Shifts estimation with M-estimators

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- Presentation of the problem
- Registering curves
- A semiparametric approach
- Main Theorems
    - Consistency
    - Asymptotic law
- Application to data

Observations : numerous and for different classes of subjects
$\longrightarrow$ The outcome of a study is a sample of noisy curve. There exists a function representing the common behaviour of the experiment and the data are deviations of this structural effect.

$$Y_{ij} = f \circ h_j(t_{ij}) + \sigma W_{ij},\ j = 1, \dots, J,\ i = 1, \dots, n_j.$$

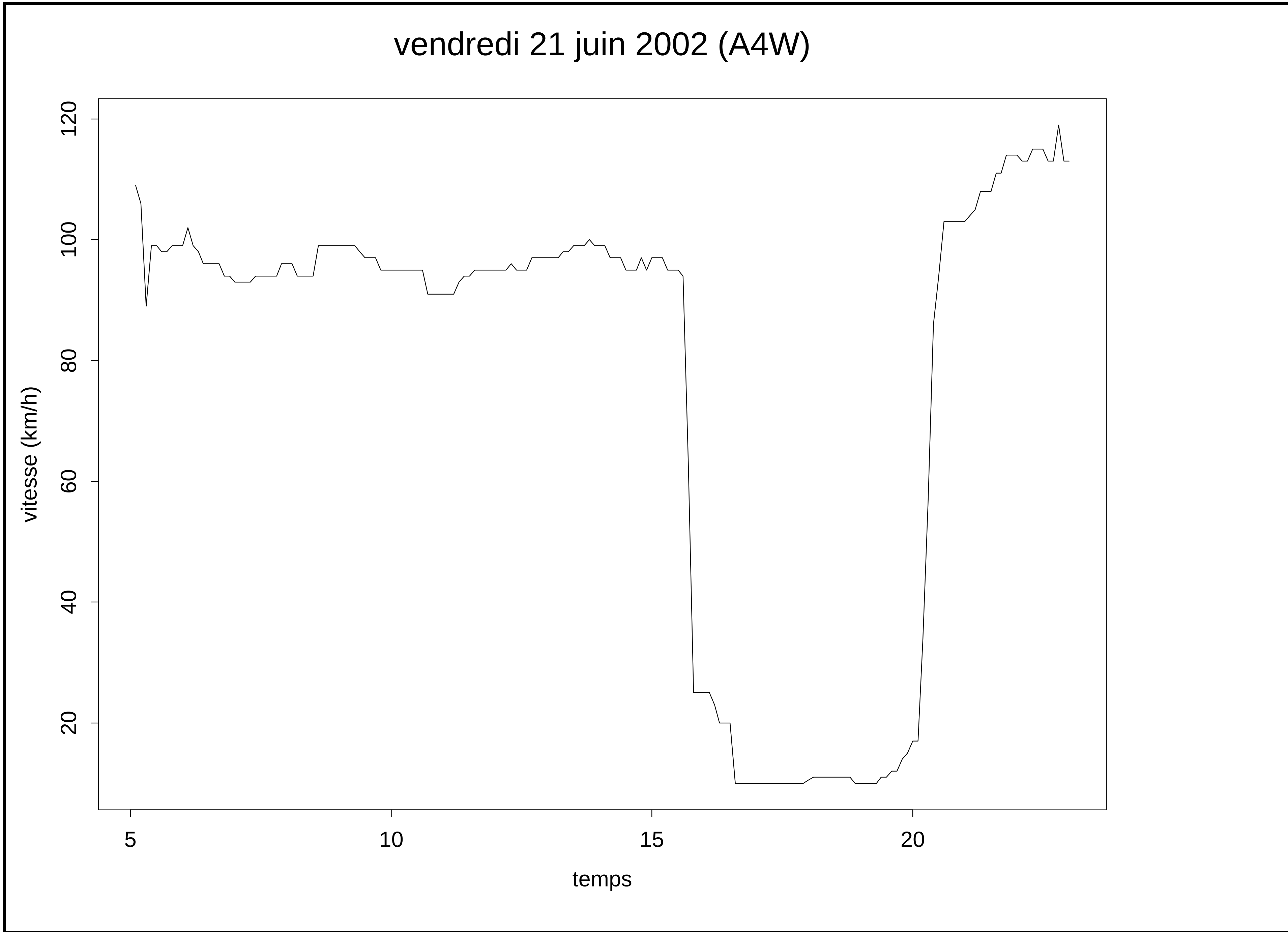
f feature studied in the experiment,
$j = 1, \dots, J$ number of different groups, $i = 1, \dots, n_j$ number of observations for one type j,
h_j warping functions, W_{ij} independent observation errors.

