An inference method for global sensitivity analysis

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Outline

Global sensitivity analysis

An inference method

Computational aspects

Discussion
Let $f(\theta_1, \ldots, \theta_d)$ be the output of some function $f$. 

Uncertainty quantification
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- This uncertainty is modeled by independent random variables $(\Theta_1, \ldots, \Theta_d) =: \Theta$. 
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- This uncertainty is modeled by independent random variables $(\Theta_1, \ldots, \Theta_d) =: \Theta$.
- The output, therefore, is also a random variable $f(\Theta_1, \ldots, \Theta_d) = f(\Theta)$.
- The output has a variance $\text{Var}_f(\Theta)$, which represents its uncertainty.
Global sensitivity analysis [Sobol (1993); Saltelli et al (2000)]

- What are the most important parameters?
Global sensitivity analysis [Sobol (1993); Saltelli et al (2000)]

- What are the most important parameters?
- If $E f(\Theta)^2 < \infty$, then

\[
 f(\Theta) = f_1(\Theta_1) + \cdots + f_d(\Theta_d) \\
 + f_{1,2}(\Theta_1, \Theta_2) + \cdots + f_{d-1,d}(\Theta_{d-1}, \Theta_d) \\
 + \cdots \\
 + f_{1,\ldots,d}(\Theta_1, \ldots, \Theta_d).
\]
Global sensitivity analysis [Sobol (1993); Saltelli et al (2000)]

- What are the most important parameters?
- If $E f(\Theta)^2 < \infty$, then

$$Var f(\Theta) = Var f_1(\Theta_1) + \cdots + Var f_d(\Theta_d)$$
$$+ Var f_{1,2}(\Theta_1, \Theta_2) + \cdots + Var f_{d-1,d}(\Theta_{d-1}, \Theta_d)$$
$$+ \cdots$$
$$+ Var f_{1,,\ldots,d}(\Theta_1, \ldots, \Theta_d).$$
Global sensitivity analysis [Sobol (1993); Saltelli et al (2000)]

- What are the most important parameters?
- If $\mathbb{E} f(\Theta)^2 < \infty$, then

$$\text{Var} f(\Theta) = \underbrace{\text{Var} f_1(\Theta_1)}_{\sigma^*\{\{1\}\}} + \cdots + \underbrace{\text{Var} f_d(\Theta_d)}_{\sigma^*\{\{d\}\}} + \underbrace{\text{Var} f_{1,2}(\Theta_1, \Theta_2)}_{\sigma^*\{\{1,2\}\}} + \cdots + \underbrace{\text{Var} f_{d-1,d}(\Theta_{d-1}, \Theta_d)}_{\sigma^*\{\{d-1,d\}\}} + \cdots + \underbrace{\text{Var} f_{1,\ldots,d}(\Theta_1, \ldots, \Theta_d)}_{\sigma^*\{\{1,\ldots,d\}\}}.$$
Sobol indices

- The expected amount of variance that could be reduced by randomly fixing the $j$th parameter is given by

$$\sigma^*(j) = \text{Var} f_j(\Theta_j) = \mathbb{E} (\text{Var}[f(\Theta)] - \text{Var}[f(\Theta)|\Theta_j]).$$
Sobol indices

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\[ \sigma^*(j) = \text{Var} f_j(\Theta_j) = E(\text{Var}[f(\Theta)] - \text{Var}[f(\Theta)|\Theta_j]). \]

- Higher-order Sobol indices quantify *interactions.*
Total indices [Homma & Saltelli (1996)]

The sum of all Sobol indices that “intersect” \(A \subset \{1, \ldots, d\}\) is the total index associated with \(A\)

\[
\tau(A) = \sum_{B \cap A \neq \emptyset} \sigma^*(B)
\]
Total indices [Homma & Saltelli (1996)]

The sum of all Sobol indices that “intersect” $A \subset \{1, \ldots, d\}$ is the *total index* associated with $A$

$$
\tau(A) = \sum_{B \cap A \neq \emptyset} \sigma^*(B)
$$

$$
= \mathbb{E} \text{Var}[f(\Theta)|\Theta_{\complement A}]
$$

and is *the expected variance induced by a random change in $\Theta_A$*. 
Dual total indices (closed Sobol indices)

