

On Interpretability in Data Analytics

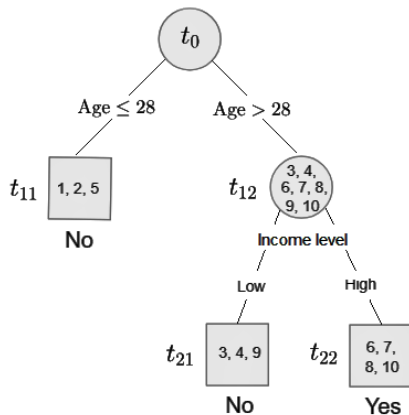
Emilio Carrizosa, IMUS - Instituto de Matemáticas de la Universidad de Sevilla

Nizhny Novgorod, 21st November 2020

Classification and regression with trees

CARTs (Breiman et al. 1984)

Applicant	Age	Income level	Loan granted
1	22	Low	No
2	26	High	No
3	30	Low	Yes
4	32	Low	No
5	20	High	No
6	45	High	Yes
7	60	High	No
8	54	High	Yes
9	50	Low	No
10	48	High	Yes



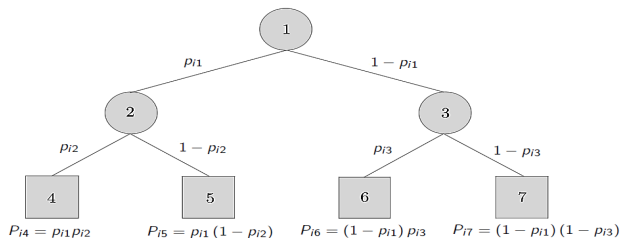
Blanquero, Carrizosa, Molero-Río, Romero Morales, EJOR, 2019

We have a sample $I = \{(\mathbf{x}_i, y_i)\}_{1 \leq i \leq n}$, where $\mathbf{x}_i \in [0, 1]^p$ and $y_i \in \{1, \dots, K\}$.

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A maximal binary tree of depth D . Nodes: Branch $t \in \tau_B$, Leaf $t \in \tau_L$.



Optimal Randomized Classification Trees

(Mixed-Integer Non-Linear Optimization Problem)

$$\begin{aligned} \min \quad & \sum_{k=1}^K \sum_{i \in I_k} \sum_{t \in \tau_L} P_{it} \sum_{k' \neq k} C_{k't} W_{kk'} \\ \text{s.t.} \quad & \sum_{j=1}^p a_{jt} = 1, \quad t \in \tau_B, \\ & \sum_{k=1}^K C_{kt} = 1, \quad t \in \tau_L, \\ & \sum_{t \in \tau_L} C_{kt} \geq 1, \quad k = 1, \dots, K, \\ & a_{jt} \in \{0, 1\}, \quad j = 1, \dots, p, \quad t \in \tau_B, \\ & C_{kt} \in \{0, 1\}, \quad k = 1, \dots, K, \quad t \in \tau_L, \\ & \alpha_t \in A, \quad t \in \tau_B. \end{aligned}$$

Optimal Randomized Classification Trees

(Continuous Non-Linear Optimization Problem)

OBLIQUE splits

$$\min \sum_{k=1}^K \sum_{i \in I_k} \sum_{t \in \tau_L} P_{it} \sum_{k' \neq k} C_{k't} W_{kk'}$$

s.t.

$$\sum_{k=1}^K C_{kt} = 1, \quad t \in \tau_L,$$

(ORCT)

$$\sum_{t \in \tau_L} C_{kt} \geq 1, \quad k = 1, \dots, K,$$

$$a_{jt} \in [-1, 1], \quad j = 1, \dots, p, \quad t \in \tau_B,$$

$$C_{kt} \in [0, 1], \quad k = 1, \dots, K, \quad t \in \tau_L,$$

$$\alpha_t \in A, \quad t \in \tau_B.$$

A new unlabeled observation $\mathbf{x}$



Once the optimization problem has been solved



the decision variables are used for predicting its class:

$$m_n(\mathbf{x}) = \arg \max_k \left\{ \sum_{t \in \tau_L} \mathbb{P}(\mathbf{x} \in k | \mathbf{x} \in t) \mathbb{P}(\mathbf{x} \in t) \right\} = \arg \max_k \left\{ \sum_{t \in \tau_L} C_{kt} \cdot P_{\mathbf{x}t} \right\}$$

UCI Machine Learning Repository

Data set	n	p	K	Class distribution
Connectionist-bench-sonar	208	60	2	55% - 45%
Wisconsin	569	30	2	63% - 37%
Credit-approval	653	37	2	55% - 45%
Pima-indians-diabetes	768	8	2	65% - 35%
Statlog-project-German-credit	1000	48	2	70% - 30%
Ozone-level-detection-one	1848	72	2	97% - 3%
Spambase	4601	57	2	61% - 39%
Iris	150	4	3	33.3%-33.3%-33.3%
Wine	178	13	3	40%-33%-27%
Seeds	210	7	3	33.3%-33.3%-33.3%
Thyroid-disease-ann-thyroid	3772	21	3	92.5%-5%-2.5%
Car-evaluation	1728	15	4	70%-22%-4%-4%

- Logistic CDF:

$$F(\cdot; \mu, \gamma) = \frac{1}{1 + \exp(-(\cdot - \mu)\gamma)}, \quad \mu \in \mathbb{R}, \quad \gamma > 0.$$

$$\mu_t \in [-1, 1], \quad t \in \tau_L, \quad \gamma_t = \gamma = 512, \quad t \in \tau_L.$$

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- Equal misclassification weights,

$$W_{kk'} = 0.5, \quad k, k' = 1, \dots, K, \quad k \neq k'.$$

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- 10 hold-out runs: training subset (75%) and test subset (25%).

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- Equal misclassification weights,

$$W_{kk'} = 0.5, \quad k, k' = 1, \dots, K, \quad k \neq k'.$$

- 10 hold-out runs: training subset (75%) and test subset (25%).
- Performance measure: average accuracy over the 10 test subsets.

ORCT compared with:

- **CART** (Breiman et al. 1984).
- **OCT-H** (Bertsimas and Dunn 2017).
- **RF** (Breiman 2001).

$$D = 1$$

Data set	ORCT average time (in secs)	Out-of-sample accuracy			
		ORCT	CART	OCT-H	RF
Connectionist-bench-sonar	22	76.3	70.0	70.4	83.1
Wisconsin	24	96.4	92.0	93.1	95.5
Credit-approval	22	83.7	85.7	87.9	86.7
Pima-indians-diabetes	21	75.8	74.2	71.6	76.3
Statlog-project-German-credit	28	72.8	72.1	71.6	75.2
Ozone-level-detection-one	94	96.7	95.6	96.8	96.4
Spambase	72	89.8	89.2	83.6	95.1

$D = 1$

Data set	ORCT average time (in secs)	Out-of-sample accuracy			
		ORCT	CART	OCT-H	RF
Connectionist-bench-sonar	22	76.3	70.0	70.4	83.1
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Spambase	72	89.8	89.2	83.6	95.1

$D = 2$

Data set	ORCT average time (in secs)	Out-of-sample accuracy			
		ORCT	CART	OCT-H	RF
Iris	17	95.9	92.7	95.1	95.4
Wine	23	96.6	88.6	91.1	98.6
Seeds	20	94.2	90.2	90.6	92.5
Thyroid-disease-ann-thyroid	145	92.2	99.1	92.5	99.1
Car-evaluation	71	90.8	88.1	87.5	88.0

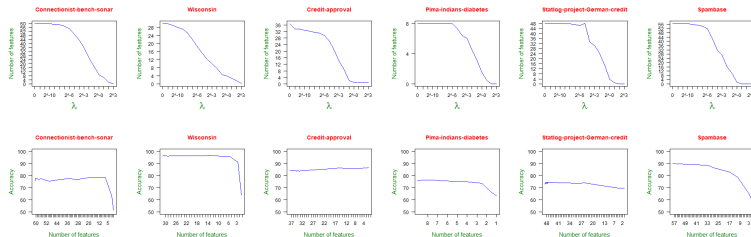
Sparsity on ORCTs at depth 1

$$\begin{aligned} \min \quad & \sum_{k=1}^2 \sum_{i \in I_k} \sum_{t \in \tau_L} P_{it} \sum_{k' \neq k} C_{k't} W_{kk'} \\ \text{s.t.} \quad & C_{12} + C_{22} = 1, \\ & C_{13} + C_{23} = 1, \\ & C_{12} + C_{13} \geq 1, \\ & C_{22} + C_{23} \geq 1, \\ & a_{j1} \in [-1, 1], \quad j = 1, \dots, p, \\ & C_{12}, C_{13}, C_{22}, C_{23} \in [0, 1], \\ & \mu_1 \in [-1, 1]. \end{aligned}$$

A lasso penalization to ORCT

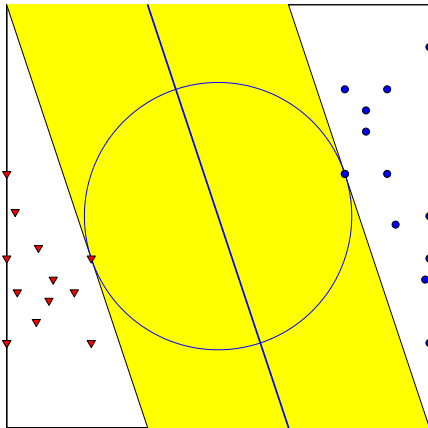
$$\begin{aligned} \min \quad & \sum_{k=1}^2 \sum_{i \in I_k} \sum_{t \in \tau_L} P_{it} \sum_{k' \neq k} C_{k't} W_{kk'} + \lambda \|\mathbf{a}_1\|_1 \\ \text{s.t.} \quad & C_{12} + C_{22} = 1, \\ & C_{13} + C_{23} = 1, \\ & C_{12} + C_{13} \geq 1, \\ & C_{22} + C_{23} \geq 1, \\ & a_{j1} \in [-1, 1], \quad j = 1, \dots, p, \\ & C_{12}, C_{13}, C_{22}, C_{23} \in [0, 1], \\ & \mu_1 \in [-1, 1]. \end{aligned}$$

