Sobol pick freeze (and FAST) methods in the Costa BRAVA sauce

Fabrice Gamboa

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SAMO Nice

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Special thanks

- COSTA BRAVA researchers
- Nice University and Organizers of Nice SAMO Conference
- Very special thanks
  - → French SA Guru : B. Iooss

  - → One of the most famous french designer : L. Pronzato

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Agenda

Overview

Costa Brava project

- Mathematical Statistics with Industrial Partners
  - → Industrial partners : CEA, IFP
  - → Academic partners : LJK, IMT
- Object of study and problematics
  - → High dimensional complicated regression models modeling a computer code $F(X)$ (X is a d-dimensional vector)
  - → Tell things on F by only using a small sample $(X_i, F(X_i))$

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What are we dealing with ?

Big computer codes= F **black box**

$$Y = F(X)$$

- Code inputs : X high dimension object (vectors or curves).
- Code outputs Y (scalar, vectorial, functional, ...).

X complex structure and/or uncertain

$\Rightarrow$ **seen as random**

STOCHASTIC APPROACH

Questions mainly addressed on the general model

- **Sensitivity analysis=**
  what coordinates of $\mathbb{X}$ have most effects on $\mathbb{F}$?
  - $\rightarrow$ Model Reduction
  - $\rightarrow$ Comprehensive analysis of the model

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Preamble

Hoeffding-Antoniadis-Efron & Morris- Sobol decomposition-FANOVA

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- **The Arnold Principle :** If a notion bears a personal name, then this name is not the name of the inventor.
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Hoeffding decomposition in a nutshell : ideal 2d-ANOVA

Ideal ANOVA $d = 2$

- $F(X^1, X^2)$ scalar response depending on discrete factors X^1, X^2,
- $X^1 \in \{1, \cdots, l_1\}$ $X^2 \in \{1, \cdots, l_2\}$

If one have at hand all $F(i_1, i_2)$ $\forall (i_1, i_2) \in \{1, \cdots, l_1\} \times \{1, \cdots, l_2\}$
Then unique *orthogonal decomposition*

$$F(X^1, X^2) = F_\emptyset + F_1(X^1) + F_2(X^2) + F_{1,2}(X^1, X^2)$$

$$F_\emptyset = \frac{1}{l_1 l_2} \sum_{i_1, i_2} F(i_1, i_2)$$

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Hoeffding decomposition : easy example ideal 2d-ANOVA

Ideal ANOVA $d = 2$

- $F(X^1, X^2)$ depending on independent random factors X^1, X^2,
- X^1 uniform on $\{1, \cdots, l_1\}$, X^2 uniform on $\in \{1, \cdots, l_2\}$

Stochastic decomposition

Then unique L^2 *orthogonal decomposition*

$$F(X^1, X^2) = F_\emptyset + F_1(X^1) + F_2(X^2) + F_{1,2}(X^1, X^2)$$

$$F_\emptyset = \mathbb{E}(F(X))$$

$$F_1(X^1) = \mathbb{E}(F(X)|X^1) - F_\emptyset$$

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Classical Hoeffding decomposition

Functional ANOVA : pioneering works of Antoniadis (1984) and Sobol (1990) (F square integrable)

X =independent components (component may be anything : scalar, vector, curve...) $X \sim \bigotimes_{i=1}^{d} \mathbb{P}_{X_i}$

Theorem (decomposition in $L^2(\bigotimes_{i=1}^{d} \mathbb{P}_{X_i})$)

F *may be written in an unique way as a sum of uncorrelated terms :*

$$F(X) = \sum_{A \subset \{1,\dots,d\}} F_A(X^A).$$

Here, $X^A := (X^i, i \in A)$. *Hence,*

$$\mathit{Var}\, F(X) = \sum_{A \subset \{1,\dots,d\}} \mathit{Var}\, F_A(X^A).$$

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Classical Hoeffding decomposition

Functional ANOVA : pioneering works of Antoniadis (1984) and Sobol (1990) (F square integrable)
$\rightarrow$ X has independent components (component may be anything : scalar, vector, curve...)

