Transformations and Invariance in Global Sensitivity Analysis

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- More severe: estimation of global sensitivity statistics used to identify the key drivers of uncertainty
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*Transformations alter the input-factor model-response mapping*
Setup

Model output of interest $y$ computed through a complex code and is dependent on $k$ uncertain input factors $x$,

$$g : x \mapsto y, \quad \Omega_x \subseteq \mathbb{R}^k \rightarrow \Omega_y \subseteq \mathbb{R},$$
Setup

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Local methods
Properties around $\mathbf{x}^0 \in \Omega_x$.
- Not responsive to uncertainty in the input factors
- Only a limited exploration of the input factor space
Global Methods: The Golden Standard

Probabilistic formulation
Input \( \mathbf{x} = (x_1, \ldots, x_k) \sim \mathbf{X} = (X_1, \ldots, X_k) \), RVec on \((\Omega_\mathbf{x}, \mathcal{A}, \mathbb{P}_\mathbf{x})\)
Output \( Y = g(\mathbf{X}) \) is RV on \((\Omega_Y, \mathcal{B}, \mathbb{P}_Y)\), \( \mathbb{P}_Y(B) = \mathbb{P}_\mathbf{x}(g^{-1}[B]) \)

\[ F_\mathbf{x}(\mathbf{x}) = \mathbb{P}_\mathbf{x}(\bigcap_{i=1}^{k} [X_i \leq x_i]) \text{ and } F_Y = \mathbb{P}_Y(Y \leq y) \] CDFs of \( \mathbf{X} \) and \( Y \)

\[ f_\mathbf{x}(\mathbf{x}) \text{ and } f_Y(y) \] PDFs of \( \mathbf{X} \) and \( Y \)
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Input distributions are known!
Global Methods II: Categories

- Linear regression (also with rank and other transformations)
- Screening methods [5]
- Variance-based methods [8]
- Expected value of information-based methods [9]
- Distribution-based methods [2]

Variance-based methods have been the most widely studied both from the theoretical and numerical viewpoints: ANOVA decomposition
Variance-Based Method

Main effects and total effects

\[ \eta_1^Y (X_i) = \frac{\text{Var}[E[Y|X_i]]}{\text{Var}[Y]}, \quad \eta_T^Y (X_i) = \frac{E[\text{Var}[Y|X_{\sim i}]]}{\text{Var}[Y]} \]

Here \( X_{\sim i} \): Vector \( X \) without \( i \)th component
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Example

\[ Y = \exp(X_1 + 2 \cdot X_2) \quad \text{with} \quad X_1, X_2 \sim \mathcal{N}(0, 1) \quad \text{iid.} \]

\( \eta_1^Y(X_i) \) and \( \eta_T^Y(X_i) \) \((i = 1, 2)\) computed with [7]'s estimator varying the number of model evaluations \( M \)
Convergence Issues, Interpretation Problems

Main effects

Total effects

Raw Data

Log Trafo

Rank Trafo

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Invariance GSA
Issues and Problems II

- No convergence on the raw data: Analytically

\[ \eta^Y_1(X_1) = 0.012, \quad \eta^Y_1(X_2) = 0.364, \]
\[ \eta^Y_T(X_1) = 0.637, \quad \eta^Y_T(X_2) = 0.988. \]
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- Convergence on the log-transformed data
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Transformations: Model structure changes from multiplicative to additive:
\[ \hat{\eta}_1^{\log(Y)}(X_i) = \hat{\eta}_T^{\log(Y)}(X_i) \]

Calculations do not readily translate back!
A decision-maker’s state of knowledge is represented by the probability law $P_Y$ of the random variable of interest $Y$. 

A Generalized Framework for GSA
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**Sensitivity summarizes two states of knowledge**
Before and after knowing that $X_i = x_i$

More on this idea: [3].
A Generalized Framework

Definition (Sensitivity Measure)

Let $d(\cdot, \cdot)$ measure a shift (discrepancy, distance) between the unconditional probability $\mathbb{P}_Y$ and the probability $\mathbb{P}_{Y|X_i=x_i}$ conditional to a realization $X_i = x_i$. The associated sensitivity measure is defined as an expected shift of the conditional probabilities,

$$
\gamma_d(X_i) = \mathbb{E} \left[ d(\mathbb{P}_Y, \mathbb{P}_{Y|X_i}) \right] \tag{1}
$$
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$$\gamma_d(X_i) = E \left[ d(P_Y, P_{Y|X_i}) \right] \quad (1)$$

First order effect: $d(P_Y, P_{Y|X_i=x_i}) = \nabla[Y]^{-1} (\nabla[Y] - \nabla[Y|X_i = x_i])$
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\gamma^Y_d(X_i) = \mathbb{E} \left[ d(P_Y, P_{Y|X_i}) \right] \quad (1)
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First order effect: $d(P_Y, P_{Y|X_i=x_i}) = \nabla [Y]^{-1} (\nabla [Y] - \nabla [Y|X_i = x_i])$