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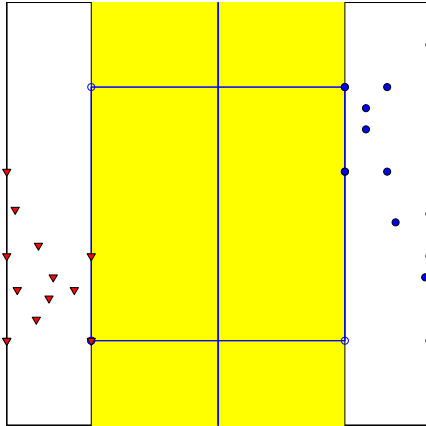


Support Vector Machines

- Roughly speaking, SVM finds the hyperplane $\omega_1 x_1 + \dots + \omega_m x_m + \beta = 0$ **separating most** the sets $\{x_i : i \in I, y_i = 1\}$ and $\{x_i : i \in I, y_i = -1\}$



SVM (ℓ_1)



Convex quadratic optimization problem with linear constraints:

$$\begin{array}{ll} \min_{\omega, \beta, \xi} & \|\omega\|^2 + \sum_{i \in I} \xi_i \\ \text{s.t.} & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\ & \xi_i \geq 0 \quad i \in I \end{array}$$



C., and Romero Morales, "Supervised classification and mathematical optimization", *Computers & Operations Research*, 2013.



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$$\begin{array}{ll} \max_{\lambda} & \sum_{i \in I} \lambda_i - \frac{1}{2} \sum_{ij} \lambda_i y_i \lambda_j y_j x_i^\top x_j \\ \text{s.t.} & \sum_{i \in I} \lambda_i y_i = 0 \\ & 0 \leq \lambda_i \leq \frac{1}{2} \quad i \in I \end{array}$$



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$$\begin{array}{ll} \max_{\lambda} & \sum_{i \in I} \lambda_i - \frac{1}{2} \sum_{ij} \lambda_i y_i \lambda_j y_j K(x_i, x_j) \\ \text{s.t.} & \sum_{i \in I} \lambda_i y_i = 0 \\ & 0 \leq \lambda_i \leq \frac{1}{2} \quad i \in I \end{array}$$

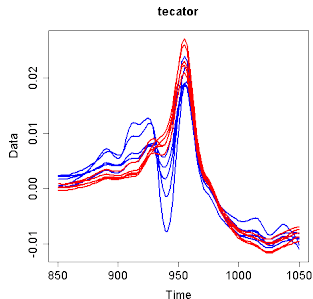


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Classification with functional data



- $x \in \mathcal{C}^0([0, T])$
- $x \approx (x(t_1), \dots, x(t_m)) \in \mathbb{R}^m$
- $(x(t_1), \dots, x(t_m)) \approx x \in \mathcal{C}^0([0, T])$



Ferraty and Vieu. *Nonparametric functional data analysis: theory and practice*, 2006.

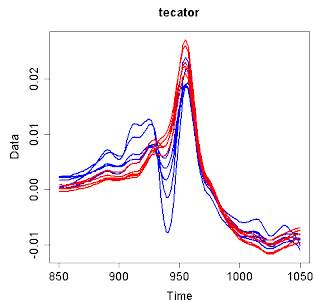


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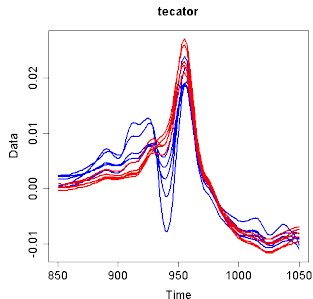


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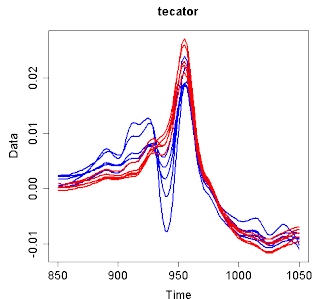


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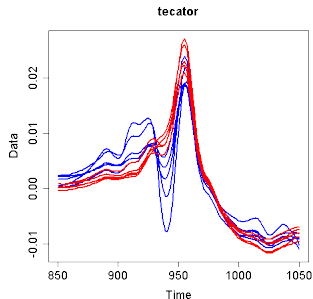


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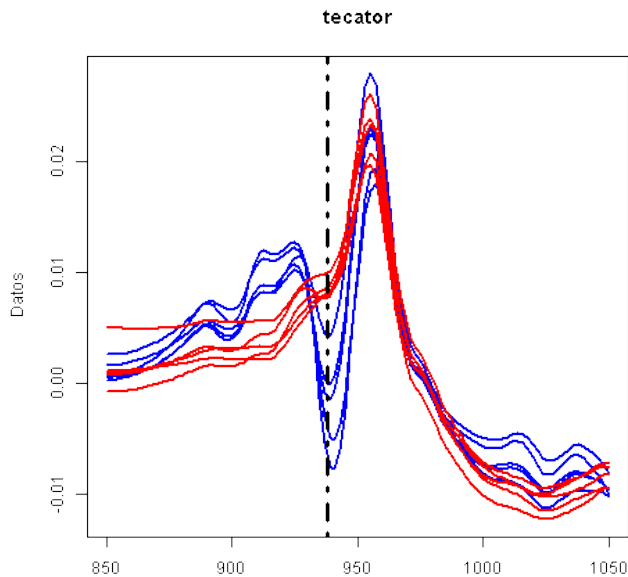


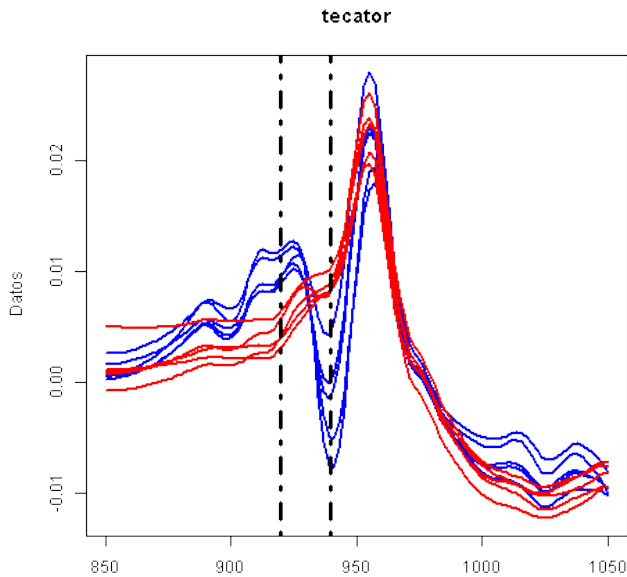
Blanquero, C., Jiménez-Cordero, Martín-Barragán. Variable Selection in Classification for Multivariate Functional Data. Researchgate, 2018.



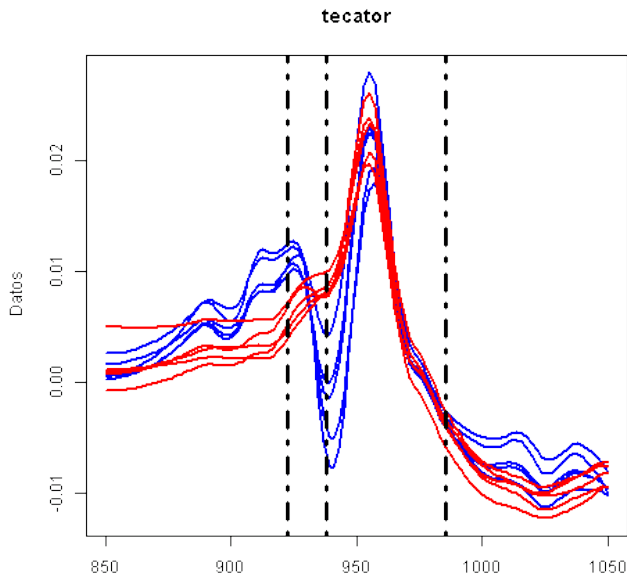
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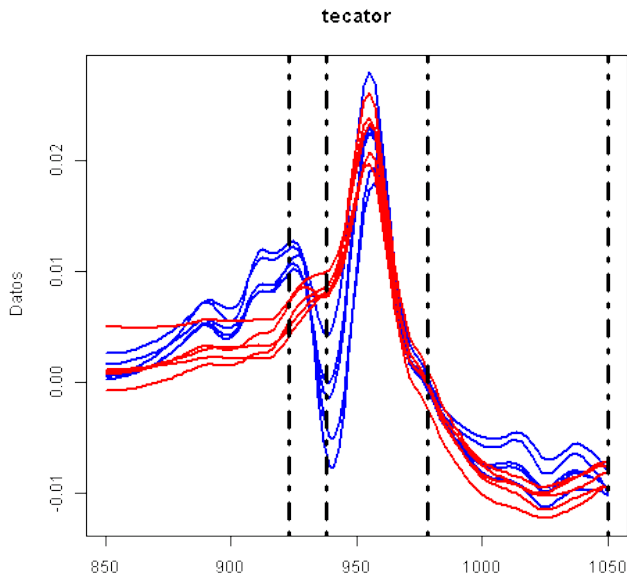
SVM with functional data





SVM with functional data





Cost-sensitive SVM

The performance measure

$$\begin{array}{ll} \min_{\omega, \beta, \xi} & \|\omega\|^2 + \sum_{i \in I} \xi_i \\ \text{s.t.} & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\ & \xi_i \geq 0 \quad i \in I \end{array}$$

ω, β, C

The performance measure

- $\{(x_i, y_i) : i \in I\}$: seen as a random sample of (X, Y)
- **Accuracy**: $\text{acc} = P(Y(\omega^\top X + \beta) > 0)$
- Distribution of (X, Y) :

The performance measure

$$\begin{array}{ll} \min_{\omega, \beta, \xi} & \|\omega\|^2 + C \sum_{i \in I} \xi_i \\ \text{s.t.} & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\ & \xi_i \geq 0 \quad i \in I \end{array}$$

$$\omega, \beta, C$$

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(Asymmetric) costs



C., Martín-Barragán, Romero Morales. "Multi-group support vector machines with measurement costs: A biobjective approach". Discrete Applied Mathematics, 2008.



