Efficient estimation of Sobol' indices of any order from a single input/output sample

Joint work with S. Da Veiga, F. Gamboa, T. Klein, and C. Prieur

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Outline of the talk

Introduction
- Framework and Sobol' indices
- The classical Pick-Freeze estimation
- Estimation from a single input/output sample

Efficient estimation from a single input/output sample
- Derivation of our estimator
- Two main ingredients
- Our efficient mirrored high-order kernel-based estimate
- Main results

Numerical applications

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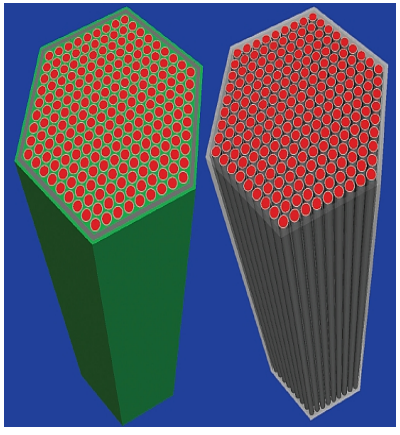
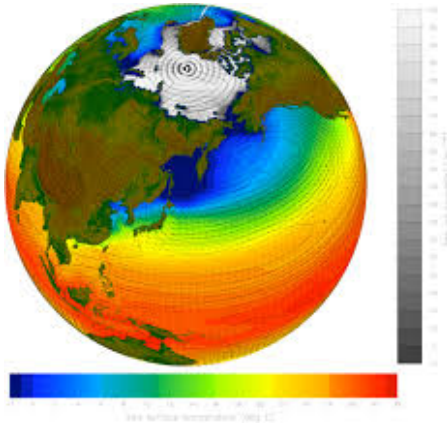
Motivation : computer models

Computer models have become essential in science and industry !





For clear reasons : cost reduction, possibility to explore hazardous or extreme scenarios...

Computer models as expensive functions

A computer model can be seen as a deterministic function

$$f : \mathbb{R}^p \to \mathbb{R}^k$$
$$v = (v_1, \ldots, v_p) \mapsto y = f(v) = (v_1, \ldots, v_p)$$

- the inputs v_i for $i = 1, \ldots p$ are objects = tunable simulation parameters (e.g. aircraft geometry, wind),
- the output y is a vector = quantity of interest (e.g. energetic efficiency, fuel consumption).

Computer models as expensive functions

Generally, the deterministic function f is

- continuous (at least) and non-linear but not analytically known $\Rightarrow$ black-box model ;
- only available through evaluations $f(v_1, \ldots, v_p)$;
- computationally expensive to evaluate.

Wishes

1. Evaluate y for any value of the p-uplet $(v_1, \ldots, v_p)$.
2. Identify the most important variables to be able to fix the less important ones to their nominal value.

Probabilistic frame

In order to quantify the influence of a variable, it is common to assume that the inputs are random :

$$V := (V_1, \ldots, V_p) \in \mathscr{E}^p.$$

Then $f : \mathscr{E}^p \to \mathbb{R}^k$ is a deterministic measurable function evaluable on runs and the output code Y becomes random too :

$$Y = f(V_1, \ldots, V_p).$$

Main assumptions

1. *The inputs $V_1, \ldots, V_p \in \mathscr{E}$ are independent.*
2. *The output Y has a finite second moment.*

First toy example

Let have a look on a simple example :

$$(V_1, V_2, V_3) \in \mathbb{R}^3 \mapsto Y = V_1 + V_1 V_2.$$

Obviously,

1. Y is not depending on V_3 ;
2. V_1 should be more influent than V_2 as it appears once alone (term V_1) and once related to V_2 (term $V_1 V_2$).

An input variable is influent if its variations leads to strong variations on the output.

$\Rightarrow$ *Build an index of influence on the variance of the output*

The so-called Sobol' indices

Quantification of the amount of randomness that a variable or a group of variables bring to Y => so-called Sobol' indices.

Such indices stem from the Hoeffding decomposition of the variance of f (or equivalently Y) that is assumed to be real-valued and to lie in L^2 in the sequel.

Let $\mathbf{u}$ be a subset of $\{1,\ldots,p\}$ and $\sim\mathbf{u}$ its complementary in $\{1,\ldots,p\}$: $\sim\mathbf{u} = \{1,\cdots,p\} \setminus \mathbf{u}$.

Let denote $V_{\mathbf{u}} = (V_i, i \in \mathbf{u})$ and $V_{\sim\mathbf{u}} = (V_i, i \in \sim\mathbf{u})$.

From Hoeffding decomposition to Sobol' indices

The decomposition of the output Y gives

$$Y := f(V) = \underbrace{\mathbb{E}[Y]}_{\text{Mean effect}} + \underbrace{\mathbb{E}[Y|V_{\mathbf{u}}] - \mathbb{E}[Y] + \mathbb{E}[Y|V_{\sim\mathbf{u}}]) - \mathbb{E}[Y]}_{\text{First order effects}} + \underbrace{Y - (\mathbb{E}[Y] + \mathbb{E}[Y|V_{\mathbf{u}}] - \mathbb{E}[Y] + \mathbb{E}[Y|V_{\sim\mathbf{u}}] - \mathbb{E}[Y])}_{\text{Second order effects or interaction:}=IA}.$$

Factors in the decomposition being orthogonal in L^2, one may compute the variance on both sides,

$$\mathrm{Var}(Y) = \mathrm{Var}\left(\mathbb{E}[Y|V_{\mathbf{u}}]\right) + \mathrm{Var}\left(\mathbb{E}[Y|V_{\sim\mathbf{u}}]\right) + \mathrm{Var}\left(IA\right).$$

From Hoeffding decomposition to Sobol' indices

This is the so-called Hoeffding decomposition of f. Dividing by $\mathrm{Var}(Y)$, one gets

$$1 = \frac{\mathrm{Var}\left(\mathbb{E}[Y|V_{\mathbf{u}}]\right)}{\mathrm{Var}(Y)} + \frac{\mathrm{Var}\left(\mathbb{E}[Y|V_{\sim\mathbf{u}}]\right)}{\mathrm{Var}(Y)} + \frac{\mathrm{Var}(IA)}{\mathrm{Var}(Y)}$$
$$:= S^{\mathbf{u}} + S^{\sim\mathbf{u}} + S^{\mathbf{u},\sim\mathbf{u}} \quad \Rightarrow \quad \text{Sobol}' \text{ indices}$$

☞ $S^{\mathbf{u}} = \frac{\mathrm{Var}(\mathbb{E}[Y|V_{\mathbf{u}}]))}{\mathrm{Var}(Y)}$ *quantifies the first order effect of* $V_{\mathbf{u}}$,

while $1 - S^{\sim\mathbf{u}} = S^{\mathbf{u}} + S^{\mathbf{u},\sim\mathbf{u}}$ *quantifies the total effect of* $V_{\mathbf{u}}$.

First toy example (continued)

We consider again

$$Y = f(V) = V_1 + V_1 V_2$$

where $V = (V_1, V_2, V_3) \sim \mathcal{N}_3(0, I_3)$. Then

$$(S^1, S^2, S^3) = (1/2, 0, 0)$$

and

$$(S^{1,Tot}, S^{2,Tot}, S^{3,Tot}) = (1, 1/2, 0).$$

Pick-Freeze estimation of Sobol' indices (I)

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

- draw $V = (V_1, V_2, V_3, V_4, V_5)$,
- build $V^{\mathbf{u}} = (V_1, V_2, V_3', V_4', V_5')$.

