A Variance-based Spectral Method
Polynomial Chaos Expansion: Part I

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- Why PCE? The main idea
- Why PCE? A simple example

PCE for any function

- PCE in 1-2 dimension
- PCE in d-dimension

Why PCE?
The Main Idea

Why PCE?- The Main Idea

The ANOVA representation: If $\mathbb{E}\left[f^2(\boldsymbol{u})\right] < +\infty$ with $\boldsymbol{u} = (u_1, u_2, u_3)$ a vector of independent input random variables, then we can always write:

$$f(u_1, u_2, u_3) = f_0 + f_1(u_1) + f_2(u_2) + f_3(u_3) + \dots$$
$$f_{12}(u_1, u_2) + f_{13}(u_1, u_3) + f_{23}(u_2, u_3) + f_{123}(u_1, u_2, u_3)$$

where $\mathbb{E}\left[f_{\boldsymbol{\alpha}}(\boldsymbol{u}) f_{\boldsymbol{\beta}}(\boldsymbol{u})\right] = V_{\boldsymbol{\alpha}} \delta_{\boldsymbol{\alpha}\boldsymbol{\beta}}$, with $\boldsymbol{\alpha}, \boldsymbol{\beta} \subseteq (1, 2, 3)$

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Consequently, we obtain the variance decomposition:
$$\mathrm{Var}\left[f(\boldsymbol{u})\right] = 0 + V_1 + V_2 + V_3 + V_{12} + V_{13} + V_{23} + V_{123}$$

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Polynomial chaos expansion (the present talk) tries to estimate $f_{\boldsymbol{\alpha}}, \forall \boldsymbol{\alpha} \subseteq (1, 2, 3) \rightarrow$ Computationally cheap

Why PCE ?
A simple example

Why PCE?- A simple example

Consider the following model, $f(\boldsymbol{u}) = u_1 + 10\left(u_2 - \frac{1}{2}\right)\left(u_3 - \frac{1}{2}\right)$ with $u_j \sim \mathcal{U}(0,1)$

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Let us make the following transformation:
$\psi_1(u_j) = \sqrt{3}(2u_j - 1) \Leftrightarrow u_j = \frac{\psi_1(u_j)+\sqrt{3}}{2\sqrt{3}} = \frac{\psi_1(u_j)}{2\sqrt{3}} + \frac{1}{2}$

Note that,

$$\mathbb{E}\left[\psi_1(u_j)\right] = \int_0^1 \sqrt{3}(2u_j - 1)\mathrm{d}u_j = 0 \text{ centered}$$

$$\mathrm{Var}\left[\psi_1(u_j)\right] = \int_0^1 \left(\sqrt{3}(2u_j - 1)\right)^2 \mathrm{d}u_j = 1 \text{ normalised}$$

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Because $\mathbb{E}\left[\psi_1(u_j)\right] = 0$ we obtain, the following ANOVA decomposition:

$$f(\boldsymbol{u}) = \frac{1}{2} + \frac{\psi_1(u_1)}{2\sqrt{3}} + 10\left(\frac{\psi_1(u_2)}{2\sqrt{3}}\right)\left(\frac{\psi_1(u_3)}{2\sqrt{3}}\right)$$

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The PC representation of $f(\boldsymbol{u}) = u_1 + 10\left(u_2 - \frac{1}{2}\right)\left(u_3 - \frac{1}{2}\right)$ with $u_j \sim \mathcal{U}(0,1)$

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$S_1 + S_{23} = 1$ the function is non-additive and $S_1 = T_1$, $T_2 = T_3 = S_{23}$

What-if the function
is non-polynomial?

