

# Introduction to Polynomial Chaos

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The polynomial chaos expansion method<sup>1</sup> is a tool used for uncertainty quantification (UQ), which is concerned with understanding the uncertainty in models of complex systems. Oftentimes, one has a model of some phenomena, which takes a set of parameters as inputs. However, the values of these inputs are not known with certainty and one wishes to understand how that uncertainty affects the outputs of the model. For models with modest computational demands, this uncertainty propagation (UP) can often be analyzed using monte carlo simulation (MCS), where a distribution is assumed for each parameter, and random realizations of the parameter set are used to simulate the model, which provides a distribution of the model outputs given the distributions of inputs. However, for computationally demanding models, it might not be feasible to run a large number of independent simulations of the model, so alternative approaches with lower computational demands are needed. The polynomial chaos expansion method is often used when analyzing uncertainty propagation.

This paper provides a brief introduction to polynomial chaos (PC) for graduate students in engineering and applied science, who would like to gain some rudimentary understanding of the technique. More detailed treatment of the material can be found in Xiu [4] (or Xiu [3]), which is more technical in nature but still quite accessible. Before covering polynomial chaos, we start with an example of the solution to a simple ODE, where we review concepts such as orthogonality and series representation of functions. This gives us the foundation to cover polynomial chaos. The latest version of this paper along with an accompanying python notebook with solutions to all examples can be found here:

<https://github.com/dcline1/PolynomialChaos>

## 1 Review of Fourier Series Methods for Solving ODEs

It's helpful to provide an example of function expansions in a familiar deterministic context before presenting the main material of these notes. This section is based on (Haberman [1], sec. 2.3), but the material is standard and can be found in any introductory text on PDEs or ODEs containing Fourier series methods. We consider the following second order ordinary differential equation (ODE)

$$\frac{d^2 u(x)}{dx^2} = -\lambda u(x), \quad (1.1)$$

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<sup>1</sup>Also known as the spectral method or stochastic spectral method.

subject to boundary conditions  $u(0) = 0$  and  $u(L) = 0$  and some initial condition  $f(x)$  for  $0 \leq x \leq L$ . If we guess  $u(x)$  has the form  $u(x) = e^{rx}$ , we get

$$\frac{du(x)}{dx} = re^{rx} = ru(x), \quad \frac{d^2u(x)}{dx^2} = r^2e^{rx} = r^2u(x),$$

Setting  $r^2 = -\lambda$  gives us (1.1), and we have  $r = \pm\sqrt{-\lambda} = \pm i\sqrt{\lambda}$ , where  $i = \sqrt{-1}$ . Therefore, solutions of (1.1) have the form  $u(x) = ce^{\pm i\sqrt{\lambda}x}$  for some constant  $c$ . For simplicity, we only consider the case where  $\lambda > 0$ . Using the relationships  $e^{i\alpha x} = \cos \alpha x + i \sin \alpha x$  and  $e^{-i\alpha x} = \cos \alpha x - i \sin \alpha x$ , we may write the solutions in the following form

$$\begin{aligned} u(x) &= c_1 e^{i\sqrt{\lambda}x} = c_1(\cos \sqrt{\lambda}x + i \sin \sqrt{\lambda}x), \\ u(x) &= c_2 e^{-i\sqrt{\lambda}x} = c_2(\cos \sqrt{\lambda}x - i \sin \sqrt{\lambda}x), \end{aligned}$$

for some arbitrary (possibly complex) constants  $c_1$  and  $c_2$ . Since linear combinations of solutions of ODEs are also solutions, we may alternatively write

$$\begin{aligned} u(x) &= c_1(\cos \sqrt{\lambda}x + i \sin \sqrt{\lambda}x) + c_2(\cos \sqrt{\lambda}x - i \sin \sqrt{\lambda}x) \\ &= a \cos \sqrt{\lambda}x + b \sin \sqrt{\lambda}x, \end{aligned} \tag{1.2}$$

where  $a = (c_1 + c_2)$  and  $b = (c_1 - c_2)i$ . Note that since  $c_1$  and  $c_2$  can be complex, we can take  $b$  to be real.<sup>2</sup> We say that (1.2) is the real solution of (1.1). Applying the first boundary condition,  $u(0) = 0$ , we immediately get  $a = 0$ , since  $\cos 0 = 1$ . Applying the second boundary condition gives

$$u(L) = b \sin \sqrt{\lambda}L = 0,$$

which is only true if  $b = 0$  (the trivial solution) or  $\sin \sqrt{\lambda}L = 0$ , which can only occur when  $\sqrt{\lambda}L = n\pi$ , where  $n$  is an integer (the graph of  $\sin$  only crosses zero at  $n\pi$ ). We therefore have

$$\lambda = \left(\frac{n\pi}{L}\right)^2.$$

Plugging this back into (1.2), we see the real solution to have the form

$$u(x) = b \sin \frac{n\pi x}{L}.$$

Again, since linear combinations of solutions of ODEs are themselves solutions, we have the general solution

$$u(x) = \sum_{n=1}^p b_n \Phi_n(x), \tag{1.3}$$

for some  $p > 0$  where we've introduced

$$\Phi_n(x) = \sin \frac{n\pi x}{L}$$

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<sup>2</sup>For example, take  $c_1 = (a - bi)/2$  and  $c_2 = (a + bi)/2$ , where  $a, b \in \mathbb{R}$ .

