Polynomial Chaos Expansion

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Literature

Based on

- Asmussen, Søren, Pierre-Olivier Goffard, und Patrick J. Laub. „Orthonormal Polynomial Expansions and Lognormal Sum Densities“. In *Risk and Stochastics*, von Pauline Barrieu. WORLD SCIENTIFIC (EUROPE), 2019. https://doi.org/10.1142/9781786341952_0008.
- Sudret, Bruno. *Polynomial Chaos Expansions in 90 Minutes*. ETH Zurich, 7. Oktober 2021, 101 p. Application/pdf, 101 p. https://doi.org/10.3929/ETHZ-B-000508852.
- Sudret, B., Marelli, S., & Wiart, J. (2017). Surrogate models for uncertainty quantification: An overview. *2017 11th European Conference on Antennas and Propagation (EUCAP)*, 793–797. https://doi.org/10.23919/EuCAP.2017.7928679
- Sudret, B. (2016). *Uncertainty propagation using polynomial chaos expansions*.

Notation

- Input random variables: joint PDF $f_{\mathrm{X}}(x)$ (in our case, independently sampled)
- Response: $\mathcal{M}\left(\mathbf{x}^{(\mathbf{i})}\right)$
- Response sample set: $\mathbf{M} = \{\mathcal{M}\left(\mathbf{x}^{(1)}\right), \mathcal{M}\left(\mathbf{x}^{(2)}\right), \ldots, \mathcal{M}\left(\mathbf{x}^{(n)}\right)\}^{\top}$

See Sudret (2021).

Idea

We can expand the random model response as an infinite series:

$$Y = \sum_{\alpha \in \mathbb{N}^d} y_\alpha \Psi_\alpha(\boldsymbol{X})$$

with

- $\Psi_\alpha(X)$: basic functions (multivariate orthonormal polynomials)
- y_α: coefficients to be computed (“coordinates”)
- In particular, the coordinates are not our quantities of interest.

Taken and abridged from Sudret (2021).

Orthogonal polynomials

- In PCA the distributions of the input variables are associated with a family of orthogonal polynomials
- Only for a few distributions, the corresponding orthogonal polynomials are known

- Standard distributions and orthogonal polynomials:

Distribution	Orthogonal Polynomial
Normal	Hermite
Uniform	Legendre
Exponential	Laguerre
Beta	Jacobi

Orthogonal polynomials: Other distributions

- We may transform input variables from other distributions so that we obtain variables from distributions with known orthogonal polynomials
- **Isoprobabilistic transforms** transform any samples from a random variable with continuous distribution to a sample from a simpler distribution, e.g. Uniform or Normal, of which we know the orthogonal polynomials.

For our project:

- Lognormal to $\mathcal{N}(0, 1)$ (Hermite Polynomial)
- $\mathcal{U}[a, b]$ to $\mathcal{U}[-1, 1]$ (Legendre Polynomial)
- Gumbel to $\mathcal{U}[-1, 1]$ (Legendre Polynomial)

Other methods to obtain orthogonal polynomials

1. Use orthogonal polynomials derived in research papers for certain distributions (for example orthogonal polynomial for lognormal distribution from Asmussen et al. 2019)

2. Numerical Methods

Other methods Lognormal

Theorem 1.1. *The polynomials orthonormal with respect to the lognormal distribution are given by*

$$Q_k(x) = \frac{\mathrm{e}^{-\frac{k^2\sigma^2}{2}}}{\sqrt{\left[\mathrm{e}^{-\sigma^2}, \mathrm{e}^{-\sigma^2}\right]_k}} \sum_{i=0}^{k} (-1)^{k+i} \mathrm{e}^{-i\mu - \frac{i^2\sigma^2}{2}} e_{k-i}\left(1, \ldots, \mathrm{e}^{(k-1)\sigma^2}\right) x^i, \tag{1.2.10}$$

for $k \in \mathbb{N}_0$ *where*

$$e_i\left(X_1, \ldots, X_k\right) = \begin{cases} \sum_{1 \le j_1 < \ldots < j_i \le k} X_{j_1} \ldots X_{j_i}, & \text{for } i \le k, \\ 0, & \text{for } i > k, \end{cases} \tag{1.2.11}$$

are the elementary symmetric polynomials and $[x, q]_n = \prod_{i=0}^{n-1}\left(1 - xq^i\right)$ *is the Q-Pochhammer symbol.*

Source: Asmussen et al. (2019).

Choose number of multivariate polynomials

- In practice, we can't compute infinite series expansion, thus we need to truncate

Standard procedure:

N...sample size

n...number of input variables

P...number of multivariate polynomials

p...highest polynomial order

$$P = \binom{n+p}{p} \qquad N \geq P$$

Taken from Sudret (2021)

Choose number of multivariate polynomials

In our project, we have:

N = 200

n = 7

Thus, we may choose p = 2 or p = 3, resulting in

$$\mathrm{P} = \binom{9}{2} = 36 \text{ or } \mathrm{P} = \binom{10}{3} = 120$$

See Sudret (2021).