Approach allows for estimates: Analogously to Correlation Ratio estimation of first order effects.
Monotonic Transformations

Consider a monotonic transformation of $y,$

$$u : \Omega_Y \to \Omega_U \subseteq \mathbb{R}, \ y \mapsto u(y) \text{ and } u \circ g : \Omega_X \to \mathbb{R}, \ x \mapsto u(g(x))$$
Monotonic Transformations

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$$ u : \Omega_Y \rightarrow \Omega_U \subseteq \mathbb{R}, \ y \mapsto u(y) \text{ and } u \circ g : \Omega_X \rightarrow \mathbb{R}, \ x \mapsto u(g(x)) $$

When $x$ is uncertain, $u$ becomes a random variable (denoted by $U$) induced by $\mathbb{P}_X$ through the composition of $u$ with $g$.

$\gamma^U(X_i)$: sensitivity statistics of $X_i$ with respect to $U = u(Y)$. 

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Invariance GSA
Monotonic Invariance

A sensitivity measure is monotonic invariant, if \( \gamma^U(X_i) = \gamma^Y(X_i) \) for all suitable models \( Y = g(X) \) and transformations \( U = u: g(X) \).
Monotonic Invariance

A sensitivity measure is monotonic invariant, if $\gamma^U(X_i) = \gamma^Y(X_i)$ for all suitable models $Y = g(X)$ and transformations $U = u: g(X)$

**Theorem**

A sensitivity measure $\gamma_d$ is monotonic invariant if its shift $d$ is monotonic invariant.

Decision Theory: Sensitivity measure independent under choice of utility function [1]
Invariant shifts

**Definition**
Let $\mathbb{P}$ and $\mathbb{Q}$ be probability measures on $(\Omega, \mathcal{A})$. Let $h : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ be a continuous and non-decreasing function with $h(0) = 0$ and $\sup_t \frac{h(2t)}{h(t)} < \infty$ (Orlicz condition for generalized triangle inequality). Then, we define

$$d(\mathbb{P}, \mathbb{Q}) = \sup_{A \in \mathcal{A}} h \left( \left| \mathbb{P}(A) - \mathbb{Q}(A) \right| \right)$$  \hspace{1cm} (2)

**Theorem**
Such a $d(\cdot, \cdot)$ is monotonic invariant.
Invariant shifts: PDF based

Example
For \( h(t) = t \) and \( f \) and \( g \) PDFs of \( P \) and \( Q \): From (2)

\[
\sup_{A \in A} |P(A) - Q(A)| = \sup_{A \in A} \left| \int_A (f(y) - g(y)) dy \right| \\
= \frac{1}{2} \int_Y |f(y) - g(y)| dy
\]

(Consider \( A = \{y : f(y) \geq g(y)\}\))

Hence: Borgonovo importance measure is transformation invariant,

\[
\delta^Y(X_i) = \frac{1}{2} \int_{X_i} f_{X_i}(x_i) \int_Y |f_Y(y) - f_{Y|X_i=x_i}(y)| dy dx_i
\]
Monotonic invariant shifts: CDF based

Consider only half-rays $A(y) = \{ z \leq y \}$ in (2):

$$d(P, Q) = \sup_{y \in \mathbb{R}} h(|F(y) - G(y)|)$$

(3)

where $F(y) = P(z \leq y)$ and $G(y) = Q(z \leq y)$ are the CDFs.

Transformation invariance: Birnbaum-Orlicz family of metrics

$h(t) = t$: Kolmogorov-Smirnov distance,

$$\beta^Y(X_i) = \int_{\mathcal{X}} f_{X_i}(x_i) \sup_{y \in \mathcal{Y}} \left| F_Y(y) - F_{Y|X_i=x_i}(y) \right| \, dx_i$$
Example revisited

\[ Y = \exp(X_1 + 2 \cdot X_2) \quad \text{with} \quad X_1, X_2 \sim \mathcal{N}(0, 1) \quad \text{iid}. \]
Example revisited

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Level E Geosphere Transport Model

Sensitivity of total dose over time: QMC sample, size 8192:

Main Effects

Main Effects on Log

Kolmogorov Smirnov Sensitivity

Borgonovo Sensitivity

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Conclusions

- Uncertainty is coded in the probability in general, not only in the variance: Need for stronger sensitivity measures
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- Uncertainty is coded in the probability in general, not only in the variance: Need for stronger sensitivity measures
- General Framework: Estimators from given data are available
- Transformation invariance: no change of interpretation
- Suitable domain for estimation: gain in numerical precision
Thank you!

Any questions?

More details: [4]
Estimation from given data: [6]

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