Sobol sensitivity analysis
Recent statistical result overview
Kick and follow for network construction

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CARTABLE

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Special thanks

- My collaborators in sensitivity analysis: G. Chastaing, S. Da Veiga, B. Iooss, A. Janon, T. Klein, A. Lagnoux, P. Lemaitre, M. Nodet, A.L. Popelin, C. Prieur
- INRA and Organizers of CARTABLE Conference for the invitation

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Overview

1 Sensitivity analysis: the Costa Brava consortium

2 Hoeffding decomposition

3 Sobol indices

4 Hoeffding decomposition revisited

5 Openness to other problems

6 End

7 Bibliography

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- Mathematical Statistics with Industrial Partners-Project ended 2013
  - → 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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Hoeffding-Antoniadis-Efron & Morris- Sobol decomposition-FANOVA

From Barry Simon: CMV matrices: Five years after (2007)

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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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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:*

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

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

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

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

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

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2. Hoeffding decomposition
3. Sobol indices
4. Hoeffding decomposition revisited
5. Openness to other problems
6. End
7. Bibliography

Definition and intuition beyond

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

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

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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

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

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Plugging approach

- Plugging approach developped in S. Da Veiga, F. Wahl and FG Technometrics, [3]
- 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. Da Veiga and FG Journal of nonparametric statistics [2]
One wish to estimate

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

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 [11]: expansion of $T(g)$ around a preliminary estimator $\hat{g}$ and optimal estimation of a quadratic functional

Expansion of $T(g)$

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

$$
\begin{aligned}
&= \iint H(\hat{g},x,y)g(x,y)dxdy + \iiint K(\hat{g},x,y,z)g(x,y)g(x,z)dxdydz \\
&+ \Gamma_n
\end{aligned}
$$

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

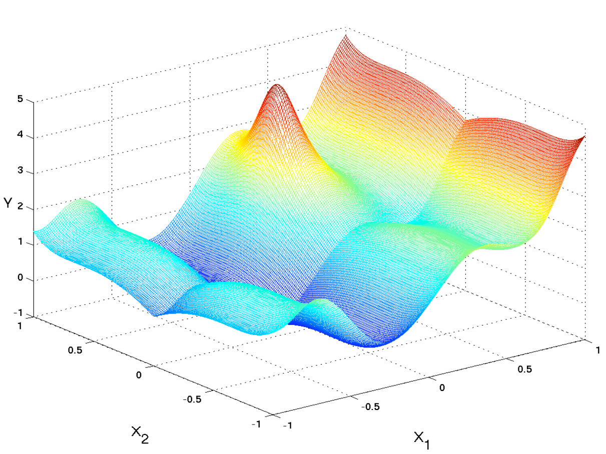
$\widehat{T(g)}$ *is convergent and asymptotically Gaussian. Its asymptotic variance is*

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

This is the optimal variance (semiparametric efficiency!!)

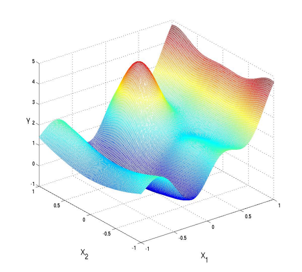
Analytical example

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

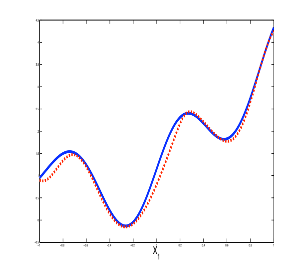


Kriging (theoretical curve, approximation)

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



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



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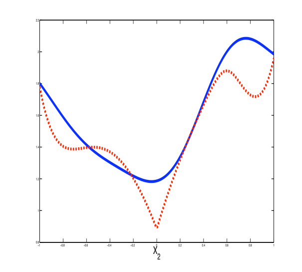
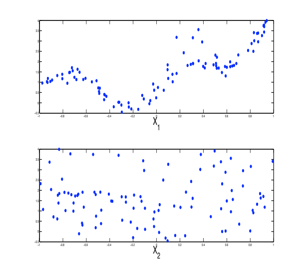


Local polynomial (theoretical curve, approximation)

Marginal samples



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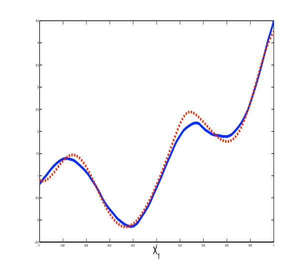

