

Algorithms for Uncertainty Quantification

Tutorial 6: Polynomial chaos approximation 1: the pseudo-spectral approach

In this worksheet, we focus on the generalized polynomial chaos approximation and the pseudo-spectral approach.

Orthogonal polynomials

In the lecture, we saw that the generalized polynomial chaos (gPC) approximation is defined in terms of orthogonal polynomials. Given a weight function ρ , two polynomials $\phi_i(x)$ and $\phi_j(x)$ are called orthogonal with respect to ρ if

$$\langle \phi_i(x), \phi_j(x) \rangle_\rho = \int \phi_i(x) \phi_j(x) \rho(x) dx = \gamma_i \delta_{ij},$$

where $\gamma_i = \langle \phi_i(x), \phi_i(x) \rangle_\rho \in \mathbb{R}$ and δ_{ij} is Kronecker's delta function.

Two polynomials $\phi_i(x)$ and $\phi_j(x)$ are called orthonormal with respect to ρ if

$$\langle \phi_i(x), \phi_j(x) \rangle_\rho = \int \phi_i(x) \phi_j(x) \rho(x) dx = \delta_{ij}.$$

Note that orthogonal polynomials can be easily transformed into orthonormal polynomials via

$$\phi_i(x) := \frac{\phi_i(x)}{\sqrt{\gamma_i}}.$$

A scheme to compute orthogonal polynomials is Stieltjes' three-terms recursion relation

$$\begin{aligned}\phi_{-1}(x) &\equiv 0 \\ \phi_0(x) &\equiv 1 \\ \phi_{n+1}(x) &= (A_n x + B_n) \phi_n(x) - C_n \phi_{n-1}(x) \quad n \geq 0,\end{aligned}$$

where A_n, B_n, C_n are some constants.

Fortunately, we do not need to implement this scheme from scratch. In `chaospy`, it is easy to generate orthogonal polynomials based on a given probability distribution ρ . In the following code snippet, we assume that the underlying distribution is uniform. To generate orthogonal polynomials up to degree N , the `python + chaospy` syntax is

```
import chaospy as cp

# create a uniform distribution object
distr = cp.Uniform()

# generate N orthonormal polynomials based on distr
orth_poly = cp.orth_ttr(N, distr, normed=True)
# when you want unnormalized polynomials, i.e. normed=False, to
  compute the normalization constants, the syntax is
orth_poly, norm_consts = cp.orth_ttr(N, distr, retall=True)

# to compute the inner product, i.e. the expectation of the
  product of two polynomials of degrees i and j, use
expect = cp.E(orth_poly[i]*orth_poly[j], distr)
```

Assignment 1

Let $\rho_1 = \mathcal{U}(-1,1)$ and $\rho_2 = \mathcal{N}(10,1)$. Moreover, let $N = [2, 5, 8]$. Write a `python` program to generate orthonormal polynomials of degree up to N with respect to ρ_1 and ρ_2 . Check their orthonormality by computing $\langle \phi_i(x), \phi_j(x) \rangle_\rho$, $i, j = 0, \dots, N$, i.e. $\mathbb{E}[\phi_i(x) \cdot \phi_j(x)]$. What do you observe?

Probabilistic collocation: the pseudo-spectral approach

In the methodology that follows, the assumption is that the weight function ρ is a probability density function. In the lecture, we saw that, given a function $f(x, \omega)$, where x denotes the deterministic inputs and ω denotes the stochastic inputs, the degree N gPC approximation of f reads

$$f(x, \omega) \approx f^N(x, \omega) = \sum_{i=0}^{N-1} \hat{f}_i(x) \phi_i(\omega), \quad (1)$$

where $\phi_i(\omega)$, $i = 0, \dots, N - 1$ are orthogonal polynomials with respect to the probability distribution ρ of ω and $\hat{f}_i(x)$ are the expansion's coefficients. In this tutorial, we compute $\hat{f}_i(x)$ via

