Introduction to Uncertainty Quantification (UQ)

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FLOW Winter School on Machine Learning and Data-Driven Methods

HANDS-ON, PCE

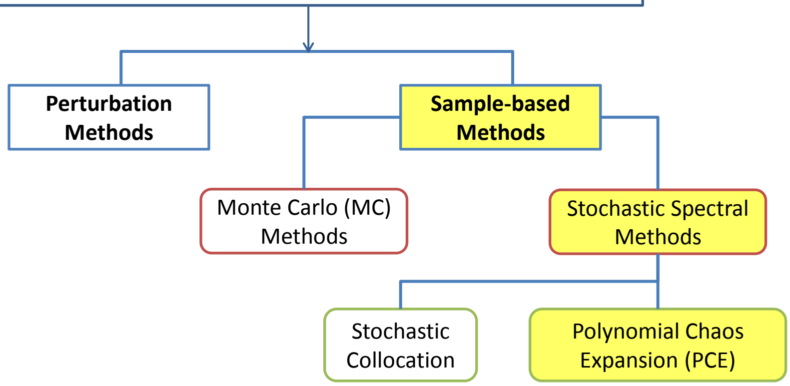
… Recap

UQ FWD Problem - Roadmap

- Estimates for mean and variance of the model response:

$$\mathbb{E}[f(\chi,\mathbf{q})] := \mu = \int_{\mathbb{Q}} f(\chi,\mathbf{q})\rho_{\mathbf{Q}}(\mathbf{q})\mathrm{d}\mathbf{q}$$

$$\mathbb{V}[f(\chi,\mathbf{q})] = \int_{\mathbb{Q}} \left(f(\chi,\mathbf{q})^2 - \mu^2\right)\rho_{\mathbf{Q}}(\mathbf{q})\mathrm{d}\mathbf{q}$$



Polynomial Chaos Expansion (PCE)

- PCE is widely used in UQ studies.
- PCE can be very efficient.
- PCE: Spectral representation of a stochastic problem:

$$\tilde{f}(\chi,q) = \sum_{k=0}^{K} \hat{f}_k(\chi)\psi_k(q)$$

Coefficients,
to be determined

Bases are chosen

Outline

1. Basics
2. How to choose the bases
3. Extension to multi-dimensional parameter space (in Hands-on)
4. How to implement PCE and compute the coefficients

See e.g. Le Maitre and Knio 2010, Xiu 2007, Xiu and Karniadakis 2002, 2003, Smith 2014, McClarren 2018

PCE

➢ **Basics**

- Consider a random variable $\xi \in \Gamma$
- For two functions $f(\xi),\, g(\xi)$ in a Hilbert space, the following weighted inner product is defined:

$$\langle f(\xi),\, g(\xi)\rangle_\rho = \int_{\mathrm{supp}(\rho)} f(\xi) g(\xi) \rho(\xi) \mathrm{d}\xi$$

- **Orthogonality** w.r.t. $\rho(\xi)$: $\langle f(\xi),\, g(\xi)\rangle_\rho = 0$

PCE

➢ **Basics**

- Consider a set of bases $\{\psi_i(\xi)\}_{i=0}^{N-1}$ which are

1. Orthogonal w.r.t $\rho(\xi)$

$$\langle \psi_i(\xi),\, \psi_j(\xi)\rangle_\rho = \int_{\mathrm{supp}(\rho)} \psi_i(\xi)\psi_j(\xi)\rho(\xi)\mathrm{d}\xi = \gamma_i \delta_{ij}$$

$$\gamma_i = \langle \psi_i(\xi)\psi_i(\xi)\rangle_\rho$$

Kronecker Delta

2. For the first basis: $\mathbb{E}(\psi_0(\xi)) = \int_{\mathrm{supp}(\rho)} \psi_0(\xi)\rho(\xi)\mathrm{d}\xi = 1$

Recall, PCE: $\tilde{f}(\chi, \xi) = \sum_{k=0}^{K} \hat{f}_k(\chi)\psi_k(\xi)$

PCE-Choose the Bases

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➢ **How to choose the bases?**

- To get the fastest convergence in the expansion, optimal bases are chosen corresponding to the distribution.

Distribution	Density, $\rho(\xi)$	Polynomial	Support Range
Uniform	$\frac{1}{2}$	Legendre	$[-1,1]$
*Normal	$\frac{1}{\sqrt{2\pi}}e^{\frac{-\xi^2}{2}}$	Hermite	$[-\infty,\infty]$
Beta	$\frac{(1-\xi)^\alpha(1+\xi)^\beta}{2^{\alpha+\beta+1}B(\alpha+1,\beta+1)}$	Jacobi	$[-1,1]$
Exponential	$e^{-\xi}$	Laguerre	$[0,\infty]$
Gamma	$\frac{\xi^\alpha e^{-\xi}}{\Gamma(\alpha+1)}$	Generalized Laguerre	$[0,\infty]$