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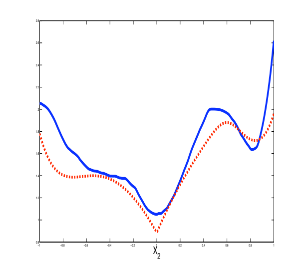

Analytical example

		Kriging	Loc poly	Eff. est
		100 pts	100 pts	100 pts
$\mathrm{Var}(\mathbb{E}(Y\|X^1))$	1.0932	1.0539	1.0643	1.1701
$\mathrm{Var}(\mathbb{E}(Y\|X^2))$	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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$$\text{Cov}\,(F_{1,2}(X^1, X^2)), F_{1,2}(X^1, X'^{,2})) =$$
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Continuation Obviously

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Sobol pick freeze estimator of S_i

$$S_i = \frac{\text{Cov}(F(X), F(\tilde{X}))}{\frac{\text{Var}[F(X)]+\text{Var}[F(\tilde{X})]}{2}}$$

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Further results: sharp asymptotic

Theorem (F. G, A. Janon, T. Klein, A. Lagnoux, C. Prieur Statistics [5])

$\widehat{S}_i$ 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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Euclidean and Hilbert extensions

Theorem (F. G, A. Janon, T. Klein, A. Lagnoux EJS [6])

- *Sobol indice may be generalized in an Euclidean and Hilbertian context, imposing isometric invariance*
- *Pick freeze method has Euclidean and Hilbertian extensions (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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Theorem (F. G, A. Janon, T. Klein, A. Lagnoux EJS [6])

- *Sobol indice may be generalized in an Euclidean and Hilbertian context, imposing isometric invariance*
- *Pick freeze method has Euclidean and Hilbertian extensions (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)

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Euclidean and Hilbert extensions-Continuation

- Hoeffding still holds (one dimensional by duality)

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

- Set $\mathrm{Var}(\langle u, Z \rangle) = \langle u, (\mathrm{Var}\, Z) u \rangle$. Z is a L^2 r.v. in $\mathbb{H}$ and $u \in \mathbb{H}$

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

- Isometric invariance+ sum to 1 again!! $1 = \sum_{A \subset \{1,\ldots,d\}} S_A$
- Indices first discussed in M. Lamboni, H. Monod, and D. Makowski RESS [10]

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A very fast journey on FAST

Very nice work using Weyl Theorem and harmonic analysis

- $X_1, \ldots, X_N$, $X_j := (R_{\alpha_1}(X^1_{j-1}), R_{\alpha_2}(X^2_{j-1}), \cdots, R_{\alpha_d}(X^d_{j-1}))$
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1. Sensitivity analysis: the Costa Brava consortium
2. Hoeffding decomposition
3. Sobol indices
4. Hoeffding decomposition revisited
5. Openness to other problems
6. End
7. Bibliography

Hoeffding decomposition revisited

Functional ANOVA: case of dependent inputs (Hooker [7])

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

Theorem (G. Chasaing, F. G, C. Prieur EJS [1])

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

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

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

example: $d = 2$

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

$$F_\emptyset \perp F_i, \;\; F_{1,2} \perp F_i, \;\; F_{1,2} \perp F_\emptyset$$

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

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Openness to other problems

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  - → Following: I. Sobol, S. Kucherenko Maths and Computers in Simulation (Gaussian and uniform cases)[12]
  - → Make use of world expertise of *Institut de Mathématiques de Toulouse* on functional inequalities
  - → Bound on Sobol global index by using Poincaré inequality
- From variance to Cramér von Mises distance (F. G, A. Lagnoux, T. Klein Arxiv [4])
  - → Hoeffding decomposition of $\mathbf{1}_{\{F(X)\leqslant t\}}$
  - → Cramér von Mises distance between the laws of $F(X)$ and $F(X)$ knowing X_j
  - → Normalized indices and Pick Freeze algorithm
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Kick and follow for network construction

- Y a response variable. X a vector of explicative variables
- Does the value of Y depends on the coinfluence of X_i and X_j?
- Compute an estimate of the order two Sobol index S_{ij}
- Threshold this estimate to build a network (if $\widehat{S}_{ij} > c$ draw an edge between i and j)

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This is the end

CAM ON

Thank you

Gracias

MERCI

Obrigado

Grazie

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