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

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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

- Two main ingredients
- Our efficient mirrored high-order kernel-based estimate
- Main results

Sketch of the proofs

Numerical applications

- The Bratley function
- The g-Sobol function

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Framework

Complicated function f valued in $\mathbb{R}^k$ depending on several variables :

$$y = f(v_1, \ldots, v_p) \in \mathbb{R}^k$$

where

1. the inputs v_i pour $i = 1, \ldots p$ are objects ;
2. f is deterministic and unknown. It is called a black-box model.

Aim

Generally,

1. f is not analytically known ;
2. given $(v_1, \ldots, v_p)$, the computer code gives $y = f(v_1, \ldots, v_p)$;
3. computing $y = f(v_1, \ldots, v_p)$ may be costly.

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 :

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

Then $f : \mathcal{E}^p \to \mathbb{R}^k$ 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 $V_1, \ldots, V_p \in \mathcal{E}$ are independent.*
2. *The output Y is scalar with a finite second moment.*

First toy example

Let have a look on a simple example :

$$(V_1, V_2, V_3) \mapsto Y = V_1 + V_1 V_2.$$

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 lie in L^2.

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

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

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

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

From Hoeffding decomposition to Sobol indices

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

$$1 = \frac{\mathrm{Var}\left(\mathbb{E}[Y|V_{\mathbf{u}}]\right)}{\mathrm{Var}(Y)} + \frac{\mathrm{Var}\left(\mathbb{E}[Y|V_{\sim\mathbf{u}}]\right)}{\mathrm{Var}(Y)} + \frac{\mathrm{Var}(IA)}{\mathrm{Var}(Y)}$$

$$:= S^{\mathbf{u}} + S^{\sim\mathbf{u}} + S^{\mathbf{u},\sim\mathbf{u}} \qquad \Rightarrow \quad \text{Sobol indices}$$

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

while $S^{\mathbf{u}} + S^{\mathbf{u},\sim\mathbf{u}}$ *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

$$\left(S^1, S^2, S^3, S^{1,2}\right) = (1/2, 0, 0, 1/2).$$

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 $V^{\mathbf{u}}=\left(V_1,V_2,V_3',V_4',V_5'\right)$.

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

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

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* $(X_j, Y_j)_{j=1,\dots,n}$ *of the pair* (X, Y).

Our estimator

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

$$T_{n,\text{oracle}} = \frac{1}{n}\sum_{i=1}^{n}(2Y_i - m(X_i))m(X_i).$$

• 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 theorem.

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

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,

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

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

For kernel density estimation, bias is (multivariate Taylor)

$$Bias = \mathbb{E}[\widehat{f}(x)] - f(x) = \sum_{1 \leqslant |\beta| < \nu} \frac{h^{|\beta|}}{\beta\,!} \frac{\partial^\beta f}{\partial x^\beta}(x) \kappa_{1,\beta}(k)$$

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

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

☞ f ($=$ density of X in the sequel) with sufficient regularity.

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

For kernel density estimation, bias is (multivariate Taylor)

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

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

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 ? (III)

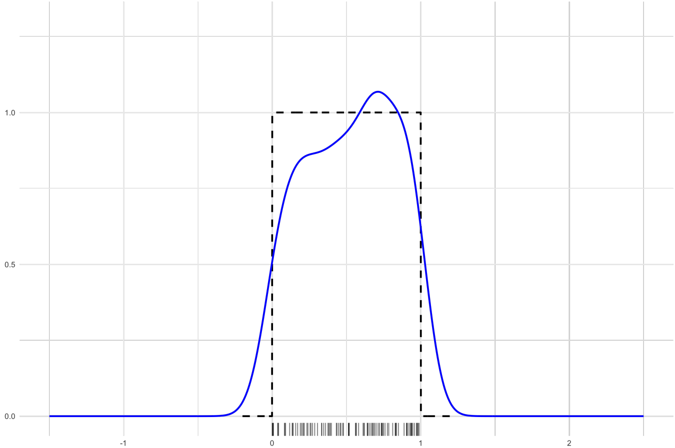
By analysing the variance (skipped here), with a high-order kernel, we finally get

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

☞ kernel with high enough order.

