Global Sensitivity Analysis

How to perform comprehensive, efficient, and robust Global Sensitivity Analysis?

Debraj Roy

Computational Science Lab, University of Amsterdam

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Introduction

Global Sensitivity Analysis (GSA)

To understand GSA we need to be clear about the following:

- The shortcomings of OFAT
- The objective of GSA
- Formulation of GSA

Global sensitivity analysis

Which parameters are most significant *over the entire input range?*

Applications of GSA

Factor prioritization

which factors determine output the most

Factor fixing

which factors can be removed from the model

Variance cutting

which factors, made more certain, would make output more certain

Factor mapping

which factors are most important for causing good/bad outputs

"Good" global sensitivity index should satisfy

- To be global, i.e. to consider parameter variations in the entire feasible space.
- To be quantitative, i.e. computable through a numerical, reproducible procedure.
- To be model independent, i.e. applicable independently of the form of the input—output relationship, e.g. linear or non-linear, additive or non-additive, etc.
- To be unconditional on any assumed input value.
- To be easy to interpret, compute and stable.
- To be moment-independent.

Variance-based Sensitivity

Indices

Consider a model:

$$Y = f(X_1, X_2, X_3,, X_k)$$

What would happen to the uncertainty of Y if we could fix a factor.

Imagine that we fix factor X_i at a particular value x_i^* .

 $Y = f(X_1, X_2, X_3,, X_k)$ Let $V_{X_{\sim i}}(Y|X_i = x_i^*)$ be the resulting variance of Y, taken over $X_{\sim i}$ (all factors but X_i). We call this a conditional variance, as it is conditional on X_i being fixed to x_i^* .

$$Y = f(X_1, X_2, X_3,, X_k)$$

We would imagine that, having frozen one potential source of variation (X_i) , the resulting variance $V_{X_{\sim i}}(Y|X_i=x_i^*)$ will be less than the corresponding total or unconditional variance V(Y)

$$Y = f(X_1, X_2, X_3,, X_k)$$

 $V_{X_{\sim i}}(Y|X_i = x_i^*)$ could be a potential indicator of sensitivity of parameter X_i , reasoning that the smaller the remaining variance - $V_{X_{\sim i}}(Y|X_i = x_i^*)$, the greater the influence of X_i .

$$Y = f(X_1, X_2, X_3,, X_k)$$

There are few problem though in using $V_{X_{\sim i}}(Y|X_i=x_i^*)$ as a measure for sensitivity:

- First, it makes the sensitivity measure dependent on the position of point x_i* for each input factor, which is impractical
- one can design a model that for particular factors X_i and fixed point x_i^* yields $V_{X_{\sim i}}(Y|X_i=x_i^*)>V(Y)$

Solution:

- If we take instead the average of this measure over all possible points x_i^* , the dependence on x_i^* will disappear.
- We write this as $E_{X_i}(V_{X_{\sim i}}(Y|X_i=x_i^*))$. This is always lower or equal to V(Y)

Solution:

- If we take instead the average of this measure over all possible points x_i^* , the dependence on x_i^* will disappear.
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$$E_{X_i}(V_{X_{\sim i}}(Y|X_i)) + V_{X_i}(E_{X_{\sim i}}(Y|X_i)) = V(Y)$$

First-order Sensitivity Index

$$S_i = rac{V_{X_i}(E_{X_{\sim i}}(Y|X_i))}{V(Y)}, 0 \leq S_i \leq 1$$

A high value signals an important variable. And vice versa? Does a small value of S_i flag a non-important variable?

Higher-order Sensitivity Indices

We continue our game with conditioned variances by playing with two factors instead of one.

$$\frac{V_{X_i,X_j}(E_{X_{\sim ij}}(Y|X_i,X_j))}{V(Y)}$$

Higher-order Sensitivity Indices

We continue our game with conditioned variances by playing with two factors instead of one.

$$V(E(Y|X_i,X_j)) = V_i + V_j + V_{ij}$$

The term V_{ij} is the interaction term between factors X_i, X_j . It captures that part of the response of Y to X_i, X_j that cannot be written as a superposition of effects separately due to X_i, X_j

What is a total effect term? Let us again use our model, and ask what we would obtain if we were to compute:

$$\frac{V_{\sim i}(E_{X_i}(Y|X_{\sim i}))}{V(Y)}$$

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$$\frac{V_{\sim i}(E_{X_i}(Y|X_{\sim i}))}{V(Y)}$$

We are conditioning now on all factors but X_i . In other words, we ask the question what variance would remain if we fix everything but X_i .