$$\hat{f}_i(x) = \int_{\text{supp}(\rho)} f(x) \phi_i(x) \rho(x) dx \approx \sum_{k=0}^{K-1} f(x_k) \phi_i(x_k) w_k, \quad (2)$$

where $\{x_k, w_k\}_{k=0}^{K-1}$ denotes the set of nodes and weights associated to ρ . For simplicity, we assume that the orthogonal polynomials are orthonormal. After we obtain the gPC expansion coefficients, statistics such as expectation and variance can be easily computed via

$$\mathbb{E}[f(x, \omega)] = \hat{f}_0(x), \quad \text{Var}[f(x, \omega)] = \sum_{i=1}^{N-1} \hat{f}_i^2(x). \quad (3)$$

Assignment 2

For fixed x , show that the mean of $f^N(x, \omega) = \sum_{i=0}^{N-1} \hat{f}_i(x) \phi_i(\omega)$ is given as

$$\mathbb{E}[f(x, \omega)] = \hat{f}_0(x) \quad (4)$$

and its variance as

$$\text{Var}[f(x, \omega)] = \sum_{i=1}^{N-1} \hat{f}_i^2(x). \quad (5)$$

Hint: $\phi_0(\omega) = 1$

Solution 2

$$\begin{aligned}\mathbb{E}[f^N(x, \omega)] &= \mathbb{E}\left[\sum_{i=0}^{N-1} \hat{f}_i(x) \phi_i(\omega)\right] \\ &= \sum_{i=0}^{N-1} \hat{f}_i(x) \mathbb{E}[\phi_i(\omega)] \\ &= \sum_{i=0}^{N-1} \hat{f}_i(x) \int_{\Omega} \phi_i(\omega) p_{\Omega}(\omega) d\omega \\ &= \sum_{i=0}^{N-1} \hat{f}_i(x) \int_{\Omega} \phi_i(\omega) \cdot 1 p_{\Omega}(\omega) d\omega \\ &= \sum_{i=0}^{N-1} \hat{f}_i(x) \int_{\Omega} \phi_i(\omega) \cdot \phi_0(\omega) p_{\Omega}(\omega) d\omega \\ (\phi_i(\omega) \text{ orthonormal}) &= \sum_{i=0}^{N-1} \hat{f}_i(x) \delta_{i0} \\ &= \hat{f}_0(x)\end{aligned}$$

$$\begin{aligned}
\text{Var}[f^N(x, \omega)] &= \mathbb{E}\left[\left(\sum_{i=0}^{N-1} \hat{f}_i(x)\phi_i(\omega) - \mathbb{E}[f^N(x, \omega)]\right)^2\right] \\
&= \mathbb{E}\left[\left(\sum_{i=0}^{N-1} \hat{f}_i(x)\phi_i(\omega) - \hat{f}_0(x)\right)^2\right] \\
&= \mathbb{E}\left[\left(\sum_{i=1}^{N-1} \hat{f}_i(x)\phi_i(\omega)\right)^2\right] \\
&= \mathbb{E}\left[\left(\sum_{i=1}^{N-1} \hat{f}_i(x)\phi_i(\omega)\right)\left(\sum_{i=1}^{N-1} \hat{f}_i(x)\phi_i(\omega)\right)\right] \\
(\text{defining } \hat{f}_i\phi_i &:= \hat{f}_i(x)\phi_i(\omega)) = \mathbb{E}[\hat{f}_1\phi_1\hat{f}_1\phi_1 + \hat{f}_1\phi_1\hat{f}_2\phi_2 + \cdots + \hat{f}_1\phi_1\hat{f}_{N-1}\phi_{N-1} + \\
&\quad \hat{f}_2\phi_2\hat{f}_1\phi_1 + \hat{f}_2\phi_2\hat{f}_2\phi_2 + \cdots + \hat{f}_2\phi_2\hat{f}_{N-1}\phi_{N-1} + \\
&\quad \vdots \\
&\quad \hat{f}_{N-1}\phi_{N-1}\hat{f}_1\phi_1 + \hat{f}_{N-1}\phi_{N-1}\hat{f}_2\phi_2 + \cdots + \hat{f}_{N-1}\phi_{N-1}\hat{f}_{N-1}\phi_{N-1}] \\
(\text{linearity of } \mathbb{E}:) &= \hat{f}_1\hat{f}_1\mathbb{E}[\phi_1\phi_1] + \hat{f}_1\hat{f}_2\mathbb{E}[\phi_1\phi_2] + \cdots + \hat{f}_1\hat{f}_{N-1}\mathbb{E}[\phi_1\phi_{N-1}] + \\
&\quad \vdots \\
&\quad \hat{f}_{N-1}\hat{f}_1\mathbb{E}[\phi_{N-1}\phi_1] + \hat{f}_{N-1}\hat{f}_2\mathbb{E}[\phi_{N-1}\phi_2] + \cdots + \hat{f}_{N-1}\hat{f}_{N-1}\mathbb{E}[\phi_{N-1}\phi_{N-1}] \\
&\quad (\mathbb{E}[\phi_i\phi_j] = \delta_{ij}:) = \sum_{i=1}^{N-1} \hat{f}_i^2
\end{aligned}$$