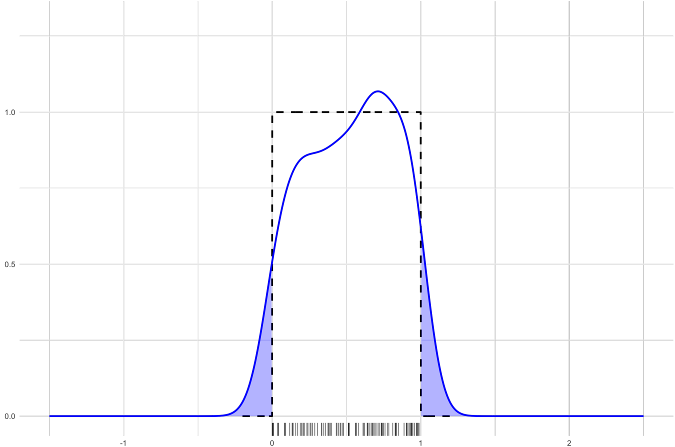
KDE boundary issues (I)

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



KDE boundary issues (II)

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



A partial solution

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

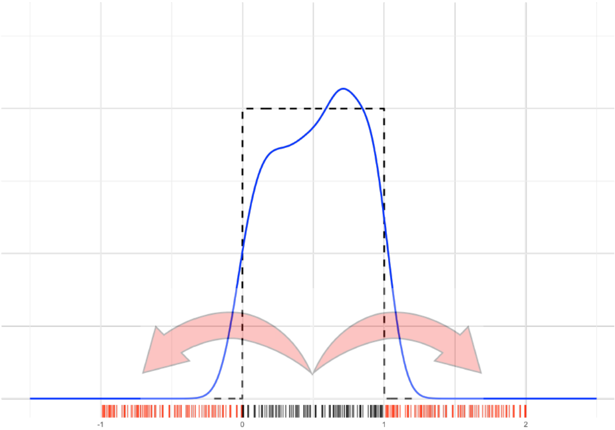
$$T^{\text{trunc},\varepsilon} = \mathbb{E}[\mathbb{E}[Y|X]^2 \mathbb{1}_{X\in(\varepsilon,1-\varepsilon)^d}].$$

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.

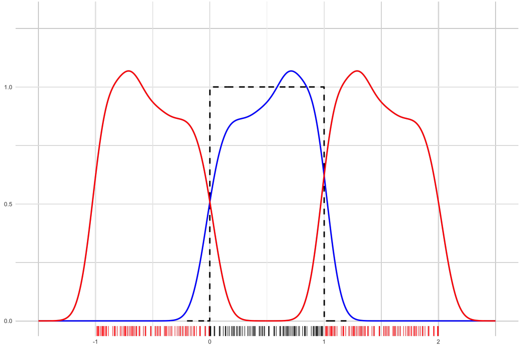
Second ingredient : mirror transformation (I)

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



Second ingredient : mirror transformation (II)

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

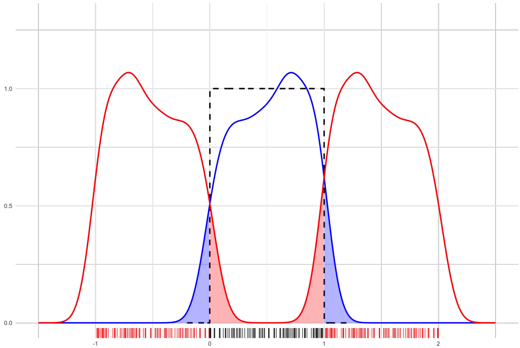


$\widehat{f}_{\text{lower}}(x) = \frac{1}{nh}\sum_{i=1}^{n} k\left(\frac{x-(-X_i)}{h}\right)$

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

Second ingredient : mirror transformation (III)