What is a total effect term? Let us again use our model, and ask what we would obtain if we were to compute:

$$S_{T_i} = 1 - \frac{V_{X_{\sim i}}(E_{X_i}(Y|X_{\sim i}))}{V(Y)}$$

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To consider a different example, for a generic three-factor model, one would have:

$$S_{T_1} = 1 - \frac{V_{X_{\sim 1}}(E_{X_1}(Y|X_{\sim 1}))}{V(Y)} = S_1 + S_{12} + S_{13} + S_{123}$$

High Dimensional Model

decomposition

High dimensional model representation

$$Y = f(X_1, X_2, X_3,, X_k)$$

$$Y = f_0 + \sum_i f_i(X_i) + \sum_{i,j} f_{ij}(X_i, X_j) + ...$$

where f_0 is a constant and f_i is a function of X_i , f_{ij} a function of X_i and X_j , etc. Assuming [?],

$$\int_0^1 f_{i_1 i_2 \dots i_s}(X_{i_1}, X_{i_2}, \dots, X_{i_s}) dX_k = 0, \text{ for } k = i_1, \dots, i_s$$

High dimensional model representation

$$Y = f_0 + \sum_{i} f_i(X_i) + \sum_{i,j} f_{ij}(X_i, X_j) + \dots$$

Taking unconditional expectation on both sides:

$$f_0 = E(Y)$$

Taking conditional expectation $X_i = x_i$

$$f_i(x_i) = E(Y|X_i = x_i) - f_0$$

 f_i is the effect of varying X_i alone (known as the main effect of X_i)

High dimensional model representation

$$Y = f_0 + \sum_i f_i(X_i) + \sum_{i,j} f_{ij}(X_i, X_j) + \dots$$

Taking conditional expectation $X_i = x_i, X_j = x_j$ $f_{ii}(x_i, x_j) = E(Y|X_i = x_i, X_i = x_j) - f_i(x_i) - f_i(x_j) - f_0$

 f_{ij} is the effect of varying X_i and X_j simultaneously, additional to the effect of their individual variations. This is known as a second-order interaction. Higher-order terms have analogous definitions.

Can you derive the third-order interaction?

Variance decomposition

If inputs are independent, V distributes over this!
$$Var(Y) = \sum_{i} V(Y|X_i) + \sum_{i,j} V(Y|X_i,X_j) + \dots$$

$$Var(Y) = \sum_{i=1}^{d} V_i + \sum_{i < j}^{d} V_{ij} + \dots + V_{12...d}$$

$$V_i = Var_{X_i} \left(E_{\mathbf{X}_{\sim i}}(Y \mid X_i) \right)$$

$$V_{ij} = Var_{X_{ij}} \left(E_{\mathbf{X}_{\sim ij}}(Y \mid X_i,X_j) \right) - V_i - V_j$$

First-Order Sensitivity Index

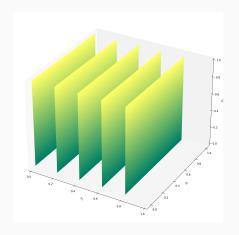
First-order sensitivity index", or "main effect index" $S_i = \frac{V_i}{V(Y)}$. it measures the effect of varying X_i alone, but averaged over variations in other input parameters.

$$V(Y) = \sum_{i=1}^{d} V_i + \sum_{i < j}^{d} V_{ij} + \dots + V_{12...d}$$

Dividing both sides by
$$Var(Y)$$
:

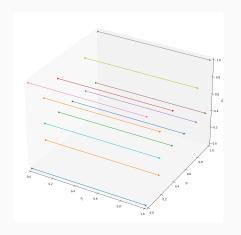
$$\sum_{i=1}^{d} S_i + \sum_{i< j}^{d} S_{ij} + \dots + S_{12...d} = 1$$

