Sobol-Hoeffding Decomposition with Application to Global Sensitivity Analysis

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PhD course on UQ - DTU
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**$L_2$ functions over unit-hypercubes**

Let $L_2(\mathcal{U}^d)$ be the space of real-valued **squared-integrable functions** over the $d$-dimensional hypercube $\mathcal{U}$:

$$
\forall f : \mathbf{x} \in \mathcal{U}^d \mapsto f(\mathbf{x}) \in \mathbb{R}, \quad f \in L_2(\mathcal{U}^d) \iff \int_{\mathcal{U}^d} f(\mathbf{x})^2 d\mathbf{x} < \infty.
$$

$L_2(\mathcal{U}^d)$ is equipped with the inner product $\langle \cdot, \cdot \rangle$,

$$
\forall f, g \in L_2(\mathcal{U}^d), \quad \langle u, v \rangle := \int_{\mathcal{U}^d} f(\mathbf{x})g(\mathbf{x}) d\mathbf{x},
$$

and norm $\| \cdot \|_2$,

$$
\forall f \in L_2(\mathcal{U}^d), \quad \| f \|_2 := \langle f, f \rangle^{1/2}.
$$
**$L_2$ functions over unit-hypercubes**

Let $L_2(\mathcal{U}^d)$ be the space of real-valued **squared-integrable functions** over the $d$-dimensional hypercube $\mathcal{U}$:

$$f : \mathbf{x} \in \mathcal{U}^d \mapsto f(\mathbf{x}) \in \mathbb{R}, \quad f \in L_2(\mathcal{U}^d) \iff \int_{\mathcal{U}^d} f(\mathbf{x})^2 d\mathbf{x} < \infty.$$

**NB:** all subsequent developments immediately extend to product-type situations, where

$$\mathbf{x} \in \mathbf{A} = A_1 \times \cdots \times A_d \subseteq \mathbb{R}^d,$$

and weighted spaces $L_2(\mathbf{A}, \rho)$,

$$\rho : \mathbf{x} \in \mathbf{A} \mapsto \rho(\mathbf{x}) \geq 0, \quad \rho(\mathbf{x}) = \rho_1(x_1) \times \cdots \times \rho_d(x_d).$$

(e.g.: $\rho$ is a pdf of a random vector $\mathbf{x}$ with mutually independent components.)
Ensemble notations

Let $\mathcal{D} = \{1, 2, \ldots, d\}$.
Given $i \subseteq \mathcal{D}$, we denote $i_\sim := \mathcal{D} \setminus i$ its complement set in $\mathcal{D}$, such that

$$i \cup i_\sim = \mathcal{D}, \quad i \cap i_\sim = \emptyset.$$ 

For instance

- $i = \{1, 2\}$ and $i_\sim = \{3, \ldots, d\}$,
- $i = \mathcal{D}$ and $i_\sim = \emptyset$. 

Ensemble notations

Let $\mathcal{D} = \{1, 2, \ldots, d\}$. Given $i \subseteq \mathcal{D}$, we denote $i_\sim := \mathcal{D} \setminus i$ its complement set in $\mathcal{D}$, such that

$$i \cup i_\sim = \mathcal{D}, \quad i \cap i_\sim = \emptyset.$$

Given $\mathbf{x} = (x_1, \ldots, x_d)$, we denote $\mathbf{x}_i$ the vector having for components the $x_{i \in i}$, that is

$$\mathcal{D} \supseteq i = \{i_1, \ldots, i_{|i|}\} \Rightarrow \mathbf{x}_i = (x_{i_1}, \ldots, x_{i_{|i|}}),$$

where $|i| := \text{Card}(i)$. For instance

$$\int_{\mathcal{U}^{|i|}} f(\mathbf{x}) d\mathbf{x}_i = \int_{\mathcal{U}^{|i|}} f(x_1, \ldots, x_d) \prod_{i \in i} dx_i,$$

and

$$\int_{\mathcal{U}^{d-|i|}} f(\mathbf{x}) d\mathbf{x}_{i_\sim} = \int_{\mathcal{U}^{d-|i|}} f(x_1, \ldots, x_d) \prod_{i \in \mathcal{D}} dx_i,$$
Sobol-Hoeffding decomposition

Any $f \in L_2(\mathcal{U}^d)$ has a unique hierarchical orthogonal decomposition of the form

$$f(x) = f(x_1, \ldots, x_d) = f_0 + \sum_{i=1}^{d} f_i(x_i) + \sum_{i=1}^{d} \sum_{j=i+1}^{d} f_{i,j}(x_i, x_j) + \sum_{i=1}^{d} \sum_{j=i+1}^{d} \sum_{k=j+1}^{d} f_{i,j,k}(x_i, x_j, x_k) + \cdots + f_1, \ldots, d(x_1, \ldots, x_d).$$

Hierarchical: 1st order functionals $(f_i) \rightarrow$ 2nd order functionals $(f_{i,j}) \rightarrow$ 3rd order functionals $(f_{i,j,l}) \rightarrow \cdots \rightarrow$ $d$-th order functional $(f_1, \ldots, d)$.

