## Around Supervised Learning with Weighted Total-Variation Penalization

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## Part 0

## Supervised Learning in High-Dimensions

## Supervised learning: framework



#### Setting

- Data  $x_i \in \mathcal{X} = \mathbb{R}^p$ ,  $y_i \in \mathcal{Y}$  for i = 1, ..., n. The  $x_i$  are called **features** and the  $y_i$  are called **labels**.
- The labels are scalar numbers. We assume that  $\mathcal{Y} \subset \mathbb{R}$ .  $\mathcal{Y} = \{-1, +1\}, \mathcal{Y} = \{0, 1\}$  for binary classification.  $\mathcal{Y} = \mathbb{R}$  for regression.
- Usually the data D<sub>n</sub> = {(x<sub>i</sub>, y<sub>i</sub>) : i = 1, ..., n} is supposed to be i.i.d.

#### Goal

• Based on (*x<sub>i</sub>*, *y<sub>i</sub>*), learn a function that predicts *y* based on a new *x* (generalization property).

#### **High-dimension**

• p is larger than n.

## Work-flow of supervised learning



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## Supervised learning: empirical risk + penalization

Minimize with respect to  $f : \mathbb{R}^{p} \to \mathbb{R}$ 

 $R_n(f) + \gamma pen(f)$ 

where

$$R_n(f) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, f(x_i))$$

is a **goodness-of-fit**, or **empirical risk**, where  $\ell$  is a **loss** function.

- pen is a penalization function, that encodes a prior assumption on *f*.
- γ > 0 is a tuning parameter, that balances good-of-fitness and penalization.
- **Simplification**: choose a linear function *f*:

$$f(x) = x^{\top}\beta = \sum_{j=1}^{p} x_{j}\beta_{j},$$

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## Supervised learning: empirical risk + penalization

• We end up with:

$$\hat{\beta} \in \underset{\beta \in \mathbb{R}^{p}}{\operatorname{argmin}} \{ R_{n}(\beta) + \lambda \operatorname{pen}(\beta) \},\$$

where

$$R_n(\beta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, x_i^\top \beta)$$

and pen( $\beta$ ) is a penalization on  $\beta$ .

• Choice of penalization !

## Supervised learning: Lasso penalization and its derivatives

- $L_0$ -quasi-norm: pen $(\beta) = \|\beta\|_0 = \#\{j : \beta_j \neq 0\}.$
- Lasso ( $L_1$ -norm): pen( $\beta$ ) =  $\|\beta\|_1 = \sum_{j=1}^{p} |\beta_j|$  [Tibshirani (1996)].
- Elastic-Net (( $L_1 + L_2^2$ )-norm): pen( $\beta$ ) =  $\|\beta\|_1 + \|\beta\|_2^2$  [Zou and Hastie (2005)].
- Fused Lasso  $(L_1 + TV)$ : pen $(\beta) = \|\beta\|_1 + \|\beta\|_{TV}$  [Tibshirani et al. (2005)] where  $\|\cdot\|_{TV}$  is the total-variation penalization defined as

$$\|\beta\|_{\mathsf{TV}} = \sum_{j=2}^{p} |\beta_j - \beta_{j-1}|.$$

 For a chosen positive vector of weights ω̂, we define the (discrete) weighted total-variation (TV) by

$$\|\beta\|_{\mathsf{TV},\hat{\omega}} = \sum_{j=2}^{p} \hat{\omega}_{j} |\beta_{j} - \beta_{j-1}|.$$

• If  $\hat{\omega} \equiv 1$ , then we define the unweighted (simple) TV by

$$\|\beta\|_{\mathsf{TV},1} = \|\beta\|_{\mathsf{TV}} = \sum_{j=2}^{p} |\beta_j - \beta_{j-1}|.$$

- Appropriate for multiple change-points estimation.