1D

The 1-dimensional case:

Consider the following polynomials:
$L_0 = 1$
$L_1(x) = \sqrt{3}x$
$L_2(x) = \frac{\sqrt{5}}{2}\left(3x^2 - 1\right)$
known as the first three (normalised) Legendre polynomials

1D

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If $x \sim \mathcal{U}(-1,1)$, then, we have the following properties:

$$\mathbb{E}\left[L_j(x)\right] = \frac{1}{2}\int_{-1}^{1} L_j(x)\mathrm{d}x = 0,\ \forall j > 0 \qquad \text{(centered)}$$

$$\mathrm{Var}\left[L_j(x)\right] = \frac{1}{2}\int_{-1}^{1} L_j^2(x)\mathrm{d}x = 1,\ \forall j > 0 \qquad \text{(normalised)}$$

Consequently, $\mathbb{E}\left[L_i(x)L_j(x)\right] = \delta_{ij}$ (orthonormality)

1D

For some probability law of x, $\exists$ an infinite polynomial set that satisfies the previous properties called a **polynomial chaos**.

For instance, $x \sim \mathcal{N}(0,1) \rightarrow$ (normalised) Hermite polynomials:
$H_0 = 1$
$H_1(x) = x$
$H_2(x) = \sqrt{2}\left(x^2 - 1\right)$
$\vdots$

For instance, $x \sim \Gamma(a,1), (x,a) > 0 \rightarrow$ (normalised) Laguerre polynomials: $L_0^{(a)} = 1$
$L_1^{(a)}(x) = \frac{1}{\sqrt{\Gamma(1+a)}}\left(x - a\right)$
$L_2^{(a)}(x) = \frac{1}{\sqrt{\Gamma(2+a)}}\left(\frac{1}{2}x^2 - (1+a)x - \frac{1}{2}a(1+a)\right)$
$\vdots$ see Xiu & Karniadakis (2002) for other RVs.

1D

RV arbitrary distributed: Let $x \sim p_x$ be arbitrary distributed and denote F_x its associated CDF. If you ignore the orthogonal polynomial basis associated to p_x, then choose one of the following options,

- Transform $x \sim p_x$ into $u \sim \mathcal{U}(0,1)$ with the integral transformation $u = F_x(x)$, and cast $y = f(u)$ onto the shifted-Legendre polynomial
- Build the orthogonal polynomial up to degree p with the modified Gram-Schmidt transformation

In Siml@b, the second option is used.

1D

For any $\mathcal{M} : \mathbb{E}\left[\mathcal{M}^2(x)\right] < +\infty$, it is possible to write,

$$\mathcal{M}(x) = \sum_{\alpha \in \mathbb{N}} a_\alpha \psi_\alpha(x)$$

where ψ_α denotes one possible polynomial chaos family of degree α. This is called a **polynomial chaos expansion (PCE).**

N.B.: The rate of convergence of the series depends on the smoothness of f (see Cameron & Martin, 1947).

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Advantage of such a representation: Any statistical moment of $\mathcal{M}(x)$ can be easily computed

$\mathbb{E}\left[\mathcal{M}(x)\right] = a_0$

$\mathbb{E}\left[\mathcal{M}^2(x)\right] = \sum_{\alpha \in \mathbb{N}} a_\alpha^2$

$\mathrm{Var}\left[\mathcal{M}(x)\right] = \sum_{\alpha \in \mathbb{N}} a_\alpha^2 - a_0^2$

$\vdots$

2D

The 2-dimensional case:

Let $\mathcal{M} : \mathbb{E}\left[\mathcal{M}^2(x_1, x_2) < +\infty\right]$ with $x_1 \sim \mathcal{U}(-1, 1)$ and $x_2 \sim \mathcal{N}(0, 1)$, then, we can write

$$\mathcal{M}(x_1, x_2) = \sum_{(\alpha_1, \alpha_2) \in \mathbb{N}^2} a_{\alpha_1 \alpha_2} \psi_{\alpha_1 \alpha_2}(x_1, x_2)$$

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that we simply write,

$$\mathcal{M}(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha}\in\mathbb{N}^2} a_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$$

with $\boldsymbol{x} = (x_1, x_2)$, $\boldsymbol{\alpha} = \alpha_1\alpha_2$ and $\psi_{\alpha_1\alpha_2}(\boldsymbol{x}) = L_{\alpha_1}(x_1)H_{\alpha_2}(x_2)$