Decomposition in a sum of $2^k$ functionals

Using ensemble notations:

$$f(x) = \sum_{i \subseteq \Omega} f_i(x_i).$$
Sobol-Hoeffding decomposition

Any $f \in L_2(U^d)$ has a **unique hierarchical orthogonal decomposition** of the form

$$f(x) = \sum_{i \subseteq \Omega} f_i(x_i).$$

**Orthogonal:** the functionals if the S-H decomposition verify the following orthogonality relations:

$$\int_{U^d} f_i(x_i) dx_j = 0, \quad \forall i \subseteq \Omega, j \in i,$$

$$\int_{U^d} f_i(x_i) f_j(x_j) dx = \langle f_i, f_j \rangle = 0, \quad \forall i, j \subseteq \Omega, i \neq j.$$

It follows the hierarchical construction

$$f_{\emptyset} = \int_{U^d} f(x) dx = \langle f \rangle_{\emptyset} = \emptyset$$

$$f_{\{i\}} = \int_{U^{d-1}} f(x) dx_{\{i\}} - f_{\emptyset} = \langle f \rangle_{\Omega \setminus \{i\}} - f_{\emptyset} \quad i \in \Omega$$

$$f_i = \int_{U^{|i|}} f(x) dx_{i^\sim} - \sum_{j \subseteq i} f_j = \langle f \rangle_{i^\sim} - \sum_{j \subseteq i} f_j \quad i \in \Omega, |i| \geq 2.$$
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Parametric sensitivity analysis

Consider $x$ as a set of $d$ independent random parameters uniformly distributed on $\mathcal{U}^d$, and $f(x)$ a model-output depending on these random parameters. It is assumed that $f$ is a 2nd order random variable: $f \in L_2(\mathcal{U}^d)$. Thus, $f$ has a unique S-H decomposition

$$f(x) = \sum_{i \subseteq \mathcal{D}} f_i(x_i).$$

Further, the integrals of $f$ with respect to $i_\sim$ are in this context conditional expectations,

$$E[f|x_i] = \int_{\mathcal{U}|i_\sim} f(x) dx_{i_\sim} = g(x_i) \quad \forall i \subseteq \mathcal{D},$$

so the S-H decomposition follows the hierarchical structure

$$f_{\emptyset} = E[f]$$
$$f_{\{i\}} = E[f|x_{\{i\}}] - E[f] \quad i \in \mathcal{D}$$
$$f_i = E[f|x_i] - \sum_{j \subset i} f_j \quad i \subseteq \mathcal{D}, |i| \geq 2.$$
Variance decomposition

Because of the orthogonality of the S-H decomposition the variance $\nabla [f]$ of the model-output can be decomposed as

$$\nabla [f] = \sum_{i \neq \emptyset} \nabla [f_i], \quad \nabla [f_i] = \langle f_i, f_i \rangle.$$

$\nabla [f_i]$ is interpreted as the contribution to the total variance $\nabla [f]$ of the interaction between parameters $x_{i \in i}$.

The S-H decomposition thus provide a rich mean of analyzing the respective contributions of individual or sets of parameters to model-output variability. However, as there are $2^d - 1$ contributions, so one needs more "abstract" characterizations.
Sensitivity indices

To facilitate the hierarchization of the respective influence of each parameter $x_i$, the partial variances $\nabla [f_i]$ are normalized by $\nabla [f]$ to obtain the sensitivity indices:

$$S_i(f) = \frac{\nabla [f_i]}{\nabla [f]} \leq 1, \quad \sum_{i \neq \emptyset} S_i(f) = 1.$$ 

The order of the sensitivity indices $S_i$ is equal to $|i| = \text{Card}(i)$.

