Modélisation statistique pour données fonctionnelles : approches non-asymptotiques et méthodes adaptatives.

Angelina Roche
thèse effectuée sous la direction d'Elodie Brunel et André Mas

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Institut de Mathématiques et de Modélisation de Montpellier
UNIVERSITÉ MONTPELLIER 2
SCIENCES ET TECHNIQUES
ECOLE DOCTORALE I2S

Statistical framework

- **Aim:** study the link between two random variables.
  - $Y \in \mathbb{R}$ a variable of interest.
  - $X \in \mathbb{H}$ an explanative (functional) variable, with $(\mathbb{H}, \langle ., . \rangle, \|.\|)$ a separable Hilbert space.

    Typically $\mathbb{H} = L^2([a,b])$, $\mathbb{H} =$ a Sobolev space...

- **Observations**: $(X_i, Y_i)_{i \in \{1,\dots,n\}}$ a sample following the same distribution as (X, Y).

Models and problems considered

- **Functional linear model**: $Y = \langle \beta, X \rangle + \varepsilon$,
  with $\beta \in \mathbb{H}$ and ε a noise term, centred, independent of X, with finite variance.

- **Model without structural constraint**

- ***Nonparametric* regression** : $Y = m(X) + \varepsilon$,
  with $m : \mathbb{H} \to \mathbb{R}$ a function and ε a noise term.

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- **Model without structural constraint**

  Estimation of the conditional cumulative distribution function

$$\begin{array}{rcl} F : \mathbb{H} \times \mathbb{R} & \longrightarrow & \mathbb{R} \\ (x, y) & \mapsto & F^x(y) = \mathbb{P}\left(Y \leq y | X = x\right). \end{array}$$

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  Minimisation of the conditional expectation :

$$x^* = \arg\min_{x \in \mathcal{C}} \{m(x)\}.$$

Outline

1. Prediction in the functional linear model
   - Estimation procedure
   - Theoretical results
   - Simulation results
2. Adaptive estimation of the conditional c.d.f
   - Bias-variance decomposition of the risk
   - Bandwidth selection device
   - Optimal estimation in the minimax sense
   - Simulation study
3. Response surface methodology for functional data
   - Response surface methodology
   - Extension to the functional setting

Outline

Functional linear model

We suppose that

$$Y = \langle \beta, X \rangle + \varepsilon, \tag{1}$$

with

- X a centred random variable with values in a separable Hilbert space $(\mathbb{H}, \langle \cdot, \cdot \rangle, \| \cdot \|)$ with infinite dimension;
- β, the slope function: an unknown element of $\mathbb{H}$;
- ε a noise term, centred, independent of X and with **unknown** variance σ^2.

Aim: estimate the slope function β using the information of the sample $\{(X_i, Y_i), i = 1, \ldots, n\}$ following (1).

Covariance operator

Multiplying the model equation $Y = \langle \beta, X \rangle + \varepsilon$ by $X(s)$ and taking expectation we obtain

$$\begin{array}{ccc} \mathbb{E}[YX] & = & \mathbb{E}[\langle \beta, X \rangle X] \\ \shortparallel & & \shortparallel \\ g \in \mathbb{H} & = & \Gamma \beta \end{array}$$

where

$$\Gamma : f \in \mathbb{H} \mapsto \mathbb{E}[\langle X, f \rangle X]$$

is the covariance operator associated to X.

- Γ positive compact self-adjoint
  $\Rightarrow$ basis $(\psi_j)_{j\geq 1}$ of eigenfunctions
  $(\lambda_j)_{j\geq 1}$ associated eigenvalues, non-increasing sequence.
- $\lambda_j \searrow 0 \Rightarrow$ ill-posed inverse problem.
- For identifiability, we suppose that

$$\mathrm{Ker}(\Gamma) = \{0\} \Leftrightarrow \lambda_j > 0 \text{ for all } j.$$

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Risk considered

Definition

The prediction error of an estimator $\widehat{\beta}$ is the quantity

$$\mathbb{E}\left[\left(\widehat{Y}_{n+1} - \mathbb{E}\left[Y_{n+1}|X_{n+1}\right]\right)^2 |(X_1, Y_1), \ldots, (X_n, Y_n)\right]$$

$$= \mathbb{E}\left[\langle \widehat{\beta} - \beta, X_{n+1}\rangle^2 |(X_1, Y_1), \ldots, (X_n, Y_n)\right]$$

$$= \langle \Gamma(\widehat{\beta} - \beta), \widehat{\beta} - \beta\rangle =: \|\widehat{\beta} - \beta\|_\Gamma^2$$

with

- (X_{n+1}, Y_{n+1}) a copy of (X, Y) independent of the sample;
- $\widehat{Y}_{n+1}$ the prediction of Y_{n+1} with the estimator $\widehat{\beta}$:

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Short overview of existing work

- **Estimation by projection or by roughness regularization**.
  On fixed basis : Fourier , B-splines, general o.n.b...
  On data-driven basis : functional PCA.
- **Numerous results with asymptotic point of view:** Cardot, Ferraty and Sarda (1999), Cai and Hall (2006), Hall and Horowitz (2007),...

  ... but very few non-asymptotic results : Cardot and Johannes (2010, lower bounds on general $\mathbb{L}^2$-risks), Comte and Johannes (2010, 2012; adaptive estimators).
- **Comte and Johannes (2010, 2012):**
  - $\rightarrow$ projection estimators on fixed basis;
  - $\rightarrow$ oracle-type inequalities for general weighted $\mathbb{L}^2$ norms without including the prediction error;
  - $\rightarrow$ minimax convergence rates.

Goal: define an adaptive estimator by projection on the PCA basis.

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Outline

fPCA

functional Principal Components Regression

Aim:

Define an approximation space S_m of dimension D_m minimising the mean distance between X and its projection on S_m.

$$S_m = \text{Vect}\{\psi_1, \dots, \psi_{D_m}\}$$

By induction:

$$\psi_{k+1} \in \arg\min_{f \in \mathbb{H}} \mathbb{E}\left[\|X - \Pi_k X - \langle X, f\rangle f\|^2\right],$$

under the constraint $\langle \psi_{k+1}, \psi_j\rangle = 0$, for all $j \le k$ et $\|\psi_{k+1}\| = 1$ (Π_k: projector $\text{Vect}\{\psi_1, \dots, \psi_k\}$).

The family $(\psi_j)_{j\ge1}$ is a o.n.b of $\mathbb{H}$ of eigenfunctions of the covariance operator

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Least-squares estimators

Case 1: the basis $(\psi_j)_{j\geq 1}$ is known

$$\widehat{\beta}_m^{(KB)} = \arg\min_{f\in S_m}\gamma_n(f),$$

with $S_m = \text{span}\{\psi_1, \ldots, \psi_{D_m}\}$,

where $(\psi_j)_{j\geq 1}$ are the eigenfunctions of the covariance operator

$$\Gamma : f \in \mathbb{H} \mapsto \mathbb{E}\left[\langle f, X\rangle X\right].$$

Case 2: the basis $(\psi_j)_{j\geq 1}$ is unknown

$$\widehat{\beta}_m^{(FPCR)} = \arg\min_{f\in \widehat{S_m}}\gamma_n(f),$$

with $\widehat{S_m} = \text{span}\{\widehat{\psi}_1, \ldots, \widehat{\psi}_{D_m}\}$,

where $(\widehat{\psi}_j)_{j\geq 1}$ are the eigenfunction of the empirical covariance operator

$$\Gamma_n : f \in \mathbb{H} \mapsto \frac{1}{n}\sum_{i=1}^{n}\langle f, X_i\rangle X_i.$$

- $\gamma_n : f \mapsto \frac{1}{n}\sum_{i=1}^{n}\left(Y_i - \langle f, X_i\rangle\right)^2$ is the *least-squares contrast*.
- $(D_m)_{m\geq 1}$ is a strictly increasing sequence such that $D_1 \geq 1$ (e.g. $D_m = m$ or $D_m = 2m+1$).

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Dimension selection (I)

Problem:

How to choose the dimension D_m ?