He, Ma. *Imbalanced learning: foundations, algorithms, and applications*. Wiley, 2013.



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Prati, Batista, Duarte Silva. "Class imbalance revisited: a new experimental setup to assess the performance of treatment methods". Knowledge and Information Systems. 2015.



Turney. "Types of cost in inductive concept learning". 2002.

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ω, β, C

Performance measures $\pi(\omega, \beta)$:

- **Accuracy:** $\text{acc} = P(Y(\omega^\top X + \beta) > 0)$
- **Sensitivity:** $\text{TPR} = P(\omega^\top X + \beta > 0 | Y = 1)$
- **Specificity:** $\text{TNR} = P(\omega^\top X + \beta < 0 | Y = -1)$
- **Youden's index:**
 $J = \text{TPR} + \text{TNR} - 1 = P(\omega^\top X + \beta > 0 | Y = 1) + P(\omega^\top X + \beta < 0 | Y = -1) - 1$
- **Positive Predictive Value:** $\text{PPV} = P(Y = 1 | \omega^\top X + \beta > 0)$
- **Negative Predictive Value:** $\text{NPV} = P(Y = -1 | \omega^\top X + \beta < 0)$
- ...

$$\begin{array}{ll} \min_{\omega, \beta, \xi} & \|\omega\|^2 + \sum_{i \in I} \xi_i \\ \text{s.t.} & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\ & \xi_i \geq 0 \quad i \in I \end{array}$$

ω, β, C

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Benítez Peña, Blanquero, C., Ramírez-Cobo. "On Support Vector Machines under a multiple-costs scenario", *Advances in Data Analysis and Classification* 2019. 2018.



Benítez Peña, Blanquero, C., Ramírez-Cobo. "Cost-sensitive Feature Selection for Support Vector Machines", *Computers & OR* 2018.

- Performance measures $\pi_\ell(\omega, \beta), \ell \in L$
- Threshold values γ_ℓ for $\pi_\ell, \ell \in L$
- I : training sample $\{(x_i, y_i) : i \in I\}$
- J : **anchor sample** $\{(x_j, y_j) : j \in J\}$ ($J \cap I = \emptyset$)
- Estimates of performance measures: $\hat{\pi}_\ell(\omega, \beta; J), \ell \in L$
- Desired: $\pi_\ell(\omega, \beta) \geq \gamma_\ell, \ell \in L$
- Imposed: $\hat{\pi}_\ell(\omega, \beta; J) \geq \gamma_\ell^*, \ell \in L$



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- Desired: $\pi_\ell(\omega, \beta) \geq \gamma_\ell, \ell \in L$
- Imposed: $\hat{\pi}_\ell(\omega, \beta; J) \geq \gamma_\ell^*, \ell \in L$



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Standard approach

$$\begin{array}{ll} \min_{\omega, \beta, \xi} & \|\omega\|^2 + \sum_{i \in I} \xi_i \\ \text{s.t.} & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\ & \xi_i \geq 0 \quad i \in I \end{array}$$

Constrained approach

$$\begin{array}{ll} \min_{\omega, \beta, \xi} & \|\omega\|^2 + \sum_{i \in I} \xi_i \\ \text{s.t.} & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\ & \xi_i \geq 0 \quad i \in I \\ & \hat{\pi}_\ell(\omega, \beta; J) \geq \gamma_\ell^* \quad \ell \in L \end{array}$$

Adding constraints to an SVM model

$$\begin{aligned} \min_{\omega, \beta, \xi} \quad & \|\omega\|^2 + C \sum_{i \in I} \xi_i \\ \text{s.t.} \quad & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\ & \xi_i \geq 0 \quad i \in I \\ & (\omega, \beta) \in \Omega \end{aligned}$$

Ω : some (polyhedral) regions forced to be in one side of the separating hyperplane



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- **Desired:** $\pi_\ell(\omega, \beta) \geq \gamma_\ell, \ell \in L$
- **Imposed:** $\hat{\pi}_\ell(\omega, \beta; J) \geq \gamma_\ell^*, \ell \in L$
- γ_ℓ^* : so that H_0 cannot be rejected in the test hypothesis

$$\begin{cases} H_0 : & \pi_\ell(\omega, \beta) \geq \gamma_\ell \\ H_1 : & \pi_\ell(\omega, \beta) < \gamma_\ell \end{cases}$$

Building γ_ℓ^*

- Hoeffding's inequality: for $Z_1, \dots, Z_n$ i.i.d., $Be(p)$, $P(\bar{Z} - p \geq c) \leq e^{-2nc^2}$.
- 100(1 - α)% CI for p :

$$\left(\bar{Z} - \sqrt{\frac{\log \alpha}{-2n}}, 1 \right)$$

- Imposing $p_0 \in CI$ means

$$\bar{Z} \geq p_0 + \sqrt{\frac{\log \alpha}{-2n}}$$

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- $\gamma_\ell^* = \gamma_\ell + \sqrt{\frac{\log \alpha}{-2|J|}}$

$$\begin{aligned}
& \min_{\omega, \beta, \xi} \quad \|\omega\|^2 + \textcolor{blue}{C} \sum_{i \in I} \xi_i \\
& \text{s.t.} \quad y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\
& \quad \xi_i \geq 0 \quad i \in I \\
& \quad \textcolor{red}{\widehat{\pi}_\ell(\omega, \beta; J) \geq \gamma_\ell^*} \quad \ell \in L
\end{aligned}$$

$$z_j = \begin{cases} 1, & \text{if } y_j (\omega^\top x_j + \beta) \geq 1 \\ 0, & \text{else} \end{cases} \quad j \in J$$

$$\begin{aligned}
& \min_{\omega, \beta, \xi, z} \quad \|\omega\|^2 + C \sum_{i \in I} \xi_i \\
& \text{s.t.} \quad y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\
& \quad \xi_i \geq 0 \quad i \in I \\
& \quad a_\ell^\top z \geq b_\ell \quad \ell \in L \\
& \quad z_\ell \in \{0, 1\} \quad \ell \in L \\
& \quad y_j (\omega^\top x_j + \beta) \geq 1 - M(1 - z_j) \quad j \in J
\end{aligned}$$

$$\begin{array}{ll}
\min_{\omega, \beta, \xi} & \|\omega\|^2 + C \sum_{i \in I} \xi_i \\
\text{s.t.} & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\
& \xi_i \geq 0 \quad i \in I \\
& \widehat{\pi}_\ell(\omega, \beta; J) \geq \gamma_\ell^* \quad \ell \in L
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\end{aligned}$$

$$z_j = \begin{cases} 1, & \text{if } y_j (\omega^\top x_j + \beta) \geq 1 \\ 0, & \text{else} \end{cases} \quad j \in J$$

$$\widehat{TPR}(\omega, \beta; J) \geq \gamma$$

$$\sum_{j \in J: y_j = 1} z_j \geq \gamma \# (\{j \in J : y_j = 1\})$$

$$\begin{aligned}
& \min_{\omega, \beta, \xi, z} \quad \|\omega\|^2 + C \sum_{i \in I} \xi_i \\
& \text{s.t.} \quad y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\
& \quad \xi_i \geq 0 \quad i \in I \\
& \quad a_\ell^\top z \geq b_\ell \quad \ell \in L \\
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\min_{\omega, \beta, \xi} \quad & \|\omega\|^2 + \sum_{i \in I} \xi_i \\
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& \widehat{\pi}_\ell(\omega, \beta; J) \geq \gamma_\ell^* \quad \ell \in L
\end{aligned}$$

$$z_j = \begin{cases} 1, & \text{if } y_j (\omega^\top x_j + \beta) \geq 1 \\ 0, & \text{else} \end{cases} \quad j \in J$$

$$\widehat{TNR}(\omega, \beta; J) \geq \gamma$$

$$\sum_{j \in J: y_j = -1} z_j \geq \gamma \# (\{j \in J : y_j = -1\})$$

$$\begin{aligned}
\min_{\omega, \beta, \xi, z} \quad & \|\omega\|^2 + C \sum_{i \in I} \xi_i \\
\text{s.t.} \quad & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\
& \xi_i \geq 0 \quad i \in I \\
& a_\ell^\top z \geq b_\ell \quad \ell \in L \\
& z_\ell \in \{0, 1\} \quad \ell \in L \\
& y_j (\omega^\top x_j + \beta) \geq 1 - M(1 - z_j) \quad j \in J
\end{aligned}$$

$$\begin{aligned}
& \min_{\omega, \beta, \xi} \quad \|\omega\|^2 + \sum_{i \in I} \xi_i \\
& \text{s.t.} \quad y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\
& \quad \xi_i \geq 0 \quad i \in I \\
& \quad \widehat{\pi}_\ell(\omega, \beta; J) \geq \gamma_\ell^* \quad \ell \in L
\end{aligned}$$

$$z_j = \begin{cases} 1, & \text{if } y_j (\omega^\top x_j + \beta) \geq 1 \\ 0, & \text{else} \end{cases} \quad j \in J$$