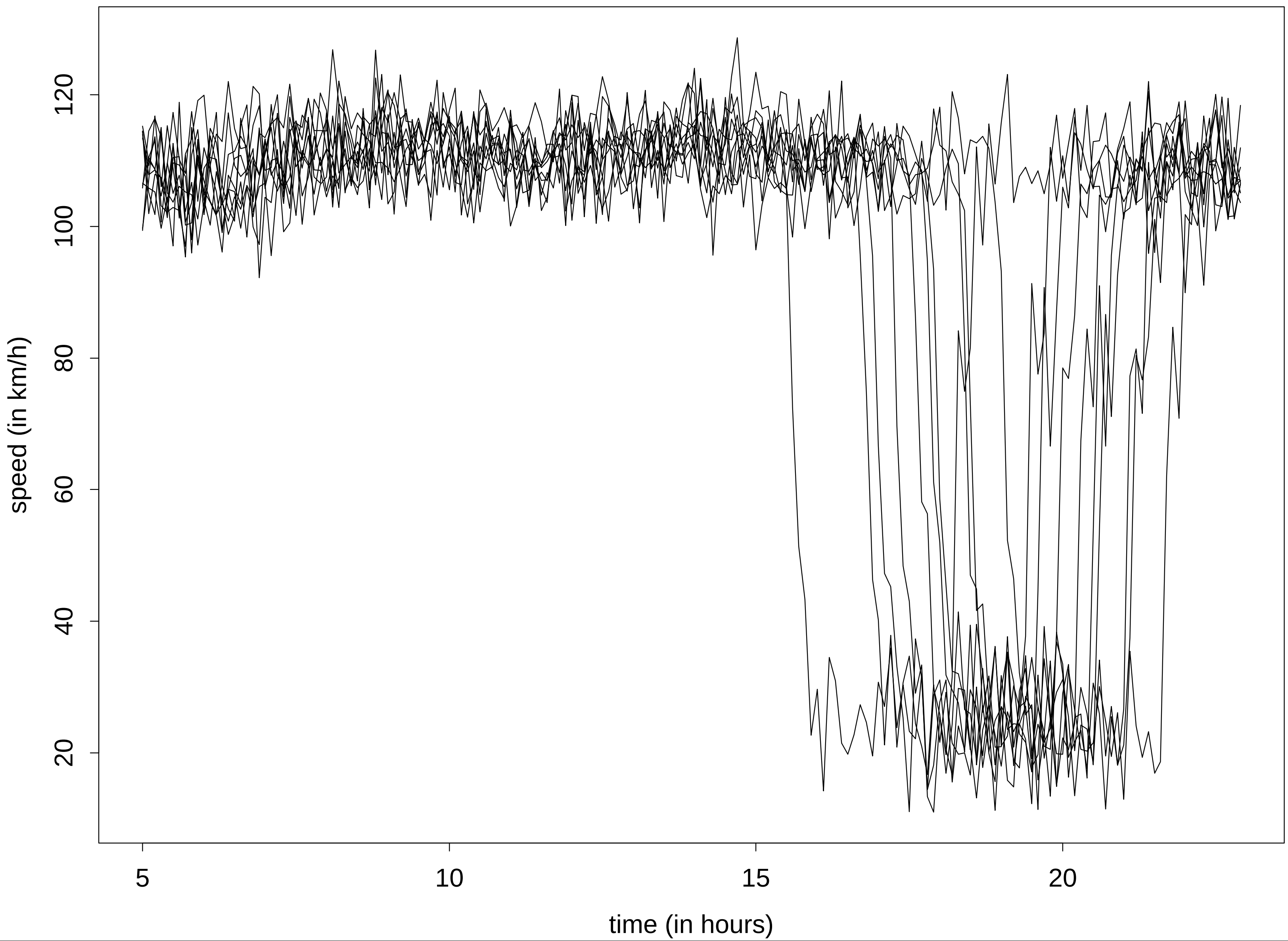
Examples :

- Velocity on the motorway after classification Lavielle, Loubes, Maza (2004)
- Growth curves.

Before estimating the trend f, necessity to rescale the data to prevent oversmoothing effects and to keep the structure of the feature.

One velocicty curve




speed (in km/h)
20
40
60
80
100
120
5
10
15
20
time (in hours)

- GOAL : estimate the structure of functions in the shift case where $f \circ h_j(.) = f(. - \theta_j^*)$, for θ_j^*, $j = 1, \ldots, J$
  Model : shift functions

$$Y_{ij} = f(t_{ij} - \theta_j^*) + \epsilon_{ij},\ j = 1, \ldots, J,\ i = 1, \ldots, n_j$$

  J is the number of curves (in each cluster) and n_i the number of observations for the j^{th}-curve. Take $n_j = n$, $\forall j$ and study the asymptotics $n \to \infty$. $\epsilon_{ij} \sim \mathcal{N}(0, \sigma^2)$, i.i.d
  Objective : provide estimates of the shifts $\hat{\theta}_j$, $j = 1, \ldots, J$, then estimate the function f using the rescaled observations.
  Provide a method that can be used in practie.

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  The unknown function f is a nuisance parameter that prevents the estimation of the parameter θ
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- Pattern recognition when the function f is known or one of the pattern is fixed. The problem tends into finding deformations of time, warping functions, that shift all the functions towards the chosen template. Work by Azencott (1994), Grenander (1991) or Piccioni and Trouvé (1998). But our function is **unknown**.