1st order sensitivity indices. The $d$ first order indices $S_{\{i\} \in \mathcal{D}}$ characterize the fraction of the variance due the parameter $x_i$ only, i.e. without any interaction with others. Therefore,

$$1 - \sum_{i=1}^{d} S_{\{i\}}(f) \geq 0,$$

measures globally the effect on the variability of all interactions between parameters. If $\sum_{i=1}^{d} S_{\{i\}} = 1$, the model is said additive, because its S-H decomposition is

$$f(x_i, \ldots, x_d) = f_0 + \sum_{i=1}^{d} f_i(x_i),$$

and the impact of the parameters can be studied separately.
Sensitivity indices

To facilitate the hierarchization of the respective influence of each parameter $x_i$, the partial variances $\nabla [f_i]$ are normalized by $\nabla [f]$ to obtain the sensitivity indices:

$$S_i(f) = \frac{\nabla [f_i]}{\nabla [f]} \leq 1, \quad \sum_{i \subseteq \mathcal{D}} S_i(f) = 1.$$ 

The order of the sensitivity indices $S_i$ is equal to $|i| = \text{Card}(i)$.

**Total sensitivity indices.** The first order SI $S\{i\}$ measures the variability due to parameter $x_i$ alone. The total SI $T\{i\}$ measures the variability due to the parameter $x_i$, including all its interactions with other parameters:

$$T\{i\} := \sum_{i \ni i} S_i \geq S\{i\}.$$ 

**Important point:** for $x_i$ to be deemed non-important or non-influent on the model-output, $S\{i\}$ and $T\{i\}$ have to be negligible. Observe that $\sum_{i \ni \mathcal{D}} T\{i\} \geq 1$, the excess from 1 characterizes the presence of interactions in the model-output.
Sobol-Hoeffding decomposition

Application to Global S.A.

Computation of the SI

Sensitivity indices

\[
\begin{align*}
S_{1,2,3} & \quad T_{1,2,3} \\
S_{1,2} & \quad S_{1,3} \\
S_{1} & \quad S_{2,3} \\
T_{1} & \quad T_{2,3}
\end{align*}
\]

\[
\begin{align*}
\cos \theta & = \frac{d}{d=3} \\
\sum S_i & = 1 \\
\sum S_{i,j} & \leq 1 \\
\sum T_{i,j} & > 1
\end{align*}
\]
Sensitivity indices

In many uncertainty problem, the set of uncertain parameters can be naturally grouped into subsets depending on the process each parameter accounts for. For instance, boundary conditions BC, material property $\varphi$, external forcing $F$, and $\mathcal{D}$ is the union of these distinct subsets:

$$
\mathcal{D} = \mathcal{D}_{BC} \cup \mathcal{D}_{\varphi} \cup \mathcal{D}_{F}.
$$

The notion of first order and total sensitivity indices can be extended to characterize the influence of the subsets of parameters. For instance,

$$
S_{\mathcal{D}_{\varphi}} = \sum_{i \subseteq \mathcal{D}_{\varphi}} S_i,
$$

measures the fraction of variance induced by the material uncertainty alone, while

$$
T_{\mathcal{D}_{F}} = \sum_{i \cap \mathcal{D}_{F} \neq \emptyset} S_i.
$$

measures the fraction of variance due to the external forcing uncertainty and all its interactions.
Let \((\xi_1, \xi_2)\) be two independent centered, normalized random variables

\[
\xi_i \sim \mathcal{N}(0, 1), \quad i = 1, 2.
\]

Consider the model-output \(f : (\xi_1, \xi_2) \in \mathbb{R}^2 \mapsto \mathbb{R}\) given by

\[
f(\xi_1, \xi_2) = (\mu_1 + \sigma_1 \xi_1) + (\mu_2 + \sigma_2 \xi_2).
\]

1. Determine the S-H decomposition of \(f\)
2. Compute the 1st order and total sensitivity indices of \(f\)
3. Comment
4. Repeat for \(f(\xi_1, \xi_2) = (\mu_1 + \sigma_1 \xi_1)(\mu_2 + \sigma_2 \xi_2)\).
Sobol-Hoeffding decomposition

**Example**

\[ f(\xi_1, \xi_2) = \mu_1 + \mu_2 + \sigma_1 \xi_1 + \sigma_2 \xi_2 \]