The pseudo-spectral approach in ChaosPy

It is straightforward to implement the gPC + pseudospectral approach in `chaospy`. The following code snippet assumes that the input probability distribution is uniform.

```

import chaospy as cp

# create a uniform distribution object
distr = cp.Uniform()

# generate K Gaussian nodes and weights based on distr

```

```

nodes , weights = cp.generate_quadrature(K, distr , rule='G')

# generate N orthonormal polynomials based on distr
orth_poly = cp.orth_ttr(N, distr , normed=True)
# when you want unnormalized polynomials , i.e. normed=False , to
  compute the normalization constants , the syntax is
orth_poly , norm_consts = cp.orth_ttr(N, distr , retall=True)

# assume that you evaluated your underlying model M at all
  quadrature nodes (see Eq. (2) and stored the values in a
  vector M_eval

# find the gPC approximation of your model M
gPC_M = cp.fit_quadrature(orth_poly , nodes , weights , M_eval)
# to return the gPC expansion coefficients , too
gPC_M , gPC_coeff = cp.fit_quadrature(orth_poly , nodes , weights ,
  M_eval , retall=True)

# finally , compute the expectation and the variance of your
  model M
expect = cp.E(gPC_M, distr)
var     = cp.Var(gPC_M, distr)

```

Assignment 3

Consider the model problem, the linear damped oscillator

$$\begin{cases} \frac{d^2y}{dt^2}(t) + c\frac{dy}{dt}(t) + ky(t) = f \cos(\omega t) \\ y(0) = y_0 \\ \frac{dy}{dt}(0) = y_1. \end{cases} \quad (6)$$

Considering $t \in [0, 20]$, $\Delta t = 0.01$, $c = 0.5$, $k = 2.0$, $f = 0.5$, $y_0 = 0.5$, $y_1 = 0.0$, use the `odeint`¹ function from `scipy.integrate` to discretize the model from Eq. (6). For the upcoming experiments, the output that we are interested in is $y(10)$. Assume that $\omega \sim \mathcal{U}(0.95, 1.05)$. Write a python program to propagate the uncertainty in ω through the model in Eq. (6) using the gPC expansion method from Eq. (1). Compute the expansion

¹see <https://docs.scipy.org/doc/scipy-0.17.0/reference/generated/scipy.integrate.odeint.html>

coefficients from Eq. (2) using the pseudo-spectral approach. Consider $K = [2, 4, 6]$ and $N = [1, 2, 3]$; the correspondence is one-to-one. Initially, write your own implementation of the pseudo-spectral approach. Afterwards, use `chaospy`'s `fit_quadrature` function. Based on these coefficients, compute the expectation and the variance of $y(10)$.