Homework 4

NE 795-001: Fall 2023

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Contents

Problem 1 - UQ with gPCE

The Generalized Polynomial Chaos Expansion (gPCE) is a method used to represent uncertain parameters in a stochastic system. It allows us to express the uncertain parameters as a series of orthogonal polynomials with respect to the probability distribution of the underlying random variables. Let's denote ω as the random variable with a known probability distribution, and $\alpha(\omega)$ and $\gamma(\omega)$ as the uncertain parameters in the Lotka-Volterra equations.

The Lotka-Volterra equations with stochastic parameters are:

$$\frac{dx}{dt} = \alpha(\omega)x - \beta xy$$
$$\frac{dy}{dt} = \delta xy - \gamma(\omega)y$$

To apply the gPCE to these equations, we first need to expand the uncertain parameters $\alpha(\omega)$ and $\gamma(\omega)$ into a polynomial chaos series:

$$\alpha(\omega) = \sum_{i=0}^{P} a_i \Psi_i(\omega)$$
$$\gamma(\omega) = \sum_{i=0}^{P} g_i \Psi_i(\omega)$$

where a_i and g_i are the deterministic coefficients of the expansion, $\Psi_i(\omega)$ are the orthogonal polynomials with respect to the probability distribution of ω, and P is the order of the expansion.

Next, we also expand the state variables $x(t, \omega)$ and $y(t, \omega)$ into gPCE series:

$$x(t,\omega) = \sum_{i=0}^{P} x_i(t)\Psi_i(\omega)$$

$$y(t,\omega) = \sum_{i=0}^{P} y_i(t)\Psi_i(\omega)$$

Substituting these expansions into the Lotka-Volterra equations, we get:

$$\frac{d}{dt}\left(\sum_{i=0}^{P} x_i(t)\Psi_i(\omega)\right) = \left(\sum_{i=0}^{P} a_i\Psi_i(\omega)\right)\left(\sum_{j=0}^{P} x_j(t)\Psi_j(\omega)\right) - \beta\left(\sum_{k=0}^{P} x_k(t)\Psi_k(\omega)\right)\left(\sum_{l=0}^{P} y_l(t)\Psi_l(\omega)\right)$$

$$\frac{d}{dt}\left(\sum_{i=0}^{P} y_i(t)\Psi_i(\omega)\right) = \delta\left(\sum_{k=0}^{P} x_k(t)\Psi_k(\omega)\right)\left(\sum_{l=0}^{P} y_l(t)\Psi_l(\omega)\right) - \left(\sum_{i=0}^{P} g_i\Psi_i(\omega)\right)\left(\sum_{j=0}^{P} y_j(t)\Psi_j(\omega)\right)$$

Now, we apply the Galerkin projection, which involves multiplying both sides of the equations by $\Psi_m(\omega)$ and integrating over the probability space of ω:

$$\int \Psi_m(\omega)\frac{d}{dt}\left(\sum_{i=0}^{P} x_i(t)\Psi_i(\omega)\right)d\mathbb{P}(\omega) = \int \Psi_m(\omega)\left[\left(\sum_{i=0}^{P} a_i\Psi_i(\omega)\right)\left(\sum_{j=0}^{P} x_j(t)\Psi_j(\omega)\right) - \beta\left(\sum_{k=0}^{P} x_k(t)\Psi_k(\omega)\right)\left(\sum_{l=0}^{P} y_l(t)\Psi_l(\omega)\right)\right]d\mathbb{P}(\omega)$$

$$\int \Psi_m(\omega)\frac{d}{dt}\left(\sum_{i=0}^{P} y_i(t)\Psi_i(\omega)\right)d\mathbb{P}(\omega) = \int \Psi_m(\omega)\left[\delta\left(\sum_{k=0}^{P} x_k(t)\Psi_k(\omega)\right)\left(\sum_{l=0}^{P} y_l(t)\Psi_l(\omega)\right) - \left(\sum_{i=0}^{P} g_i\Psi_i(\omega)\right)\left(\sum_{j=0}^{P} y_j(t)\Psi_j(\omega)\right)\right]d\mathbb{P}(\omega)$$

Since the polynomials $\Psi_i(\omega)$ are orthogonal with respect to the probability distribution of ω, the integrals of the products of different polynomials are zero, and the integral of the square of a polynomial is not zero. This property simplifies the above equations significantly.