The dual index of $A$

$$\tau^*(A) = \text{Var} \ E[f(\Theta)|\Theta_A]$$

is the expected amount of variance that could be reduced by randomly fixing the parameters indexed by $A$. 
Dual total indices (closed Sobol indices)

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▶ $\tau^*(j) = \sigma^*(j)$
Global sensitivity analysis

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- $\tau^*(j) = \sigma^*(j)$

- $\tau^*(A) = \text{Var} f(\Theta) - E \text{Var}[f(\Theta)|\Theta_A] = \tau(\{1, \ldots, d\}) - \tau(CA)$
Shapley indices [Shapley (1951); Owen (2014)]

- Shapley index of singleton \( \{ j \} \):

\[
\phi(\{ j \}) = \frac{1}{d} \sum_{B: j \notin B} \frac{1}{(d-1)|B|} (\tau(B \cup \{ j \}) - \tau(B)).
\]
Shapley indices [Shapley (1951); Owen (2014)]

- Shapley index of singleton \( \{j\} \):

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- \( \tau \) can be replaced by \( \tau^* \).
Shapley indices [Shapley (1951); Owen (2014)]

- Shapley index of singleton \{j\}:

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\phi(\{j\}) = \frac{1}{d} \sum_{B : j \notin B} \frac{1}{(d-1)(|B|)} (\tau(B \cup \{j\}) - \tau(B)).
\]

- \(\tau\) can be replaced by \(\tau^*\).

- Takes into account the fact that the variability caused by \{j\} depends on the presence/absence of the other parameters.
Questions

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- If interactions are of interest, how can we make inferences about them? How can we compute them?
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- While there are a plethora of methods to estimate and compute first-order Sobol and total indices, there is much less work on interactions.
- If interactions are of interest, how can we make inferences about them? How can we compute them?
- We assume we have a sample of model outputs.
An inference method

There is a *simple* method that

- estimates all combinations/interaction effects of all sensitivity indices;
- makes *inferences* (confidence intervals, pvalues, hypothesis testing);
- does this with a *single* sample of $n2^d$ model runs;
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Program:

1. Build $\hat{\tau}$ such that $\sqrt{n}(\hat{\tau} - \tau) \rightarrow N(0, T)$
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1. Build $\hat{\tau}$ such that $\sqrt{n}(\hat{\tau} - \tau) \rightarrow N(0, T)$
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3. $\hat{\sigma}^* = M^*\hat{\tau}^*$
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3. \( \hat{\sigma}^* = M^*\hat{\tau}^* \)
4. \( \hat{\phi} = N^*\hat{\sigma}^* \)
Step 0: sample of model outputs

For $i = 1, \ldots, n$

Draw $\Theta^{(i)}, \tilde{\Theta}^{(i)}$

For $A \in \{1, \ldots, d\}$

Compute $f(\tilde{\Theta}_A^{(i)}, \Theta_{\bar{C}_A}^{(i)})$. 
Step 1: build $\hat{\tau}$

- It holds that\(^1\)

$$
\tau(A) = E \text{Var}[f(\Theta)|\Theta_{\complement A}] = \frac{1}{2} E \left( f(\Theta) - f(\tilde{\Theta}_A, \Theta_{\complement A}) \right)^2.
$$

\(^1\)Jansen (1999)
Step 1: build $\hat{\tau}$

- It holds that
  \[ \tau(A) = \mathbb{E} \text{Var}[f(\Theta)|\Theta_{\mathcal{C}A}] = \frac{1}{2} \mathbb{E} \left( f(\Theta) - f(\tilde{\Theta}_A, \Theta_{\mathcal{C}A}) \right)^2. \]

- An estimator is
  \[ \hat{\tau}(A) = \frac{1}{n} \sum_{i=1}^{n} \left( f(\Theta^{(i)}) - f(\tilde{\Theta}_A^{(i)}, \Theta_{\mathcal{C}A}^{(i)}) \right)^2. \]

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  \]

- It holds $\sqrt{n}(\hat{\tau} - \tau) \rightarrow \text{N}(0, T)$ for some variance-covariance matrix $T$ which can be consistently estimated from the sample.