Then, we compute

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

A small miracle

$$\mathrm{Var}(\mathbb{E}[Y|V_{\mathbf{u}}]) = \mathrm{Cov}(Y, Y^{\mathbf{u}}) \text{ so that } S^{\mathbf{u}} = \frac{\mathrm{Cov}(Y, Y^{\mathbf{u}})}{\mathrm{Var}(Y)}.$$

Pick-Freeze estimation of Sobol' indices (II)

In practice, generate two n-samples :

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

Compute the code on both samples :

- $Y_j = f(V_j)$ for $j = 1, \dots, n$,
- $Y_j^{\mathbf{u}} = f(V_j^{\mathbf{u}})$ for $j = 1, \dots, n$.

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

$$S^{\mathbf{u}}_{n,PF} = \frac{\frac{1}{n}\sum_{j=1}^n Y_j Y_j^{\mathbf{u}} - \left(\frac{1}{n}\sum_{j=1}^n Y_j\right)\left(\frac{1}{n}\sum_{j=1}^n Y_j^{\mathbf{u}}\right)}{\frac{1}{n}\sum_{j=1}^n (Y_j)^2 - \left(\frac{1}{n}\sum_{j=1}^n Y_j\right)^2}$$

Pick-Freeze scheme (III) : some statistical properties

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

- Is it consistent ? YES SLLN.
- If yes, at which rate of convergence ? YES CLT (cv in $\sqrt{n}$).
- Is it asymptotically efficient ? YES.
- Is it possible to measure its performance for a fixed n ?
  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 ($dim(\mathscr{E}) = d = 1$)

and we want to estimate the Sobol' index with respect to $X = V_i$:

$$S^i = \frac{\mathrm{Var}(\mathbb{E}[Y|V_i])}{\mathrm{Var}(Y)} = \frac{\mathrm{Var}(\mathbb{E}[Y|X])}{\mathrm{Var}(Y)}.$$

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

$$(X_1, Y_1), (X_2, Y_2), \ldots, (X_n, Y_n).$$

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

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

Mighty estimation based on ranks (II)

We introduce

$$S^i_{n,Rank} = \frac{\frac{1}{n}\sum_{j=1}^{n-1} Y_{(j)} Y_{(j+1)} - \left(\frac{1}{n}\sum_{j=1}^{n} Y_j\right)^2}{\frac{1}{n}\sum_{j=1}^{n} Y_j^2 - \left(\frac{1}{n}\sum_{j=1}^{n} Y_j\right)^2}.$$

Statistical properties - only for $d = 1$ and first-order Sobol' indices
Consistency and CLT : 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

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_i, Y)
- $n_2 = n - n_1 \approx n \Rightarrow$ *Monte-Carlo estimation of the integral involved in the quantity of interest.*

Statistical properties - only for $d = 1$ and first-order Sobol' indices
Consistency, CLT, and asymptotic efficiency : OK.

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

Estimation based on nearest neighbors

Here the input $X = V_{\mathbf{u}}$, $\mathbf{u} \subset \{1, \cdots, p\}$ with respect we want to compute the Sobol' index is allowed to have dimension $d \geqslant 1$.

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

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

Statistical properties - Consistency and CLT : OK only for $d \leqslant 3$.

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

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Framework

Recall that

$$S^X = \frac{\mathrm{Var}(\mathbb{E}[Y|X])}{\mathrm{Var}(Y)} = \frac{\mathbb{E}[\mathbb{E}[Y|X]^2] - \mathbb{E}[Y]^2}{\mathrm{Var}(Y)}$$

allowing a multidimensional $X = V_{\mathbf{u}}$ with $\mathbf{u} \subset \{1, \cdots, p\}$:
$X \in \mathscr{D} = [0,1]^d$.

☞ *Thus we focus on the estimation of* $T = \mathbb{E}[\mathbb{E}[Y|X]^2]$ *from the* n*-sample* $(X_j, Y_j)_{j=1,\ldots,n}$ *of the pair* (X, Y).

Our estimator

• Starting point - if the regression function m is known, an asymptotically efficient estimator is (see Lagnoux et al. (2024))

$$T_{n,\text{oracle}} = \frac{1}{n}\sum_{i=1}^{n}(2Y_i - m(X_i))m(X_i) \quad \text{with } m(x) = \mathbb{E}[Y|X=x].$$

• Our goal - build an estimator such that $\widehat{T}_n = T_{n,\text{oracle}} + o_{\mathbb{P}}(n^{-1/2})$.
$\Rightarrow$ CLT/AE through CLT/AE of oracle and Slutsky's lemma.

• Idea - a plug-in estimator of the form

$$\widehat{T}_n = \frac{1}{n}\sum_{i=1}^{n}(2Y_i - \widehat{m}_n(X_i))\widehat{m}_n(X_i).$$

Of course, there is a lot of work to obtain the required control !

Two main ingredients

We propose to estimate the regression function m with a kernel-based estimator.

1. Standard Nadaraya-Watson with usual kernels is doomed by dimensionality.

☞ *We rely on high-order kernels with regularity assumptions on the output.*

2. If inputs have compact support, kernels have known boundary issues.

☞ *We leverage mirror transformations and derive new useful convergence lemmas.*

First ingredient : high-order kernels

(Symmetric) high-order kernels in a nutshell : $k : [-1,1] \to \mathbb{R}$ bounded : $\|k\|_\infty < \infty$ is a univariate kernel of order $\nu+1$ if :

$$\int_{-1}^{1} k(u)du = 1,$$
$$\int_{-1}^{1} u^\ell k(u)du = 0, \text{ for any } \ell \in \mathbb{N} \text{ such that } 0 < \ell \leq \nu$$
$$\int_{-1}^{1} u^{\nu+1} k(u)du \neq 0.$$

Commonly used kernels (Gaussian, Epanechnikov,...) are of order 2. Finally,

$$K_h(u) = \frac{1}{h^d} K(\frac{u}{h}) = \frac{1}{h^d} \prod_{k=1}^{d} k(\frac{u_k}{h}), \forall u \in [-1,1]^d.$$

First ingredient : why high-order kernels ? (I)

For kernel density estimation, bias is (by a multivariate Taylor expansion)

$$Bias = \mathbb{E}[\widehat{f}(x)] - f(x) = \sum_{1 \leqslant |\beta| < \nu} \frac{h^{|\beta|}}{\beta!} \frac{\partial^\beta f}{\partial x^\beta}(x) \underbrace{\kappa_{1,\beta}(k)}_{\substack{\text{with a high-order kernel,} \\ \text{this term can cancel}}}$$

$$+ h^\nu \sum_{|\beta|=\nu} \underbrace{\kappa_{2,\beta}(k)}_{\text{remainder term}} \quad \text{as } h \to 0$$

with the multi-index notation : $\beta = (\beta_1, \ldots, \beta_d) \in \mathbb{R}_+^d$, $|\beta| = \beta_1 + \cdots + \beta_d$, and $\beta! = \beta_1! \ldots \beta_d!$.