- \( \mathbb{E}[f] = (\mu_1 + \mu_2) \)
- \( \mathbb{E}[f|\xi_1] = (\mu_1 + \mu_2) + \sigma_1 \xi_1 \) \( \Rightarrow f_1(\xi_1) = \mathbb{E}[f|\xi_1] - \mathbb{E}[f] = \sigma_1 \xi_1 \)
- \( \mathbb{E}[f|\xi_2] = (\mu_1 + \mu_2) + \sigma_2 \xi_2 \) \( \Rightarrow f_2(\xi_2) = \mathbb{E}[f|\xi_2] - \mathbb{E}[f] = \sigma_2 \xi_2 \)
- \( \mathbb{E}[f|\xi_1,\xi_2] = f(\xi_1, \xi_2) \) \( \Rightarrow f_{1,2}(\xi_1, \xi_2) = \mathbb{E}[f|\xi_1,\xi_2] - \mathbb{E}[f] - f_1(\xi_1) - f_2(\xi_2) = 0 \)

- Then, \( \nabla [f] = \sigma_1^2 + \sigma_2^2 \), so

\[ S_1 = T_1 = \frac{\sigma_1^2}{\sigma_1^2 + \sigma_2^2} \quad \text{and} \quad S_2 = T_2 = \frac{\sigma_2^2}{\sigma_1^2 + \sigma_2^2} \]

- Comment: obvious case, as \( f \) is a linear (additive) model.
Example

\[ f(\xi_1, \xi_2) = \mu_1 \mu_2 + \mu_2 \sigma_1 \xi_1 + \mu_1 \sigma_2 \xi_2 + \sigma_1 \sigma_2 \xi_1 \xi_2. \]

- \( \mathbb{E} [f] = \mu_1 \mu_2 \)
- \( \mathbb{E} [f|\xi_1] = \mu_1 \mu_2 + \mu_2 \sigma_1 \xi_1 \)
  \[ \Rightarrow f_1(\xi_1) = \mathbb{E} [f|\xi_1] - \mathbb{E} [f] = \mu_2 \sigma_1 \xi_1 \]
- \( \mathbb{E} [f|\xi_2] = \mu_1 \mu_2 + \mu_1 \sigma_2 \xi_2 \)
  \[ \Rightarrow f_2(\xi_2) = \mathbb{E} [f|\xi_2] - \mathbb{E} [f] = \mu_1 \sigma_2 \xi_2 \]
- \( \mathbb{E} [f|\xi_1, \xi_2] = f(\xi_1, \xi_2) \)
  \[ \Rightarrow f_{1,2}(\xi_1, \xi_1) = \mathbb{E} [f|\xi_1, \xi_2] - \mathbb{E} [f] - f_1(\xi_1) - f_2(\xi_2) = \sigma_1 \sigma_2 \xi_1 \xi_2 \]

Then, \( \forall [f] = \mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2 + \sigma_1^2 \sigma_2^2 \), so

\[ S_1 = \frac{\mu_2^2 \sigma_1^2}{\mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2 + \sigma_1^2 \sigma_2^2} \] \text{ and } \[ S_2 = \frac{\mu_1^2 \sigma_2^2}{\mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2 + \sigma_1^2 \sigma_2^2}, \]

\[ T_1 = \frac{\mu_2^2 \sigma_1^2 + \sigma_1 \sigma_2}{\mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2 + \sigma_1^2 \sigma_2^2} \] \text{ and } \[ T_2 = \frac{\mu_1^2 \sigma_2^2 + \sigma_1 \sigma_2}{\mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2 + \sigma_1^2 \sigma_2^2}, \]

- Comment: fraction of variance due to interactions is

\[ \sigma_1^2 \sigma_2^2 / (\mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2 + \sigma_1^2 \sigma_2^2) \]
Sobol-Hoeffding decomposition

Application to Global S.A.

Computation of the SI

Example

\[ f(\xi_1, \xi_2) = \mu_1 \mu_2 + \mu_2 \sigma_1 \xi_1 + \mu_1 \sigma_2 \xi_2 + \sigma_1 \sigma_2 \xi_1 \xi_2. \]

Then, \( \nabla [f] = \mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2 + \sigma_1^2 \sigma_2^2 \), so

\[ S_1 = \frac{\mu_1^2 \sigma_1^2}{\mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2 + \sigma_1^2 \sigma_2^2} \quad \text{and} \quad S_2 = \frac{\mu_1^2 \sigma_2^2}{\mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2 + \sigma_1^2 \sigma_2^2}, \]

\[ T_1 = \frac{\mu_1^2 \sigma_2^2 + \sigma_1 \sigma_2}{\mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2 + \sigma_1^2 \sigma_2^2} \quad \text{and} \quad T_2 = \frac{\mu_1^2 \sigma_1^2 + \sigma_1 \sigma_2}{\mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2 + \sigma_1^2 \sigma_2^2}, \]

