Binarsity: a penalization for one-hot encoded features in linear supervised learning

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Supervised learning: framework

Setting

- Data $D_n = \{(X_i, Y_i) : i = 1, \ldots, n\}$ supposed to be i.i.d.
- $X_i \in \mathcal{X} = \mathbb{R}^p$, $Y_i \in \mathcal{Y}$ for $i = 1, \ldots, n$. The X_i are called **features** and the Y_i are called **labels**.
- The labels are scalar numbers. We assume that $\mathcal{Y} \subset \mathbb{R}$. $\mathcal{Y} = \mathbb{R}$ for regression, $\mathcal{Y} = \{-1, +1\}$ for binary classification.

High-dimension

- p is larger, (say $p \geq 10^4$)

Big data

- n is larger, (say $n \geq 10^6$)

Goal

- Based on (x_i, y_i), learn a function that predicts y based on a new x (generalization property).

Supervised learning: empirical risk + penalization

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

$$R_n(f) + \lambda \text{pen}(f)$$

where

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

  is an **empirical risk**, where ℓ is a **loss** function.
- pen is a penalization function, that encodes a prior assumption on f.
- $\lambda > 0$ is a **tuning parameter**, that balances good-of-fitness and penalization.
- **Simplification**: choose a **linear** function f:

  $$f(x) = x^\top \theta = \sum_{j=1}^{p} x_j \theta_j,$$

  for a parameter $\theta \in \mathbb{R}^p$ to be trained.

Supervised learning: empirical risk + penalization

- We end up with:

$$\hat{\theta} \in \underset{\theta \in \mathbb{R}^p}{\operatorname{argmin}} \{ R_n(\theta) + \lambda \text{pen}(\theta) \},$$

where

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

and $\text{pen}(\theta)$ is a penalization on θ.

- Choice of penalization !

Supervised learning: Lasso penalization and its derivatives

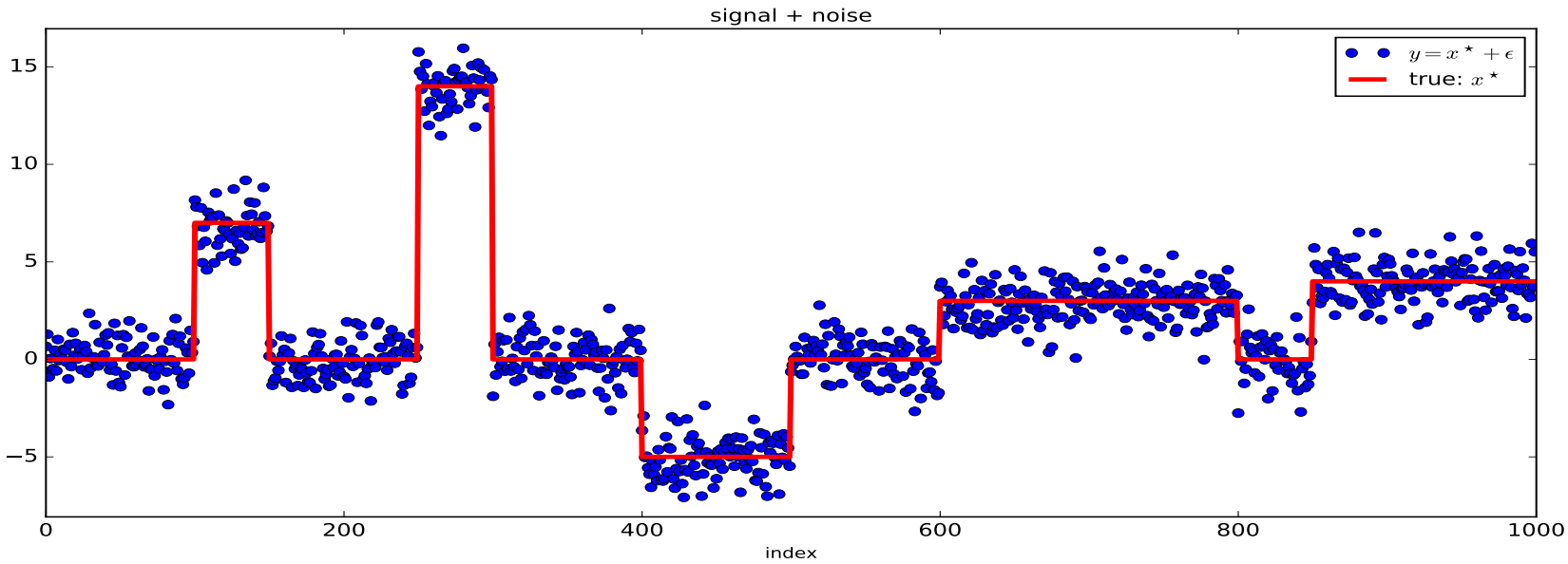
- ℓ_0-quasi-norm: $\text{pen}(\theta) = \|\theta\|_0 = \#\{j : \theta_j \neq 0\}$.
- Lasso (ℓ_1-norm): $\text{pen}(\theta) = \|\theta\|_1 = \sum_{j=1}^{p} |\theta_j|$ [Tibshirani (1996)].
- Elastic-Net ($(\ell_1 + \ell_2^2)$-norm): $\text{pen}(\theta) = \|\theta\|_1 + \|\theta\|_2^2$ [Zou and Hastie (2005)].
- Fused Lasso (ℓ_1 + TV): $\text{pen}(\theta) = \|\theta\|_1 + \|\theta\|_{\text{TV}}$ [Tibshirani et al. (2005)] where $\|\cdot\|_{\text{TV}}$ is the (discrete) total-variation penalization (TV) defined as

