

Estimation non paramétrique dans un modèle de régression additif avec réponse et covariables fonctionnelles

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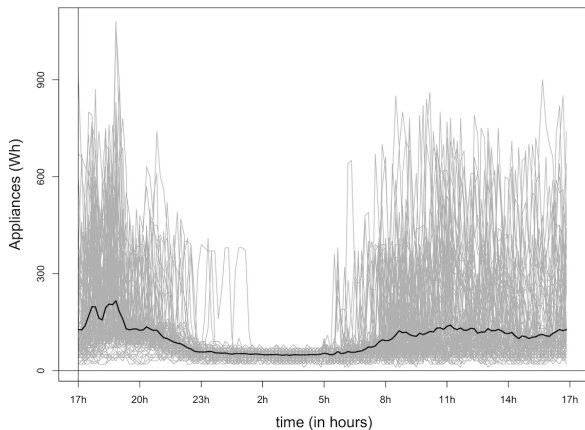


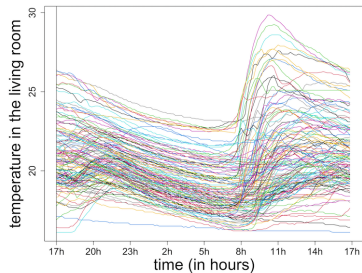
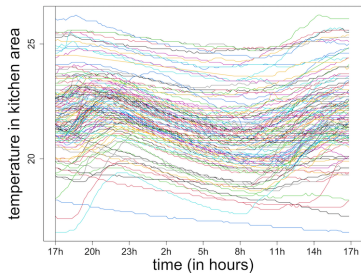
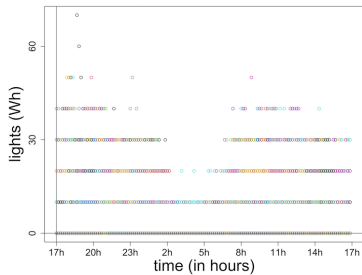
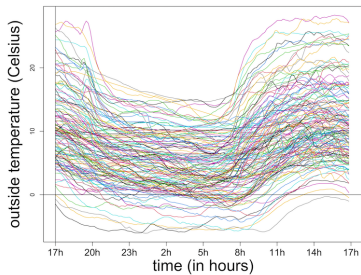
Fabienne

Previous works

- Functional data : Ramsay & Silverman, 2005.
- Important literature in the "functional linear model," meaning a **real response variable** with **functional covariates** : Cai et al. 2006 ; Cardot et al. 2007 ; Li and Hsing 2007 ; Ferraty et al. (2012), Hilgert et al. 2013 ; Cai and Yuan 2012 ; Brunel et al., 2016.
- The case where the **response variable is also functional** is less studied : "concurrent regression model" : Crambes & Mas 2013, Chagny et al. 2024.

We observe for $i = 1, \dots, N$ individuals the N independent trajectories of a process $Y_i(t)$ (the functional response) and of K processes $(X_{i,1}(t), \dots, X_{i,K}(t))$ (the functional explanatory variables) for $t \in [0, \tau]$, a fixed time interval.





- 1 Model
- 2 Least Squares Estimators
- 3 Study of the risk
- 4 Choice of the bases
- 5 Model selection
- 6 Numerical examples

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We consider the regression model with functional responses and explanatory variables ("concurrent regression model") as follows :

$$Y_i(t) = \sum_{j=1}^K b_j(t) X_{i,j}(t) + \sigma(t, \mathbf{X}_i(t)) \varepsilon_i(t), \quad t \in [0, \tau], \quad i = 1, \dots, N,$$

For $i = 1, \dots, N$,

- The processes $(\varepsilon_i(t))_{t \in [0, \tau]}$ are centered, independent, and identically distributed (i.i.d.), with $\mathbb{E}(\varepsilon_1^2(t)) = 1$;
- The processes $(\mathbf{X}_i(t) = (X_{i,1}(t) \dots X_{i,K}(t)))_{t \in [0, \tau]}$ are i.i.d. and independent of $(\varepsilon_i(t))_{t \in [0, \tau]}$.
- The integer K is known and small compared to N : it is the number of explanatory processes.
- We may consider the homoscedastic case $\sigma(t, \mathbf{x}) = \sigma$.
The model coefficients $b_1(t), \dots, b_K(t)$ are deterministic functions, unknown and to be estimated.