First ingredient : why high-order kernels ? (II)

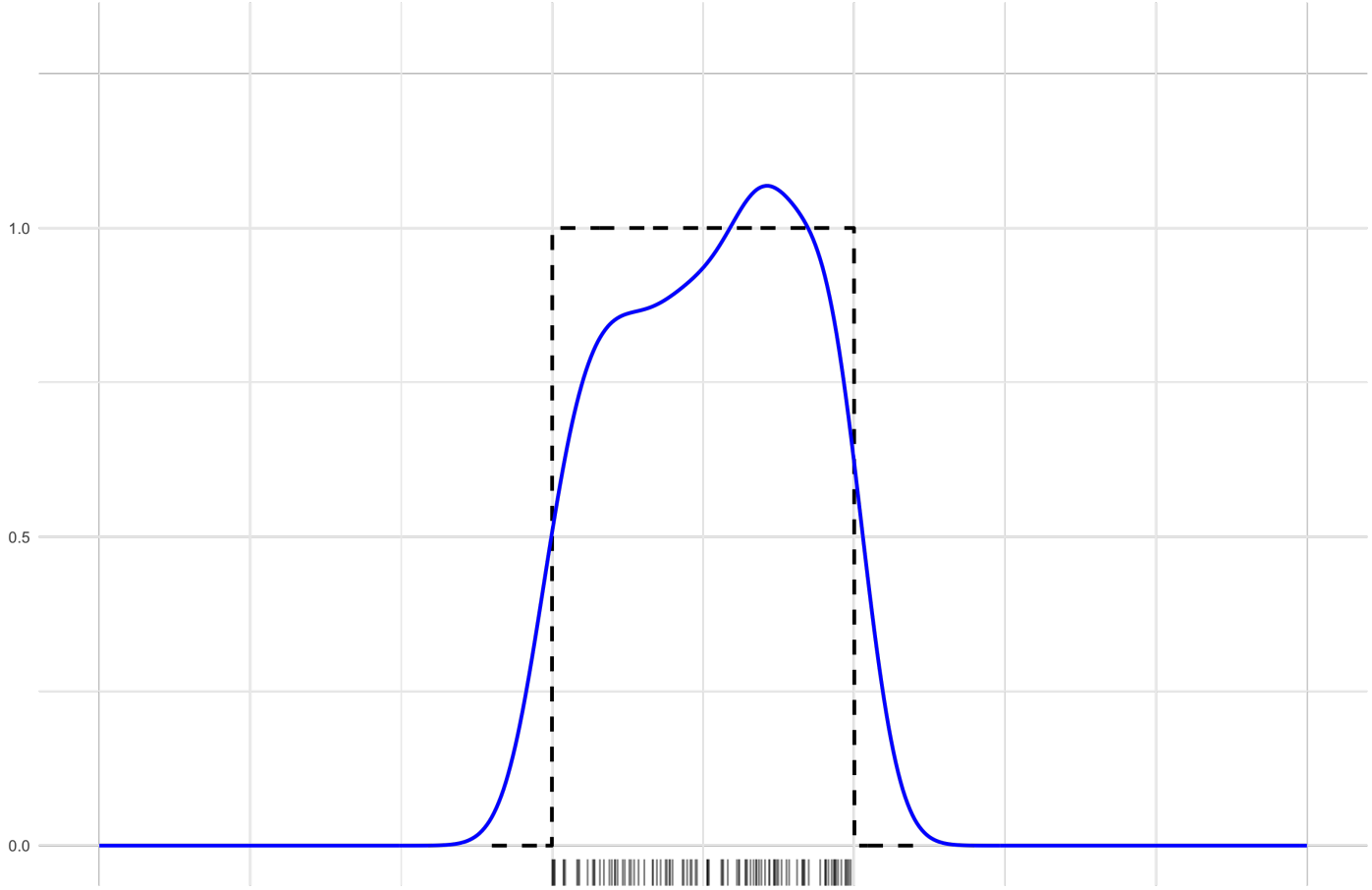
By analysing the variance (skipped here), with a high-order kernel, we finally get

$$\begin{aligned} AMISE &= \int_{\mathbb{R}^d} \mathbb{E}[(\widehat{f}(x) - f(x))^2]dx \\ &= O(n^{-\frac{2\nu}{2\nu+d}}) \quad \text{if } h = O(n^{-\frac{1}{2\nu+d}}) \text{ (optimal bandwidth)} \\ &= o(n^{-\frac{1}{2}}) \qquad \text{if } \nu > d/2 \end{aligned}$$

☞ kernel with high-enough order.

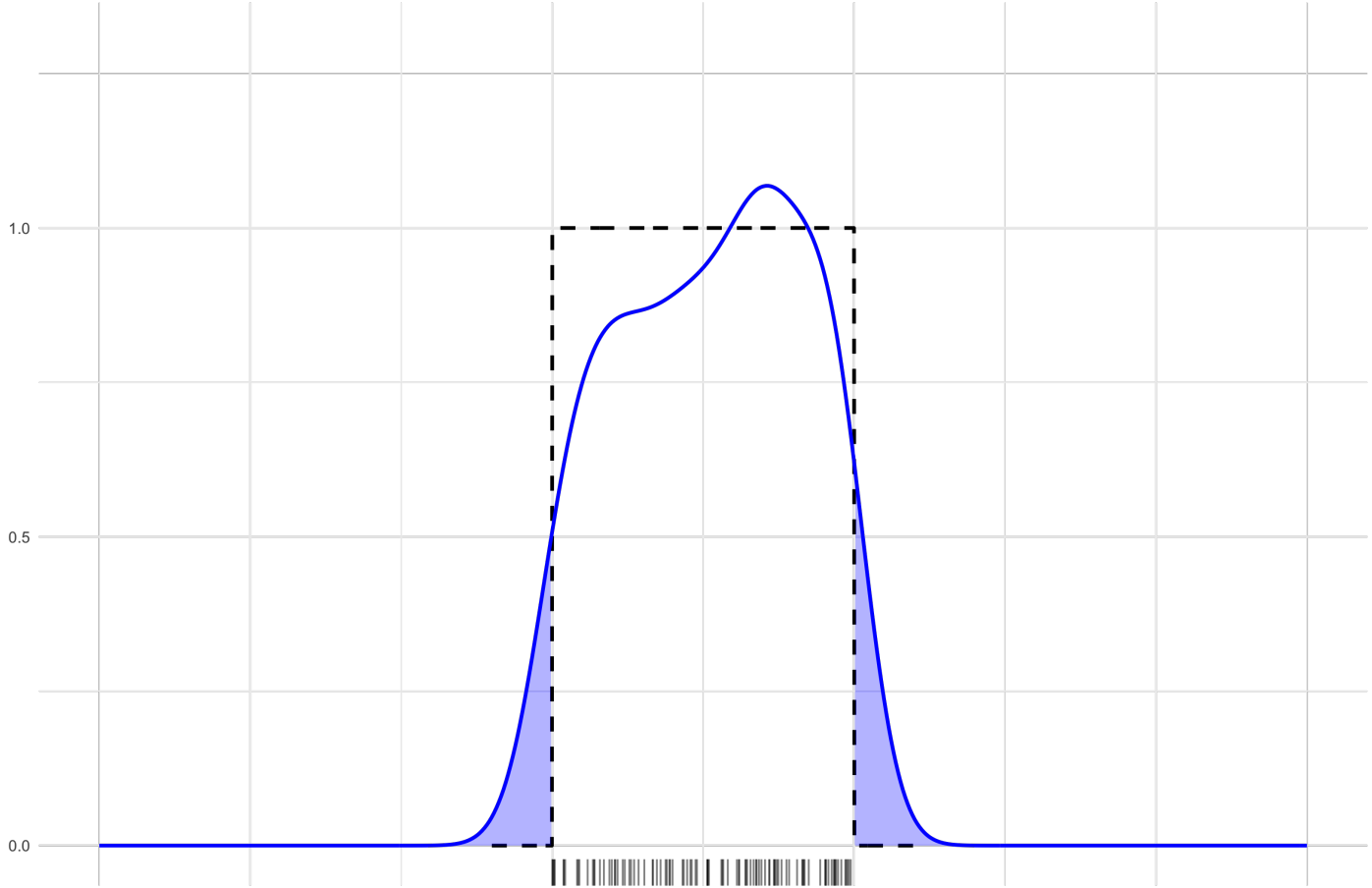
KDE boundary issues (I)

$$\widehat{f}(x) = \frac{1}{nh} \sum_{i=1}^{n} k\left(\frac{x - X_i}{h}\right) \quad \text{and} \quad \int_{-\infty}^{\infty} \widehat{f}(x) = 1$$