See Xiu and Karniadakis 2002 and Eldred & Burkardt 2009
* Weiner 1938

- Standardize the uncertain parameter to use Weiner-Askey scheme:

$$\begin{cases} q\sim\mathcal{U}[a,b] \\ \xi=-1+2(q-a)/(b-a) \end{cases} \Rightarrow \xi\sim\mathcal{U}[-1,1]$$

$$\begin{cases} q\sim\mathcal{N}(\mu,\sigma) \\ q=\mu+\sigma\xi \end{cases} \Rightarrow \xi\sim\mathcal{N}(0,1)$$

PCE-Legendre Polynomials

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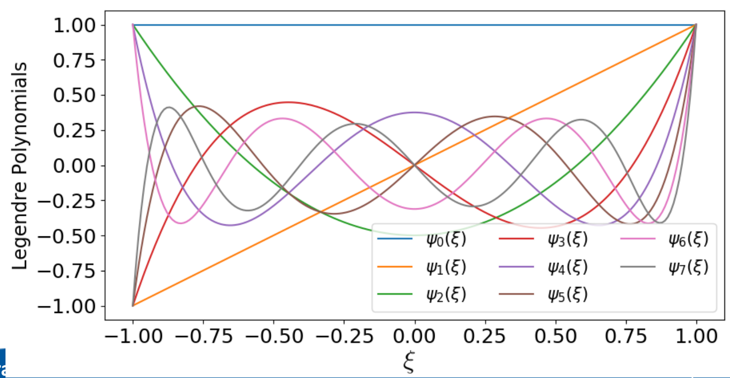
Example: Legendre polynomials

$$\begin{aligned}
\psi_0(\xi) &= 1 \\
\psi_1(\xi) &= \xi \\
\psi_2(\xi) &= (3\xi^2-1)/2 \\
\psi_3(\xi) &= (5\xi^3-3\xi)/2 \\
\psi_4(\xi) &= (35\xi^4-30\xi^2+3)/8
\end{aligned}$$



Non-Intrusive PCE-Pseudo-Spectral Method

- No need to change the deterministic code
- Take n samples from parameter space and evaluate model function at each

$$\mathcal{R}^{(i)} = f(\chi, \mathbf{q}^{(i)}), \quad i = 1, 2, \cdots, n$$

➢ **Pseudo-spectral or Discrete Projection Method** $\tilde{f}(\chi, \boldsymbol{\xi}) = \sum_{k=0}^{K} \hat{f}_k(\chi)\Psi_k(\boldsymbol{\xi})$

$$\begin{aligned}
\hat{f}_k(\chi) &= \frac{\langle f(\chi,\boldsymbol{\xi})\Psi_k(\boldsymbol{\xi})\rangle_\rho}{\langle \Psi_k(\boldsymbol{\xi})\Psi_k(\boldsymbol{\xi})\rangle_\rho} \qquad \text{(weighted projection)} \\
&= \frac{\int_\Gamma f(\chi,\boldsymbol{\xi})\Psi_k(\boldsymbol{\xi})\rho(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi}}{\int_\Gamma \Psi_k(\boldsymbol{\xi})\Psi_k(\boldsymbol{\xi})\rho(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi}} = \frac{\mathbb{E}[f(\chi,\boldsymbol{\xi})\Psi_k(\boldsymbol{\xi})]}{\mathbb{E}[\Psi_k(\boldsymbol{\xi})\Psi_k(\boldsymbol{\xi})]} \\
&\approx \frac{\sum_i \mathcal{R}^{(i)}\Psi_k(\boldsymbol{\xi}^{(i)})W_i}{\sum_i \Psi_k(\boldsymbol{\xi}^{(i)})\Psi_k(\boldsymbol{\xi}^{(i)})W_i} \quad \longleftarrow \quad \text{Quadrature Rule}
\end{aligned}$$

- Samples: Quadrature nodes
- e.g. Gauss-Legendre, Gauss-Hermite, … rules

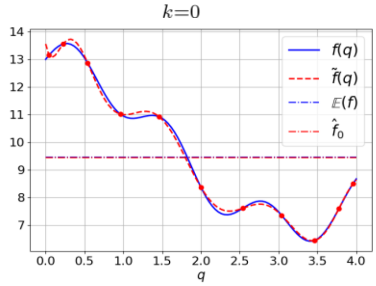
Recall: Using m quadrature nodes, polynomials up to degree (2m-1) can be exactly integrated.