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Least Squares Estimators

Let $(\varphi_j)_{j \geq 1}$ be a basis of $\mathbb{L}_\tau^2 := \mathbb{L}^2([0, \tau])$ of measurable functions such that $\int_0^\tau \varphi_j^2(x) dx \leq 1$, and let S_m be the subspace spanned by $(\varphi_j)_{1 \leq j \leq m}$. Our estimator of $\mathbf{b}(t) = (b_1(t), \dots, b_K(t))^T$ is constructed on the product space $S_{\mathbf{m}} := S_{m_1} \times \dots \times S_{m_K}$, $\mathbf{m} = (m_1, \dots, m_K)$, i.e.,

$$\hat{\mathbf{b}}_{\mathbf{m}}(t) = (\hat{b}_1(t), \dots, \hat{b}_K(t))^T \quad \text{where} \quad \hat{b}_k(t) = \sum_{j=1}^{m_k} \hat{\beta}_{k,j} \varphi_j(t),$$

For $i = 1, \dots, N$, $(Y_i(t), \mathbf{X}_i(t))_{0 \leq t \leq \tau}$ and $\mathbf{X}_i(t) = (X_{i,1}(t), \dots, X_{i,K}(t))^T$ and $\mathbf{h} = (h_1, \dots, h_K)^T \in (\mathbb{L}_\tau^2)^K$

$$\hat{\mathbf{b}}_{\mathbf{m}}(t) = \arg \min_{\mathbf{h} \in S_{\mathbf{m}}} \frac{1}{N} \sum_{i=1}^N \int_0^\tau (Y_i(t) - \mathbf{h}(t)^T \mathbf{X}_i(t))^2 dt$$

Minimizing with respect to $\mathbf{h}$ the contrast

$\frac{1}{N} \sum_{i=1}^N \int_0^\tau (Y_i(t) - \mathbf{h}(t)^T \mathbf{X}_i(t))^2 dt$ is equivalent to minimizing :

$$U_N(\mathbf{h}) = \frac{1}{N} \sum_{i=1}^N \int_0^\tau (\mathbf{h}(t)^T \mathbf{X}_i(t))^2 dt - \frac{2}{N} \sum_{i=1}^N \int_0^\tau Y_i(t) \mathbf{h}(t)^T \mathbf{X}_i(t) dt$$

and taking the expectation :

$$\begin{aligned} \mathbb{E}[U_N(\mathbf{h})] &= \mathbb{E} \left\{ \int_0^\tau (\mathbf{h}(t)^T \mathbf{X}_1(t))^2 dt \right\} - 2 \mathbb{E} \left[\int_0^\tau Y_1(t) \mathbf{h}(t)^T \mathbf{X}_1(t) dt \right] \\ &= \int_0^\tau \mathbf{h}(t)^T \underbrace{\mathbb{E}[\mathbf{X}_1(t) \mathbf{X}_1(t)^T]}_{:= \Gamma(t)} \mathbf{h}(t) dt - 2 \int_0^\tau \mathbf{b}(t)^T \mathbb{E}[\mathbf{X}_1(t) \mathbf{X}_1(t)^T] \mathbf{h}(t) dt \\ &:= \|\mathbf{h}\|_\Gamma^2 - 2 \langle \mathbf{b}; \mathbf{h} \rangle_\Gamma = \|\mathbf{h} - \mathbf{b}\|_\Gamma^2 - \|\mathbf{b}\|_\Gamma^2 \end{aligned}$$

Thus, $\mathbb{E}[U_N(\mathbf{h})]$ is minimized for $\mathbf{h} = \mathbf{b}$ and $\|\cdot\|_\Gamma$ appears as the natural semi-norm (or norm if Γ is invertible) of the problem.