Best dimension for prediction error:

D_{m^*} with

$$m^* \in \arg\min_{m=1,\ldots,N_n} \mathbb{E}\left[\left\|\widehat{\beta}_m^{(FPCR)} - \beta\right\|_\Gamma^2\right]$$

$\to$ unknown in practice !!!

$\widehat{\beta}_{m^*}^{(FPCR)}$ is the best estimator it is possible to select in the family $\left\{\widehat{\beta}_m, m = 1, \ldots, N_n\right\}$. We call it *oracle*.

Dimension selection (II)

Bias-variance decomposition of the risk

$$\mathbb{E}\left[\left\|\widehat{\beta}_m^{(FPCR)} - \beta\right\|_\Gamma^2\right] = \mathbb{E}\left[\left\|\widehat{\Pi}_m\beta - \beta\right\|_\Gamma^2\right] + \mathbb{E}\left[\left\|\widehat{\beta}_m^{(FPCR)} - \widehat{\Pi}_m\beta\right\|_\Gamma^2\right],$$

where $\hat{\Pi}_m\beta$ is the orthogonal projection on $\text{span}\{\widehat{\psi}_1, \ldots, \widehat{\psi}_{D_m}\}$.

Approximation error $\leftrightsquigarrow$ bias term:

- decreases with the dimension D_m;
- order unknown in practice (depends on the regularity of β).

Estimation error $\leftrightsquigarrow$ variance term: $\simeq \sigma^2 \frac{D_m}{n}$ $\quad$ σ^2: noise variance

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Dimension selection (III)

Dimension selection criterion

We select

$$\widehat{m} \in \arg\min_{m=1,\dots,N_n} \left\{ \gamma_n\big(\widehat{\beta}_m^{(FPCR)}\big) + \kappa \widehat{\sigma}_m^2 \frac{D_m}{n} \right\}$$

with

$$\widehat{\sigma}_m^2 := \frac{1}{n}\sum_{i=1}^{n}\left(Y_i - \langle \widehat{\beta}_m^{(FPCR)}, X_i\rangle\right)^2 = \gamma_n\big(\widehat{\beta}_m^{(FPCR)}\big)$$

an estimator of the noise variance σ^2.

Outline

Assumptions

- **Assumption on the noise:** there exists $p > 4$, such that $\mathbb{E}[\varepsilon^p] < +\infty$.
- **Assumption on the target function β:** there exists $r, R > 0$ such that

$$\beta \in \mathcal{W}_r^R := \left\{ f \in \mathbb{H}, \sum_{j\geq 1} j^r < f, \psi_j >^2 \leq R^2 \right\}$$

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- **Assumptions on the process X:**
  - **on the principal components scores:**
    - $\sup_{j\geq 1} \mathbb{E}\left[\frac{\langle X, \psi_j\rangle^{2\ell}}{\lambda_j^\ell}\right] \leq \ell! b^{\ell-1}$, for all $\ell \geq 1$
    - For all $j \neq k$, $\langle X, \psi_j\rangle$ is independent of $\langle X, \psi_k\rangle$.

    $\rightarrow$ Verified for all Gaussian processes
  - **on the eigenvalues of Γ:**
    - $\lambda_1 > \lambda_2 > \dots$
    - $cj^{-a} \leq \lambda_j \leq Cj^{-a}$ with $a > 1$, $c, C > 0$ (polynomial decrease) or $ce^{-j^a} \leq \lambda_j \leq Ce^{-j^a}$, $a, c, C > 0$ (exponential decrease).
    - There exists a constant $\gamma > 0$ such that $(j\lambda_j \max\{\ln^{1+\gamma}(j), 1\})_{j\geq 1}$ is decreasing.

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Oracle inequality and rates

Theorem

Under the previous assumptions and if $a + r/2 > 2$ (for the polynomial decrease),

$$\mathbb{E}\left[\left\|\widehat{\beta}_{\widehat{m}}^{(FPCR)} - \beta\right\|_{\Gamma}^{2}\right] \leq C_1 \min_{m=1,\dots,N_n}\left\{\mathbb{E}\left[\left\|\widehat{\Pi}_m\beta - \beta\right\|_{\Gamma}^{2}\right] + \kappa\sigma^2\frac{D_m}{n}\right\} + \frac{C_2}{n},$$

where $C_1, C_2 > 0$ are independent of n and β and $\widehat{\Pi}_m$ is the orthogonal projector onto $\widehat{S}_m$.

Rates of convergence

	Polynomial decrease $cj^{-a} \leq \lambda_j \leq Cj^{-a}$	Exponential decrease $ce^{-j^a} \leq \lambda_j \leq Ce^{-j^a}$
$\sup_{\beta\in\mathcal{W}_r^R}\mathbb{E}\left[\left\|\widehat{\beta}_{\widehat{m}}^{(FPCR)} - \beta\right\|_{\Gamma}^{2}\right]$	$\leq Cn^{-(a+r)/(a+r+1)}$	$\leq Cn^{-1}(\ln(n))^{1/a}$

→ coincides with the lower-bounds established by Cardot and Johannes (2010).

→ The estimator is optimal in the minimax sense

Oracle inequality and rates

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→ The estimator is optimal in the minimax sense

Outline

Simulation of X

$$X = \sum_{j=1}^{100} \sqrt{\lambda_j} \xi_j \psi_j,$$

with $\xi_1, ..., \xi_{100}$ independent realizations of $\mathcal{N}(0,1)$ and $\psi_j(x) = \sqrt{2}\sin(\pi(j-0.5)x)$.

$\lambda_j = j^{-2}$ $\quad\quad$ $\lambda_j = j^{-3}$ $\quad\quad$ $\lambda_j = e^{-j}$

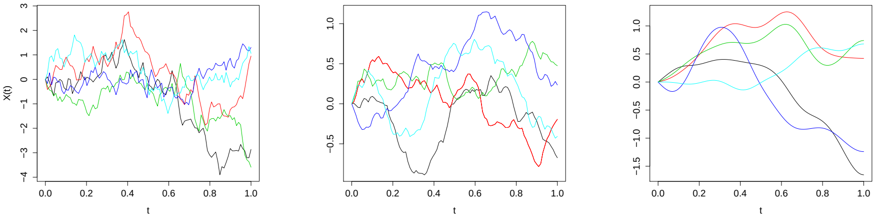
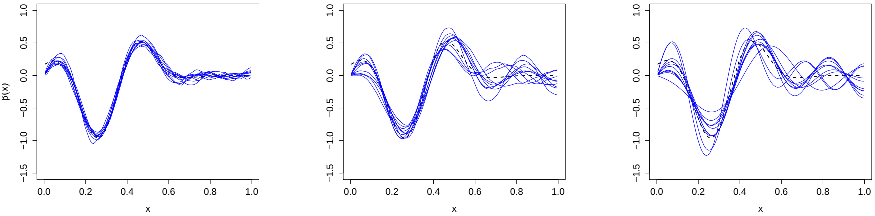


Figure: Sample of 5 random curves

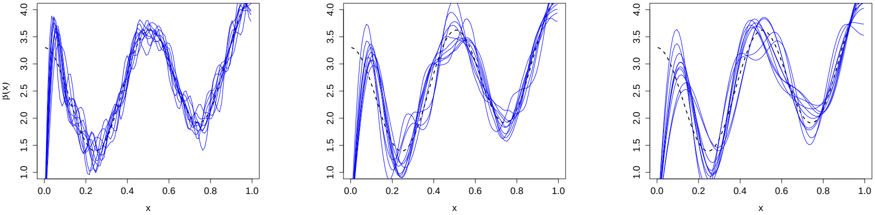
$\beta_1(t) = \exp\left(-(t-0.3)^2/0.05\right)\cos(4\pi t)$, $n = 1000$

$\lambda_j = j^{-2}$ $\qquad$ $\lambda_j = j^{-3}$ $\qquad$ $\lambda_j = \exp(-j)$



$\beta_2(t) = \ln(15t^2 + 10) + \cos(4\pi t)$, $n = 1000$

$\lambda_j = j^{-2}$ $\qquad$ $\lambda_j = j^{-3}$ $\qquad$ $\lambda_j = \exp(-j)$



Comparison with cross-validation

We compare our selection criterion with other methods:

- Cross validation:

$$\widehat{m}^{CV} := \arg\min_{m=1,\dots,N_n} \frac{1}{n}\sum_{i=1}^{n}\left(Y_i - \widehat{Y}_i^{(m,-i)}\right)^2,$$

  where $\widehat{Y}_i^{(m,-i)}$ is the prediction of Y made from the sample $\{(X_j, Y_j), j \neq i\}$.