KDE boundary issues (II)

$$\widehat{f}(x) = \frac{1}{nh} \sum_{i=1}^{n} k\left(\frac{x - X_i}{h}\right) \quad \text{and} \quad \int_0^1 \widehat{f}(x) < 1$$



A partial solution

Doksum and Samorov (1995) estimated a truncated version of T defined as

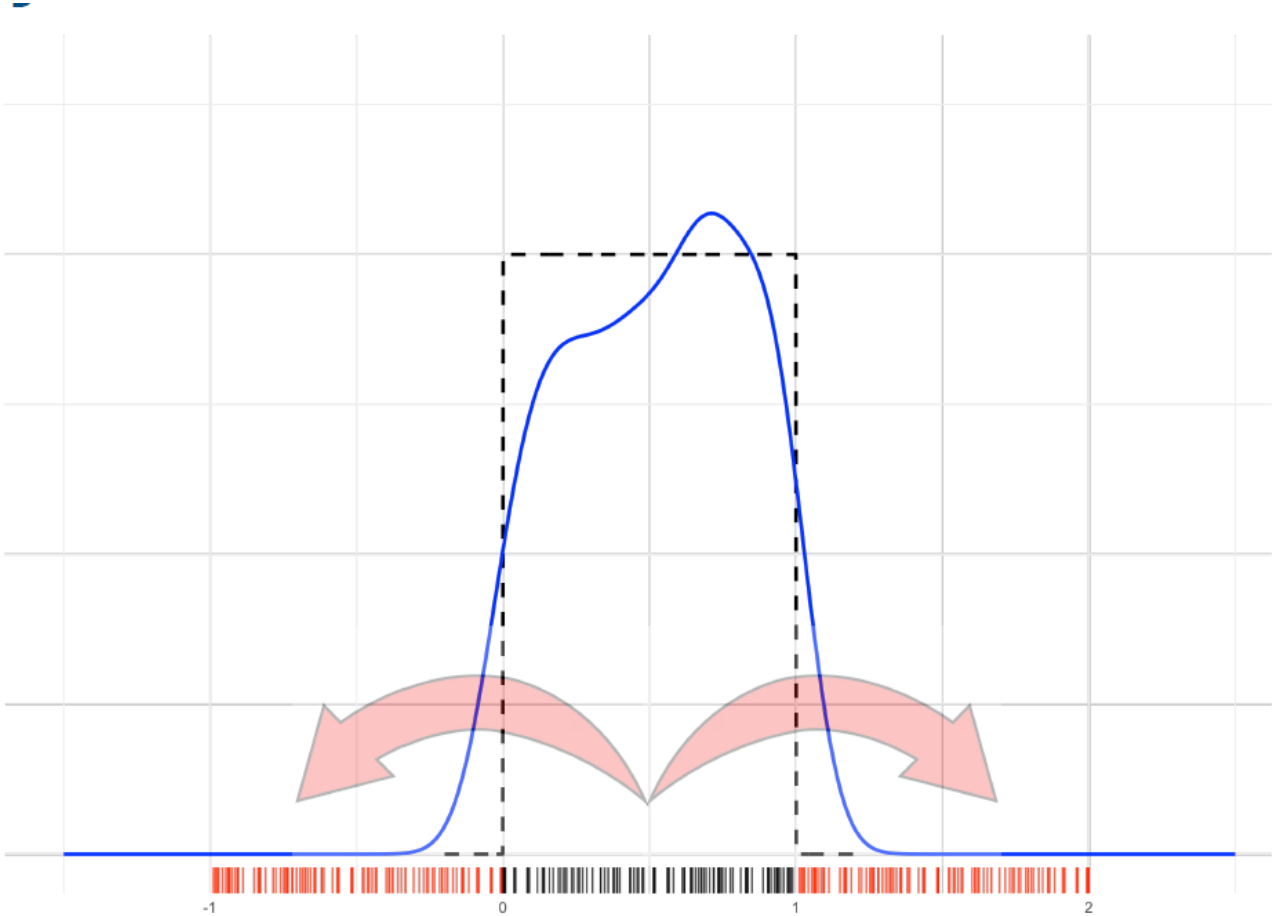
$$T^{\text{trunc},\varepsilon} = \mathbb{E}[\mathbb{E}[Y|X]^2 \mathbb{1}_{X \in (\varepsilon, 1-\varepsilon)^d}].$$

Even if $T^{\text{trunc},\varepsilon} \to T$ as $\varepsilon \to 0$ under mild assumptions, the practical tuning of the parameter ε depends on the unknown function f and its choice has a large impact.

Here, we therefore focus on mirror-type kernel estimators to estimate T rather than a truncated version of it. Such mirror-type estimators have been proposed recently to efficiently handle boundary effects inherent to kernel estimation.

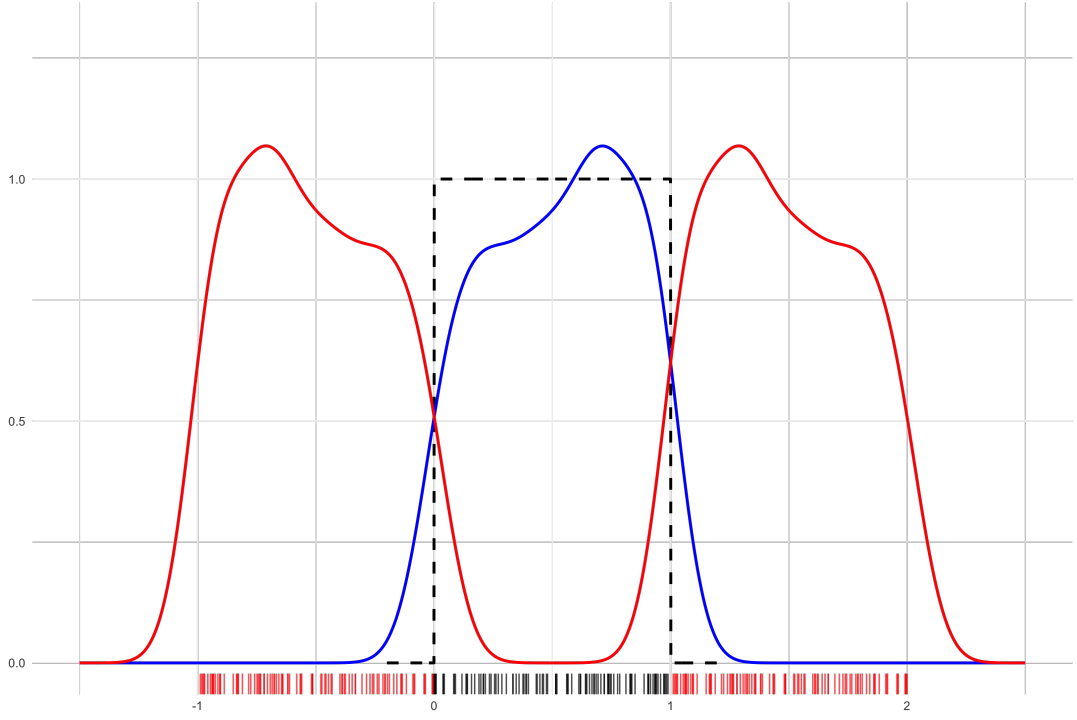
Second ingredient : mirror transformation (I)

$$\widehat{f}(x) = \frac{1}{nh}\sum_{i=1}^{n} k\left(\frac{x - X_i}{h}\right) \quad \text{and} \quad \int_{-\infty}^{\infty} \widehat{f}(x) = 1$$