$$\widehat{J}(\omega, \beta; J) \geq \gamma$$

$$\sum_{j \in J} z_j \geq \gamma \#(J)$$

$$\begin{aligned}
& \min_{\omega, \beta, \xi, z} \quad \|\omega\|^2 + C \sum_{i \in I} \xi_i \\
& \text{s.t.} \quad y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\
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& \quad a_\ell^\top z \geq b_\ell \quad \ell \in L \\
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$$\begin{aligned}
\min_{\omega, \beta, \xi} \quad & \|\omega\|^2 + C \sum_{i \in I} \xi_i \\
\text{s.t.} \quad & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\
& \xi_i \geq 0 \quad i \in I \\
& \widehat{\pi}_\ell(\omega, \beta; J) \geq \gamma_\ell^* \quad \ell \in L
\end{aligned}$$

$$z_j = \begin{cases} 1, & \text{if } y_j (\omega^\top x_j + \beta) \geq 1 \\ 0, & \text{else} \end{cases} \quad j \in J$$

$$\widehat{TPR}_m(\omega, \beta; J) \geq \gamma$$

$$\sum_{j \in J: u_j = m} z_j \geq \gamma \# (\{j \in J : u_j = m\})$$

$$\begin{aligned}
\min_{\omega, \beta, \xi, z} \quad & \|\omega\|^2 + C \sum_{i \in I} \xi_i \\
\text{s.t.} \quad & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\
& \xi_i \geq 0 \quad i \in I \\
& a_\ell^\top z \geq b_\ell \quad \ell \in L \\
& z_\ell \in \{0, 1\} \quad \ell \in L \\
& y_j (\omega^\top x_j + \beta) \geq 1 - M(1 - z_j) \quad j \in J
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\min_{\omega, \beta, \xi} \quad & \|\omega\|^2 + C \sum_{i \in I} \xi_i \\
\text{s.t.} \quad & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\
& \xi_i \geq 0 \quad i \in I \\
& \widehat{\pi}_\ell(\omega, \beta; J) \geq \gamma_\ell^* \quad \ell \in L
\end{aligned}$$

$$z_j = \begin{cases} 1, & \text{if } y_j (\omega^\top x_j + \beta) \geq 1 \\ 0, & \text{else} \end{cases} \quad j \in J$$

$$\widehat{PPV}(\omega, \beta; J) \geq \gamma$$

$$(1 - \gamma) \text{prev}_+ \sum_{j \in J: y_j = 1} z_j - \gamma (1 - \text{prev}_+) \sum_{j \in J: y_j = -1} (1 - z_j) \geq 0$$

$$\begin{aligned}
\min_{\omega, \beta, \xi, z} \quad & \|\omega\|^2 + C \sum_{i \in I} \xi_i \\
\text{s.t.} \quad & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\
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$$\begin{array}{ll}
\min_{\omega, \beta, \xi} & \|\omega\|^2 + C \sum_{i \in I} \xi_i \\
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& \widehat{\pi}_\ell(\omega, \beta; J) \geq \gamma_\ell^* \quad \ell \in L
\end{array}$$

$$z_j = \begin{cases} 1, & \text{if } y_j (\omega^\top x_j + \beta) \geq 1 \\ 0, & \text{else} \end{cases} \quad j \in J$$

$$\widehat{NPV}(\omega, \beta; J) \geq \gamma$$

$$(1 - \gamma) \text{prev}_- \sum_{j \in J: y_j = -1} z_j - \gamma (1 - \text{prev}_-) \sum_{j \in J: y_j = 1} (1 - z_j) \geq 0$$

$$\begin{array}{ll}
\min_{\omega, \beta, \xi, z} & \|\omega\|^2 + C \sum_{i \in I} \xi_i \\
\text{s.t.} & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\
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$$\widehat{\pi}_\ell(\omega, \beta; J) \geq \gamma_\ell^*$$

$$\mathbf{a}_\ell^\top \mathbf{z} \geq b_\ell$$

$$\begin{aligned}
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& \quad z_\ell \in \{0, 1\} \quad \ell \in L \\
& \quad y_j (\omega^\top \mathbf{x}_j + \beta) \geq 1 - \mathbf{M}(1 - z_j) \quad j \in J
\end{aligned}$$

$$\begin{array}{ll}
\min_{\omega, \beta, \xi} & \|\omega\|^2 + \textcolor{blue}{C} \sum_{i \in I} \xi_i \\
\text{s.t.} & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\
& \xi_i \geq 0 \quad i \in I \\
& \hat{\pi}_\ell(\omega, \beta; J) \geq \gamma_\ell^* \quad \ell \in L
\end{array}$$

$$z_j = \begin{cases} 1, & \text{if } y_j (\omega^\top x_j + \beta) \geq 1 \\ 0, & \text{else} \end{cases} \quad j \in J$$

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$$\mathbf{a}_\ell^\top \mathbf{z} \geq b_\ell$$

$$\begin{array}{llll}
\min_{\omega, \beta, \xi, \mathbf{z}} & \|\omega\|^2 + \textcolor{blue}{C} \sum_{i \in I} \xi_i & & \\
\text{s.t.} & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i & i \in I & \\
& \xi_i \geq 0 & i \in I & \\
& \mathbf{a}_\ell^\top \mathbf{z} \geq b_\ell & \ell \in L & \\
& z_\ell \in \{0, 1\} & \ell \in L & \\
& y_j (\omega^\top x_j + \beta) \geq 1 - \textcolor{blue}{M}(1 - z_j) & j \in J &
\end{array}$$

- Denote $J(z) = \{j \in J : z_j = 1\}$

$$\begin{array}{ll}
 \min_{\omega, \beta, \xi, z} & \|\omega\|^2 + C \sum_{i \in I} \xi_i \\
 \text{s.t.} & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\
 & \xi_i \geq 0 \quad i \in I \\
 & a_l^\top z \geq b_l \quad l \in L \\
 & z_\ell \in \{0, 1\} \quad \ell \in L \\
 & y_j (\omega^\top x_j + \beta) \geq 1 - M(1 - z_j) \quad j \in J
 \end{array}$$

- Denote $J(z) = \{j \in J : z_j = 1\}$

$\min_z$

s.t. $z_\ell \in \{0, 1\} \quad \ell \in L$
 $a_\ell^\top z \geq b_\ell \quad \ell \in L$

$\min_{\omega, \beta, \xi}$

s.t. $\omega^\top \omega + C \sum_{i \in I} \xi_i$
 $y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I$
 $y_j (\omega^\top x_j + \beta) \geq 1 \quad j \in J(z)$
 $\xi_i \geq 0 \quad i \in I$

- Denote $J(z) = \{j \in J : z_j = 1\}$

$$\begin{array}{ll}
 \min_z & \\
 \text{s.t.} & z_\ell \in \{0, 1\} \quad \ell \in L \\
 & a_\ell^\top z \geq b_\ell \quad \ell \in L
 \end{array}
 \quad
 \begin{array}{ll}
 \min_{\omega, \beta, \xi} & \omega^\top \omega + C \sum_{i \in I} \xi_i \\
 \text{s.t.} & y_i (\omega^\top x_i + \beta) \geq 1 - \xi_i \quad i \in I \\
 & y_j (\omega^\top x_j + \beta) \geq 1 \quad j \in J(z) \\
 & \xi_i \geq 0 \quad i \in I
 \end{array}$$

KKT conditions for inner problem (z fixed)

$$\begin{array}{ll}
 \omega & = \sum_{s \in I} \lambda_s y_s x_s + \sum_{t \in J(z)} \mu_t y_t x_t \\
 0 & = \sum_{s \in I} \lambda_s y_s + \sum_{t \in J(z)} \mu_t y_t \\
 0 & \leq \lambda_s \leq C/2 \quad s \in I \\
 0 & \leq \mu_t \quad t \in J(z)
 \end{array}$$

- Denote $J(z) = \{j \in J : z_j = 1\}$

$$\begin{array}{ll}
 \min_z & \\
 \text{s.t.} & z_\ell \in \{0, 1\} \quad \ell \in L \\
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 0 & \leq \lambda_s \leq C/2 \quad s \in I \\
 0 & \leq \mu_t \leq M z_t \quad t \in J
 \end{array}$$

(Partial) Dual

$$\begin{array}{ll} \min_{\lambda, \mu, \beta, \xi, z} & \left(\sum_{s \in I} \lambda_s y_s x_s + \sum_{t \in J} \mu_t y_t x_t \right)^\top \left(\sum_{s \in I} \lambda_s y_s x_s + \sum_{t \in J} \mu_t y_t x_t \right) \\ & + C \sum_{i \in I} \xi_i \\ \text{s.t.} & z_\ell \in \{0, 1\} \quad \ell \in L \\ & \mathbf{a}_\ell^\top \mathbf{z} \geq b_\ell \quad \ell \in L \\ & y_i \left(\left(\sum_{s \in I} \lambda_s y_s x_s + \sum_{t \in J} \mu_t y_t x_t \right)^\top x_i + \beta \right) \geq 1 - \xi_i \quad i \in I \\ & y_j \left(\left(\sum_{s \in I} \lambda_s y_s x_s + \sum_{t \in J} \mu_t y_t x_t \right)^\top x_j + \beta \right) \geq 1 - M(1 - z_j) \quad j \in J \\ & \xi_i \geq 0 \quad i \in I \\ & 0 \leq \lambda_i \leq C/2 \quad i \in I \\ & 0 \leq \mu_j \leq Mz_j \quad j \in J \end{array}$$