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- Curve fitting and characteristic points
  There exit characteristic points that locate maxima of the functions $f_j(.) = f(. - \theta_j^*)$, z_{jk}, $k = 1, \ldots, p$. Such methods estimate these points by a preliminary functional estimation then align all the points in a mean position. Work by Kneip and Gasser (1998)

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- Registered curve Work by Wang and Gasser (1999) or Ramsay (2001). Recursive method to solve the variational problem

$$\min_{\psi_j,\, j=1,\ldots,J} \int |\hat{f}_{j_0} \circ \psi_{j_0}(t) - \frac{1}{J} \sum_{k \neq j_0} \hat{f}_k \circ \psi_k(t)|^2 dt$$

$\longrightarrow$ Drawback : parametric estimation blurred by non parametric effect

Set $\hat{f}_j$, $j = 1, \ldots, m$ **kernel estimators** of the functions f_j.

- **Particular Point Method**

$$\forall k = 1, \ldots, p, \; \hat{z}_{jk} \text{ solutions of } \hat{f}_j'(z) = 0.$$

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$$\mathbf{E}[\hat{\psi}_i(t) - \psi_i(t)]^2 = O\left(b_n^2 + \sqrt{\frac{\log n}{n b_n^2}}\right)$$

with $b_n^2 = \mathbf{E}\|\hat{f}_j - f_j\|_2^2$.

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$\longrightarrow$ Non parametric rate of convergence.

First, we periodize the functions with C^∞ junction at the border. Let $T = 24$ hour be the period. Using the FFT algorithm, we consider :

Model of Fourier coefficients

$$d_{jl} = \exp(-il\alpha_j^*)c_l(f) + w_{jl},\ l = -\frac{n-1}{2}, \ldots, \frac{n-1}{2},\ j = 1, \ldots, J.$$

$w_{jl} \sim \mathcal{N}(0, \frac{\sigma^2}{n})$, i.i.d : random noise
$c_l(f), \in \mathbb{Z}$: Fourier coefficients of the true function f.
$\alpha_j^* = \frac{2\pi}{T}\theta_j^*$ the shift to be estimated, $\alpha^* = (\alpha_j^*)'_{j=1,\ldots,J}$
Objective : contruction of an estimator directly from the data d_{jl} without prior functional estimation. For this, define for $\alpha = (\alpha_1, \ldots, \alpha_J)' \in [0, T]^J$ the rescaled observations and their mean

$$\tilde{d}_{jl}(\alpha) = \exp(il\alpha_j)d_{jl} = \exp(il[\alpha_j - \alpha_j^*])c_l(f) + \exp(il\alpha_j)w_{jl},$$

$$\hat{d}_l = \frac{1}{J}\sum_{j=1}^{J}\tilde{d}_{jl}(\alpha).$$

Minimum contrast method : $\hat{\alpha} = \arg \min_{[0,T]^J} \left(M_n(\alpha) + \lambda_n^2 \sum_{j=1}^{J} |\alpha_j| \right)$

- Choice of empirical contrast.

  $\forall l \in \mathbb{Z}^*$, set $\delta_l \to 0$ and define :

$$\forall \alpha \in \mathbb{R}^J,\ M_n(\alpha) = \sum_{l=-\frac{n-1}{2}}^{\frac{n-1}{2}} \frac{1}{J} \sum_{j=1}^{J} \quad |\tilde{d}_{jl} - \frac{1}{J} \sum_{j=1}^{J} \tilde{d}_{jl}|^2.$$

Minimum contrast method : $\hat{\alpha} = \arg\min_{[0,T]^J} \left(M_n(\alpha) + \lambda_n^2 \sum_{j=1}^{J} |\alpha_j| \right)$

- Choice of empirical contrast. Smoothing effect

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Necessity of δ_l to have consistency and build a smooth contrast that can be minimized(links with Bayesian methodology of Dalayan, Golubev, Tsybakov)