Comment: fraction of variance due to interactions is

\[ \sigma_1^2 \sigma_2^2 / (\mu_1^2 \sigma_2^2 + \mu_2^2 \sigma_1^2 + \sigma_1^2 \sigma_2^2) \]

Example: \((\mu_1, \sigma_1) = (1, 3)\) and \((\mu_2, \sigma_2) = (2, 2)\), so

\[ S_1 = 9/19, \quad S_2 = 1/19, \quad S_{1,2} = 9/19. \]

One can draw the conclusions:

- \( \xi_1 \) is the most influential variable as \( S_1 > S_2 \) and \( T_1 > T_2 \).
- Interactions are important as \( 1 - S_1 - S_2 = 9/19 \approx 0.5 \), especially for \( \xi_2 \) for which \( (T_2 - S_2) / T_2 = 9/10 \approx 1 \).
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   - Monte-Carlo estimation
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1-st order sensitivity indices by Monte-Carlo sampling.

The $S_i$ can be computed by MC sampling as follow. Recall that

$$S_i(f) = \frac{\nabla{[f_{\{i\}}]}}{\nabla{[f]}} = \frac{\nabla{[E[f|x_i]]}}{\nabla{[f]}} = \frac{E[E[f|x_i]^2] - E[E[f|x_i]]^2}{\nabla{[f]}}.$$

Observe: $E[E[f|x_i]] = E[f]$.

$E[f]$ and $\nabla{[f]}$ can be estimated using MC sampling. Let $\chi_M = \{x^{(1)}, \ldots, x^{(M)}\}$ be a set of independent samples drawn uniformly in $\mathcal{U}^d$, the mean and variance estimators are:

$$\hat{E}[f] = \frac{1}{M} \sum_{l=1}^{M} f(x^{(l)}), \quad \hat{\nabla}{[f]} = \frac{1}{M-1} \sum_{l=1}^{M} (f(x^{(l)}))^2 - \hat{E}[f]^2.$$

It now remains to compute the variance of conditional expectations, $\nabla{[E[f|x_{\{i\}}]]}$.

Any idea?
Monte-Carlo estimator for variance of conditional expectation.

Observe:

\[
\int_{d+|i\sim|} f(x_i, x_i\sim)f(x_i, x'_i\sim)dx_i\,dx_i\sim\,dx_i',
\]

\[
= \int_{d|i\sim|} dx_i \int_{d|i\sim|} f(x_i, x_i\sim)dx_i\sim \int_{d|\sim|} f(x_i, x'_i\sim)dx'_i\sim
\]

\[
= \int_{d|i\sim|} dx_i \left[ \int_{d|\sim|} f(x_i, x_i\sim)dx_i\sim \right]^2.
\]
Monte-Carlo estimator for variance of conditional expectation.

Observe:

\[
\int_{\mathcal{U}^{d+|i\sim|}} f(x_i, x_{i\sim}) f(x_i, x'_{i\sim}) \, dx_i \, dx_{i\sim} \, dx'_{i\sim},
\]

\[
= \int_{\mathcal{U}^{d|\sim|}} dx_i \, \int_{\mathcal{U}^{d|\sim|}} f(x_i, x_{i\sim}) \, dx_{i\sim} \, \int_{\mathcal{U}^{d|\sim|}} f(x_i, x'_{i\sim}) \, dx'_{i\sim},
\]

\[
= \int_{\mathcal{U}^{d|\sim|}} dx_i \, \left[ \int_{\mathcal{U}^{d|\sim|}} f(x_i, x_{i\sim}) \, dx_{i\sim} \right]^2.
\]

\[
\text{Variance: } \text{V}\left[ \mathbb{E}[f|\{x_i\}] \right] = \mathbb{E}\left[ \mathbb{E}[f|\{x_i\}]^2 \right] - \mathbb{E}\left[ \mathbb{E}[f|\{x_i\}] \right]^2 = \mathbb{E}\left[ \mathbb{E}[f|\{x_i\}]^2 \right] - \mathbb{E}[f]^2.
\]
Monte-Carlo estimator for variance of conditional expectation.