   —> Partitioning a nonstationary signal into several contiguous
   stationary segments of variable duration [Harchaoui and
   Lévy-Leduc (2010)].
- Widely used in sparse signal processing and imaging (2D) [Chambolle et al. (2010)].
- Enforces sparsity in the discrete gradient, which is desirable for applications with features ordered in some meaningful way [Tibshirani et al. (2005)].

## Toy example: recovery of piecewise constant signal



## Part I

## Learning the Intensity of Time Events with Change-Points [A., Gaïffas, Guilloux (2015), published in IEEE TIT]

## Counting process: stochastic setup

•  $N = \{N(t)\}_{0 \le t \le 1}$  is a counting process.





• Doob-Meyer decomposition:



• The intensity of N is defined by

 $\lambda_0(t)dt = d\Lambda_0(t) = \mathbb{P}[N \text{ has a jump in } [t, t + dt)|\mathcal{F}(t)],$ 

where  $\mathcal{F}(t) = \sigma(N(s), s \leq t)$ .

## Piecewise constant intensity

Assume that

$$\lambda_0(t) = \sum_{\ell=1}^{L_0} eta_{0,\ell} \mathbbm{1}_{( au_{0,\ell-1}, au_{0,\ell}]}(t), \, 0 \leq t \leq 1.$$

- $\{\tau_{0,0} = 0 < \tau_{0,1} < \dots < \tau_{0,L_0-1} < \tau_{0,L_0} = 1\}$ : set of true change-points.
- $\{\beta_{0,\ell} : 1 \leq \ell \leq L_0\}$ : set of jump sizes of  $\lambda_0$ .
- L<sub>0</sub> : number of true change-points.



#### Data

We observe n i.i.d copies of N on [0,1], denoted  $N_1, \ldots, N_n$ .

- We define  $\overline{N}_n(I) = \frac{1}{n} \sum_{i=1}^n N_i(I)$ ,  $N_i(I) = \int_I dN_i(t)$ , for any interval  $I \subset [0, 1]$ .
- This assumption is equivalent to observing a single process N with intensity nλ<sub>0</sub> (only used to have a notion of growing observations with an increasing n).

## A procedure based on weighted TV penalization

• We introduce the least-squares functional

$$R_n(\lambda) = \int_0^1 \lambda(t)^2 dt - \frac{2}{n} \sum_{i=1}^n \int_0^1 \lambda(t) dN_i(t),$$

[Reynaud-Bouret (2003, 2006), Gaïffas and Guilloux (2012)].

- Fix  $m = m_n \ge 1$ , an integer that shall go to infinity as  $n \to \infty$ .
- We approximate  $\lambda_0$  in the set of nonnegative piecewise constant functions on [0,1] given by

$$\Lambda_m = \Big\{\lambda_\beta = \sum_{j=1}^m \beta_{j,m} \lambda_{j,m} : \beta = [\beta_{j,m}]_{1 \le j \le m} \in \mathbb{R}_+^m \Big\},\$$

where

$$\lambda_{j,m} = \sqrt{m} \mathbb{1}_{I_{j,m}}$$
 et  $I_{j,m} = \left(\frac{J-1}{m}, \frac{J}{m}\right]$ 

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## A procedure based on weighted TV penalization

• The estimator of  $\lambda_0$  is defined by

$$\hat{\lambda} = \lambda_{\hat{\beta}} = \sum_{j=1}^{m} \hat{\beta}_{j,m} \lambda_{j,m}.$$

where  $\hat{\beta}$  is giving by

$$\hat{\beta} = \operatorname*{argmin}_{\beta \in \mathbb{R}^m_+} \Big\{ R_n(\lambda_\beta) + \|\beta\|_{\mathsf{TV},\hat{\omega}} \Big\}.$$

• We consider the dominant term

$$\hat{\omega}_j = \mathcal{O}\left(\sqrt{\frac{m\log m}{n}} \bar{N}_n\left(\left(\frac{j-1}{m},1\right]\right)\right).$$