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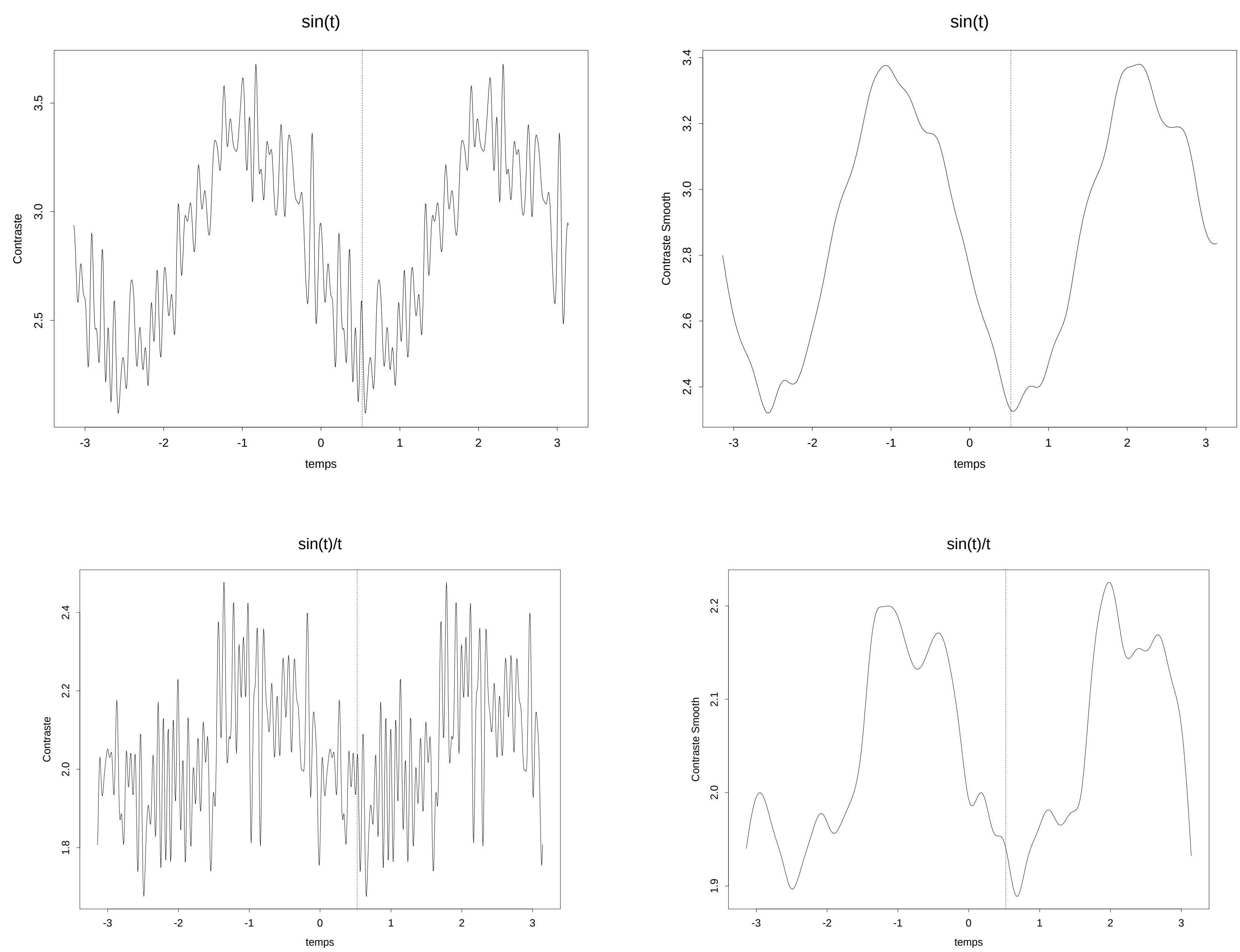
- Assumptions (A) $\quad \sum_l |c_l(f)|^2 < +\infty$

$$\sum_l l^2 |\delta_l|^2 < +\infty.$$


sin(t)
Contraste
temps
sin(t)
Contraste Smooth
temps
sin(t)/t
Contraste
temps
sin(t)/t
Contraste Smooth
temps

If $\alpha \notin \mathbb{Q}$, the dynamical system $T : X \to X + \alpha$ over $\mathbb{T}$ has an invariant measure λ and the only stable sets are $\mathbb{T}$ and the null space.

$\longrightarrow$ **ergodic theorem**

$T: \quad [0,T]^J \longrightarrow [0,T]^J, \quad (\theta_1, \ldots, \theta_J) \longrightarrow (\theta_1 + \alpha_1, \ldots, \theta_J + \alpha_J)$

$$\text{empirical process} : Z_n(\alpha) = \frac{1}{\sqrt{n}} \sum_{l=-n}^{n} \cos(l\alpha)\xi_l$$

$$\mathrm{Var}(Z_n(\alpha)) \to \kappa \int_0^{2\pi} \cos^2\theta \, d\theta = \sigma^2,$$

$$\mathrm{Cov}(Z_n(\alpha) Z_n(\alpha^{'})) \to \kappa \int_{[0,2\pi]^2} \cos\theta_1 \; \cos\theta_2 d\theta_1 d\theta_2 = 0.$$

“Convergence” of the marginals to a **white noise**

$$(Z_n(\alpha_1), \ldots, Z_n(\alpha_J)) \xrightarrow{\mathcal{L}} \mathcal{N}_J(0, \sigma^2 Id_J).$$

But no rate of convergence for process.