for notational convenience. It just so happens that, with moderate restrictions, any piecewise-smooth function  $f(x)$  on the interval  $x \in [0, L]$  can be represented as

$$f(x) = \sum_{n=1}^{\infty} b_n \Phi_n(x), \quad (1.4)$$

which is known as the Fourier series of  $f(x)$ . In order to satisfy the initial condition, we therefore just need to determine the coefficients  $b_n$ . This is done using the orthogonality of sin functions<sup>3</sup>

$$\langle \Phi_m(x) \Phi_n(x) \rangle = \int_0^L \Phi_m(x) \Phi_n(x) dx = \begin{cases} L/2, & m = n \\ 0, & m \neq n \end{cases}, \quad (1.5)$$

where  $\langle \cdot \cdot \rangle$  denotes our chosen inner product (in this case just the integral over our domain with no weighting function). It's common to write (1.5) more concisely as

$$\langle \Phi_m(x) \Phi_n(x) \rangle = \frac{L}{2} \delta_{mn} \quad (1.6)$$

where

$$\delta_{mn} = \begin{cases} 1, & m = n \\ 0, & m \neq n \end{cases}$$

is the Kronecker delta function. Now to determine the  $m^{\text{th}}$  coefficient,  $b_m$ , we simply multiply both sides of (1.4) by  $\Phi_m(x)$  and integrate over our domain to get

$$\begin{aligned} \int_0^L f(x) \Phi_m(x) dx &= \int_0^L \left( \sum_{n=1}^{\infty} b_n \Phi_n(x) \right) \Phi_m(x) dx \\ &= \sum_{n=1}^{\infty} b_n \left( \int_0^L \Phi_n(x) \Phi_m(x) dx \right) \\ &= \sum_{n=1}^{\infty} b_n \langle \Phi_n(x) \Phi_m(x) \rangle \\ &= b_m \langle \Phi_m(x) \Phi_m(x) \rangle \\ &= b_m \frac{L}{2} \end{aligned}$$

since  $\langle \Phi_m(x) \Phi_m(x) \rangle = \langle \Phi_m^2(x) \rangle = L/2$  by (1.6) and we've used the orthogonality of sines to drop all other terms. Solving for  $b_m$ , we get

$$b_m = \frac{2}{L} \int_0^L f(x) \Phi_m(x) dx, \quad (1.7)$$

or more compactly,

$$b_m = \frac{\langle f(x) \Phi_m(x) \rangle}{\langle \Phi_m^2(x) \rangle}. \quad (1.8)$$

In this section, we introduced the Fourier series representation of a function and used the orthogonality of functions to obtain the coefficients. These concepts are fundamental to polynomial chaos.

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<sup>3</sup>see, e.g., this video for a proof.

## 2 Polynomial Expansions

Similar to Fourier series expansions of functions as linear combinations of orthogonal trigonometric functions,  $\Phi_j(x)$ , we can also represent functions using linear combinations of orthogonal polynomials

$$f(x) = \sum_{j=0}^{\infty} a_j \Psi_j(x) \quad (2.1)$$

where  $\{\Psi_j(x) \mid j = 0, 1, \dots\}$  is a family of orthogonal polynomials, often referred to as the polynomial basis, satisfying

$$\langle \Psi_m(x) \Psi_n(x) \rangle = \int \Psi_m(x) \Psi_n(x) w(x) dx = \gamma_m \delta_{mn} \quad (2.2)$$

where the inner product is defined with respect to some weighting function  $w(x)$  and  $\gamma_m$  is a normalization constant. Note the similarity with (1.6), but while Fourier series use orthogonal periodic functions for the basis, polynomial expansions use orthogonal polynomials, which are not periodic.

Following the same procedure as we used for the Fourier series, we can solve for the coefficients by multiplying both sides of (2.1) by  $\Psi_i(x)$  and integrating to get

$$\begin{aligned} \int f(x) \Psi_i(x) dx &= \int \left( \sum_{j=0}^{\infty} a_j \Psi_j(x) \right) \Psi_i(x) dx \\ &= \sum_{j=0}^{\infty} a_j \left( \int \Psi_j(x) \Psi_i(x) dx \right) \\ &= \sum_{j=0}^{\infty} a_j \langle \Psi_j(x) \Psi_i(x) \rangle \\ &= a_i \langle \Psi_i^2(x) \rangle \end{aligned}$$

where we used polynomial orthogonality to drop all terms other than  $i$ . Solving for  $a_i$ , we get

$$a_i = \frac{\langle f(x) \Psi_i(x) \rangle}{\langle \Psi_i^2(x) \rangle}, \quad (2.3)$$

which is analogous to (1.8). In practice, we truncate (2.1) at some positive integer  $p$ , which gives us the following approximation

$$f(x) \approx f_p(x) = \sum_{j=0}^p a_j \Psi_j(x) \quad (2.4)$$

The weighting function,  $w(x)$ , is often chosen to be a probability density function, and certain classes of polynomials are orthogonal with respect to well-known probability density functions. Examples of orthogonal polynomials (and the distribution, or *germ*, corresponding to their weighting function) include Legendre (uniform), Hermite (Gaussian), and Laguerre (exponential or Gamma)

polynomials. We will focus on Hermite polynomials in this paper, but the results are easily extended to the others.

