Locating Hyperplanes for Multiclass Classification

Víctor Blanco[1], **Alberto Japón**[2] y Justo Puerto[2]

Universidad de Granada[1]
Universidad de Sevilla[2]

Contents

Data

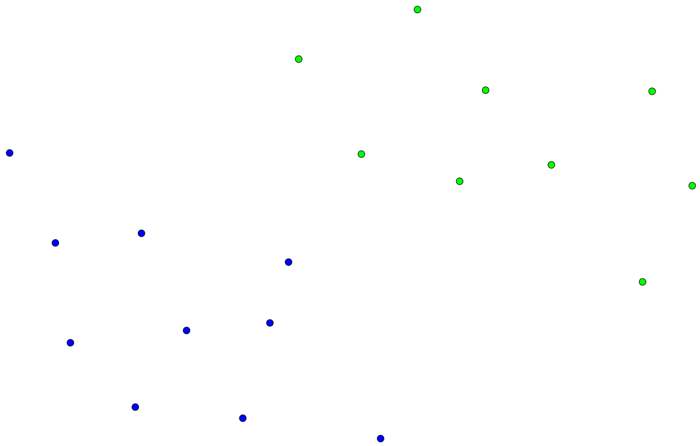
- Random sample of size n
- p predictor variables

$$x_i \in \mathbb{R}^p, \; i = 1, \ldots, n$$

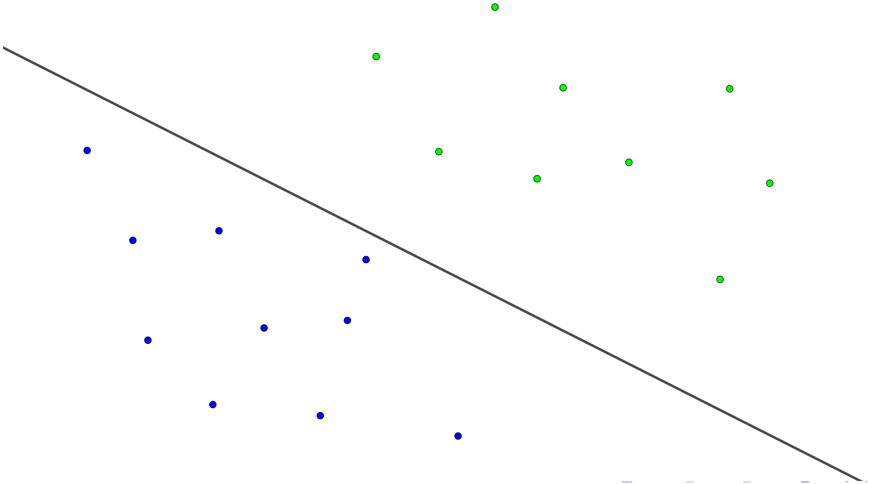
- One target variable with k classes