First-Order Sensitivity Index



$$\sum_{i=1}^{d} S_i + \sum_{i< j}^{d} S_{ij} + \dots + S_{12...d} = 1$$

$$\begin{split} S_{\mathit{Ti}} &= \frac{\mathit{E}_{\mathsf{X}_{\sim i}} \left(\mathsf{Var}_{\mathit{X_i}}(\mathit{Y} | \mathsf{X}_{\sim i}) \right)}{\mathsf{Var}(\mathit{Y})} = 1 - \frac{\mathsf{Var}_{\mathsf{X}_{\sim i}} \left(\mathit{E}_{\mathit{X_i}}(\mathit{Y} | \mathsf{X}_{\sim i}) \right)}{\mathsf{Var}(\mathit{Y})} \\ \text{and} \\ \sum_{i=1}^{d} S_{\mathit{Ti}} &\geq 1 \end{split}$$



$$\sum_{i=1}^d S_{Ti} \geq 1$$

Estimating Sensitivity Indicies

Estimating Sensitivity

Consider a model:

If the factors to the model $y = f(X_1, X_2, X_3,, X_k)$ is composed of independent random variables, the joint probability density function of the factors is:

$$P(X_1, X_2, X_3,, X_k) = \prod_{i=1}^k p_i(x_i)$$

Expectation and Variance

Mean and variance of y can be computed as:

$$E(y) = \int \cdots \int_{k} f(X_1, X_2, X_3,, X_k) \prod_{i=1}^{k} p_i(x_i) dx_i$$

$$V(y) = \int \cdots \int_{k} (f(X_{1}, X_{2}, X_{3}, \dots, X_{k}) - E(y))^{2} \prod_{i=1}^{k} p_{i}(x_{i}) dx_{i}$$

$$= \int \cdots \int_{k} f^{2}(X_{1}, X_{2}, X_{3}, \dots, X_{k}) \prod_{i=1}^{k} p_{i}(x_{i}) dx_{i} - E^{2}(y)$$

If one of the input factors x_j is fixed to a generic value \tilde{x}_j , the resulting variance of y will be equal to:

$$V(y|x_{j} = \tilde{x}_{j}) = \int \cdots \int_{k} (f(X_{1}, X_{2}, X_{3}, \dots, X_{k}) - E(y|x_{j} = \tilde{x}_{j}))^{2} \prod_{\substack{i=1\\i \neq j}}^{k} p_{i}(x_{i}) dx_{i}$$

$$= \int \cdots \int_{k} f^{2}(X_{1}, X_{2}, X_{3}, \dots, X_{k}) \prod_{\substack{i=1\\i \neq j}}^{k} p_{i}(x_{i}) dx_{i} - E^{2}(y|x_{j} = \tilde{x}_{j})$$

Estimating First-order Sensitivity

For the purpose of sensitivity analysis one is interested in eliminating the dependence upon the value \tilde{x}_j by integrating $V(y|x_j=\tilde{x}_j)$ over the probability density function of \tilde{x}_j , obtaining:

$$E(V(y|x_j)) = \int \cdots \int_k f^2(X_1, X_2, X_3, \dots, X_k) \prod_{i=1}^k p_i(x_i) dx_i - \int E^2(y|x_j = \tilde{x}_j) p_j(x_j) d\tilde{x}_j$$

$$V(y) = \int \cdots \int_{k} f^{2}(X_{1}, X_{2}, X_{3},, X_{k}) \prod_{i=1}^{k} p_{i}(x_{i}) dx_{i} - E^{2}(y)$$

$$E(V(y|x_j)) = \int \cdots \int_k f^2(X_1, X_2, X_3, \dots, X_k) \prod_{i=1}^k p_i(x_i) dx_i - \int E^2(y|x_j = \tilde{x}_j) p_j(x_j) d\tilde{x}_j$$