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The estimator $\hat{\mathbf{b}}_{\mathbf{m}}(t) = (\hat{b}_1(t), \dots, \hat{b}_K(t))^T$ where $\hat{b}_k(t) = \sum_{j=1}^{m_k} \hat{\beta}_{k,j} \varphi_j(t)$, or equivalently the coefficients :

$$\hat{B}_{\mathbf{m}} = (\underbrace{\hat{\beta}_{1,1}, \dots, \hat{\beta}_{1,m_1}}_{b_1(t)}, \underbrace{\hat{\beta}_{2,1}, \dots, \hat{\beta}_{2,m_2}}_{b_2(t)}, \dots, \underbrace{\hat{\beta}_{K,1}, \dots, \hat{\beta}_{K,m_K}}_{b_K(t)})^T$$

are obtained by algebraic resolution through a standard gradient calculation associated with the least squares contrast : $\vec{\nabla} U_N(\hat{B}_{\mathbf{m}}) = \vec{0}$ which leads to

$$\underbrace{\begin{pmatrix} \hat{\Psi}_{m_1, m_1} & \cdots & \hat{\Psi}_{m_1, m_K} \\ \vdots & & \vdots \\ \hat{\Psi}_{m_K, m_1} & \cdots & \hat{\Psi}_{m_K, m_K} \end{pmatrix}}_{:= \hat{\Psi}_{\mathbf{m}}} \begin{pmatrix} \hat{\beta}_{1,1} \\ \vdots \\ \hat{\beta}_{1, m_1} \\ \vdots \\ \hat{\beta}_{K,1} \\ \vdots \\ \hat{\beta}_{K, m_K} \end{pmatrix} = \underbrace{\begin{pmatrix} \hat{V}_{1, m_1} \\ \vdots \\ \hat{V}_{K, m_K} \end{pmatrix}}_{\hat{V}_{\mathbf{m}}}$$

$$\text{with, } \hat{\Psi}_{m_j, m_k} = \left(\int_0^\tau \varphi_p(t) \varphi_q(t) \frac{1}{N} \sum_{i=1}^N X_{i,j}(t) X_{i,k}(t) dt \right)_{1 \leq p \leq m_j; 1 \leq q \leq m_k}.$$

$$\text{and } \hat{V}_{j, m_j} = \left(\frac{1}{N} \int_0^\tau \varphi_p(t) \sum_{i=1}^N X_{i,j}(t) Y_i(t) dt \right)_{1 \leq p \leq m_j}$$

In order to ensure the existence of the estimator, conditions for the invertibility of $\hat{\Psi}_m$ must be imposed.

Recall that the semi-norm associated with the contrast is

$$\|\mathbf{h}\|_{\Gamma}^2 = \int_0^{\tau} \mathbf{h}(t)^T \Gamma(t) \mathbf{h}(t) dt \text{ with } \Gamma(t) = \mathbb{E}[\mathbf{X}_1(t) \mathbf{X}_1(t)^T]$$

and its empirical equivalent $\|\mathbf{h}\|_N^2 = \int_0^{\tau} \mathbf{h}(t)^T \Gamma_N(t) \mathbf{h}(t) dt$ with $\Gamma_N(t) := \left(\frac{1}{N} \sum_{i=1}^N X_{i,j}(t) X_{i,k}(t) \right)_{1 \leq j, k \leq K}$ and $\mathbb{E}[\Gamma_N(t)] = \Gamma(t)$.