$$y_i \in \{y_{i1}, \ldots, y_{ik}\}, \; i = 1, \ldots, n$$

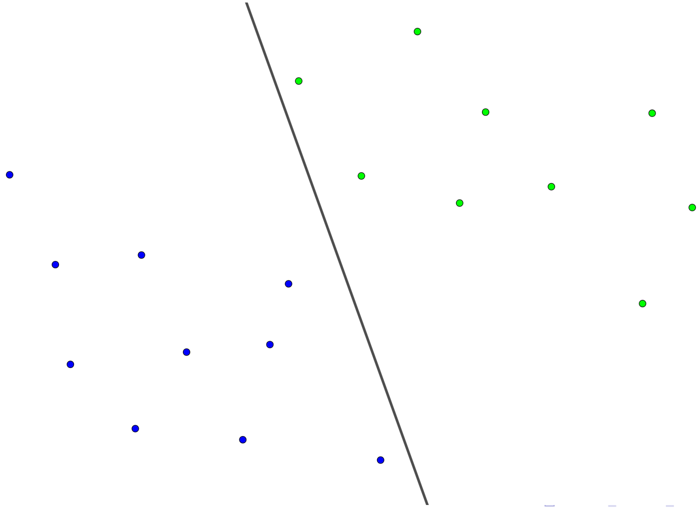
SVM



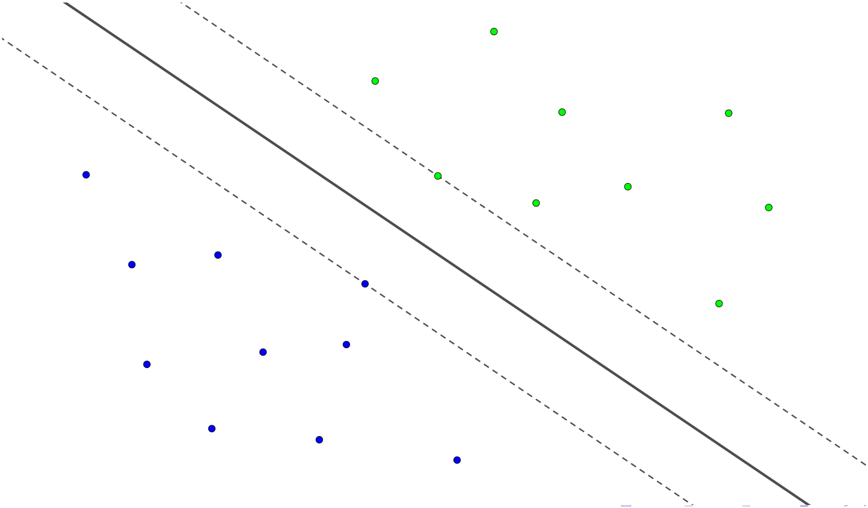
SVM



SVM



SVM



Basic SVM formulation

$$\min \frac{1}{2}\|\omega\|_2^2$$

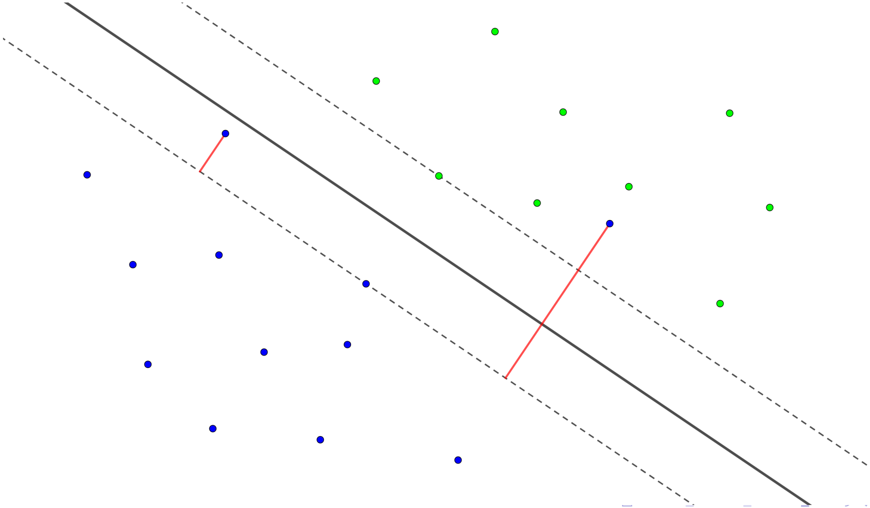
$$\begin{aligned} \text{s.t:} \quad & y_i(\omega' x_i + \omega_0) \geq 1 \qquad && \forall i = 1, \ldots, n \\ & \omega \in \mathbb{R}^p, \; \omega_0 \in \mathbb{R} \end{aligned}$$