Second ingredient : mirror transformation (II)

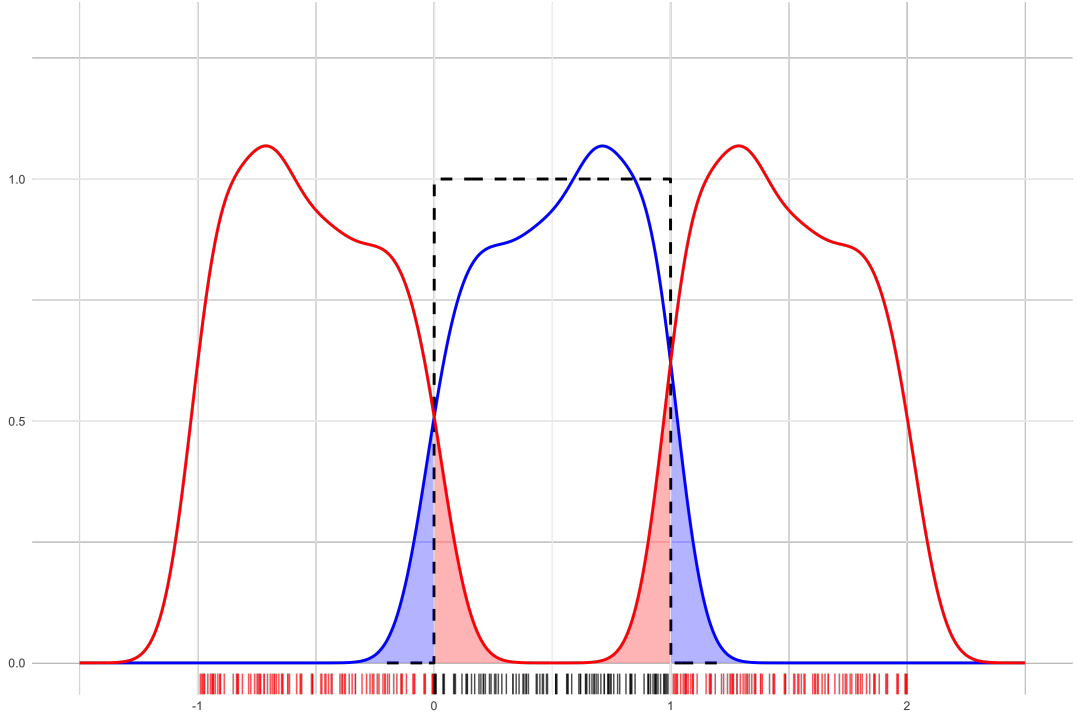
$$\widehat{f}(x) = \frac{1}{nh}\sum_{i=1}^{n} k\left(\frac{x - X_i}{h}\right) \quad \text{and} \quad \int_{-\infty}^{\infty} \widehat{f}(x) = 1$$



$$\widehat{f}_{\text{lower}}(x) = \frac{1}{nh}\sum_{i=1}^{n} k\left(\frac{x-(-X_i)}{h}\right) \qquad \widehat{f}_{\text{upper}}(x) = \frac{1}{nh}\sum_{i=1}^{n} k\left(\frac{x-(2-X_i)}{h}\right)$$

Second ingredient : mirror transformation (III)

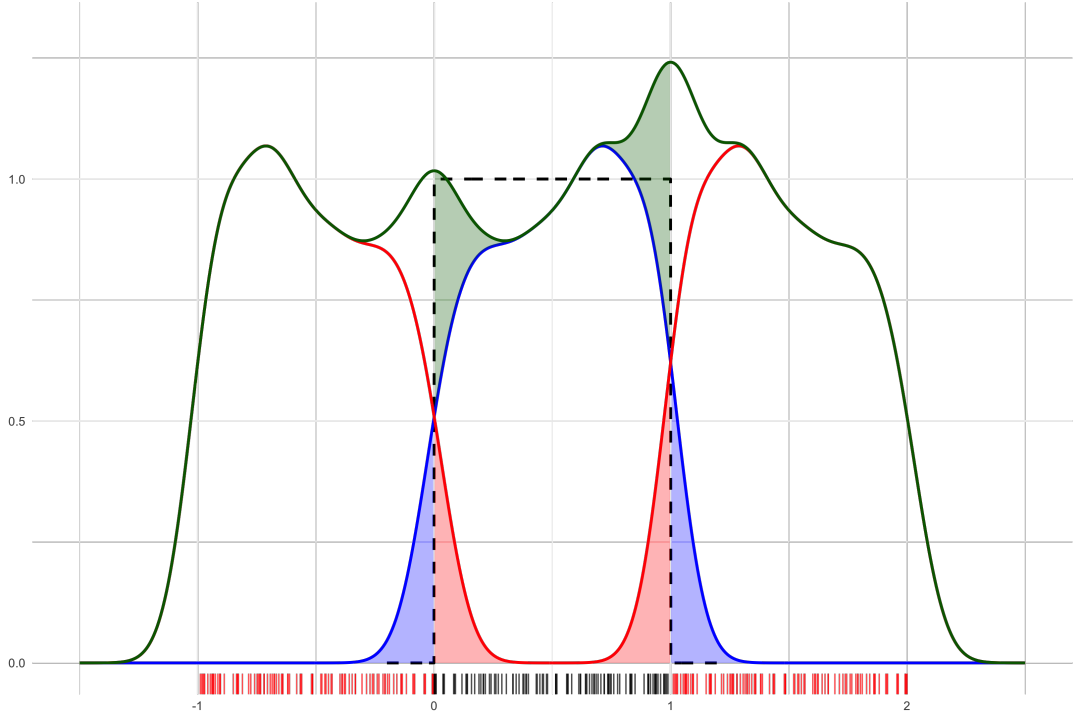
$$\widehat{f}(x) = \frac{1}{nh}\sum_{i=1}^{n} k\left(\frac{x - X_i}{h}\right) \quad \text{and} \quad \int_{-\infty}^{\infty} \widehat{f}(x) = 1$$



$$\widehat{f}_{\text{lower}}(x) = \frac{1}{nh}\sum_{i=1}^{n} k\left(\frac{x-(-X_i)}{h}\right) \qquad \widehat{f}_{\text{upper}}(x) = \frac{1}{nh}\sum_{i=1}^{n} k\left(\frac{x-(2-X_i)}{h}\right)$$

Second ingredient : mirror transformation (IV)

$$\widehat{f}_{\text{mirror}}(x) = \widehat{f}(x) + \widehat{f}_{\text{lower}}(x) + \widehat{f}_{\text{upper}}(x)$$