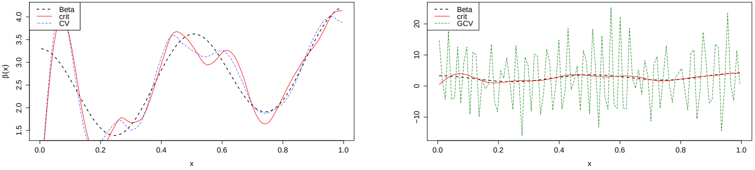
- Generalized cross-validation:

$$\widehat{m}^{GCV} := \arg\min_{m=1,\dots,N_n} \frac{\gamma_n(\widehat{\beta}_m)}{\left(1 - \frac{\mathrm{tr}(H_m)}{n}\right)^2},$$

  where $\widehat{Y}_i^{(m)} := \langle \widehat{\beta}_m, X_i \rangle$ (prediction of Y) and H_m is the Hat matrix defined by $\widehat{\mathbf{Y}}^{(m)} = H_m \mathbf{Y}$;

Comparison with cross-validation

Estimation of β_1



Estimation of β_2

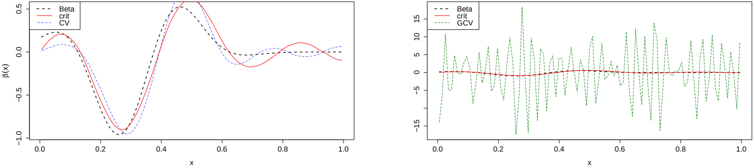


Figure: Left: comparison of estimators $\hat{\beta}_m$ when m is selected by minimization of the penalized criterion or the CV criterion. Right: comparison with the GCV criterion. $n = 2000$, $\lambda_j = j^{-3}$.

Comparison with cross-validation

Comparison of risks

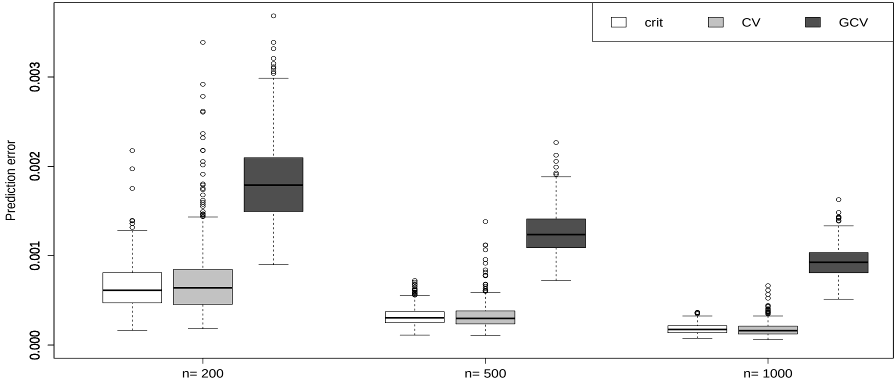


Figure: Boxplot of prediction errors calculated from 500 independent samples. Estimation of β_1, $\lambda_j = j^{-3}$.

Comparison with cross-validation

Ratio to the oracle

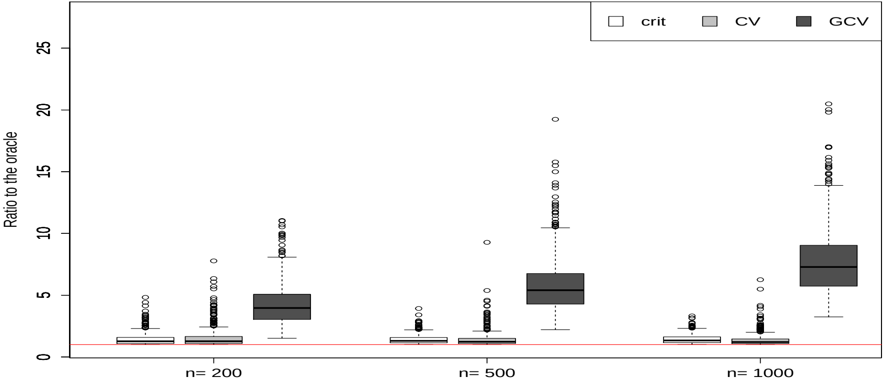


Figure: Ratio $\|\widehat{\beta}_{\widehat{m}} - \beta\|_\Gamma^2 / \|\widehat{\beta}_{m^*} - \beta\|_\Gamma^2$ where $\|\widehat{\beta}_{m^*} - \beta\|_\Gamma^2 = \min_{1,\dots,N_n} \left\{ \|\widehat{\beta}_m - \beta\|_\Gamma^2 \right\}$.
Estimation of β_1, $\lambda_j = j^{-3}$.

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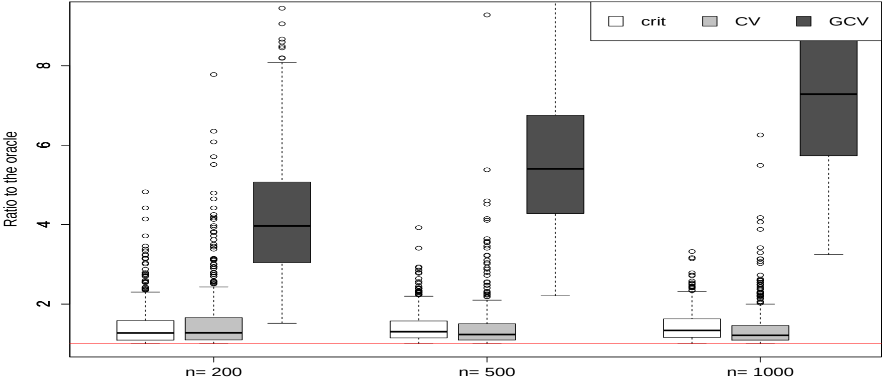

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Estimation of β_1, $\lambda_j = j^{-3}$.

Outline

Goal

Aim: estimate the conditional distribution function

$$F^x(y) = \mathbb{P}(Y \leq y | X = x)$$

using the information of the sample $\{(X_i, Y_i), i = 1, \ldots, n\}$ following the same distribution as (X, Y).

Estimation method

- **Kernel estimation**

$$\widehat{F}^x_{h,d}(y) = \frac{\sum_{i=1}^n K_h\left(d(X_i, x)\right) \mathbf{1}_{\{Y_i \le y\}}}{\sum_{i=1}^n K_h\left(d(X_i, x)\right)}$$

where

- $K : \mathbb{R} \to \mathbb{R}_+$ is a kernel function. It verifies $\int_{\mathbb{R}} K(t)dt = 1$.
- $h > 0$ is a bandwidth.
- $d : \mathbb{H}^2 \to \mathbb{R}_+$ is a general pseudometric.

- **Reference:** Ferraty *et al.* (2006, 2010) :
  - Almost complete and uniform almost complete convergence (with bias-variance decomposition).
  - Rates of convergence on some examples of processes.
- **Purposes**
  - **provide a data-driven choice for the bandwidth h with nonasymptotic theoretical results;**
  - discuss the choice of the semi-metric d in the kernel;
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Outline

Considered risk

- For the main part of the talk: $d(x,x') = \|x - x'\|$, $(x,x') \in \mathbb{H}$.

$$\widehat{F}_h^x(y) := \widehat{F}_{h,d}^x(y) = \frac{\sum_{i=1}^n K_h(\|X_i - x\|)\mathbf{1}_{\{Y_i \le y\}}}{\sum_{i=1}^n K_h(\|X_i - x\|)}$$

- **Integrated risk**

$$\mathcal{R}(\widehat{F}_h, F) := \mathbb{E}\left[\int_B \left(\int_D \left(\widehat{F}_h^x(y) - F^x(y)\right)^2 dy\right) d\mathbb{P}_X(x)\right] = \mathbb{E}\left[\|\widehat{F}_h^{X'} - F^{X'}\|_D^2 \mathbf{1}_B(X')\right]$$

with

- X' is a copy of X, independent of the data-sample.
- D is a compact subset of $\mathbb{R}$;
- B is a bounded subset of $\mathbb{H}$.