Theorem

F *may be written in an unique way as a sum of uncorrelated terms :*

$$F(X) = \sum_{A \subset \{1,\dots,d\}} F_A(X^A).$$

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example : $d = 2$

$$F(X^1, X^2) = F_\emptyset + F_1(X^1) + F_2(X^2) + F_{1,2}(X^1, X^2)$$

$$F_\emptyset = \mathbb{E}(F(X)), \quad F_i(X^i) = \mathbb{E}(F(X)|X^i) - F_\emptyset$$

$$\begin{aligned} F_{1,2}(X^1, X^2) &= F(X^1, X^2) - [F_\emptyset + F_1(X^1) + F_2(X^2)] \\ &= F(X^1, X^2) - \mathbb{E}(F(X)|X^1) - \mathbb{E}(F(X)|X^2) + \mathbb{E}(F(X)). \end{aligned}$$

Othogonality

$$\begin{aligned} \mathbb{E}[F_{1,2}(X^1, X^2)F_1(X^1)] &= \mathbb{E}[F_{1,2}(X^1, X^2)F_2(X^2)] = \mathbb{E}[F_{1,2}(X^1, X^2)] = 0 \\ \mathbb{E}[F_1(X^1)F_2(X^2)] &= \mathbb{E}[F_1(X^1)] = \mathbb{E}[F_2(X^2)] = 0 \end{aligned}$$

Overview

Definition and intuition beyond

Important assumption X has independent components (component may be anything)

→Want to know the most influent components (having most effects on F)

Sobol indices of first order

$$S_i := \frac{\mathrm{Var}(\mathbb{E}[F(X)|X_i])}{\mathrm{Var}F(X)} = \frac{\mathrm{Var}F_i(X^i)}{\mathrm{Var}F(X)}$$

Sobol total indices

$$S_i^{\mathrm{tot}} := 1 - \frac{\mathrm{Var}(\mathbb{E}[F(X)|X^{\sim i}])}{\mathrm{Var}F(X)} = \sum_{A \subset \{1,\cdots,d\}: i \in A} \frac{\mathrm{Var}F_A(X^A)}{\mathrm{Var}F(X)}$$

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Statistical problems

$Y = F(X)$, $X_1, \cdots X_N$ some *sample* of X and $Y_1, \cdots X_N$ at hand

- Give estimators of S_i and S_i^{tot},
- Develop mathematical tools to quantify accuracy of estimators (limit Theorem, confidence regions...)
- Build *optimal* estimation procedures.

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A crucial question : Sampling

- How we should sample the system $Y = F(X)$?
- Completely random ?
- Structured random ?
- Ergodic ?

- Here in our discussion :
- Completely random : $X_1, \dots, X_N$ I.I.D.
- Structured random : Sobol Pick Freeze method
  $\to X_1, \dots, X_N, F(X_1), \dots, F(X_N)$,
  $\to \tilde{X}_1, \dots, \tilde{X}_N$. $\tilde{X} = (X^i, X'^{,\sim i})$. $X'^{,\sim i}$ independent copy of $X^{\sim i}$.
- Ergodic : FAST. Use of Weyl Theorem
  $\to X_1, \dots, X_N, X_j := (R_{\alpha_1}(X^1_{j-1}), R_{\alpha_2}(X^2_{j-1}), \cdots, R_{\alpha_d}(X^d_{j-1}))$

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A crucial question : Sampling

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Frame I.I.D. Sample

- X scalar components
- $Y = F(X)$, $X_1, \cdots X_N$ independent copies of X and $Y_1, \cdots X_N$ at hand
- Assume that (X, Y) has a smooth probability density $g(x, y)$

$$Y = r_i(X^i) + \varepsilon_i$$

- $r_i(X^i) := \mathbb{E}[F(X)|X^i] = F_i(X^i) + \mathbb{E}[F(X)]$ and $\varepsilon_i := F(X) - \mathbb{E}[F(X)|X^i] - \mathbb{E}[F(X)]$
- We have

$$r_i(x) = \frac{\int yg(x,y)dy}{\int g(x,y)dy} \quad S_i = \frac{\text{Var } r_i(X^i)}{\text{Var } Y} = 1 - \frac{\text{Var } \varepsilon_i}{\text{Var } Y} = 1 - \frac{\mathbb{E}[\mathbb{E}(\varepsilon_i^2|X^i)]}{\text{Var } Y}$$

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Plugging approach

- Plugging approach developped in S. Daveiga, F. Wahl and FG Technometrics, 2009
- Plugging estimators based on nonparametric estimates of $r_i(x)$ or of $\mathbb{E}(\varepsilon_i^2|X^i = x)$ (local polynomial) and a second sample $X_1, \cdots, X_{N'}$

$$\widehat{S}_i = \frac{\mathrm{Var}_{N'} \widehat{r}_i(X^i)}{\mathrm{Var}_{N'} Y}$$