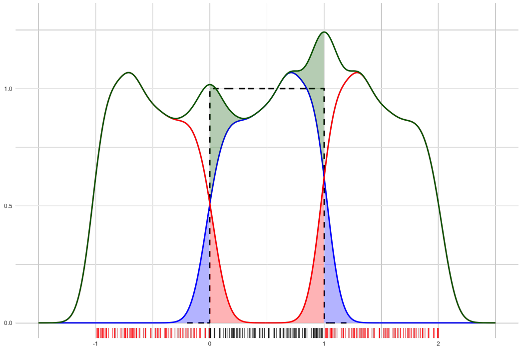
$$\widehat{f}(x) = \frac{1}{nh}\sum_{i=1}^{n} k\left(\frac{x - X_i}{h}\right) \quad \text{and} \quad \int_{-\infty}^{\infty} \widehat{f}(x) = 1$$



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

Second ingredient : mirror transformation (IV)

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

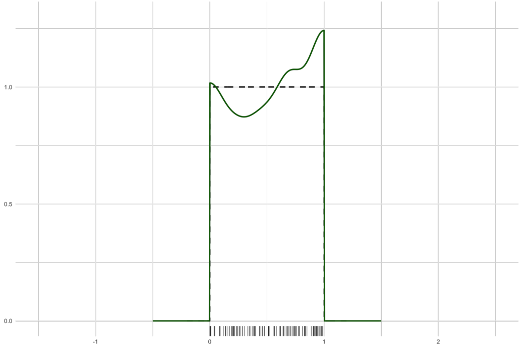


$$\widehat{f}_{\text{lower}}(x) = \frac{1}{nh}\sum_{i=1}^{n} k\left(\frac{x-(-X_i)}{h}\right)$$

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

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 :

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

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

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

and its leave-one-out version :

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

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 - $k : [-1,1] \to \mathbb{R}$ 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

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

- 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).

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`.

Using the delta method, we are now able to get the asymptotic behaviour of the estimation of S^X, letting

$$\widehat{S}_{n,h_n} = \frac{\widehat{T}_{n,h_n} - \left(\frac{1}{n}\sum_{j=1}^n Y_j\right)^2}{\frac{1}{n}\sum_{j=1}^n Y_j^2 - \left(\frac{1}{n}\sum_{j=1}^n Y_j\right)^2}.$$

Corollary (CLT & AE for the estimation of the Sobol' indices)

Under all the assumptions of the theorem, one has (i)

$$\sqrt{n}\left(\widehat{S}_{n,h_n} - S^X\right) \xrightarrow[n\to\infty]{\mathscr{L}} \mathcal{N}(0,\sigma^2),$$

where the limit variance σ^2 has an explicit expression.

(ii) $\widehat{S}_{n,h_n}$ is asymptotically efficient to estimate S^X from an i.i.d. sample $(X_i, Y_i)_{i=1,\cdots,n}$ of the pair (X, Y).

Let us denote S^i the first-order Sobol index associated to the i-th input and its estimator $\widehat{S}^i$ given by :

$$\widehat{S}^i_{n,h_n} = \frac{\widehat{T}^i_{n,h_n} - \left(\frac{1}{n}\sum_{j=1}^n Y_j\right)^2}{\frac{1}{n}\sum_{j=1}^n Y_j^2 - \left(\frac{1}{n}\sum_{j=1}^n Y_j\right)^2}.$$

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

Under all the assumptions of the theorem, one has

$$\sqrt{n}\Big((\widehat{S}^1_{n,h_n},\ldots,\widehat{S}^p_{n,h_n})^T - (S^1,\ldots,S^p)^T\Big) \xrightarrow[n\to\infty]{\mathscr{D}} \mathscr{N}(0,\Sigma),$$

where the limit variance Σ has an explicit expression. Furthermore, such estimation is asymptotically efficient.

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
- Two main ingredients
- Our efficient mirrored high-order kernel-based estimate
- Main results

Sketch of the proofs

Numerical applications
- The Bratley function
- The g-Sobol function

Sketch of the proof : CLT

Following the same lines as in the proof of Theorem 2.1 in Doksum (1995), we aim at proving that

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

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.

Sketch of the proof : asymptotic efficiency

The influence efficient function of ψ at P, as stated in Doksum (1995), is given by (see Klein (2024) for the details) :

$$\widetilde{\psi}_P(x,y) = (2y - m(x))m(x) - \mathbb{E}[Ym(X)].$$

Moreover, we deduce from (1) that

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

and conclude using Condition (25.22) of Van der Vaart (2000).