Observe:

\[
\int_{\mathcal{U}d+\mid \sim} f(x_i, x_{i\sim})f(x_i, x'_{i\sim})dx_{i\sim}dx_{i\sim},
\]

\[
= \int_{\mathcal{U}\mid i\sim} dx_i \int_{\mathcal{U}\mid i\sim} f(x_i, x_{i\sim})dx_{i\sim} \int_{\mathcal{U}\mid i\sim} f(x_i, x'_{i\sim})dx'_{i\sim}
\]

\[
= \int_{\mathcal{U}\mid i\sim} dx_i \left[ \int_{\mathcal{U}\mid i\sim} f(x_i, x_{i\sim})dx_{i\sim} \right]^2.
\]

\[
\mathbb{V} \left[ \mathbb{E} \left[ f \mid x_{\{i\}} \right] \right] = \mathbb{E} \left[ \mathbb{E} \left[ f \mid x_{\{i\}} \right]^2 \right] - \mathbb{E} \left[ \mathbb{E} \left[ f \mid x_{\{i\}} \right]^2 \right] = \mathbb{E} \left[ \mathbb{E} \left[ f \mid x_{\{i\}} \right]^2 \right] - \mathbb{E} [f]^2
\]

\[
= \lim_{M \to \infty} \frac{1}{M} \sum_{l=1}^{M} f \left( x_{\{i\}}^{(l)} , x_{\{i\}}^{(l)} \right) f \left( \tilde{x}_{\{i\}}^{(l)} , x_{\{i\}}^{(l)} \right) - \mathbb{E} [f]^2
\]

\[
\left( \text{independent samples } x_{\{i\}}^{(l)} , \tilde{x}_{\{i\}}^{(l)} \text{ and } x_{\{i\}}^{(k)} \right)
\]
Monte-Carlo estimators for 1st order SI $S_{\{i\}}$.

1. Draw 2 independent sample sets, with size $M$, $\chi_M$ and $\tilde{\chi}_M$
2. Compute estimators $\hat{E}[f]$ and $\hat{V}[f]$ from $\chi_M$ (or $\tilde{\chi}_M$) [M model evaluations]
3. For $i = 1, 2, \ldots, d$:
   - Estimate variance of conditional expectation through
     \[
     \hat{V}[\hat{E}[f|\xi_{\{i\}}]] = \frac{1}{M} \sum_{l=1}^{M} f\left(x^{(l)}_{\{i\}} \sim \tilde{x}^{(l)}_{\{i\}}, x^{(l)}_{\{i\}} \sim x^{(l)}_{\{i\}}\right) \left(\hat{E}[f] - \hat{E}[f]\right)^2
     \]
     [M new model evaluations at $(\tilde{x}^{(l)}_{\{i\}} \sim , x^{(l)}_{\{i\}})$]
   - Estimator of the 1-st order SI:
     \[
     \hat{S}_{\{i\}}(f) = \frac{\hat{V}[\hat{E}[f|\xi_{\{i\}}]]}{\hat{V}[f]}.\]

Requires $(d + 1) \times M$ model evaluations.
\[ \nabla \left[ \mathbb{E} \left[ f(x_{\{i\}}) \right] \right] \approx \frac{1}{M} \sum_{l=1}^{M} f(x_{\{i\}} \sim, x_{\{i\}} \sim) f(\tilde{x}_{\{i\}} \sim, x_{\{i\}} \sim) - \left( \frac{1}{M} \sum_{l=1}^{M} f(x_{\{i\}} \sim, x_{\{i\}} \sim) \right)^2. \]
Total sensitivity indices by Monte-Carlo sampling.

The $T_{\{i\}}$ can be computed by MC sampling as follow. Recall that

$$T_{\{i\}}(f) = \sum_{i \ni \{i\}} S_i(f) = 1 - \sum_{i \subseteq D \setminus \{i\}} S_i(f) = 1 - \frac{\mathbb{V}[\mathbb{E}[f|x_{\{i\} \sim}]]}{\mathbb{V}[f]}.$$ 

As for $\mathbb{V}[\mathbb{E}[f|x_{\{i\} \sim}]]$, we can derive the following Monte-Carlo estimator for $\mathbb{V}[\mathbb{E}[f|x_{\{i\} \sim}]]$, using the two independent sample sets $\chi_M$ and $\tilde{\chi}_M$

$$\mathbb{V}[\mathbb{E}[f|x_{\{i\} \sim}]] = \frac{1}{M} \sum_{l=1}^{M} f\left(\mathbf{x}_{\{i\} \sim}^{(l)}, \mathbf{x}_{\{i\} \sim}^{(l)}\right) f\left(\mathbf{x}_{\{i\} \sim}^{(l)}, \tilde{\mathbf{x}}_{\{i\} \sim}^{(l)}\right) - \mathbb{E}[f]^2,$$

so finally

$$\hat{T}_{\{i\}}(f) = 1 - \frac{1}{\mathbb{V}[f]} \left(\frac{1}{M} \sum_{l=1}^{M} f\left(\mathbf{x}_{\{i\} \sim}^{(l)}, \mathbf{x}_{\{i\} \sim}^{(l)}\right) f\left(\mathbf{x}_{\{i\} \sim}^{(l)}, \tilde{\mathbf{x}}_{\{i\} \sim}^{(l)}\right) - \mathbb{E}[f]^2\right).$$

