Prediction and testing of mixtures of features issued from a continuous dictionary

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Industrial motivation: spectroscopy

Wave numbers (cm-1)	Peak assignment
3690-3400-3364-3200-3014	-OH
2952-2920-2850	$\nu - CH_2, CH_3$ Aliphatic
1731	$\nu - C = O$
1647	$\nu - C = C \text{ de } HC = CH_2$
1540	$\nu - C = C \text{ de R-CR} = \text{CH-R}, \delta \text{ CH2}$ Aliphatic
1419	δCH_2 , δ -CH Aliphatic
1160-1082	ν Si-O (SiO ₂)
1009-909	ν Si-O (Si-OH)
825	C-Cl
664	CH Aromatic

Location of absorption spikes of chemical components for polychloroprene samples ([Tchalla, 2017]).





Goal: recover from y the parameters β^* and $\vartheta^* = (\theta_1^*, \cdots, \theta_s^*)$.

Motivation : low-pass filter



• I The model

• II Estimation and Prediction

• III Tests

I The model

The model

We observe a random element y of a Hilbert space H_T (e.g.: \mathbb{R}^T , $L^2(\lambda_T),...$) with scalar product $\langle \cdot, \cdot \rangle_T$ (and norm $\|\cdot\|_T$).



Notations

- *T* increases with the amount of information of the observation (number of grid points, 1/noise level...).
- $\theta_k^{\star} \in \Theta \subset \mathbb{R}$ and $\beta_k^{\star} \in \mathbb{R}$, for all k.
- Continuous dictionary (φ_T(θ), θ ∈ Θ) of elements of H_T of norm 1. The map φ_T is continuous on Θ.
- w_T Gaussian process.

The model: Gaussian noise (I)

Assumptions on the noise (H1)

For all $f \in H_T$, the random variable $\langle f, w_T \rangle_T$ is centered Gaussian with:

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\operatorname{Var}\left(\langle f, w_T \rangle_T\right) \leq \Delta_T \|f\|_T^2.
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Ex: spectroscopy

- Regular grid: $t_1 < \cdots < t_T$ on \mathbb{R} with step-size $\Delta_T = \frac{t_T - t_1}{T}$.
- Observations: y(t_i) = signal(t_i) + w_T(t_i), 1 ≤ i ≤ T.
- Noise: $w_T(t_i)$ i.i.d $\sim \mathcal{N}(0, 1)$.

$$\begin{array}{lll} H_{\mathcal{T}} &=& L^2(\lambda_{\mathcal{T}}) & \text{where} & \lambda_{\mathcal{T}}(\mathrm{d} t) &= \\ \Delta_{\mathcal{T}} \sum_{j=1}^{\mathcal{T}} \delta_{t_j}(\mathrm{d} t). & \end{array}$$



 $\Delta_T = \text{step-size}$.

The model: Gaussian noise (II)

Assumptions on the noise (H1)

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 $\operatorname{Var}\left(\langle f, w_T \rangle_T\right) \leq \Delta_T \|f\|_T^2.$

Ex: low-pass filter

- Observations: (y(t), t ∈ ℝ/ℤ) s.t y ∈ L²(Leb).
- Truncated white noise: $w_T = \frac{1}{\sqrt{T}} \sum_{k=1}^T G_k \psi_k,$

 $-G_k \text{ i.i.d} \sim \mathcal{N}(0, 1),$ $-(\psi_k, k \in \mathbb{N}) \text{ o.n.b. of } L^2(\text{Leb}).$

Thus $||w_T||_{L^2(\text{Leb})}$ is of order 1.