L_{α_1}: α_1-th Legendre polynomial degree
H_{α_2}: α_2-th Hermite polynomial degree

2D

Once again we can compute:

$\mathbb{E}\left[\mathcal{M}(\boldsymbol{x})\right] = a_{00}$

$\mathrm{Var}\left[\mathcal{M}(\boldsymbol{x})\right] = \sum_{\boldsymbol{\alpha}\in\mathbb{N}^2} a_{\boldsymbol{\alpha}}^2 - a_{00}^2$

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Further, we can show that

$\mathbb{E}\left[\mathcal{M}(\boldsymbol{x})|x_1\right] = \sum_{\alpha_1\in\mathbb{N}} a_{\alpha_1 0}\psi_{\alpha_1 0}(x_1, x_2) = \sum_{\alpha_1\in\mathbb{N}} a_{\alpha_1 0} L_{\alpha_1}(x_1)$

$\mathbb{E}\left[\mathcal{M}(\boldsymbol{x})|x_2\right] = \sum_{\alpha_2\in\mathbb{N}} a_{0\alpha_2}\psi_{0\alpha_2}(x_1, x_2) = \sum_{\alpha_2\in\mathbb{N}} a_{0\alpha_2} H_{\alpha_2}(x_2)$

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This is important for assessing the first-order effect:

$S_i = \frac{\mathrm{Var}[\mathbb{E}[\mathcal{M}(\boldsymbol{x})|x_i]]}{\mathrm{Var}[\mathcal{M}(\boldsymbol{x})]}$

2D

The ANOVA decomposition:

Recalling the ANOVA decomposition of $\mathcal{M}$,

$$\mathcal{M}(\boldsymbol{x}) = \mathcal{M}_0 + \mathcal{M}_1(x_1) + \mathcal{M}_2(x_2) + \mathcal{M}_{12}(x_1, x_2)$$

with $\mathbb{E}\left[\mathcal{M}(\boldsymbol{x})\right] = \mathcal{M}_0$

$\mathbb{E}\left[\mathcal{M}(\boldsymbol{x})|x_1\right] = \mathcal{M}_1(x_1) + \mathcal{M}_0$

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$\mathbb{E}\left[\mathcal{M}(\boldsymbol{x})|x_2\right] = \mathcal{M}_2(x_2) + \mathcal{M}_0$

We see that $\mathcal{M}_0 = a_{00}$

$\mathcal{M}_1(x_1) = \sum_{\alpha_1 \in \mathbb{N}^*} a_{\alpha_1 0} L_{\alpha_1}(x_1) \rightarrow$ main effect of x_1

$\mathcal{M}_2(x_2) = \sum_{\alpha_2 \in \mathbb{N}^*} a_{0\alpha_2} H_{\alpha_2}(x_2) \rightarrow$ main effect of x_2

$\mathcal{M}_{12}(x_1, x_2) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^* \times \mathbb{N}^*} a_{\alpha_1\alpha_2} \psi_{\alpha_1\alpha_2}(x_1, x_2) \rightarrow$ interaction effect

2D

The Sobol' sensitivity indices:

It is straightforward to compute the Sobol' indices,

$$S_1 = \frac{\mathrm{Var}\left[\mathbb{E}\left[\mathcal{M}(\boldsymbol{x})|x_1\right]\right]}{\mathrm{Var}\left[\mathcal{M}(\boldsymbol{x})\right]} = \frac{\mathrm{Var}\left[\mathcal{M}_1(x_1)\right]}{\mathrm{Var}\left[\mathcal{M}(\boldsymbol{x})\right]} = \frac{\sum_{\alpha_1\in\mathbb{N}^*} a_{\alpha_1 0}^2}{\sum_{\boldsymbol{\alpha}\in\mathbb{N}^2} a_{\boldsymbol{\alpha}}^2 - a_{00}^2}$$