- The linear space  $\Lambda_m$  is endowed by the norm  $\|\lambda\| = \sqrt{\int_0^1 \lambda^2(t) dt}.$
- Let  $\hat{S}$  to be the support of the discrete gradient of  $\hat{\beta}$ ,

$$\hat{S} = \{j : \hat{\beta}_{j,m} \neq \hat{\beta}_{j-1,m} \text{ for } j = 2, \dots, m\}.$$

• Let  $\hat{L}$  to be the estimated number of change-points defined by:

$$\hat{L}=|\hat{S}|.$$

#### The estimator $\hat{\lambda}$ satisfies the following:

#### Theorem 1

Fix x > 0 and let the data-driven weights  $\hat{\omega}$  defined as above. Assume that  $\hat{L}$  satisfies  $\hat{L} \leq L_{max}$ . Then, we have

$$\begin{split} \|\hat{\lambda}-\lambda_0\|^2 &\leq \inf_{eta\in\mathbb{R}^m_+} \left\|\lambda_eta-\lambda_0
ight\|^2 + 6(L_{\max}+2(L_0-1))\max_{1\leq j\leq m}\hat{\omega}_j^2 \ &+ C_1rac{\|\lambda_0\|_\inftyig(x+L_{\max}(1+\log m))}{n} \ &+ C_2rac{mig(x+L_{\max}(1+\log m)ig)^2}{n^2}, \end{split}$$

with a probability larger than  $1 - L_{max}e^{-x}$ .

## Trade-off bias and variance

• Let  $\Delta_{\beta,\max} = \max_{1 \le \ell, \ell' \le L_0} |\beta_{0,\ell} - \beta_{0,\ell'}|$ , be the maximum of jump size of  $\lambda_0$ .

Corollary

We have

$$\|\lambda_{eta} - \lambda_{\mathbf{0}}\|^2 \leq rac{2L_{\mathbf{0}}\Delta_{eta,\max}^2}{m}.$$

• Our procedure has a fast rate of convergence of order

$$\frac{(L_{\max} \vee L_0)m\log m}{n}.$$

• An optimal tradeoff between approximation and complexity is given by the choice:

If 
$$L_{\max} = \mathcal{O}(m) \Rightarrow m = \mathcal{O}(n^{1/3})$$
.  
If  $L_{\max} = \mathcal{O}(1) \Rightarrow m = \mathcal{O}(n^{1/2})$ .

## Consistency of change-points detection

- There is an unavoidable non-parametric bias of approximation.
- The approximate change-points sequence  $(\frac{j_{\ell}}{m})_{0 \leq \ell \leq L_0}$  is defined as the right-hand side boundary of the unique interval  $I_{j_{\ell},m}$  that contains the true change-point  $\tau_{0,\ell}$ .
- $\tau_{0,\ell} \in \left(\frac{j_\ell-1}{m}, \frac{j_\ell}{m}\right]$ , for  $\ell = 1, \ldots, L_0 1$ , where  $j_0 = 0$  and  $j_{L_0} = m$  by convention.



- Let  $\hat{S} = \{\hat{j}_1, \dots, \hat{j}_{\hat{L}}\}$  with  $\hat{j}_1 < \dots < \hat{j}_{\hat{L}}$ , and  $\hat{j}_0 = 0$  and  $\hat{j}_{\hat{L}+1} = m$ .
- We define simply

$$\hat{ au}_\ell = rac{\hat{j}_\ell}{m} ext{ for } \ell = 1, \dots, \hat{ extsf{L}}.$$

## Consistency of change-points detection

 We can't recover the exact position of two change-points if they lie on the same interval I<sub>j,m</sub>.

#### Minimal distance between true change-points

Assume that there is a positive constant  $c \ge 8$  such that

$$\min_{1 \le \ell \le L_0} |\tau_{0,\ell} - \tau_{0,\ell-1}| > \frac{c}{m}.$$

 $\longrightarrow$  The change-points of  $\lambda_0$  are sufficiently far apart.  $\longrightarrow$  There cannot be more than one change-point in the "high-resolution" intervals  $I_{j,m}$ .

