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

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Outline

Notations & Assumptions

Why PCE? The main idea

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

Notations & Assumptions

- $y = f(\boldsymbol{x})$ the scalar QoI
- $\boldsymbol{x} = (x_1, x_2, \ldots, x_d) \sim p_x$
- $x_i \sim p_{x_i} = \dfrac{\mathrm{d}F_{x_i}}{\mathrm{d}x_i}$, the marginal pdf ($F_{x_i}$ cdf) of x_i
- $\mathcal{D} = \{0, 1, \ldots, d\}$, $\mathcal{D}_{-i} \bigcap \{i\} = \emptyset$, $\mathcal{D}_{+i} \bigcap \{i\} \neq \emptyset$

<u>Assumptions</u>: $\mathbb{E}\left[f^2\right] = \int_{\mathbb{R}^d} f^2(\boldsymbol{x}) p_x \mathrm{d}\boldsymbol{x} < \infty$ and $p_x = \prod_{i=1}^{d} p_{x_i}$

ANOVA HDMR
Variance-based Sensitivity Indices

Isoprobabilistic Transformation

$\boldsymbol{x} \sim p_x$ can be transformed into $\boldsymbol{u} \sim \mathcal{U}(0,1)^d$ as follows,

$$\begin{cases} u_1 = F_{x_1}(x_1) \\ u_2 = F_{x_2}(x_2) \\ \vdots \\ u_d = F_{x_d}(x_d) \end{cases} \tag{1}$$

- The transformation is unique
- It requires the knowledge of the cdf's
- It is a special case of Rosenblatt transformations (adequate when $p_x \neq \prod_{i=1}^{d} p_{x_i}$)

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- It requires the knowledge of the cdf's
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As a consequence, $f(\boldsymbol{x}) = f(F_{x_1}^{-1}(u_1), \ldots, F_{x_d}^{-1}(u_d)) = g(\boldsymbol{u})$
The sensitivity of $f(\boldsymbol{x})$ to x_i = The sensitivity of $g(\boldsymbol{u})$ to u_i

Sobol' HDMR

Under the previous assumptions, Sobol' (1993) shows that it is possible to cast $g(\boldsymbol{u})$ as follows,

$$
\begin{aligned}
g(\boldsymbol{u}) &= g_0 + \sum_{i_1=1}^{d} g_{i_1}(u_{i_1}) + \sum_{i_2>i_1}^{d} g_{i_1,i_2}(u_{i_1}, u_{i_2}) \cdots + g_{1,\ldots,d}(u_1, \ldots, u_d) \quad (2) \\
&= \sum_{\alpha \subseteq \mathcal{D}} g_\alpha(\boldsymbol{u}_\alpha) \quad (3)
\end{aligned}
$$

with $g_0 = \mathbb{E}\left[g(\boldsymbol{u})\right]$, and, $\int_0^1 g_\alpha(\boldsymbol{u}_\alpha)\mathrm{d}u_k = 0, \forall k \in \alpha$

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As a result:

- **Sobol's hdmr is unique under our assumptions**
- **The g_α's are pairwise $\perp$:** $\mathbb{E}[g_\alpha g_\beta] = V_\alpha \delta_{\alpha\beta}$

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Consequently, the total variance of y can be decomposed as a sum of partial variances,

$$V_y = \sum_{i_1=1}^{d} V_{i_1} + \sum_{i_2>i_1}^{d} V_{i_1,i_2} + \cdots + V_{1,\ldots,d} \quad (4)$$

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$$1 = \sum_{i_1=1}^{d} S_{i_1} + \sum_{i_2>i_1}^{d} S_{i_1,i_2} + \cdots + S_{1,\ldots,d}$$

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- $S_i = \frac{\mathbb{V}[\mathbb{E}[y|x_i]]}{\mathbb{V}[y]}$ is the first-order effect of x_i also called correlation ratio
- the remainders are called interaction effects.
- $T_i = \frac{\mathbb{E}[\mathbb{V}[y|\boldsymbol{x}_{-i}]]}{\mathbb{V}[y]} = \sum_{\alpha\subset\mathcal{D}_{+i}} S_\alpha$ is the total-order effect of x_i
- $Sh_i = \sum_{\alpha\subset\mathcal{D}_{+i}} \frac{S_\alpha}{|\alpha|}$ is called the Shapley effect of x_i

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introducing the so-called Sobol' indices.
We have the following relations:

- $T_i \geq Sh_i \geq S_i$
- $\sum_{i=1}^{d} S_i \leq 1$, $\sum_{i=1}^{d} T_i \geq 1$, $\sum_{i=1}^{d} Sh_i = 1$

Why PCE?
The Main Idea

1D

<u>The 1-dimensional case</u>:

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

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

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

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

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

For convergence properties see, Cameron & Martin (1947) and Ernst et al. (2012).