Condition $(\mathcal{A}_S)$ (Identifiability)

(i) $\forall t \in [0, \tau]$, the matrix $\Gamma(t)$ is invertible and

$$f_{\Gamma} := \sup_{t \in [0, \tau]} \|\Gamma(t)^{-1}\|_{\text{op}} < +\infty.$$

(ii) $\forall t \in [0, \tau]$, $\forall N \geq 1$, $\Gamma_N(t)$ is almost surely invertible.

$(\mathcal{A}_S)$ implies that $\|\cdot\|_{\Gamma}$ and $\|\cdot\|_N$ are norms.

Proposition

If the condition $(\mathcal{A}_5)$ is satisfied, then the matrix $\hat{\Psi}_{\mathbf{m}}$ (resp. $\Psi_{\mathbf{m}}$) is symmetric positive definite.

Thus, the least squares estimator

$$\hat{\mathbf{b}}_{\mathbf{m}}(t) = (\hat{b}_1(t), \dots, \hat{b}_K(t))^T \quad \text{where} \quad \hat{b}_k(t) = \sum_{j=1}^{m_k} \hat{\beta}_{k,j} \varphi_j(t),$$

or equivalently the vector of coefficients :

$\hat{B}_{\mathbf{m}} = (\hat{\beta}_{1,1}, \dots, \hat{\beta}_{1,m_1}, \hat{\beta}_{2,1}, \dots, \hat{\beta}_{2,m_2}, \dots, \hat{\beta}_{K,1}, \dots, \hat{\beta}_{K,m_K})^T$ are obtained by :

$$\hat{B}_{\mathbf{m}} = \hat{\Psi}_{\mathbf{m}}^{-1} \hat{V}_{\mathbf{m}}$$

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We further assume that :

Condition $(\mathcal{A}_{X,p})$

- a) There exists an integer $p \geq 1$, such that

$$G_p^p := \max_{j=1,\dots,K} \sup_{t \in [0,\tau]} \mathbb{E}[|X_{1,j}|^p(t)] < +\infty.$$
- b) ... and some other technical conditions satisfied by gaussian processes or Poisson processes...

Condition $(\mathcal{A}_b)$

The functions $b_k : \mathbb{R}^+ \rightarrow \mathbb{R}$, $k = 1, \dots, K$, are measurable and bounded on $[0, \tau]$ (so they belong to $\mathbb{L}_\tau^2$).

Condition $(\mathcal{A}_\varphi)$

There exists $\omega > 0$, and $\exists c_\varphi > 0$ such that

$$L(S_m) := \sup_{t \in [0,\tau]} \sum_{j=1}^m \varphi_j^2(t) \leq c_\varphi m^\omega, \text{ for all } m \geq 1.$$

We study a truncated version of the estimator :

$$\tilde{\mathbf{b}}_{\mathbf{m}} = \hat{\mathbf{b}}_{\mathbf{m}} \mathbf{1}_{\Lambda_N},$$

where $\Lambda_N = \{\forall t \in [0, \tau], \|\Gamma_N(t)^{-1}\|_{\text{op}} \leq c_1 N^{c_2}\}$, and $c_1, c_2 > 0$.

Théorème

Suppose that $(\mathcal{A}_S)$, $(\mathcal{A}_{X,p})$, $(\mathcal{A}_b)$ and $(\mathcal{A}_\varphi)$ are satisfied, and let $\mathbf{m} = (m_1, \dots, m_K)$ such that $|\mathbf{m}| := m_1 + \dots + m_K \leq N$,

Moreover, suppose that

$$\sup_{t \in [0, \tau]} \mathbb{E}[\varepsilon^4(t)] < +\infty \text{ and } \sup_{j=1, \dots, K} \sup_{t \in [0, \tau]} \mathbb{E}[X_{1,j}^4(t) \sigma^4(t, \mathbf{X}_1(t))] < +\infty,$$

$$\text{and } \sup_{t \in [0, \tau], x \in \mathbb{R}^K} \sigma^2(t, x) := \|\sigma\|_\infty^2 < +\infty.$$