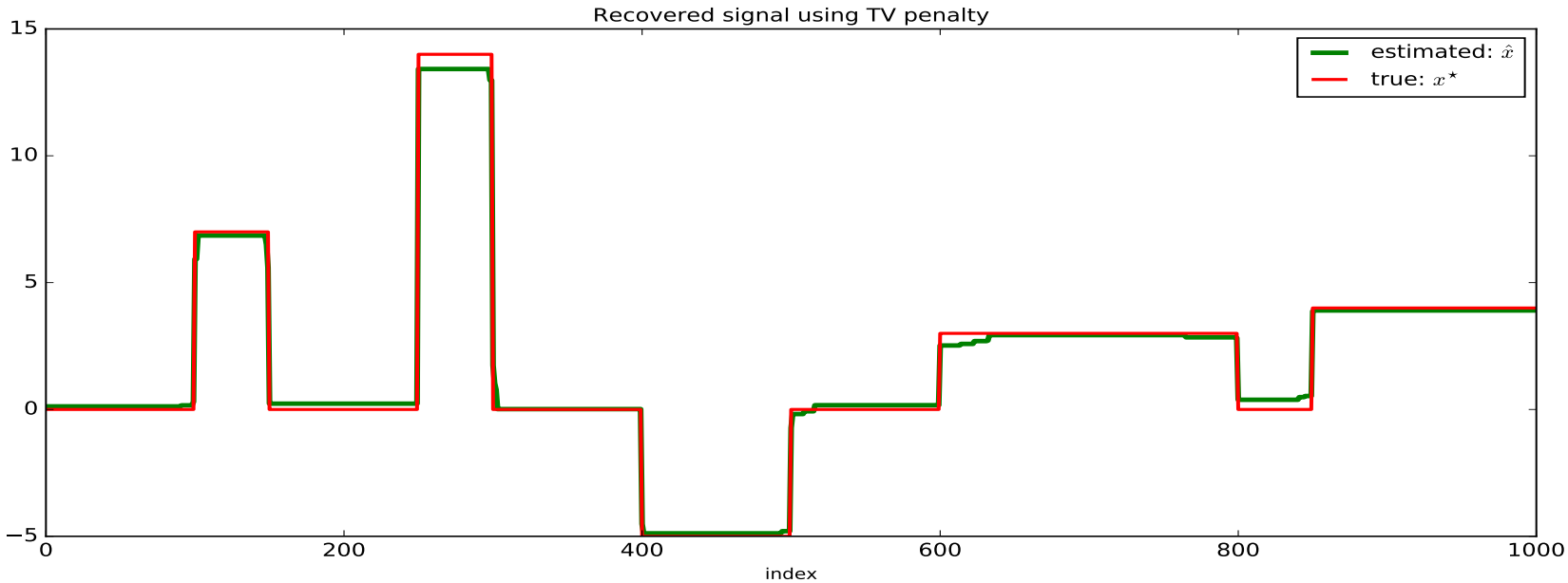
$$\|\theta\|_{\text{TV}} = \sum_{j=2}^{p} |\theta_j - \theta_{j-1}|, \text{ for all } \theta \in \mathbb{R}^p.$$

Motivations for using TV

- Appropriate for multiple change-points estimation.
  $\longrightarrow$ 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 using TV





Weighted TV

- For a chosen positive vector of weights $\hat{\omega}$, we define the weighted TV by

$$\|\theta\|_{\mathrm{TV},\hat{\omega}} = \sum_{j=2}^{p} \hat{\omega}_j |\theta_j - \theta_{j-1}|.$$

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

$$\|\theta\|_{\mathrm{TV},1} = \|\theta\|_{\mathrm{TV}} = \sum_{j=2}^{p} |\theta_j - \theta_{j-1}|.$$

Proximal operator of weighted TV penalization

- We are interested in computing a solution

$$\hat{\theta} = \underset{\theta}{\operatorname{argmin}}\{g(\theta) + h(\theta)\},$$

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

- The proximal operator prox_h of a proper, lower semi-continuous, convex function $h : \mathbb{R}^n \to (-\infty, \infty]$, is defined as

$$\operatorname{prox}_h(y) = \underset{\theta \in \mathbb{R}^n}{\operatorname{argmin}} \left\{ \frac{1}{2}\|y - \theta\|_2^2 + h(\theta) \right\}, \text{ for all } y \in \mathbb{R}^n.$$

- Proximal gradient descent (PGD) algorithm is based on

$$\theta^{(t+1)} = \operatorname{prox}_{\varepsilon_t h}\left(\theta^{(t)} - \eta_t \nabla g(\theta^{(t)})\right).$$

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

Proximal operator of weighted TV penalization

- We have

$$\hat{\theta} = \text{prox}_{\|\cdot\|_{\text{TV},\hat{\omega}}}(y) = \underset{\theta \in \mathbb{R}^n}{\text{argmin}} \left\{ \frac{1}{2} \| Y - \theta \|_2^2 + \| \theta \|_{\text{TV},\hat{\omega}} \right\}.$$

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

Algorithm 1: $\hat{\theta} = \text{prox}_{\|\cdot\|_{\text{TV},\hat{\omega}}}(y)$