---

\(^1\)Jansen (1999)
Step 2: $\hat{\tau}^*$

- Recall $\tau^*(A) = \tau(\{1, \ldots, d\}) - \tau(\mathcal{C}A)$
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- Recall $\tau^*(A) = \tau(\{1, \ldots, d\}) - \tau(\complement A)$
- There is a matrix $L$ such that $\hat{\tau}^* = L\hat{\tau}$
Step 2: \( \hat{\tau}^* \)

- Recall \( \tau^*(A) = \tau(\{1, \ldots, d\}) - \tau(\mathcal{C}A) \)
- There is a matrix \( L \) such that \( \hat{\tau}^* = L\hat{\tau} \)
- Hence \( \sqrt{n}(\hat{\tau}^* - \tau^*) \to N(0, LTL^\top) \).
Step 3: $\hat{\sigma}^*$ (Möbius inversion formula)

- If $\sigma^*$ and $\tau^*$ are two real maps on $2^D$ such that $\tau^*(\emptyset) = 0$ then

\[
\tau^*(A) = \sum_{B \subseteq A} \sigma^*(B) \quad \text{and} \quad \sigma^*(A) = \sum_{B \subseteq A} (-1)^{|A \setminus B|} \tau^*(B)
\]

are equivalent.

\[\text{2}^{\text{See Owen (2006) for an application of the Möbius inversion formulas to sensitivity analysis}}\]
Step 3: $\hat{\sigma}^*$ (Möbius inversion formula)

- If $\sigma^*$ and $\tau^*$ are two real maps on $\mathbb{2}^D$ such that $\tau^*(\emptyset) = 0$ then

$$\tau^*(A) = \sum_{B \subseteq A} \sigma^*(B) \text{ and } \sigma^*(A) = \sum_{B \subseteq A} (-1)^{|A \setminus B|} \tau^*(B)$$

are equivalent.

- Therefore, $\hat{\sigma}^* = M^*\hat{\tau}^*$ and hence

$$\sqrt{n}(\hat{\sigma}^* - \sigma^*) \rightarrow N(0, M^*LTL^\top M^*^\top).$$

\[^2\text{See Owen (2006) for an application of the Möbius inversion formulas to sensitivity analysis.}\]
Hypothesis testing

Test the contribution of $\sigma^*(A_1), \ldots, \sigma^*(A_k)$
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Test the contribution of $\sigma^*(A_1), \ldots, \sigma^*(A_k)$

$$H_0 : \sum_{i=1}^{k} \sigma^*(A_i) \leq (1 - \eta) \text{Var } f(X)$$

$\Leftrightarrow H_0 : \sum_{i=1}^{2^d - 1} c_i \sigma^*(A_i) \leq 0$

$\Leftrightarrow H_0 : c^\top \sigma \leq 0$
Hypothesis testing

Test the contribution of $\sigma^*(A_1), \ldots, \sigma^*(A_k)$

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$$\iff H_0 : \sum_{i=1}^{2^d-1} c_i \sigma^*(A_i) \leq 0$$

$$\iff H_0 : c^\top \sigma \leq 0$$

Test statistic: $\frac{\sqrt{nc^\top \hat{\sigma}^*}}{c^\top M^* LTL^\top M^*^\top c}$
Step 3: Find $\hat{\phi}$

- Shapley indices can be expressed\(^3\) as

$$\phi(j) = \sum_{B \cap \{j\} \neq \emptyset} \frac{\sigma^*(B)}{|B|},$$

\(^3\)Owen (2014)
Step 3: Find $\hat{\phi}$

- Shapley indices can be expressed\(^3\) as

$$\phi(j) = \sum_{B \cap \{j\} \neq \emptyset} \frac{\sigma^*(B)}{|B|},$$

- $\hat{\phi} = N^* \hat{\sigma}^*$

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- Shapley indices can be expressed as
  \[
  \phi(j) = \sum_{B \cap \{j\} \neq \emptyset} \frac{\sigma^*(B)}{|B|},
  \]

- $\hat{\phi} = N^*\hat{\sigma}^*$

- $\sqrt{n}(\hat{\phi} - \phi) \to N(0, N^*M^*LTL^TM^*^TN^*^T)$

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$^3$Owen (2014)
Boolean model of cell fate decision

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4Zinovyev et al (2012)
Sensitivity analysis \((n = 1000, d = 12)\)

- \(n = 1000\) “observations” were drawn.
- \(d = 12\) inputs were considered.

Histogram of outputs:
Statements as “activation of proteins C8 and RIP1 contribute to more 85% of apoptosis total variance ($p$–value $\leq 0.03$)” can be made.
We need to compute

\[
\begin{aligned}
\hat{\sigma}^* &= \frac{\hat{T}^*}{2^d \times 1} \\
&= \frac{M^* \hat{T}^*}{2^d \times 2^d} \\
\hat{\phi} &= \frac{N^* \hat{\sigma}^*}{d \times 2^d} \\
&= \frac{N^* \hat{\Sigma}^*}{d \times 2^d} \\
\hat{T}^* &= \frac{M^* T^* M^*\top}{2^d \times 2^d} \\
\hat{\Sigma}^* &= \frac{N^* \hat{\Sigma}^* N^*\top}{2^d \times 2^d}
\end{aligned}
\]
We need to compute

$$\begin{array}{c|c|c|c}
\hline
n2^d & \hat{\tau}^* & \hat{T}^* & n4^d \\
4^d & \sigma^* = M^* \hat{\tau}^* & \Sigma^* = M^* T^* M^*\top & 8^d \\
d2^d & \phi = N^* \sigma^* & N^* \Sigma^* N^*\top & d4^d \\
\hline
\end{array}$$

How can we do this efficiently?
Computational aspects

We need to compute

\[
\begin{align*}
 n2^d & | \hat{T}^* \in [2^d \times 1] \\
 4^d & | M^* \hat{T}^* \in [2^d \times 2^d][2^d \times 1] \\
 d2^d & | \hat{\sigma}^* = N^* \hat{\sigma}^* \in [d \times 2^d][2^d \times 1] \\
 & | \hat{T}^* \in [2^d \times 2^d] \\
 & | \hat{\Sigma}^* = \hat{\sigma}^* \hat{T}^* \hat{T}^* M^* \in [2^d \times 2^d][2^d \times 2^d][2^d \times 2^d] \\
 & | \hat{\sigma}^* \hat{\Sigma}^* \hat{\Sigma}^* \in [2^d \times 2^d][2^d \times 2^d][2^d \times d] \\
 n4^d & | M^* \in [2^d \times 2^d] \\
 8^d & | T^* M^* \in [2^d \times 2^d][2^d \times 2^d][2^d \times 2^d] \\
 d4^d & | \in [d \times 2^d][2^d \times 2^d][2^d \times d]
\end{align*}
\]

How can we do this efficiently?
### Computational aspects

We need to compute

\[
\begin{align*}
\hat{\tau}^* & \quad [2^d \times 1] \\
\hat{\sigma}^* & = M^* \quad [2^d \times 2^d] \\
\hat{\phi} & = N^* \quad [d \times 2^d]
\end{align*}
\]

\[
\begin{align*}
\hat{T}^* & \quad [2^d \times 2^d] \\
\hat{\Sigma}^* & = M^* T^* M^*^\top \\
N^* & \quad [d \times 2^d]
\end{align*}
\]

How can we do this efficiently?
### Computational aspects

We need to compute

\[
\begin{align*}
    n2^d & : \hat{\tau}^* \in [2^d \times 1] \\
    3^d & : \hat{\sigma}^* = M^* \hat{\tau}^* \in [2^d \times 2^d][2^d \times 1] \\
    d2^d & : \hat{\phi} = N^* \hat{\sigma}^* \in [d \times 2^d][2^d \times 1]
\end{align*}
\]

\[
\begin{align*}
    \hat{T}^* & = \begin{bmatrix} \hat{T}^* \\ \hat{\tau}^* \end{bmatrix} \in [2^d \times 2^d] \\
    \hat{\Sigma}^* & = \begin{bmatrix} \hat{\Sigma}^* \\ \hat{\tau}^* \end{bmatrix} \in [2^d \times 2^d][2^d \times 2^d] \\
    \hat{\Sigma}^* & = \begin{bmatrix} \hat{\Sigma}^* \\ \hat{\tau}^* \end{bmatrix} \in [2^d \times 2^d][2^d \times 2^d][2^d \times 2^d] \\
    N^* & = \begin{bmatrix} N^* \\ \hat{\tau}^* \end{bmatrix} \in [d \times 2^d][2^d \times 2^d][2^d \times d]
\end{align*}
\]