To simplify the equations obtained from the Galerkin projection, we will use the orthogonality property of the polynomial basis $\Psi_i(\omega)$. The orthogonality condition states that:

$$\int \Psi_i(\omega)\Psi_j(\omega)d\mathbb{P}(\omega) = \begin{cases} 0 & \text{if } i \neq j \\ \langle \Psi_i^2 \rangle & \text{if } i = j \end{cases}$$

where $\langle \Psi_i^2 \rangle$ is the expected value of $\Psi_i^2(\omega)$, which is a constant.

Let's simplify the first equation after applying the Galerkin projection:

$$\int \Psi_m(\omega)\frac{d}{dt}\left(\sum_{i=0}^{P} x_i(t)\Psi_i(\omega)\right)d\mathbb{P}(\omega) = \int \Psi_m(\omega)\left[\left(\sum_{i=0}^{P} a_i\Psi_i(\omega)\right)\left(\sum_{j=0}^{P} x_j(t)\Psi_j(\omega)\right) - \beta\left(\sum_{k=0}^{P} x_k(t)\Psi_k(\omega)\right)\left(\sum_{l=0}^{P} y_l(t)\Psi_l(\omega)\right)\right]d\mathbb{P}(\omega)$$

We can take the time derivative outside of the integral and the summation because it does not depend on ω:

$$\sum_{i=0}^{P}\frac{dx_i(t)}{dt}\int \Psi_m(\omega)\Psi_i(\omega)d\mathbb{P}(\omega) = \sum_{i=0}^{P}\sum_{j=0}^{P} a_i x_j(t)\int \Psi_m(\omega)\Psi_i(\omega)\Psi_j(\omega)d\mathbb{P}(\omega) - \beta\sum_{k=0}^{P}\sum_{l=0}^{P} x_k(t)y_l(t)\int \Psi_m(\omega)\Psi_k(\omega)\Psi_l(\omega)d\mathbb{P}(\omega)$$

Using the orthogonality condition, the integrals simplify to:

$$\frac{dx_m(t)}{dt}\langle\Psi_m^2\rangle = \sum_{i=0}^{P} a_i x_i(t)\langle\Psi_m\Psi_i\rangle - \beta\sum_{k=0}^{P} x_k(t)y_k(t)\langle\Psi_m^2\rangle$$

Since $\langle\Psi_m\Psi_i\rangle$ is zero for $i \neq m$ and $\langle\Psi_m^2\rangle$ for $i = m$, we can simplify further:

$$\frac{dx_m(t)}{dt}\langle\Psi_m^2\rangle = a_m x_m(t)\langle\Psi_m^2\rangle - \beta x_m(t)y_m(t)\langle\Psi_m^2\rangle$$

Dividing both sides by $\langle\Psi_m^2\rangle$:

$$\frac{dx_m(t)}{dt} = a_m x_m(t) - \beta x_m(t)y_m(t)$$

We can perform a similar simplification for the second equation:

$$\frac{dy_m(t)}{dt} = \delta x_m(t)y_m(t) - g_m y_m(t)$$

These are the simplified deterministic ODEs for the coefficients $x_m(t)$ and $y_m(t)$ in the gPCE expansion of the state variables $x(t,\omega)$ and $y(t,\omega)$. The resulting system of ODEs can be solved to find the evolution of the moments of $x(t,\omega)$ and $y(t,\omega)$.

After simplifying the equations using the orthogonality property of the polynomial basis $\Psi_i(\omega)$, we obtain a system of deterministic ordinary differential equations (ODEs) for the coefficients $x_m(t)$ and $y_m(t)$ in the gPCE expansion of the state variables $x(t,\omega)$ and $y(t,\omega)$. The final form of these ODEs is:

For the prey population $x(t,\omega)$:

$$\frac{dx_m(t)}{dt} = a_m x_m(t) - \beta\sum_{k=0}^{P}\sum_{l=0}^{P} C_{mkl}x_k(t)y_l(t)$$

For the predator population $y(t,\omega)$:

$$\frac{dy_m(t)}{dt} = \delta\sum_{k=0}^{P}\sum_{l=0}^{P} C_{mkl}x_k(t)y_l(t) - g_m y_m(t)$$

where C_{mkl} are the triple product integrals of the polynomial basis:

$$C_{mkl} = \int \Psi_m(\omega)\Psi_k(\omega)\Psi_l(\omega)d\mathbb{P}(\omega)$$

These triple product integrals are typically nonzero only for certain combinations of indices m, k, and l, depending on the specific polynomial basis used and the probability distribution of ω. The coefficients a_m and g_m are the gPCE coefficients for the uncertain parameters $\alpha(\omega)$ and $\gamma(\omega)$, respectively.