1. **set** $k = k_0 = k_- = k_+ \leftarrow 1$; $\theta_{\min} \leftarrow y_1 - \hat{\omega}_2$; $\theta_{\max} \leftarrow y_1 + \hat{\omega}_2$; $u_{\min} \leftarrow \hat{\omega}_2$; $u_{\max} \leftarrow -\hat{\omega}_2$;
2. **if** $k = n$ **then**
   $\hat{\theta}_n \leftarrow \theta_{\min} + u_{\min}$;
3. **if** $y_{k+1} + u_{\min} < \theta_{\min} - \hat{\omega}_{k+2}$ **then** /* negative jump */
   $\hat{\theta}_{k_0} = \cdots = \hat{\theta}_{k_-} \leftarrow \theta_{\min}$; $k = k_0 = k_- = k_+ \leftarrow k_- + 1$;
   $\theta_{\min} \leftarrow y_k - \hat{\omega}_{k+1} + \hat{\omega}_k$; $\theta_{\max} \leftarrow y_k + \hat{\omega}_{k+1} + \hat{\omega}_k$; $u_{\min} \leftarrow \hat{\omega}_{k+1}$; $u_{\max} \leftarrow -\hat{\omega}_{k+1}$;
4. **else if** $y_{k+1} + u_{\max} > \theta_{\max} + \hat{\omega}_{k+2}$ **then** /* positive jump */
   $\hat{\theta}_{k_0} = \ldots = \hat{\theta}_{k_+} \leftarrow \theta_{\max}$; $k = k_0 = k_- = k_+ \leftarrow k_+ + 1$;
   $\theta_{\min} \leftarrow y_k - \hat{\omega}_{k+1} - \hat{\omega}_k$; $\theta_{\max} \leftarrow y_k + \hat{\omega}_{k+1} - \hat{\omega}_k$; $u_{\min} \leftarrow \hat{\omega}_{k+1}$; $u_{\max} \leftarrow -\hat{\omega}_{k+1}$;
5. **else** /* no jump */
   set $k \leftarrow k + 1$; $u_{\min} \leftarrow y_k + \hat{\omega}_{k+1} - \theta_{\min}$; $u_{\max} \leftarrow y_k - \hat{\omega}_{k+1} - \theta_{\max}$;
   if $u_{\min} \geq \hat{\omega}_{k+1}$ **then**
      $\theta_{\min} \leftarrow \theta_{\min} + \frac{u_{\min} - \hat{\omega}_{k+1}}{k - k_0 + 1}$; $u_{\min} \leftarrow \hat{\omega}_{k+1}$; $k_- \leftarrow k$;
   if $u_{\max} \leq -\hat{\omega}_{k+1}$ **then**
      $\theta_{\max} \leftarrow \theta_{\max} + \frac{u_{\max} + \hat{\omega}_{k+1}}{k - k_0 + 1}$; $u_{\max} \leftarrow -\hat{\omega}_{k+1}$; $k_+ \leftarrow k$;
6. **if** $k < n$ **then**
   go to 3.;
7. **if** $u_{\min} < 0$ **then**
   $\hat{\theta}_{k_0} = \cdots = \hat{\theta}_{k_-} \leftarrow \theta_{\min}$; $k = k_0 = k_- \leftarrow k_- + 1$; $\theta_{\min} \leftarrow y_k - \hat{\omega}_{k+1} + \hat{\omega}_k$;
   $u_{\min} \leftarrow \hat{\omega}_{k+1}$; $u_{\max} \leftarrow y_k + \hat{\omega}_k - v_{\max}$; **go to 2.**;
8. **else if** $u_{\max} > 0$ **then**
   $\hat{\theta}_{k_0} = \cdots = \hat{\theta}_{k_+} \leftarrow \theta_{\max}$; $k = k_0 = k_+ \leftarrow k_+ + 1$; $\theta_{\max} \leftarrow y_k + \hat{\omega}_{k+1} - \hat{\omega}_k$;
   $u_{\max} \leftarrow -\hat{\omega}_{k+1}$; $u_{\min} \leftarrow y_k - \hat{\omega}_k - u_{\min}$; **go to 2.**;
9. **else**
   $\hat{\theta}_{k_0} = \cdots = \hat{\theta}_n \leftarrow \theta_{\min} + \frac{u_{\min}}{k - k_0 + 1}$;

Features binarization

- Supervised training dataset $(x_i, y_i)_{i=1,\dots,n}$ containing features $x_i = (x_{i,1}, \dots, x_{i,p})^\top \in \mathbb{R}^p$ and labels $y_i \in \mathcal{Y} \subset \mathbb{R}$, that are i.i.d.
- We denote $\boldsymbol{X} = [x_{i,j}]_{1 \leq i \leq n; 1 \leq j \leq p}$ the $n \times p$ features matrix.
- Let $\boldsymbol{X}_{\bullet,j}$ be the j-th feature column of $\boldsymbol{X}$.
- The binarized matrix $\boldsymbol{X}^B$ is a matrix with an extended number $d > p$ of columns (only binary).
- The j-th column $\boldsymbol{X}_{\bullet,j}$ is replaced by a number $d_j \geq 2$ of columns $\boldsymbol{X}^B_{\bullet,j,1}, \dots, \boldsymbol{X}^B_{\bullet,j,d_j}$ containing only zeros and ones.