How can we do this efficiently?
Möbius inversion formula recast as Kronecker auto-products

\[ \sigma^*(A) = \sum_{B \subseteq A} (-1)^{|A \setminus B|} \tau^*(A). \]

\[
\begin{pmatrix}
\sigma^*(0) \\
\sigma^*(1) \\
\sigma^*(2) \\
\sigma^*(3) \\
\sigma^*(12) \\
\sigma^*(13) \\
\sigma^*(23) \\
\sigma^*(123)
\end{pmatrix} =
\begin{pmatrix}
1 & -1 & 1 \\
-1 & 1 & \\
-1 & 1 & 1 \\
1 & -1 & -1 & 1 \\
1 & -1 & -1 & \\
1 & -1 & -1 & 1 \\
1 & -1 & 1 & 1 \\
-1 & 1 & 1 & 1 \\
\end{pmatrix} \begin{pmatrix}
\tau^*(0) \\
\tau^*(1) \\
\tau^*(2) \\
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\]
\[
\begin{pmatrix}
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1 & 1 \\
-1 & 1 \\
-1 & 1 \\
1 & -1 & -1 & 1 \\
-1 & 1 & -1 & 1 \\
1 & -1 & -1 & 1 \\
-1 & 1 & 1 & -1 & 1 \\
1 & -1 & -1 & 1 & 1
\end{pmatrix} \begin{pmatrix}
\tau^*(0) \\
\tau^*(3) \\
\tau^*(2) \\
\tau^*(23) \\
\tau^*(1) \\
\tau^*(13) \\
\tau^*(12) \\
\tau^*(123)
\end{pmatrix}
\]
“Boolean” order

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<table>
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<td>110</td>
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</table>

Let $\sigma^*$ and $\tau^*$ satisfy M"{o}bius inversion formula

\[
\sigma^*(A) = \sum_{B \subset A} (-1)^{|A \setminus B|} \tau^*(A).
\]

If $\sigma^*$ and $\tau^*$ have their components arranged in the “Boolean” order, then 

\[
\sigma^* = (\otimes_d M) \tau^*,
\]

where

\[
M = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}.
\]

Therefore, the cost of computing $\hat{\sigma}^*$ and $\hat{\Sigma}^*$ are $\Theta(d^2)$ and $\Theta(d^4)$, respectively.
“Boolean” order

Let $\sigma^*$ and $\tau^*$ satisfy Möbius inversion formula

$$\sigma^*(A) = \sum_{B \subset A} (-1)^{|A\setminus B|} \tau^*(A).$$

If $\sigma^*$ and $\tau^*$ have their components arranged in the “Boolean” order, then $\sigma^* = (\otimes^d M)\tau^*$, where

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Therefore, the cost of computing $\hat{\sigma}^*$ and $\hat{\Sigma}^*$ are $\Theta(d2^d)$ and $\Theta(d4^d)$, respectively.
## Computational aspects

We need to compute

$$n2^d$$

$$3^d$$

$$d2^d$$

How can we do this efficiently?
Computational aspects

We need to compute

\[
\begin{align*}
n2^d & \quad \hat{\tau}^* \quad [2^d \times 1] \quad \hat{T}^* \quad [2^d \times 2^d] \quad n4^d \\
d2^d & \quad \hat{\sigma}^* = M^* \hat{\tau}^* \quad [2^d \times 2^d][2^d \times 1] \quad \hat{\Sigma}^* = M^* T^* M^*\top \quad d4^d \\
d2^d & \quad \hat{\phi} = N^* \hat{\sigma}^* \quad [d \times 2^d][2^d \times 1] \quad N^* \hat{\Sigma}^* N^*\top \quad d4^d
\end{align*}
\]

How can we do this efficiently?
Discussion I

- Thanks to Möbius and Kronecker, it is straightforward to make *inferences* for *all* types of sensitivity indices and *all* interactions/combinations.

- But most of the computational burden of a sensitivity analysis comes from model runs.
Discussion II

- We did *not* use the Sobol-Hoeffding decomposition!
- What are the “axioms” of sensitivity analysis?
- What are interactions?
- What are sensitivity indices?