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Numerical applications
The Bratley function
The g-Sobol function

For all test cases :

- first-order and total-order 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.

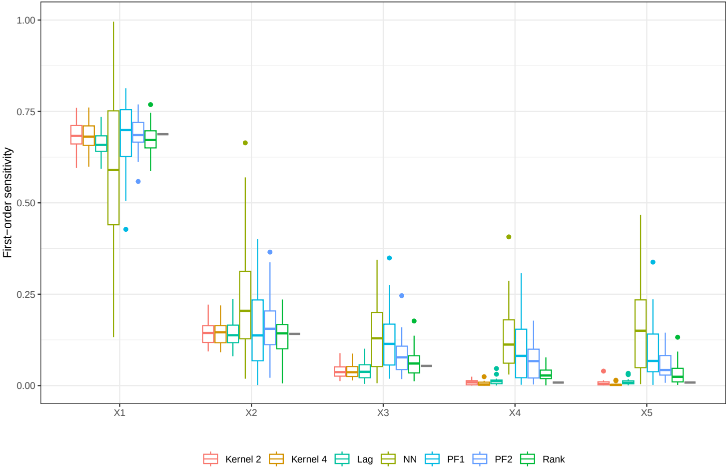
The Bratley function

First, we consider the Bratley function defined by :

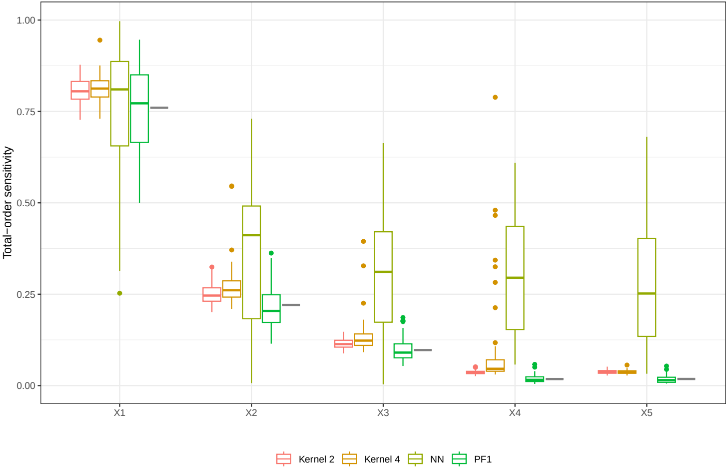
$$g_{\text{Bratley}}(V_1,\ldots,V_p) = \sum_{i=1}^{p} (-1)^i \prod_{j=1}^{i} V_j,$$

with $V_i \sim \mathscr{U}([0,1])$ i.i.d. and $p = 5$.

The Bratley function - first-order indices - $n = 500$



The Bratley function - total-order indices - $n = 500$



The g-Sobol function

We investigate the g-Sobol function defined by

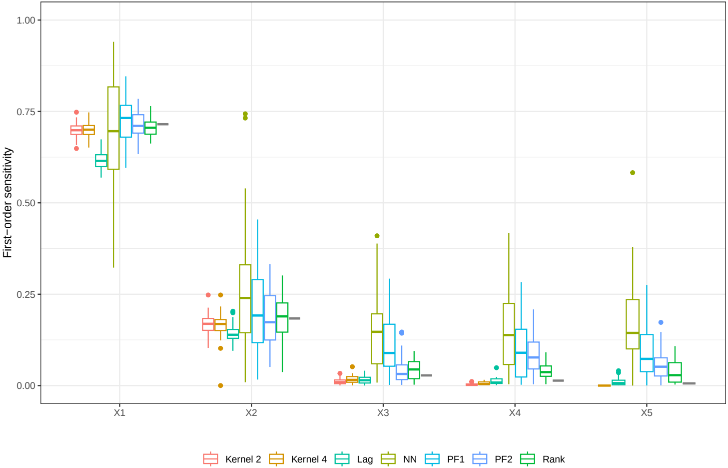
$$g_{\text{g-Sobol}}(V_1,\dots,V_p) = \prod_{i=1}^{p} \frac{|4V_i - 2| + a_i}{1 + a_i},$$

with $V_i \sim \mathscr{U}([0,1])$ i.i.d., $p = 5$ and $a = (0,1,4.5,9,99)$.