General SVM formulation

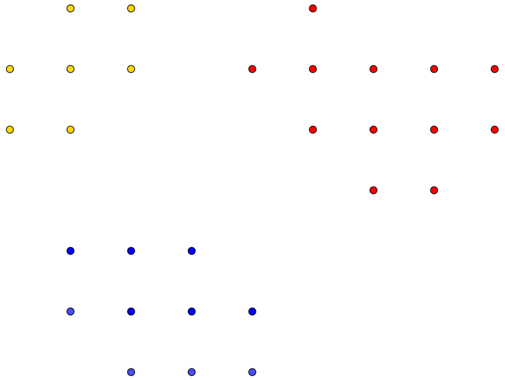
$$\min\left\{\frac{1}{2}\|\omega\|_2^2 + C\sum_{i=1}^{n} d_i\right\}$$

$$\begin{aligned}
\text{s.t:}\quad & y_i(\omega' x_i + \omega_0) \geq 1 - d_i && \forall i = 1,\dots,n\\
& \omega \in \mathbb{R}^p,\ \ \omega_0 \in \mathbb{R} && \\
& d_i \in \mathbb{R}^+ && \forall i = 1,\dots,n
\end{aligned}$$

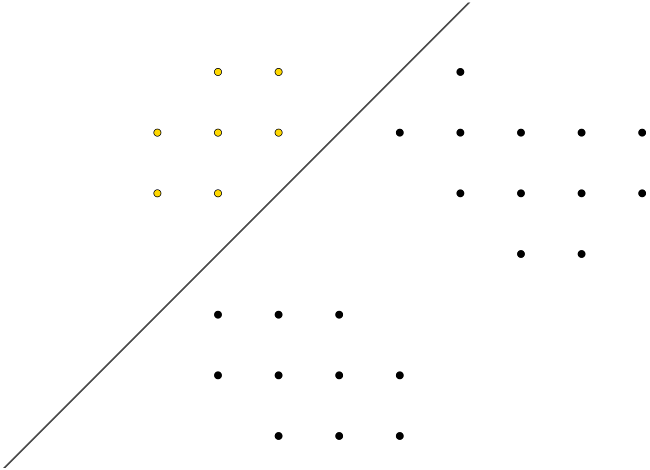
SVM



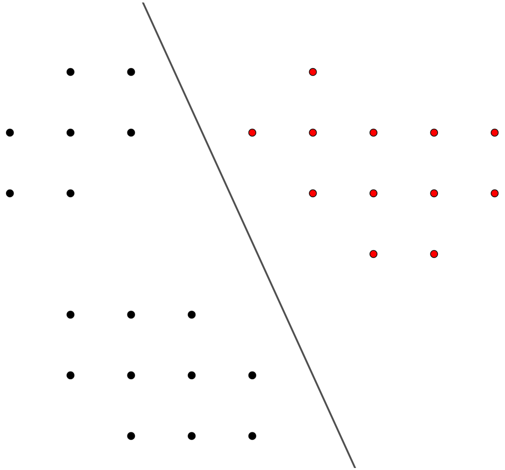