2D

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$$S_2 = \frac{\mathrm{Var}\left[\mathbb{E}\left[\mathcal{M}(\boldsymbol{x})|x_2\right]\right]}{\mathrm{Var}\left[\mathcal{M}(\boldsymbol{x})\right]} = \frac{\mathrm{Var}\left[\mathcal{M}_2(x_2)\right]}{\mathrm{Var}\left[\mathcal{M}(\boldsymbol{x})\right]} = \frac{\sum_{\alpha_2 \in \mathbb{N}^*} a_{0\alpha_2}^2}{\sum_{\boldsymbol{\alpha} \in \mathbb{N}^2} a_{\boldsymbol{\alpha}}^2 - a_{00}^2}$$

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$$S_{12} = \frac{\mathrm{Var}\left[\mathcal{M}_{12}(x_1, x_2)\right]}{\mathrm{Var}\left[\mathcal{M}(\boldsymbol{x})\right]} = \frac{\sum_{\boldsymbol{\alpha} \in \mathbb{N}^* \times \mathbb{N}^*} a^2_{\alpha_1 \alpha_2}}{\sum_{\boldsymbol{\alpha} \in \mathbb{N}^2} a^2_{\boldsymbol{\alpha}} - a^2_{00}}$$

knowing the PCE coefficients $a_{\boldsymbol{\alpha}}$.

The d-dimensional PCE

d-dimension

Let $\mathcal{M}(\boldsymbol{x}) \in \mathcal{L}^2$ with $\boldsymbol{x} = (x_1, \ldots, x_d)$, its PCE writes:

$$\mathcal{M}(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^d} a_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) \tag{1}$$

which is called the Polynomial Chaos Expansion of $\mathcal{M}(\boldsymbol{x})$ with $\boldsymbol{\alpha} = \alpha_1 \alpha_2 \ldots \alpha_d$ with $\alpha_j \in \mathbb{N}$ and we denote the polynomial degree, $|\boldsymbol{\alpha}| = \sum_{i=1}^{d} \alpha_i$.

The $|\boldsymbol{\alpha}|$-th degree multi-dimensional basis element writes:

$$\psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) = \prod_{i=1}^{d} \psi_{\alpha_i}(x_i)$$

d-dimension

PCE and Sobol' indices

From the PCE: $\mathcal{M}(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^d} a_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$ it can be guessed that,

- $\mathrm{Var}\left[\mathcal{M}(\boldsymbol{x})\right] = \sum_{\boldsymbol{\alpha}:|\boldsymbol{\alpha}|>0} a_{\boldsymbol{\alpha}}^2$
- $S_i = \dfrac{\sum_{\alpha_i>0} a^2_{0\ldots\alpha_i\ldots0}}{\sum_{\boldsymbol{\alpha}:|\boldsymbol{\alpha}|>0} a_{\boldsymbol{\alpha}}^2}$
- $S_{ij} = \dfrac{\sum_{\alpha_i>0}\sum_{\alpha_j>0} a^2_{0\ldots\alpha_i 0\ldots\alpha_j\ldots0}}{\sum_{\boldsymbol{\alpha}:|\boldsymbol{\alpha}|>0} a_{\boldsymbol{\alpha}}^2}$
- $\vdots$
- $T_i = \dfrac{\sum_{\boldsymbol{\alpha}:\boldsymbol{\alpha}_i>0} a_{\boldsymbol{\alpha}}^2}{\sum_{\boldsymbol{\alpha}:|\boldsymbol{\alpha}|>0} a_{\boldsymbol{\alpha}}^2}$

Conclusion: Performing GSA with PCE = Assessing the PC coefficients $a_{\boldsymbol{\alpha}}$.

d-dimension

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In practice, only a truncated and sparse PCE is investigated:

$$\mathcal{M}(\boldsymbol{x}) \simeq \sum_{\boldsymbol{\alpha} \in \mathcal{A}} a_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$$

where $\mathcal{A}$ is a non-empty **finite** subset of $\mathbb{N}^d$.

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Question 1: How to compute the PCE coefficients $\boldsymbol{a}_{\mathcal{A}}$?

Question 2: How to find the optimal subset $\mathcal{A}$?

Answer in Part II

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