Contrast : $\forall \alpha \in \mathbb{R}^J$, $M_n(\alpha) = \sum_{l=-\frac{n-1}{2}}^{\frac{n-1}{2}} \frac{1}{J}\sum_{j=1}^{J} \delta_l^2 |\tilde{d}_{jl} - \frac{1}{J}\sum_{j=1}^{J} \tilde{d}_{jl}|^2.$

Theorem 1 For δ_l satisfying assumptions (A), and $\lambda_n^2 \to 0$ we get

$$M_n(\alpha) \xrightarrow{P_{\alpha^*}} K(\alpha, \alpha^*) \sim -\int_0^T |\frac{1}{J}\sum_{j=1}^{J} f * \psi(u + \theta_j - \theta_j^*)|^2 du$$

For $W(n, \eta) = \sup\{|M_n(\alpha) - M_n(\beta)|,\ \|\alpha - \beta\| \leq \eta\}$, for any $\epsilon_k \to 0$ and $\eta_k \to 0$ we have

$$\lim_{n\to\infty} \mathbf{P}_{\alpha^*}[W(n, \eta_k) > \epsilon_k] = 0.$$

$$\Longrightarrow \hat{\alpha}_n = \arg \min_{\alpha \in [0,T]^J} \left(M_n(\alpha) + \lambda_n^2 \sum_{j=1}^{J} |\alpha_j| \right) \xrightarrow{P_{\alpha^*}} \alpha^*.$$

Consistency of the penalized M-estimator

$M_n(\alpha) = \sum_{l=-\frac{n-1}{2}}^{\frac{n-1}{2}} \frac{1}{J} \sum_{j=1}^{J} \delta_l^2 |\tilde{d}_{jl} - \frac{1}{J} \sum_{j=1}^{J} \tilde{d}_{jl}|^2 =$ determinist term + stochastic term. Set ξ_l^x, ξ_l^y i.i.d $\mathcal{N}(0,1)$, and $\kappa_1, \kappa_2, \kappa_3$ constants such that

- $\kappa_1 \frac{1}{n} \sum_{l=-\frac{n-1}{2}}^{\frac{n-1}{2}} \delta_l^2 \frac{1}{J} \sum_{j=1}^{J} (|\xi_l^x|^2 + |\xi_l^y|^2) \rightarrow$ constant by LLN.

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- $\kappa_2 \frac{1}{\sqrt{n}} \sum_{l=-\frac{n-1}{2}}^{\frac{n-1}{2}} \delta_l^2 |c_l| \xi_l^x \xrightarrow{P_{\alpha^*}} 0$ since $\| \sum_l \delta_l^2 c_l(f) \xi_l^x \|_2^2 < \infty$, due to regularity conditions on f.

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- $\kappa_3 \frac{1}{n} \sum_{l=-\frac{n-1}{2}}^{\frac{n-1}{2}} \frac{1}{J^2} \sum_{j,k=1}^{J} \delta_l^2 \cos(l[\alpha_j + \alpha_k]) \xi_{jl}^x \xi_{kl}^y \xrightarrow{P_{\alpha^*}} 0$ due to concentration and choice of δ_l to gain uniformity of the convergene.

$\longrightarrow$ the penalized M-estimator

$\hat{\alpha}_n = \arg\min_{\alpha \in [0,T]^J} \left(M_n(\alpha) + \lambda_n^2 \sum_{j=1}^{J} |\alpha_j| \right)$ is convergent.

All the results are given for $J \geq 3$.

By Taylor's expansion we get :

Theorem 2 Under the assumption that $\sqrt{n}\lambda_n^2 \to 0$, we get the asymptotic normality of $\hat{\alpha}_n$.

$$\sqrt{n}(\hat{\alpha}_n - \alpha^*) \xrightarrow{\mathcal{L}} \mathcal{N}(0, \Gamma),$$

with

$$\Gamma = \frac{(J-1)\sum_{l\in\mathbb{Z}} l^2\delta_l^2}{J^6(J-2)^2(\sum_{l\in\mathbb{Z}} \delta_l l^2 |c_l(f)|)^2} V(J).$$

The variance depends on the choice of δ_l, $l \in \mathbb{Z}^*$ and least favorable case is :

$$\sqrt{nI_n(f)}(\hat{\alpha}_n - \alpha^*) \xrightarrow{\mathcal{L}} \mathcal{N}(0, V(J))$$

where $I_n(f) = \sum_l l^2 c_l(f)^2 = \|f'\|^2$ and a choice $\delta_l \approx c_l(f)$.

So the assumption over δ_l leads to $\boxed{\sum_l l^2 c_l(f)^2 < +\infty}$

$$\frac{\partial}{\partial \alpha_k} M_n(\alpha) = \sum_l l\delta_l(V_l + W_l) = \frac{2(J-1)}{J^2} \sum_{l=-\frac{n-1}{2}}^{\frac{n-1}{2}} l \,\mathrm{Im}\left[\overline{\hat{d}_l}(\alpha)\tilde{d}_{kl}(\alpha)\right].$$

Lemma 1 A be a symetric matrix such that $I - 2A > 0$

$$\log \mathbf{E}(e^{<t,X>+X'AX}) = \frac{1}{2}\|(I-2A)^{-\frac{1}{2}}t\|^2 - \frac{1}{2}\log\det(I-2A)$$