II Estimation and Prediction

Estimators

Estimators

 $\begin{aligned} & (\hat{\beta}, \hat{\vartheta}) \in \operatornamewithlimits{argmin}_{\beta \in \mathbb{R}^{K}, \vartheta \in \Theta_{T}^{K}} \quad \frac{1}{2} \| y - \beta \Phi_{T}(\vartheta) \|_{T}^{2} + \kappa \| \beta \|_{\ell_{1}}. \qquad (\mathcal{P}_{1}(\kappa)) \\ \bullet \ K \text{ is an upper bound for } s. \qquad \Phi_{T}(\vartheta) \in H_{T}^{K} \text{ is defined by:} \\ \bullet \ \Theta_{T} \text{ is a compact interval.} \qquad \Phi_{T}(\vartheta) = (\phi_{T}(\theta_{1}), \dots, \phi_{T}(\theta_{K}))^{\top}. \end{aligned}$

• $\kappa > 0$ tuning parameter.

Estimators

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 $(\hat{\beta}, \hat{\vartheta}) \in \operatorname{argmin}_{\beta \in \mathbb{R}^{K}, \vartheta \in \Theta_{T}^{K}} \quad \frac{1}{2} \|y - \beta \Phi_{T}(\vartheta)\|_{T}^{2} + \kappa \|\beta\|_{\ell_{1}}. \qquad (\mathcal{P}_{1}(\kappa))$ • K is an upper bound for s. $\Phi_{T}(\vartheta) \in H_{T}^{K} \text{ is defined by:}$

 $\Phi_{\mathcal{T}}(\vartheta) = (\phi_{\mathcal{T}}(\theta_1), \dots, \phi_{\mathcal{T}}(\theta_K))^{\top}.$

- Θ_T is a compact interval.
- $\kappa > 0$ tuning parameter.







$$\Phi_{\mathcal{T}}(\hat{\vartheta}) = (\phi_{\mathcal{T}}(\hat{\theta}_1), \dots, \phi_{\mathcal{T}}(\hat{\theta}_{\mathcal{K}}))^\top,$$



Estimation: estimation risks (I)



Estimation: estimation risks (II)

Estimators Let $(\hat{\beta}, \hat{\vartheta}) \in \mathbb{R}^{K} \times \Theta^{K}$ be measurable functions of y solutions of $(\mathcal{P}_{1}(\kappa))$ "approximating" $(\beta^{\star} = (\beta_{1}^{\star}, \cdots, \beta_{s}^{\star}), \vartheta^{\star} = (\theta_{1}^{\star}, \cdots, \theta_{s}^{\star}))$. We define: **Estimation risks (II)**





The Beurling Lasso [De Castro & Gamboa, 2012]

$$\min_{\mu \in \mathcal{M}(\Theta_{T})} \quad \frac{1}{2} \| y - \langle \phi_{T}, \mu \rangle \|_{T}^{2} + \kappa \| \mu \|_{TV}. \tag{$\mathcal{P}_{2}(\kappa)$}$$

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$$\mathcal{P}_1(\kappa)$$
 and $\mathcal{P}_2(\kappa)$

- Existence of a solution to $\mathcal{P}_2(\kappa)$ [Bredies & Pikkarainen, 2013].
- If $\mathcal{P}_2(\kappa)$ admits a solution $\hat{\mu} = \sum_{k=1}^{K} \hat{\beta}_k \delta_{\hat{\theta}_k}$ then $(\hat{\beta}, \hat{\vartheta})$ is a solution to $\mathcal{P}_1(\kappa)$.
- If H_T has finite dimension K, then there exists a solution to P₂(κ) with K atoms at most, [Boyer et al, 2019].

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Ex : low-pass filter

The observation space is $H_T = L^2$ (Leb).



$$\min_{\mu \in \mathcal{M}(\Theta_{\mathcal{T}})} \quad \frac{1}{2} \| y - \langle \phi_{\mathcal{T}}, \mu \rangle \|_{\mathcal{T}}^2 + \kappa \| \mu \|_{\mathcal{T}V}. \tag{$\mathcal{P}_2(\kappa)$}$$

 $\mathcal{P}_1(\kappa)$ and $\mathcal{P}_2(\kappa)$

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Numerical implementation

 Modified Frank-Wolfe algorithm [Boyd, Schiebinger & Recht, 2017], [Denoyelle, Duval, Peyré & Soubies 2020], [Globabae & Poon, 2022].