Linear algebra provides some intuition for (2.1). In linear algebra, an  $n$ -dimensional vector can be represented as a linear combination of  $n$  basis vectors. If we instead have a function, we can construct a vector as a discretized version of a function by taking function values at a discrete set of points. As we increase the resolution of the sampling points, we get an infinite dimensional vector in the limit. Therefore, functions can be thought of as infinite dimensional vectors, and we see that the linear combination of an infinite number of orthogonal polynomials for functions is analogous to a linear combination of  $n$  orthogonal basis vectors for  $n$ -dimensional vectors.

### 3 Hermite Polynomials

As mentioned above, orthogonal Hermite polynomials use a Gaussian weighting function. We will therefore use  $z$  to denote the independent variable when discussing Hermite polynomials.

Polynomial expansions using Hermite polynomials have the following form

$$\begin{aligned}
f(z) &= a_0 H_0 \\
&+ \sum_{i_1=1}^d a_{i_1} H_1(z_{i_1}) \\
&+ \sum_{i_1=1}^d \sum_{i_2=1}^{i_1} a_{i_1 i_2} H_2(z_{i_1}, z_{i_2}) \\
&+ \sum_{i_1=1}^d \sum_{i_2=1}^{i_1} \sum_{i_3=1}^{i_2} a_{i_1 i_2 i_3} H_3(z_{i_1}, z_{i_2}, z_{i_3}) \\
&+ \dots
\end{aligned} \tag{3.1}$$

where

$$H_n(z_{i_1}, \dots, z_{i_n}) = e^{\frac{1}{2}z^T z} (-1)^n \frac{\partial^n}{\partial z_{i_1} \dots \partial z_{i_n}} e^{-\frac{1}{2}z^T z}, \tag{3.2}$$

and  $z = (z_1, \dots, z_d) \in \mathbb{R}^d$  is a  $d$ -dimensional vector. We may write (3.1) in the form of (2.1) by defining a one-to-one mapping between the  $a_j$  and  $a_{i_1 \dots i_n}$  coefficients and a one-to-one mapping between the  $\Psi_n(z)$  polynomials and the  $H_n(z_{i_1}, \dots, z_{i_n})$  basis functions.

The notation in (3.1) and (3.2) is standard, but can be quite confusing. Let's work through the details for 1-dimensional variables Hermite polynomials.<sup>4</sup> We start with a scalar  $z$  and consider the following Gaussian-type equation

$$e^{-\frac{1}{2}z^2} \tag{3.3}$$

Taking the derivative, we get

$$\frac{d}{dz} e^{-\frac{1}{2}z^2} = -z e^{-\frac{1}{2}z^2}$$

Taking the derivative again, we get

$$\frac{d^2}{dz^2} e^{-\frac{1}{2}z^2} = \frac{d}{dz} \left( -z e^{-\frac{1}{2}z^2} \right) = (z^2 - 1) e^{-\frac{1}{2}z^2}$$

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<sup>4</sup>See Appendix A for 2-dimensional Hermite polynomials.

And again, we get

$$\begin{aligned}
\frac{d^3}{dz^3} e^{-\frac{1}{2}z^2} &= \frac{d}{dz} (z^2 - 1) e^{-\frac{1}{2}z^2} \\
&= 2ze^{-\frac{1}{2}z^2} + (z^2 - 1)(-z)e^{-\frac{1}{2}z^2} \\
&= -(z^3 - 3z)e^{-\frac{1}{2}z^2}
\end{aligned}$$

Using the following assignments for the polynomials on the right hand sides

$$\begin{aligned}
H_1(z) &= z \\
H_2(z) &= z^2 - 1 \\
H_3(z) &= z^3 - 3z
\end{aligned}$$

leads to the following general definition

$$H_n(z) = e^{\frac{1}{2}z^2} (-1)^n \frac{d^n}{dz^n} e^{-\frac{1}{2}z^2}, \quad (3.4)$$

which also satisfies  $H_0(z) = 1$ . By assigning  $H_1(z) = H_1(z)$ ,  $H_2(z) = H_2(z, z)$ ,  $H_3(z) = H_3(z, z, z)$ , and so on, we see that (3.4) fits the form given in (3.2), since  $H_n(z)$  is just  $H_n(z_{i_1}, \dots, z_{i_n})$  for  $d = 1$ . These are the Hermite polynomials for scalar  $z$ .<sup>5</sup>

It turns out that Hermite polynomials are orthogonal.<sup>6</sup> More concretely, it can be shown that the inner product has the following closed-form solution

$$\langle H_m(z) H_n(z) \rangle = \int_{-\infty}^{\infty} H_m(z) H_n(z) \phi(z) dz = n! \delta_{mn} \quad (3.5)$$

where

$$\phi(z) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}z^2}$$

is the standard normal density function. Note that (3.5) is zero whenever  $m \neq n$ , as required.