(Partial) Dual: The kernel trick

$$\begin{array}{ll} \min & \sum_{s,s' \in I} \lambda_s y_s \lambda_{s'} y_{s'} K(x_s, x_{s'}) + \sum_{t,t' \in J} \mu_t y_t \mu_{t'} y_{t'} K(x_t, x_{t'}) \\ & + 2 \sum_{s \in I, t \in J} \lambda_s y_s \mu_t y_t K(x_s, x_t) + C \sum_{i \in I} \xi_i \\ \text{s.t.} & z_\ell \in \{0, 1\} & \ell \in L \\ & \mathbf{a}_\ell^\top \mathbf{z} \geq b_\ell & \ell \in L \\ & y_i \left(\sum_{s \in I} \lambda_s y_s K(x_s, x_i) + \sum_{t \in J} \mu_t y_t K(x_t, x_i) + \beta \right) \geq 1 - \xi_i & i \in I \\ & y_j \left(\sum_{s \in I} \lambda_s y_s K(x_s, x_j) + \sum_{t \in J} \mu_t y_t K(x_t, x_j) + \beta \right) \geq 1 - M(1 - z_j) & j \in J \\ & \xi_i \geq 0 & i \in I \\ & 0 \leq \lambda_i \leq C/2 & i \in I \\ & 0 \leq \mu_j \leq Mz_j & j \in J \end{array}$$

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Parameters involved:

- C , to be **tuned**
- M , to be **fixed**

Experiments

- RBF kernel, parameters tuned by grid search
- Python + Gurobi
- $M = 100$, $\text{time.limit} = 300 \text{ sec}$

Data sets

Name	$ \Omega $	V	$ \Omega_+ $	(%)
australian	690	14	383	(55.5%)
votes	435	16	267	(61.4%)
wisconsin	567	30	357	(62.7%)
german	1000	45	700	(70%)
pageBlocks	5472	10	558	(10.2%)
biodeg	1055	41	356	(33.7%)

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Results

Name		SVM	SVM(C_+, C_-)	Sliding β	CSVM
		Mean (Std)	Mean (Std)	Mean (Target) (Std)	Mean (Target) (Std)
australian	TPR	0.83 (0.071)	0.806 (0.093)	0.821 (0.855) (0.073)	0.903 (0.855) (0.05)
	TNR	0.863 (0.079)	0.878 (0.088)	0.855 (0.068)	0.772 (0.081)
votes	TPR	0.963 (0.04)	0.945 (0.042)	0.971 (0.988) (0.037)	0.978 (0.988) (0.026)
	TNR	0.951 (0.031)	0.941 (0.037)	0.91 (0.063)	0.922 (0.04)
wisconsin	TPR	0.948 (0.049)	0.962 (0.027)	0.989 (0.973) (0.017)	0.965 (0.973) (0.037)
	TNR	0.99 (0.017)	0.931 (0.07)	0.953 (0.045)	0.945 (0.045)
german	TPR	0.464 (0.103)	0.89 (0.08)	0.043 (0.65) (0.023)	0.671 (0.65) (0.164)
	TNR	0.847 (0.031)	0.407 (0.069)	0.996 (0.009)	0.668 (0.111)
pageBlocks	TPR	0.807 (0.03)	0.557 (0.361)	0.819 (0.832) (0.981)	0.859 (0.832) (0.045)
	TNR	0.988 (0.004)	0.901 (0.088)	0.981 (0.006)	0.965 (0.012)
biodeg	TPR	0.783 (0.084)	0.793 (0.083)	0.797 (0.808) (0.095)	0.852 (0.808) (0.057)
	TNR	0.909 (0.032)	0.839 (0.037)	0.891 (0.037)	0.833 (0.05)

Cost-sensitive SVM Feature Selection

Aim

- Find a minimum-cost (e.g. minimum-cardinality) set of features
 - Attaining $\hat{\pi}_\ell(\omega, \beta) \geq \gamma_\ell^*, \ell \in L$
 - Hoping $\pi_\ell(\omega, \beta; I) \geq \gamma_\ell, \ell \in L$
- Once identified the features, solve an SVM

$$\begin{aligned} \min_{\mathbf{w}, \beta, \mathbf{z}, \zeta} \quad & \sum_{k=1}^N \delta_k z_k \\ \text{s.t.} \quad & y_i(\mathbf{w}^\top \mathbf{x}_i + \beta) \geq 1 - L(1 - \zeta_i), & \forall i \in I \\ & \sum_{i \in I} \zeta_i(1 - y_i) \geq \lambda_{-1} \sum_{i \in I} (1 - y_i) \\ & \sum_{i \in I} \zeta_i(1 + y_i) \geq \lambda_1 \sum_{i \in I} (1 + y_i) \\ & |w_k| \leq M z_k & \forall k \in 1, \dots, N \\ & \zeta_i \in \{0, 1\} & \forall i \in I \\ & z_k \in \{0, 1\} & \forall k \in 1, \dots, N \end{aligned}$$

Results. Linear kernel

Name		SVM		FS		Feature reduction
		Mean	Std	Mean	Std	
wisconsin	Acc	0.975	0.021	0.947	0.025	30 → 2 (0 Std)
	TPR	0.992	0.013	0.973	0.031	
	TNR	0.943	0.051	0.905	0.063	
votes	Acc	0.954	0.033	0.949	0.036	32 → 2 (0 Std)
	TPR	0.955	0.038	0.928	0.059	
	TNR	0.947	0.059	0.979	0.036	
nursery	Acc	1	0	1	0	19 → 1 (0 Std)
	TPR	1	0	1	0	
	TNR	1	0	1	0	
Australian	Acc	0.848	0.051	0.855	0.057	34 → 1 (0 Std)
	TPR	0.798	0.083	0.801	0.087	
	TNR	0.912	0.05	0.926	0.041	
careval	Acc	0.956	0.017	0.946	0.019	15 → 9 (0 Std)
	TPR	0.96	0.022	0.963	0.017	
	TNR	0.948	0.024	0.907	0.04	
leukemia	Acc	0.972	0.164	0.875	0.331	7128 → 3.139 (1.205 Std)
	TPR	0.979	0.196	0.896	0.305	
	TNR	0.96	0.144	0.833	0.373	
gastrointestinal	Acc	0.895	0.307	0.829	0.379	698 → 1 (0 Std)
	TPR	0.929	0.258	0.839	0.367	
	TNR	0.8	0.4	0.8	0.4	

Results. Radial kernel

Discrete-Level SVM



E. Carrizosa, A. Nogales-Gómez and D. Romero Morales

Strongly Agree or Strongly Disagree?: Rating Features in Support Vector Machines, *Information Sciences*, 2015



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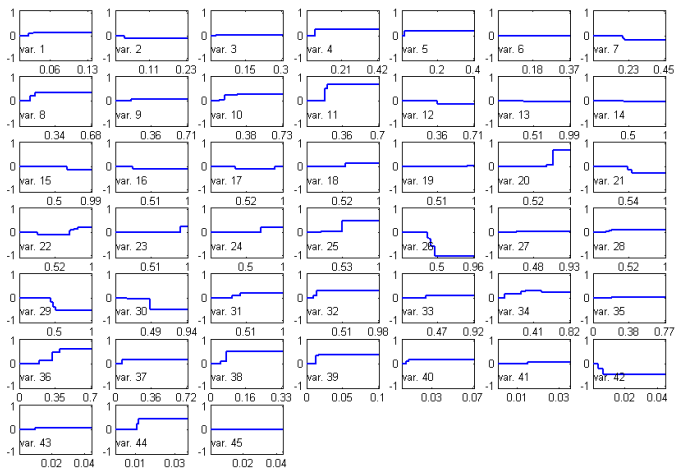
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Romero Morales, D., J. Wang.

"Forecasting cancellation rates for services booking revenue management using data mining", *EJOR*, 2010.



C., Nogales-Gómez, Romero Morales. *Information Science*, 2015

Impose $\omega_j \in \mathcal{A}$, finite, e.g., $\mathcal{A} = \{-a, 0, a\}$

The following features contribute to being a good customer:		Strongly agree	Neutral	Strongly Disagree
Status of existing checking account	... < 0 DM 0 ≤ ... < 200 DM ... ≥ 200 DM		X	
Credit duration	No checking account	X		
Credit history	no credits taken/all credits paid back duly			X
	all credits at this bank paid back duly			X
	existing credits paid back duly till now		X	
	delay in paying off in the past		X	
Purpose	critical account/other credits existing (not at this bank)	X		
	new car			X
	used car		X	
	furniture/equipment		X	
	radio/television		X	
	domestic appliances			X
	repairs		X	
	education			X
	vacation		X	
	retaining	X		
	business		X	
	others			X
Credit amount	...			
Saving accounts	... < 100 DM 100 ≤ ... < 500 500 ≤ ... < 1000 ... ≥ 1000		X	
	unknown/no saving accounts	X		
Duration of present employment	unemployed		X	
	... < 1 year			X
	1 ≤ ... < 4 years			X
	4 ≤ ... < 7 years			X
	... ≥ 7 years		X	
Installment rate in % of disposable income	...			
Personal status and sex	male (divorced/separated)			X
	female (divorced/separated/married)		X	
	male (single)		X	
	male (married/widowed)		X	
	female (single)		X	
Other debtors/guarantors	none		X	
	co-applicant	X		
	guarantor		X	
Duration of present residence	...			
Property	real estate		X	
	building society savings agreement/life insurance		X	
	car/other		X	
	unknown/no property			X
Age	...			
Other installment plans	bank	X		
	store		X	
	none		X	
Housing	rent		X	
	own		X	
	for free	X		
Number of existing credits at this bank	...			
Job	unemployed/unskilled (not-existent)		X	
	unskilled (resident)		X	
	skilled employee/official		X	
	management/self-employed/highly qualified employee officer		X	
Number of people being liable to provide maintenance for	...			
Telephone	None		X	
	Yes		X	
Foreign worker	Yes		X	
	No	X		

C., Nogales-Gómez, Romero Morales. *Information Science*, 2015

Impose $\omega_j \in \mathcal{A}$, finite, e.g., $\mathcal{A} = \{-b, -a, 0, a, b\}$