Estimation: why gridless methods



- Discrete grid of K points $\vartheta^{\mathcal{G}} = (\theta_1^{\mathcal{G}}, \cdots, \theta_K^{\mathcal{G}}).$
- Solve the Lasso problems:

$$\hat{\beta} \in \operatorname*{argmin}_{\beta \in \mathbb{R}^{K}} \quad \frac{1}{2} \| y - \beta \Phi_{\mathcal{G}} \|_{T}^{2} + \kappa \| \beta \|_{\ell_{1}},$$

where $\Phi_{\mathcal{G}} = (\phi_{\mathcal{T}}(\theta_1^{\mathcal{G}}), \cdots, \phi_{\mathcal{T}}(\theta_K^{\mathcal{G}}))^{\top}$.



Estimation: why gridless methods



Inconvenients related to the refinement of the grid on $\boldsymbol{\Theta}$

- Strong correlations between the lines $\Phi_{\mathcal{G}} \implies$ numerical problems.
- The size of the grid grows exponentially with d when $\Theta \subset \mathbb{R}^d$.
- In the location model: clusters of spikes in the neighbourhood of the true spikes [Duval & Peyré, 2017].

Estimation: numerical aspects (Blasso V Lasso on a grid)

- Numerical experiment

• Signal in $H_T = \mathbb{R}^T$ with T = 100, mixture of two Gaussian-shaped spikes with $\theta_1^{\star} = 0$ and $\theta_2^{\star} = 3$ and amplitudes in [-10,10] uniformly distributed, corrupted by i.i.d. centered Gaussian r. v. with $\sigma = 0.1$.





Estimation: gridless methods



Estimation: assumptions (I)

Smoothness of the dictionary functions (H2)

• $\phi_T(\theta) = \varphi_T(\theta) / \|\varphi_T(\theta)\|_T$.

• $\varphi_T : \Theta \to H_T$ is C^3 . • $\|\varphi_T(\theta)\|_T > 0$ on Θ .

• $\|\partial_{\theta}\phi_T(\theta)\|_T^2 > 0$ on Θ .



Estimation: assumptions (II)

Kernel and approximating kernel

We define a kernel on Θ^2 to measure the correlation between components of the dictionary:

$$\mathcal{K}_{\mathcal{T}}(\theta, \theta') = \langle \phi_{\mathcal{T}}(\theta), \phi_{\mathcal{T}}(\theta') \rangle_{\mathcal{T}},$$

and an approximating symmetric kernel $\mathcal{K}^{\text{prox}}$ sur Θ_{∞}^2 .

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Ex: spectroscopy

If $\Delta_T \rightarrow 0$ and $\sigma_T = cst$,

$$\mathcal{K}^{\mathsf{prox}} = \lim_{T \to +\infty} \mathcal{K}_T.$$

Assumptions on the approximating (H3)

The kernel $\mathcal{K}^{\text{prox}}$ is $\mathcal{C}^{3,3}$ with bounded derivatives + other smoothness assumptions. It is locally concave on the diagonal and strictly less than 1 outside the diagonal.

Estimation: assumptions (III)

Fisher-Rao metric on the space of parameters

$$\mathfrak{d}_{\mathcal{K}}(heta, heta') = \inf_{\gamma} \int_{0}^{1} |\dot{\gamma}_{s}| \sqrt{\partial_{x,y} \mathcal{K}(\gamma_{s},\gamma_{s})} \, \mathrm{d}s$$

inf. on the set of smooth paths $\gamma : [0,1] \to \Theta$ such that $\gamma_0 = \theta$ and $\gamma_1 = \theta'$. $\to \text{invariance } \mathfrak{d}_{\mathcal{K}_{\varphi}}(\theta, \theta') = \mathfrak{d}_{\mathcal{K}_{\varphi \circ h}}(h^{-1}(\theta), h^{-1}(\theta')).$

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Univariate examples

• Translated spikes model (spectroscopy / low-pass filter):

 $\mathfrak{d}_{\mathcal{K}_{\mathcal{T}}}(\theta, \theta') \sim |\theta - \theta'|$ (Euclidean distance).