• The procedure will be able to recover the (unique) intervals  $I_{j_{\ell},m}$ , for  $\ell = 0, \dots, L_0$ , where the change-point belongs.

## Consistency of change-points detection

- $\Delta_{j,\min} = \min_{1 \le \ell \le L_0 1} \left| \frac{j_{\ell+1}}{m} \frac{j_{\ell}}{m} \right|$ , the minimum distance between two consecutive terms in the change-points of  $\lambda_0$ .
- $\Delta_{\beta,\min} = \min_{1 \le q \le m-1} |\beta_{0,q+1,m} \beta_{0,q,m}|$ , the smallest jump size of the projection  $\lambda_{0,m}$  of  $\lambda_0$  onto  $\Lambda_m$ .
- (ε<sub>n</sub>)<sub>n≥1</sub>, a non-increasing and positive sequence that goes to zero as n → ∞.

#### **Technical Assumptions**

We assume that  $\Delta_{j,\min}$ ,  $\Delta_{\beta,\min}$  and  $(\varepsilon_n)_{n\geq 1}$  satisfy

$$\frac{\sqrt{nm}\Delta_{j,\min}\Delta_{\beta,\min}}{\sqrt{\log m}} \to \infty \text{ and } \frac{\sqrt{nm}\varepsilon_n\Delta_{\beta,\min}}{\sqrt{\log m}} \to \infty.$$

#### Theorem 2

Under the given Assumptions, and if  $\hat{L} = L_0$ , then the change-points estimators  $\{\hat{\tau}_1, \ldots, \hat{\tau}_{\hat{l}}\}$  satisfy

$$\mathbb{P}\Big[\max_{1\leq\ell\leq \boldsymbol{L_0}}|\hat{\tau}_{\ell}-\tau_{0,\ell}|\leq \varepsilon_n\Big]\to 1, \text{ as } n\to\infty.$$

If m ≈ n<sup>1/3</sup>, Theorem 2 holds with ε<sub>n</sub> ≈ n<sup>-1/3</sup>, Δ<sub>β,min</sub> = n<sup>-1/6</sup> et Δ<sub>j,min</sub> ≈ n<sup>-1/3</sup>.
m ≈ n<sup>1/2</sup>, Theorem 2 holds with ε<sub>n</sub> ≈ n<sup>-1/2</sup>, Δ<sub>β,min</sub> ≈ n<sup>-1/6</sup> et Δ<sub>j,min</sub> ≈ n<sup>-1/2</sup>.

## Implementation: proximal operator

• We are interested in computing a solution

$$x^{\star} = \operatorname*{argmin}_{x \in \mathbb{R}^p} \{g(x) + h(x)\},$$

where g is smooth and h is simple (prox-calculable).

 The proximal operator prox<sub>h</sub> of a proper, lower semi-continuous, convex function h : ℝ<sup>m</sup> → (-∞, ∞], is defined as

$$\operatorname{prox}_{h}(v) = \operatorname{argmin}_{x \in \mathbb{R}^{m}} \left\{ \frac{1}{2} \|v - x\|_{2}^{2} + h(x) \right\}, \text{ for all } v \in \mathbb{R}^{m}.$$

• Proximal gradient descent (PGD) algorithm is based on

$$x^{(k+1)} = \operatorname{prox}_{\varepsilon_k h} \left( x^{(k)} - \varepsilon_k \nabla g(x^{(k)}) \right).$$

[Daubechies et al. (2004) (ISTA) , Beck and Teboulle (2009) (FISTA)]

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## Proximal operator of the weighted TV penalization