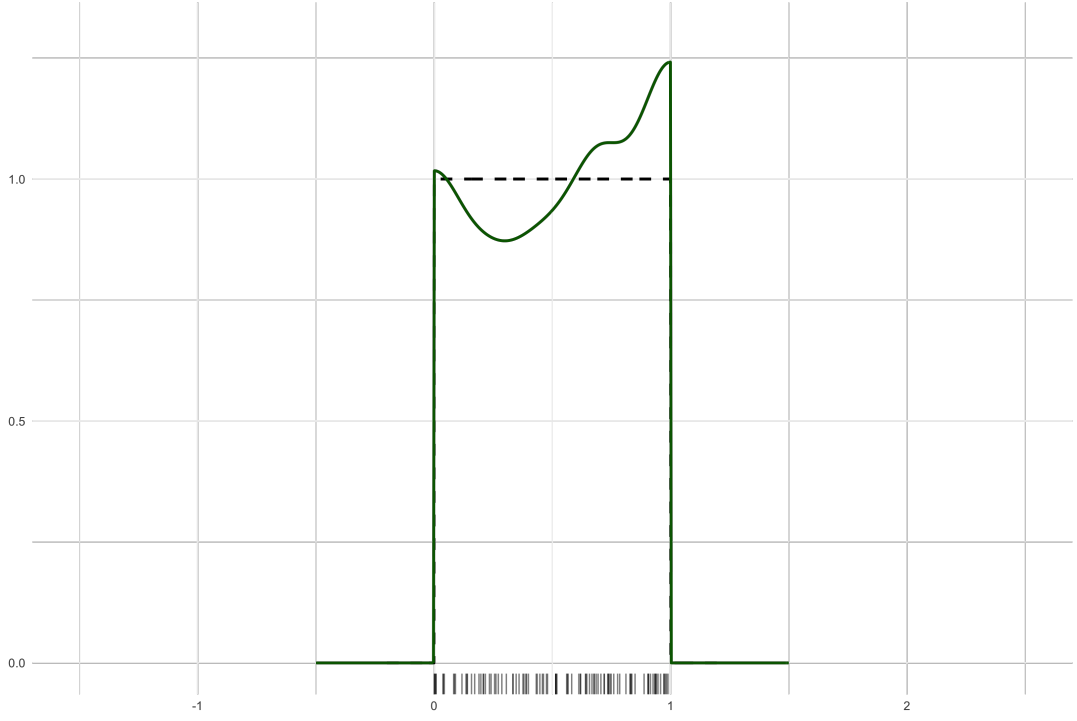


$$\widehat{f}_{\text{lower}}(x) = \frac{1}{nh}\sum_{i=1}^{n} k\left(\frac{x-(-X_i)}{h}\right)$$

$$\widehat{f}_{\text{upper}}(x) = \frac{1}{nh}\sum_{i=1}^{n} k\left(\frac{x-(2-X_i)}{h}\right)$$

Second ingredient : mirror transformation (V)

$$\widehat{f}_{\text{mirror}}(x) = \left(\widehat{f}(x) + \widehat{f}_{\text{lower}}(x) + \widehat{f}_{\text{upper}}(x)\right) \times \mathbb{1}_{x\in[0,1]} \quad \text{and} \quad \int_0^1 \widehat{f}_{\text{mirror}}(x) = 1$$



$$\widehat{f}_{\text{lower}}(x) = \frac{1}{nh}\sum_{i=1}^{n} k\left(\frac{x-(-X_i)}{h}\right) \qquad \widehat{f}_{\text{upper}}(x) = \frac{1}{nh}\sum_{i=1}^{n} k\left(\frac{x-(2-X_i)}{h}\right)$$

Our efficient mirrored high-order kernel-based estimate

As Pujol (2022), we consider the following 1D-transformations :

$$\forall z \in [0,1],\ m^{-1}(z) = -z, \quad m^0(z) = z, \quad \textit{and} \quad m^1(z) = 2 - z$$

and, for any $a \in \{-1,0,1\}^d$ and $x \in [0,1]^d$, the d-dimensional vector

$$M^a(x) = (m^{a_1}(x_1), \cdots, m^{a_d}(x_d))$$

of mirrors in all possible directions.

Our efficient mirrored high-order kernel-based estimate

The mirrored density estimate of the density f_X of X is

$$\widehat{f}_{mirror}(x) = \frac{1}{nh_n^d} \sum_{j=1}^{n} \sum_{a\in\{-1,0,1\}^d} \prod_{l=1}^{d} k\Big(\frac{x_l - m^{a_l}(X_j)}{h_n}\Big)$$
$$= \frac{1}{n} \sum_{j=1}^{n} \sum_{a\in\{-1,0,1\}^d} K_{h_n}(x - M^a(X_j))$$

and its leave-one-out version :

$$\widehat{f}_{n,h_n,i}(x) = \frac{1}{n} \sum_{j\neq i} \sum_{a\in\{-1,0,1\}^d} K_{h_n}(x - M^a(X_j)).$$

Our efficient mirrored high-order kernel-based estimate

Similarly, the leave-one-out (mirrored) Nadaraya-Watson estimate of the regression function is :

$$\widehat{m}_{n,h_n,i}(X_i) = \frac{\sum_{j\neq i} Y_j \sum_{a\in\{-1,0,1\}^d} K_{h_n}(X_i - M^a(X_j))}{\sum_{j\neq i} \sum_{a\in\{-1,0,1\}^d} K_{h_n}(X_i - M^a(X_j) -)} = \frac{\widehat{g}_{n,h_n,i}(X_i)}{\widehat{f}_{n,h_n,i}(X_i)}.$$

The associated plug-in estimator then becomes :

$$\widehat{T}_{n,h_n} = \frac{1}{n}\sum_{i=1}^{n}(2Y_i - \widehat{m}_{n,h_n,i}(X_i))\widehat{m}_{n,h_n,i}(X_i).$$

Assumptions

($\mathscr{A}1$) Support - The support of $(V_1,\ldots,V_p)$ is $[0,1]^p$ and that of X is $[0,1]^d$.

($\mathscr{A}2$) Absolute continuity - X is absolutely continuous with respect to the Lebesgue measure on $[0,1]^d$ with density function f_X and $\exists\delta>0$ such that $\inf_{x\in[0,1]^d} f_X(x)\geqslant\delta$ for some $\delta>0$.

($\mathscr{A}3$) Bounded moments - $\mathbb{E}[Y^4]<\infty$ and $\sigma^2(x)=\mathrm{Var}(Y|X=x)$ is bounded on $[0,1]^d$.

($\mathscr{A}4$) Smoothness of f_X - $f_X\in\mathscr{C}^\alpha([0,1]^d)$ for some $\alpha>0$ and its derivatives of order β $(0<\beta\leq\lfloor\alpha\rfloor)$ vanish near the boundary.

($\mathscr{A}5$) Smoothness of m - The regression function m belongs to $\mathscr{C}^\alpha([0,1]^d)$.

($\mathscr{A}6$) Kernel - $k\colon[-1,1]\to\mathbb{R}$ is a bounded univariate kernel of order $(\nu+1)$ $(\nu=\lfloor\alpha\rfloor)$.

Under the previous assumptions and an additional technical one, for all $i \in \{1, \cdots, d\}$, we get :

- bias and variance controls

$$\left\| \mathbb{E}\left[\widehat{f}_{n,h_n,i}\right] - f_X \right\|_\infty = O\left(h_n^\alpha\right),$$

$$\mathbb{E}\Big[\int_{[0,1]^d} \left(\widehat{f}_{n,h_n,i}(x) - f_X(x)\right)^2 dx\Big] = o(n^{-1/2}),$$

- lower control

$$\frac{1}{\inf_{x\in[0,1]^d} \left|\widehat{f}_{n,h_n,i}(x)\right|} = O_{\mathbb{P}}(1),$$

when $nh_n^{2d} \to \infty$ and $nh_n^{4\alpha} \to 0$ as $n \to \infty$.

