first equation of (6.7):  $\dot{X} = \alpha(\boldsymbol{\xi})X - \beta XY$  :

$$\sum_{k=0}^P \dot{X}_k(t) \Psi_k(\boldsymbol{\xi}) = \alpha(\boldsymbol{\xi}) \sum_{k=0}^P X_k(t) \Psi_k(\boldsymbol{\xi}) - \beta \left( \sum_{j=0}^P X_j(t) \Psi_j(\boldsymbol{\xi}) \right) \left( \sum_{k=0}^P Y_k(t) \Psi_k(\boldsymbol{\xi}) \right) \quad (6.10)$$

Now we take the inner product of both sides of the above equation with  $\Psi_i$  for  $i = 0, \dots, k$ :

Left hand side:

$$\left\langle \sum_{k=0}^P \dot{X}_k(t) \Psi_k(\boldsymbol{\xi}), \Psi_i(\boldsymbol{\xi}) \right\rangle = \dot{X}_i \langle \Psi_i(\boldsymbol{\xi}), \Psi_i(\boldsymbol{\xi}) \rangle = \dot{X}_i \mathbb{E} [\Psi_i^2(\boldsymbol{\xi})]. \quad (6.11)$$

Right hand side:

$$\left\langle \alpha(\boldsymbol{\xi}) \sum_{k=0}^P X_k(t) \Psi_k(\boldsymbol{\xi}), \Psi_i(\boldsymbol{\xi}) \right\rangle - \left\langle \beta \sum_{j,k=0}^P X_j(t) Y_k \Psi_j(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi}), \Psi_i(\boldsymbol{\xi}) \right\rangle$$

Using  $\alpha(\boldsymbol{\xi}) = a_1 + b_1 \xi_1$ , we have

$$\left\langle \alpha(\boldsymbol{\xi}) \sum_{k=0}^P X_k(t) \Psi_k(\boldsymbol{\xi}), \Psi_i(\boldsymbol{\xi}) \right\rangle = a_1 X_i(t) \mathbb{E} [\Psi_i^2(\boldsymbol{\xi})] + b_1 \sum_{k=0}^P X_k(t) \mathbb{E} [\xi_1 \Psi_i(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi})]$$

On the other hand,

$$\left\langle \beta \sum_{j,k=0}^P X_j(t) Y_k \Psi_j(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi}), \Psi_i(\boldsymbol{\xi}) \right\rangle = \beta \sum_{j,k=0}^P X_j(t) Y_k(t) \mathbb{E} [\Psi_i(\boldsymbol{\xi}) \Psi_j(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi})]$$

Thus, the right hand side of (6.10) is given by,

$$a_1 X_i(t) \mathbb{E} [\Psi_i^2(\boldsymbol{\xi})] + b_1 \sum_{k=0}^P X_k(t) \mathbb{E} [\xi_1 \Psi_i(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi})] - \beta \sum_{j,k=0}^P X_j(t) Y_k(t) C_{ijk}, \quad (6.12)$$

where

$$C_{ijk} = \mathbb{E} [\Psi_i(\boldsymbol{\xi}) \Psi_j(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi})].$$

Putting (6.11) and (6.12) together, we get:

$$\dot{X}_i \mathbb{E} [\Psi_i^2(\boldsymbol{\xi})] = a_1 X_i(t) \mathbb{E} [\Psi_i^2(\boldsymbol{\xi})] + b_1 \sum_{k=0}^P X_k(t) \mathbb{E} [\xi_1 \Psi_i(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi})] - \beta \sum_{j,k=0}^P X_j(t) Y_k(t) C_{ijk},$$

Therefore, we get

$$\dot{X}_i = a_1 X_i(t) + \frac{b_1}{\mathbb{E} [\Psi_i^2(\boldsymbol{\xi})]} \sum_{k=0}^P X_k(t) \mathbb{E} [\xi_1 \Psi_i(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi})] - \frac{\beta}{\mathbb{E} [\Psi_i^2(\boldsymbol{\xi})]} \sum_{j,k=0}^P X_j(t) Y_k(t) C_{ijk},$$

Through a similar calculation we get,

$$\dot{Y}_i = -a_2 Y_i(t) - \frac{b_2}{\mathbb{E} [\Psi_i^2(\boldsymbol{\xi})]} \sum_{k=0}^P Y_k(t) \mathbb{E} [\xi_1 \Psi_i(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi})] + \frac{\delta}{\mathbb{E} [\Psi_i^2(\boldsymbol{\xi})]} \sum_{j,k=0}^P X_j(t) Y_k(t) C_{ijk},$$

Therefore, to solve for the modes  $X_i$  and  $Y_i$  in the PC expansions  $X$  and  $Y$  we need to solve the following coupled system of  $2(P+1)$  equations (here  $P+1 = \frac{(2+p)!}{2!p!}$  where  $p$  is the polynomial order of the expansion):

$$\begin{cases} \dot{X}_i = a_1 X_i(t) + \frac{b_1}{\mathbb{E} [\Psi_i^2(\boldsymbol{\xi})]} \sum_{k=0}^P X_k(t) \mathbb{E} [\xi_1 \Psi_i(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi})] - \frac{\beta}{\mathbb{E} [\Psi_i^2(\boldsymbol{\xi})]} \sum_{j,k=0}^P X_j(t) Y_k(t) C_{ijk}, \\ \dot{Y}_i = -a_2 Y_i(t) - \frac{b_2}{\mathbb{E} [\Psi_i^2(\boldsymbol{\xi})]} \sum_{k=0}^P Y_k(t) \mathbb{E} [\xi_1 \Psi_i(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi})] + \frac{\delta}{\mathbb{E} [\Psi_i^2(\boldsymbol{\xi})]} \sum_{j,k=0}^P X_j(t) Y_k(t) C_{ijk}, \end{cases}$$