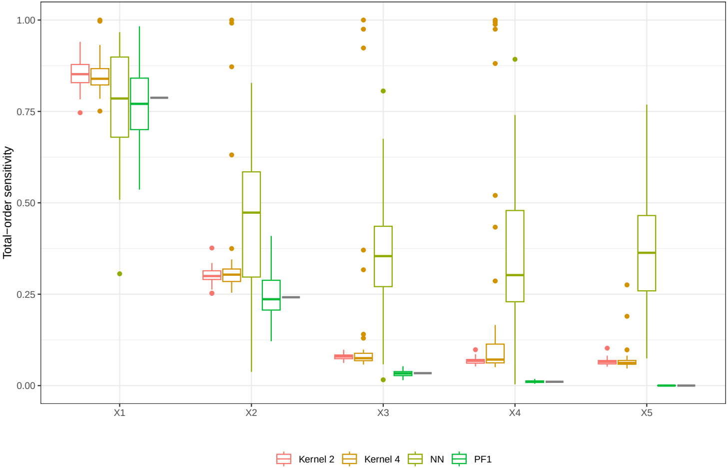
Notice that it is non-differentiable at any input value with a component equal to 0.5, but the impact on our estimator performance is negligible for first-order indices.

Except for the degraded performance of the lag estimator, the conclusions are the same as for the Bratley function, even for total indices.

The g-Sobol function - first-order indices - $n = 500$



The g-Sobol function - total-order 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.

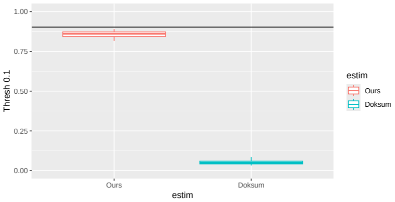
We consider Example 3.2 from Doksum and Samarov (1995) :

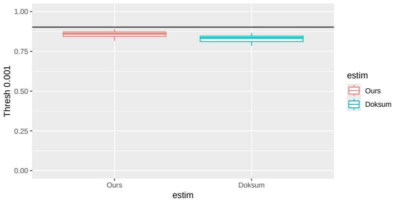
$$Y = \frac{1}{2} + 4X_1 + 4(X_2 - \frac{1}{2})^2 + 4X_3^{1/2} + \tau e,$$

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 $\epsilon = 10^{-1}$ and 10^{-3}.

Tuning of parameter ϵ





When ϵ is equal to 10^{-3}, the performance of both estimators are similar. However when $\epsilon = 10^{-1}$, 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 with respect to this parameter limits its practical use.

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.”. Available on Hal and Arxiv (2024).
https://hal.science/hal-04052837v2.

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Efficient influence function and asymptotic efficiency

Let $\mathscr{P}$ be the set of absolutely continuous probability distributions on $[0,1]^d \times \mathbb{R}$ and $P_0 \in \mathscr{P}$ be the probability distribution of (X, Y), such that we can write our target $T = \psi(P_0)$ where $\psi : \mathscr{P} \to \mathbb{R}$.

If ψ is differentiable at all $P \in \mathscr{P}$, the efficient influence function $\widetilde{\psi}_P : [0,1]^d \times \mathbb{R} \to \mathbb{R}$ is the gradient with smallest variance among all gradients of ψ at P with zero mean w.r.t. to P.

The link with efficient estimators is the following : a sequence of estimators T_n of $T = \psi(P_0)$ is asymptotically efficient iif

$$T_n - T = T_n - \psi(P_0) = \frac{1}{n}\sum_{i=1}^{n} \widetilde{\psi}_{P_0}(X_i, Y_i) + o_{P_0}\left(\frac{1}{\sqrt{n}}\right),$$

See Eq.(25.22) in van der Vaart (2000).