Assumptions to control the risk

- **Assumptions on the kernel**
  - $\text{supp}(K) \subset [0;1]$
  - $0 < c_K \leq K(t) \leq C_K < +\infty,\ t \in [0;1]$

- **Assumption on the target function F:**

$$\exists \beta \in (0;1), \quad \exists C_D > 0, \quad \forall x, x' \in \mathbb{H}, \quad \|F^x - F^{x'}\|_D \leq C_D \|x - x'\|^\beta$$

$\longrightarrow$ F belongs to a Hölder space with smoothness index β.

- **Assumption on the process X:**
  - through the small ball probabilities

$$\varphi(h) := \mathbb{P}(\|X\| \leq h) \text{ and } \varphi^{x_0}(h) := \mathbb{P}(\|X - x_0\| \leq h), \quad x_0 \in \mathbb{H}.$$

  - $\exists c_\varphi, C_\varphi > 0$, such that

$$\forall h > 0,\ \forall x_0 \in B,\ c_\varphi \varphi(h) \leq \varphi^{x_0}(h) \leq C_\varphi \varphi(h).$$

Upper-bound for the risk

Proposition

Under the previous assumptions, there exists $C > 0$, such that, for any $h > 0$,

$$\mathcal{R}(\widehat{F}_h, F) \leq C\left(h^{2\beta} + \frac{1}{n\varphi(h)}\right),$$

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Unknown oracle choice

$$h^* = \arg\min_{h \in \mathcal{H}_n} \mathcal{R}(\widehat{F}_h, F)$$

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Question: How to choose h without the knowledge of β and $\varphi(h)$?

Outline

1. Prediction in the functional linear model
   - Estimation procedure
   - Theoretical results
   - Simulation results

2. Adaptive estimation of the conditional c.d.f
   - Bias-variance decomposition of the risk
   - Bandwidth selection device
   - Optimal estimation in the minimax sense
   - Simulation study

3. Response surface methodology for functional data
   - Response surface methodology
   - Extension to the functional setting

Bandwidth selection device

Inspired from the work of Goldenshluger and Lepski (2011)

Bias-variance decomposition of the risk

$$\mathcal{R}\left(\widehat{F}_h, F\right) = \mathbb{E}\left[\|F^{X'} - \mathbb{E}\left[\widehat{F}_h^{X'}|X'\right]\|_D^2 \mathbf{1}_B(X')\right] + \mathbb{E}\left[\|\mathbb{E}\left[\widehat{F}_h^{X'}|X'\right] - \widehat{F}_h^{X'}\|_D^2 \mathbf{1}_B(X')\right].$$

- Variance term of order $\frac{1}{n\varphi(h)}$ $\rightarrow$ can be estimated:

$$\widehat{V}(h) = \kappa \frac{\ln n}{n\widehat{\varphi}(h)} \text{ where } \widehat{\varphi}(h) = \frac{1}{n}\sum_{i=1}^{n} \mathbf{1}_{\{\|X\| \leq h\}}.$$

- How to approximate the bias term ?

$$\widehat{A}(h) = \max_{h' \in \mathcal{H}_n} \left(\|\widehat{F}_{h'}^{X'} - \widehat{F}_{h' \vee h}^{X'}\|_D^2 - \widehat{V}(h')\right)_+$$

- Finally $\hat{h} = \arg\min_{h \in \mathcal{H}_n} \left\{\widehat{A}(h) + \widehat{V}(h)\right\} \Rightarrow \widehat{F}_{\hat{h}}^{X'}$.

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Main result: nonasymptotic adaptive risk bound

Theorem

Under the previous assumptions, and if the collection $\mathcal{H}_n$ is not too large, there exist 2 constants $c, C > 0$ such that

$$\mathcal{R}(\widehat{F}_{\hat{h}}, F) \leq c \min_{h \in \mathcal{H}_n} \left\{ h^{2\beta} + \frac{\ln(n)}{n\varphi(h)} \right\} + \frac{C}{n}.$$

Outline

Additional assumption on the small ball probability

$$\varphi(h) = \mathbb{P}\left(\|X\| \leq h\right), \ h > 0.$$

3 possible assumptions on the decay of the s.b.p.

- **Fast decay**

$$\varphi(h) \asymp h^{\gamma} \exp\left(-ch^{-\alpha}\right), \quad \gamma \in \mathbb{R}, \alpha > 0.$$

Ex: if X is a brownian motion, assumption satisfied with $\alpha = 2$.

- **Intermediate decay**

$$\varphi(h) \asymp h^{\gamma} \exp\left(-c \ln^{-\alpha}(1/h)\right), \quad \gamma \in \mathbb{R}, \alpha > 1.$$

- **Low decay**

$$\varphi(h) \asymp h^{\gamma}, \quad \gamma > 0.$$

Ex: if $X \in \mathbb{R}^d$ (random vector), assumption satisfied with $\gamma = d$.

Rates of convergence

	Fast decay for $\varphi(h)$ (slow rates)	Intermediate decay for $\varphi(h)$ (intermediate)	Low decay for $\varphi(h)$ (fast rates)
(a) $\mathcal{R}(\widehat{F}_{\hat{h}}, F) \lesssim \cdots$ (adaptive rate)	$(\ln(n))^{-2\beta/\alpha}$	$\exp\left(-\frac{2\beta}{c_2^{1/\alpha}} \ln^{1/\alpha}(n)\right)$	$\left(\frac{n}{\ln(n)}\right)^{-\frac{2\beta}{2\beta+\gamma}}$

$\longrightarrow$ similar rates to the ones obtained by Ferraty *et al.* (2006), but for an adaptive bandwidth.

Rates of convergence

	Fast decay for $\varphi(h)$ (slow rates)	Intermediate decay $\varphi(h)$ (intermediate)	Low decay $\varphi(h)$ (fast rates)
(a) $\mathcal{R}(\widehat{F}_{\hat{h}}, F) \lesssim \cdots$ (adaptive rate)	$(\ln(n))^{-2\beta/\alpha}$	$\exp\left(-\frac{2\beta}{c_2^{1/\alpha}} \ln^{1/\alpha}(n)\right)$	$\left(\frac{n}{\ln(n)}\right)^{-\frac{2\beta}{2\beta+\gamma}}$
(b) Minimax rate $\inf_{\widetilde{F}} \sup_{F,X\ldots} \mathcal{R}(\widetilde{F}, F) \gtrsim \cdots$ (lower bound)	$(\ln(n))^{-2\beta/\alpha}$	$\exp\left(-\frac{2\beta}{c_2^{1/\alpha}} \ln^{1/\alpha}(n)\right)$	$n^{-\frac{2\beta}{2\beta+\gamma}}$

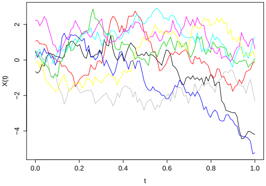
$\longrightarrow$ similar rates to the ones obtained by Mas (2012) for regression estimation.
$\longrightarrow$ the estimator is then optimal in the minimax sense, up to the extra $\ln(n)$ factor.

Outline

Implementation

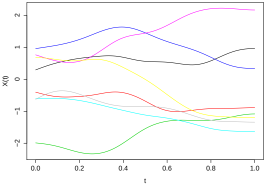
- **Choice of K:** uniform kernel $K = \mathbf{1}_{[0,1]}$.
- **Choice of $\mathcal{H}_n$:** $\mathcal{H}_n = \{C/k,\ 1 \leq k \leq k_{\max}\}$.
- **Simulation of X:**
  - $(W(t))_t$ a brownian motion,
  - $(\xi_j)_{j\geq 0}$ *i.i.d.* $\mathcal{N}(0,1)$.