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Efficient estimation of non linear functional

S. Daveiga and FG Journal of nonparametric statistics 2013
One wish to estimate

$$\text{Var}\,(\mathbb{E}(Y|X^i)) = \mathbb{E}(\mathbb{E}(Y|X^i)^2) - (\mathbb{E}(Y))^2.$$

One wish to estimate

$$T(g) = \mathbb{E}(\mathbb{E}(Y|X^i)^2) = \int\int \left(\frac{\int y\ g(x,y)dy}{\int g(x,y)dy} \right)^2\ g(x,y)dxdy.$$

We follow a method developed by B. Laurent in Annals of Stats 1996 : expansion of $T(g)$ around a preliminary estimator $\hat{g}$ and optimal estimation of a quadratic functional

Expansion of $T(g)$

$$
\begin{aligned}
T(g) = & \int\int \left[2y\widehat{r}_i(x) - \widehat{r}_i(x)^2\right] g(x,y)dxdy \\
+ & \int\int\int \frac{1}{\left(\int \hat{g}(x,y)dy\right)} \left[yz + \widehat{r}_i(x)^2 - (y+z)\widehat{r}_i(x)\right] g(x,y)g(x,z)dxdydz \\
+ & \Gamma_n \\
= & \int\int H(\hat{g},x,y)g(x,y)dxdy + \int\int\int K(\hat{g},x,y,z)g(x,y)g(x,z)dxdydz \\
+ & \Gamma_n
\end{aligned}
$$

Here

$$
\begin{aligned}
H(\hat{g},x,y) &= 2y\widehat{r}_i(x) - \widehat{r}_i(x)^2 \\
K(\hat{g},x,y,z) &= \frac{1}{\left(\int \hat{g}(x,y)dy\right)} \left[yz + \widehat{r}_i(x)^2 - (y+z)\widehat{r}_i(x)\right].
\end{aligned}
$$

$$\widehat{T(g)} == \int\int H(\hat{g}, x, y)\widehat{g(x, y)}dxdy + \int\int\int K(\hat{g}, x, y, z)\widehat{g(x, y)g}(x, z)dxdydz$$

Theorem

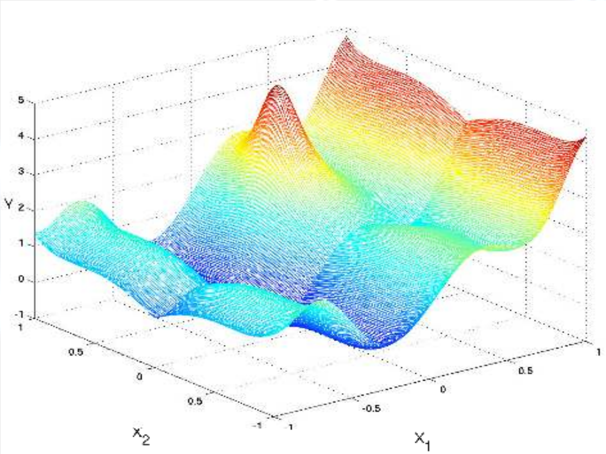
$\widehat{T(g)}$ *is convergent and asymptotically Gaussian. Its asymptotic variance is*

$$C(f) = 4\mathbb{E}\left(\mathit{Var}(Y|X^i)\mathbb{E}(Y|X^i)^2\right) + \mathit{Var}\ \left(\mathbb{E}(Y|X^i)^2\right).$$

This is the optimal variance (semiparametric efficiency ! !)

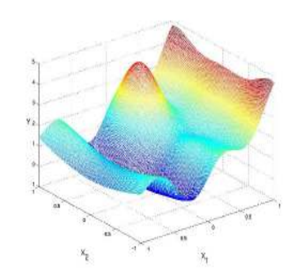
Analytical example

$$
\begin{aligned}
Y \quad = \quad & 0.2\exp(X^1-3)+2.2|X^2|+1.3(X^2)^6-2(X^2)^2-0.5(X^2)^4-0.5(X^1)^4 \\
& +2.5(X^1)^2+0.7(X^1)^3+\frac{3}{(8X^1-2)^2+(5X^2-3)^2+1}+\sin(5X^1)\cos(3(X^1)^2)
\end{aligned}
$$