The initial conditions are given by

$$\begin{cases} X_0(0) = a_1, X_1(0) = b_1, X_2(0) = 0, \dots, X_P(0) = 0, \\ Y_0(0) = a_2, Y_1(0) = b_2, Y_2(0) = 0, \dots, Y_P(0) = 0. \end{cases}$$

Note that the reformulated system of the intrusive method is much larger and a lot more complex than the original system. The main take home message here is that we need to solve this system only once so we get the coefficients  $X_k$  and  $Y_k$  of the chaos expansions for  $X$  and  $Y$ ; we can then sample the expansion of  $X$  and  $Y$  as many times as we would like at a very cheap computational cost.

On the other hand, a naive Monte-Carlo approach would require solving the original (deterministic) dynamical system for a large collection (say about 10,000) of sample points in the parameters space to generate the distribution for  $X$  and  $Y$  over time. In the case of a system as simple as the predator-prey model here, a naive Monte-Carlo approach maybe manageable, but for more complicated systems with more random parameters, cost of Monte-Carlo simulations can become prohibitive.

## 6.6 The non-intrusive method

Consider the PC expansion of  $X$  and  $Y$ :

$$X(t, \boldsymbol{\xi}) = \sum_{k=0}^P X_k(t) \Psi_k(\boldsymbol{\xi}), \quad (6.13)$$

$$Y(t, \boldsymbol{\xi}) = \sum_{k=0}^P Y_k(t) \Psi_k(\boldsymbol{\xi}), \quad (6.14)$$

where we recall that  $\boldsymbol{\xi} = (\xi_1, \xi_2)$  with  $\xi_1$  and  $\xi_2$  standard normal random variables. Let us the expansion for  $X$  for example. Note that using the orthogonality of  $\Psi_k$  we can directly get,

$$X_k(t) = \frac{\langle X(t, \boldsymbol{\xi}), \Psi_k(\boldsymbol{\xi}) \rangle}{\langle \Psi_k(\boldsymbol{\xi}), \Psi_k(\boldsymbol{\xi}) \rangle} = \frac{\mathbb{E}[X(t, \boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi})]}{\mathbb{E}[\Psi_k^2(\boldsymbol{\xi})]}.$$

Now the moment  $\mathbb{E}[\Psi_k^2(\boldsymbol{\xi})]$  can be computed analytically, because  $\Psi_k$  is none but a multivariate Hermite Polynomial. However, we cannot compute the moment in the numerator because we do not have  $X(t, \boldsymbol{\xi})$  (if we did have  $X(t, \boldsymbol{\xi})$  there would be nothing to solve for anyway). Note however, that

$$\begin{aligned} \mathbb{E}[X(t, \boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi})] &= \int_{\Omega} X(t, \boldsymbol{\xi}(\omega)) \Psi_k(\boldsymbol{\xi}(\omega)) dP(\omega) \\ &= \int_{\mathbb{R}^2} X(t, \mathbf{x}) \Psi_k(\mathbf{x}) f_{\boldsymbol{\xi}}(\mathbf{x}) d\mathbf{x}, \end{aligned} \quad (6.15)$$

where  $f_{\boldsymbol{\xi}}$  is joint PDF of  $\xi_1$  and  $\xi_2$ . Thus, we can compute the moments  $\mathbb{E}[X(t, \boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi})]$  by computing the integral in (6.15) numerically. In this case, a natural integration scheme would be Gauss-Hermite quadrature (in 2D):

$$\int_{\mathbb{R}^2} X(t, \mathbf{x}) \Psi_k(\mathbf{x}) f_{\boldsymbol{\xi}}(\mathbf{x}) d\mathbf{x} = \sum_{j=1}^N w^j X(t, \mathbf{x}^j) \Psi_k(\mathbf{x}^j).$$

Where  $\mathbf{x}^j$  and  $w^j$  are multi-dimensional nodes and weights for Gauss Hermite quadrature (in 2D). To complete the computations then, one needs to solve for  $X(t, \mathbf{x}^j)$  by solving the original predator prey system (6.7) with  $\boldsymbol{\xi} = \mathbf{x}^j$ ,  $j = 1, \dots, N$ ; that is, solve (6.7) with

$$\alpha = a_1 + b_1 x_1^j, \quad \gamma = a_2 + b_2 x_2^j,$$

to get  $X(\cdot, \mathbf{x}^j)$ ,  $j = 1, \dots, N$ . Then, the coefficients  $X_k$  of the chaos expansion of  $X$  can be computed through the above procedure. This method of computing the coefficients in the chaos expansion, via numerical integrations, is what is known as the NISP method.

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