Efficient influence function and asymptotic efficiency

In our case, the efficient influence function at any $P \in \mathscr{P}$ writes

$$\widetilde{\psi}_P(x,y) = (2y - m(x))m(x) - \psi(P).$$

where m is the regression function under P : $m(x) = \mathbb{E}_P[Y|X=x]$, see Klein, Lagnoux, Rochet (2024).

Then, if m under P_0 is known, taking

$$T_{n,oracle} = \frac{1}{n}\sum_{i=1}^{n}(2Y_i - m(X_i))m(X_i)$$

leads to an asymptotically efficient estimator of T.

Plug-in estimation

A first point of view consists in seeing

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

as a plug-in version of

$$T_{n,oracle} = \frac{1}{n}\sum_{i=1}^{n}(2Y_i - m(X_i))m(X_i)$$

where the difference $m - \widehat{m}_n$ needs to be controlled to still have

$$\widehat{T}_n = \psi(P_0) + \frac{1}{n}\sum_{i=1}^{n}\widetilde{\psi}_{P_0}(X_i, Y_i) + o_{P_0}\Big(\frac{1}{\sqrt{n}}\Big).$$

One-step estimation

A second point of view relies on one-step estimators, that consider a first-order bias correction of an initial estimator $\psi(\widehat{P})$ where $\widehat{P}$ is a smoothed estimate of P_0.

More precisely, a simple Taylor expansion of $\psi(P_0)$ around $\psi(\widehat{P})$ involves the efficient influence function $\widetilde{\psi}$ at $\widehat{P}$:

$$\psi(P_0) - \psi(\widehat{P}) = \mathbb{E}_{P_0}[\widetilde{\psi}_{\widehat{P}}] - \overbrace{\mathbb{E}_{\widehat{P}}[\widetilde{\psi}_{\widehat{P}}]}^{=0} + r_2(\widehat{P}, P) = \mathbb{E}_{P_0}[\widetilde{\psi}_{\widehat{P}}] + r_2(\widehat{P}, P)$$

since by definition, $\mathbb{E}_P[\widetilde{\psi}_P] = 0$ for all P. Thus, if $r_2(\widehat{P}, P) = o(1)$,

$$\psi(\widehat{P}) + \mathbb{E}_{P_0}[\widetilde{\psi}_{\widehat{P}}] \sim \psi(P_0).$$

One-step estimation

Thus it is possible to improve $\psi(\widehat{P})$ by considering an estimate of this first-order bias $\mathbb{E}_{P_0}[\widetilde{\psi}_{\widehat{P}}]$: for instance, $\mathbb{E}_{P_n}[\widetilde{\psi}_{\widehat{P}}]$ where P_n is the empirical distribution of the observations $(X_i, Y_i)_{i=1,\ldots,n}$.

In our particular case, this induces an estimator given by

$$\widehat{T}_n = \psi(\widehat{P}) + \mathbb{E}_{P_n}[\widetilde{\psi}_{\widehat{P}}] = \frac{1}{n}\sum_{i=1}^{n}(2Y_i - \widehat{m}(X_i))\widehat{m}(X_i)$$

where $\widehat{m}$ is the regression function under $\widehat{P}$, that is precisely a smoothing estimate of m. We can then hope that $\widehat{T}_n$ will be asymptotically efficient if the difference $\widehat{P} - P_0$ converges to 0 at an appropriate rate.

Construction of high-order kernels

The kernel k is typically chosen as a symmetric second-order kernel (Epanechnikov, Gaussian, ...) with the following properties :

$$\int k(u)du = 1, \quad \int uk(u)du = 0, \quad \int u^2 k(u) > 0.$$

The terminology second-order refers to the fact that the first non-zero moment of k is the second one (except for the zero-th order one which ensures the kernel is normalized).

Construction of high-order kernels

More generally, a high-order kernel of order r satisfies

$$\int k(u)du = 1, \quad \int u^j k(u)du = 0, \ \forall j = 1, \ldots, r-1, \quad \int u^r k(u) > 0.$$

Here, we will focus on high-order kernels with compact support, which are used together with mirror-type transformations to avoid boundary effects appearing when the domain is compact.