The MC estimation of the $T_{\{i\}}$ needs $d \times M$ additional model evaluations.
\[ \chi_M : \begin{bmatrix} x_1^{(1)} & \ldots & x_i^{(1)} & \ldots & x_d^{(1)} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ x_1^{(l)} & \ldots & x_i^{(l)} & \ldots & x_d^{(l)} \\
\vdots & \ddots & \vdots & \ddots & \vdots \\ x_1^{(M)} & \ldots & x_i^{(M)} & \ldots & x_d^{(M)} \end{bmatrix} \]

\[ \tilde{\chi}_M : \begin{bmatrix} \tilde{x}_1^{(1)} & \ldots & \tilde{x}_i^{(1)} & \ldots & \tilde{x}_d^{(1)} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \tilde{x}_1^{(l)} & \ldots & \tilde{x}_i^{(l)} & \ldots & \tilde{x}_d^{(l)} \\
\vdots & \ddots & \vdots & \ddots & \vdots \\ \tilde{x}_1^{(M)} & \ldots & \tilde{x}_i^{(M)} & \ldots & \tilde{x}_d^{(M)} \end{bmatrix} \]

\[ \tilde{\chi}_M^{\{i\}} : \begin{bmatrix} x_1^{(1)} & \ldots & \tilde{x}_i^{(1)} & \ldots & x_d^{(1)} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \tilde{x}_1^{(l)} & \ldots & \tilde{x}_i^{(l)} & \ldots & x_d^{(l)} \\
\vdots & \ddots & \vdots & \ddots & \vdots \\ x_1^{(M)} & \ldots & \tilde{x}_i^{(M)} & \ldots & x_d^{(M)} \end{bmatrix} \]

\[ \mathbb{V} \left[ \mathbb{E} \left[ f | \mathbf{x}^{\{i\}} \right] \right] \approx \frac{1}{M} \sum_{l=1}^{M} f(\mathbf{x}^{\{i\}} \sim, \mathbf{x}^{\{i\}} \sim) f(\mathbf{x}^{\{i\}} \sim, \tilde{\mathbf{x}}^{\{i\}} \sim) - \left( \frac{1}{M} \sum_{l=1}^{M} f(\mathbf{x}^{\{i\}} \sim, \mathbf{x}^{\{i\}} \sim) \right)^2. \]
MC estimation of 1st order and total sensitivity indices:

- requires $M \times (2d + 1)$ simulations
- convergence of estimators in $\mathcal{O}(1/\sqrt{M})$
- slow convergence, but $d$-independent
- convergence not related to smoothness of $f$
- works also (in practice) with advanced sampling schemes (QMC, LHS, ...). How to proceed with QMC/LHS?
S-H decomposition from PC expansions.
Consider the model-output $f : \xi \in \Xi \subset \mathbb{R}^d \rightarrow \mathbb{R}$, where $\xi = (\xi_1, \ldots, \xi_d)$ are independent real-valued r.v. with joint-probability density function

$$p_\xi(x_1, \ldots, x_d) = \prod_{i=1}^{d} p_i(x_i).$$

Let $\{ \Psi_\alpha \}$ be the set of $d$-variate orthogonal polynomials,

$$\Psi_\alpha(\xi) = \prod_{i=1}^{d} \psi^{(i)}_{\alpha_i}(\xi_i),$$

with $\psi^{(i)}_{i \geq 0} \in \pi_i$ the uni-variate polynomials mutually orthogonal with respect to the density $p_i$.

If $f \in L_2(\Xi, p_\xi)$, it has a convergent PC expansion

$$f(\xi) = \lim_{N_0 \rightarrow \infty} \sum_{|\alpha| \leq N_0} \Psi_\alpha(\xi) f_\alpha, \quad |\alpha| = \sum_{i=1}^{d} |\alpha_i|. $$
S-H decomposition from PC expansions.