Features binarization: setup

- If $X_{\bullet,j}$ takes values (modalities) in the set $\{1, \ldots, M_j\}$ with cardinality M_j, we take $d_j = M_j$, and use a binary coding of each modality by defining

$$x^B_{i,j,k} = \begin{cases} 1, & \text{if } x_{i,j} = k, \\ 0, & \text{otherwise,} \end{cases}$$

- If $X_{\bullet,j}$ is quantitative, then d_j we consider a partition of intervals $I_{j,1}, \ldots, I_{j,d_j}$ for the range of values of $\boldsymbol{X}_{\bullet,j}$ and define

$$x^B_{i,j,k} = \begin{cases} 1, & \text{if } x_{i,j} \in I_{j,k}, \\ 0, & \text{otherwise,} \end{cases}$$

- The i-th raw of $\boldsymbol{X}^B$ is written

$$x^B_i = (x^B_{i,1,1}, \ldots, x^B_{i,1,d_1}, x^B_{i,2,1}, \ldots, x^B_{i,2,d_2}, \ldots, x^B_{i,p,1}, \ldots, x^B_{i,p,d_p})^\top \in \mathbb{R}^d$$

Features binarization: setup

- A natural choice of intervals is given by the quantiles, namely we can typically choose $I_{j,k} = \left(q_j(\frac{k-1}{d_j}), q_j(\frac{k}{d_j})\right]$ for $k = 1, \ldots, d_j$, where $q_j(\alpha)$ denotes a quantile of order $\alpha \in [0, 1]$ for $\boldsymbol{X}_{\bullet,j}$.
- To each binarized feature $\boldsymbol{X}^B_{\bullet,j,k}$ 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

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

Features binarization

- The one-hot-encodings satisfy $\sum_{k=1}^{d_j} \boldsymbol{X}_{i,j,k} = 1$ for all j, meaning that the columns of each block sum to $\mathbf{1}_n$.
  $\rightarrow \boldsymbol{X}^B$ is not of full rank by construction.
- Some of the raw features $\boldsymbol{X}_{\bullet,j}$ might not be relevant for the prediction task, so we want to select raw features from their one-hot encodings,
  $\rightarrow$ **block-sparsity** in θ.
- In our penalization term, we impose $\sum_{k=1}^{d_j} \theta_{j,k} = 0$ for all $j = 1, \ldots, p$ (**sum-to-zero-constraint**).
- We remark that within each block, binary features are ordered.
  $\rightarrow$ We use a within block weighted total-variation penalization

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

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

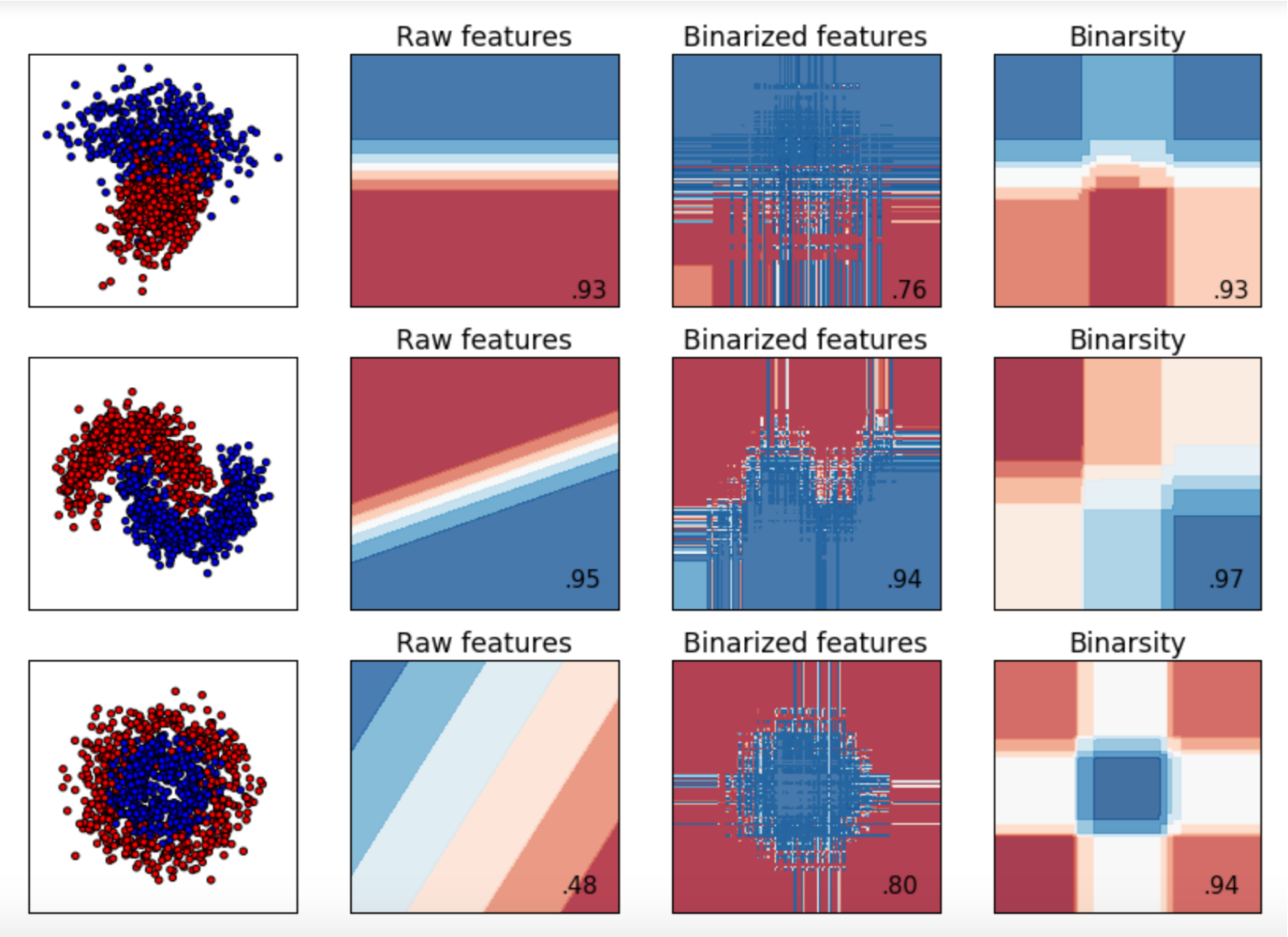
$$\text{bina}(\theta) = \sum_{j=1}^{p} \Big(\sum_{k=2}^{d_j} \hat{\omega}_{j,k} |\theta_{j,k} - \theta_{j,k-1}| + \delta_1(\theta_{j,\bullet}) \Big),$$