Starting with (3.1), we may plug in (3.2) for a 1-dimensional  $z$ , which is just (3.4), to get

$$\begin{aligned}
f(z) &= a_0 H_0 + a_1 H_1(z) + a_{11} H_2(z, z) + a_{111} H_3(z, z, z) + \dots \\
&= a_0 H_0 + a_1 H_1(z) + a_{11} H_2(z) + a_{111} H_3(z) + \dots
\end{aligned} \quad (3.6)$$

or, equivalently,

$$f(z) = a_0 + a_1 z + a_{11} (z^2 - 1) + a_{111} (z^3 - 3z) + \dots \quad (3.7)$$

Assigning  $\{a_1 = a_1, a_2 = a_{11}, a_3 = a_{111}, \dots\}$  and  $\Psi_n(z) = H_n(z)$ , we can recast this in the form of (2.1) as

$$f(z) = \sum_{j=0}^{\infty} a_j H_j(z). \quad (3.8)$$

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<sup>5</sup>Specifically, the *probabilist's* Hermite polynomials. We could instead use  $e^{-z^2}$  in place of  $e^{-\frac{1}{2}z^2}$ , which are known as the *physicist's* Hermite polynomials.

<sup>6</sup>see, e.g., these videos for a proof.

**Exercise 3.a** Plot the first 3, 5, and 8 Hermite polynomials. What can be said about them?

**Exercise 3.b** Construct the Hermite polynomial expansion of  $f(z) = 10 + 2z$ .

**Exercise 3.c** Construct the Hermite polynomial expansion of  $f(z) = \sin(4z)/z$ .

**Exercise 3.d** Construct the Hermite polynomial expansion of  $f(z) = |z|$ .

## 4 Polynomial Chaos Expansions of Random Variables

We've seen how to represent an arbitrary deterministic function as a linear combination of orthogonal basis functions, for both the Fourier basis and for orthogonal polynomial bases. It turns out, we can also represent functions of random variables using orthogonal polynomial bases in (2.1). As might be expected, constructing orthogonal polynomials with respect to probability densities allows for some analytical results.

For random variables with known probability distributions, the natural choice of orthogonal polynomial basis is the class for which  $w(x)$  in (2.2) is related to the probability density function of the random variable  $X$ . For instance, the natural choice of orthogonal polynomial basis for a Gaussian random variable,  $Z$ , is the Hermite polynomial basis  $\Psi_j = H_j$ .

**Exercise 4.a** Construct the Hermite polynomial expansion of  $f(Z) = Z$  where  $Z \sim N(0, 1)$ . What are the values of the coefficients?

**Exercise 4.b** Construct the Hermite polynomial expansion of  $f(Z) = 10 + 2Z$  where  $Z \sim N(0, 1)$ . What are the values of the coefficients?

**Exercise 4.c** Construct the Hermite polynomial expansion of  $f(Z) = e^{\mu + \sigma Z}$ , where  $\mu = 1$ ,  $\sigma = 0.1$ , and  $Z \sim N(0, 1)$ . What are the values of the coefficients?

This works well for functions of standard classes of known probability distributions. But what if we have an arbitrary random variable  $Y$  with cumulative distribution function  $F_Y(y) = P(Y \leq y)$ ? In this case, not only might  $Y$  not be a function of a known random variable  $X$ , as we saw above, but the cdf might not even have an analytical form (e.g. an empirical distribution). By transforming  $X$  into a uniform random variable, we can generalize the inner product  $\langle Y, \Psi_i(x) \rangle$  to handle any arbitrary  $Y$ .

We start by transforming  $X$  into a  $U \sim U(0, 1)$  uniform random variable using the cdf  $F_X(x) = P(X \leq x)$ , since  $F_X(X) \sim U$ . Then given the CDF of  $Y$ , we can transform  $U$  into a  $Y$  random variable using the inverse transform  $Y \sim F_Y^{-1}(U)$ . In other words, we can use the mapping  $Y(X) = F_Y^{-1}(F_X(X))$ . This gives us the following inner product

$$\int_{-\infty}^{\infty} Y(x) \Psi_k(x) w(x) dx = \int_{-\infty}^{\infty} F_Y^{-1}(F_X(x)) \Psi_k(z) w(x) dx \quad (4.1)$$

and we can rewrite (2.3) as

$$a_i = \frac{\langle F_Y^{-1}(F_X(x)) \Psi_i(x) \rangle}{\langle \Psi_i^2(x) \rangle}. \quad (4.2)$$