Proposition 1 Let c_l, $l \in \mathbb{Z}^*$, $\sum_l \|c_l\|^2 < +\infty$. Let $Y_1, \ldots, Y_n$ be an i.i.d sample of Y a centered random variable, $B_l \in \mathcal{M}_{k\times k}(\mathbb{R})$ a symetric matrix such that $\mathbf{E}(X'B_lX) = 0$, $\forall l$. Set $T_n = \left(\sum_{l=1}^n < c_l, Y_l >, \frac{1}{\sqrt{n}} \sum_{l=1}^n Y_l' B_l Y_l\right)'$, we get :

$$T_n \xrightarrow{\mathcal{L}} \mathcal{N}_2\left(0, V\right) \quad \text{where,}$$

$$V \in M_{2\times 2}(\mathbb{R}),\ V_{12} = V_{21} = 0,\ V_{11} = \sum_{l=1}^{\infty} |c_l|^2,\ V_{22} = \sum_{l=1}^{\infty} \mathbf{E}(X'B_lX)^2.$$

$$W_l = \sum_{j=1}^{J} \sin[l(\alpha_k^* - \alpha_j^*)](w_{kl}^x w_{jl}^x + w_{kl}^y w_{jl}^y) + \cos[l(\alpha_k^* - \alpha_j^*)](w_{kl}^y w_{jl}^x - w_{kl}^x w_{jl}^y)$$

$$= Y^{'} B_l Y = Y^{'} \underbrace{\frac{B_l + B_l^{'}}{2}}_{B_l^s} Y$$

with $Y = (w_{1l}^x \dots w_{Jl}^x \, w_{1l}^y \dots w_{Jl}^y)^{'}$ and B defined by blocks $B = (L_1, \dots, L_{2J})^{'}$

$L_k =$

$(\sin(l(\alpha_k^* - \alpha_1^*)), \dots, \sin(l(\alpha_k^* - \alpha_J^*)), -\cos(l(\alpha_k^* - \alpha_1^*)), \dots, -\cos(l(\alpha_k^* - \alpha_J^*)))$

$L_{k+J} =$

$(\cos(l(\alpha_k^* - \alpha_1^*)), \dots, \sin(l(\alpha_k^* - \alpha_1^*)), \dots, \sin(l(\alpha_k^* - \alpha_J^*)), \dots, \cos(l(\alpha_k^* - \alpha_J^*)))$

Proof of Theorem : let $v \in \mathbb{R}$ such that $I - \frac{2v}{\sqrt{n}} B_l^s > 0, \ \forall l \in \mathbb{Z}^*$. Set

$W = (u, v)^{'}$

$$\log \mathbf{E}\left(e^{<W,T_n>}\right) = \frac{1}{2} \sum_{j=1}^{n} \|(I - \frac{2v}{\sqrt{n}} B_l^s)^{-1/2} u c_l\|^2 - \frac{n}{2} \sum_{l} \log\det(I - 2\frac{2v}{\sqrt{n}} B_l^s)$$

With the definition of the symetrized version of the weight matrix B_l^s, $l \in \mathbb{Z}^*$

$$\mathrm{Trace}(B_l^s) = (J-1)l\delta_l^2, \quad \rho(B_l^s) \leq 2Jl\delta_l^2$$

Set to apply the previous lemmas to

$$T_n^{'} = \left(\sum_{l=1}^{n} < l\delta_l^2 c_l, Y_l >, \frac{1}{\sqrt{n}} \sum_{l=1}^{n} Y_l^{'} B_l^s Y_l \right)$$

and get the following asymptotic behaviour

$$T_n \xrightarrow{\mathcal{L}} \mathcal{N}_2 \left(0, \begin{pmatrix} \sum_l l^2 \delta_l^4 |c_l|^2 & 0 \\ 0 & \sigma^2 (J-1) \sum_l l\delta_l^2 \end{pmatrix} \right)$$

For the second derivative we get :

$$\frac{\partial^2}{\partial \alpha_j \partial \alpha_k} M_n(\alpha) = \frac{J-1}{J^3} \sum_{l=-\frac{n-1}{2}}^{\frac{n-1}{2}} 2l^2 \delta_l^2 \mathrm{Re}(e^{il(\alpha_k - \alpha_j)} \bar{d}_{jl} d_{kl}).$$

3 terms to study :

- $$\sum_{l=-\frac{n-1}{2}}^{\frac{n-1}{2}} l^2\delta_l^2|c_l|^2\cos[l(\alpha_k-\alpha_k^*+\alpha_j^*-\alpha_j)]$$

- $$\sum_{l=-\frac{n-1}{2}}^{\frac{n-1}{2}} l^2\delta_l^2\cos[l(\alpha_k-\alpha_j)]\epsilon_{jl}^x\epsilon_{kl}^x=\frac{1}{n}\sum_{l=-\frac{n-1}{2}}^{\frac{n-1}{2}} l^2\delta_l^2\cos[l(\alpha_k-\alpha_j)]\xi_{jl}^x\xi_{kl}^x$$

- $$\sum_{l=-\frac{n-1}{2}}^{\frac{n-1}{2}} l^2\delta_l^2c_l^x\cos(l\alpha_j^*)\epsilon_{kl}^x=\frac{1}{\sqrt{n}}\sum_{l=-\frac{n-1}{2}}^{\frac{n-1}{2}} l^2\delta_l^2c_l^x\cos(l\alpha_j^*)\xi_{kl}^x.$$

Under the assumptions over δ_l, $l\in\mathbb{Z}^*$ and c_l, $l\in\mathbb{Z}^*$, concentration of empirical process give uniform convergence to an invertible matrix.