Multiclass problem



One Vs All



One Vs All



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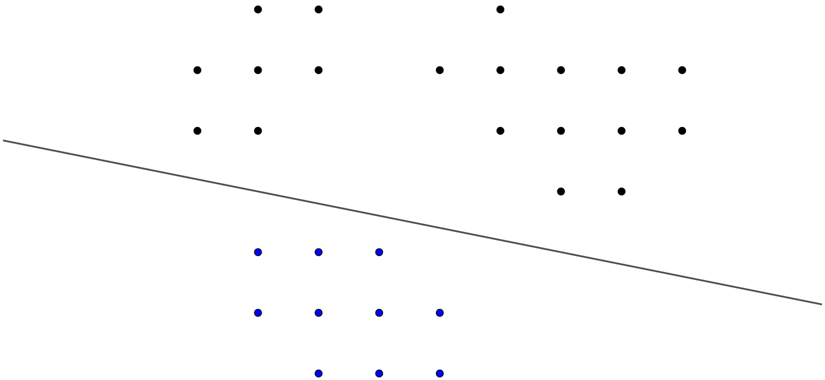
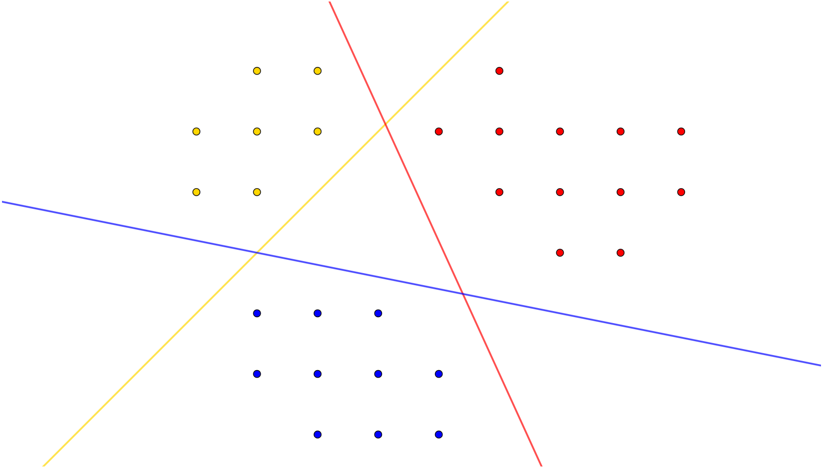
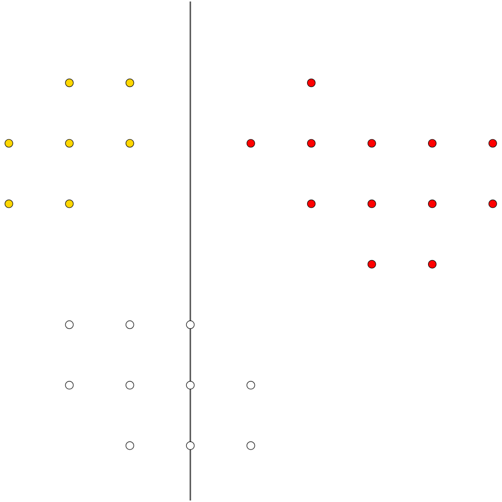


One Vs All



One Vs One



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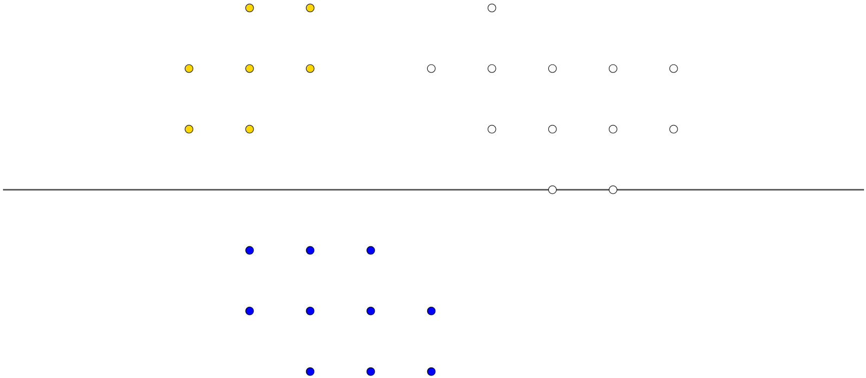

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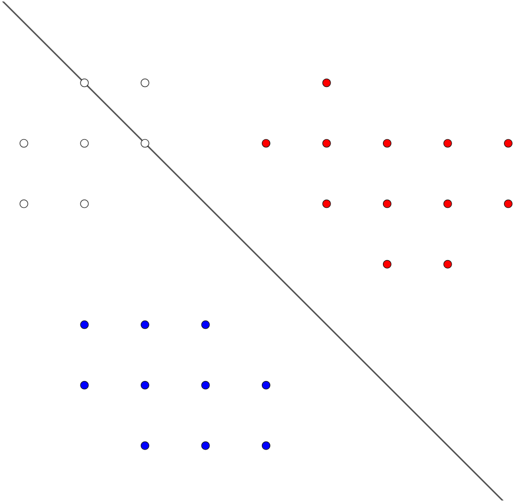