We have dropped the dependence \tilde{x}_j due to the integration, therefore:

$$V(y) - E(V(y|x_j)) = \int E^2(y|x_j = \tilde{x}_j) p_j(\tilde{x}_j) d\tilde{x}_j - E^2(y)$$

We have dropped the dependence \tilde{x}_j due to the integration, therefore:

$$V(y) - E(V(y|x_j)) = \int E^2(y|x_j = \tilde{x}_j) p_j(\tilde{x}_j) d\tilde{x}_j - E^2(y)$$

The left-hand side of the above equation is also equal to $V_{X_i}(E_{X_{\sim i}}(Y|X_i))$ and is a good measure of the sensitivity of y with respect to factor x_j . If one divides it by the unconditional variance V(y), one obtains the so-called first-order sensitivity index:

$$S_i = \frac{V_{X_i}(E_{X_{\sim i}}(Y|X_i))}{V(Y)}, 0 \leq S_i \leq 1$$

$$V(y) - E(V(y|x_j)) = \int E^2(y|x_j = \tilde{x}_j) p_j(\tilde{x}_j) d\tilde{x}_j - E^2(y)$$

The the computational question reduces to estimating the integral $\int E^2(y|x_j=\tilde{x_j})p_j(\tilde{x_j})d\tilde{x_j}$

$$\int E^{2}(y|x_{j} = \tilde{x}_{j})p_{j}(\tilde{x}_{j})d\tilde{x}_{j} =$$

$$\int \left\{ \int \cdots \int f(x_{1}, x_{2}, x_{3}, \dots, x_{k}) \prod_{\substack{i=1\\i\neq j}}^{k} p_{i}(x_{i})dx_{i} \right\}^{2} p_{j}(\tilde{x}_{j})d\tilde{x}_{j}$$

$$\int E^{2}(y|x_{j} = \tilde{x}_{j})p_{j}(\tilde{x}_{j})d\tilde{x}_{j}$$

$$= \int \left\{ \int \cdots \int f(x_{1}, x_{2}, x_{3}, \dots, x_{k}) \prod_{\substack{i=1\\i \neq j}}^{k} p_{i}(x_{i})dx_{i} \right\}^{2} p_{j}(\tilde{x}_{j})d\tilde{x}_{j}$$

$$= \int \cdots \int f(x_{1}, x_{2}, x_{3}, \dots, x_{k}) \prod_{\substack{i=1\\i \neq j}}^{k} p_{i}(x_{i})dx_{i}$$

$$f(x'_{1}, x'_{2}, x'_{3}, \dots, x'_{k}) \prod_{\substack{i=1\\i \neq j}}^{k} p_{i}(x'_{i})dx'_{i}p_{j}(\tilde{x}_{j})d\tilde{x}_{j}$$

$$\int E^{2}(y|x_{j} = \tilde{x}_{j})p_{j}(\tilde{x}_{j})d\tilde{x}_{j}$$

$$= \int \left\{ \int \cdots \int f(x_{1}, x_{2}, x_{3}, \dots, x_{k}) \prod_{\substack{i=1\\i \neq j}}^{k} p_{i}(x_{i})dx_{i} \right\}^{2} p_{j}(\tilde{x}_{j})d\tilde{x}_{j}$$

$$= \int \cdots \int f(x_{1}, x_{2}, \dots, \tilde{x}_{j}, \dots, x_{k})f(x'_{1}, x'_{2}, \dots, \tilde{x}_{j}, \dots, x'_{k}) \prod_{i=1}^{k} p_{i}(x_{i})dx_{i} \prod_{\substack{i=1\\i \neq j}}^{k} p_{i}(x'_{i})dx'_{i}$$

The integral can be computed using a single Monte Carlo loop. The Monte Carlo procedure that follows was proposed by Saltelli et al. Two input sample matrices A and B are generated:

$$A = \begin{bmatrix} x_{11} & \dots & x_{1k} \\ \vdots & \ddots & \vdots \\ x_{n1} & & x_{nK} \end{bmatrix} \qquad B = \begin{bmatrix} x'_{11} & \dots & x'_{1k} \\ \vdots & \ddots & \vdots \\ x'_{n1} & \dots & x'_{nk} \end{bmatrix}$$

Then a new matrix B_A^j can be defined as:

$$B_{A}^{j} = \begin{bmatrix} x'_{11} & x'_{12} & \dots & x_{1j} & \dots & x'_{1k} \\ \vdots & \dots & \ddots & & & \\ x'_{n1} & x'_{n2} & \dots & x_{nj} & \dots & x'_{nk} \end{bmatrix}$$

If one thinks of matrix A as the "sample" matrix, and of B as the "re-sample" matrix, then A_B^j a matrix where all factors except x_j are re-sampled.

$$\int E^{2}(y|x_{j} = \tilde{x}_{j})p_{j}(\tilde{x}_{j})d\tilde{x}_{j} = \frac{1}{n}\sum_{i=1}^{n}f(A)_{i}f(B_{A}^{j})_{i}$$

$$E^{2}(y) = \frac{1}{n}\sum_{i=1}^{n}f(A)_{i}f(B)_{i}$$

In this way the computational cost associated with a full set of first order indices S_i is n(k+2).

Estimating Total-order Sensitivity

$$S_{T_i} = 1 - \frac{V_{X_{\sim i}}(E_{X_i}(Y|X_{\sim i}))}{V(Y)}$$

We need to estimate $V_{X_{\sim i}}(E_{X_i}(Y|X_{\sim i}))$

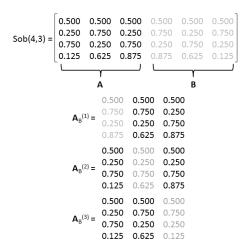
Estimating Total-order Sensitivity

$$\int E^{2}(y|x_{j} = \sim \tilde{x}_{j})\rho_{j}(\sim \tilde{x}_{j})d(\sim \tilde{x_{j}}) = \frac{1}{n}\sum_{i=1}^{n}f(B)_{i}f(B_{A}^{j})_{i}$$

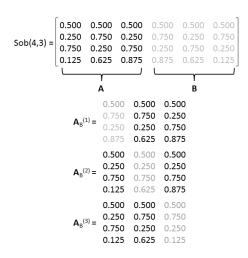
$$E^{2}(y) = \frac{1}{n}\sum_{i=1}^{n}f(A)_{i}f(B)_{i}$$

Homework: Work it out yourself. What is the computational cost?

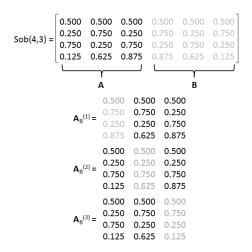
Generate an N \times 2d sample matrix, i.e. each row is a sample point in the hyperspace of 2d dimensions. Sample from pdf [?].



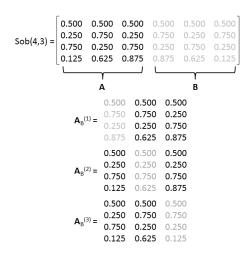
Use the first d columns of the matrix as matrix \mathbf{A} , and the remaining d columns as matrix \mathbf{B} .



Build d further N × d matrices A_B^i , for i = 1,2,...,d, such that the ith column of A_B^i = the ith column of B, and the remaining columns are from



N(d+2) points in the input space (one for each row).corresponding f(A), f(B) and $f(A_B^i)$ values.

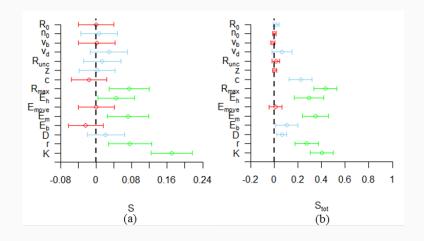


$$Var_{X_i}(E_{\mathbf{X}_{\sim i}}(Y|X_i)) \approx \frac{1}{N} \sum_{j=1}^{N} f(\mathbf{B})_j \left(f(\mathbf{A}_B^i)_j - f(\mathbf{A})_j \right)$$