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: $L_0^{(a)} = 1$
$L_1^{(a)}(x) = \frac{1}{\sqrt{\Gamma(1+a)}}(x-a)$
$L_2^{(a)}(x) = \frac{1}{\sqrt{\Gamma(2+a)}}\left(\frac{1}{2}x^2 - (1+a)x - \frac{1}{2}a(1+a)\right)$
$\vdots$ see Xiu & Karniadakis (2002) for other RVs.

1D

RV arbitrary distributed: If the orthogonal polynomial basis associated to p_x is unknown, 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 $y = f(x) = g(u)$ 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 $f : \mathbb{E}\left[f^2(x)\right] < +\infty$, it is possible to write,

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

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

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Advantage of such a representation: Any statistical moment of $f(x)$ can be easily computed

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

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

$\mathbb{V}\left[f(x)\right] = \sum_{\alpha \in \mathbb{N}} a_\alpha^2 - a_0^2$

$\vdots$

2D

<u>The 2-dimensional case</u>:

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

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

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that we simply write,

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

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:
$\mathbb{E}\left[f(\boldsymbol{x})\right] = a_{00}$
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Further, we can show that

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

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

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This is important for assessing the first-order effect:

$S_i = \frac{\mathbb{V}[\mathbb{E}[f(\boldsymbol{x})|x_i]]}{\mathbb{V}[f(\boldsymbol{x})]}$

2D

The ANOVA decomposition:

Recalling the ANOVA decomposition of f,

$$f(\boldsymbol{x}) = f_0 + f_1(x_1) + f_2(x_2) + f_{12}(x_1, x_2)$$

with $\mathbb{E}[f(\boldsymbol{x})] = f_0$

$$\mathbb{E}[f(\boldsymbol{x})|x_1] = f_1(x_1) + f_0$$

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We see that $f_0 = a_{00}$

$f_1(x_1) = \sum_{\alpha_1 \in \mathbb{N}^*} a_{\alpha_1 0} L_{\alpha_1}(x_1) \rightarrow$ main effect of x_1

$f_2(x_2) = \sum_{\alpha_2 \in \mathbb{N}^*} a_{0\alpha_2} H_{\alpha_2}(x_2) \rightarrow$ main effect of x_2

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

2D

The Sobol' sensitivity indices:

It is straightforward to compute the Sobol' indices,

$$S_1 = \frac{\mathbb{V}\left[\mathbb{E}\left[f(\boldsymbol{x})|x_1\right]\right]}{\mathbb{V}\left[f(\boldsymbol{x})\right]} = \frac{\mathbb{V}\left[f_1(x_1)\right]}{\mathbb{V}\left[f(\boldsymbol{x})\right]} = \frac{\sum_{\alpha_1 \in \mathbb{N}^*} a_{\alpha_1 0}^2}{\sum_{\boldsymbol{\alpha} \in \mathbb{N}^2} a_{\boldsymbol{\alpha}}^2 - a_{00}^2}$$

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$$S_{12} = \frac{\mathbb{V}\left[f_{12}(x_1, x_2)\right]}{\mathbb{V}\left[f(\boldsymbol{x})\right]} = \frac{\sum_{\boldsymbol{\alpha} \in \mathbb{N}^* \times \mathbb{N}^*} a_{\alpha_1 \alpha_2}^2}{\sum_{\boldsymbol{\alpha} \in \mathbb{N}^2} a_{\boldsymbol{\alpha}}^2 - a_{00}^2}$$

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

The d-dimensional PCE

d-dimension

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

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^d} a_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) \tag{5}$$

which is called the Polynomial Chaos Expansion of $f(\boldsymbol{x})$ 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: $f(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha}\in\mathbb{N}^d} a_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$ it can be inferred that,

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

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

d-dimension

Truncated PCE

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

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

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

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If $\mathcal{A} = \left\{\boldsymbol{\alpha} \in \mathbb{N}^d : |\boldsymbol{\alpha}| \leq p\right\}$ then

$$\mathrm{Card}\,(\mathcal{A}) = P = \frac{(p+d)!}{p!d!}, \text{ not optimal}$$

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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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