Given the truncated PC expansion of $f$,

$$\hat{f}(\xi) = \sum_{|\alpha| \leq A} \Psi_\alpha(\xi)f_\alpha,$$

one can readily obtain the PC approximation of the S-H functionals through

$$\hat{f}_i(\xi_i) = \sum_{|\alpha| \leq A(i)} \Psi_\alpha(\xi_i)f_\alpha,$$

where the multi-index set $A(i)$ is given by

$$A(i) = \{ \alpha \in A; \alpha_i > 0 \text{ for } i \in i, \alpha_i = 0 \text{ for } i \notin i \}/A.$$

For the sensitivity indices it comes

$$S_i(\hat{f}) = \frac{\sum_{\alpha \in A(i)} f^2_\alpha \langle \Psi_\alpha, \Psi_\alpha \rangle}{\sum_{\alpha \in A} f^2_\alpha \langle \Psi_\alpha, \Psi_\alpha \rangle}, \quad T_{\{i\}}(\hat{f}) = \frac{\sum_{\alpha \in T(i)} f^2_\alpha \langle \Psi_\alpha, \Psi_\alpha \rangle}{\sum_{\alpha \in A} f^2_\alpha \langle \Psi_\alpha, \Psi_\alpha \rangle},$$

where

$$T(i) = \{ \alpha \in A; \alpha_i > 0 \text{ for } i \in i \}$$
Subsets of PC multi-indices for S-H functionals
Example: Let \((\xi_1, \xi_2)\) be two independent random variables with uniform distributions on the unit interval. Consider the model-output \(f : (\xi_1, \xi_2) \in [0, 1]^2 \mapsto \mathbb{R}\) given by

\[ f(\xi_1, \xi_2) = \tanh(3(\xi_1 - 0.2\xi_2 - 0.5)(1 + \xi_2)). \]
S-H decomposition at $N_0 = 3$ ($P = 10$):
S-H decomposition at $N_0 = 5$: ($P = 21$)
Sobol-Hoeffding decomposition

Application to Global S.A.

Computation of the SI

S-H decomposition at $N_0 = 7$: ($P = 36$)
S-H decomposition at $N_0 = 9$: ($P = 55$)
Convergence of sensitivity indices:

<table>
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<th>No</th>
<th>Card($\mathcal{A}$)</th>
<th>$S_{{1}}(\hat{f})$</th>
<th>$S_{{2}}(\hat{f})$</th>
<th>$S_{{1,2}}(\hat{f})$</th>
<th>$|\hat{f} - f|_2$</th>
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<tr>
<td>3</td>
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<td>2.545 (−2)</td>
<td>1.676 (−2)</td>
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<td>7</td>
<td>36</td>
<td>9.572 (−1)</td>
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<td>9</td>
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<tr>
<td>15</td>
<td>136</td>
<td>9.571 (−1)</td>
<td>2.542 (−2)</td>
<td>1.748 (−2)</td>
<td>1.9 (−4)</td>
</tr>
</tbody>
</table>
Convergence of sensitivity indices for \textbf{naive} MC sampling:
Homework: Homma-Saltelli function

\[ f(x_1, x_2, x_3) = \sin(x_1) + a \sin^2(x_2) + bx_3^4 \sin(x_1), \]

where \( x_1, x_2 \) and \( x_3 \) are i.i.d. random variables uniformly distributed on \([-\pi, \pi]\).

Letting \( \langle \cdot \rangle \) be the expectation (over \([-\pi, \pi]^3\)), we have

\[ \langle \sin \rangle = 0, \quad \langle \sin^2 \rangle = 1/2, \quad \langle \sin^4 \rangle = 3/8, \quad \langle x^n \rangle = \begin{cases} \frac{\pi^n}{n+1}, & n \text{ even}, \\ 0, & n \text{ odd}. \end{cases} \]

1. Compute the SH decomposition of \( f \) and the associated sensitivity indices.
   Solution:
   \[ f(x_1, x_2, x_3) = \frac{a}{2} + \sin(x_1)(1 + b\pi^2/4) + a(\sin^2(x_2) - 1/2) + b\sin(x_1)(x_3^4 - \pi^4/5)). \]

2. Compute PC expansion of \( f \) by non-intrusive spectral projection for polynomial degrees 1 to 6 and extract 1st order and total sensitivity indices for \( a = 7 \) and \( b = 0.1 \).

3. Compute 1-st order and total sensitivity indices by Monte-Carlo simulation.
Further readings: