# New estimation of Sobol' indices using kernels 

 Joint work with Fabrice, Thierry Klein, Clémentine Prieur, and Sébastien da Veiga
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## Outline of the talk

## Introduction

Framework and Sobol' indices

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Estimation survey
The classical Pick-Freeze estimation
Estimation from a unique sample
Kernel-based estimations
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New estimation based on kernels
Notation and setting
Estimation using kernels and main results
Sketch of the proof
Numerical applications

## Framework

In this talk, we consider the following black-box model :

$$
Y=f\left(V_{1}, \ldots, V_{p}\right),
$$

where $f: E=E_{1} \times E_{2} \times \cdots \times E_{p} \rightarrow \mathbb{R}^{k}$ is an unknown and deterministic function.

Main assumptions
(1) $V_{1}, \ldots, V_{p}$ are independent.
(2) $\mathbb{E}\left[\|Y\|^{2}\right]<\infty$.
(3) $Y$ is scalar (here, for sake of simplicity).

## The so-called Sobol' indices

Classically to quantify the amount of randomness that a variable or a group of variables bring to $Y$, one computes the so-called Sobol' indices.

For instance, the first order Sobol' and the total Sobol' indices with respect to $V_{\mathbf{u}}=\left(V_{i}, i \in \mathbf{u}\right)$ is given by

$$
S^{\mathbf{u}}=\frac{\operatorname{Var}\left(\mathbb{E}\left[Y \mid V_{\mathbf{u}}\right]\right)}{\operatorname{Var}(Y)} \quad \text { and } \quad S^{\mathbf{u}, \text { Tot }}=1-S^{\sim \mathbf{u}}=1-\frac{\operatorname{Var}\left(\mathbb{E}\left[Y \mid V_{\sim \mathbf{u}}\right]\right)}{\operatorname{Var}(Y)}
$$

(assuming $Y$ is scalar).
Such indices stem from the Hoeffding decomposition of the variance of $f$ (or equivalently $Y$ ) that is assumed to lie in $L^{2}$.

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## Pick-Freeze estimation of Sobol' indices (I)

To fix ideas assume for example $p=5, \mathbf{u}=\{1,2\}$ so that
$\sim \mathbf{u}=\{3,4,5\}$.
We consider the Pick-Freeze variable $Y_{\mathbf{u}}$ defined as follows:

- draw $V=\left(V_{1}, V_{2}, V_{3}, V_{4}, V_{5}\right)$,
- build $V^{\mathbf{u}}=\left(V_{1}, V_{2}, V_{3}^{\prime}, V_{4}^{\prime}, V_{5}^{\prime}\right)$.

Then, we compute

- $Y=f(V)$,
- $Y^{\mathbf{u}}=f\left(V^{\mathbf{u}}\right)$.

A small miracle

$$
\operatorname{Var}(\mathbb{E}[Y \mid X])=\operatorname{Var}\left(\mathbb{E}\left[Y \mid V_{\mathbf{u}}\right]\right)=\operatorname{Cov}\left(Y, Y^{\mathbf{u}}\right) \text { so that } S^{\mathbf{u}}=\frac{\operatorname{Cov}\left(Y, Y^{\mathbf{u}}\right)}{\operatorname{Var}(Y)}
$$

## Pick-Freeze estimation of Sobol' indices (II)

In practice, generate two $n$-samples:

- one $n$-sample of $V:\left(V_{j}\right)_{j=1, \ldots, n}$,
- one $n$-sample of $V^{\mathbf{u}}:\left(V_{j}^{\mathbf{u}}\right)_{j=1, \ldots, n}$.

Compute the code on both samples:

- $Y_{j}=f\left(V_{j}\right)$ for $j=1, \ldots, n$,
- $Y_{j}^{\mathbf{u}}=f\left(V_{j}^{\mathbf{u}}\right)$ for $j=1, \ldots, n$.

Then estimate $S^{\mathbf{u}}$ by

$$
S_{n, P F}^{\mathbf{u}}=\frac{\frac{1}{n} \sum_{j=1}^{n} Y_{j} Y_{j}^{\mathbf{u}}-\left(\frac{1}{n} \sum_{j=1}^{n} Y_{j}\right)\left(\frac{1}{n} \sum_{j=1}^{n} Y_{j}^{\mathbf{u}}\right)}{\frac{1}{n} \sum_{j=1}^{n}\left(Y_{j}\right)^{2}-\left(\frac{1}{n} \sum_{j=1}^{n} Y_{j}\right)^{2}}
$$

## Pick-Freeze scheme (III) : some statistical properties

Is the Pick-Freeze estimator a "good" estimator of the Sobol' index?

- Is it consistent? Response : YES SLLN.
- If yes, at which rate of convergence? Resp. : YES CLT (cv in $\sqrt{n}$ ).
- Is it asymptotically efficient? Resp. : YES.
- Is it possible to measure its performance for a fixed $n$ ? Response : YES Berry-Esseen and/or concentration inequalities.

Ref. : A. Janon, T. Klein, A. Lagnoux, M. Nodet, and C. Prieur. " Asymptotic normality et efficiency of a Sobol' index estimator", ESAIM P\&S, 2013.
F. Gamboa, A. Janon, T. Klein, A. Lagnoux, and C. Prieur. "Statistical Inference for Sobol’ Pick Freeze Monte Carlo method", Statistics, 2015.

## Drawbacks of the Pick-Freeze estimation

- The cost (= number of evaluations of the function $f$ ) of the estimation of the $p$ first-order Sobol' indices is quite expensive : $(p+1) n$.
- This methodology is based on a particular design of experiment that may not be available in practice. For instance, when the practitioner only has access to real data.

We are interested in an estimator based on a n-sample only.

## Mighty estimation based on ranks (I)

Here we assume that the inputs $V_{i}$ for $i=1, \ldots, p$ are scalar and we want to estimate the Sobol' index $S^{i}$ with respect to $X=V_{i}$ :

$$
S^{i}=\frac{\operatorname{Var}\left(\mathbb{E}\left[Y \mid V_{i}\right]\right)}{\operatorname{Var}(Y)}=\frac{\operatorname{Var}(\mathbb{E}[Y \mid X])}{\operatorname{Var}(Y)}
$$

To do so, we consider a $n$-sample of the input/output pair $(X, Y)$ given by

$$
\left(X_{1}, Y_{1}\right),\left(X_{2}, Y_{2}\right), \ldots,\left(X_{n}, Y_{n}\right)
$$

The pairs $\left(X_{(1)}, Y_{(1)}\right),\left(X_{(2)}, Y_{(2)}\right), \ldots,\left(X_{(n)}, Y_{(n)}\right)$ are rearranged in such a way that

$$
X_{(1)}<\ldots<X_{(n)} .
$$

## Mighty estimation based on ranks (II)

We introduce

$$
S_{n, R a n k}^{i}=\frac{\frac{1}{n} \sum_{j=1}^{n-1} Y_{(j)} Y_{(j+1)}-\left(\frac{1}{n} \sum_{j=1}^{n} Y_{j}\right)^{2}}{\frac{1}{n} \sum_{j=1}^{n} Y_{j}^{2}-\left(\frac{1}{n} \sum_{j=1}^{n} Y_{j}\right)^{2}}
$$

Statistical properties

- Consistency: OK.
- Central Limit Theorem: OK.

Ref. : S. Chatterjee. "A new coefficient of Correlation", JASA, 2020.
F. Gamboa, P. Gremaud, T. Klein, and A. Lagnoux. " Global Sensitivity Analysis : a new generation of mighty estimators based on rank statistics",
Bernoulli. 2022.

## Efficient estimation based on kernels

Ref. : S. da Veiga and F. Gamboa. "Efficient estimation of sensitivity indices", Journal of Nonparametric Statistics, 2013.

Here again we assume that the inputs $V_{i}$ for $i=1, \ldots, p$ are scalar.
To do so, the initial $n$-sample is split into two samples of sizes

- $n_{1}=\lfloor n / \log n\rfloor \Rightarrow$ estimation of the joint density of $(V, Y)$
- $n_{2}=n-n_{1} \approx n \Rightarrow$ Monte-Carlo estimation of the integral involved in the quantity of interest.

Statistical properties

- Consistency: OK.
- Central Limit Theorem: OK.
- Asymptotic efficiency: OK.


## Estimation based on nearest neighbors

Ref. : L. Devroye, L. Györfi, G. Lugosi, and H. Walk. "A nearest neighbor estimate of the residual variance", EJS, 2018.

Here the input $X$ with respect we want to compute the Sobol' index is allowed to have dimension $d$.

To do so, the initial $n$-sample is split into two samples of sizes

- $n / 2 \Rightarrow$ estimation of the regression function $\mathbb{E}[Y \mid X=x]$ using the first NN of $x$ among the points of the first sample;
- $n / 2 \Rightarrow$ plug-in estimator.


## Statistical properties

- Consistency: OK
- Central Limit Theorem: OK only for $d \leqslant 3$.


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Introduction

Recall that

$$
S^{X}=\frac{\operatorname{Var}(\mathbb{E}[Y \mid X])}{\operatorname{Var}(Y)}
$$

allowing a multidimensional $X$ living in a compact set: $X \in \mathscr{D} \subset \mathbb{R}^{d}$.
To estimate $\mathbb{E}[Y]$ and $\operatorname{Var}(Y)$ from the $n$-sample $\left(Y_{j}\right)_{j=1, \ldots, n}$ of the output $Y$, we will naturally use the classical empirical mean and variance respectively.

Thus we focus on the estimation of $\mathbb{E}\left[\mathbb{E}[Y \mid X]^{2}\right]$ from the $n$-sample $\left(X_{j}, Y_{j}\right)_{j=1, \ldots, n}$ of the pair $(X, Y)$.

## Introduction

A natural estimator inspired from the NN and kernel-based plug-in estimators would be

$$
\binom{n}{2}^{-1} \sum_{1 \leqslant j<j^{\prime} \leqslant n} \frac{Y_{j} Y_{j^{\prime}}}{2}\left(\frac{K_{h_{n}}\left(X_{j^{\prime}}-X_{j}\right)}{f_{X}\left(X_{j}\right)}+\frac{K_{h_{n}}\left(X_{j}-X_{j^{\prime}}\right)}{f_{X}\left(X_{j^{\prime}}\right)}\right)
$$

for a bandwidth $h_{n}>0$ and a kernel $K_{h_{n}}$.
Nevertheless, boundary issues appear when the input domain is compact.

## New estimation based on kernels

To bypass this issue, we consider the following kernel-based estimator

$$
T_{n, h_{n}}=\binom{n}{2}^{-1} \sum_{1 \leqslant j<j^{\prime} \leqslant n} \frac{Y_{j} Y_{j^{\prime}}}{2}\left(\frac{K_{h_{n}} \circ A_{X_{j}}\left(X_{j^{\prime}}-X_{j}\right)}{f_{X}\left(X_{j}\right)}+\frac{K_{h_{n}} \circ A_{X_{j^{\prime}}}\left(X_{j}-X_{j^{\prime}}\right)}{f_{X}\left(X_{j^{\prime}}\right)}\right)
$$

for a bandwidth $h_{n}>0$, a mirror-type transformation $A_{x}$, and a kernel $K_{h_{n}}$.

We introduce the functions

$$
g_{1}(x)=\mathbb{E}[Y \mid X=x] \quad \text { and } \quad g_{2}(x)=\mathbb{E}\left[Y^{2} \mid X=x\right] .
$$

The supremum norm is denoted by $\|\cdot\|_{\infty}$.

Multi-index notation and smoothness
For any $d$ and $\beta=\left(\beta_{1}, \ldots, \beta_{d}\right) \in \mathbb{R}_{+}^{d}$, we define the integer part of $\beta$ by

$$
\lfloor\beta\rfloor=\left(\left\lfloor\beta_{1}\right\rfloor, \ldots,\left\lfloor\beta_{d}\right\rfloor\right)=: \gamma \in \mathbb{N}^{d} .
$$

In addition, we introduce, for any $v \in \mathbb{R}^{d}$,

$$
|\gamma|=\gamma_{1}+\cdots+\gamma_{d}, \quad \gamma!=\gamma_{1}!\cdots \gamma_{d}!, \quad \text { and } \quad v^{\beta}=v_{1}^{\beta_{1}} \ldots v_{d}^{\beta_{d}} .
$$

Let $\alpha>0$. We define $\mathscr{C}^{\alpha}(\mathscr{D})=\{\phi: \mathscr{D} \rightarrow \mathbb{R}$ with derivatives up to order $\lfloor\alpha\rfloor$ and partial derivative of order $\lfloor\alpha\rfloor$ is $\alpha-\lfloor\alpha\rfloor$-Hölder $\}$. Namely, there exists $C_{\phi}>0$ such that, for any $x$ and $x^{\prime} \in \mathscr{D}$, one has

$$
\left|\frac{\partial^{\beta} \phi}{\partial x^{\beta}}(x)-\frac{\partial^{\beta} \phi}{\partial x^{\beta}}\left(x^{\prime}\right)\right| \leqslant C_{\phi}\left\|x-x^{\prime}\right\|_{\infty}^{\alpha-\lfloor\alpha\rfloor}
$$

for any $\beta \in \mathbb{N}^{d}$ such that $|\beta|=\lfloor\alpha\rfloor$.

## Assumptions

( $\mathscr{A} 1$ ) Support The support of inputs $V=\left(V_{1}, \ldots, V_{p}\right)$ is of the form $\left[B_{1}, C_{1}\right] \times \cdots \times\left[B_{p}, C_{p}\right]$ where $B_{i}<C_{i}$ for all $1 \leqslant i \leqslant p$.
$(\mathscr{A} 2)$ Absolute continuity The distribution of the random vector $(V, Y) \in \mathbb{R}^{P} \times \mathbb{R}$ is absolutely continuous with respect to the Lebesgue measure. The marginal pdf of $(X, Y), V, X$, and $W$ are denoted by $f_{X, Y}, f_{V}, f_{X}$, and $f_{W}$ respectively.
( $\mathscr{A} 3)$ Kernel Let $K: \mathbb{R}^{d} \rightarrow \mathbb{R}$ be a kernel with support included in $\mathscr{D}$ such that $\|K\|_{\infty}<+\infty$ and $\int_{\mathscr{D}} K(u) d u=1$. We assume that $K$ is of order $\lfloor\alpha\rfloor$ which means that $\int_{\mathscr{D}} \|^{\beta} K(u) d u=0$ for any $\beta \in \mathbb{N}^{d}$ such that $0<|\beta| \leqslant\lfloor\alpha\rfloor$. Finally, we define $K_{h}(x)=K(x / h) / h^{d}$ for any $x \in \mathscr{D}$.
$(\mathscr{A} 4)$ Bandwidth The sequence $\left(h_{n}\right)_{n \in \mathbb{N}}$ of bandwidths is positive and $h_{n} \rightarrow 0$ as $n \rightarrow \infty$.

## Mirror-type transformation

The next definition allows to circumvent the boundary issues.
$(\mathscr{D} 1)$ For $x \in \mathscr{D}$, we define

$$
A_{x}:\left\{\begin{array}{ccc}
\mathbb{R}^{d} & \rightarrow & \mathbb{R}^{d} \\
u=\left(u_{1}, \ldots, u_{d}\right) & \mapsto & \left(\sigma_{1}\left(x_{1}\right) u_{1}, \ldots, \sigma_{d}\left(x_{d}\right) u_{d}\right)
\end{array}\right.
$$

with $\sigma_{i}(s):=1-2 \mathbb{1}_{\left(\frac{B_{i}+c_{i}}{2}, c_{i}\right)}(s) \in\{-1,1\}$.
Observe that $\mathscr{A}=\left\{A_{x}, x \in \mathscr{D}\right\}$ is a finite subset of $G L_{d}(\mathbb{R})$, $\mathscr{A}=\left\{A_{1}, \ldots, A_{\kappa}\right\}$, with cardinal $\kappa=2^{d}$. Moreover, it satisfies
(i) for any $\ell=1, \ldots, \kappa,\left|\operatorname{det}\left(A_{\ell}\right)\right|=1$;
(ii) Mirror condition : for any $x \in \mathscr{D}$, there exists $A_{\ell} \in \mathscr{A}$ such that $A_{x}=A_{\ell}$ and $x+A_{x}^{-1}\left([0,1 / 2]^{d}\right) \subset \mathscr{D}$.

Mirror-type transformation
$\mathscr{D}=[0,1]^{2}$
$x=(1 / 3,3 / 4)$
$y=(2 / 3,1 / 5)$


## Theorem (Bias and quadratic controls)

I.1. Assume that $g_{1} \in \mathbb{L}^{1}(\mathscr{D}), g_{1} f_{X} \in \mathscr{C}^{\alpha}(\mathscr{D})$, and
$\int_{\mathscr{D}}\left|g_{1}(x) \frac{\partial^{\beta}\left(g_{1} f_{x}\right)}{\partial x^{\beta}}(x)\right| d x<\infty$ for any $\beta$ such that $1 \leqslant|\beta|<\lfloor\alpha\rfloor$. Then we have

$$
\left|\mathbb{E}\left[T_{n, h_{n}}\right]-\mathbb{E}\left[\mathbb{E}[Y \mid X]^{2}\right]\right| \leqslant C h_{n}^{\alpha} .
$$

I.2. Assume in addition that $g_{1} \in \mathscr{C}^{\alpha}(\mathscr{D}), g_{2} / f_{X} \in \mathbb{L}^{1}(\mathscr{D}) \cap \mathbb{L}^{2}(\mathscr{D})$ and $g_{2} f_{X} \in \mathbb{L}^{2}(\mathscr{D})$, and $\int_{\mathscr{D}} g_{2}(x)\left|\frac{\partial^{\beta}\left(g_{1} f_{X}\right)}{\partial x^{\beta}}(x) \frac{\partial^{\beta^{\prime}}\left(g_{1} f_{X}\right)}{\partial x^{\beta^{\prime}}}(x)\right| d x<\infty$ for any $\beta$ and $\beta^{\prime}$ such that $1 \leqslant|\beta|,\left|\beta^{\prime}\right|<\lfloor\alpha\rfloor$. Then we have

$$
\mathbb{E}\left[\left(T_{n, h_{n}}-\mathbb{E}\left[T_{n, h_{n}}\right]-\frac{1}{n} \sum_{j=1}^{n} Z_{j}\right)^{2}\right] \leqslant C h_{n}^{2 \alpha}+\frac{C}{h_{n}^{d} n^{2}}
$$

where, for $j=1, \ldots, n, Z_{j}=2\left(Y_{j} g_{1}\left(X_{j}\right)-\mathbb{E}\left[\mathbb{E}[Y \mid X]^{2}\right]\right)$.

## Theorem (Central Limit Theorem)

II. Assuming in addition that $\mathbb{E}\left[Y^{4}\right]<\infty, \alpha>d / 2, h_{n} \underset{n \rightarrow \infty}{ } 0$, $n h_{n}^{d} \underset{n \rightarrow \infty}{ } \infty$, and $n h_{n}^{2 \alpha} \underset{n \rightarrow \infty}{ } 0$, we get

$$
\sqrt{n}\left(T_{n, h_{n}}-\mathbb{E}\left[\mathbb{E}[Y \mid X]^{2}\right]\right) \xrightarrow[n \rightarrow \infty]{\mathscr{D}} \mathscr{N}\left(0,4 \tau^{2}\right)
$$

with $\tau^{2}=\operatorname{Var}\left(Y g_{1}(X)\right)$.

Ref. : F. Gamboa, T. Klein, A. Lagnoux, C. Prieur, and S. da Veiga. "New estimation of Sobol' indices based on kernels". Available on Hal and Arxiv (2023). https://hal.science/hal-04052837.

Using the delta method, we are now able to get the asymptotic behavior of the estimation of $S^{X}$.

Corollary (CLT for the estimation of the Sobol' indices)
Under all the assumptions of the theorem (II included), one has

$$
\sqrt{n}\left(\frac{T_{n, h_{n}}-\left(\frac{1}{n} \sum_{j=1}^{n} Y_{j}\right)^{2}}{\frac{1}{n} \sum_{j=1}^{n} Y_{j}^{2}-\left(\frac{1}{n} \sum_{j=1}^{n} Y_{j}\right)^{2}}-S^{X}\right) \underset{n \rightarrow \infty}{\stackrel{\mathscr{D}}{\longrightarrow}} \mathscr{N}\left(0, \sigma^{2}\right)
$$

where the limit variance $\sigma^{2}$ has an explicit expression.

Using one more time the delta method, we deduce the asymptotic behavior of the vector containing the $p$ first-order Sobol' indices. Let us denote $S^{i}$ the first-order Sobol index associated to the $i$-th input and its estimator $\widehat{S}^{i}$ given by :

$$
\widehat{S}^{i}=\frac{T_{n, h_{n}}-\left(\frac{1}{n} \sum_{j=1}^{n} Y_{j}\right)^{2}}{\frac{1}{n} \sum_{j=1}^{n} Y_{j}^{2}-\left(\frac{1}{n} \sum_{j=1}^{n} Y_{j}\right)^{2}}
$$

## Corollary (CLT for the global estimation of the $p$ first-order Sobol' indices)

Under all the assumptions of the theorem (II included), one has

$$
\sqrt{n}\left(\left(\widehat{S}^{1}, \ldots, \widehat{S}^{p}\right)^{T}-\left(S^{1}, \ldots, S^{p}\right)^{T}\right) \xrightarrow[n \rightarrow \infty]{\mathscr{D}} \mathscr{N}(0, \Sigma)
$$

where the limit variance $\Sigma$ has an explicit expression.

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## Also in the paper...

- A procedure for bandwidth selection inspired from Delyon and Portier in 2016.
- An extension to unknown density $f_{X}$ in which we consider
- parametric estimation of $f_{X}$,
- nonparametric estimation of $f_{X}$.


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## Sketch of the proof (I)

Since $Y \in \mathbb{L}^{2}(\mathbb{R})$, one has

$$
\begin{aligned}
\mathbb{E}\left[T_{n, h}\right] & =\iint_{\mathscr{D}^{2}} \frac{K_{h} \circ A_{x_{1}}\left(x_{2}-x_{1}\right)}{f_{X}\left(x_{1}\right)} f_{X}\left(x_{1}\right) f_{X}\left(x_{2}\right) g_{1}\left(x_{1}\right) g_{1}\left(x_{2}\right) d x_{1} d x_{2} \\
& =\int_{\mathscr{D}} \int_{\mathscr{D}_{X}} K(u) g_{1}(x) g_{1}\left(x+h A_{x}^{-1}(u)\right) f_{X}\left(x+h A_{x}^{-1}(u)\right) d u d x .
\end{aligned}
$$

In addition,
$\mathbb{E}\left[\mathbb{E}[Y \mid X]^{2}\right]=\mathbb{E}\left[g_{1}^{2}(X)\right]=\int_{\mathscr{D}} g_{1}(x)^{2} f_{X}(x) d x=\iint_{\mathscr{D}^{2}} K(u) g_{1}(x)^{2} f_{X}(x) d x d u$
leading to $\mathbb{E}\left[T_{n, h}\right]-\mathbb{E}\left[\mathbb{E}[Y \mid X]^{2}\right]$

$$
=\iint_{\mathscr{D}^{2}} K(u) g_{1}(x)\left(g_{1}\left(x+h A_{x}^{-1}(u)\right) f_{X}\left(x+h A_{x}^{-1}(u)\right)-g_{1}(x) f_{X}(x)\right) d x d u
$$

## Sketch of the proof (II)

For all $j, j^{\prime}=1, \ldots, n$, we introduce the symmetric function given by

$$
R\left(\binom{x_{j}}{y_{j}},\binom{x_{j^{\prime}}}{y_{j^{\prime}}}\right)=\frac{y_{j} y_{j^{\prime}}}{2}\left(\frac{K_{h_{n}} \circ A_{x_{j}}\left(x_{j^{\prime}}-x_{j}\right)}{f_{X}\left(x_{j}\right)}+\frac{K_{h_{n}} \circ A_{x_{j^{\prime}}}\left(x_{j}-x_{j^{\prime}}\right)}{f_{X}\left(x_{j^{\prime}}\right)}\right) .
$$

Then the Hoeffding projections of $R$ are given by (see Pena 1999)

$$
\begin{aligned}
\pi_{1} R\binom{x}{y}= & \mathbb{E}\left[R\left(\binom{x}{y},\binom{X_{2}}{Y_{2}}\right)\right]-\mathbb{E}\left[R\left(\binom{X_{1}}{Y_{1}},\binom{X_{2}}{Y_{2}}\right)\right] \\
\pi_{2} R\left(\binom{x_{1}}{y_{1}},\binom{x_{2}}{y_{2}}\right)= & R\left(\binom{l_{1}}{y_{1}},\binom{x_{2}}{y_{2}}\right)-\mathbb{E}\left[R\left(\binom{x_{1}}{y_{1}},\binom{X_{2}}{Y_{2}}\right)\right] \\
& -\mathbb{E}\left[R\left(\binom{x_{2}}{y_{2}},\binom{X_{2}}{Y_{2}}\right)\right]+\mathbb{E}\left[R\left(\binom{X_{1}}{Y_{1}},\binom{X_{2}}{Y_{2}}\right)\right] .
\end{aligned}
$$

## Sketch of the proof (III)

Hence the Hoeffding decomposition writes

$$
\begin{aligned}
& T_{n, h_{n}}- \mathbb{E}\left[T_{\left.n, h_{n}\right]=2 U_{n}^{(1)}\left(\pi_{1} R\right)+U_{n}^{(2)}\left(\pi_{2} R\right)}^{=}\right. \\
&=\frac{1}{n} \sum_{j=1}^{n} \underbrace{2\left(Y_{j} g_{1}\left(X_{j}\right)-\mathbb{E}\left[\mathbb{E}[Y \mid X]^{2}\right]\right)}_{=Z_{j}} \\
&+\underbrace{2 U_{n}^{(1)}\left(\pi_{1} R\right)-\frac{2}{n} \sum_{j=1}^{n}\left(Y_{j} g_{1}\left(X_{j}\right)-\mathbb{E}\left[\mathbb{E}[Y \mid X]^{2}\right]\right)}_{=S_{1}}+\underbrace{U_{n}^{(2)}\left(\pi_{2} R\right)}_{=S_{2}} .
\end{aligned}
$$

with $\quad U_{n}^{(1)}\left(\pi_{1} R\right)=\frac{1}{n} \sum_{j=1}^{n}\left(\pi_{1} R\right)\binom{X_{j}}{Y_{j}}$
$U_{n}^{(2)}\left(\pi_{2} R\right)=\frac{2}{n(n-1)} \sum_{1 \leqslant j<j^{\prime} \leqslant n}^{n}\left(\pi_{2} R\right)\left(\binom{X_{j}}{Y_{j}},\binom{X_{j^{\prime}}}{Y_{j^{\prime}}}\right.$ (Giné, Nikl '08).

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## Ishigami function

The Ishigami model is given by :

$$
Y=f(V)=f\left(V_{1}, V_{2}, V_{3}\right)=\sin \left(V_{1}\right)+7 \sin ^{2}\left(V_{2}\right)+0.1 V_{3}^{4} \sin \left(V_{1}\right)
$$

where $\left(V_{j}\right)_{j=1,2,3}$ are i.i.d. uniform random variables on $[-\pi ; \pi]$.
One has

$$
S^{1}=0.3139, S^{2}=0.4424, S^{3}=0
$$



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## Bratley function

Let us consider the Bratley function defined by :

$$
g\left(V_{1}, \ldots, V_{p}\right)=\sum_{i=1}^{p}(-1)^{i} \prod_{j=1}^{i} V_{j}
$$

with $V_{i} \sim \mathscr{U}([0,1])$ i.i.d. After some tedious calculations, one gets

$$
\begin{aligned}
\operatorname{Var}(Y) & =\frac{1}{18}-\frac{2}{45}\left(-\frac{1}{2}\right)^{p}+\frac{1}{10} \frac{1}{3^{p}}-\frac{1}{9} \frac{1}{2^{2 p}} \\
S^{i} & =\frac{\operatorname{Var}\left[\mathbb{E}\left(Y \mid V_{i}\right)\right]}{\operatorname{Var}(Y)}=\frac{1}{\operatorname{Var}(Y)} \frac{\left(2^{p-i+1}-(-1)^{p-i+1}\right)^{2}}{2^{2 p} \times 3^{3}} .
\end{aligned}
$$

Now let us compute the total indices for $i=1$ and 2 and $p=5$,

$$
S^{1, \text { Tot }}=1-\frac{1111}{3^{4} \times 2^{10} \times \operatorname{Var}(Y)} \approx 0.77, \quad S^{2, \text { tot }}=1-\frac{3703}{3^{4} \times 2^{10} \times \operatorname{Var}(Y)} \approx 0.22 .
$$

Estimation survey 0

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Numerical applications 0000