- Curse of dimensionality: $K+1 = \prod_{i=1}^{p} n_i$ (Full-tensor product)

PCE – Estimated Statistics

1. Use sampling approaches for $\tilde{f}(\chi, q)$, see e.g. *
2. Use analytical estimates (here) †

$$\tilde{f}(\chi, \boldsymbol{\xi}) = \sum_{k=0}^{K} \hat{f}_k(\chi)\Psi_k(\boldsymbol{\xi})$$



$$\begin{aligned}
\mathbb{E}(\tilde{f}(\chi,\boldsymbol{\xi})) &= \mathbb{E}\left(\sum_{k=0}^{K}\hat{f}_k(\chi)\Psi_k(\boldsymbol{\xi})\right) \\
&= \hat{f}_0(\chi) \\
\mathbb{V}(\tilde{f}(\chi,\boldsymbol{\xi})) &= \mathbb{E}\left(\left(\sum_{k=0}^{K}\hat{f}_k(\chi)\Psi_k(\boldsymbol{\xi}) - \hat{f}_0(\boldsymbol{\xi})\right)^2\right) \\
&= \mathbb{E}\left(\left(\sum_{k=1}^{K}\hat{f}_k(\chi)\Psi_k(\boldsymbol{\xi})\right)^2\right) \\
&= \sum_{k=1}^{K}\hat{f}_k^2(\chi)\gamma_k \quad \text{where} \quad \gamma_k = \langle \Psi_k(\boldsymbol{\xi}), \Psi_k(\boldsymbol{\xi})\rangle_\rho
\end{aligned}$$

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* Eldred and Burkardt J. 2009

† see Xiu and Karniadakis 2003, Le Maitre and Knio 2010, Smith 2014, McClarren 2018

Tasks 1, 2

1. For the 1D parameter q, estimate mean and variance of an algebraic model function using PCE method. To this end, complete the missing lines in `pce1D(…)`
2. Study the convergence of the estimated moments to the corresponding exact values as number of samples (in both PCE and MC) increases.

PCE-Multi-dimensional parameter space

- **Extension to p-D parameter space**
  - Consider $\mathbf{q}=\{q_1,q_2,\cdots,q_p\}, \qquad q_i \in \mathbb{Q}_i$
  - Therefore, $\mathbf{q}\in\mathbb{Q}\subset\mathbb{R}^p$ where $\mathbb{Q}=\otimes_{i=1}^p \mathbb{Q}_i$
  - Assume parameters are <u>independent</u>, therefore,

$$\rho_{\mathbf{Q}}(\mathbf{q})=\prod_{i=1}^p \rho_{Q_i}(q_i)$$

  - Map $q_i \to \xi_i$ and $\mathbb{Q}_i \to \Gamma_i \Rightarrow \Gamma=\otimes_{i=1}^p \Gamma_i$

PCE: $\tilde{f}(\chi,\boldsymbol{\xi})=\sum_{k=0}^{K}\hat{f}_k(\chi)\Psi_k(\boldsymbol{\xi})\,,\ \Psi_k(\boldsymbol{\xi})=\psi_{k_1}(\xi_1)\psi_{k_2}(\xi_2)\cdots\psi_{k_p}(\xi_p)$

1. Create index set and specify truncation of the expansion
2. Choose the bases
3. Compute the unknown coefficients

See e.g. Le Maitre and Knio 2010; Xiu 2007; Xiu and Hesthaven 2005

PCE – Index Set & Truncation

$$\tilde{f}(\chi, \boldsymbol{\xi}) = \sum_{k=0}^{K} \hat{f}_k(\chi)\Psi_k(\boldsymbol{\xi}) \, , \; \Psi_k(\boldsymbol{\xi}) = \psi_{k_1}(\xi_1)\psi_{k_2}(\xi_2)\cdots\psi_{k_p}(\xi_p)$$

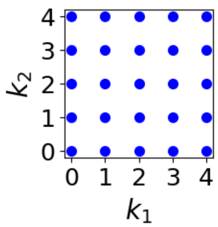
L_i : Maximum polynomial order in *i*-th parameter space

$\mathbf{k} = \{k_1, k_2, \cdots, k_p\}$: Multi-index

- **Tensor Product**

Index set=$\{\mathbf{k} : \max_{1 \le i \le p} k_i \le L_i\}$

$$K + 1 = \prod_{i=1}^{p}(L_i + 1)$$



Ex.

$L_1 = L_2 = 4 \Rightarrow K = 24$

$k_1, k_2 = \{0, 1, 2, 3, 4\}$

$$\begin{aligned} \Psi_0(\boldsymbol{\xi}) &= \psi_0(\xi_1)\psi_0(\xi_2) \\ \Psi_1(\boldsymbol{\xi}) &= \psi_1(\xi_1)\psi_0(\xi_2) \\ &\cdots \\ \Psi_{24}(\boldsymbol{\xi}) &= \psi_4(\xi_1)\psi_4(\xi_2) \end{aligned}$$

Task 3 (Extra)

1. Complete `PCE2D_TP_constructor()` to construct a PCE for Rosenbrock's function. Consider tensor product over the parameter space.

$$f(q_1, q_2) = 100(q_2 - q_1^2)^2 + (1 - q_1)^2$$

$$q_1, \, q_2 \sim \mathcal{U}[-2, 2]$$

2. If the exact $\mathbb{E}[f(q_1, q_2)] = 455.6666$, plot the reduction of the error in the estimated mean value when increasing the number of samples.