The optimization algorithm is a quadratic minimization of a functional of J variables

Using Krylov's methods such as conjugate gradient algorithm
$\longrightarrow$ Fourier transform of the model, via an FFT algorithm.
$\longrightarrow$ convergence in J steps.

- Efficient method for curve regitration

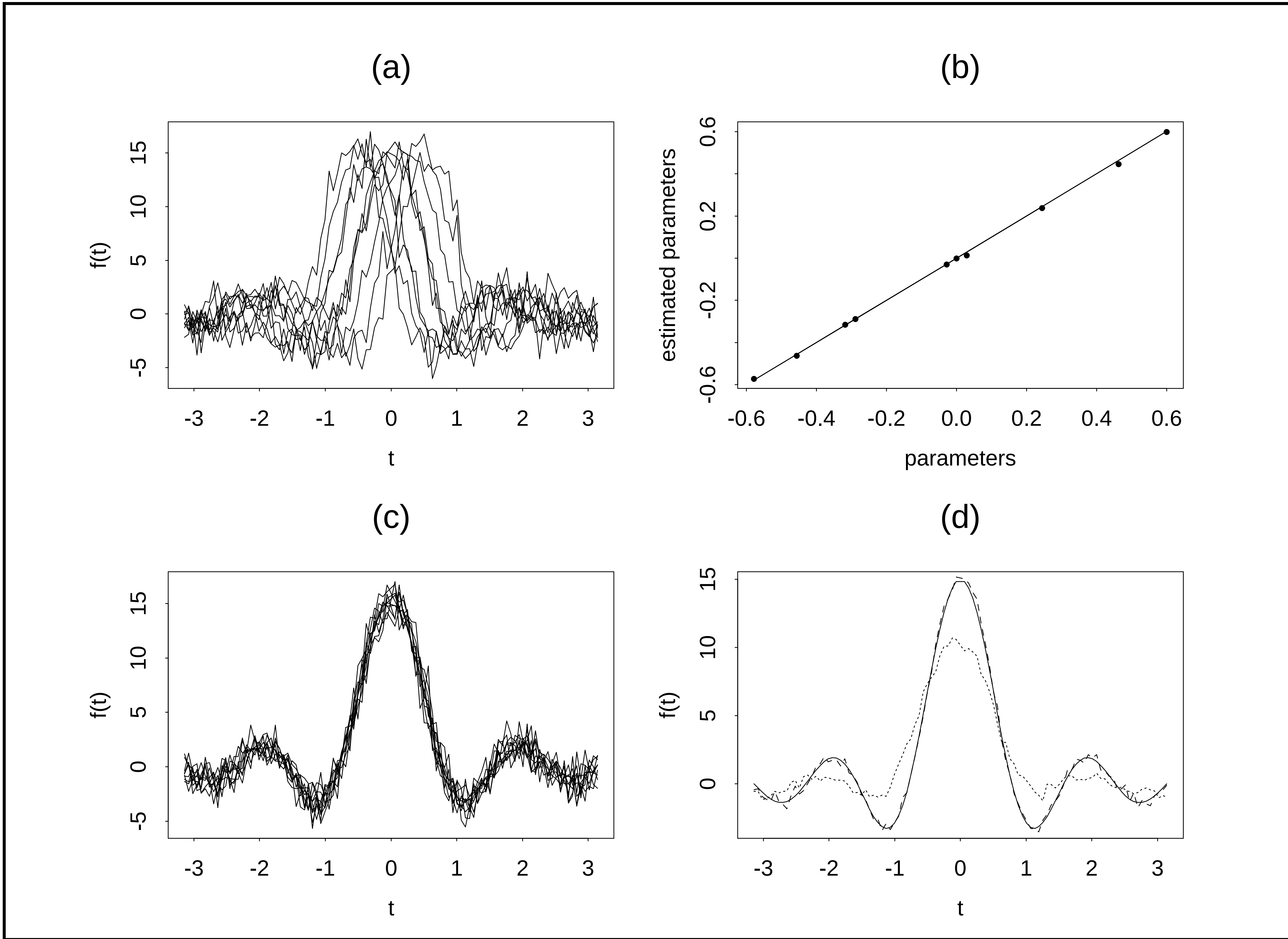
  For simulated data as well as real data
  in the cases where $f = f_j$ (the functions differ slightly).