Fast decay for $\varphi(h)$



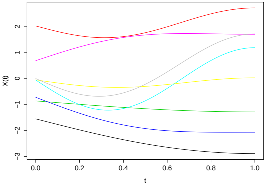
$X(t) = W(t) + \xi_0$

Intermediate decay for $\varphi(h)$



$X(t) = \xi_0$
$+\sqrt{2}\sum_{j=1}^{150} \xi_j \frac{e^{-j}}{\sqrt{j}} \sin(\pi(j-0.5)t)$

Low decay for $\varphi(h)$



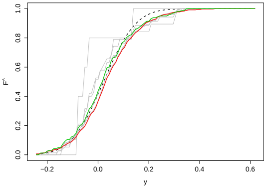
$X(t) = \xi_0 + \sqrt{2}\xi_1 \sin(\pi t/2)$
$+\xi_2 \sin(3\pi t/2)/\sqrt{2}$

Estimators

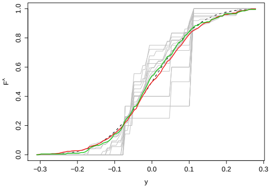
Conditional c.d.f estimation in a regression model

Observations: $(X_i, Y_i)_{i \in \{1,\dots,500\}}$ such that $Y_i = \left(\int_0^1 \beta(t) X_i(t) dt \right)^2 + \varepsilon_i$ with $\beta(t) = \sin(4\pi t)$ and $\varepsilon_i \sim \mathcal{N}(0, 0.1)$.

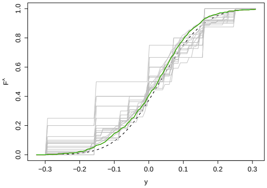
Fast decay for $\varphi(h)$



Intermediate decay for $\varphi(h)$



Low decay for $\varphi(h)$



.. true conditional c.d.f. | — estimators $(\widehat{F}_h)_{h \in \mathcal{H}_n}$,

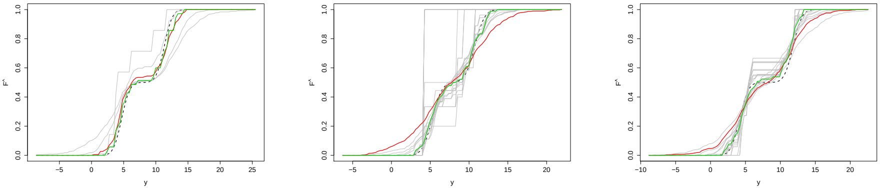
— oracle estimator $\widehat{F}_{h^*}$, | — adaptive estimator $\widehat{F}_{\widehat{h}}$.

Estimators

Conditional c.d.f estimation in a Gaussian mixture model

Observations: $(X_i, Y_i)_{i \in \{1,\dots,500\}}$ such that
$Y_i | X_i = x \sim 0.5\mathcal{N}(8 - 4\|x\|, 1) + 0.5\mathcal{N}(8 + 4\|x\|, 1)$,

Fast decay for $\varphi(h)$ | Intermediate decay for $\varphi(h)$ | Low decay for $\varphi(h)$



.. true conditional c.d.f. | — estimators $(\widehat{F}_h)_{h \in \mathcal{H}_n}$,
— oracle estimator $\widehat{F}_{h^*}$, | — adaptive estimator $\widehat{F}_{\widehat{h}}$.

Outline

Outline

Response surface methodology

Brief history

- Box and Wilson (1950): optimal conditions for chemical experimentation → widely used in industry.
- Sacks *et. al* (1989): Extension to numerical experiments
  - ↪ Bates *et. al* (1996): conception of electrical circuit;
  - ↪ Lee and Hajela (1996): conception of rotor blades...
- Recent advances: Facer and Müller (2003), Khuri and Mukhopadhyay (2010), Georgiou, Stylianou and Aggarwal (2014).

Methodology

Goal: minimisation of $(x_1, \ldots, x_n) \mapsto m(x_1, \ldots, x_d)$, **unknown**.
Information available:

$y_i = m(x_{1,i}, \ldots, x_{d,i}) + \varepsilon_i, i = 1, \ldots, n,$

$(x_{1,i}, \ldots, x_{d,i})_{i=1}^n$ **chosen by the user** and n **as small as possible**.

Example:

- $m(x_1, x_2) = x_1^2 + x_2^2;$
- $\varepsilon \sim \mathcal{N}(0, 1).$

Methodology

Goal: minimisation of $(x_1, \ldots, x_n) \mapsto m(x_1, \ldots, x_d)$, **unknown**.
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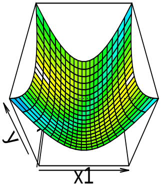

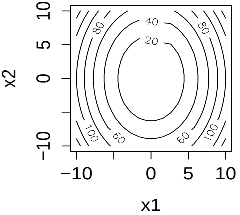

Example:

- $m(x_1, x_2) = x_1^2 + x_2^2$;
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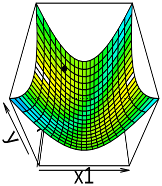
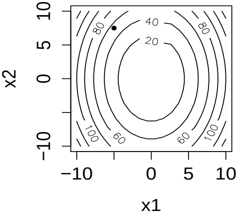




Example:

- $m(x_1, x_2) = x_1^2 + x_2^2$;
- $\varepsilon \sim \mathcal{N}(0, 1)$.

Legend:

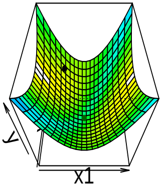
- Initial point

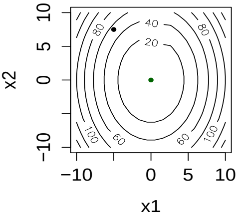
Methodology

Goal: minimisation of $(x_1, \ldots, x_n) \mapsto m(x_1, \ldots, x_d)$, **unknown**.
Information available:

$y_i = m(x_{1,i}, \ldots, x_{d,i}) + \varepsilon_i$, $i = 1, \ldots, n$,

$(x_{1,i}, \ldots, x_{d,i})_{i=1}^n$ **chosen by the user** and n **as small as possible**.





Example:

- $m(x_1, x_2) = x_1^2 + x_2^2$;
- $\varepsilon \sim \mathcal{N}(0, 1)$.

Legend:

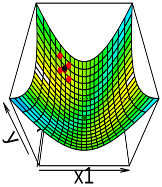
- ● Initial point
- ● Minimal point (target)

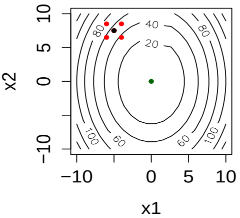
Methodology

Goal: minimisation of $(x_1, \ldots, x_n) \mapsto m(x_1, \ldots, x_d)$, **unknown**.
Information available:

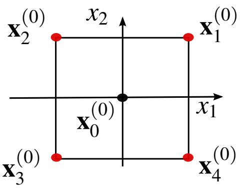
$y_i = m(x_{1,i}, \ldots, x_{d,i}) + \varepsilon_i$, $i = 1, \ldots, n$,

$(x_{1,i}, \ldots, x_{d,i})_{i=1}^{n}$ **chosen by the user** and n **as small as possible**.





Factorial 2^2 design: 4 points



Example:

- $m(x_1, x_2) = x_1^2 + x_2^2$;
- $\varepsilon \sim \mathcal{N}(0, 1)$.

Legend:

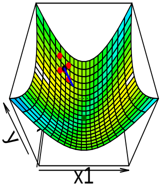
- Initial point (black)
- Minimal point (target) (green)
- Factorial design points (red)

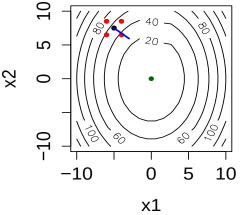
Methodology

Goal: minimisation of $(x_1, \ldots, x_n) \mapsto m(x_1, \ldots, x_d)$, **unknown**.
Information available:

$y_i = m(x_{1,i}, \ldots, x_{d,i}) + \varepsilon_i$, $i = 1, \ldots, n$,

$(x_{1,i}, \ldots, x_{d,i})_{i=1}^{n}$ **chosen by the user** and n **as small as possible**.