How to estimate the PCE?

- We have from slide 4 that we can write our model as an infinite series.
- In estimation, we regard this expansion as the sum of a truncated series and a residual:

$$Y \coloneqq \mathcal{M}(\boldsymbol{X}) = \sum_{\alpha \in \mathcal{A}} y_{\alpha} \Psi_{\alpha}(\boldsymbol{X}) + \varepsilon_P \equiv \boldsymbol{Y}^{\top} \boldsymbol{\Psi}(\boldsymbol{X}) + \varepsilon_P(\boldsymbol{X})$$

$$\boldsymbol{Y} = \{y_{\alpha}, \boldsymbol{\alpha} \in \mathcal{A}\} \equiv \{y_0, y_1, \dots, y_{P-1}\}$$

$$\boldsymbol{\Psi}(\boldsymbol{x}) = \{\Psi_0(\boldsymbol{x}), \Psi_1(\boldsymbol{x}), \dots, \Psi_{\mathrm{P}-1}(\boldsymbol{x})\}$$

$$\boldsymbol{\varepsilon}_{\mathbf{P}}(\boldsymbol{X}) = \mathcal{M}(\boldsymbol{X}) - \sum_{\alpha \in \mathcal{A}} y_{\alpha} \Psi_{a}(\boldsymbol{X})$$

Taken and abridged from Sudret (2021).

How to estimate the PCE?

The estimation problem reduces to a least-square minimisation:

$$\widehat{\mathrm{Y}} = \arg\min_{\mathrm{y}_\alpha} \mathrm{E}[\varepsilon_P^2(\boldsymbol{X})] = \arg\min_{\mathrm{y}_\alpha} \mathrm{E}[(\boldsymbol{Y}^\top \boldsymbol{\Psi}(\boldsymbol{X}) - \mathcal{M}(\boldsymbol{X}))^2]$$

We can solve this using that the coefficient y_α is the projection of the model onto $\Psi_\alpha(\boldsymbol{X})$:

$$\hat{\mathrm{y}}_\alpha = \mathrm{E}[\mathcal{M}(\boldsymbol{X})\Psi_\alpha(\boldsymbol{X})]$$

Taken and abridged from Sudret (2021, 2016).

Summary of the least-squares estimation

1. Collect the model responses for the design points:

$$M = \{\mathcal{M}(\boldsymbol{x}^{(1)}), \mathcal{M}(\boldsymbol{x}^{(2)}), \dots, \mathcal{M}(\boldsymbol{x}^{(n)})\},$$

where the $\boldsymbol{x}^{(i)}$ are the design points of the experimental design

2. Compute the *experimental matrix*:

$$A_{ij} = \Psi_{\mathrm{j}}\left(\boldsymbol{x}^{(i)}\right), \quad i = 1, \dots, n; \quad j = 0, \dots, P-1,$$

where the Ψ_{j} are the basic functions.

3. Solve the linear system:

$$\widehat{\boldsymbol{Y}} = (\boldsymbol{A}^{\top}\boldsymbol{A})^{-1}\boldsymbol{A}^{\top}\boldsymbol{M}$$

See Sudret (2021).

What next?

- We are not really interested in the coefficients of the PCE
- Rather, we want to get statistics from the distribution of our response.

Mean value and variance

As the basic functions are orthonormal, we have that

$$\mathrm{E}[\Psi_{\alpha}(\boldsymbol{X})] = 0, \qquad \mathrm{E}[\Psi_{\alpha}(\boldsymbol{X})\Psi_{\beta}(\boldsymbol{X})] = 0, \alpha \neq \beta$$

Thus, we get

$$\mu_Y = y_0$$

$$\widehat{\sigma}_{\alpha}^2 = \sum_{\alpha \in \mathcal{A} \setminus \mathbf{0}} y_{\alpha}^2$$

See Sudret (2021).

Approximating the PDF

- We can consider the polynomial series expansion as an *analytical function of the input variables* after the isoprobabilistic transform, $\boldsymbol{\xi}$
- We draw a large sample set from $\boldsymbol{\xi}$ of size $10^5 \leq n_{sim} \leq 10^6$:

$$\mathcal{X}_{sim} = \{\boldsymbol{\xi}_j, j = 1, \ldots, n_{sim}\}$$

- We simulate response values using our coordinates and base functions:

$$\mathcal{Y} = \{\mathscr{y}_j = \sum_{\alpha \in \mathcal{A}} y_\alpha \, \Psi_\alpha(\boldsymbol{\xi}_j), \qquad j = 1, \ldots, n_{sim}\}$$

- In a last step, we use kernel density estimation to get a „smooth“ PDF:

$$\hat{f}_Y(y) = \frac{1}{n_{sim} h} \sum_{j=1}^{n_{sim}} K\left(\frac{y - \mathscr{y}_j}{h}\right)$$

with a $\mathcal{N}(0, 1)$ kernel and some bandwidth h.

See Sudret (2021).