While the above transformations are theoretically sound, they have a tendency to be numerically unstable due to numerical errors in the tails of (4.1). However, since  $F_X(X) \sim U(0, 1)$  and  $X \sim F_X^{-1}(U)$ , we can transform the inner product in (4.1) with respect to  $X$  into the following inner product with respect to a  $U(0, 1)$  random variable

$$\int_{-\infty}^{\infty} F_Y^{-1}(F_X(x)) \Psi_k(z) w(x) dx = \int_0^1 F_Y^{-1}(u) \Psi_k(F_X^{-1}(u)) du \quad (4.3)$$

since the weighting function (i.e. probability density function) in the inner product for the  $U(0, 1)$  uniform distribution is  $w(u) = 1$ . The coefficients are therefore

$$a_i = \frac{\langle F_Y^{-1}(u) \Psi_i(F_X^{-1}(u)) \rangle_u}{\langle \Psi_i^2(x) \rangle} \quad (4.4)$$

where  $\langle \cdot \rangle_u$  is the inner product for the uniform distribution. Note that no adjustments are needed for the denominator, since we may continue to use the orthogonality of  $\Psi_i(x)$  just as we did before. While (4.1) and (4.3) are mathematically equivalent, (4.3) avoids numerical errors in the tails, since the integral is taken from  $[0, 1]$  instead of  $(-\infty, \infty)$ .

The polynomial expansion in (2.1) then becomes

$$f(u) = \sum_{j=0}^{\infty} a_j \Psi_j(F_X^{-1}(u)) \quad (4.5)$$

**Exercise 4.d** Using the uniform transformation in (4.3)–(4.5), construct the Hermite polynomial expansion of  $f(Z) = e^{\mu + \sigma Z}$ , where  $\mu = 1$ ,  $\sigma = 0.1$ , and  $Z \sim N(0, 1)$ . What are the values of the coefficients?

**Exercise 4.e** Using the uniform transformation in (4.3)–(4.5), construct the Hermite polynomial expansion of  $Y \sim \text{Beta}(\alpha, \beta)$ , where  $\alpha = \beta = 0.5$ . What are the values of the coefficients?

#### 4.1 Statistical Moments

Note that the right side of (2.4) is an *analytical* surrogate to function  $f$  on the left. This opens up the possibility of analytically calculating the approximate moments of  $f(X)$ . When the weighting function in the inner product is a probability density function and the orthogonal polynomials are normalized such that  $\Psi_0(X) = 1$ , we can directly use the inner products to calculate expected



values, since  $\langle \cdot \rangle = E[\cdot]$ . This gives us

$$\begin{aligned}
E[f(X)] &\approx E[f_p(X)] \\
&= E[f_p(X)\Psi_0(X)] \\
&= E\left[\left(\sum_{j=0}^p a_j \Psi_j(X)\right) \Psi_0(X)\right] \\
&= \sum_{j=0}^p E[a_j \Psi_j(X)\Psi_0(X)] \\
&= \sum_{j=0}^p a_j \langle \Psi_j(X)\Psi_0(X) \rangle \\
&= a_0
\end{aligned} \tag{4.6}$$

and we see that  $E[f(X)] \approx a_0$ . Note that this is a general result and holds regardless of the class of orthogonal polynomials used in (2.4). Similarly,

$$\begin{aligned}
E[f^2(X)] &\approx E[f_p^2(X)] \\
&= E\left[\left(\sum_{j=0}^p a_j \Psi_j(X)\right) \left(\sum_{j=0}^p a_j \Psi_j(X)\right)\right] \\
&= \left\langle \left(\sum_{j=0}^p a_j \Psi_j(X)\right) \left(\sum_{j=0}^p a_j \Psi_j(X)\right) \right\rangle \\
&= \left\langle \sum_{j=0}^p a_j^2 \Psi_j^2(X) \right\rangle \\
&= \sum_{j=0}^p a_j^2 \langle \Psi_j^2(X) \rangle.
\end{aligned}$$

The variance is therefore

$$\begin{aligned}
Var(f(X)) &= E[f^2(X)] - E^2[f(X)] \\
&\approx E[f_p^2(X)] - E^2[f_p(X)] \\
&= \sum_{j=0}^p a_j^2 \langle \Psi_j^2(X) \rangle - a_0^2 \\
&= \sum_{j=1}^p a_j^2 \langle \Psi_j^2(X) \rangle
\end{aligned} \tag{4.7}$$

since  $\langle \Psi_0^2(X) \rangle = 1$ . Again, this holds regardless of the chosen orthogonal polynomial basis. Therefore, once we solve for the coefficients of our polynomial chaos representation of  $f$ , the average response and confidence intervals are essentially automatic using (4.6) and (4.7).

**Exercises 4.1.a-e** Calculate the mean and variance of all random variables in exercises 4.a-e using (4.6) and (4.7). Do they match the closed-form statistics for these distributions?

## 5 Polynomial Expansions of Functions with Random Parameters

We will use the following simple equation as our example model

$$\frac{dv(t)}{dt} = -r v(t), \quad v(0) = v_0 = 3 \quad (5.1)$$

where the model parameter  $r$  is random. This problem could be calculated using monte carlo simulation, but that requires many simulations of the model. If the model is expensive to evaluate, this might be prohibitive.

Alternatively, we could use polynomial chaos, which can be applied in two main ways: intrusive and non-intrusive. We will cover both approaches below.