Least-squares fit of a first order model:

$$y = \beta_1 x_1 + \beta_2 x_2 + \varepsilon'.$$

Direction of steepest descent estimated :

$$(-\widehat{\beta}_1, -\widehat{\beta}_2).$$

Example:

- $m(x_1, x_2) = x_1^2 + x_2^2$;
- $\varepsilon \sim \mathcal{N}(0, 1)$.

Legend:

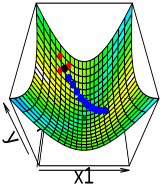
- ● (black) Initial point
- ● (green) Minimal point (target)
- ● (red) Factorial design points
- — (blue) direction of descent

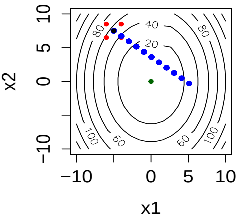
Methodology

Goal: minimisation of $(x_1, \ldots, x_n) \mapsto m(x_1, \ldots, x_d)$, **unknown**.
Information available:

$$y_i = m(x_{1,i}, \ldots, x_{d,i}) + \varepsilon_i, \; i = 1, \ldots, n,$$

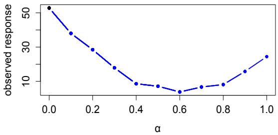
$(x_{1,i}, \ldots, x_{d,i})_{i=1}^{n}$ **chosen by the user** and n **as small as possible**.





Observed response:

$$y = f(x_1 - \alpha\widehat{\beta}_1, x_2 - \alpha\widehat{\beta}_2) + \varepsilon$$



Example:

- $m(x_1, x_2) = x_1^2 + x_2^2$;
- $\varepsilon \sim \mathcal{N}(0, 1)$.

Legend:

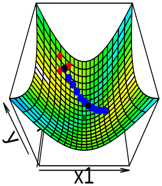
- Initial point (black)
- Minimal point (target) (green)
- Factorial design points (red)
- Descent steps (blue)

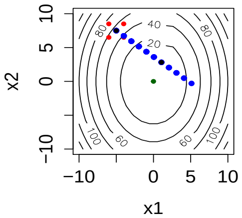
Methodology

Goal: minimisation of $(x_1, \ldots, x_n) \mapsto m(x_1, \ldots, x_d)$, **unknown**.
Information available:

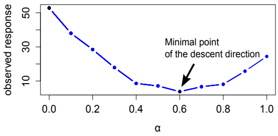
$y_i = m(x_{1,i}, \ldots, x_{d,i}) + \varepsilon_i, i = 1, \ldots, n,$

$(x_{1,i}, \ldots, x_{d,i})_{i=1}^{n}$ **chosen by the user** and n **as small as possible**.





Observed response:
$y = f(x_1 - \alpha\widehat{\beta}_1, x_2 - \alpha\widehat{\beta}_2) + \varepsilon$



Example:

- $m(x_1, x_2) = x_1^2 + x_2^2$;
- $\varepsilon \sim \mathcal{N}(0, 1)$.

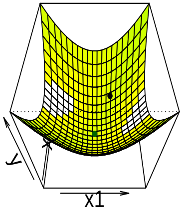
Legend:

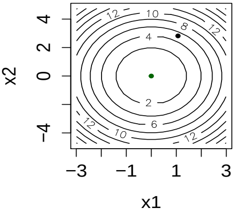
- ● (black) Initial point
- ● (green) Minimal point (target)
- ● (red) Factorial design points
- ● (blue) Descent steps

Methodology

Goal: minimisation of $(x_1,\ldots,x_n) \mapsto m(x_1,\ldots,x_d)$, **unknown**.
Information available:

$y_i = m(x_{1,i},\ldots,x_{d,i}) + \varepsilon_i$, $i = 1,\ldots,n$,
$(x_{1,i},\ldots,x_{d,i})_{i=1}^n$ **chosen by the user** and n **as small as possible**.





Example:

- $m(x_1,x_2) = x_1^2 + x_2^2$;
- $\varepsilon \sim \mathcal{N}(0,1)$.

Legend:

- ● (black) Minimal point of the descent direction
- ● (green) Minimal point (target)

Methodology

Goal: minimisation of $(x_1, \ldots, x_n) \mapsto m(x_1, \ldots, x_d)$, **unknown**.
Information available:

$y_i = m(x_{1,i}, \ldots, x_{d,i}) + \varepsilon_i$, $i = 1, \ldots, n$,
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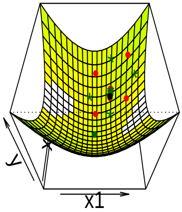
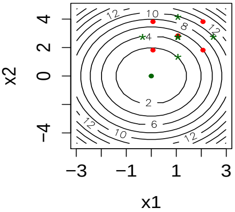
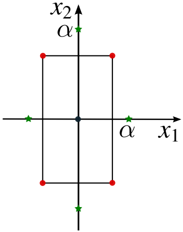




Central Composite Design: 8 points



Example:

- $m(x_1, x_2) = x_1^2 + x_2^2$;
- $\varepsilon \sim \mathcal{N}(0, 1)$.

Legend:

- ● Minimal point of the descent direction
- ● Minimal point (target)
- ● Factorial design points
- ★ CCD axial points

Methodology

Goal: minimisation of $(x_1,\ldots,x_n) \mapsto m(x_1,\ldots,x_d)$, **unknown**.
Information available:

$y_i = m(x_{1,i},\ldots,x_{d,i}) + \varepsilon_i$, $i = 1,\ldots,n$,

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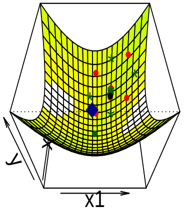

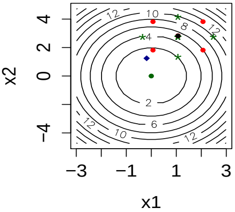

Least-squares fit of a second-order model:

$$y = \beta_1 x_1 + \beta_2 x_2 + (x_1, x_2) B (x_1, x_2)^t + \varepsilon''.$$

Stationary point:

$$(x_1^*, x_2^*) = \frac{1}{2}\widehat{B}^{-1}(\widehat{\beta}_1, \widehat{\beta}_2)^t$$

.

Example:

- $m(x_1, x_2) = x_1^2 + x_2^2$;
- $\varepsilon \sim \mathcal{N}(0,1)$.

Legend:

- ● Minimal point of the descent direction
- ● Minimal point (target)
- ● Factorial design points
- ★ CCD axial points
- ◆ Stationary point (estimated minimal point)

Methodology

Goal: minimisation of $(x_1, \ldots, x_n) \mapsto m(x_1, \ldots, x_d)$, **unknown**.
Information available:

$y_i = m(x_{1,i}, \ldots, x_{d,i}) + \varepsilon_i$, $i = 1, \ldots, n$,

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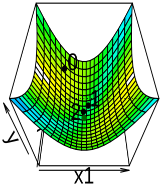

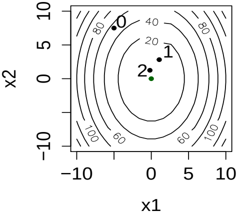

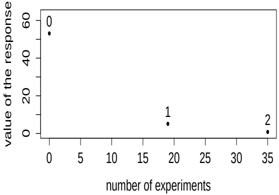

Example:

- $m(x_1, x_2) = x_1^2 + x_2^2$;
- $\varepsilon \sim \mathcal{N}(0, 1)$.

Legend:

- ● Step points
- ● Minimal point (target)

Outline

Problems raised by the functional context

- First and second-order models can be defined easily but
  ... How to define functional design of experiments ?
- One possible answer: combine dimension reduction with classical finite-dimensional design of experiments
  - $(\mathbf{x}_0^{(i)} = (x_{0,1}^{(i)}, \ldots, x_{0,d}^{(i)}) \in \mathbb{R}^d, i = 1, \ldots, n_0)$ d-dimensional design of experiments;
  - $\{\varphi_1, \ldots, \varphi_d\}$ orthonormal family of $\mathbb{H}$

$$x_o^{(i)} = x_0 + \sum_{j=1}^{d} x_{0,j}^{(i)} \varphi_j,$$

$\longrightarrow$ functional design of experiments.