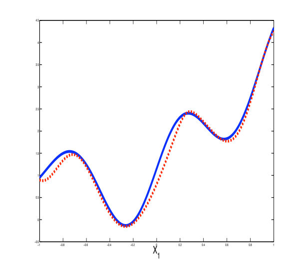


Kriging (theoretical curve, approximation)

$F(X^1, X^2)$



$\mathbb{E}(Y|X^1)$



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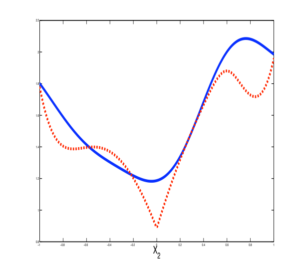
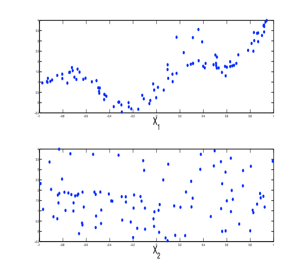


Local polynomial (theoretical curve, approximation)

Marginal samples



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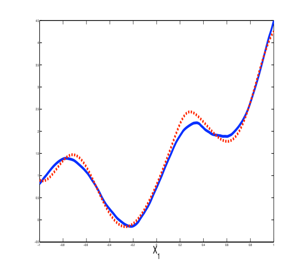

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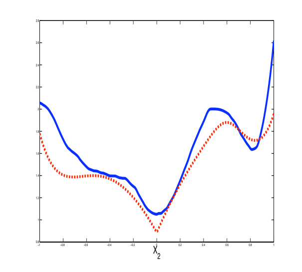

Analytical example

		Kriging	Loc poly	Eff. est
		100 pts	100 pts	100 pts
$\mathrm{Var}(\mathbb{E}(Y\mid X^1))$	1.0932	1.0539	1.0643	1.1701
$\mathrm{Var}(\mathbb{E}(Y\mid X^2))$	0.0729	0.1121	0.0527	0.0939

X^1 : quite identical results

X^2 : *marginal approximations* are better

Sobol Pick freeze sampling scheme

- $X_1, \ldots, X_N, F(X_1), \ldots, F(X_N),$
- $\tilde{X}_1, \ldots, \tilde{X}_N \; F(\tilde{X}_1), \ldots, F(\tilde{X}_N)$. With $\tilde{X} = (X^i, X'^{,\sim i})$. $X'^{,\sim i}$ is an independent copy of $X^{\sim i}$.

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Why this sampling scheme ?

Intuition beyond. Example d=2

- In hand : $((X^1_1, X^2_N), \cdots, (X^1_N, X^2_N))$ and $((X^1_1, X'^2_N), \cdots, (X^1_N, X'^{,2}_N))$
- Hoeffding decomposition

  $\rightarrow F(X^1, X^2) = F_\emptyset + F_1(X^1) + F_2(X^2) + F_{1,2}(X^1, X^2)$

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- Obviously

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Continuation Obviously

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Sobol pick freeze estimator of S_i

$$S_i = \frac{\mathrm{Cov}(F(X), F(\tilde{X}))}{\mathrm{Var}\left(\frac{F(X)+F(\tilde{X})}{\sqrt{2}}\right)}$$

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Further results : sharp asymptotic

Theorem (F. G, A. Janon, T. Klein, A. Lagnoux, C. Prieur Arxiv (2013))

$\widehat{S}_i$ satisfies both exponential inequalities and a Berry-Esseen Theorem .

- Exponential inequality $\mathbb{P}(|\widehat{S}_i - S_i| \geqslant t) \leqslant \exp(-N\psi(t)), \ \psi(t) > 0.$
- Berry-Esseen Theorem : precise bound on the error made when using CLT.

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Concentration inequalities for $\hat{S}_i$

Proposition

Let $\mathbb{P} = \mu_1 \otimes \ldots \otimes \mu_N$ *be a proability measure on the cartesian product* $\chi = \chi_1 \times \ldots \times \chi_N$ *of metric spaces* (χ_i, d_i) *with finite diameters* D_i*,* $i = 1 \ldots N$*, equipped with the* l^1*-metric* $d = \sum_{i=1}^{N} d_i$*. Then if* G *is a 1-Lipschitz function on* (X, d)*, for every* $r \geqslant 0$*,*

$$\mathbb{P}\left(G \geqslant \int G\,dP + r\right) \leqslant \exp\{-\frac{r^2}{2D^2}\}$$

where $D^2 = \sum_{i=1}^{N} D_i^2$*.*

see M. Ledoux, *The concentration of measure phenomenon*,**Mathematical Surveys and Monographs**, Vol 89, 2001.