• Scale model: $H = L^2(\text{Leb})$ and $\varphi(\theta) = e^{-\cdot\theta}$ with $\Theta = \mathbb{R}^*_+$ and

 $\mathfrak{d}_{\mathcal{K}_{\mathcal{T}}}(\theta, \theta') \propto |\log(\theta/\theta')|.$

We have $\mathfrak{d}_{\mathcal{K}_{\mathcal{T}}}(\theta, \theta + \varepsilon) \xrightarrow[\theta \to 0]{} + \infty$ (\neq Euclidean distance).

Estimation: assumptions (IV)

Proximity of $\mathcal{K}_{\mathcal{T}}$ and $\mathcal{K}^{\text{prox}}$

• Proximity between kernels:

$$\mathcal{V}_{\mathcal{T}} = \max_{i,j \in \{0,\cdots,3\}} \sup_{\Theta_{\mathcal{T}}^2} |\mathcal{K}_{\mathcal{T}}^{[i,j]} - \mathcal{K}^{\mathsf{prox}[i,j]}|.$$

• equivalent metrics $: \mathfrak{d}_{\mathcal{K}_{\mathcal{T}}}$ and $\mathfrak{d}_{\mathcal{K}^{\text{prox}}} : = \mathfrak{d}_{\mathcal{K}^{\text{prox}}} / \rho_{\mathcal{T}} \leq \mathfrak{d}_{\mathcal{K}_{\mathcal{T}}} \leq \rho_{\mathcal{T}} \mathfrak{d}_{\mathcal{K}^{\text{prox}}}$

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Proximity assumptions between $\mathcal{K}_{\mathcal{T}}$ and $\mathcal{K}^{\text{prox}}$ (H4)

 $s \mathcal{V}_T \leq C$ and $\rho_T \leq \rho$.

Estimation: assumptions (IV)

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Proximity assumptions between $\mathcal{K}_{\mathcal{T}}$ and $\mathcal{K}^{\text{prox}}$ (H4)

$$s \mathcal{V}_T \leq C$$
 and $\rho_T \leq \rho$.



Estimation: bounds on prediction and estimation errors

Theorem 1

We observe $y \in H_T$ with unknown parameters $\beta^* \in \mathbb{R}^s$ and $\vartheta^* = (\theta_1^*, \cdots, \theta_s^*) \in \Theta_T^s$ avec $s \leq K$ such that assumptions H1-H4 are checked and, for all $\ell \neq k$,

 $\mathfrak{d}_{\mathcal{K}_{\mathcal{T}}}(\theta_{\ell}^{\star}, \theta_{k}^{\star}) \gtrsim \delta(s)$ (séparation).

Then, the estimators $\hat{\beta}$ and $\hat{\vartheta}$ defined by $\mathcal{P}_1(\kappa)$ with

 $\kappa \geq \mathcal{C}_1 \sqrt{\Delta_T \log \tau} \quad \text{ and } \quad \tau > 1,$

with the following bounds on the prediction and estimation risks:

$$\begin{split} \left\| \beta^{\star} \, \Phi_{T}(\vartheta^{\star}) - \hat{\beta} \, \Phi_{T}(\hat{\vartheta}) \right\|_{T} &\leq \mathcal{C}_{0} \, \sqrt{s} \, \kappa, \\ \sum_{k=1}^{s} \left| |\beta_{k}^{\star}| - \sum_{\ell \in S_{k}(r)} |\hat{\beta}_{\ell}| \right| &+ \sum_{k=1}^{s} \left| \beta_{k}^{\star} - \sum_{\ell \in S_{k}(r)} \hat{\beta}_{\ell} \right| &+ \left\| \hat{\beta}_{S(r)^{c}} \right\|_{\ell_{1}} &\leq \mathcal{C}_{0} \, \kappa \, s. \end{split}$$
with probability larger than: $1 - \mathcal{C}_{2} \left(\frac{|\Theta_{T}|_{\partial T}}{\tau \sqrt{\log \tau}} \vee \frac{1}{\tau} \right).$

Remark: the bounds do not depend on K!