The following features contribute to being a good customer:		Strongly agree	Agree	Neutral	Disagree	Strongly Disagree
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Credit duration	no credit taken; all credits paid back duly all credits at this bank paid back duly existing credits paid back duly till now delay in paying off in the past critical account (other credits existing (not at this bank))					
Credit history						
Purpose	new car used car furniture/equipment radio/television domestic appliances repairs education vacation retraining business others					
Credit amount	... < 100 DM 100 ≤ ... < 500 500 ≤ ... < 1000 ... ≥ 1000					
Saving accounts	unknown/no saving accounts					
Duration of present employment	unemployed ... < 1 year 1 ≤ ... < 4 years 4 ≤ ... < 7 years ... ≥ 7 years					
Installment rate in % of disposable income						
Personal status and sex	male (divorced/separated) female (divorced/separated/married) male (single) male (married/widowed) female (single)					
Other debtors/guarantors	none co-applicant guarantor					
Duration of present residence						
Property	own estate building society savings agreement/life insurance car/others unknown/no property					
Age						
Other installment plans	bank stores none					
Housing	rent own for free					
Number of existing credits at this bank						
Job	unemployed (unskilled) (non-resident) unskilled (resident) skilled employee/official management/self-employed/highly qualified employee/officer					
Number of people being liable to provide maintenance for						
Employer	None Yes No					
Foreign worker						

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$$\begin{aligned} \min \quad & \omega^\top \omega + C \sum_{i=1}^n \xi_i \\ & y_i(\omega^\top x_i + \beta) \geq 1 - \xi_i, \quad i, i = 1, 2, \dots, n \\ & \xi_i \geq 0, \quad i, i = 1, 2, \dots, n \\ & \omega \in \mathbb{R}^d, \beta \in \mathbb{R}. \end{aligned}$$

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- Define

$$z_{ja} = \begin{cases} 1, & \text{if } \omega_j = a \\ 0, & \text{else} \end{cases}$$

DiLSVM problem:

$$\begin{aligned}
 \min \quad & \sum_{j=1}^d \sum_{a \in \mathcal{A}} a^2 z_{ja} + C \sum_{i=1}^n \xi_i \\
 & y_i \left(\sum_{j=1}^d \sum_{a \in \mathcal{A}} a z_{ja} x_{ij} + \beta \right) \geq 1 - \xi_i \quad i = 1, 2, \dots, n \\
 & \sum_{a \in \mathcal{A}} z_{ja} = 1 \quad j = 1, \dots, d \\
 & \xi_i \geq 0 \quad i = 1, 2, \dots, n \\
 & z_{ja} \in \{0, 1\} \quad \forall j = 1, \dots, d, a \in \mathcal{A} \\
 & \beta \in \mathbb{R}.
 \end{aligned}$$

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 & z_{ja} \in \{0, 1\} \quad \forall j = 1, \dots, d, a \in \mathcal{A} \\
 & \beta \in \mathbb{R}.
 \end{aligned}$$

Performance of the DILSVM⁽¹⁾ classifier

Name	SVM		CKZ	
	Accuracy	Sparsity	$C = \infty, a_1 = 1$	
	Accuracy	Sparsity	Accuracy	Sparsity
adult	84.89	0.00	82.93	55.93
mushroom	99.98	0.00	99.98	49.08
german	72.96	4.12	72.52	51.43
ijcnn1	91.37	0.00	90.18	81.82
careval	95.05	0.00	86.92	30.00
gamma	79.32	0.00	70.37	31.00
abalone	79.52	0.00	74.28	15.00
shuttle	98.17	0.00	80.83	15.55
cod-rna	93.86	0.00	66.56	87.50
calhous	83.59	0.00	63.57	0.00

Name	MILP		RSVM		RR	
	$a_1 \in \{2^0, \dots, 2^{10}\}$		$a_1 \in \{2^0, \dots, 2^{10}\}$		$a_1 \in \{2^0, \dots, 2^{10}\}$	
	Accuracy	Sparsity	Accuracy	Sparsity	Accuracy	Sparsity
adult	<u>90.43</u>	79.27	75.81	<u>100.00</u>	82.33	97.36
mushroom	<u>100.00</u>	91.60	52.01	<u>100.00</u>	99.47	97.56
german	<u>75.32</u>	70.95	69.24	<u>98.89</u>	69.28	93.02
ijcnn1	<u>90.17</u>	<u>100.00</u>	<u>90.18</u>	<u>98.18</u>	90.17	96.59
careval	<u>96.21</u>	59.52	82.03	62.86	87.61	<u>81.19</u>
gamma	<u>79.09</u>	50.00	77.95	<u>80.00</u>	78.31	73.00
abalone	<u>78.28</u>	70.00	77.19	72.00	76.91	<u>75.50</u>
shuttle	<u>97.32</u>	63.33	84.30	<u>75.56</u>	93.75	68.33
cod-rna	<u>78.17</u>	87.50	71.05	88.75	76.13	<u>93.75</u>
calhous	<u>81.98</u>	31.25	78.60	50.00	78.17	<u>65.00</u>

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Name	MILP vs SVM		RSVM		RR	
	$a_1 \in \{2^0, \dots, 2^{10}\}$		$a_1 \in \{2^0, \dots, 2^{10}\}$		$a_1 \in \{2^0, \dots, 2^{10}\}$	
	Accuracy	Sparsity	Accuracy	Sparsity	Accuracy	Sparsity
adult	B	B	75.81	<u>100.00</u>	82.33	97.36
mushroom		B	52.01	<u>100.00</u>	99.47	97.56
german	B	B	69.24	<u>98.89</u>	69.28	93.02
ijcnn1	W	B	<u>90.18</u>	<u>98.18</u>	90.17	96.59
careval	B	B	82.03	62.86	87.61	<u>81.19</u>
gamma		B	77.95	<u>80.00</u>	78.31	73.00
abalone	W	B	77.19	72.00	76.91	<u>75.50</u>
shuttle		B	84.30	<u>75.56</u>	93.75	68.33
cod-rna	W	B	71.05	88.75	76.13	<u>93.75</u>
calhous	W	B	78.60	50.00	78.17	<u>65.00</u>

Performance of the DILSVM⁽²⁾ classifier

Name	SVM		CKZ $C = \infty, a_1 = 1$	
	Accuracy	Sparsity	Accuracy	Sparsity
adult	84.89	0.00	82.93	55.93
mushroom	99.98	0.00	99.98	49.08
german	72.96	4.12	72.52	51.43
ijcnn1	91.37	0.00	90.18	81.82
careval	95.05	0.00	86.92	30.00
gamma	79.32	0.00	70.37	31.00
abalone	79.52	0.00	74.28	15.00
shuttle	98.17	0.00	80.83	15.55
cod-rna	93.86	0.00	66.56	87.50
calhous	83.59	0.00	63.57	0.00

Name	MILP $a_1 \in \{2^0, \dots, 2^{10}\}$ $a_2 \in \{a_1/2, a_1/2^2\}$		RSVM $a_1 \in \{2^0, \dots, 2^{10}\}$ $a_2 \in \{a_1/2, a_1/2^2\}$		RR $a_1 \in \{2^0, \dots, 2^{10}\}$ $a_2 \in \{a_1/2, a_1/2^2\}$		fixing $\bar{C}, \bar{a}_1$ $a_2 \in \{\bar{a}_1/2, \bar{a}_1/2^2\}$	
	Accuracy	Sparsity	Accuracy	Sparsity	Accuracy	Sparsity	Accuracy	Sparsity
adult	<u>90.56</u>	77.40	77.88	90.33	89.04	<u>93.33</u>	<u>89.08</u>	67.07
mushroom	<u>100.00</u>	91.60	99.41	95.80	<u>100.00</u>	<u>100.00</u>	<u>100.00</u>	91.60
german	<u>75.96</u>	55.87	70.92	<u>57.78</u>	73.00	54.76	71.60	35.56
ijcnn1	90.18	95.46	<u>90.46</u>	65.91	90.25	70.45	90.17	<u>100.00</u>
careval	98.71	35.72	89.81	43.34	<u>98.76</u>	<u>53.81</u>	96.84	51.90
gamma	79.31	50.00	78.28	52.00	79.19	<u>57.00</u>	<u>79.36</u>	32.00
abalone	<u>79.05</u>	55.00	78.28	57.00	77.64	<u>65.00</u>	78.43	61.00
shuttle	<u>97.59</u>	45.55	92.16	43.33	96.30	43.33	97.32	<u>47.78</u>
cod-rna	<u>90.64</u>	42.50	73.94	<u>82.50</u>	80.10	62.50	81.32	<u>46.25</u>
calhous	<u>83.03</u>	17.50	80.14	<u>25.00</u>	80.47	17.50	82.25	20.00

Performance of the DILSVM⁽²⁾ classifier

Name	SVM		CKZ $C = \infty, a_1 = 1$	
	Accuracy	Sparsity	Accuracy	Sparsity
adult	84.89	0.00	82.93	55.93
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Name	MILP vs SVM $a_1 \in \{2^0, \dots, 2^{10}\}$ $a_2 \in \{a_1/2, a_1/2^2\}$		RSVM $a_1 \in \{2^0, \dots, 2^{10}\}$ $a_2 \in \{a_1/2, a_1/2^2\}$		RR $a_1 \in \{2^0, \dots, 2^{10}\}$ $a_2 \in \{a_1/2, a_1/2^2\}$		fixing $\bar{C}, \bar{a}_1$ $a_2 \in \{\bar{a}_1/2, \bar{a}_1/2^2\}$	
	Accuracy	Sparsity	Accuracy	Sparsity	Accuracy	Sparsity	Accuracy	Sparsity
adult	B	B	77.88	90.33	89.04	<u>93.33</u>	<u>89.08</u>	67.07
mushroom		B	99.41	95.80	<u>100.00</u>	<u>100.00</u>	<u>100.00</u>	91.60
german	B	B	70.92	<u>57.78</u>	73.00	54.76	71.60	35.56
ijcnn1	W	B	<u>90.46</u>	65.91	90.25	70.45	90.17	<u>100.00</u>
careval	B	B	89.81	43.34	<u>98.76</u>	<u>53.81</u>	96.84	51.90
gamma		B	78.28	52.00	79.19	<u>57.00</u>	<u>79.36</u>	32.00
abalone		B	78.28	57.00	77.64	<u>65.00</u>	78.43	61.00
shuttle		B	92.16	43.33	96.30	43.33	97.32	<u>47.78</u>
cod-rna	W	B	73.94	<u>82.50</u>	80.10	62.50	81.32	<u>46.25</u>
calhous		B	80.14	<u>25.00</u>	80.47	17.50	82.25	20.00