where the indicator function

$$\delta_1(u) = \begin{cases} 0 & \text{if} \quad \mathbf{1}^\top u = 0, \\ \infty & \text{otherwise.} \end{cases}$$

- If a raw feature j is statistically not relevant for predicting the labels, then the full block $\theta_{j,\bullet}$ should be zero.
- If a raw feature j is relevant, then the number of different values for the coefficients of $\theta_{j,\bullet}$ should be kept as small as possible, in order to balance bias and variance.

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



Weights in Binarsity

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

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

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

$$y|x \mapsto f^0(y|x) = \exp\left(\frac{y m^0(x) - b(m^0(x))}{\varphi} + c(y)\right),$$

- The functions $b(\cdot)$ and $c(\cdot)$ are known, while the natural parameter function $m^0(x)$ is *unknown*.
- We have

$$m^0(x) = g(\mathbb{E}[Y_i|X_i = x_i]), \qquad \text{where } b' = g^{-1}.$$

- 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

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

  where $m_\theta(x_i) = \theta^\top x_i^B$.
- ℓ is the generalized linear model loss function and is given by

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

- 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

$$\hat{\theta} \in \underset{\theta \in \mathbb{R}^d}{\operatorname{argmin}} \big\{ R_n(\theta) + \operatorname{bina}(\theta) \big\}.$$

Fast oracle inequality in GLM with binarsity scenario

Assumption

Assume that b is three times continuously differentiable, and that there exist constants $C_n > 0$, and $0 < L_n \leq U_n$ such that
$C_n = \max_{i=1,\dots,n} |m^0(x_i)| < \infty$ *and* $L_n \leq \max_{i=1,\dots,n} b''\big(m^0(x_i)\big) \leq U_n$.

For all $\theta \in \mathbb{R}^d$, let $J(\theta) = \big[J_1(\theta), \dots, J_p(\theta)\big]$ be the concatenation of the support sets relative to the total-variation penalization, that is

$$J_j(\theta) = \big\{k : \theta_{j,k} \neq \theta_{j,k-1}, \text{ for } k = 2, \dots, d_j\big\}.$$

Assumption

Let $K = [K_1, \dots, K_p]$ be a concatenation of index sets. Assume

$$\kappa(K) \in \inf_{u \in \mathscr{C}_{\mathrm{TV},\hat{\omega}}(K) \setminus \{\mathbf{0}_d\}} \left\{ \frac{\|\boldsymbol{X} u\|_2}{\sqrt{n}\|u_K\|_2} \right\} > 0$$

with $\mathscr{C}_{\mathrm{TV},\hat{\omega}}(K) = \left\{ u \in \mathbb{R}^d : \sum_{j=1}^p \|(u_j)_{K_j^\complement}\|_{\mathrm{TV},\hat{\omega}_{j,\bullet}} \leq 2 \sum_{j=1}^p \|(u_j)_{K_j}\|_{\mathrm{TV},\hat{\omega}_{j,\bullet}} \right\}$.

Fast oracle inequality in GLM with binarsity scenario

To evaluate the quality of the estimation, we shall use the *excess risk* of $\hat{m}$,

$$R(\hat{m}) - R(m^0(\boldsymbol{X})) = \mathbb{E}_{\mathscr{L}(Y|X)}[R_n(\hat{m}) - R_n(m^0)].$$