In particular, we will study symmetric kernels on $[-1,1]$ and non-symmetric ones on $[0,1]$.

Construction of high-order kernels

In order to build a kernel of order r with compact support $[-1,1]$, there are at least two approaches, which are described below.

Legendre orthonormal polynomials. The first construction relies on the (normalized) Legendre orthonormal polynomials on $[-1,1]$ denoted by $\{P_m(\cdot)\}_{m\in\mathbb{N}}$. Then we define the kernel k as

$$k(u) = \sum_{m=0}^{r+1} P_m(0) P_m(u) \mathbb{1}_{u\in[-1,1]}, \tag{2}$$

see Comte (2017).

Construction of high-order kernels

High-order Epanechnikov kernel. Hansen (2005) proposes a high-order generalization of smooth and second-order kernels on $[-1,1]$ including the uniform, biweight, and Epanechnikov ones. Focusing on the latter, the kernel

$$k(u) = B_r(u) k_e(u) \tag{3}$$

where $k_e(u) = \frac{3}{4}(1-u^2)\mathbb{1}_{u \in [-1,1]}$ and

$$B_r(u) = \frac{\left(\frac{3}{2}\right)_{r/2-1}\left(\frac{5}{2}\right)_{r/2-1}}{(2)_{r/2-1}} \sum_{k=0}^{r/2-1} \frac{(-1)^k \left(\frac{r+3}{2}\right)_k u^{2k}}{k!(r/2-1-k)!\left(\frac{3}{2}\right)_k}$$

is of order r for odd r where $(x)_a$ is the Pochhammer's symbol.

Construction of high-order kernels

As for kernels with compact support $[0,1]$, the two following methods can be envisioned.

Shifted Legendre orthonormal polynomials. Similarly to the first construction above, we can also consider the shifted Legendre orthonormal polynomials on $[0,1]$, denoted by $\{Q_m(\cdot)\}_{m\in\mathbb{N}}$, leading to

$$k(u) = 2\sum_{m=0}^{r+1} Q_m(0)Q_m(u)\mathbb{1}_{u\in[0,1]}. \tag{4}$$

Construction

Dilatation. Another approach, due to Kerkyacharian (2001), relies on dilatations of an integrable function $g : \mathbb{R} \to \mathbb{R}$:

$$k(u) = \sum_{k=1}^{r} \binom{r}{k} (-1)^{k+1} \frac{1}{k} g\left(\frac{u}{k}\right). \tag{5}$$

If g has support $[a, b]$, then k has support $[a, rb]$ and is of order r.

To obtain a kernel with support $[0, 1]$, one can for example take a shifted Epanechnikov kernel k_{shift} on $[0, 1/r]$:

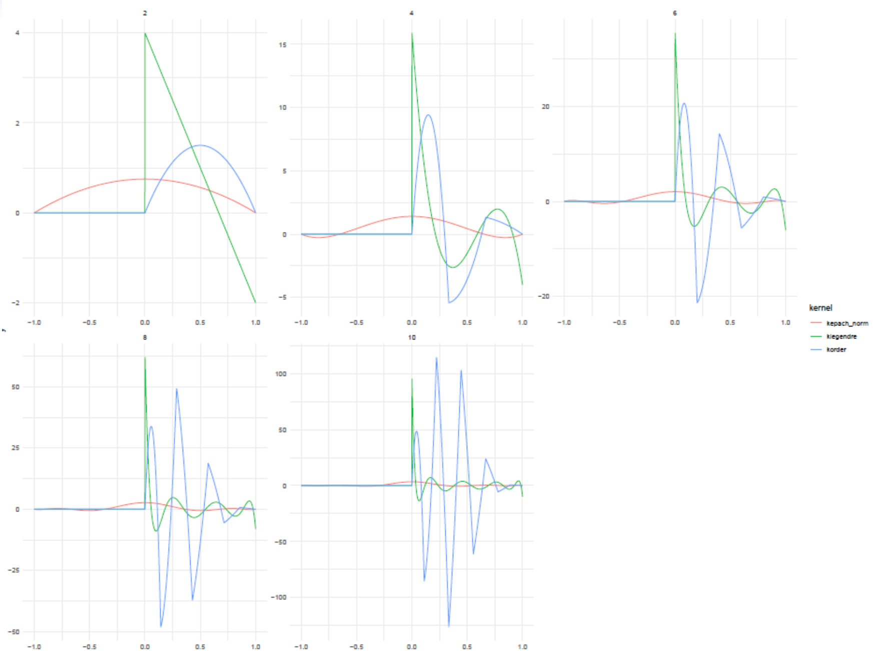
$$k_{\mathrm{shift}}(u) = 6u(1 - ru)r^2 \mathbb{1}_{u \in [0,1/r]}.$$