• We have

$$\hat{\boldsymbol{\beta}} = \operatorname*{argmin}_{\boldsymbol{\beta} \in \mathbb{R}^m_+} \Big\{ \frac{1}{2} \| \mathbf{N} - \boldsymbol{\beta} \|_2^2 + \| \boldsymbol{\beta} \|_{\mathsf{TV},\hat{\boldsymbol{\omega}}} \Big\},$$

where  $\boldsymbol{\mathsf{N}}=[\boldsymbol{\mathsf{N}}_{j}]_{1\leq j\leq m}\in\mathbb{R}_{+}^{m}$  is given by

$$\mathbf{N} = \left(\sqrt{m}\bar{N}_n(I_{1,m}),\ldots,\sqrt{m}\bar{N}_n(I_{m,m})\right).$$

Then

$$\hat{eta} = \operatorname{prox}_{\|\cdot\|_{\mathsf{TV},\hat{\omega}}}(\mathsf{N}).$$

- Modification of Condat's algorithm [Condat (2013)].
- If we have a feasible dual variable <sup>û</sup>, we can compute the primal solution β̂, by Fenchel duality.
- The Karush-Kuhn-Tucker (KKT) optimality conditions characterize the unique solutions  $\hat{\beta}$  and  $\hat{u}$ .

Algorithm 1:  $\beta = \operatorname{prox}_{\|\cdot\|_{\mathsf{TV},\alpha}}(\mathsf{N})$ 1. set  $k = k_0 = k_- = k_+ \leftarrow 1$ ;  $\beta_{\min} \leftarrow N_1 - \hat{\omega}_2$ ;  $\beta_{\max} \leftarrow N_1 + \hat{\omega}_2$ ;  $\theta_{\min} \leftarrow \hat{\omega}_2$ ;  $\theta_{\max} \leftarrow -\hat{\omega}_2$ ; 2. if k = m then  $\hat{\beta}_m \leftarrow \beta_{\min} + \theta_{\min};$ 3. if  $N_{k+1} + \theta_{\min} < \beta_{\min} - \hat{\omega}_{k+2}$  then /\* negative jump \*/  $\begin{array}{c} \lambda_{+1} + \delta_{\min} \sim \rho_{\min} \quad \lambda_{k+2} + \delta_{\min}; \quad k = k_0 = k_- = k_+ \leftarrow k_- + 1; \\ \beta_{\min} \leftarrow \mathbf{N}_k - \hat{\omega}_{k+1} + \hat{\omega}_k; \quad \beta_{\max} \leftarrow \mathbf{N}_k + \hat{\omega}_{k+1} + \hat{\omega}_k; \quad \theta_{\min} \leftarrow \hat{\omega}_{k+1}; \quad \theta_{\max} \leftarrow -\hat{\omega}_{k+1}; \end{array}$ 4. else if  $N_{k+1} + \theta_{max} > \beta_{max} + \hat{\omega}_{k+2}$  then /\* positive jump \*/  $\begin{array}{l} \hat{\beta}_{k_{1}}^{\star+1} & \cdots & \hat{\beta}_{k_{1}} & \leftarrow \beta_{\max}; \ k = k_{0} = k_{-} = k_{+} \leftarrow k_{+} + 1; \\ \beta_{\min} \leftarrow \mathbf{N}_{k} - \hat{\omega}_{k+1} - \hat{\omega}_{k}; \ \beta_{\max} \leftarrow \mathbf{N}_{k} + \hat{\omega}_{k+1} - \hat{\omega}_{k}; \ \theta_{\min} \leftarrow \hat{\omega}_{k+1}; \ \theta_{\max} \leftarrow -\hat{\omega}_{k+1}; \end{array}$ 5. else /\* no jump \*/ set  $k \leftarrow k+1$ ;  $\theta_{\min} \leftarrow \mathbf{N}_k + \hat{\omega}_{k+1} - \beta_{\min}$ ;  $\theta_{\max} \leftarrow \mathbf{N}_k - \hat{\omega}_{k+1} - \beta_{\max}$ ;  $\begin{vmatrix} \mathbf{if} \ \theta_{\min} \geq \hat{\omega}_{k+1} \ \mathbf{then} \\ \beta_{\min} \leftarrow \beta_{\min} + \frac{\theta_{\min} - \hat{\omega}_{k+1}}{k - k_0 + 1}; \ \theta_{\min} \leftarrow \hat{\omega}_{k+1}; \ k_- \leftarrow k; \end{vmatrix}$  $\begin{array}{l} \text{if } \theta_{\max} \leq -\hat{\omega}_{k+1} \text{ then} \\ \mid \beta_{\max} \leftarrow \beta_{\max} + \frac{\theta_{\max} + \hat{\omega}_{k+1}}{k - k_0 + 1}; \, \theta_{\max} \leftarrow -\hat{\omega}_{k+1}; \, k_+ \leftarrow k; \end{array}$ 6. if k < m then go to 3.; 7. if  $\theta_{\min} < 0$  then  $\begin{array}{l} & \underset{\beta_{k_0}}{\overset{\text{min}}{\underset{\beta_{k_1}}}{\underset{\beta_{k_1}}}{\underset{\beta_{k_1}}}{\underset{\beta_{k_1}}}{\underset{\beta_{k_1}}}{\underset{\beta_{k_1}}{\underset{\beta_{k_1}}}{\underset{\beta_{k_1}}{\underset{\beta_{k_1}}}{\underset{\beta_{k_1}}}{\underset{\beta_{k_1}}{\underset{\beta_{k_1}}{\underset{\beta_{k_1}}{\underset{\beta_{k_1}}}{\underset{\beta_{k_1}}}}}}}}}}}}}}}}}}}}}}}}}}$ 8. else if  $\theta_{max} > 0$  then 
$$\begin{split} \hat{\boldsymbol{\beta}}_{k_0} &= \cdots = \hat{\boldsymbol{\beta}}_{k_+} \leftarrow \boldsymbol{\beta}_{\text{max}}; \, k = k_0 = k_+ \leftarrow k_+ + 1; \, \boldsymbol{\beta}_{\text{max}} \leftarrow \mathbf{N}_k + \hat{\boldsymbol{\omega}}_{k+1} - \hat{\boldsymbol{\omega}}_k; \\ \boldsymbol{\theta}_{\text{max}} \leftarrow - \hat{\boldsymbol{\omega}}_{k+1}; \, \boldsymbol{\theta}_{\text{min}} \leftarrow \mathbf{N}_k - \hat{\boldsymbol{\omega}}_k - \boldsymbol{\theta}_{\text{min}}; \, \text{go to } 2.; \end{split}$$
9. else  $\hat{\beta}_{k_0} = \cdots = \hat{\beta}_m \leftarrow \beta_{\min} + \frac{\theta_{\min}}{k - k_0 + 1};$ 