The system of ODEs can be solved numerically to obtain the time evolution of the coefficients $x_m(t)$ and $y_m(t)$, which in turn provide the statistical moments of the prey and predator populations. This approach allows us to analyze the impact of uncertainty in the parameters $\alpha(\omega)$ and $\gamma(\omega)$ on the dynamics of the Lotka-Volterra system.

Problem 3 - SA for the Sobol' G function

The Sobol' G function is defined as a product of individual functions $g_i(X_i)$ for each input factor X_i, where each $g_i(X_i)$ is given by:

$$g_i(X_i) = \frac{|4X_i - 2| + a_i}{1 + a_i}$$

where a_i is a non-negative parameter that determines the importance of the corresponding input factor X_i. The range of X_i is from 0 to 1, as they are uniformly distributed in the unit cube I_d.

1. Range of Variation of $g_i(X_i)$ as a function of a_i

To find the range of variation of $g_i(X_i)$ as a function of a_i, we need to consider the minimum and maximum values that $g_i(X_i)$ can take.

The minimum value of $|4X_i - 2|$ occurs when $X_i = 0.5$, which gives $|4 \cdot 0.5 - 2| = 0$. The maximum value occurs at the endpoints of the interval $X_i = 0$ or $X_i = 1$, which gives $|4 \cdot 0 - 2| = |4 \cdot 1 - 2| = 2$.

Therefore, the range of $g_i(X_i)$ is:

$$\min(g_i(X_i)) = \frac{0 + a_i}{1 + a_i} = \frac{a_i}{1 + a_i}$$

$$\max(g_i(X_i)) = \frac{2 + a_i}{1 + a_i}$$

The range of variation of $g_i(X_i)$ is then:

$$\max(g_i(X_i)) - \min(g_i(X_i)) = \frac{2 + a_i}{1 + a_i} - \frac{a_i}{1 + a_i} = \frac{2}{1 + a_i}$$

This range of variation indicates how much $g_i(X_i)$ can change as X_i varies from 0 to 1. The sensitivity of the overall function G with respect to each X_i is influenced by the range of variation of $g_i(X_i)$. A larger range of variation implies that changes in X_i can have a more significant impact on the value of G, indicating higher sensitivity. The parameter a_i plays a crucial role in determining the sensitivity. As a_i increases, the range of variation $\frac{2}{1+a_i}$ decreases, which means that the function $g_i(X_i)$ becomes less sensitive to changes in X_i. Conversely, when a_i is small (especially when a_i is close to 0), the function $g_i(X_i)$ is more sensitive to changes in X_i.

Therefore, the sensitivity of the Sobol' G function with respect to each input factor X_i is inversely related to the corresponding parameter a_i. A smaller a_i results in higher sensitivity, while a larger a_i results in lower sensitivity. This property makes the Sobol' G function useful for sensitivity analysis, as it allows for the control of the influence of each input factor on the output by adjusting the corresponding a_i parameter.

2. Prove that, for each of the $g_i(X_i)$ functions, $\int_0^1 g_i(X_i)\,dX_i = 1$

To prove that the integral of each $g_i(X_i)$ function over the interval [0, 1] is equal to 1, we need to evaluate the following integral:

$$\int_0^1 g_i(X_i)\,dX_i = \int_0^1 \frac{|4X_i - 2| + a_i}{1 + a_i}\,dX_i$$

First, we can simplify the integral by taking the constant term $1 + a_i$ outside of the integral, as it does not depend on X_i:

$$\int_0^1 g_i(X_i)\,dX_i = \frac{1}{1 + a_i}\int_0^1 (|4X_i - 2| + a_i)\,dX_i$$

Next, we need to split the integral into two parts to handle the absolute value function. The expression $|4X_i - 2|$ changes at $X_i = 0.5$, where it equals zero. Therefore, we split the integral at $X_i = 0.5$:

$$\int_0^1 g_i(X_i)\,dX_i = \frac{1}{1 + a_i}\left(\int_0^{0.5} (2 - 4X_i + a_i)\,dX_i + \int_{0.5}^1 (4X_i - 2 + a_i)\,dX_i\right)$$

Now, we can evaluate each integral separately:

For the first integral, from 0 to 0.5:

$$\int_0^{0.5} (2 - 4X_i + a_i)\,dX_i = \left[2X_i - 2X_i^2 + a_iX_i\right]_0^{0.5} = \left[(2\cdot 0.5 - 2\cdot(0.5)^2 + a_i\cdot 0.5) - (0 - 0 + 0)\right]$$

$$= 1 - 0.5 + 0.5a_i = 0.5 + 0.5a_i$$

For the second integral, from 0.5 to 1:

$$\int_{0.5}^1 (4X_i - 2 + a_i)\,dX_i = \left[2X_i^2 - 2X_i + a_iX_i\right]_{0.5}^1 = \left[(2\cdot 1^2 - 2\cdot 1 + a_i\cdot 1) - (2\cdot(0.5)^2 - 2\cdot 0.5 + a_i\cdot 0.5)\right]$$

$$= (2 - 2 + a_i) - (0.5 - 1 + 0.5a_i) = a_i + 0.5 - 0.5a_i = 0.5 + 0.5a_i$$

Adding both parts together:

$$\int_0^1 g_i(X_i)\,dX_i = \frac{1}{1 + a_i}\left((0.5 + 0.5a_i) + (0.5 + 0.5a_i)\right) = \frac{1}{1 + a_i}\cdot(1 + a_i)$$

$$= \frac{1 + a_i}{1 + a_i} = 1$$

Thus, we have proven that the integral of each $g_i(X_i)$ function over the interval [0, 1] is equal to 1:

$$\int_0^1 g_i(X_i)\,dX_i = 1$$

3. What is the mean value of the G function, $E[G]$?

To find the mean value of the Sobol' G function, $E[G]$, we need to integrate the function over the d-dimensional unit cube I_d. The mean value is given by the expected value of the function, which is the integral of the function over its domain, normalized by the measure of the domain. Since each X_i is uniformly distributed over [0, 1], the measure of the domain is 1 for each dimension, and the mean value is simply the integral of the function over the domain.

The Sobol' G function is defined as:

$$G(X_1, X_2, ..., X_d) = \prod_{i=1}^{d} \frac{|4X_i - 2| + a_i}{1 + a_i}$$

The expected value of G is:

$$E[G] = \int_{I_d} G(X_1, X_2, ..., X_d)\, dX_1\, dX_2 \ldots dX_d$$

Since the X_i are independent and identically distributed, we can separate the integrals:

$$E[G] = \int_0^1 \frac{|4X_1 - 2| + a_1}{1 + a_1}\, dX_1 \int_0^1 \frac{|4X_2 - 2| + a_2}{1 + a_2}\, dX_2 \ldots \int_0^1 \frac{|4X_d - 2| + a_d}{1 + a_d}\, dX_d$$

From the previous step, we know that the integral of each $g_i(X_i)$ over [0, 1] is 1:

$$\int_0^1 g_i(X_i)\, dX_i = 1$$

Therefore, the expected value of G simplifies to:

$$E[G] = 1 \cdot 1 \cdot \ldots \cdot 1 = 1$$

So, the mean value of the Sobol' G function, $E[G]$, is 1.

4. What is the variance of the G function, Var(G)?

Given the G function:

$$G(X_1, X_2, ..., X_d) = \prod_{i=1}^{d} g_i(X_i)$$

where

$$g_i(X_i) = \frac{|4X_i - 2| + a_i}{1 + a_i}$$

and $E[g_i(X_i)] = 1$, as shown in the previous steps.

The variance of the product of independent random variables $g_i(X_i)$ is given by:

$$\mathrm{Var}\left(\prod_{i=1}^{d} g_i(X_i)\right) = \prod_{i=1}^{d}(\mathrm{Var}(g_i(X_i)) + E^2[g_i(X_i)]) - \prod_{i=1}^{d} E^2[g_i(X_i)]$$

Since $E[g_i(X_i)] = 1$, the formula simplifies to:

$$\mathrm{Var}(G) = \prod_{i=1}^{d}(\mathrm{Var}(g_i(X_i)) + 1) - 1$$

Now, we need to calculate $\mathrm{Var}(g_i(X_i))$:

$$\mathrm{Var}(g_i(X_i)) = E[g_i(X_i)^2] - E^2[g_i(X_i)]$$

We already know that $E^2[g_i(X_i)] = 1$, so we need to find $E[g_i(X_i)^2]$:

$$E[g_i(X_i)^2] = \int_0^1 \left(\frac{|4X_i - 2| + a_i}{1 + a_i}\right)^2 dX_i$$

Splitting the integral to handle the absolute value:

$$E[g_i(X_i)^2] = \int_0^{0.5} \left(\frac{2 - 4X_i + a_i}{1 + a_i}\right)^2 dX_i + \int_{0.5}^1 \left(\frac{4X_i - 2 + a_i}{1 + a_i}\right)^2 dX_i$$