Estimation: separation between parameters



Estimation: separation between parameters



Estimation: separation between parameters



Estimation: bounds on the prediction risk



Estimation: bounds on the prediction risk



 \rightarrow The upper bound is of the same order as that for the Lasso estimator in the linear regression model.



III Tests

Tests: $\beta^* \Phi_T(\vartheta^*) = \beta^0 \Phi_T(\vartheta^0)$



Tests: $\beta^* \Phi_T(\vartheta^*) = \beta^0 \Phi_T(\vartheta^0)$

Goodness-of-fit: Let $(\beta^0, \vartheta^0) \in (\mathbb{R}^*)^{s^0} \times \Theta_T^{s^0}$ (known) and $(\beta^*, \vartheta^*) \in (\mathbb{R}^*)^s \times \Theta_T^s$ (unknown). $\begin{cases} H_0 & : \quad \beta^* \Phi_T(\vartheta^*) = \beta^0 \Phi_T(\vartheta^0), \\ H_1(\rho) & : \quad \left\|\beta^* \Phi_T(\vartheta^*) - \beta^0 \Phi_T(\vartheta^0)\right\|_T \ge \rho. \end{cases}$

Testing risk and minimal separation

A test Ψ is a measurable function y taking values in $\{0, 1\}$: $\Psi = 0$ accept H_0 and $\Psi = 1$ reject H_0 .

• The maximal testing risk:

$$R_{\rho}(\Psi) = \underbrace{\sup_{\substack{(\beta^{\star}, \vartheta^{\star}) \in H_{0} \\ \text{1st type error prob.}}} \mathbb{E}_{\beta^{\star}, \vartheta^{\star})[\Psi]}_{\text{1st type error prob.}} + \underbrace{\sup_{\substack{(\beta^{\star}, \vartheta^{\star}) \in H_{1}(\rho) \\ 2\text{nd type error prob.}}} \mathbb{E}_{\beta^{\star}, \vartheta^{\star})[1-\Psi]}_{\text{2nd type error prob.}}$$

• The minimax separation distance for testing at $\alpha \in (0, 1)$:

$$\rho^{\star}(\alpha) = \inf\{\rho > 0 : \inf_{\Psi} R_{\rho}(\Psi) \leq \alpha\}.$$





Corollary 1

Discrete process on a regular grid of T points on \mathbb{R}/\mathbb{Z} with $w_T(t_j)$ i.i.d $\sim \mathcal{N}(0,1)$ for $1 \leq j \leq T$.

$$egin{cases} H_0 & : & oldsymbol{s} = 0, \ H_1(
ho) & : & \left\|eta^\star
ight\|_{\ell_2} \geq
ho \end{cases}$$

The bound becomes:

$$\rho^{\star}(\alpha) \lesssim \min\left(\frac{1}{(\alpha T)^{rac{1}{4}}}, \sqrt{rac{s}{T}}\log\left(rac{c}{\alpha \sigma_{T}}
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Remarks

• In the sparse linear regression model, a third regime appears with the rate $\frac{K^{1/4}}{\sqrt{T}}$; Ingster, Verzelen, Tsybakov (2010), Nickl and van de Geer, (2013), showed that the minimax testing rate is $\frac{1}{T^{1/4}} \wedge \sqrt{\frac{s \log(K)}{T}} \wedge \frac{K^{1/4}}{\sqrt{T}}$.

Conclusion and perspectives

Estimation and tests

Under least separation conditions between the true non linear parameters:

- Prediction risks of the same order as for the Lasso-type estimators when ϑ^{\star} is known.
- Testing separation rate is of the same order as for signal detection when ϑ^{\star} is given.
- (Simultaneous reconstruction (analogous to group-Lasso) when many signals share a common structure).

Perspectives

- $\Theta \subseteq \mathbb{R}^d$
- Improve on the non-linear parameter separation conditions in general
- Extend the testing problems