... How can we define the directions $\{\varphi_1, \ldots, \varphi_d\}$?
- Possible basis of approximation
  - Fixed basis: Fourier, B-splines, wavelets,...
  - If a training sample exists: data driven basis
    - PCA basis;
    - PLS basis Wold (1975), Preda and Saporta (2005), Delaigle and Hall (2012): allows to take into account the interaction between x and y.

Problems raised by the functional context

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Example of functional design of experiments

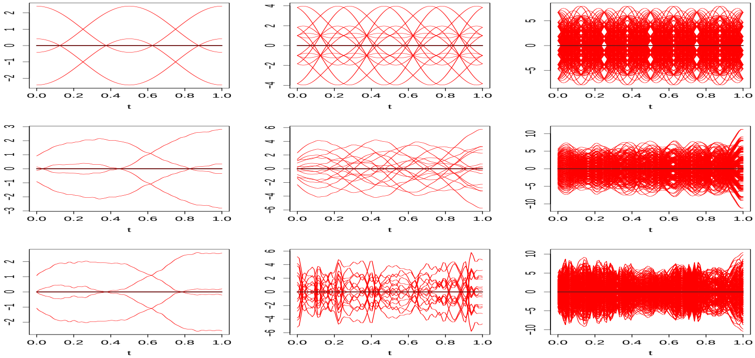
Factorial 2^d design in $\mathbb{H} = \mathbb{L}^2([0,1])$

$d = 2$, 16 curves | $d = 4$, 32 curves | $d = 8$, 280 curves

Fourier

PCA[1]

PLS[2]

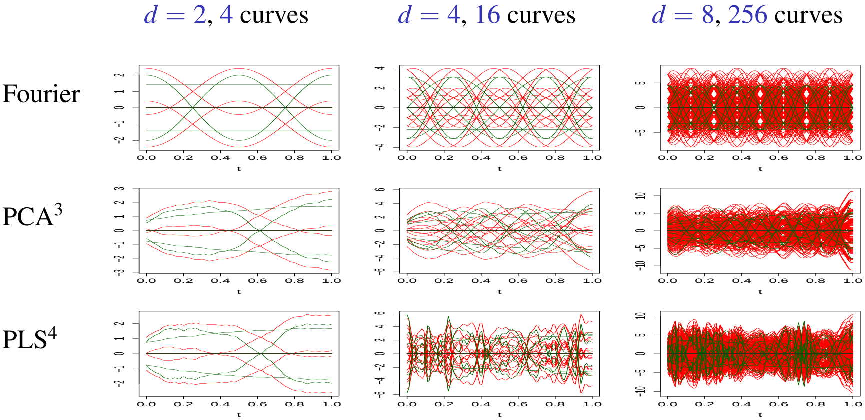


X brownian motion, $Y = \|X - f\|^2 + \varepsilon, f(t) = \cos(4\pi t) + 3\sin(\pi t) + 10, \varepsilon \sim \mathcal{N}(0, 0.01)$

[1] calculated from $(X_i)_{i=1}^{500}$
[2] calculated from $(X_i, Y_i)_{i=1}^{500}$

Example of functional design of experiments

Central Composite Designs in $\mathbb{H} = \mathbb{L}^2([0,1])$



X brownian motion, $Y = \|X - f\|^2 + \varepsilon, f(t) = \cos(4\pi t) + 3\sin(\pi t) + 10, \varepsilon \sim \mathcal{N}(0, 0.01)$

---

[3] calculated from $(X_i)_{i=1}^{500}$
[4] calculated from $(X_i, Y_i)_{i=1}^{500}$

Methodology

Adaptation to a functional context

Goal: minimisation of $x \mapsto m(x)$, **unknown**.

Example:

- $m(x) = \|x - f\|^2$ with

$f(t) = \cos(4\pi t) + 3\sin(\pi t) + 10$;

- $\varepsilon \sim \mathcal{N}(0, 10)$.

Methodology

Adaptation to a functional context

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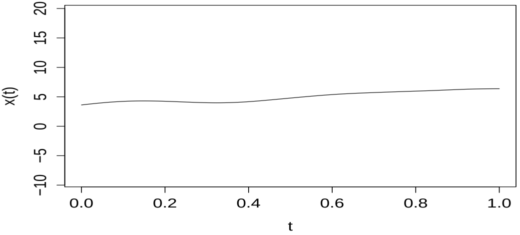


Example:

- $m(x) = \|x - f\|^2$ with $f(t) = \cos(4\pi t) + 3\sin(\pi t) + 10$;
- $\varepsilon \sim \mathcal{N}(0, 10)$.

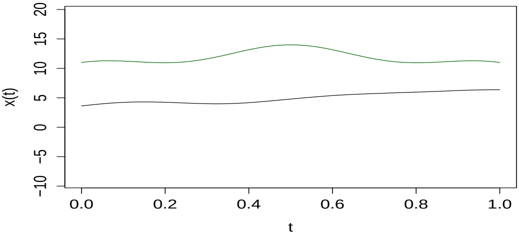
Legend:

— Initial point

Methodology

Adaptation to a functional context

Goal: minimisation of $x \mapsto m(x)$, **unknown**.



Example:

- $m(x) = \|x - f\|^2$ with $f(t) = \cos(4\pi t) + 3\sin(\pi t) + 10$;
- $\varepsilon \sim \mathcal{N}(0, 10)$.

Legend:

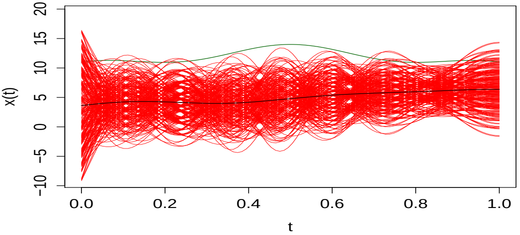
— Initial point

— Minimal point $f(t)$ (target)

Methodology

Adaptation to a functional context

Goal: minimisation of $x \mapsto m(x)$, **unknown**.



Example:

- $m(x) = \|x - f\|^2$ with $f(t) = \cos(4\pi t) + 3\sin(\pi t) + 10$;
- $\varepsilon \sim \mathcal{N}(0, 10)$.

Legend:

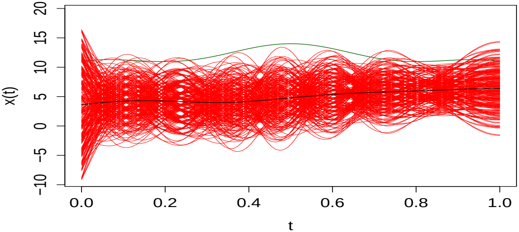
- — Initial point
- — Minimal point $f(t)$ (target)
- — 2^8 factorial design[5]

[5] directions : PLS basis calculated from $(X_i, m(X_i) + \varepsilon_i)_{i=1}^{500}$ (X_i brownian motion)

Methodology

Adaptation to a functional context

Goal: minimisation of $x \mapsto m(x)$, **unknown**.



Least-squares fit of a first order model → estimation of direction of steepest descent

Example:

- $m(x) = \|x - f\|^2$ with $f(t) = \cos(4\pi t) + 3\sin(\pi t) + 10$;
- $\varepsilon \sim \mathcal{N}(0, 10)$.

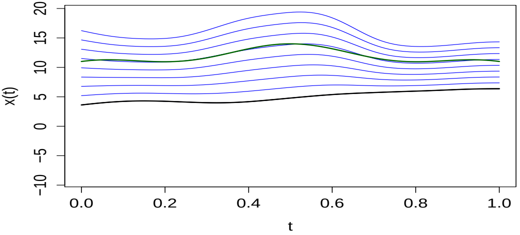
Legend:

- — (black) Initial point
- — (green) Minimal point $f(t)$ (target)

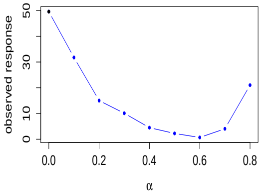
Methodology

Adaptation to a functional context

Goal: minimisation of $x \mapsto m(x)$, **unknown**.