The estimator $\tilde{\mathbf{b}}_{\mathbf{m}}$ of $\mathbf{b}(t) = (b_1(t), \dots, b_K(t))^T$ satisfies, for $p \geq (2c_2 + 3) \vee 4$ and a constant $c > 0$,

$$\mathbb{E}[\|\tilde{\mathbf{b}}_{\mathbf{m}} - \mathbf{b}\|_N^2] \leq \inf_{\mathbf{h} \in S_{\mathbf{m}}} \|\mathbf{h} - \mathbf{b}\|_\Gamma^2 + 2\tau \|\sigma\|_\infty^2 \frac{|\mathbf{m}|}{N} + \frac{c}{N},$$

Convergence Rate

With a regularity hypothesis on the functions $b_1, \dots, b_K$, we control the approximation error (bias).

Proposition

Suppose that for all $j \in \{1, \dots, K\}$, the function b_j belongs to a function space such that $\inf_{h \in S_{m_j}} \|b_j - h\|^2 \leq L_j m_j^{-2s_j}$. If we choose each $m_j = O(N^{1/(2s_j+1)})$ and with $s_{(1)} = \min_{j=1, \dots, K} s_j$, there exists a constant $C > 0$ such that,

$$\mathbb{E}[\|\tilde{\mathbf{b}}_{\mathbf{m}} - \mathbf{b}\|_F^2] \leq C N^{-2s_{(1)}/(2s_{(1)}+1)}.$$

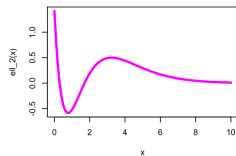
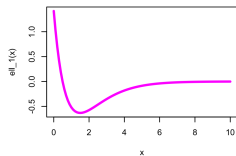
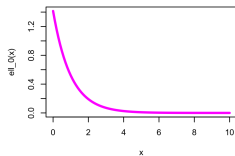
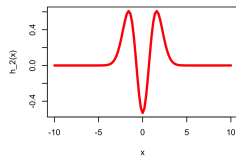
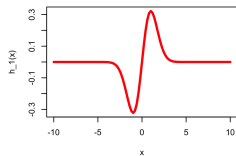
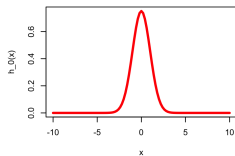
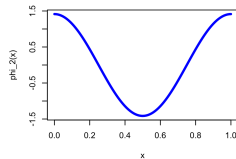
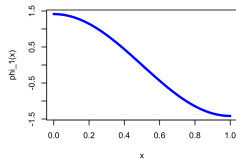
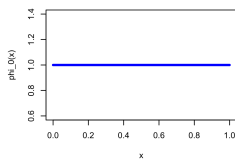
Example : Sobolev space associated with the (orthonormal) basis $(\varphi_j)_j$.
 $W(s, L) = \{f = \sum_{j \geq 0} \theta_j \varphi_j, \text{ such that } \forall J \geq 1, \sum_{j \geq J} \theta_j^2 \leq L^2 J^{-2s}\}.$

If $b_j \in W(s_j, L_j)$, $j \in \{1, \dots, K\}$, we can establish that

$$\inf_{h \in S_{m_j}} \|b_j - h\|^2 \leq L_j^2 m_j^{-2s_j}.$$

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First bases functions **Trigo [T]**, **Hermite [H]** et **Laguerre [L]**.

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Model Selection

We need to choose the dimension $\mathbf{m} = (m_1, \dots, m_K)$ from the family of dimensions :

$$\mathcal{M}_N = \{ \mathbf{m} \in \{1, \dots, N\}^K, \quad \forall i \in \{1, \dots, K\}, m_i \leq N \}.$$

And we select

$$\hat{\mathbf{m}} \in \arg \min_{\mathbf{m} \in \mathcal{M}_N} \left[U_N(\hat{\mathbf{b}}_{\mathbf{m}}) + \text{pen}(\mathbf{m}) \right], \quad \text{pen}(\mathbf{m}) = \kappa \|\sigma\|_{\infty}^2 \frac{|\mathbf{m}|}{N},$$

i.e., penalizing the least squares criterion with a term $\text{pen}(\mathbf{m})$ of the order of the variance.