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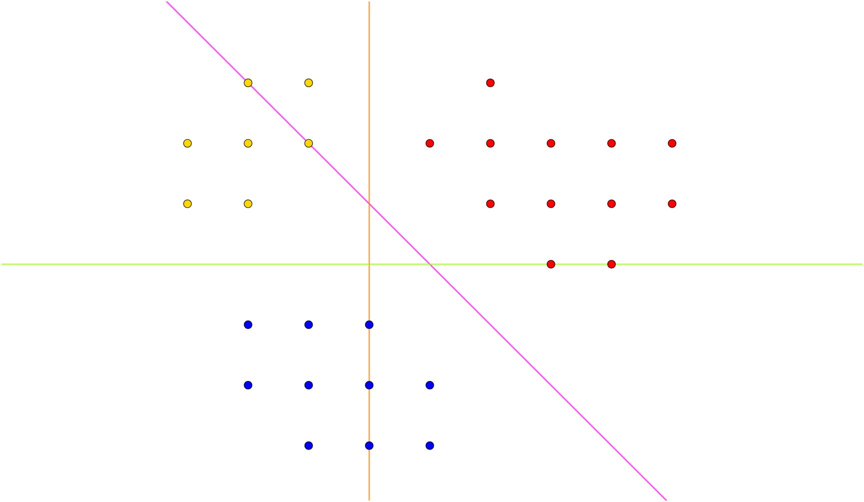

1. Support Vector Machine (SVM)

2. Multiclass methods for SVM
   - Sequential methods
   - Global methods

3. MCSVM
   - The model
   - Results

Weston-Watkins

$$\min \left\{ \sum_{r=1}^{k} \frac{\omega_r' \omega_r}{2} + C \sum_{i=1}^{n} \sum_{j \neq y_i} \xi_i^j \right\}$$

$$\begin{aligned}
\text{s.t:} \quad & \omega_{y_i}' x_i + \omega_{y_i 0} \geq \omega_j' x_i + \omega_{j0} + 2 - \xi_i^j && \forall i = 1, \ldots, n,\ j \in \{1, \ldots, k\} \setminus y_i \\
& \xi_i^j \geq 0 && \forall i = 1, \ldots, n,\ j \in \{1, \ldots, k\} \setminus y_i \\
& \omega_r \in \mathbb{R}^p, \omega_{r0} \in \mathbb{R} && \forall r = 1, \ldots, k
\end{aligned}$$

Crammer-Singer

$$\min \left\{ \sum_{r=1}^{k} \frac{\omega_r' \omega_r}{2} + C \sum_{i=1}^{n} \xi_i \right\}$$

$$\begin{aligned}
\text{s.t:}\quad & \omega_{y_i}' x_i + \delta_{y_i j} - \omega_j' x_i \geq 1 - \xi_i^j && \forall i = 1, \dots, n,\ j \in \{1, \dots, k\} \\
& \xi_i \geq 0 && \forall i = 1, \dots, n \\
& \omega_r \in \mathbb{R}^p, \omega_{r0} \in \mathbb{R} && \forall r = 1, \dots, k \\
& \delta_{y_i j} \in \{0, 1\} && \forall y_i, j \in \{1, \dots, k\}
\end{aligned}$$