Observed response on descent path:



Example:

- $m(x) = \|x - f\|^2$ with $f(t) = \cos(4\pi t) + 3\sin(\pi t) + 10$;
- $\varepsilon \sim \mathcal{N}(0, 10)$.

Legend:

- — Initial point
- — Minimal point $f(t)$ (target)
- — Points of the descent direction

Methodology

Adaptation to a functional context

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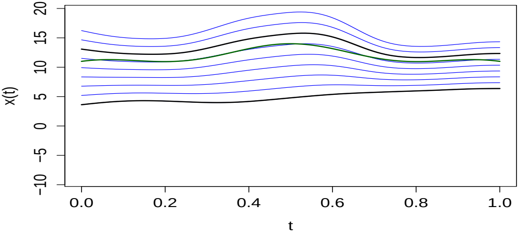
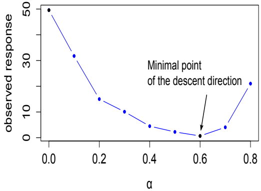


Observed response on descent path:



Example:

- $m(x) = \|x - f\|^2$ with

$f(t) = \cos(4\pi t) + 3\sin(\pi t) + 10$;

- $\varepsilon \sim \mathcal{N}(0, 10)$.

Legend:

- Black line: Minimal point of the descent direction
- Green line: Minimal point $f(t)$ (target)
- Blue line: Points of the descent direction

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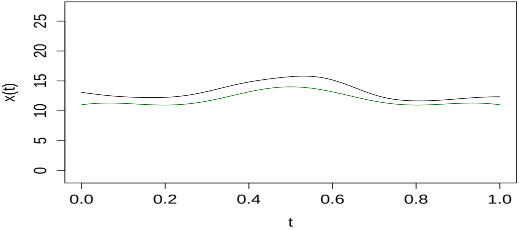
Adaptation to a functional context

Goal: minimisation of $x \mapsto m(x)$, **unknown**.



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Legend:

— Minimal point of the descent direction

— Minimal point $f(t)$ (target)

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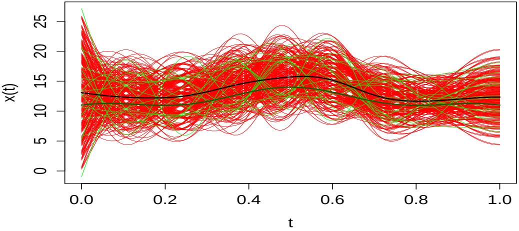

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- $m(x) = \|x - f\|^2$ with $f(t) = \cos(4\pi t) + 3\sin(\pi t) + 10$;
- $\varepsilon \sim \mathcal{N}(0, 10)$.

Legend:

- Black line: Minimal point of the descent direction
- Dark green line: Minimal point $f(t)$ (target)
- Red and light green lines: } Central Composite Design[5]

[5] directions : PLS basis calculated from $(X_i, m(X_i) + \varepsilon_i)_{i=1}^{500}$ (X_i brownian motion, $d = 8$)

Methodology

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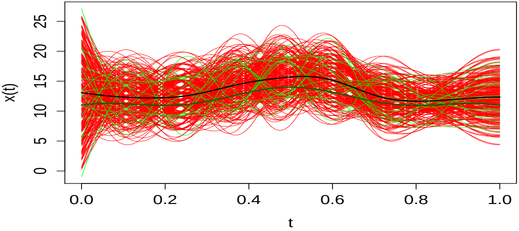

Least-squares fit of a second order model $\to$ estimation of stationary point

Example:

- $m(x) = \|x - f\|^2$ with $f(t) = \cos(4\pi t) + 3\sin(\pi t) + 10$;
- $\varepsilon \sim \mathcal{N}(0, 10)$.

Legend:

- black — Minimal point of the descent direction
- dark green — Minimal point $f(t)$ (target)
- red, light green — } Central Composite Design[5]

[5] directions : PLS basis calculated from $(X_i, m(X_i) + \varepsilon_i)_{i=1}^{500}$ (X_i brownian motion, $d = 8$)

Methodology

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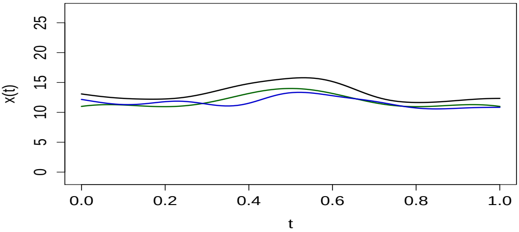
Goal: minimisation of $x \mapsto m(x)$, **unknown**.



Example:

- $m(x) = \|x - f\|^2$ with $f(t) = \cos(4\pi t) + 3\sin(\pi t) + 10$;
- $\varepsilon \sim \mathcal{N}(0, 10)$.

Legend:

- — (black) Minimal point of the descent direction
- — (green) Minimal point $f(t)$ (target)
- — (blue) Stationary point (estimation of the minimal point)

Methodology

Adaptation to a functional context

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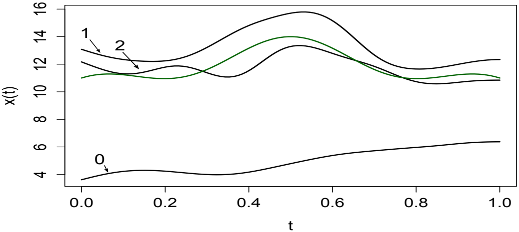

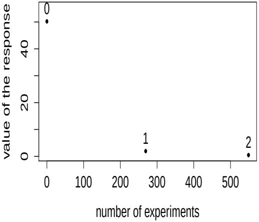

Example:

- $m(x) = \|x - f\|^2$ with

$f(t) = \cos(4\pi t) + 3\sin(\pi t) + 10$;

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Legend:

— Step points

— Minimal point $f(t)$ (target)

Conclusion

- **Model selection for functional principal component regression**

  $\rightarrow$ faster and more stable than usual cross-validation

  ... with non-asymptotic control of the prediction error.

- **Bandwidth selection for kernel estimation**

  $\rightarrow$ first adaptive estimation procedure in *nonparametric* estimation for functional data

  $\rightarrow$ precise lower bounds and convergence rates.

$\longrightarrow$ both estimation procedures leads to minimax optimal estimators.

- **First attempt to adapt Response Surface Methodology to functional data**.

  $\rightarrow$ definition of functional design of experiments.

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Perspectives

- **Response surface methodology:** minimisation of the probability of failure of a nuclear reactor vessel (CEA Cadarache);

- **Functional single-index model:** $Y = g(\langle \beta, X \rangle) + \varepsilon$. Is it possible to define a projection based estimator which is adaptive ?

- **Kernel estimators in high/infinite dimension (with Gaëlle Chagny):**
  - How to choose *relevant* metrics for kernels ?
  - Theoretical study of resulting estimators.

- **Functional linear model**: Adaptive parameter selection for the roughness regularization method.

$$\widehat{\beta}_\rho \in \arg\min_{f \in S} \left\{ \frac{1}{n} \sum_{i=1}^{n} (Y_i - \langle f, X_i \rangle)^2 + \rho \|f\|_S^2 \right\},$$

with ρ a smoothing parameter, $S \subset \mathbb{H}$ and $\|\cdot\|_S$ a seminorm on S.

Thank you for your attention!

- **Penalized contrast estimation in functional linear models with circular data.**
  É. Brunel and A. Roche, accepted for publication in *Statistics*.
- **Non-asymptotic Adaptive Prediction in Functional Linear Models.**
  É. Brunel, A. Mas and A. Roche, submitted.
- **Adaptive and minimax estimation of the cumulative distribution function given a functional covariate.**
  G. Chagny and A. Roche, in revision.
- **Response surface methodology for functional data : application to nuclear safety**
  Work in progress.
- **Adaptive estimation in functional generalized linear models**
  Work in progress.