**Exercise 5.a** Assuming  $r \sim N(\mu, \sigma^2)$ , where  $\mu = 0.2$  and  $\sigma = 0.05$ , and  $v_0 = 3$ , draw  $N = 10,000$  random realizations of  $r$ , and for each one, evaluate (5.1) numerically over  $t = [0, 10]$  using 10,000 timesteps. Calculate the sample mean and standard deviation at each timestep. Plot all model runs, along with the mean and 95% confidence intervals through time.

### 5.1 Intrusive Approach

The intrusive approach applies polynomial chaos expansions directly to both the model parameters *and* model equations. Intrusive methods therefore require full knowledge of the model equations. The most common intrusive approach is known as stochastic Galerkin projection.

Given our example model, we start by applying the polynomial chaos expansion method to both  $r$  and  $v(t)$  using the same polynomial basis for both as follows

$$r(x) \approx \sum_{i=0}^p \hat{r}_i \Psi_i(x) \quad (5.2)$$

$$v(x, t) \approx \sum_{j=0}^p \hat{v}_j(t) \Psi_j(x) \quad (5.3)$$

Taking the derivative of (5.3) with respect to time gives

$$\frac{dv(x, t)}{dt} \approx \frac{d}{dt} \left( \sum_{j=0}^p \hat{v}_j(t) \Psi_j(x) \right) = \sum_{j=0}^p \frac{d\hat{v}_j(t)}{dt} \Psi_j(x). \quad (5.4)$$

Similar to the derivation in Section 2, we multiply (5.4) by  $\Psi_k(x)$  for some  $0 \leq k \leq p$  and take the

inner product to get

$$\begin{aligned}
\int \frac{dv(x, t)}{dt} \Psi_k(x) w(x) dx &\approx \int \left( \sum_{j=0}^p \frac{d\hat{v}_j(t)}{dt} \Psi_j(x) \right) \Psi_k(x) w(x) dx \\
&= \sum_{j=0}^p \int \frac{d\hat{v}_j(t)}{dt} \Psi_j(x) \Psi_k(x) w(x) dx \\
&= \sum_{j=0}^p \frac{d\hat{v}_j(t)}{dt} \int \Psi_j(x) \Psi_k(x) w(x) dx \\
&= \sum_{j=0}^p \frac{d\hat{v}_j(t)}{dt} \langle \Psi_j(x) \Psi_k(x) \rangle \\
&= \frac{d\hat{v}_k(t)}{dt} \langle \Psi_k^2(x) \rangle
\end{aligned} \tag{5.5}$$

Similarly, the inner product of the right hand side of (5.1) and  $\Psi_k(x)$  can be approximated using the polynomial chaos representations in (5.2) and (5.3) as follows

$$\begin{aligned}
-\int r(x) v(x, t) \Psi_k(x) w(x) dx &\approx -\int \left( \sum_{i=0}^p \hat{r}_i \Psi_i(x) \right) \left( \sum_{j=0}^p \hat{v}_j(t) \Psi_j(x) \right) \Psi_k(x) w(x) dx \\
&= -\int \sum_{i=0}^p \sum_{j=0}^p \hat{r}_i \hat{v}_j(t) \Psi_i(x) \Psi_j(x) \Psi_k(x) w(x) dx \\
&= -\sum_{i=0}^p \sum_{j=0}^p \int \hat{r}_i \hat{v}_j(t) \Psi_i(x) \Psi_j(x) \Psi_k(x) w(x) dx \\
&= -\sum_{i=0}^p \sum_{j=0}^p \hat{r}_i \hat{v}_j(t) \langle \Psi_i(x) \Psi_j(x) \Psi_k(x) \rangle
\end{aligned} \tag{5.6}$$

where the triple product, which has a closed-form solution, is given by

$$\langle \Psi_i(x) \Psi_j(x) \Psi_k(x) \rangle = \int \Psi_i(x) \Psi_j(x) \Psi_k(x) w(x) dx = \frac{i!j!k!}{(s-i)!(s-j)!(s-k)!} \tag{5.7}$$

where  $s \geq \min\{i, j, k\}$  and  $s = (i + j + k)/2$  is even. Equating (5.5) and (5.6), we get

$$\frac{d\hat{v}_k(t)}{dt} \langle \Psi_k^2(x) \rangle = -\sum_{i=0}^p \sum_{j=0}^p \hat{r}_i \hat{v}_j(t) \langle \Psi_i(x) \Psi_j(x) \Psi_k(x) \rangle$$

or in terms of the derivative,

$$\frac{d\hat{v}_k(t)}{dt} = -\sum_{j=0}^p \hat{v}_j(t) \left( \sum_{i=0}^p \hat{r}_i \frac{\langle \Psi_i(x) \Psi_j(x) \Psi_k(x) \rangle}{\langle \Psi_k^2(x) \rangle} \right) \tag{5.8}$$

This looks quite complicated, but note that quantity in parentheses is constant, since  $\hat{r}_i$ ,  $\langle \Psi_k^2(x) \rangle$ , and  $\langle \Psi_i(x) \Psi_j(x) \Psi_k(x) \rangle$  are all constants. Therefore, for the vector  $\hat{v} \in \mathbb{R}^p$ , we have the following  $p$ -dimensional linear system of equations

$$\frac{d\hat{v}}{dt} = A\hat{v} \quad (5.9)$$

for some  $p \times p$  matrix  $A$ . In other words, the Galerkin projection gives us a single  $p^{th}$  order ODE to solve instead of  $N$  ODE's we'd need to run for monte carlo analysis. Since  $p$  is typically small (e.g.  $p < 50$ ) and  $N$  is typically large (e.g.  $N = 10,000$ ), the savings in computational time can be substantial.