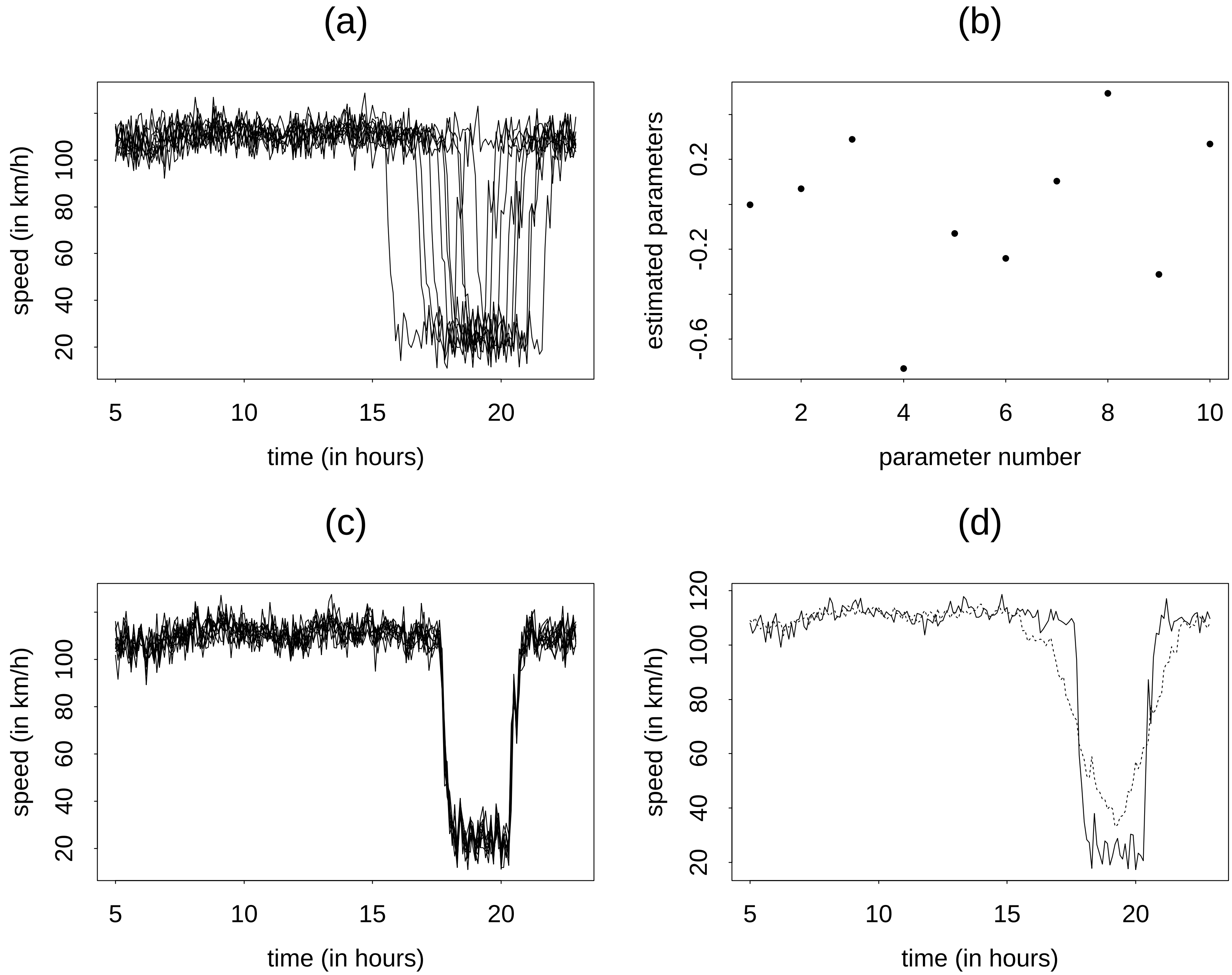
- Semi-parametric method

  The shifts estimation is not blurred by the non-parametric effect.
  Parametric rate of convergence for the parameters.

- Projects

  For growth curves or medical data, other asymptotics : $n < +\infty$ (probably small) and $J = J_m \to +\infty$.


(a)
f(t)
-5
0
5
10
15
-3
-2
-1
0
1
2
3
t
(b)
estimated parameters
-0.6
-0.2
0.2
0.6
-0.6
-0.4
-0.2
0.0
0.2
0.4
0.6
parameters
(c)
f(t)
-5
0
5
10
15
-3
-2
-1
0
1
2
3
t
(d)
f(t)
0
5
10
15
-3
-2
-1
0
1
2
3
t


(a)
speed (in km/h)
20 40 60 80 100
5 10 15 20
time (in hours)
(b)
estimated parameters
-0.6 -0.2 0.2
2 4 6 8 10
parameter number
(c)
speed (in km/h)
20 40 60 80 100
5 10 15 20
time (in hours)
(d)
speed (in km/h)
20 40 60 80 100 120
5 10 15 20
time (in hours)