In practice, we still need to estimate $\|\sigma\|_{\infty}^2$, which is unknown, by evaluating the supremum of the residual variance.

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Illustration 1 : $K = 3$ covariates

Simulation of $N = 200$ trajectories of :

$$Y_i(t) = b_1(t)X_{1,i}(t) + b_2(t)X_{2,i}(t) + b_3(t)X_{3,i}(t) + \varepsilon_i(t)$$

with

$$b_1(t) = \cos(2.8\pi t), \quad b_2(t) = 0.25 \exp(-t/3) - 2 \exp(-2t), \quad b_3(t) = 2t^2.$$

- $X_1(t) = 1$,
- $X_2(t)$ a Poisson process with parameter $\lambda = 0.5$,
- $X_{3,i}(t) = \mu_X(t) + \sum_{j=1}^{10} \rho_j \xi_{i,j} \phi_j(t)$ where $\mu_X(t) = t + \sin(t)$, and for $j \geq 1$, $\phi_j(t) = \sqrt{2} \sin((j - 1/2)\pi t)$, $\rho_j = 1/((j - 1/2)\pi)$, and the $\xi_{i,j}$ are i.i.d. $\mathcal{N}(0, 1)$.
- The noise $\varepsilon(t) = c_\varepsilon \sum_{j=11}^{20} \rho_j \xi_{i,j} \phi_j(t)$ with $c_\varepsilon = 7$ chosen to obtain a signal-to-noise ratio of approximately 2.

$$b_1(t) = \cos(2.8\pi t), \quad b_2(t) = 0.25 \exp(-t/3) - 2 \exp(-2t), \quad b_3(t) = 2t^2.$$

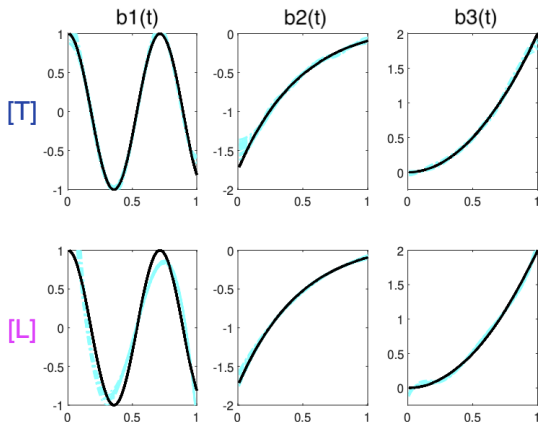


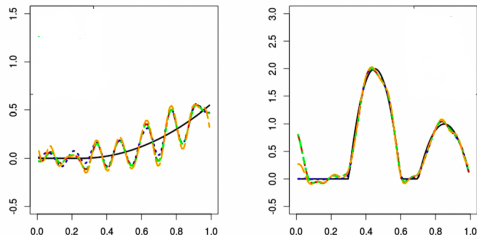
Figure – Estimation of $b_1(t)$, $b_2(t)$, and $b_3(t)$, with the $[T]$ basis (first row) and the $[L]$ basis (second row) for 25 repetitions ($N = 200$). Average dimensions selected : (5.6, 3.6, 5.5) for $[T]$ and (6.0, 2.0, 4.0) for $[L]$.