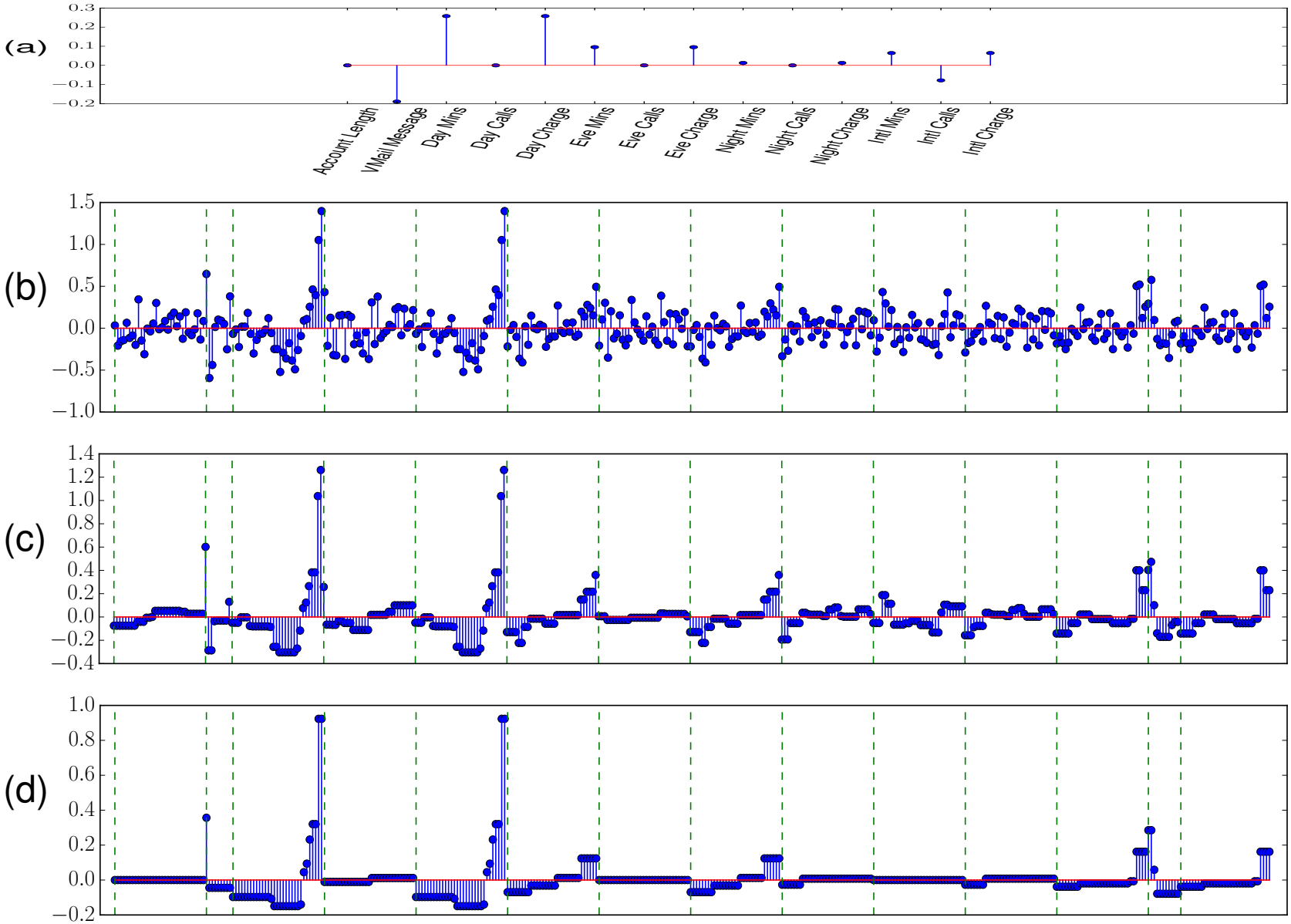
Theorem 3

With a high probability, any solution $\hat{\theta}$ of the penalized problem restricted on $B_d(\rho)$ fulfills the following risk bound

$$R(m_{\hat{\theta}}) - R(m^0) \leq (1+\zeta) \inf_{\theta \in B_d(\rho)} \left\{ R(m_\theta) - R(m^0) + \frac{\xi |J(\theta)|}{\kappa^2(J(\theta))} \max_{j=1,\dots,p} \|(\hat{\omega}_{j,\bullet})_{J_j(\theta)}\|_\infty^2 \right\},$$

where $B_d(\rho) = \{\theta \in \mathbb{R}^d : \|\theta\|_2 \leq \rho\}$, $\zeta = Cst(C_n, \rho, p, L_n, U_n) << 1$ and $\xi = Cst(C_n, \rho, p, L_n, U_n)$.

Illustration of the binarsity penalty on the "Churn" dataset.



Proximal algorithm of weighted binarsity

- Since Binarsity is separable by blocks, we have

$$\left(\operatorname{prox}_{\text{bina}}(\theta)\right)_{j,\bullet} = \operatorname{prox}_{(\|\cdot\|_{\text{TV},\hat{\omega}_{j,\bullet}}+\delta_1)}(\theta_{j,\bullet}),$$

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

- Algorithm 2 expresses $\operatorname{prox}_{\text{bina}}$ based on the proximal operator of the weighted TV penalization.

Algorithm 2:

Input: vector $\theta \in \mathbb{R}^d$ and weights $\hat{\omega}_{j,k}$ for $j = 1, \ldots, p$ and $k = 1, \ldots, d_j$

Output: vector $\eta = \operatorname{prox}_{\text{bina}}(\theta)$

for $j = 1$ **to** p **do**

  $\beta_{j,\bullet} \leftarrow \operatorname{prox}_{\|\theta_{j,\bullet}\|_{\text{TV},\hat{\omega}_{j,\bullet}}}(\theta_{j,\bullet})$ (TV-weighted prox in block j)

  $\eta_{j,\bullet} \leftarrow \beta_{j,\bullet} - \frac{1}{d_j}\sum_{k=1}^{d_j} \beta_{j,k}$ (within-block centering)