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	Accuracy	Sparsity	Accuracy	Sparsity	Accuracy	Sparsity	Accuracy	Sparsity
adult	<u>90.56</u>	77.40	77.88	90.33	89.04	<u>93.33</u>	B	B
mushroom	<u>100.00</u>	91.60	99.41	95.80	<u>100.00</u>	<u>100.00</u>	B	B
german	<u>75.96</u>	55.87	70.92	<u>57.78</u>	73.00	54.76	W	B
ijcnn1	90.18	95.46	<u>90.46</u>	65.91	90.25	70.45	W	B
careval	98.71	35.72	89.81	43.34	<u>98.76</u>	<u>53.81</u>	B	B
gamma	79.31	50.00	78.28	52.00	79.19	<u>57.00</u>		B
abalone	<u>79.05</u>	55.00	78.28	57.00	77.64	<u>65.00</u>	W	B
shuttle	<u>97.59</u>	45.55	92.16	43.33	96.30	43.33		B
cod-rna	<u>90.64</u>	42.50	73.94	<u>82.50</u>	80.10	62.50	W	B
calhous	<u>83.03</u>	17.50	80.14	<u>25.00</u>	80.47	17.50	W	B

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	Accuracy	Sparsity	Accuracy	Sparsity	Accuracy	Sparsity	Accuracy	Sparsity
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mushroom	<u>100.00</u>	91.60	99.41	95.80	<u>100.00</u>	<u>100.00</u>		B
german	<u>75.96</u>	55.87	70.92	<u>57.78</u>	73.00	54.76		B
ijcnn1	90.18	95.46	<u>90.46</u>	65.91	90.25	70.45		B
careval	98.71	35.72	89.81	43.34	<u>98.76</u>	<u>53.81</u>	B	B
gamma	79.31	50.00	78.28	52.00	79.19	<u>57.00</u>		B
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When we have categorical features ...

Suppose $x = (x', x'')$, with m_{cont} continuous and m_{cat} categorical features.

- each feature of x' : continuous
- each feature j of x'' :
 - takes K_j different values
 - which we codify as K_j dummy (0 – 1) variables $x''_{j1}, \dots, x''_{jK_j}$
- ... and we may have many categorical variables: Carrizosa, Martín-Barragán, Romero Morales, *IJOC*, 2010; Liu, Hussain, Tan, Dash, *DMKD*, 2002, ...

When we have categorical features ...

- Suppose $\mathbf{x} = (\mathbf{x}', \mathbf{x}'')$, with m_{cont} continuous and m_{cat} categorical features.
 - each feature of $\mathbf{x}'$: continuous
 - each feature j of $\mathbf{x}''$:
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 - score function:

$$\sum_{j=1}^{m_{cont}} \nu_j x'_j + \sum_{j=1}^{m_{cat}} \sum_{k \in K_j} \omega_{jk} x''_{jk} + \beta$$

- Optimization problem:

$$\begin{aligned} \min \quad & \sum_{j=1}^{m_{cont}} \nu_j^2 + \sum_{j=1}^{m_{cat}} \sum_{k \in K_j} \omega_{jk}^2 + C \sum_{i \in \Omega_{tr}} \xi_i \\ \text{s.t.} \quad & y_i \left(\sum_{j=1}^{m_{cont}} \nu_j x'_{ij} + \sum_{j=1}^{m_{cat}} \sum_{k \in K_j} \omega_{jk} x''_{ijk} + \beta \right) \geq 1 - \xi_i \quad i \in \Omega_{tr} \\ & \xi_i \geq 0 \quad i \in \Omega_{tr} \end{aligned}$$

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\end{aligned}$$

- Again, convex quadratic problem with linear constraints
- Hard to interpret if many categorical values in features
- Convenient to **reduce complexity** (= reduce number of categorical values in features) without damaging accuracy of classifier

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Strategies

- Feature selection
- Clustering values in certain categorical features

SVM and categorical features

We have ...

- $\mathbf{x} = (\mathbf{x}', \mathbf{x}'')$, with m_{cont} continuous and m_{cat} categorical features, each j of $\mathbf{x}''$: takes K_j different values

We wish ...

- $\mathbf{x} = (\mathbf{x}', \mathbf{x}'')$, with m_{cont} continuous and m_{cat} categorical features, each j of $\mathbf{x}''$: takes L_j different values, with $L_j \leq K_j$ fixed, $L_j = 2$, say
- For each categorical feature, *needed*:

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- For each categorical feature, **needed**:
 - cluster the K_j values into L_j clusters
 - Assign one weight to each cluster, i.e., assign a common weight to all values in the same cluster

We have ...

- $x = (x', x'')$, with m_{cont} continuous and m_{cat} categorical features, each j of x'' : takes K_j different values

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$$\begin{aligned} \min \quad & \sum_{j=1}^{m_{cont}} \nu_j^2 + \sum_{j=1}^{m_{cat}} \sum_{k \in K_j} \omega_{jk}^2 + C \sum_{i \in \Omega_{tr}} \xi_i \\ \text{s.t.} \quad & y_i \left(\sum_{j=1}^{m_{cont}} \nu_j x'_{ij} + \sum_{j=1}^{m_{cat}} \sum_{k \in K_j} \omega_{jk} x''_{ijk} + \beta \right) \geq 1 - \xi_i \quad i \in \Omega_{tr} \\ & \xi_i \geq 0 \quad i \in \Omega_{tr} \end{aligned}$$

Now we have ...

- Define z_{jkl} :

$$z_{jkl} = \begin{cases} 1, & \text{if, in feature } j, \text{ value } k \text{ is assigned to cluster } l \\ 0, & \text{else} \end{cases}$$

- Seek $\bar{\omega}_{jl}$: weight of **all** values of feature j allocated to cluster l

We had ...

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 \text{s.t.} \quad & y_i \left(\sum_{j=1}^{m_{cont}} \nu_j x'_{ij} + \sum_{j=1}^{m_{cat}} \sum_{l=1}^{L_j} \bar{\omega}_{jl} \sum_{k=1}^{K_j} z_{jkl} x''_{ijk} + \beta \right) \geq 1 - \xi_i \quad i \in \Omega_{tr} \\
 & \sum_{l=1}^{L_j} z_{jkl} = 1 \quad j, k \\
 & z_{jkl} \in \{0, 1\} \quad j, k, l \\
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- Mixed Integer Nonlinear **Nonconvex** Optimization Problem
- Very hard to solve, even with state-of-the-art software, e.g. Couenne
- Structural properties are obtained

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- Structural properties are obtained

$$\begin{aligned}
\min \quad & \sum_{j=1}^{m_{cont}} \nu_j^2 + \sum_{j=1}^{m_{cat}} \sum_{l=1}^{L_j} \bar{\omega}_{jl}^2 + C \sum_{i \in \Omega_{tr}} \xi_i \\
\text{s.t.} \quad & y_i \left(\sum_{j=1}^{m_{cont}} \nu_j x'_{ij} + \sum_{j=1}^{m_{cat}} \sum_{l=1}^{L_j} \bar{\omega}_{jl} \sum_{k=1}^{K_j} z_{jkl} x''_{ijk} + \beta \right) \\
& \geq 1 - \xi_i \quad i \in \Omega_{tr} \\
& \sum_{l=1}^{L_j} z_{jkl} = 1 \quad j, k \\
& z_{jkl} \in \{0, 1\} \quad j, k, l \\
& \xi_i \geq 0 \quad i \in \Omega_{tr}
\end{aligned}$$

- Mixed Integer Nonlinear **Nonconvex** Optimization Problem
- Very hard to solve, even with state-of-the-art software, e.g. Couenne
- Structural properties are obtained

Property

If, for some categorical feature j^* , an optimal solution exists with $z_{j^* kl^*} = 1$ for all $k = 1, \dots, K_j$ for some $l^* \in \{1, \dots, L_{j^*}\}$, i.e., if the trivial cluster is obtained, then $\bar{\omega}_{j^* l} = 0$ for all $l \in \{1, \dots, L_{j^*}\}$, i.e., feature j is irrelevant.