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## Real data: RNA-seq

- RNA-seq can be modelled mathematically as replications of an inhomogeneous counting process with a piecewise constant intensity [Shen and Zhang (2012)].
- We applied our method to the sequencing data of the breast tumor cell line HCC1954 7.72 million reads) and its reference cell line BL1954 (6.65 million reads) [Chiang et al. (2009)].



Binned counts of reads on the tumor data



A zoom into the sequence of reads for tumor data.

## Real data

Weighted total-variation estimator on the tumor data

#### Unweighted total-variation estimator for the tumor data



Zoom into the weighted (left) and unweighted (right) TV estimators applied to the tumor data.

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## Part II

# Binarsity: a penalization for one-hot encoded features

## Features binarization

- Supervised training dataset  $(x_i, y_i)_{i=1,...,n}$  containing features  $x_i = (x_{i,1}, \ldots, x_{i,p})^\top \in \mathbb{R}^p$  and labels  $y_i \in \mathcal{Y} \subset \mathbb{R}$ , that are i.i.d.
- We denote  $\mathbf{X} = [x_{i,j}]_{1 \le i \le n; 1 \le j \le p}$  the  $n \times p$  features matrix.
- Let **X**<sub>•,j</sub> be the *j*-th feature column of **X**.
- The binarized matrix X<sup>B</sup> is a matrix with an extended number d > p of columns (only binary).
- The *j*-th column X<sub>•,j</sub> is replaced by a number d<sub>j</sub> ≥ 2 of columns X<sup>B</sup><sub>•,j,1</sub>,..., X<sup>B</sup><sub>•,j,d<sub>j</sub></sub> containing only zeros and ones.
- The *i*-th row of  $\boldsymbol{X}^{B}$  is written

$$x_i^B = (x_{i,1,1}^B, \ldots, x_{i,1,d_1}^B, \ldots, x_{i,p,1}^B, \ldots, x_{i,p,d_p}^B)^\top \in \mathbb{R}^d.$$

## Features binarization

If X<sub>●,j</sub> takes values (modalities) in the set {1,..., M<sub>j</sub>} with cardinality M<sub>j</sub>, we take d<sub>j</sub> = M<sub>j</sub>, and use a binary coding of each modality by defining

$$x_{i,j,k}^B = egin{cases} 1, & ext{if } x_{i,j} = k, \ 0, & ext{otherwise}, \end{cases}$$

 If X<sub>●,j</sub> is quantitative, then d<sub>j</sub> we consider a partition of intervals I<sub>j,1</sub>,..., I<sub>j,d<sub>j</sub></sub> for the range of values of X<sub>●,j</sub> and define

$$x_{i,j,k}^B = egin{cases} 1, & ext{if } x_{i,j} \in I_{j,k}, \ 0, & ext{otherwise}, \end{cases}$$

## Features binarization

- A natural choice of intervals is given by the quantiles, namely we can typically choose  $I_{j,k} = (q_j(\frac{k-1}{d_j}), q_j(\frac{k}{d_j})]$  for  $k = 1, \ldots, d_j$ .
- To each binarized feature  $X^{B}_{\bullet,j,k}$  corresponds a parameter  $\theta_{j,k}$ .
- The parameters associated to the binarization of the *j*-th feature is denoted  $\theta_{j,\bullet} = (\theta_{j,1} \cdots \theta_{j,d_j})^{\top}$ .
- The full parameters vector of size  $d = \sum_{j=1}^{p} d_j$ , is simply

$$\theta = (\theta_{1,\bullet}^{\top} \cdots \theta_{p,\bullet}^{\top})^{\top} = (\theta_{1,1} \cdots \theta_{1,d_1} \theta_{2,1} \cdots \theta_{2,d_2} \cdots \theta_{p,1} \cdots \theta_{p,d_p})^{\top}.$$

- The one-hot-encodings satisfy ∑<sub>k=1</sub><sup>dj</sup> X<sub>i,j,k</sub> = 1 for all j, meaning that the columns of each block sum to 1<sub>n</sub>.
   → X<sup>B</sup> is not of full rank by construction.
- Some of the raw features X<sub>●,j</sub> might not be relevant for the prediction task, so we want to select raw features from their one-hot encodings.
  - $\rightarrow$  block-sparsity in  $\theta$ .

## Binarsity

- In our penalization term, we impose  $\sum_{k=1}^{d_j} \theta_{j,k} = 0$  for all j = 1, ..., p (sum-to-zero-constraint).
- We remark that within each block, binary features are ordered.  $\rightarrow$  We use a within block weighted total-variation penalization

$$\sum_{j=1}^{p} \|\theta_{j,\bullet}\|_{\mathsf{TV},\hat{\omega}_{j,\bullet}}$$

where

$$\|\theta_{j,\bullet}\|_{\mathsf{TV},\hat{\omega}_{j,\bullet}} = \sum_{k=2}^{d_j} \hat{\omega}_{j,k} |\theta_{j,k} - \theta_{j,k-1}|,$$