Concentration inequalities for $\widehat{S}_i$

We consider

- $\chi_i = [-1,1] \times [-1,1]$ (bounded input variables) equipped with the metric d_i defined by
$$d_i(z, z') := \|x - x'\|_2 + \|y - y'\|_2$$
for $z = (x, y)$, $z' = (x', y') \in X_i$, and $x, x', y, y' \in [-1, 1]$.
- $F/L : X \to \mathbb{R}$ 1-Lipschitz where $L := \frac{2}{N}(S_i + t + 1)$ and
$$F(x, y) = \frac{1}{N}\sum_{i=1}^{N}\left(x_i y_i - (S_i + t)\frac{x_i^2 + y_i^2}{2}\right) + \frac{S_i + t - 1}{2}\overline{x + y}_N.$$
- $r = \frac{V}{L}\left(t - \frac{1}{2N}(S_i + t - 1)(S_i + 1)\right)$.

Then
$$\mathbb{P}\left(\left|\widehat{S}_i - S_i\right| \geqslant t\right) \leqslant 2\exp\left\{-\frac{NV^2}{2}\left(\frac{t - \frac{1}{2N}(S_i + t - 1)(S_i + 1)}{8(S_i + t + 1)}\right)^2\right\}.$$

Concentration inequalities for $\widehat{S}_i$

We consider

- $\chi_i = [-1, 1] \times [-1, 1]$ (bounded input variables) equipped with the metric d_i defined by
$$d_i(z, z') := \|x - x'\|_2 + \|y - y'\|_2$$
for $z = (x, y)$, $z' = (x', y') \in X_i$, and $x, x', y, y' \in [-1, 1]$.
- $F/L : X \to \mathbb{R}$ 1-Lipschitz where $L := \frac{2}{N}(S_i + t + 1)$ and
$$F(x, y) = \frac{1}{N} \sum_{i=1}^{N} \left(x_i y_i - (S_i + t) \frac{x_i^2 + y_i^2}{2} \right) + \frac{S_i + t - 1}{2} \overline{x + y}_N .$$
- $r = \frac{V}{L} \left(t - \frac{1}{2N}(S_i + t - 1)(S_i + 1) \right)$.

Then
$$\mathbb{P}\left(\left| \widehat{S}_i - S_i \right| \geqslant t \right) \leqslant 2 \exp \left\{ -\frac{NV^2}{2} \left(\frac{t - \frac{1}{2N}(S_i + t - 1)(S_i + 1)}{8(S_i + t + 1)} \right)^2 \right\} .$$

S_i being unknown, we are looking for a bound independent of S_i which is given in the following corollary

Corollary

Since $0 \leqslant S_i \leqslant 1$,

$$\mathbb{P}\left(\left|\widehat{S}_i - S_i\right| \geqslant t\right) \leqslant 2\exp\left\{-\frac{N}{128d}\left(1-\frac{1}{N}\right)^2\left(\frac{t}{t+2}\sum_{l=1}^{d} v_l\right)^2\right\}.$$

As a consequence, let t and an error α be fixed, one has

$$\mathbb{P}\left(\left|\widehat{S}_i - S_i\right| \geqslant t\right) \leqslant \alpha \iff 2N \geqslant \beta + 2 + \sqrt{\beta(\beta+4)}$$

where $\beta := 128d\log\left(\frac{2}{\alpha}\right)\left(\frac{t}{t+2}\sum_{l=1}^{k} v_l\right)^{-2}$.

Quality at a fixed N - Berry-Esseen results

First result **(Using Pineli's Theorem)** : Assume that the random variable Y has finite moments up to order 6 and $k = 1$. Then, for all $z \in \mathbb{R}$,

$$\left| \mathbb{P}\left(\frac{\sqrt{N}}{\sigma} \left[\widehat{S}_i - S_i \right] \leqslant z \right) - \Phi(z) \right| \leqslant \frac{\kappa}{\sqrt{N}} .$$

Here σ^2 is the asymptotic variance of $\sqrt{N}\widehat{S}_i$ and κ a generic constant.