Illustration 2 : from Manrique et al. (2018)

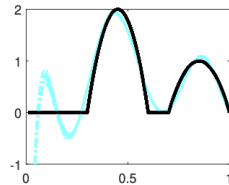
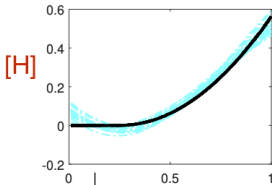
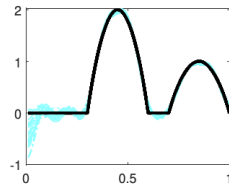
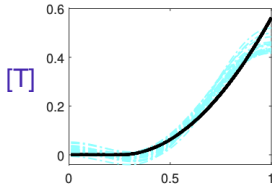
We compare our method to that of Manrique, Crambes & Hilgert (2018) :

$$Y_i(t) = b_1(t) + b_2(t)X_{i,1}(t) + \sigma(t)\varepsilon_i(t), \quad i = 1 \cdots N.$$

Figure from Manrique et al. (2018).



- $K = 1$ and the explanatory functional covariate $X_{i,1}$ is centered.
- "Ridge" regularization of the functional linear regression estimator.
- Convergence results under fairly general conditions (in particular, non-compact support).
- No guarantees of optimality and difficult to generalize for $K > 1$.



Manrique et al.

Basis [T]

Basis [H]

WASE

0.0150 (0.0097)

0.0032 (0.0015)

0.0642(0.0088)

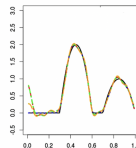
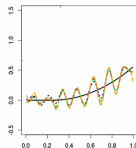


Illustration 3 : Real data

Electric consumption of devices in an eco-friendly house in Stambrugge, Belgium, from Candanedo et al. (2017)



Illustration 3 : Real data

19,728 measurements every 10 minutes over 137 days (144 measurements per day) of the electricity consumption of devices ($Y_i(t)$), $i = 1, \dots, 137$, $t \in [0, 24]$. $t = 0$ at 5 p.m, $t = 144$ at 4 :50 p.m. (+1 day)

$$X_1(t) = 100$$

$$X_2(t) : \text{outdoor temperature}$$

$$X_3(t) : \text{lighting}$$

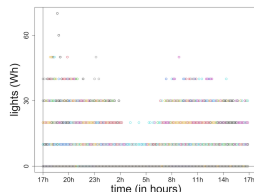
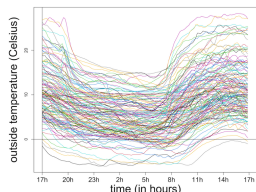
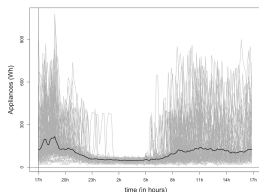


Illustration 3 : Real data

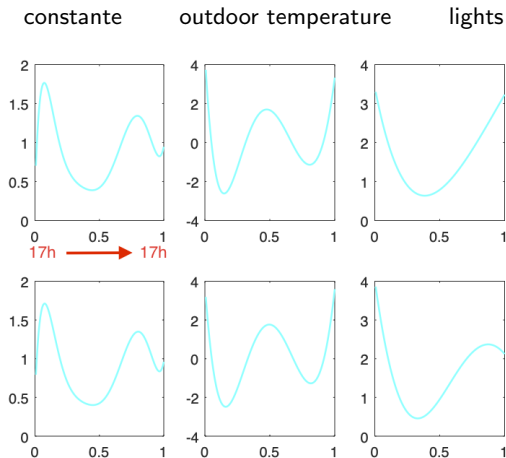


Figure – Electricity data. Estimation de $b_1(t)$ (left), $b_2(t)$ (middle) et $b_3(t)$ (right), base [L] (first line) et base [H] (second line). Selected dimensions are (8,5,5) and (8,5,4).

Conclusion

- We consider various continuous or non-continuous explanatory processes.
- Our method allows the simultaneous estimation of K functions : the method is computationally simple and fast.
- The model selection procedure allows for anisotropy.
- The convergence rates are proved to be optimal.
- Thanks to the additivity of the model, there is no curse of dimensionality. The convergence rate of $\hat{b}_m$ is associated with the lowest regularity of the functions to estimate b_k , $k = 1, \dots, K$.

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