## Binarsity

• We therefore introduce the following new penalization called *binarsity* 

$$\mathsf{bina}( heta) = \sum_{j=1}^{p} \Big( \sum_{k=2}^{d_j} \hat{w}_{j,k} | heta_{j,k} - heta_{j,k-1} | + \delta_1( heta_{j,\bullet}) \Big),$$

where the indicator function

$$\delta_1(u) = egin{cases} 0 & ext{if} \quad \mathbf{1}^ op u = 0, \ \infty & ext{otherwise}. \end{cases}$$

- If a raw feature j is statistically not relevant for predicting the labels, then the full block θ<sub>j,•</sub> should be zero.
- If a raw feature *j* is relevant, then the number of different values for the coefficients of θ<sub>j,•</sub> should be kept as small as possible, in order to balance bias and variance.

We consider the following data-driven weighted version of Binarsity given by

$$\hat{\omega}_{j,k} = \mathcal{O}\left(\sqrt{\frac{\log p}{n}}\hat{\pi}_{j,k}\right),$$

where

$$\hat{\pi}_{j,k} = \frac{\#\left(\left\{i=1,\ldots,n:x_{i,j}\in\left(q_j\left(\frac{k}{d_j}\right),q_j(1)\right]\right\}\right)}{n}.$$

 $\hat{\pi}_{j,k}$  corresponds to the proportion of 1s in the sub-matrix obtained by deleting the first k columns in the *j*-th binarized block matrix.

## Generalized linear models

• The conditional distribution of  $Y_i$  given  $X_i = x_i$  is assumed to be from one parameter exponential family

$$y|x\mapsto f^0(y|x)=\exp\Big(rac{ym^0(x)-b(m^0(x))}{arphi}+c(y)\Big),$$

- The functions b(·) and c(·) are known, while the natural parameter function m<sup>0</sup>(x) is unknown.
- We have

$$\mathbb{E}[Y_i|X_i=x_i]=b'(\boldsymbol{m}^0(x_i)).$$

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• Logistic and probit regression for binary data or multinomial regression for categorical data, Poisson regression for count data, etc ...

### Generalized linear models + binarsity

• We consider the empirical risk

$$R_n(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, m_\theta(x_i)),$$

where  $m_{\theta}(x_i) = \theta^{\top} x_i^B$ .

•  $\ell$  is the generalized linear model loss function and is given by

$$\ell(y,y') = -yy' + b(y').$$

• Our estimator of  $m^0$  is given by  $\hat{m} = m_{\hat{\theta}}$ , where  $\hat{\theta}$  is the solution of the penalized log-likelihood problem

$$\hat{ heta} \in \operatorname*{argmin}_{ heta \in \mathbb{R}^d} \{ R_n( heta) + \operatorname{bina}( heta) \}.$$

• Since Binarsity is separable by blocks, we have

$$(\operatorname{prox}_{\operatorname{bina}_{\widehat{\omega}}}(\theta))_{j,\bullet} = \operatorname{prox}_{(\|\cdot\|_{\operatorname{TV},\widehat{\omega}_{j,\bullet}}+\delta_{\mathcal{H}_i})}(\theta_{j,\bullet}),$$

for all  $j = 1, \ldots, p$ .

 Algorithm 2 expresses prox<sub>bina<sub>0</sub></sub> based on the proximal operator of the weighted TV penalization.

## Toy example $(n = 1000, p = 2, d_1 = d_2 = 100)$



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Modal'X, 11th May 2017

Supervised Learning with weighted TV



Mokhtar Z. Alaya

- We introduce a data-driven weighted total-variation penalizations for two problems: change-points detection and generalized linear models with binarized features.
- For each procedure, we give: theoretical guaranties by proving non-asymptotic oracles inequalities for the prediction error and algorithms that efficiently solve the studied convex problems.

- With S. Bussy and A. Guilloux, we study the estimation problem of high-dimensional Cox model, with covariables having multiple cut-points, using binarsity penalization.
- With T. Allart, we study the complete TV penalty, which is more stable than the simple TV penalization

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