**Exercise 5.b** Construct the Hermite polynomial expansion of  $r \sim N(\mu, \sigma^2)$ , where  $\mu = 0.2$  and  $\sigma = 0.05$  for  $p = 10$ . What are the values of the coefficients?

**Exercise 5.c** Using the coefficients from 5.b and (5.8), construct the  $A$  in (5.9) for the example model (5.1) and solve the system of equations. Plot the solutions (coefficients) through time. Calculate the mean and standard deviation through time using the solutions of the system of ODEs. Plot the mean and 95% confidence intervals through time. Compare with the monte carlo results in 5.a.

## 5.2 Non-Intrusive Approach

When we do not know the details of the model or the model is not amenable to the intrusive approach (e.g. when we aren't able to reformulate and recode the model, as is necessary with an intrusive approach), we can use a non-intrusive approach, where we essentially treat the model as a black box. In this approach, we have a set of  $N$  pairs of model parameter inputs,  $x_i$ , and model outputs,  $f_i$ , which comprise the training set  $\mathcal{D} = \{(x_i, f_i) \mid 1 \leq i \leq N\}$ . We wish to solve for the coefficients, such that the following equation is satisfied for all samples

$$\sum_{j=0}^p a_j \Psi_j(x_i) = f_i, \quad 1 \leq i \leq N. \quad (5.10)$$

Note that this function is linear in  $i$  and that  $x_i$  is transformed using the orthogonal polynomial basis functions. In other words, this problem has the following form

$$\begin{bmatrix} \Psi_0(x_1) & \cdots & \Psi_p(x_1) \\ \vdots & \ddots & \vdots \\ \Psi_0(x_N) & \cdots & \Psi_p(x_N) \end{bmatrix} \begin{bmatrix} a_0 \\ \vdots \\ a_p \end{bmatrix} = \begin{bmatrix} f_1 \\ \vdots \\ f_N \end{bmatrix} \quad (5.11)$$

or more succinctly

$$\Psi \mathbf{a} = \mathbf{f} \quad (5.12)$$

where  $\Psi$  is the  $N \times p$  design matrix,  $\mathbf{a}$  is a  $p \times 1$  column vector, and  $\mathbf{f}$  is a  $N \times 1$  column vector. We can solve for the coefficient vector,  $\mathbf{a}$ , using linear regression. Note that the polynomial basis functions can grow very large for higher-order expansions. Therefore, it might be desirable to use

some form of regularization (e.g. Ridge regression) when solving for the coefficients to limit their size.

The number of function evaluations required for fitting the coefficients is typically much lower than for monte carlo simulation. This means that it's often much faster to fit the surrogate function and calculate moments than it is to run a full monte carlo simulation. Therefore, just like intrusive methods, the savings in computational time can be substantial.

**Exercise 5.d** Taking  $N = 100$ , construct the vector  $z_i = F_Z^{-1}(u_i)$ , where  $u_i = (i + 0.5)/N$  are equally spaced points over the interval  $(0, 1)$ . For each  $z_i$ , calculate  $r_i = 0.2 + 0.05x_i$  and evaluate (5.1) numerically over  $t = [0, 10]$  using 10,000 timesteps. Construct the design matrix  $\Psi$  using  $\{z_1, \dots, z_N\}$  and Hermite polynomials as the orthogonal polynomial basis. For each timestep, solve for the coefficients  $(a_1, \dots, a_p)$  using linear regression such that the coefficients are functions of time  $(a_1(t), \dots, a_p(t))$ . Plot the solutions (coefficients) through time. Calculate the mean and standard deviation through time using the coefficients. Plot the mean and 95% confidence intervals through time. Compare with the monte carlo results in 5.a.