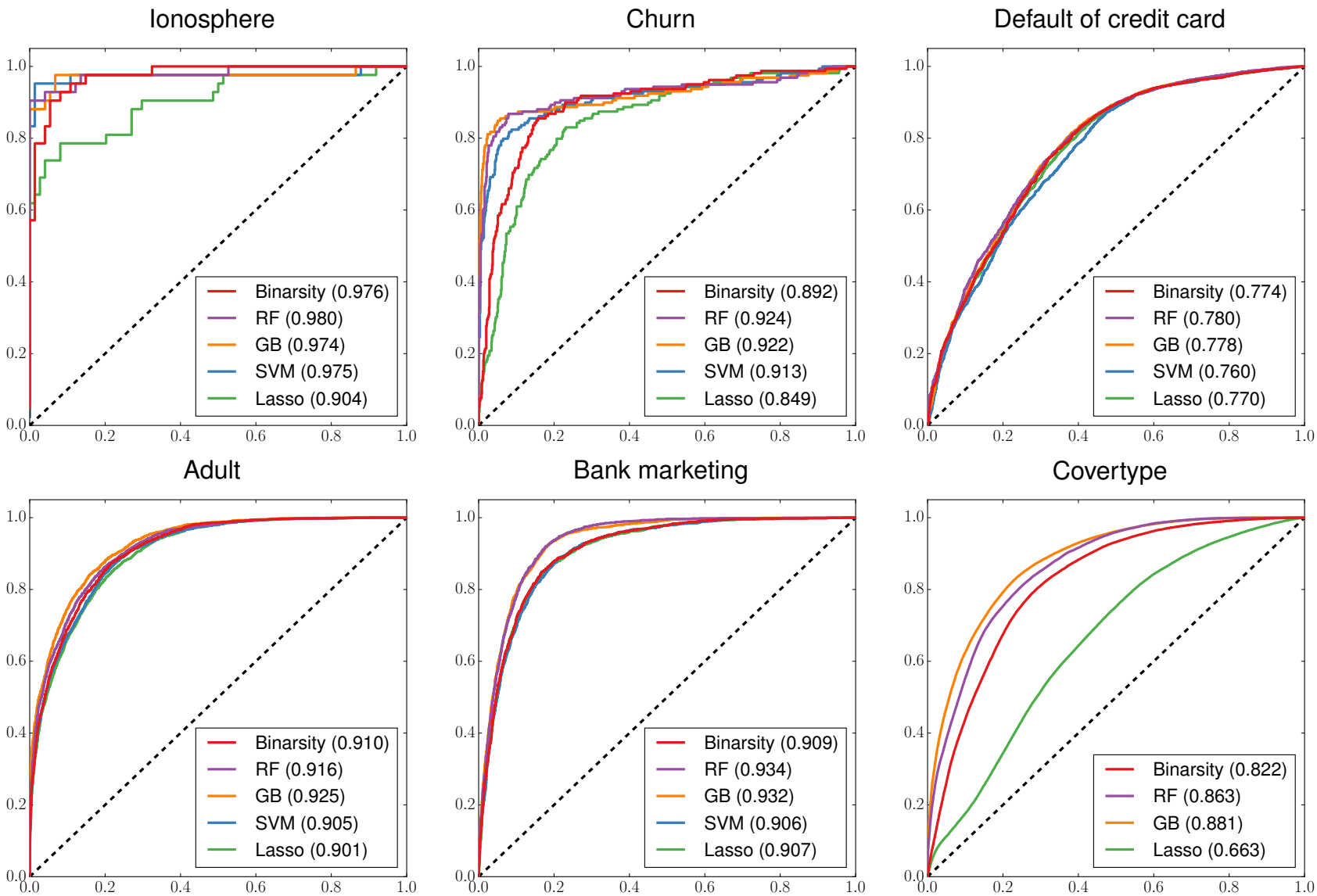
Return: η

Real data

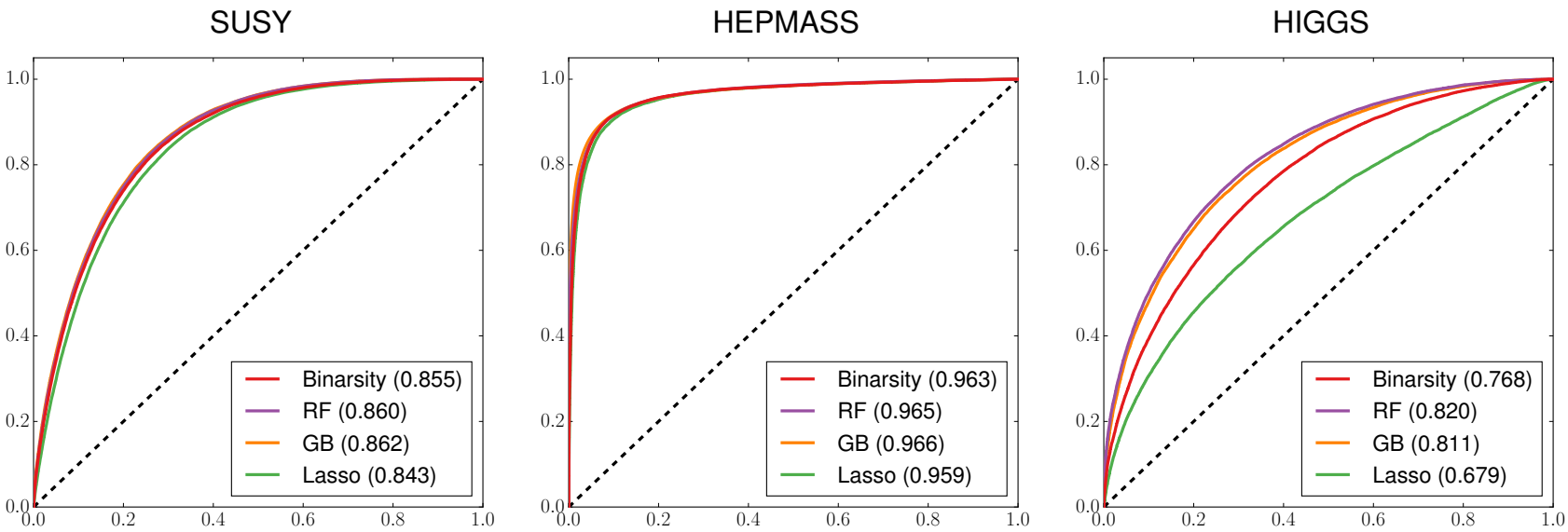
Dataset	n	p
Ionosphere	351	34
Churn	3333	21
Default of credit card	30000	24
Adult	32561	14
Bank marketing	45211	17
Covertype	550088	10
SUSY	5000000	18
HEPMASS	10500000	28
HIGGS	11000000	24