Theorem (Central Limit Theorem and asymptotic efficiency)

Under the previous assumptions, one has (i)

$$\sqrt{n}\big(\widehat{T}_{n,h_n} - \mathbb{E}[\mathbb{E}[Y|X]^2]\big) \xrightarrow[n\to\infty]{\mathscr{L}} \mathcal{N}\big(0, \mathrm{Var}((2Y - m(X))m(X))\big)$$

as soon as $\alpha > d/2$ *and* $h_n = n^{-\gamma}$ *with* $1/(4\alpha) < \gamma < 1/(2d)$ *;*

(ii) $\widehat{T}_{n,h_n}$ *is asymptotically efficient to estimate* $\mathbb{E}[\mathbb{E}[Y|X]^2]$ *from an i.i.d. sample* $(X_i, Y_i)_{i=1,\cdots,n}$ *of the pair* (X, Y)*.*

☞ The same guarantees hold for the estimation $\widehat{S}_{n,h_n}$ of S^X applying the delta method.

Ref. : S. Da Veiga, F. Gamboa, T. Klein, A. Lagnoux, C. Prieur. "Efficient estimation of Sobol' indices of any order from a single input/output sample.". Available on Hal and Arxiv (2024). `https://hal.science/hal-04052837v2`.

Sketch of the proofs

Following the same lines as in the proof of Theorem 2.1 in Doksum and Samarov (1995), we prove that

$$\widehat{T}_{n,h} = \underbrace{\frac{1}{n}\sum_{i=1}^{n}(2Y_i - m(X_i))m(X_i)}_{=T_{n,oracle}} + o_{\mathbb{P}}(n^{-1/2})$$

$$= T + \frac{1}{n}\sum_{i=1}^{n}\widetilde{\psi}_P(X_i, Y_i) + o_{\mathbb{P}}(n^{-1/2}).$$

The conclusion of the theorem will then follow directly applying the standard central limit theorem for the sum of i.i.d. random variables to the right-hand side of the previous display together with Slutsky's lemma.

Outline of the talk

Introduction
- Framework and Sobol' indices
- The classical Pick-Freeze estimation
- Estimation from a single input/output sample

Efficient estimation from a single input/output sample
- Derivation of our estimator
- Two main ingredients
- Our efficient mirrored high-order kernel-based estimate
- Main results

Numerical applications

For all test cases :

- first-order and total Sobol' indices for each input variable V_i (i.e. $X = V_i$ and $X = V_{\sim i}$ resp.) ;
- mirror-type estimator with an Epanechnikov kernel of order 2 and 4 (kernel bandwidth optimized via LOO on m) ;
- concurrent estimators :
  - PF estimator studied (Janon'12) ("PF1")
  - replicated PF estimator (Tissot'15) ("PF2")
  - rank estimator (Gamboa'20) ("Rank") for 1st-order indices
  - lag estimator (Klein'24) ("Lag") for 1st-order indices
  - nearest-neighbour estimator (Devroye 2018) ("NN") ;
- we generate a n-sample $(X_1, Y_1), \cdots, (X_n, Y_n)$ (except for PF) ;
- each experiment is repeated 50 times with $n = 500$;
- the reference value is obtained from a PF estimation with very large sample size.

A realistic flood model

The flood model used is a simplification of the 1D Saint-Venant hydrodynamic equations, assuming constant and uniform flows and very wide rectangular cross-sections. It consists of an equation involving the characteristics of the river section upstream of the industrial site :

$$S = Z_v + H - H_d - C_b$$

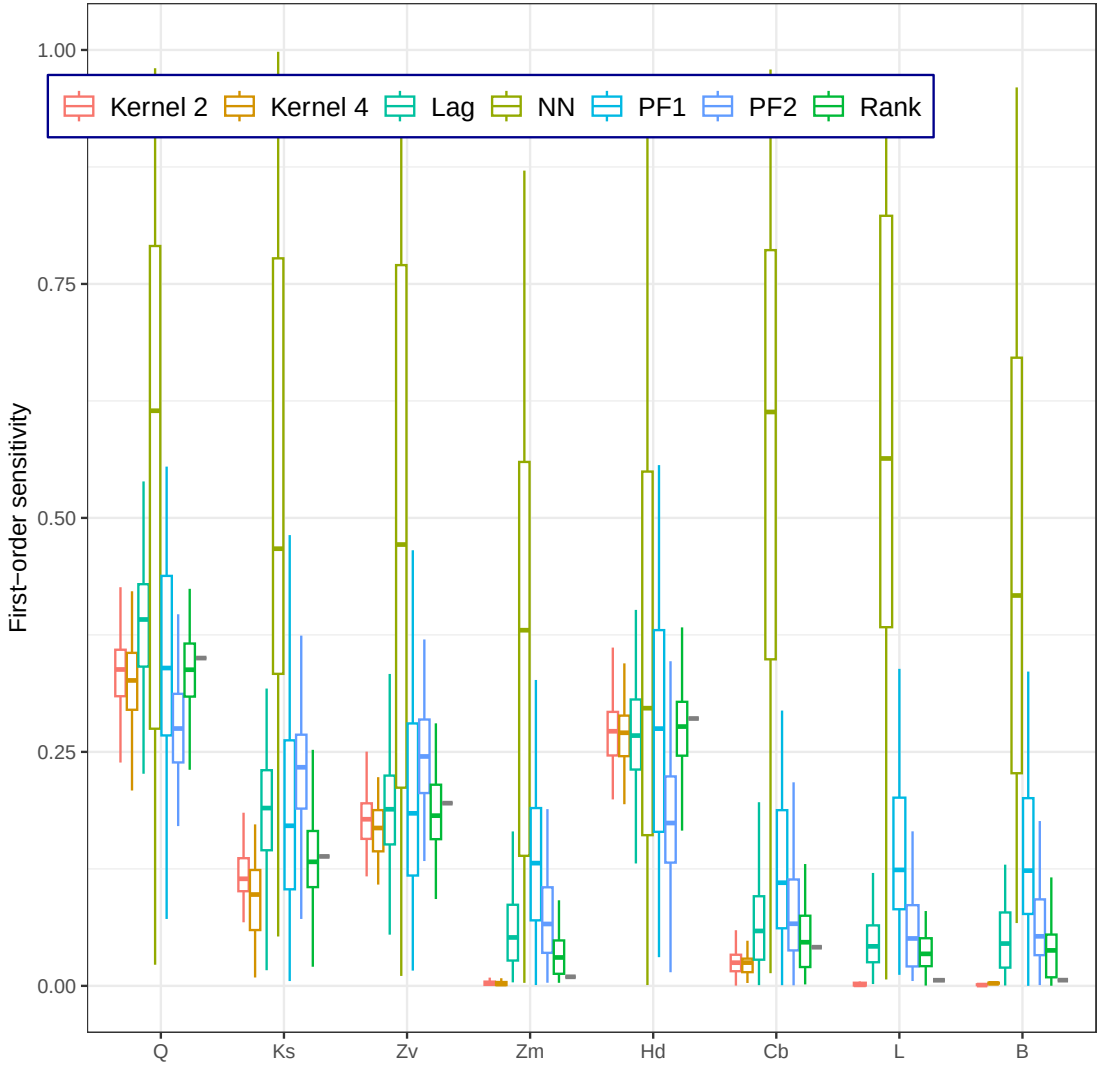
where H is calculated as :