Evaluating these integrals, as you have done, gives us:

$$E[g_i(X_i)^2] = \frac{4}{3(1 + a_i)^2} + \frac{2a_i}{(1 + a_i)^2} + \frac{a_i^2}{(1 + a_i)^2}$$

Subtracting $E^2[g_i(X_i)] = 1$ from $E[g_i(X_i)^2]$, we get:

$$\mathrm{Var}(g_i(X_i)) = \frac{4}{3(1 + a_i)^2} + \frac{2a_i}{(1 + a_i)^2} + \frac{a_i^2}{(1 + a_i)^2} - 1$$

Simplifying, we find:

$$\mathrm{Var}(g_i(X_i)) = \frac{1}{3(1 + a_i)^2}$$

Finally, we use this result to find the overall variance $\mathrm{Var}(G)$ of the G function:

$$\mathrm{Var}(G) = \prod_{i=1}^{d}\left(\frac{1}{3(1 + a_i)^2} + 1\right) - 1$$

4. Prove that the variance V_i due to each X_i is given by:

$$V_i = \mathrm{Var}_{(X_i)}[E_{(X_{\sim i})}(G|X_i)] = \frac{1}{3(1+a_i)^2}$$

To calculate V_i, the variance due to each X_i, we need to follow these steps:

1. Compute the conditional expectation of G given X_i, denoted as $E_{(X_{\sim i})}(G|X_i)$, where $X_{\sim i}$ represents all variables except X_i.

2. Compute the variance of this conditional expectation with respect to X_i, denoted as $\mathrm{Var}_{(X_i)}[E_{(X_{\sim i})}(G|X_i)]$.

Let's start with step 1:

The Sobol' G function is given by:

$$G(X_1, X_2, ..., X_d) = \prod_{i=1}^{d} g_i(X_i)$$

where

$$g_i(X_i) = \frac{|4X_i - 2| + a_i}{1 + a_i}$$

The conditional expectation of G given X_i is the product of $g_i(X_i)$ and the expectations of all other $g_j(X_j)$ for $j \neq i$:

$$E_{(X_{\sim i})}(G|X_i) = g_i(X_i) \cdot \prod_{j=1, j\neq i}^{d} E[g_j(X_j)]$$

Since we know that $E[g_j(X_j)] = 1$ for all j, the conditional expectation simplifies to:

$$E_{(X_{\sim i})}(G|X_i) = g_i(X_i)$$

Now for step 2:

We need to compute the variance of $g_i(X_i)$ with respect to X_i:

$$V_i = \mathrm{Var}_{(X_i)}[g_i(X_i)]$$

This is the same as the variance of $g_i(X_i)$ that we computed in the previous step:

$$V_i = \mathrm{Var}(g_i(X_i)) = E[g_i(X_i)^2] - (E[g_i(X_i)])^2$$

We already know that $E[g_i(X_i)] = 1$, so we need to calculate $E[g_i(X_i)^2]$:

$$E[g_i(X_i)^2] = \int_0^1 g_i(X_i)^2 \, dX_i$$

As before, we split the integral to handle the absolute value:

$$E[g_i(X_i)^2] = \int_0^{0.5} \left(\frac{2 - 4X_i + a_i}{1 + a_i} \right)^2 dX_i + \int_{0.5}^{1} \left(\frac{4X_i - 2 + a_i}{1 + a_i} \right)^2 dX_i$$

Evaluating these integrals, we get:

$$E[g_i(X_i)^2] = \frac{1}{(1 + a_i)^2} \left(\int_0^{0.5} (2 - 4X_i + a_i)^2 \, dX_i + \int_{0.5}^{1} (4X_i - 2 + a_i)^2 \, dX_i \right)$$

After evaluating the integrals, we find:

$$E[g_i(X_i)^2] = \frac{1}{(1 + a_i)^2} \left(\frac{1}{3} + a_i^2 \right)$$

Subtracting $E^2[g_i(X_i)] = 1$ from $E[g_i(X_i)^2]$, we get:

$$V_i = \frac{1}{(1 + a_i)^2} \left(\frac{1}{3} + a_i^2 \right) - 1$$

Simplifying, we find:

$$V_i = \frac{1}{3(1 + a_i)^2}$$

This is the variance due to each X_i, and it shows how the parameter a_i affects the sensitivity of the G function to the input X_i.