[Source: UCI Machine Learning Repository (https://archive.ics.uci.edu/ml/datasets/)]

Real data

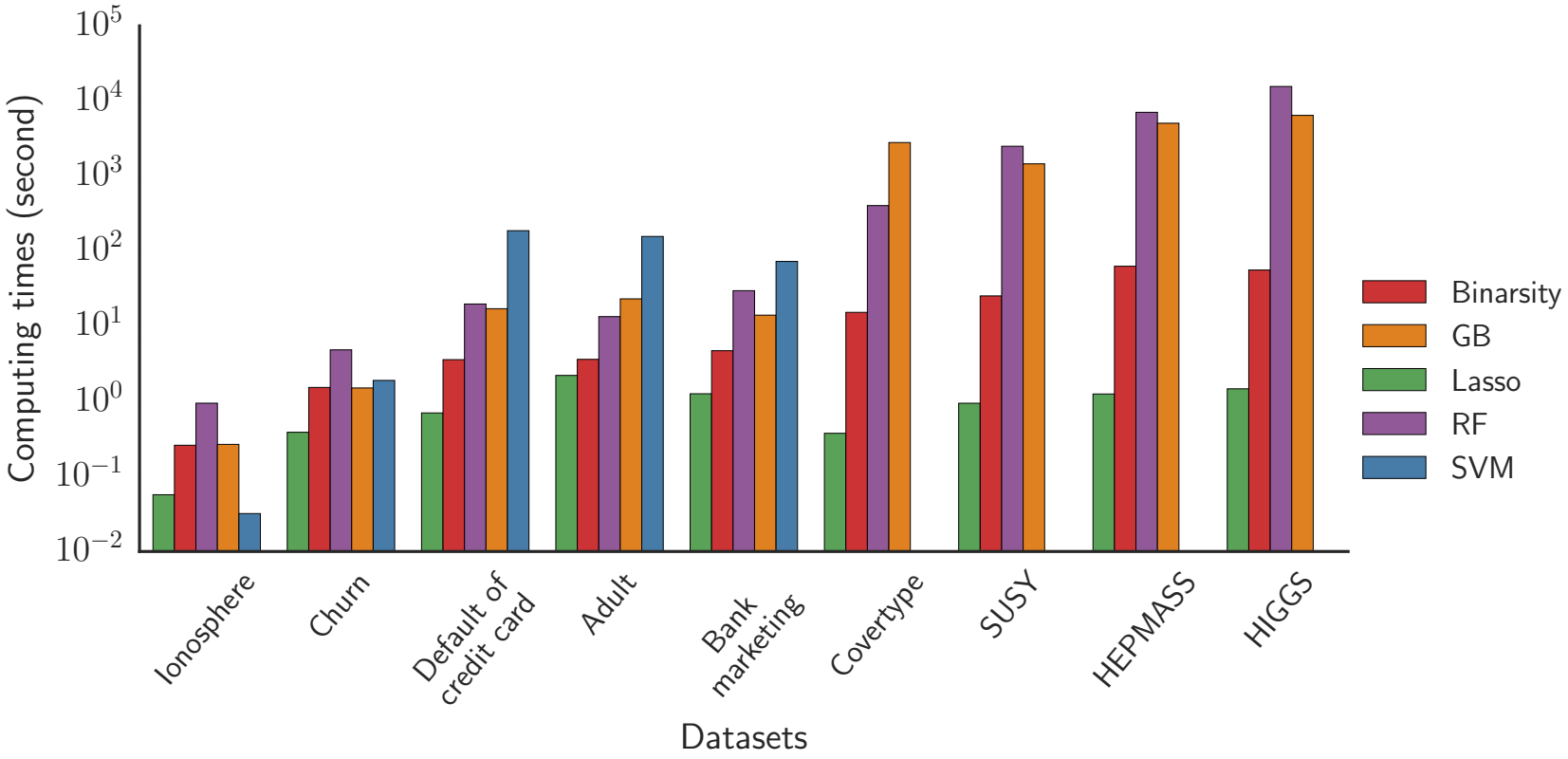

Ionosphere
Binarsity (0.976)
RF (0.980)
GB (0.974)
SVM (0.975)
Lasso (0.904)
Churn
Binarsity (0.892)
RF (0.924)
GB (0.922)
SVM (0.913)
Lasso (0.849)
Default of credit card
Binarsity (0.774)
RF (0.780)
GB (0.778)
SVM (0.760)
Lasso (0.770)
Adult
Binarsity (0.910)
RF (0.916)
GB (0.925)
SVM (0.905)
Lasso (0.901)
Bank marketing
Binarsity (0.909)
RF (0.934)
GB (0.932)
SVM (0.906)
Lasso (0.907)
Covertype
Binarsity (0.822)
RF (0.863)
GB (0.881)
Lasso (0.663)

Real data



Python library "tick" [Gaïffas et al. (2017)]
(https://x-datainitiative.github.io/tick/)

Computing time comparisons



Computing time comparisons (in seconds) between the methods on the considered datasets

Take Home Message

- We introduce a data-driven weighted TV penalization for two problems: estiamtion of intsity of a counting process and GLM with binarized features.
- For each procedure, we give: theoretical guaranties via non-asymptotic oracles inequalities for the prediction error and algorithms that efficiently solve the studied convex problems.

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Thank you!