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Variance-based methods for Sensitivity Analysis II Part - Estimations

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$$S_i = \frac{Var[E(y|x_i)]}{Var(y)}$$

First order sensitivity index

S_i can be described as the fraction of the model output variance which is caused by the input x_i alone

$$T_i = 1 - \frac{Var[E(y|\boldsymbol{x}_{-i})]}{Var(y)} = \frac{E[Var(y|\boldsymbol{x}_{-i})]}{Var(y)}$$

Total order sensitivity index

The total order sensitivity index is a measure which, for variable x_i, is the sum of all sensitivity indices which include the input x_i

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How can we compute them?

$$S_i = \frac{Var[E(y|xi)]}{Var(y)} \qquad T_i = \frac{E[Var(y|\boldsymbol{x}_{-i})]}{Var(y)}$$

$$V_1 = Var[E(y|x_1)] = \int f(x_1', x_2') \left[f(x_1', x_2) - f(x_1, x_2) \right] dx_1 dx_2 dx_1' dx_2'$$

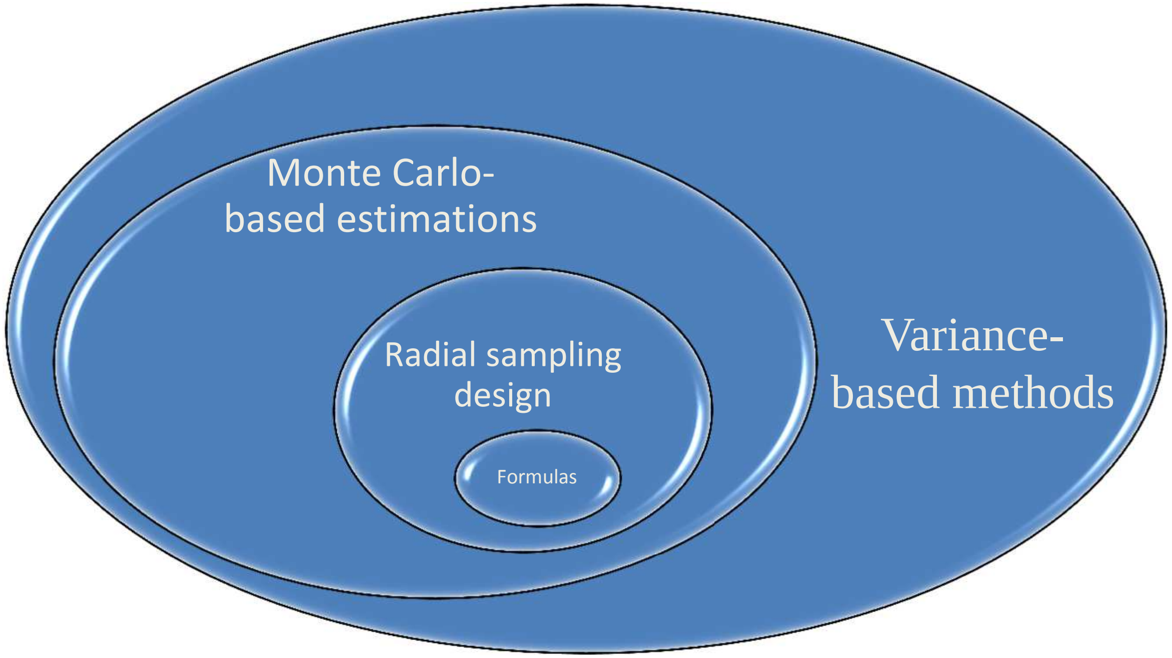
$$V_{T1} = E[Var(y|x_{-1})] = \frac{1}{2} \int \left[f(x_1, x_2) - f(x'_1, x_2) \right]^2 dx_1 dx_2 dx'_1$$

How can we compute them?

$$S_i = \frac{Var[E(y|xi)]}{Var(y)}$$

$$T_i = \frac{E[Var(y|\boldsymbol{x}_{-i})]}{Var(y)}$$

Monte Carlo estimation

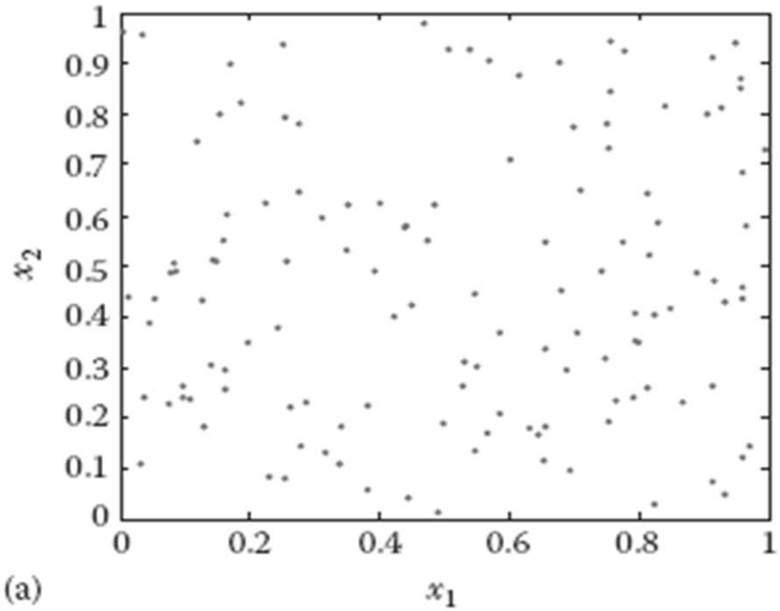


Monte Carlo is based on *random sampling**: taking random points from our input distributions

$$\begin{bmatrix} x_{11} & x_{12} & x_{1d} \\ x_{21} & x_{22} & x_{2d} \\ \vdots & & \vdots \\ x_{N1} & x_{N2} & x_{Nd} \end{bmatrix} \xrightarrow{\text{model}} \begin{bmatrix} y_1 \\ y_2 \\ \cdots \\ \cdots \\ y_N \end{bmatrix}$$

With d input variables, we can represent a sample of N points in an Nxd matrix

An example of random sampling with two dimensions



(a)

It is helpful to think of sampling inputs in terms of points in a plane (d=2), cube (d=3), hypercube (d>3)

Monte Carlo estimates

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$$S_i = \frac{Var[E(y \mid x_i)]}{Var(y)}$$

$$V_1 = Var[E(y \mid x_1)] = \int f(x_1', x_2')\left[f(x_1', x_2) - f(x_1, x_2)\right] dx_1 dx_2 dx_1' dx_2'$$

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Monte Carlo estimates

$$S_i = \frac{Var[E(y \mid x_i)]}{Var(y)}$$

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$$\Downarrow$$

$$\boxed{\hat{V}_1 = Var\left[E\left(y \mid x_1\right)\right] = \frac{1}{N} \sum_{r=1}^{N} f\left(x_{r1}', x_{r2}'\right)\left[f\left(x_{r1}', x_{r2}\right) - f\left(x_{r1}, x_{r2}\right)\right]}$$

Monte Carlo estimates

$$S_i = \frac{Var[E(y \mid x_i)]}{Var(y)}$$

$$V_1 = Var[E(y \mid x_1)] = \int f(x_1', x_2') \left[f(x_1', x_2) - f(x_1, x_2) \right] dx_1 dx_2 dx_1' dx_2'$$

$$\hat{V}_1 = Var\left[E\left(y \mid x_1\right)\right] = \frac{1}{N} \sum_{r=1}^{N} f\left(x_{r1}', x_{r2}'\right) \left[f\left(x_{r1}', x_{r2}\right) - f\left(x_{r1}, x_{r2}\right) \right]$$

MC estimates: total effects

$$T_i = 1 - \frac{Var[E(y|\boldsymbol{x}_{-i})]}{Var(y)} = \frac{E[Var(y|\boldsymbol{x}_{-i})]}{Var(y)}$$

$$V_{T1} = E[Var\ (y \mid x_{-1})] = \frac{1}{2}\int \left[\boxed{f\,(x_1, x_2)} - \boxed{f\,(x'_1\,, x_2)}\right]^2 dx_1 dx_2 d\,x'_1$$

$$\updownarrow \qquad \updownarrow$$

$$\hat{V}_{T1} = E\left[Var\left(y \mid x_{-1}\right)\right] = \frac{1}{2N}\sum_{r=1}^{N}\left[\boxed{f\left(x_{r1}, x_{r2}\right)} - \boxed{f\left(x'_{r1}, x_{r2}\right)}\right]^2$$

Monte Carlo estimates

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$$S_i = \frac{Var[E(y \mid x_i)]}{Var(y)}$$

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MC estimates: examples

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We need an ad-hoc sampling design

Example in 2-D:

$$\hat{V}_1 = \frac{1}{N}\sum_{r=1}^{N} f(x_{r1}', x_{r2}')\left[f(x_{r1}', x_{r2}) - f(x_{r1}, x_{r2})\right]$$

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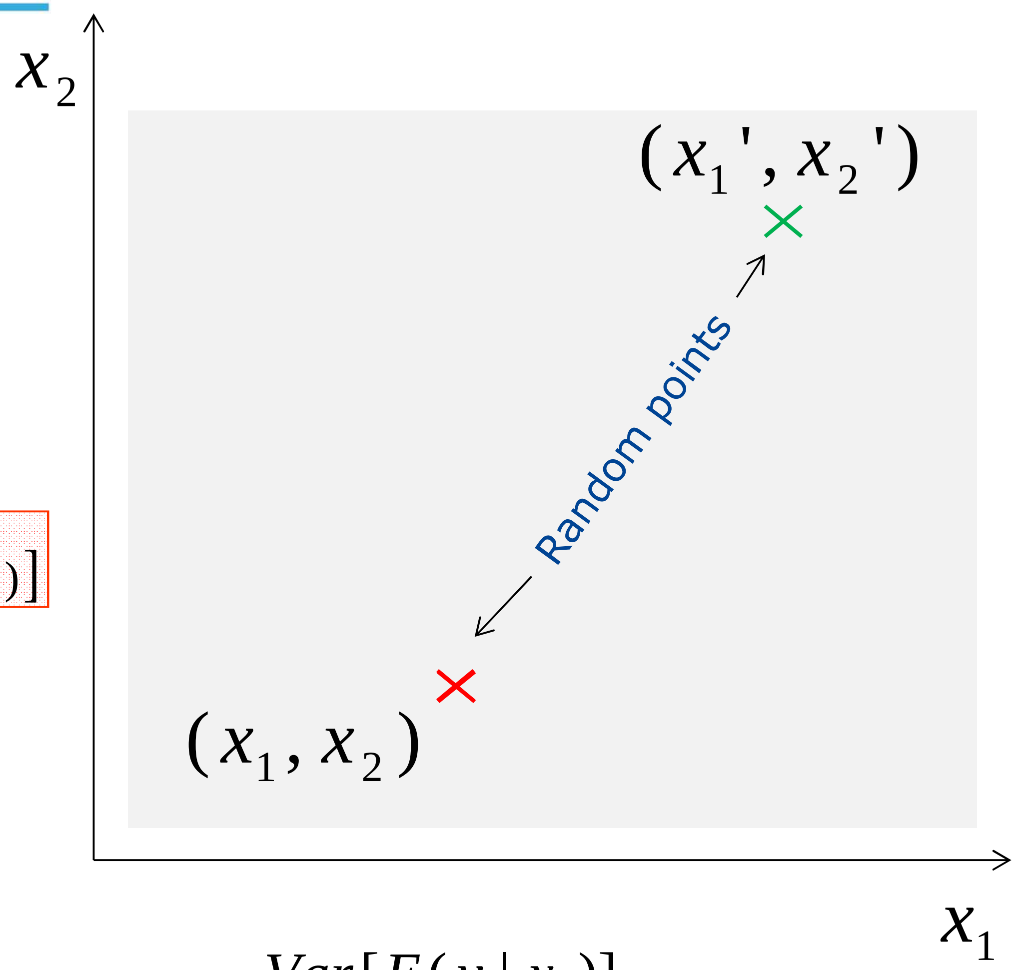

$$S_i = \frac{Var[E(y \mid x_i)]}{Var(y)}$$

MC estimates: examples

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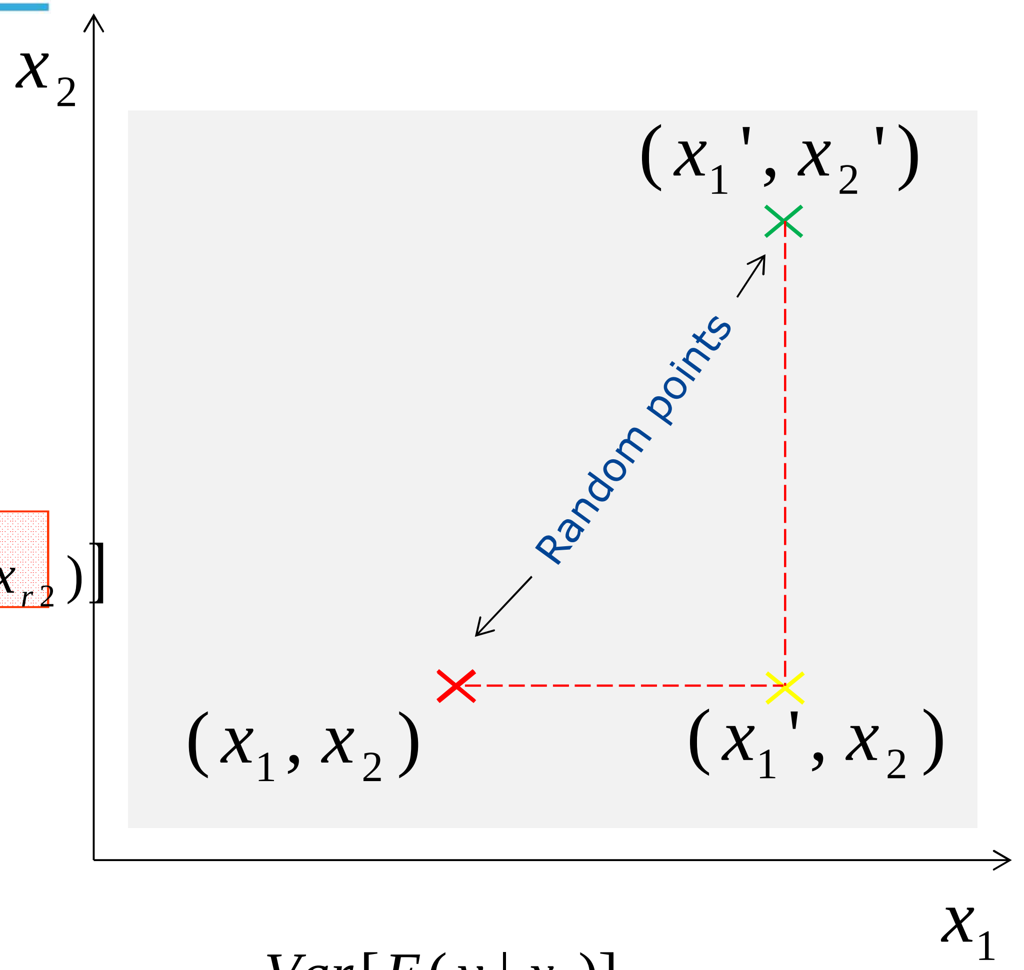

$$S_i = \frac{Var[E(y \mid x_i)]}{Var(y)}$$

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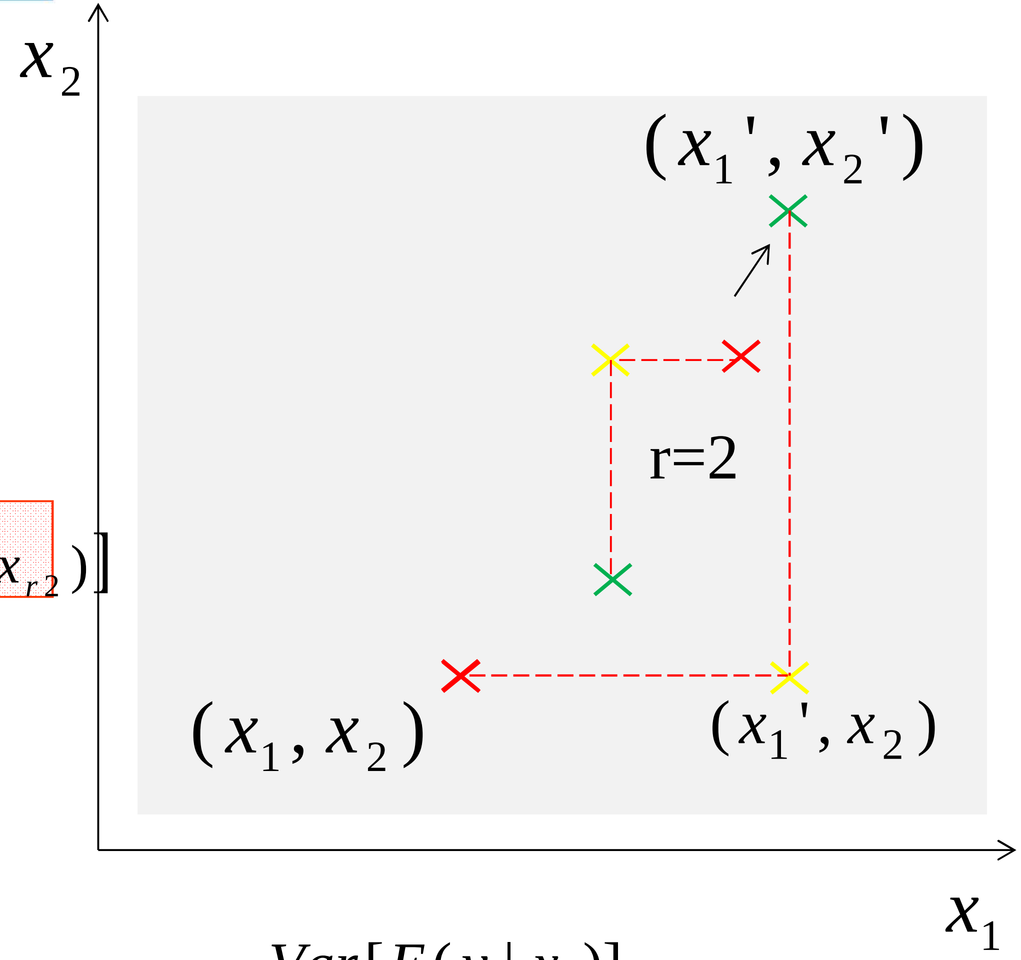

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MC estimates: examples

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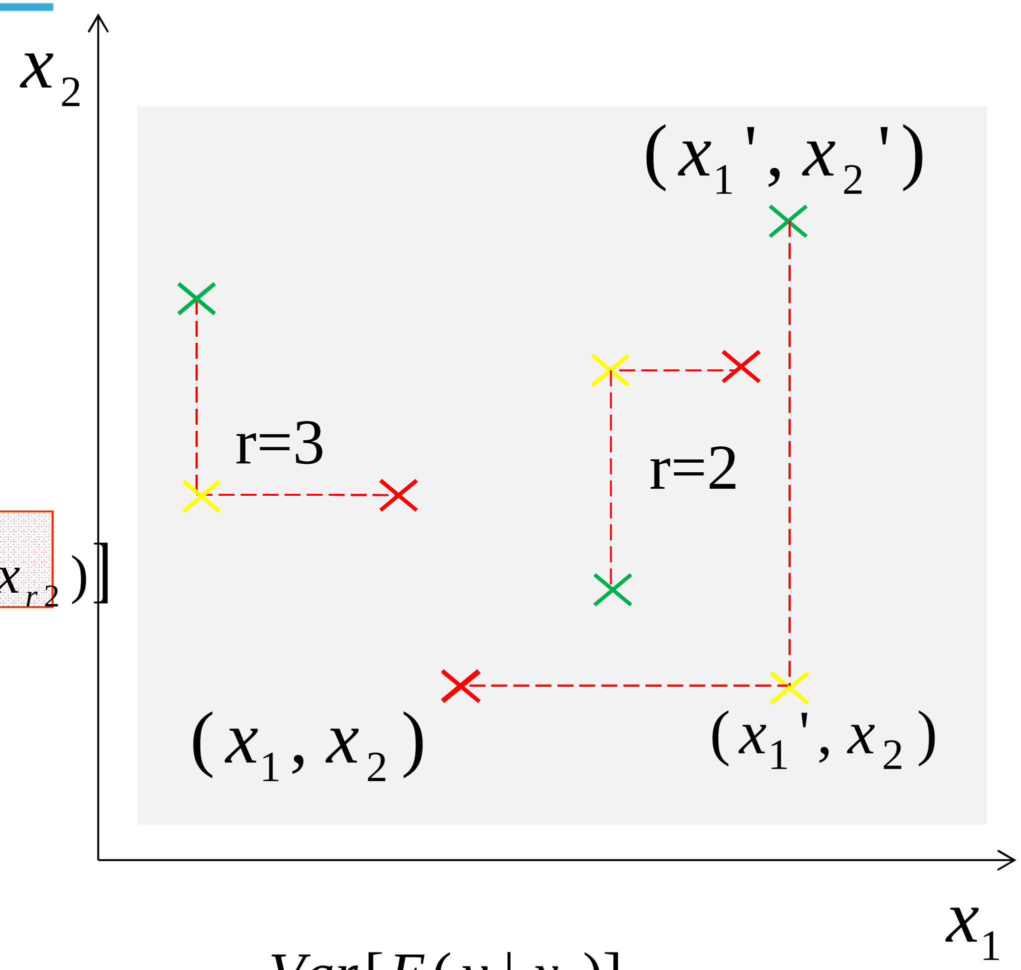
$$\hat{V}_1 = \frac{1}{N}\sum_{r=1}^{N} f(x_{r1}', x_{r2}')\left[f(x_{r1}', x_{r2}) - f(x_{r1}, x_{r2})\right]$$



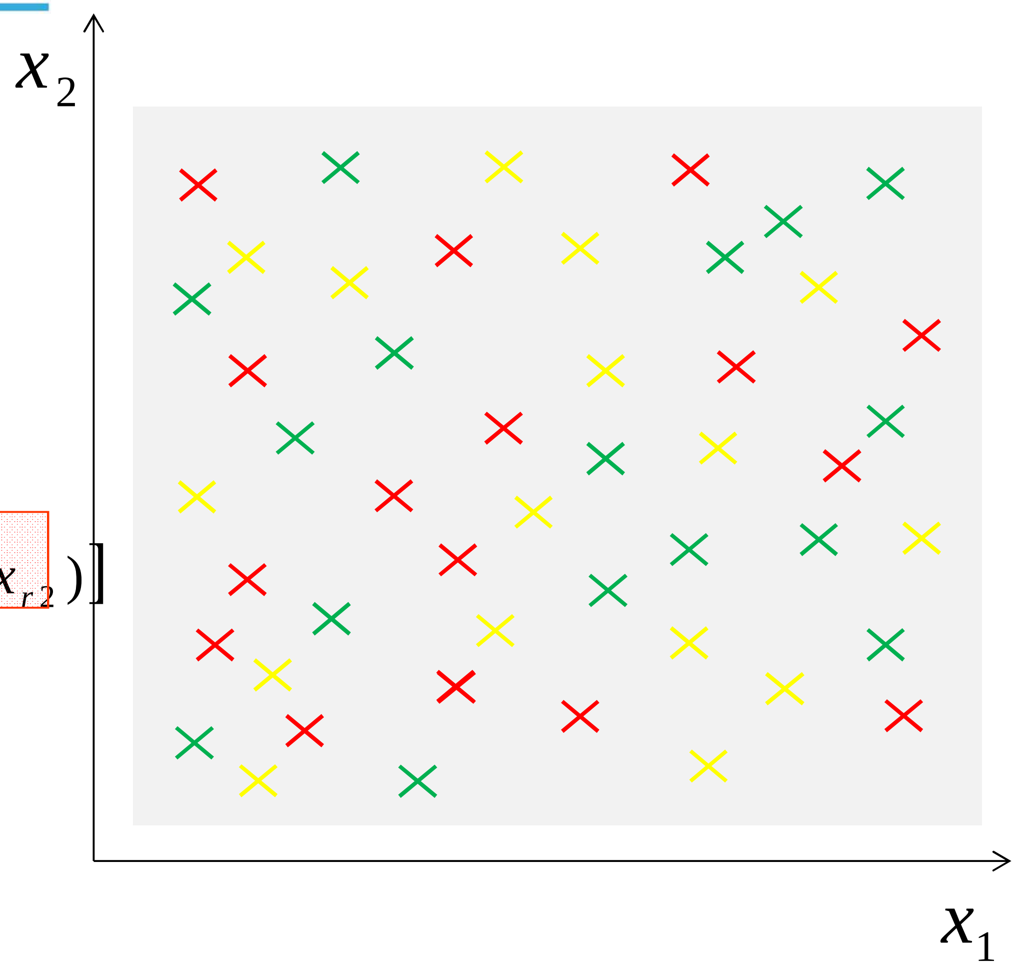
$$S_i = \frac{Var[E(y \mid x_i)]}{Var(y)}$$

MC estimates: examples

We need an ad-hoc sampling design

Example in 2-D:

$$\hat{V}_1 = \frac{1}{N}\sum_{r=1}^{N} f\boxed{(x_{r1}', x_{r2}')}\left[\boxed{f(x_{r1}', x_{r2})} - \boxed{f(x_{r1}, x_{r2})}\right]$$

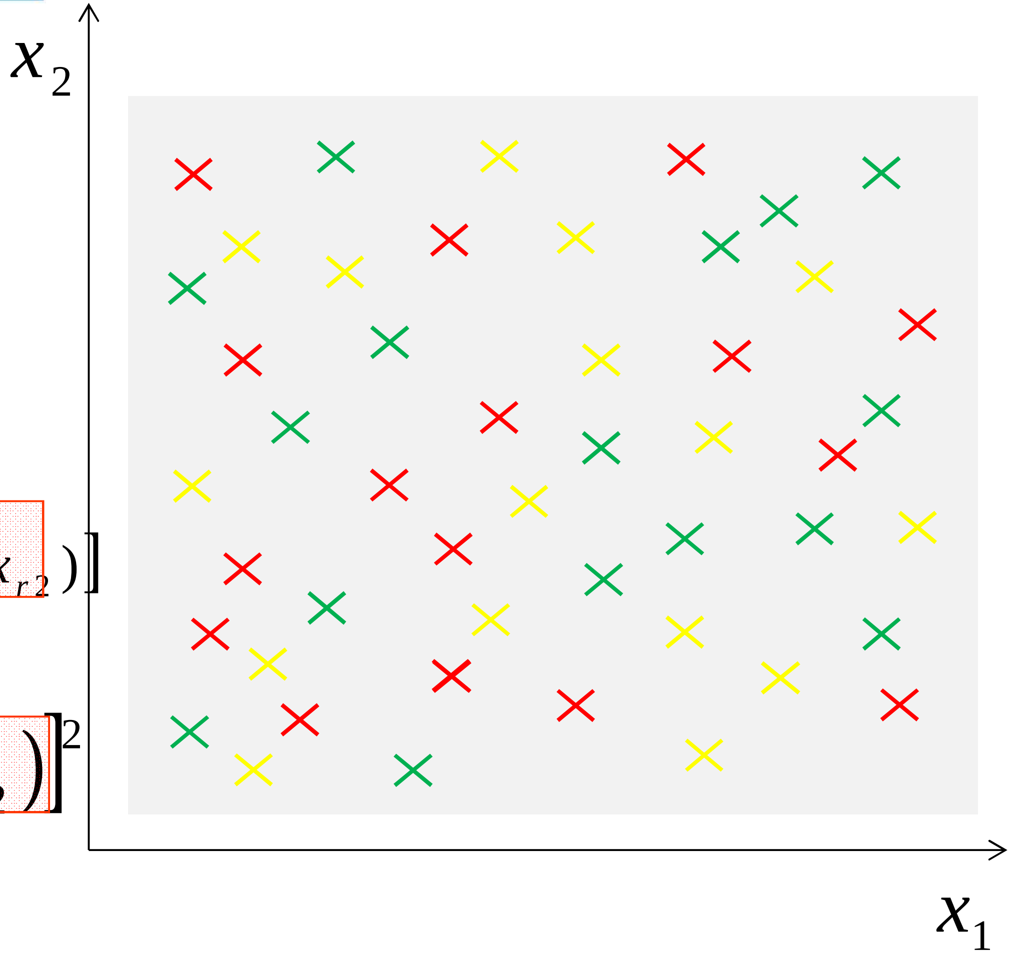


Precision increases as *N* increases
Analysis requires *N*(*d*+2) runs of the model
N limited by availability of the computational resources

MC estimates: examples

We need an ad-hoc sampling design

Example in 2-D:



$$\hat{V}_1 = \frac{1}{N}\sum_{r=1}^{N} f(x_{r1}', x_{r2}')[f(x_{r1}', x_{r2}) - f(x_{r1}, x_{r2})]$$

$$\hat{V}_{T1} = \frac{1}{2N}\sum_{r=1}^{N}\left[f\left(x_{r1}', x_{r2}\right) - f\left(x_{r1}, x_{r2}\right)\right]^2$$

Precision increases as *N* increases
Analysis requires $N(d+2)$ runs of the model
N limited by availability of the computational resources

Monte Carlo estimates

$$\hat{V}_{T1} = E\left[Var\left(y \mid x_2, x_3\right)\right] = \frac{1}{2N}\sum_{r=1}^{N}\left[f\left(x'_{r1}, x_{r2}, x_{r3}\right) - f\left(x_{r1}, x_{r2}, x_{r3}\right)\right]^2$$

$$\hat{V}_{T2} = E\left[Var\left(y \mid x_1, x_3\right)\right] = \frac{1}{2N}\sum_{r=1}^{N}\left[f\left(x_{r1}, x'_{r2}, x_{r3}\right) - f\left(x_{r1}, x_{r2}, x_{r3}\right)\right]^2$$

$$\hat{V}_{T3} = E\left[Var\left(y \mid x_1, x_2\right)\right] = \frac{1}{2N}\sum_{r=1}^{N}\left[f\left(x_{r1}, x_{r2}, x'_{r3}\right) - f\left(x_{r1}, x_{r2}, x_{r3}\right)\right]^2$$

$$\hat{V}_1 = Var\left[E\left(y \mid x_1\right)\right] = \frac{1}{N}\sum_{r=1}^{N} f\left(x'_{r1}, x'_{r2}, x'_{r3}\right)\left[f\left(x'_{r1}, x_{r2}, x_{r3}\right) - f\left(x_{r1}, x_{r2}, x_{r3}\right)\right]$$

$$\hat{V}_2 = Var\left[E\left(y \mid x_2\right)\right] = \frac{1}{N}\sum_{r=1}^{N} f\left(x'_{r1}, x'_{r2}, x'_{r3}\right)\left[f\left(x_{r1}, x'_{r2}, x_{r3}\right) - f\left(x_{r1}, x_{r2}, x_{r3}\right)\right]$$

$$\hat{V}_3 = Var\left[E\left(y \mid x_3\right)\right] = \frac{1}{N}\sum_{r=1}^{N} f\left(x'_{r1}, x'_{r2}, x'_{r3}\right)\left[f\left(x_{r1}, x_{r2}, x'_{r3}\right) - f\left(x_{r1}, x_{r2}, x_{r3}\right)\right]$$

MC estimate: first order indices →Practical Steps: matrix view

$$Var[E(y|x_1)] = \frac{1}{N}\sum_{r=1}^{N} f(x'_{r1}, x'_{r2}, x'_{r3})[f(x'_{r1}, x_{r2}, x_{r3}) - f(x_{r1}, x_{r2}, x_{r3})]$$

$$Var[E(y|x_2)] = \frac{1}{N}\sum_{r=1}^{N} f(x'_{r1}, x'_{r2}, x'_{r3})[f(x_{r1}, x'_{r2}, x_{r3}) - f(x_{r1}, x_{r2}, x_{r3})]$$

$$Var[E(y|x_3)] = \frac{1}{N}\sum_{r=1}^{N} f(x'_{r1}, x'_{r2}, x'_{r3})[f(x_{r1}, x_{r2}, x'_{r3}) - f(x_{r1}, x_{r2}, x_{r3})]$$

B $\quad$ **A**$_B$ $\quad$ **A**

A = [$x_1 \quad x_2 \quad x_3$] $\qquad$ **B** = [$x'_1 \quad x'_2 \quad x'_3$]

A = [0.500 0.750 0.800] $\qquad$ **B** = [0.123 0.056 0.701]

A$_B^{(1)}$ = [0.123 0.750 0.800]

A$_B^{(2)}$ = [0.500 0.056 0.800]

A$_B^{(3)}$ = [0.500 0.750 0.701]

Monte Carlo estimate →Practical Steps: matrix view

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$$Var[E(y \mid x_1)] = \frac{1}{N}\sum_{r=1}^{N} f\left(x'_{r1}, x'_{r2}, x'_{r3}\right)\left[f\left(x'_{r1}, x_{r2}, x_{r3}\right) - f\left(x_{r1}, x_{r2}, x_{r3}\right)\right]$$

$$Var[E(y \mid x_2)] = \frac{1}{N}\sum_{r=1}^{N} f\left(x'_{r1}, x'_{r2}, x'_{r3}\right)\left[f\left(x_{r1}, x'_{r2}, x_{r3}\right) - f\left(x_{r1}, x_{r2}, x_{r3}\right)\right]$$

$$Var[E(y \mid x_3)] = \frac{1}{N}\sum_{r=1}^{N} f\left(x'_{r1}, x'_{r2}, x'_{r3}\right)\left[f\left(x_{r1}, x_{r2}, x'_{r3}\right) - f\left(x_{r1}, x_{r2}, x_{r3}\right)\right]$$

$$\begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ \vdots & & \vdots \\ x_{N1} & x_{N2} & x_{N3} \end{bmatrix} \qquad \begin{bmatrix} x'_{11} & x'_{12} & x'_{13} \\ x'_{21} & x'_{22} & x'_{23} \\ \vdots & & \vdots \\ x'_{N1} & x'_{N2} & x'_{N3} \end{bmatrix}$$

A **B**

1. Generate TWO independent random samples with N points in d dimensions
2. Denote the first matrix $\boldsymbol{A}$ and the other one $\boldsymbol{B}$

Monte Carlo estimate
→Practical Steps: matrix view

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$$Var[E(y|x_1)] = \frac{1}{N}\sum_{r=1}^{N} \boxed{f(x'_{r1}, x'_{r2}, x'_{r3})}\left[\boxed{f(x'_{r1}, x_{r2}, x_{r3})} - \boxed{f(x_{r1}, x_{r2}, x_{r3})}\right]$$

$$Var[E(y|x_2)] = \frac{1}{N}\sum_{r=1}^{N} \boxed{f(x'_{r1}, x'_{r2}, x'_{r3})}\left[\boxed{f(x_{r1}, x'_{r2}, x_{r3})} - \boxed{f(x_{r1}, x_{r2}, x_{r3})}\right]$$

$$Var[E(y|x_3)] = \frac{1}{N}\sum_{r=1}^{N} \boxed{f(x'_{r1}, x'_{r2}, x'_{r3})}\left[\boxed{f(x_{r1}, x_{r2}, x'_{r3})} - \boxed{f(x_{r1}, x_{r2}, x_{r3})}\right]$$

$$A = \begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ \vdots & & \vdots \\ x_{N1} & x_{N2} & x_{N3} \end{bmatrix} \qquad B = \begin{bmatrix} x'_{11} & x'_{12} & x'_{13} \\ x'_{21} & x'_{22} & x'_{23} \\ \vdots & & \vdots \\ x'_{N1} & x'_{N2} & x'_{N3} \end{bmatrix}$$

1. Generate TWO independent random samples with N points in d dimensions
2. Denote the first matrix A and the other one B
3. For a given input variable x_i, construct a matrix A_{Bi} which consists of all the columns of matrix A, except the i-th column, which is taken from matrix B

$$A_B^{(1)} = \begin{bmatrix} x'_{11} & x_{12} & x_{13} \\ x'_{21} & x_{22} & x_{23} \\ \vdots & & \vdots \\ x'_{N1} & x_{N2} & x_{N3} \end{bmatrix}$$

$$A_B^{(2)} = \begin{bmatrix} x_{11} & x'_{12} & x_{13} \\ x_{21} & x'_{22} & x_{23} \\ \vdots & & \vdots \\ x_{N1} & x'_{N2} & x_{N3} \end{bmatrix}$$

$$A_B^{(3)} = \begin{bmatrix} x_{11} & x_{12} & x'_{13} \\ x_{21} & x_{22} & x'_{23} \\ \vdots & & \vdots \\ x_{N1} & x_{N2} & x'_{N3} \end{bmatrix}$$

Monte Carlo estimate: first order indices
→Practical Steps: matrix view

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$$Var\left[E(y\,|\,x_1)\right]=\frac{1}{N}\sum_{r=1}^{N} f\left(x'_{r1},x'_{r2},x'_{r3}\right)\left[f\left(x'_{r1},x_{r2},x_{r3}\right)-f\left(x_{r1},x_{r2},x_{r3}\right)\right]$$

$$Var\left[E(y\,|\,x_2)\right]=\frac{1}{N}\sum_{r=1}^{N} f\left(x'_{r1},x'_{r2},x'_{r3}\right)\left[f\left(x_{r1},x'_{r2},x_{r3}\right)-f\left(x_{r1},x_{r2},x_{r3}\right)\right]$$

$$Var\left[E(y\,|\,x_3)\right]=\frac{1}{N}\sum_{r=1}^{N} f\left(x'_{r1},x'_{r2},x'_{r3}\right)\left[f\left(x_{r1},x_{r2},x'_{r3}\right)-f\left(x_{r1},x_{r2},x_{r3}\right)\right]$$

$$\begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ \vdots & & \vdots \\ x_{N1} & x_{N2} & x_{N3} \end{bmatrix} \qquad \begin{bmatrix} x'_{11} & x'_{12} & x'_{13} \\ x'_{21} & x'_{22} & x'_{23} \\ \vdots & & \vdots \\ x'_{N1} & x'_{N2} & x'_{N3} \end{bmatrix}$$

A B

1. Generate TWO independent random samples with N points in d dimensions
2. Denote the first matrix A and the other one B
3. For a given input variable x_i, construct a matrix A_{Bi} which consists of all the columns of matrix A , except the i-th column, which is taken from matrix B
4. Now an estimation of V_i, the numerator of S_i, is given as follows:

$$\hat{V}_i=\frac{1}{N}\sum_{r=1}^{N} f(B)_r\left(f\left(A_B^i\right)_r - f(A)_r\right)$$

$$A_B^{(1)} = \begin{bmatrix} x'_{11} & x_{12} & x_{13} \\ x'_{21} & x_{22} & x_{23} \\ \vdots & & \vdots \\ x'_{N1} & x_{N2} & x_{N3} \end{bmatrix}$$

$$A_B^{(2)} = \begin{bmatrix} x_{11} & x'_{12} & x_{13} \\ x_{21} & x'_{22} & x_{23} \\ \vdots & & \vdots \\ x_{N1} & x'_{N2} & x_{N3} \end{bmatrix}$$

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Monte Carlo sampling

$$\mathbf{A} = \begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ \vdots & & \vdots \\ x_{N1} & x_{N2} & x_{N3} \end{bmatrix} \xrightarrow{M} f(\mathbf{A}) = \begin{bmatrix} f(x_{11}, x_{12}, x_{13}) \\ f(x_{21}, x_{22}, x_{23}) \\ \vdots \\ f(x_{N1}, x_{N2}, x_{N3}) \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} x'_{11} & x'_{12} & x'_{13} \\ x'_{21} & x'_{22} & x'_{23} \\ \vdots & & \vdots \\ x'_{N1} & x'_{N2} & x'_{N3} \end{bmatrix} \xrightarrow{M} f(\mathbf{B}) = \begin{bmatrix} f(x'_{11}, x'_{12}, x'_{13}) \\ f(x'_{21}, x'_{22}, x'_{23}) \\ \vdots \\ f(x'_{N1}, x'_{N2}, x'_{N3}) \end{bmatrix}$$

$$\mathbf{A}_B = \begin{bmatrix} x'_{11} & x_{12} & x_{13} \\ x'_{21} & x_{22} & x_{23} \\ \vdots & & \vdots \\ x'_{N1} & x_{N2} & x_{N3} \end{bmatrix} \xrightarrow{M} f(\mathbf{A}_B) = \begin{bmatrix} f(x'_{11}, x_{12}, x_{13}) \\ f(x'_{21}, x_{22}, x_{23}) \\ \vdots \\ f(x'_{N1}, x_{N2}, x_{N3}) \end{bmatrix}$$

In 3-D: N*(3+2)

In general: N*(d+2)

Monte Carlo estimate: first order indices
→Practical Steps: matrix view

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$$Var[E(y|x_1)] = \frac{1}{N}\sum_{r=1}^{N} f(x'_{r1}, x'_{r2}, x'_{r3})[f(x'_{r1}, x_{r2}, x_{r3}) - f(x_{r1}, x_{r2}, x_{r3})]$$

$$Var[E(y|x_2)] = \frac{1}{N}\sum_{r=1}^{N} f(x'_{r1}, x'_{r2}, x'_{r3})[f(x_{r1}, x'_{r2}, x_{r3}) - f(x_{r1}, x_{r2}, x_{r3})]$$

$$Var[E(y|x_3)] = \frac{1}{N}\sum_{r=1}^{N} f(x'_{r1}, x'_{r2}, x'_{r3})[f(x_{r1}, x_{r2}, x'_{r3}) - f(x_{r1}, x_{r2}, x_{r3})]$$

$$\begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ \vdots & & \vdots \\ x_{N1} & x_{N2} & x_{N3} \end{bmatrix} \qquad \begin{bmatrix} x'_{11} & x'_{12} & x'_{13} \\ x'_{21} & x'_{22} & x'_{23} \\ \vdots & & \vdots \\ x'_{N1} & x'_{N2} & x'_{N3} \end{bmatrix}$$

A **B**

$$\hat{V}_i = \frac{1}{N}\sum_{r=1}^{N} f(B)_r \left(f(A_B^i)_r - f(A)_r \right)$$

$$\mathbf{A_B}^{(1)} = \begin{bmatrix} x'_{11} & x_{12} & x_{13} \\ x'_{21} & x_{22} & x_{23} \\ \vdots & & \vdots \\ x'_{N1} & x_{N2} & x_{N3} \end{bmatrix}$$

$$\mathbf{A_B}^{(2)} = \begin{bmatrix} x_{11} & x'_{12} & x_{13} \\ x_{21} & x'_{22} & x_{23} \\ \vdots & & \vdots \\ x_{N1} & x'_{N2} & x_{N3} \end{bmatrix}$$

$$\mathbf{A_B}^{(3)} = \begin{bmatrix} x_{11} & x_{12} & x'_{13} \\ x_{21} & x_{22} & x'_{23} \\ \vdots & & \vdots \\ x_{N1} & x_{N2} & x'_{N3} \end{bmatrix}$$

Monte Carlo estimate →Practical Steps: matrix view

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$$S_i = \frac{Var[E(y \mid x_i)]}{Var(y)} \qquad T_i = \frac{E[Var(y|\boldsymbol{x}_{-i})]}{Var(y)}$$

$$\mathbf{A} = \begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ \vdots & & \vdots \\ x_{N1} & x_{N2} & x_{N3} \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} x'_{11} & x'_{12} & x'_{13} \\ x'_{21} & x'_{22} & x'_{23} \\ \vdots & & \vdots \\ x'_{N1} & x'_{N2} & x'_{N3} \end{bmatrix}$$

$$\hat{V}_i = \frac{1}{N}\sum_{r=1}^{N} f(B)_r \left(f\left(A_B^i\right)_r - f(A)_r \right)$$

$$\hat{V}_{Ti} = \frac{1}{2N}\sum_{r=1}^{N} \left[f\left(A_B^i\right)_r - f(A)_r \right]^2$$

$$\mathbf{A}_\mathrm{B}^{(1)} = \begin{bmatrix} x'_{11} & x_{12} & x_{13} \\ x'_{21} & x_{22} & x_{23} \\ \vdots & & \vdots \\ x'_{N1} & x_{N2} & x_{N3} \end{bmatrix}$$

$$\mathbf{A}_\mathrm{B}^{(2)} = \begin{bmatrix} x_{11} & x'_{12} & x_{13} \\ x_{21} & x'_{22} & x_{23} \\ \vdots & & \vdots \\ x_{N1} & x'_{N2} & x_{N3} \end{bmatrix}$$

$$\mathbf{A}_\mathrm{B}^{(3)} = \begin{bmatrix} x_{11} & x_{12} & x'_{13} \\ x_{21} & x_{22} & x'_{23} \\ \vdots & & \vdots \\ x_{N1} & x_{N2} & x'_{N3} \end{bmatrix}$$

MC estimate: total order indices →Practical Steps: matrix view

$$\hat{V}_{T1} = E[Var(y \mid x_2 x_3)] = \frac{1}{2N}\sum_{r=1}^{N}\left[f\left(\boxed{x'_{r1}, x_{r2}, x_{r3}}\right) - f\left(\boxed{x_{r1}, x_{r2}, x_{r3}}\right)\right]^2$$

$$\hat{V}_{T2} = E[Var(y \mid x_1 x_3)] = \frac{1}{2N}\sum_{r=1}^{N}\left[f\left(\boxed{x_{r1}, x'_{r2}, x_{r3}}\right) - f\left(\boxed{x_{r1}, x_{r2}, x_{r3}}\right)\right]^2$$

$$\hat{V}_{T3} = E[Var(y \mid x_1 x_2)] = \frac{1}{2N}\sum_{r=1}^{N}\left[f\left(\boxed{x_{r1}, x_{r2}, x'_{r3}}\right) - f\left(\boxed{x_{r1}, x_{r2}, x_{r3}}\right)\right]^2$$

$\mathbf{A}_B$ $\qquad$ $\mathbf{A}$

Jansen's formula

$\mathbf{A} = [\ x_1 \quad x_2 \quad x_3]$ $\qquad$ $\mathbf{B} = [\ x_1' \quad x_2' \quad x_3']$

A = [0.500 0.750 0.800] $\qquad$ **B** = [~~0.123 0.056 0.701~~]

$\mathbf{A}_B^{(1)}$ = [0.123 0.750 0.800]

$\mathbf{A}_B^{(2)}$ = [0.500 0.056 0.800]

$\mathbf{A}_B^{(3)}$ = [0.500 0.750 0.701]

Monte Carlo estimation – radial design

Given two random **independent** matrices **A** and B of the same size Nxd, (where **N** is the sample size and the number of factors):

$$A = \begin{bmatrix} a_{1,1} & \cdots & a_{1,j} & & a_{1,d} \\ \vdots & & a_{2,j} & & \\ & & \vdots & \ddots & \\ a_{N,1} & & a_{N,j} & & a_{N,d} \end{bmatrix} \quad B = \begin{bmatrix} b_{1,1} & \cdots & b_{1,j} & & b_{1,d} \\ \vdots & & a_{2,j} & & \\ & & \vdots & \ddots & \\ b_{N,1} & & b_{N,j} & & b_{N,d} \end{bmatrix}$$

$$A = \begin{bmatrix} a_{1,1} & \cdots & a_{1,j} & & a_{1,d} \\ \vdots & & a_{2,j} & & \\ & & \vdots & \ddots & \\ a_{N,1} & & a_{N,j} & & a_{N,d} \end{bmatrix} \quad B = \begin{bmatrix} b_{1,1} & \cdots & b_{1,j} & & b_{1,d} \\ \vdots & & a_{2,j} & & \\ & & \vdots & \ddots & \\ b_{N,1} & & b_{N,j} & & b_{N,d} \end{bmatrix}$$

Ab (*pseudo A matrix*) where all columns are from A but the *j-th* column which is replaced with *j-th* column of B

Ba (*pseudo B matrix*) where all columns are from B but the *j-th* column which is replaced with *j-th* column from A.

$$Ab = \begin{bmatrix} a_{1,1} & \cdots & b_{1,j} & & a_{1,d} \\ \vdots & & b_{2,j} & & \\ & & \vdots & \ddots & \\ a_{N,1} & & b_{N,j} & & a_{N,d} \end{bmatrix} \quad Ba = \begin{bmatrix} b_{1,1} & \cdots & a_{1,j} & & b_{1,d} \\ \vdots & & b_{2,j} & & \\ & & \vdots & \ddots & \\ b_{N,1} & & a_{N,j} & & b_{N,d} \end{bmatrix}$$

Monte Carlo estimate
→Practical Steps: matrix view

$$S_i = \frac{Var[E(y \mid x_i)]}{Var(y)} \qquad T_i = \frac{E[Var(y|\boldsymbol{x}_{-i})]}{Var(y)}$$

$$\mathbf{A} = \begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ \vdots & & \vdots \\ x_{N1} & x_{N2} & x_{N3} \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} x'_{11} & x'_{12} & x'_{13} \\ x'_{21} & x'_{22} & x'_{23} \\ \vdots & & \vdots \\ x'_{N1} & x'_{N2} & x'_{N3} \end{bmatrix}$$

A **B**

$$\hat{V}_i = \frac{1}{N}\sum_{r=1}^{N} f(A)_r \left(f\left(B_A^i\right)_r - f(B)_r\right)$$

$$\hat{V}_{Ti} = \frac{1}{2N}\sum_{r=1}^{N} \left[f\left(B_A^i\right)_r - f(B)_r\right]^2$$

$$\mathbf{B}_A{}^{(1)} = \begin{bmatrix} x'_{11} & x_{12} & x_{13} \\ x'_{21} & x_{22} & x_{23} \\ \vdots & & \vdots \\ x'_{N1} & x_{N2} & x_{N3} \end{bmatrix}$$

$$\mathbf{B}_A{}^{(2)} = \begin{bmatrix} x_{11} & x'_{12} & x_{13} \\ x_{21} & x'_{22} & x_{23} \\ \vdots & & \vdots \\ x_{N1} & x'_{N2} & x_{N3} \end{bmatrix}$$

$$\mathbf{B}_A{}^{(3)} = \begin{bmatrix} x_{11} & x_{12} & x'_{13} \\ x_{21} & x_{22} & x'_{23} \\ \vdots & & \vdots \\ x_{N1} & x_{N2} & x'_{N3} \end{bmatrix}$$

Example

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$$y = x_1 + 10\left(x_2 - \frac{1}{2}\right)\left(x_3 - \frac{1}{2}\right) \qquad x_1, x_2, x_3 \in U[0,1]$$

$$\boxed{N=1500}$$

$$\hat{V}_1 = \frac{1}{1500}\sum_{r=1}^{1500} f(B)_r\left(f\left(A_B^1\right)_r - f(A)_r\right)$$

$$\begin{bmatrix} 0.50 & 0.12 & 0.90 \\ 0.25 & 0.37 & 0.15 \\ 0.75 & 0.87 & 0.65 \\ \vdots & \vdots & \vdots \\ 0.85 & 0.11 & 0.77 \\ 0.23 & 0.98 & 0.89 \end{bmatrix} \qquad \begin{bmatrix} 0.85 & 0.63 & 0.90 \\ 0.60 & 0.38 & 0.65 \\ 0.10 & 0.88 & 0.15 \\ \vdots & \vdots & \vdots \\ 0.24 & 0.83 & 0.18 \\ 0.62 & 0.70 & 0.31 \end{bmatrix}$$

A **B**

Example

European Commission

$$y = x_1 + 10(x_2 - \frac{1}{2})(x_3 - \frac{1}{2}) \qquad x_1, x_2, x_3 \in U[0,1]$$

$\boxed{N=1500}$

$$\hat{V}_1 = \frac{1}{1500}\sum_{r=1}^{1500} f(B)_r \left(f\left(A_B^1\right)_r - f(A)_r \right)$$

$$\begin{bmatrix} 0.50 & 0.12 & 0.90 \\ 0.25 & 0.37 & 0.15 \\ 0.75 & 0.87 & 0.65 \\ \vdots & \vdots & \vdots \\ 0.85 & 0.11 & 0.77 \\ 0.23 & 0.98 & 0.89 \end{bmatrix} \qquad \begin{bmatrix} 0.85 & 0.63 & 0.90 \\ 0.60 & 0.38 & 0.65 \\ 0.10 & 0.88 & 0.15 \\ \vdots & \vdots & \vdots \\ 0.24 & 0.83 & 0.18 \\ 0.62 & 0.70 & 0.31 \end{bmatrix}$$

A **B**

$$\mathbf{A_B}^{(1)} = \begin{bmatrix} 0.85 & 0.12 & 0.90 \\ 0.60 & 0.37 & 0.15 \\ 0.10 & 0.87 & 0.65 \\ \vdots & \vdots & \vdots \\ 0.24 & 0.11 & 0.77 \\ 0.62 & 0.98 & 0.89 \end{bmatrix}$$

Monte Carlo sampling

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$$\mathbf{A} = \begin{bmatrix} 0.50 & 0.12 & 0.90 \\ 0.25 & 0.37 & 0.15 \\ 0.75 & 0.87 & 0.65 \\ \vdots & \vdots & \vdots \\ 0.85 & 0.11 & 0.77 \\ 0.23 & 0.98 & 0.89 \end{bmatrix} \xrightarrow{M} f(\mathbf{A}) = \begin{bmatrix} -0.99 \\ 0.67 \\ 1.32 \\ \vdots \\ -0.19 \\ 2.18 \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} 0.85 & 0.63 & 0.90 \\ 0.60 & 0.38 & 0.65 \\ 0.10 & 0.88 & 0.15 \\ \vdots & \vdots & \vdots \\ 0.24 & 0.83 & 0.18 \\ 0.62 & 0.70 & 0.31 \end{bmatrix} \xrightarrow{M} f(\mathbf{B}) = \begin{bmatrix} 1.38 \\ 0.41 \\ -1.20 \\ \vdots \\ -0.80 \\ 0.22 \end{bmatrix}$$

$$\mathbf{A}_B^{(1)} = \begin{bmatrix} 0.85 & 0.12 & 0.90 \\ 0.60 & 0.37 & 0.15 \\ 0.10 & 0.87 & 0.65 \\ \vdots & \vdots & \vdots \\ 0.24 & 0.11 & 0.77 \\ 0.62 & 0.98 & 0.89 \end{bmatrix} \xrightarrow{M} f(\mathbf{A}_B^{(1)}) = \begin{bmatrix} -0.64 \\ 1.03 \\ 0.68 \\ \vdots \\ -0.81 \\ 2.57 \end{bmatrix}$$

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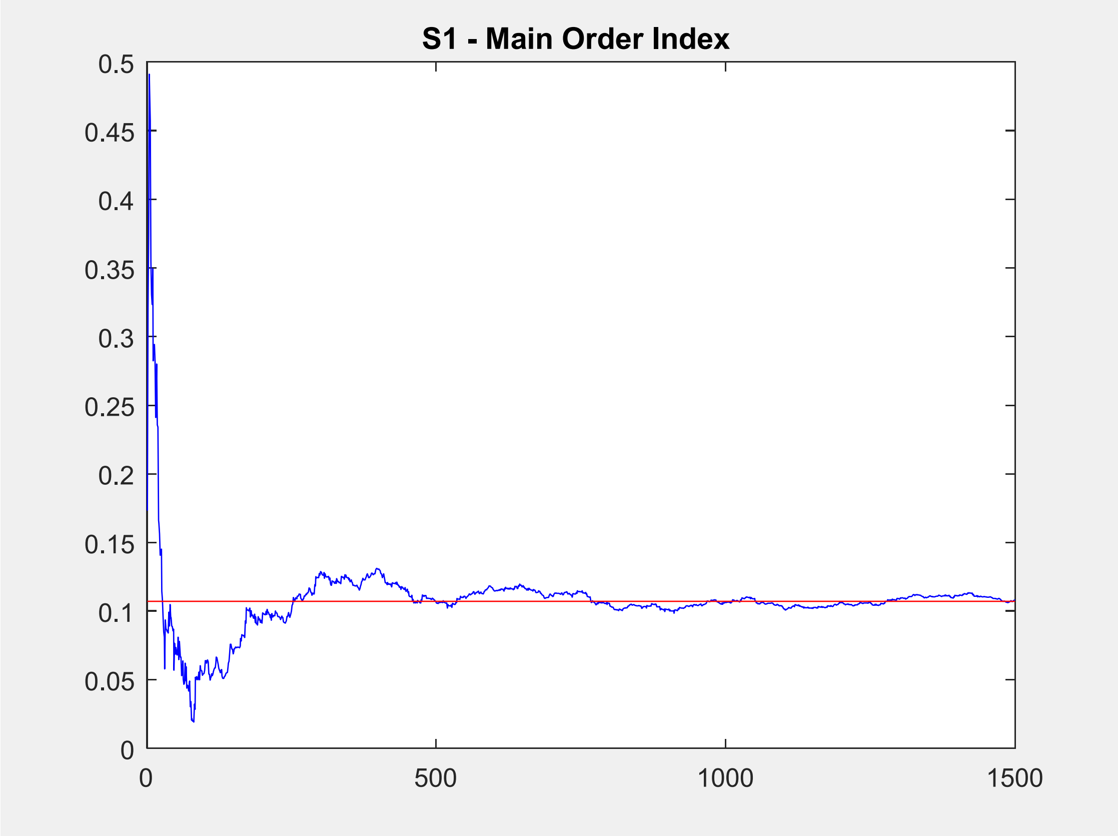
Example

$$y = x_1 + 10(x_2 - \frac{1}{2})(x_3 - \frac{1}{2}) \qquad x_1, x_2, x_3 \in U[0,1]$$



$$\hat{V}_1 = \frac{1}{1500}\sum_{r=1}^{1500} f(B)_r \left(f\left(A_B^1\right)_r - f(A)_r \right)$$

$$S_1 = 0.1071$$

N	$\hat{S}_1$	Δ
250	0.1000	0.0071
500	0.1062	0.0009
1000	0.1065	0.0006
1500	0.1079	-0.0008

$*Var = 0.777$

Note: convergence rate strongly depends on the model structure

Monte Carlo estimate: first order indices →Practical Steps: groups

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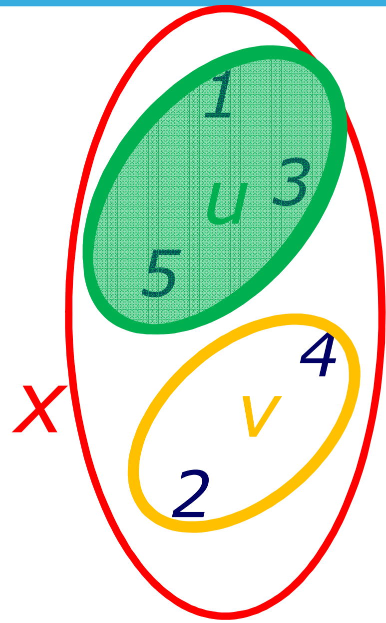
$$\hat{V}_u = Var[E(y\,|\,u)] = \frac{1}{N}\sum_{r=1}^{N} f\left(x'_{r1}, x'_{r2}, x'_{r3}, x'_{r4}, x'_{r5}\right)\left[f\left(x'_{r1}, x_{r2}, x'_{r3}, x_{r4}, x'_{r5}\right) - f\left(x_{r1}, x_{r2}, x_{r3}, x_{r4}, x_{r5}\right)\right]$$

$$\hat{V}_v = Var[E(y\,|\,v)] = \frac{1}{N}\sum_{r=1}^{N} f\left(x'_{r1}, x'_{r2}, x'_{r3}, x'_{r4}, x'_{r5}\right)\left[f\left(x_{r1}, x'_{r2}, x_{r3}, x'_{r4}, x_{r5}\right) - f\left(x_{r1}, x_{r2}, x_{r3}, x_{r4}, x_{r5}\right)\right]$$

B $\qquad$ A_B $\qquad$ A



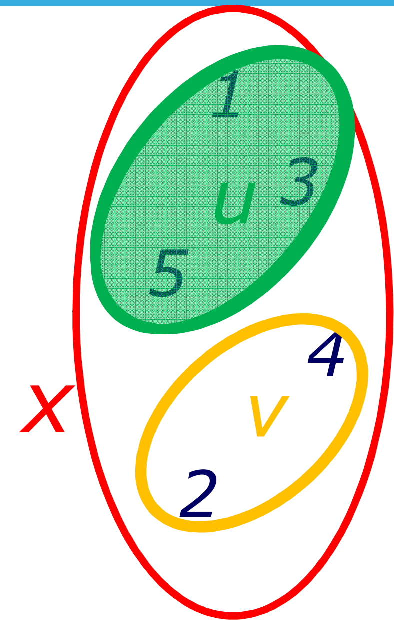
A = [x_1 x_2 x_3 x_4 x_5]   B = [x_1’ x_2’ x_3’ x_4’ x_5’]

Monte Carlo estimate: first order indices
→Practical Steps: groups

$$\hat{V}_u = Var[E(y|u)] = \frac{1}{N}\sum_{r=1}^{N} f\left(x'_{r1}, x'_{r2}, x'_{r3}, x'_{r4}, x'_{r5}\right)\left[f\left(x'_{r1}, x_{r2}, x'_{r3}, x_{r4}, x'_{r5}\right) - f\left(x_{r1}, x_{r2}, x_{r3}, x_{r4}, x_{r5}\right)\right]$$

$$\hat{V}_v = Var[E(y|v)] = \frac{1}{N}\sum_{r=1}^{N} f\left(x'_{r1}, x'_{r2}, x'_{r3}, x'_{r4}, x'_{r5}\right)\left[f\left(x_{r1}, x'_{r2}, x_{r3}, x'_{r4}, x_{r5}\right) - f\left(x_{r1}, x_{r2}, x_{r3}, x_{r4}, x_{r5}\right)\right]$$

B $\qquad$ A_B $\qquad$ A



A = [$\underline{x_1}$ $\quad x_2$ $\quad \underline{x_3}$ $\quad x_4$ $\quad \underline{x_5}$] $\qquad$ B = [x_1' $\quad x_2$' $\quad x_3$' $\quad x_4$' $\quad x_5$']

A = [0.500 0.750 0.800 0.167 0.777] $\qquad$ B = [0.123 0.056 0.701 0.107 0.432]

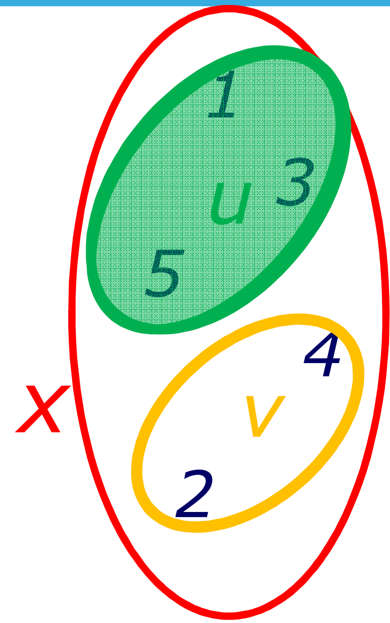
$A_B^{(u)}$ = [0.123 0.750 0.701 0.167 0.432]

Monte Carlo estimator: first order indices
→Practical Steps: groups

$$\hat{V}_u = Var[E(y\,|\,u)] = \frac{1}{N}\sum_{r=1}^{N} f\left(x'_{r1}, x'_{r2}, x'_{r3}, x'_{r4}, x'_{r5}\right)\left[f\left(x'_{r1}, x_{r2}, x'_{r3}, x_{r4}, x'_{r5}\right) - f\left(x_{r1}, x_{r2}, x_{r3}, x_{r4}, x_{r5}\right)\right]$$

$$\hat{V}_v = Var[E(y\,|\,v)] = \frac{1}{N}\sum_{r=1}^{N} f\left(x'_{r1}, x'_{r2}, x'_{r3}, x'_{r4}, x'_{r5}\right)\left[f\left(x_{r1}, x'_{r2}, x_{r3}, x'_{r4}, x_{r5}\right) - f\left(x_{r1}, x_{r2}, x_{r3}, x_{r4}, x_{r5}\right)\right]$$

B $\quad$ A_B $\quad$ A



A = [$\underline{x_1}$ x_2 $\underline{x_3}$ x_4 $\underline{x_5}$] B = [x_1' x_2' x_3' x_4' x_5']

A = [0.500 0.750 0.800 0.167 0.777] B = [0.123 0.056 0.701 0.107 0.432]

$A_B^{(u)}$ = [0.123 0.750 0.701 0.167 0.432]

$A_B^{(v)}$ = [0.500 0.056 0.800 0.107 0.777]

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Key messages:

- Versatility
- Easiness
- Model-free (i.e. nonlinear, interactions)
- Groups – discrete variables
- Implementation

- Total number of runs
- Specific sampling strategy

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OWEN formulas for first-order index

$$A=\begin{bmatrix} a_{1,1} & \cdots & a_{1,j} & & a_{1,d} \\ \vdots & & a_{2,j} & & \\ & & \vdots & & \\ & & & \ddots & \\ a_{N,1} & & a_{N,j} & & a_{N,d} \end{bmatrix} \quad B=\begin{bmatrix} b_{1,1} & \cdots & \boxed{b_{1,j}} & & b_{1,d} \\ \vdots & & b_{2,j} & & \\ & & \vdots & & \\ & & & \ddots & \\ b_{N,1} & & b_{N,j} & & b_{N,d} \end{bmatrix} \quad C=\begin{bmatrix} c_{1,1} & \cdots & \boxed{c_{1,j}} & & c_{1,d} \\ \vdots & & c_{2,j} & & \\ & & \vdots & & \\ & & & \ddots & \\ c_{N,1} & & c_{N,j} & & c_{N,d} \end{bmatrix}$$

$$Ab=\begin{bmatrix} a_{1,1} & \cdots & \boxed{b_{1,j}} & & a_{1,d} \\ \vdots & & b_{2,j} & & \\ & & \vdots & & \\ & & & \ddots & \\ a_{N,1} & & b_{N,j} & & a_{N,d} \end{bmatrix} \quad Bc=\begin{bmatrix} b_{1,1} & \cdots & \boxed{c_{1,j}} & & b_{1,d} \\ \vdots & & c_{2,j} & & \\ & & \vdots & & \\ & & & \ddots & \\ b_{N,1} & & c_{N,j} & & b_{N,d} \end{bmatrix}$$

$$\widehat{V}_i = \frac{1}{N}\sum_{j=1}^{N}\left(yB_j - yBc_j^i\right)\left(yAb_j^i - yA_j\right)$$

Improved formulas for first-order index (3)

$$\hat{S}_i^B = \frac{\frac{1}{N}\sum_{j=1}^{N} yB_j(yAb_j^i - yA_j)}{\frac{1}{N}\sum_{j=1}^{N} yB_j(yB_j - yA_j)}$$

$$\hat{S}_i^A = \frac{\frac{1}{N}\sum_{j=1}^{N} yA_j(yBa_j^i - yB_j)}{\frac{1}{N}\sum_{j=1}^{N} yA_j(yA_j - yB_j)}$$

$$\hat{S}_i^I = \frac{\hat{f}_{ABa_i} - \hat{f}_0^2}{\hat{f}_B^2 - \hat{f}_0^2} \qquad \hat{S}_i^{IV} = \frac{\hat{f}_{BAb_i} - \hat{f}_0^2}{\hat{f}_A^2 - \hat{f}_0^2}$$

$$\hat{S}_i^{II} = \frac{\hat{f}_{ABa_i} - \hat{f}_{0_i}^2}{\hat{f}_{Ba_i}^2 - \hat{f}_{0_i}^2} \qquad \hat{S}_i^{V} = \frac{\hat{f}_{BAb_i} - \hat{f}_{0_i}^2}{\hat{f}_{Ba_i}^2 - \hat{f}_{0_i}^2}$$

$$\hat{S}_i^{III} = \frac{\hat{f}_{ABa_i} - \hat{f}_{0_i}^2}{\hat{f}_{Ab_i}^2 - \hat{f}_{0_i}^2} \qquad \hat{S}_i^{VI} = \frac{\hat{f}_{BAb_i} - \hat{f}_{0_i}^2}{\hat{f}_{Ab_i}^2 - \hat{f}_{0_i}^2}$$

Individual terms for the estimation of the first-order indices	
$\hat{f}_A^2 = \left(\frac{1}{N}\sum_{j=1}^{N} yA_j\right)^2$	$\hat{f}_{Ba_i}^2 = \left(\frac{1}{N}\sum_{j=1}^{N} yBa_j^i\right)^2$
$\hat{f}_B^2 = \left(\frac{1}{N}\sum_{j=1}^{N} yB_j\right)^2$	$\hat{f}_{BAb_i} = \left(\frac{1}{N}\sum_{j=1}^{N} yB_j\, yAb_j^i\right)$
$\hat{f}_{Ab_i}^2 = \left(\frac{1}{N}\sum_{j=1}^{N} yAb_j^i\right)^2$	$\hat{f}_{ABa_i} = \left(\frac{1}{N}\sum_{j=1}^{N} yA_j\, yBa_j^i\right)$

$$\hat{S}_i^T = (\hat{S}_i^A + \hat{S}_i^B + \hat{S}_i^I + \hat{S}_i^{II} + \hat{S}_i^{III} + \hat{S}_i^{IV} + \hat{S}_i^{V} + \hat{S}_i^{VI})/8$$

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Improved formulas for first-order index (3)

$$\hat{S}_i^B = \frac{\frac{1}{N}\sum_{j=1}^{N} yB_j(yAb_j^i - yA_j)}{\frac{1}{N}\sum_{j=1}^{N} yB_j(yB_j - yA_j)}$$

$$\hat{S}_i^A = \frac{\frac{1}{N}\sum_{j=1}^{N} yA_j(yBa_j^i - yB_j)}{\frac{1}{N}\sum_{j=1}^{N} yA_j(yA_j - yB_j)}$$

$$\hat{S}_i^I = \frac{\hat{f}_{ABa_i} - \hat{f}_0^2}{\hat{f}_B^2 - \hat{f}_0^2} \qquad \hat{S}_i^{IV} = \frac{\hat{f}_{BAb_i} - \hat{f}_0^2}{\hat{f}_A^2 - \hat{f}_0^2}$$

$$\hat{S}_i^{II} = \frac{\hat{f}_{ABa_i} - \hat{f}_{0_i}^2}{\hat{f}_{Ba_i}^2 - \hat{f}_{0_i}^2} \qquad \hat{S}_i^{V} = \frac{\hat{f}_{BAb_i} - \hat{f}_{0_i}^2}{\hat{f}_{Ba_i}^2 - \hat{f}_{0_i}^2}$$

$$\hat{S}_i^{III} = \frac{\hat{f}_{ABa_i} - \hat{f}_{0_i}^2}{\hat{f}_{Ab_i}^2 - \hat{f}_{0_i}^2} \qquad \hat{S}_i^{VI} = \frac{\hat{f}_{BAb_i} - \hat{f}_{0_i}^2}{\hat{f}_{Ab_i}^2 - \hat{f}_{0_i}^2}$$

Individual terms for the estimation of the first-order indices	
$\hat{f}_A^2 = \left(\frac{1}{N}\sum_{j=1}^{N} yA_j\right)^2$	$\hat{f}_{Ba_i}^2 = \left(\frac{1}{N}\sum_{j=1}^{N} yBa_j^i\right)^2$
$\hat{f}_B^2 = \left(\frac{1}{N}\sum_{j=1}^{N} yB_j\right)^2$	$\hat{f}_{BAb_i} = \left(\frac{1}{N}\sum_{j=1}^{N} yB_j\, yAb_j^i\right)$
$\hat{f}_{Ab_i}^2 = \left(\frac{1}{N}\sum_{j=1}^{N} yAb_j^i\right)^2$	$\hat{f}_{ABa_i} = \left(\frac{1}{N}\sum_{j=1}^{N} yA_j\, yBa_j^i\right)$

$$\hat{S}_i^T = (\hat{S}_i^A + \hat{S}_i^B + \hat{S}_i^I + \hat{S}_i^{II} + \hat{S}_i^{III} + \hat{S}_i^{IV} + \hat{S}_i^{V} + \hat{S}_i^{VI})/8$$

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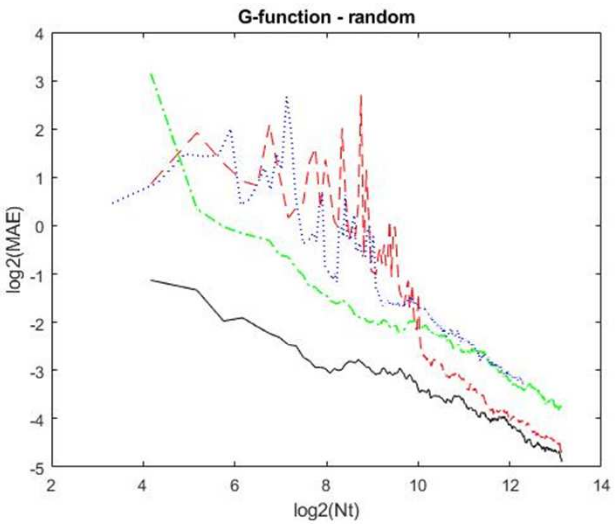
The IA-Innovative Algorithm for S_i

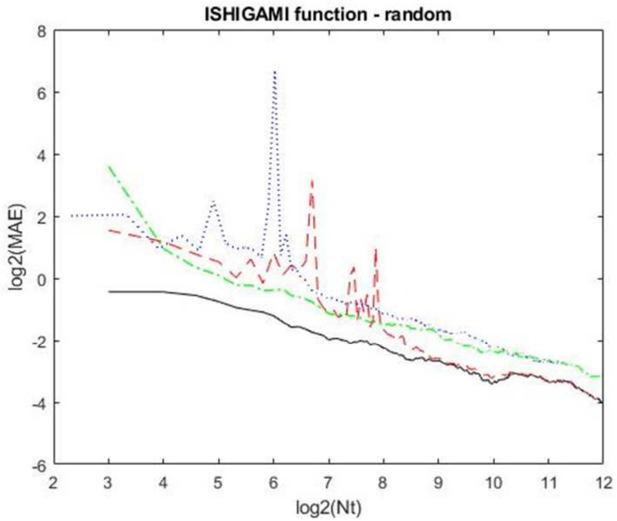
2N(d+1)

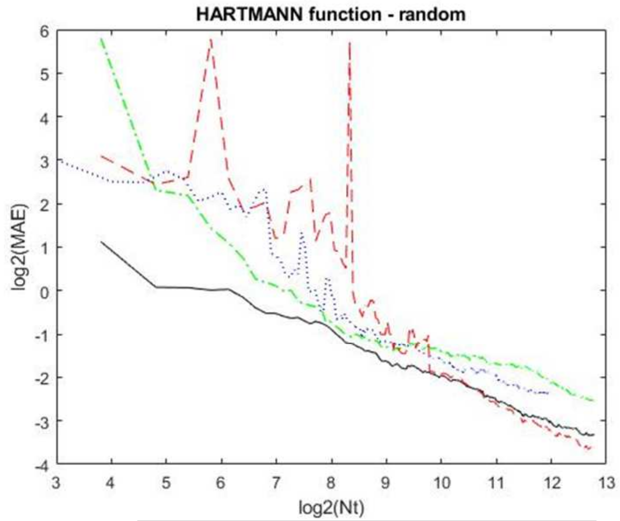
$$\hat{S}_i^{IA} = \frac{\sum_{j=1}^{N}(yA_j - yAb_j^i)(yBa_j^i - yB_j)}{\frac{1}{2}\left(\sum_{j=1}^{N}(yA_j - yB_j)^2 + (yAb_j^i - yBa_j^i)^2\right)}$$

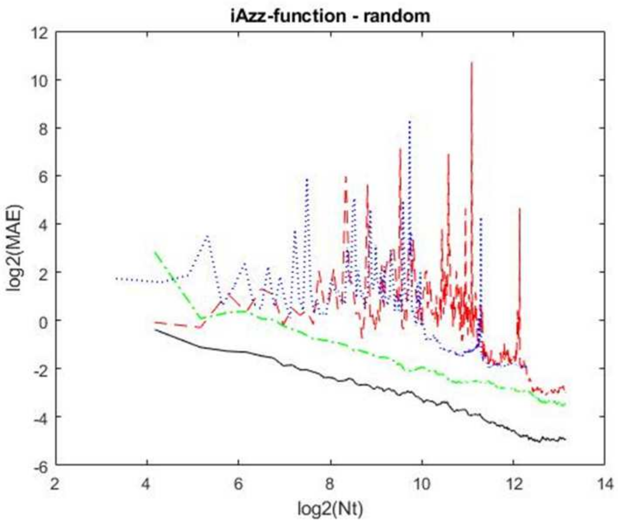
The variance is dynamically adaptive for each factor and it is estimated by the average of the contributions of independent couples of input matrices.

Tests – Monte Carlo samples









$$\boldsymbol{MAE} = \frac{\mathbf{1}}{\boldsymbol{nr}}\sum_{\boldsymbol{j=1}}^{\boldsymbol{nr}}\sum_{\boldsymbol{i}}^{\boldsymbol{k}}\left|\hat{\boldsymbol{S}}_{\boldsymbol{i}} - \boldsymbol{Se}_{\boldsymbol{i}}\right|$$

Tests were performed referring to a sample of N=500 and 20 replicas

IA-estimator with groups

a=[0 1 4.5 9 99 99 99 99]

$$\hat{S}_1^{IA} = \frac{\sum_{j=1}^{500}(yA_j - yAb_j^1)(yB_j - yBa_j^1)}{\frac{1}{2}\left(\sum_{j=1}^{500}(yA_j - yB_j)^2 + (yAb_j^1 - yBa_j^1)^2\right)} = 0{,}72$$

$$\hat{S}_2^{IA} = \frac{\sum_{j=1}^{500}(yA_j - yAb_j^2)(yB_j - yBa_j^2)}{\frac{1}{2}\left(\sum_{j=1}^{500}(yA_j - yB_j)^2 + (yAb_j^2 - yBa_j^2)^2\right)} = 0{,}21$$

$$\hat{S}_3^{IA} = \frac{\sum_{j=1}^{500}(yA_j - yAb_j^3)(yB_j - yBa_j^3)}{\frac{1}{2}\left(\sum_{j=1}^{500}(yA_j - yB_j)^2 + (yAb_j^3 - yBa_j^3)^2\right)} = 0{,}00$$

S_1=0.72 S_2=0.22 S_3=0.00

$$A = \begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} & a_{1,4} & a_{1,5} & a_{1,6} & a_{1,7} & a_{1,8} \\ \vdots & & & & & & & \\ & \ddots & a_{r,3} & & \ddots & a_{r,6} & a_{r,7} & \\ & & & & & & & \vdots \\ a_{N,1} & a_{N,2} & & a_{N,4} & a_{N,5} & & & a_{N,8} \end{bmatrix} \quad B = \begin{bmatrix} b_{1,1} & b_{1,2} & b_{1,3} & b_{1,4} & b_{1,5} & b_{1,6} & b_{1,7} & b_{1,8} \\ \vdots & & & & & & & \\ & \ddots & b_{r,3} & & \ddots & b_{r,6} & b_{r,7} & \\ & & & & & & & \vdots \\ b_{N,1} & b_{N,2} & & b_{N,4} & b_{N,5} & & & b_{N,8} \end{bmatrix}$$

$$Ab_1 = \begin{bmatrix} b_{1,1} & a_{1,2} & a_{1,3} & a_{1,4} & a_{1,5} & a_{1,6} & a_{1,7} & a_{1,8} \\ \vdots & & & & & & & \\ & \ddots & a_{r,3} & & \ddots & a_{r,6} & a_{r,7} & \\ & & & & & & & \vdots \\ b_{N,1} & a_{N,2} & & a_{N,4} & a_{N,5} & & & a_{N,8} \end{bmatrix} \quad Ba_1 = \begin{bmatrix} a_{1,1} & b_{1,2} & b_{1,3} & b_{1,4} & b_{1,5} & b_{1,6} & b_{1,7} & b_{1,8} \\ \vdots & & & & & & & \\ & \ddots & b_{r,3} & & \ddots & b_{r,6} & b_{r,7} & \\ & & & & & & & \vdots \\ a_{N,1} & b_{N,2} & & b_{N,4} & b_{N,5} & & & b_{N,8} \end{bmatrix}$$

$$Ab_2 = \begin{bmatrix} a_{1,1} & b_{1,2} & b_{1,3} & b_{1,4} & a_{1,5} & a_{1,6} & a_{1,7} & a_{1,8} \\ \vdots & & & & & & & \\ & \ddots & b_{r,3} & & \ddots & a_{r,6} & a_{r,7} & \\ & & & & & & & \vdots \\ a_{N,1} & b_{N,2} & & b_{N,4} & a_{N,5} & & & a_{N,8} \end{bmatrix} \quad Ba_2 = \begin{bmatrix} b_{1,1} & a_{1,2} & a_{1,3} & a_{1,4} & b_{1,5} & b_{1,6} & b_{1,7} & b_{1,8} \\ \vdots & & & & & & & \\ & \ddots & a_{r,3} & & \ddots & b_{r,6} & b_{r,7} & \\ & & & & & & & \vdots \\ b_{N,1} & a_{N,2} & & a_{N,4} & b_{N,5} & & & b_{N,8} \end{bmatrix}$$

$$Ab_3 = \begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} & a_{1,4} & b_{1,5} & b_{1,6} & b_{1,7} & b_{1,8} \\ \vdots & & & & & & & \\ & \ddots & a_{r,3} & & \ddots & b_{r,6} & b_{r,7} & \\ & & & & & & & \vdots \\ a_{N,1} & a_{N,2} & & a_{N,4} & b_{N,5} & & & b_{N,8} \end{bmatrix} \quad Ba_3 = \begin{bmatrix} b_{1,1} & b_{1,2} & b_{1,3} & b_{1,4} & a_{1,5} & a_{1,6} & a_{1,7} & a_{1,8} \\ \vdots & & & & & & & \\ & \ddots & b_{r,3} & & \ddots & a_{r,6} & a_{r,7} & \\ & & & & & & & \vdots \\ b_{N,1} & b_{N,2} & & b_{N,4} & a_{N,5} & & & a_{N,8} \end{bmatrix}$$

The IA-Innovative Algorithm for S_T

Estimation of the first-order index for the group 'all the factors' except *i:*

$$\hat{S}_{\sim i}^{IA} = \frac{\sum_{j=1}^{N}((yA_j - yBa_j^i)(yB_j - yAb_j^i))}{\frac{1}{2}\sum_{j=1}^{N}((yA_j - yB_j)^2 + (yAb_j^i - yBa_j^i)^2)}$$

Estimator for the Sobol' total index of input *i* can be easily derived:

$$\widehat{ST}_i^{IA} = 1 - \frac{\sum_{j=1}^{N}((yA_j - yBa_j^i)(yB_j - yAb_j^i))}{\frac{1}{2}\sum_{j=1}^{N}((yA_j - yB_j)^2 + (yAb_j^i - yBa_j^i)^2)}$$

European Commission

Thank you

Joint Research Centre

European Commission

Compute the Sobol' sensitivity indices:

$$y = x_1 + 10(x_2 - \frac{1}{2})(x_3 - \frac{1}{2})$$

$$x_1, x_2, x_3 \in U[0,1]$$

European Commission

Compute the Sobol' sensitivity indices:

$$y = x_1 + 10(x_2 - \frac{1}{2})(x_3 - \frac{1}{2})$$

$$x_1, x_2, x_3 \in U[0,1]$$

$$Y = \prod_{1}^{d} g_i(X_i) = \prod_{1}^{d} \frac{|4x_i - 2| + a_i}{1 + a_1}$$

$$\boxed{x_i \sim U(0,1)}$$

- ✓ It is a strongly non-linear and non-monotonic function.
- ✓ The values of the ai determine the range of variation of each gi.
- ✓ The higher the ai value, the more stable the function gi(Xi) the lower the importance the relative Xi.

$$a = [0 \;\; 1 \;\; 4.5 \;\; 9 \;\; 99 \;\; 99 \;\; 99 \;\; 99]$$

S = [0.7162 0.1790 0.0237 0.0072 0.0001 0.0001 0.0001 0.0001]

T = [0.7871 0.2422 0.0343 0.0105 0.0001 0.0001 0.0001 0.0001]

$$a = [99 \;\; 99 \;\; 99 \;\; 99 \;\; 99 \;\; 99 \;\; 99 \;\; 99]$$

no interactions