Property

Suppose $L_j = 2$. Then, any optimal solution satisfies

$$\bar{\omega}_{j1} \bar{\omega}_{j2} \leq 0$$

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Alternative (big-M) formulation

- Define variables $\tilde{\omega}_{jkl}$:

$$\tilde{\omega}_{jkl} = \begin{cases} \bar{\omega}_{jl}, & \text{if value } k \text{ of feature } j \text{ goes to cluster } l \\ 0, & \text{else} \end{cases}$$

$$\begin{aligned} \min \quad & \sum_{j=1}^{m_{cont}} \nu_j^2 + \sum_{j=1}^{m_{cat}} \sum_{l=1}^{L_j} \bar{\omega}_{jl}^2 + C \sum_{i \in \Omega_{tr}} \xi_i \\ \text{s.t.} \quad & y_i \left(\sum_{j=1}^{m_{cont}} \nu_j x'_{ij} + \sum_{j=1}^{m_{cat}} \sum_{l=1}^{L_j} \bar{\omega}_{jl} \sum_{k=1}^{K_j} z_{jkl} x''_{ijk} + \beta \right) \\ & \geq 1 - \xi_i & i \in \Omega_{tr} \\ & \sum_{l=1}^{L_j} z_{jkl} = 1 & j, k \\ & z_{jkl} \in \{0, 1\} & j, k, l \\ & \xi_i \geq 0 & i \in \Omega_{tr} \end{aligned}$$

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$$\begin{aligned} \min \quad & \sum_{j=1}^{m_{cont}} \nu_j^2 + \sum_{j=1}^{m_{cat}} \sum_{l=1}^{L_j} \tilde{\omega}_{jl}^2 + C \sum_{i \in \Omega_{tr}} \xi_i \\ \text{s.t.} \quad & y_i \left(\sum_{j=1}^{m_{cont}} \nu_j x'_{ij} + \sum_{j=1}^{m_{cat}} \sum_{l=1}^{L_j} \tilde{\omega}_{jk(i)l} + \beta \right) \geq 1 - \xi_i & i \in \Omega_{tr} \\ & \tilde{\omega}_{jkl} \leq \bar{\omega}_{jl} + M(1 - z_{jkl}) & j, k, l \\ & \tilde{\omega}_{jkl} \geq \bar{\omega}_{jl} - M(1 - z_{jkl}) & j, k, l \\ & \tilde{\omega}_{jkl} \leq Mz_{jkl} & j, k, l \\ & \tilde{\omega}_{jkl} \geq -Mz_{jkl} & j, k, l \\ & \sum_{l=1}^{L_j} z_{jkl} = 1 & j, k \\ & z_{jkl} \in \{0, 1\} & j, k, l \\ & \xi_i \geq 0 & i \in \Omega_{tr} \end{aligned}$$

Alternative (big-M) formulation

$$\begin{aligned} \min \quad & \sum_{j=1}^{m_{cont}} \nu_j^2 + \sum_{j=1}^{m_{cat}} \sum_{l=1}^{L_j} \tilde{\omega}_{jl}^2 + c \sum_{i \in \Omega_{tr}} \xi_i \\ \text{s.t.} \quad & y_i \left(\sum_{j=1}^{m_{cont}} \nu_j x'_{ij} + \sum_{j=1}^{m_{cat}} \sum_{l=1}^{L_j} \tilde{\omega}_{jk(i)l} + \beta \right) \geq 1 - \xi_i \quad i \in \Omega_{tr} \\ & \tilde{\omega}_{jkl} \leq \tilde{\omega}_{jl} + M(1 - z_{jkl}) \quad j, k, l \\ & \tilde{\omega}_{jkl} \geq \tilde{\omega}_{jl} - M(1 - z_{jkl}) \quad j, k, l \\ & \tilde{\omega}_{jkl} \leq M z_{jkl} \quad j, k, l \\ & \tilde{\omega}_{jkl} \geq -M z_{jkl} \quad j, k, l \\ & \sum_{l=1}^{L_j} z_{jkl} = 1 \quad j, k \\ & z_{jkl} \in \{0, 1\} \quad j, k, l \\ & \xi_i \geq 0 \quad i \in \Omega_{tr} \end{aligned}$$

- Many more variables ($\tilde{\omega}_{jkl}$) and constraints
- Convex quadratic objective + linear constraints
- Solvable (in principle) by off-the-shelf software such as Cplex

Strategies

- Exact (solving the nonlinear problem with nonconvex constraints)
- Heuristics
 - SVM^{C}
 - SVM^{RR}
 - SVM^{MRR}

Centroid-based

- 1 Solve original SVM^O
- 2 From the weights, perform 1-dim clustering (1d L_j -means)
- 3 Return SVM with clustered values

Randomized rounding

- 1 Solve the continuous relaxation of the nonlinear **nonconvex** formulation
- 2 Round (at random) the allocation variables z_{jkl}
- 3 Return SVM with clustered values

Big M Randomized rounding

- 1 Solve the continuous relaxation of the nonlinear **convex** (big M) formulation
- 2 Round (at random) the allocation variables z_{jkl}
- 3 Return SVM with clustered values

Experiments

10 data sets from the UCI ML Repository

Name	Name in Repository	$ \Omega $	n	Class split (in %)	J	J'	$\sum_{i=1}^J K_j$	K_j
census income	Census-Income (KDD) Data Set	95130	5000	94/6	31	9	491	9,52,47,17,3,7,24,15,5,10,3,6,8,6,6, 50,38,8,9,8,9,3,3,5,42,42,42,5,3,3,3
adult	Adult	30956	5000	24/76	11	3	117	5,8,5,16,5,7,14,6,5,5,41
mushrooms	Mushrooms	8124	5000	48/52	17	4	111	6,4,10,9,4,3,12,4,4,9,9,4,3,8,9,6,7
coil 2000	Insurance Company Benchmark (COIL 2000)	5822	3900	94/6	5	80	77	41,6,10,10,10
abalone	Abalone	4177	2800	50/50	1	7	3	3
molecular	Molecular Biology (Splice junction Gene Sequences)	3190	2200	52/48	60	0	480	8,8,8,...
careval	Car Evaluation	1728	1200	30/70	6	0	21	4,4,4,3,3,3
solar-c	Solar Flare Data Set	1066	800	83/17	5	5	23	7,6,4,3,3
german	Statlog (German Credit Data)	1000	700	30/70	11	9	52	4,5,11,5,5,5,3,4,3,3,4
australian	Statlog (Australian Credit Approval)	690	500	56/44	4	10	29	3,14,9,3

Accuracy

- In 7 datasets (census income, mushrooms, coil 2000, abalone, molecular, solar-c, german), at least 1 strategy: comparable to SVM^O
- In 2 (adult, australian) SVM^O : outperformed
- Just in 1 (careval) SVM^O : winner.

Complexity

Dramatic reduction in nonzero weights:

- smallest: coil 2000 (8.12 p.p.)
- remaining: at least 30 p.p. reduction (even 85.25 p.p.)

- Heursitics: just slightly higher cost than SVM^O
- Exact: rather expensive, but yielding better results.
- Trade-off accuracy/running time: needed

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<i>Name</i>	SVM ^O					
	Accuracy			Reduction		
	mean	std	med	mean	std	med
census income	<u>94.90</u>	0.00	<u>94.90</u>	36.86	0.00	36.86
adult	84.57	0.22	84.63	16.07	3.26	15.38
mushrooms	<u>100.00</u>	0.00	<u>100.00</u>	28.83	0.00	28.83
coil 2000	<u>100.00</u>	0.00	<u>100.00</u>	<u>98.70</u>	0.00	<u>98.70</u>
abalone	79.87	1.18	<u>79.72</u>	0.00	0.00	0.00
molecular	<u>94.22</u>	0.80	<u>94.04</u>	42.96	3.12	41.46
careval	<u>96.74</u>	1.34	<u>96.97</u>	0.95	2.86	0.00
solar-c	83.53	1.23	<u>83.46</u>	47.83	34.51	30.43
german	74.60	2.71	75.66	5.38	1.88	4.81
australian	84.11	3.17	84.73	13.10	4.83	10.34

	Accuracy			Reduction		
	mean	std	med	mean	std	med
census income	94.85	0.00	94.85	89.82	0.00	89.82
adult	88.22	2.44	89.59	86.24	2.21	86.32
mushrooms	<u>100.00</u>	0.00	<u>100.00</u>	76.58	0.00	76.58
coil 2000	<u>100.00</u>	0.00	<u>100.00</u>	<u>98.70</u>	0.00	<u>98.70</u>
abalone	<u>79.90</u>	1.05	79.44	<u>33.33</u>	0.00	<u>33.33</u>
molecular	93.94	0.73	93.84	<u>100.00</u>	0.00	<u>100.00</u>
careval	82.80	5.15	82.95	55.24	8.57	61.90
solar-c	83.61	1.38	<u>83.46</u>	87.83	10.43	91.30
german	74.80	2.36	75.00	57.69	0.00	57.69
australian	84.42	3.32	84.73	80.69	9.66	75.86

	Accuracy			Reduction		
	mean	std	med	mean	std	med
census income	94.84	0.04	94.82	91.69	0.33	91.45
adult	83.44	0.37	83.44	83.42	1.34	83.76
mushrooms	<u>100.00</u>	0.00	<u>100.00</u>	80.72	4.56	81.98
coil 2000	<u>100.00</u>	0.00	<u>100.00</u>	<u>98.70</u>	0.00	<u>98.70</u>
abalone	79.86	1.02	79.44	<u>33.33</u>	0.00	<u>33.33</u>
molecular	93.40	1.28	93.53	75.13	0.19	75.00
careval	92.23	1.28	92.42	58.10	12.2	61.90
solar-c	<u>83.83</u>	1.08	<u>83.46</u>	94.78	11.14	<u>100.00</u>
german	74.60	3.12	74.00	61.73	4.59	58.65
australian	84.53	3.12	84.73	84.83	11.03	86.21

	Accuracy			Reduction		
	mean	std	med	mean	std	med
census income	94.40	0.04	94.37	91.45	1.62	91.65
adult	<u>88.75</u>	2.96	<u>89.63</u>	89.83	4.36	91.45
mushrooms	98.58	0.77	98.59	78.29	5.87	77.93
coil 2000	<u>100.00</u>	0.00	<u>100.00</u>	<u>98.70</u>	0.00	<u>98.70</u>
abalone	79.87	0.96	79.66	<u>33.33</u>	0.00	<u>33.33</u>
molecular	88.04	1.68	88.38	77.29	0.90	77.50
careval	83.94	4.91	85.41	<u>70.48</u>	10.82	<u>71.43</u>
solar-c	83.76	1.02	<u>83.46</u>	<u>99.13</u>	2.61	<u>100.00</u>
german	72.53	3.77	71.66	<u>63.08</u>	4.28	<u>63.46</u>
australian	84.53	3.05	84.73	<u>94.48</u>	2.76	<u>93.10</u>

Many thanks!!!



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