Second result

Here assume $\mathbb{E}(Y) = 0$ and let $\widehat{S}_i = \frac{\frac{1}{N}\sum F(X_j)F(\tilde{X}_j)}{\frac{1}{N}\sum F(X_j)}$.
Assume that the random variable $F(X)$ has finite moment up to order 6.
Then, for all $t \in \mathbb{R}$,

$$\left| \mathbb{P}\left(\frac{\sqrt{N}}{\sigma}(\widehat{S}_i - S_i) \leqslant t \right) - \Phi(t) \right| \leqslant \frac{\kappa \mu_{3,N}}{\sqrt{N}} + \left| \Phi(t) - \Phi\left(\frac{t}{\sqrt{1 + \frac{t\nu_N}{\sigma\sqrt{N}V^2}}} \right) \right|.$$

- σ^2 is the asymptotic variance
- Φ the Gaussian cdf
- $\mu_{3,N}$ is a third order deviation moment
- ν_N is a bias term

Numerical applications for the centered case

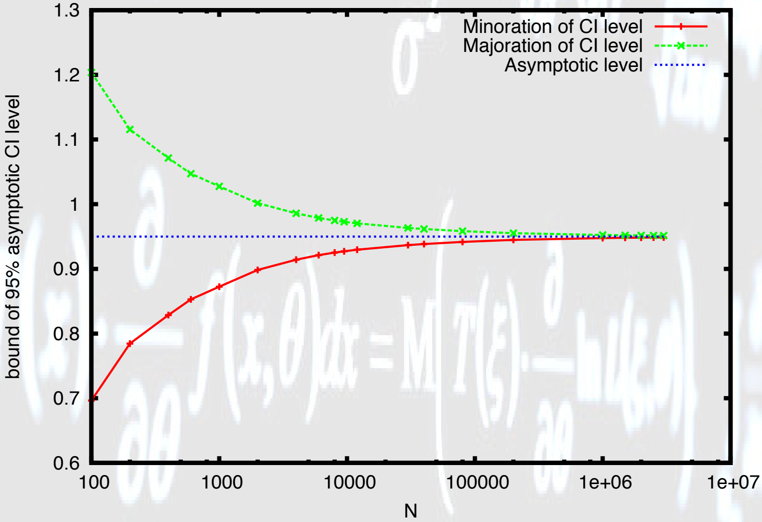
We study the Ishigami function recentered by its true mean $7/2$ defined by

$$F(X_1, X_2, X_3) = \sin X_1 + 7\sin^2 X_2 + 0.1 X_3^4 \sin X_1 - \frac{7}{2}.$$

For y, we choose $y = 1.96\frac{\widehat{\sigma^2}}{\sqrt{N}}$, where $\widehat{\sigma^2}$ is an empirical estimate of σ^2, so as to compute (estimators of) upper and lower bounds of the actual level of the 95%-level confidence interval.

We present the numerical results, as functions of N, and for $i = 1$ in the following figure (for $i = 2$ or $i = 3$), the results are very similar.

Numerical applications for the centered case



Euclidean and Hilbert extensions

Theorem (F. G, A. Janon, T. Klein, A. Lagnoux CRAS (2013))

- *Sobol indice may be generalized in an Euclidean and Hilbertian context, imposing isometric invariance*
- *Pick freeze method has Euclidean and Hilbertian extensions ($\mathbb{F}$ is vectorial or functional valued). Furthermore, the extended estimate has also many very nice properties of that obtained in the scalar case.*

- $F(X) \in \mathbb{H}$. $\mathbb{H}$ being Euclidean or Hilbert space ($\mathbb{R}^k$, L^2, ...)
- Hoeffding still holds (one dimensional by duality)

$$F(X) = \sum_{A \subset \{1,\ldots,d\}} F_A(X^A), \quad F_A(X^A) \in \mathbb{H}$$

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$$S_i := \frac{\mathrm{Tr}[\mathrm{Var}\, F_A(X^A)]}{\mathrm{Tr}[\,\mathrm{Var}\, F(X)]}$$

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Very nice work using Weyl Theorem and harmonic analysis

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Hoeffding decomposition revisited

Functional ANOVA : case of dependent inputs (pioneering works : Stone-Hooker)

→Assume that X has a lower/upper bounded density with respect to the product of its marginals

Theorem (G. Chasaing, F. G, C. Prieur Electronic Journal of Statistics(2013))

F *may be written in an unique way as a sum :*

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Where, X^A *is uncorellated with* X^B *as soon as* $A \subset B$.

example : $d = 2$

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Overview

Conclusion

Costa Brava a Winner winner game between Applied researchers and Academic statisticians

This is the end

CAM ON

Thank you

Gracias

MERCI

Obrigado

Grazie