$$H = \left(\frac{Q}{BK_s \sqrt{\frac{Z_m - Z_v}{L}}} \right)^{0.6}.$$

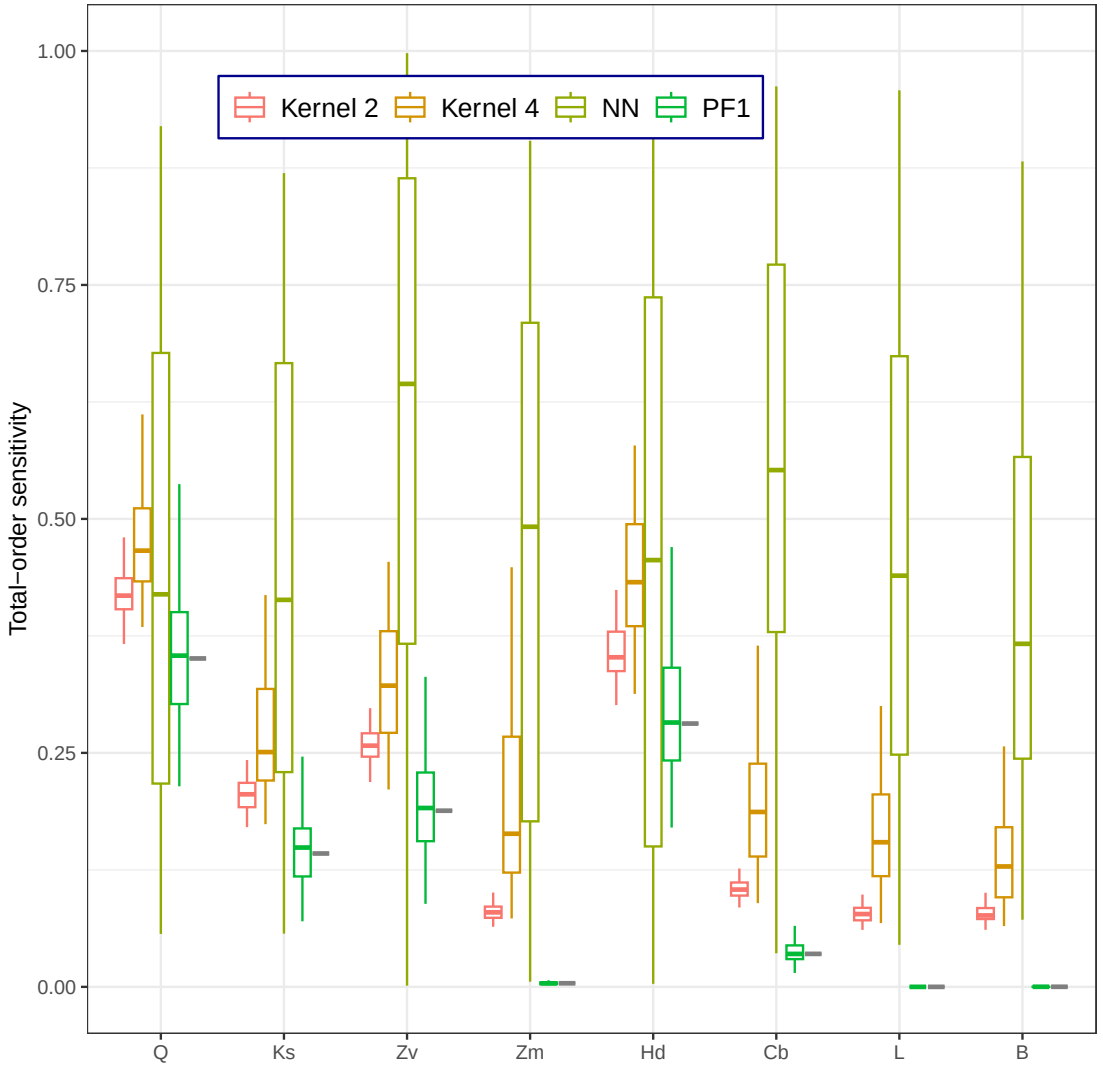
A realistic flood model - model parameters

- S : overflow (in meters), model output ;
- H : maximum annual water level (in meters) ;
- Q : maximum annual flow rate (in m^3/s) with Gumbel max distribution $Gu(1013, 558)$, truncated to be in $[500, 3000]$;
- K_s : strickler coefficient with normal distribution $\mathcal{N}(30, 8)$, truncated below at 15 ;
- Z_v : downstream riverbed elevation (in meters) with triangular distribution $T(49, 50, 51)$;
- Z_m : upstream riverbed elevation (in meters) with triangular distribution $T(54, 55, 56)$;
- H_d : dike height (in meters) with uniform distribution $\mathcal{U}(7, 9)$;
- C_b : bank elevation (in meters) with triangular distribution $T(55, 55.5, 56)$;
- L : length of the river section (in meters) with triangular distribution $T(4990, 5000, 5010)$;
- B : river width (in meters) with triangular distribution $T(295, 300, 305)$.

A realistic flood model - first-order indices - $n = 500$



A realistic flood model - total indices - $n = 500$



Tuning of parameter ϵ

We illustrate numerically that the choice of the ϵ tuning parameter of the estimator proposed in Doksum (1995) is very sensitive, thus limiting its practical use as opposed to our mirror-type estimator.

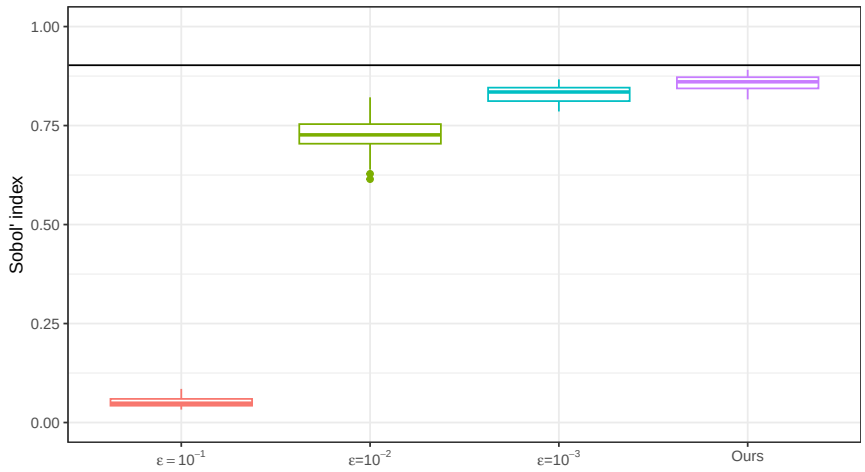
We consider Example 3.2 from Doksum and Samarov (1995) :

$$Y = \frac{1}{2} + 4X_1 + 4(X_2 - \frac{1}{2})^2 + 4X_3^{1/2} + \tau e,$$

with X_1, X_2, and X_3 i.i.d. $\sim \mathscr{U}([0,1])$ and $e \sim \mathscr{N}(0,1)$.

We test $\epsilon = 10^{-1}$, $\epsilon = 10^{-2}$ and 10^{-3}.

Tuning of parameter ϵ



When ϵ is equal to 10^{-3} (3rd), the performance of both estimators are similar. However when $\epsilon = 10^{-1}$ (1st), the bias of Doksum and Samarov (1995) can be very large.

Since in practice such an estimation problem is unsupervised, the tuning of ϵ seems highly difficult and the non-robustness of the final estimator wrt this parameter limits its practical use.

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Thanks for your attention ! Questions ?

Reference

S. Da Veiga, F. Gamboa, T. Klein, A. Lagnoux, C. Prieur. "Efficient estimation of Sobol' indices of any order from a single input/output sample". In revision at Information and Inference. Available on Hal and Arxiv (2025). `https://hal.science/hal-04052837v2`.

T. Klein, A. Lagnoux, T.M.N. Nguyen, P. Rochet. "Asymptotic efficiency for Sobol' and Cramér-von Mises indices under two designs of experiments". In revision at ESAIM P&S. `https://hal.science/hal-03477991`.