## References

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## Appendix

### A Hermite Polynomials in 2-Dimensions

To solidify our understanding, we work through the Hermite polynomial expansion for two dimensions. Take  $z = (z_1, z_2)$ . In this case, analogous to (3.3), we have

$$e^{-\frac{1}{2}z^T z} = e^{-\frac{1}{2}(z_1^2 + z_2^2)}. \quad (\text{A.1})$$

Taking the derivative with respect to  $z_1$ , we get

$$\frac{\partial}{\partial z_1} e^{-\frac{1}{2}z^T z} = -z_1 e^{-\frac{1}{2}z^T z}.$$

Applying (3.2), we get

$$H_1(z_1) = e^{-\frac{1}{2}z^T z}(-1) \left( -z_1 e^{-\frac{1}{2}z^T z} \right) = z_1. \quad (\text{A.2})$$

Similarly,  $H_1(z_2) = z_2$ . Taking the derivative again with respect to  $z_1$ , we get

$$\frac{\partial^2}{\partial z_1 \partial z_1} e^{-\frac{1}{2}z^T z} = \frac{\partial}{\partial z_1} \left( -z_1 e^{-\frac{1}{2}z^T z} \right) = (z_1^2 - 1) e^{-\frac{1}{2}z^T z}$$

which gives us

$$H_2(z_1, z_1) = e^{-\frac{1}{2}z^T z}(-1)^2(z_1^2 - 1)e^{-\frac{1}{2}z^T z} = z_1^2 - 1. \quad (\text{A.3})$$

Similarly,  $H_2(z_2, z_2) = z_2^2 - 1$ . Taking the cross derivative, we get

$$\frac{\partial^2}{\partial z_2 \partial z_1} e^{-\frac{1}{2}z^T z} = \frac{\partial}{\partial z_2} \left( -z_1 e^{-\frac{1}{2}z^T z} \right) = z_1 z_2 e^{-\frac{1}{2}z^T z},$$

which leads to

$$H_2(z_2, z_1) = e^{-\frac{1}{2}z^T z}(-1)^2(z_2 z_1) e^{-\frac{1}{2}z^T z} = z_2 z_1. \quad (\text{A.4})$$

The third-order derivative with respect to  $z_1$  is calculated as

$$\begin{aligned} \frac{\partial^3}{\partial z_1 \partial z_1 \partial z_1} e^{-\frac{1}{2}z^T z} &= \frac{\partial^2}{\partial z_1 \partial z_1} \left( -z_1 e^{-\frac{1}{2}z^T z} \right) \\ &= \frac{\partial}{\partial z_1} (z_1^2 - 1) e^{-\frac{1}{2}z^T z} \\ &= 2z_1^2 e^{-\frac{1}{2}z^T z} + (z_1^2 - 1)(-z_1) e^{-\frac{1}{2}z^T z} \\ &= -(z_1^3 + 3z_1) e^{-\frac{1}{2}z^T z}, \end{aligned} \quad (\text{A.5})$$

which gives us

$$H_3(z_1, z_1, z_1) = e^{-\frac{1}{2}z^T z}(-1)^3 \left( -(z_1^3 + 3z_1) e^{-\frac{1}{2}z^T z} \right) = z_1^3 + 3z_1. \quad (\text{A.6})$$

Similarly,  $H_3(z_2, z_2, z_2) = z_2^3 + 3z_2$ . Finally, we have

$$\begin{aligned}
\frac{\partial^3}{\partial z_2 \partial z_1 \partial z_1} e^{-\frac{1}{2} z^T z} &= \frac{\partial^2}{\partial z_2 \partial z_1} \left( -z_1 e^{-\frac{1}{2} z^T z} \right) \\
&= \frac{\partial}{\partial z_2} (z_1^2 - 1) e^{-\frac{1}{2} z^T z} \\
&= (z_1^2 - 1)(-z_2) e^{-\frac{1}{2} z^T z} \\
&= -(z_1^2 z_2 - z_2) e^{-\frac{1}{2} z^T z},
\end{aligned}$$

which leads to

$$H_3(z_2, z_1, z_1) = e^{-\frac{1}{2} z^T z} (-1)^3 \left( -(z_1^2 z_2 - z_2) e^{-\frac{1}{2} z^T z} \right) = z_1^2 z_2 - z_2 \quad (\text{A.7})$$

By symmetry, we also have  $H_3(z_2, z_2, z_1) = z_1 z_2^2 - z_1$ .

Applying (3.1) with  $z = (z_1, z_2)$ , we get

$$\begin{aligned}
f(z) &= a_0 H_0 \\
&+ a_1 H_1(z_1) + a_2 H_1(z_2) \\
&+ a_{11} H_2(z_1, z_1) + a_{21} H_2(z_2, z_1) + a_{22} H_2(z_2, z_2) \\
&+ a_{111} H_3(z_1, z_1, z_1) + a_{211} H_3(z_2, z_1, z_1) + a_{221} H_3(z_2, z_2, z_1) + a_{222} H_3(z_2, z_2, z_2) \\
&+ \dots
\end{aligned} \quad (\text{A.8})$$

or, equivalently,

$$\begin{aligned}
f(z) &= a_0 \\
&+ a_1 z_1 + a_2 z_2 \\
&+ a_{11} (z_1^2 - 1) + a_{21} z_1 z_2 + a_{22} (z_2^2 - 1) \\
&+ a_{111} (z_1^3 + 3z_1) + a_{211} (z_1^2 z_2 - z_2) + a_{221} (z_1 z_2^2 - z_1) + a_{222} (z_2^3 + 3z_2) \\
&+ \dots
\end{aligned} \quad (\text{A.9})$$

Enumerating the summands from left to right, we can represent (A.8) and (A.9) using the simplified notation in (2.1).