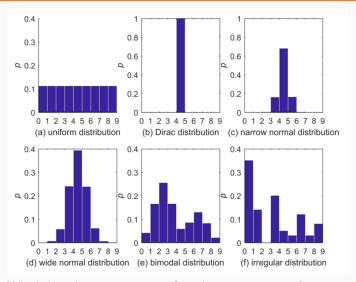
$$E_{\mathbf{X}_{\sim i}}(Var_{X_i}(Y|\mathbf{X}_{\sim i})) \approx \frac{1}{2N} \sum_{j=1}^{N} \left(f(\mathbf{A})_j - f(\mathbf{A}_B^i)_j \right)^2$$

$$Sob(4,3) = \begin{bmatrix} 0.500 & 0.500 & 0.500 & 0.500 & 0.500 & 0.500 \\ 0.250 & 0.750 & 0.250 & 0.750 & 0.250 & 0.750 \\ 0.750 & 0.250 & 0.750 & 0.250 & 0.750 & 0.250 \\ 0.125 & 0.625 & 0.875 & 0.875 & 0.625 & 0.125 \end{bmatrix}$$

$$\mathbf{A}_{\mathbf{B}}^{(1)} = \begin{bmatrix} 0.500 & 0.500 & 0.500 & 0.500 \\ 0.750 & 0.250 & 0.250 & 0.750 \\ 0.250 & 0.250 & 0.250 & 0.250 \\ 0.875 & 0.625 & 0.875 \\ 0.500 & 0.500 & 0.500 \\ 0.750 & 0.750 & 0.750 \\ 0.125 & 0.625 & 0.875 \\ 0.500 & 0.500 & 0.500 \\ 0.750 & 0.750 & 0.750 \\ 0.125 & 0.625 & 0.750 \\ 0.750 & 0.750 & 0.250 \\ 0.750 & 0.750 & 0.250 \\ 0.750 & 0.750 & 0.250 \\ 0.750 & 0.250 & 0.250 \\ 0.125 & 0.625 & 0.125 \end{bmatrix}$$

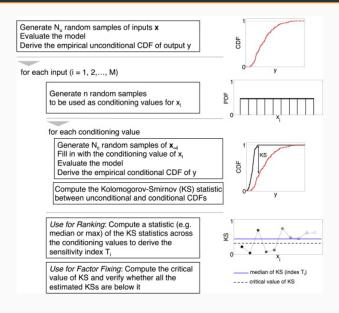


Variance-based drawback

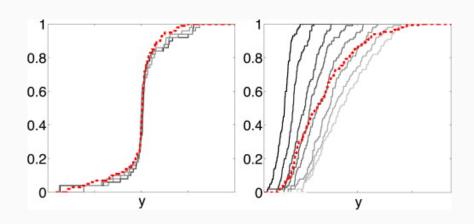


Which has the most variance? and most uncertain?

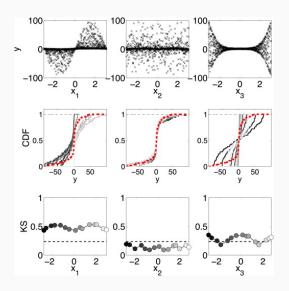
Density based methodsk

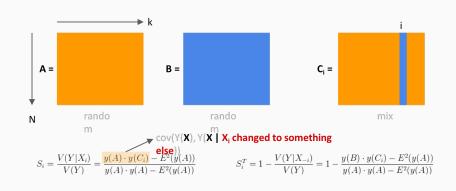


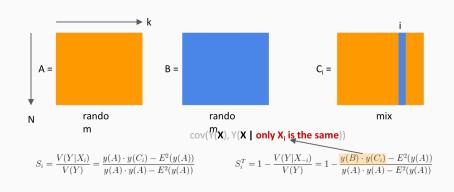
Density based methods

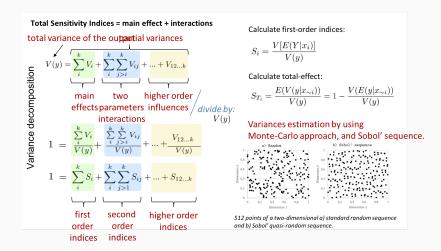


Density based methods









Questions?

References I