Numerical stability - Kernel values versus order

In what follows, we investigate numerically the high-order kernels introduced above.

Since kernels in (2) and (4) are identical up to a shift, we only focus on kernels as defined in (3) for $[-1,1]$ and (4) and (5) for $[0,1]$.

They are coded below, note that they all take as input a parameter h which corresponds to the kernel bandwidth.


2
4
6
8
10
kernel
kepach_norm
klegendre
korder

Numerical stability - Kernel values versus order

It appears clearly that non-symmetric kernels with support $[0,1]$ exhibit large variations which increase with the order, as opposed to the symmetric kernel on $[-1,1]$. This implies that numerical instabilities when computing estimators are to be expected, as illustrated below on a simple regression case.

Regression with mirror transformations

Now we consider a standard regression setting : we have access to a n-sample (X_i, Y_i) for $i = 1, \ldots, n$ with

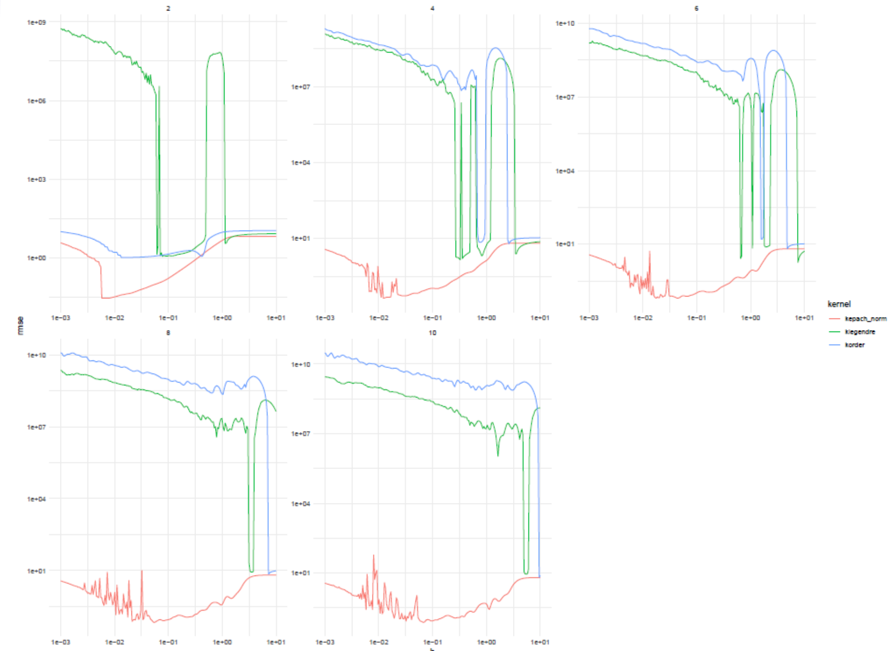
$$Y_i = m(X_i) + \epsilon_i$$

where the X_i's are i.i.d. r.v. on $[0,1]$ and ϵ_i is a centred noise.

We consider regression estimators denoted by $\widehat{m}^1$ on $[0,1]$ and $\widehat{m}^2$ on $[-1,1]$ and the Bratley function.

The only parameter which needs to be tuned is the bandwidth h.

We consider a grid of evenly-spaced values on a logarithmic scale and compute the leave-one-out mean square error for each of them.


2
4
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rmse
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kernel
kepach_norm
klegendre
korder

Regression with mirror transformations

We clearly see a very high numerical instability for the first estimator with kernels supported on $[0,1]$, even on a simple regression example in dimension 1.