1. Support Vector Machine (SVM)
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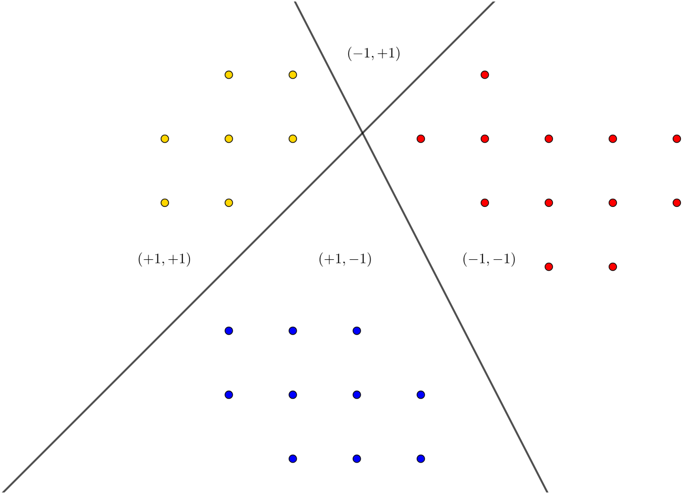
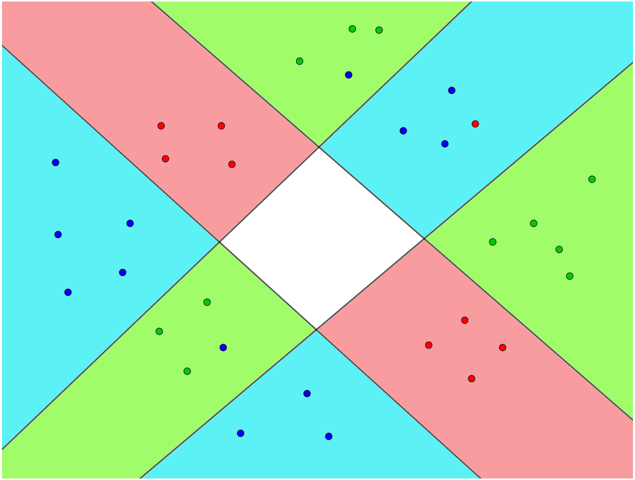
MCSVM



Class assignment through cells



Separation between classes

$$\max \min \left\{ \frac{2}{\|\omega_1\|_2}, \ldots, \frac{2}{\|\omega_m\|_2} \right\}$$

$$\min \max \left\{ \frac{1}{2}\|\omega_1\|_2^2, \ldots, \frac{1}{2}\|\omega_m\|_2^2 \right\}$$

Separation between classes

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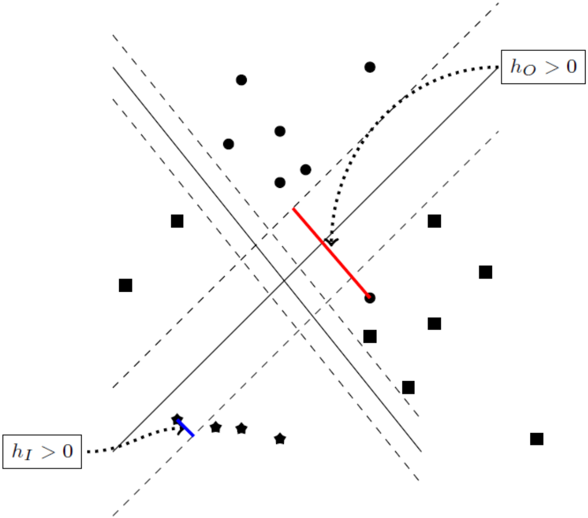
Error functions

$$h_I\left(x,y,\mathscr{H}\right)=\begin{cases}\max\{0,\min\{1,1-\mathrm{s}_r(x)(\omega_r^t x+\omega_{r0})\}\} & \text{if } x \text{ is well classified with respect to } \mathscr{H}\\ 0 & \text{otherwise}\end{cases}$$

$$h_O\left(x,y,\mathscr{H}\right)=\begin{cases}1-\mathrm{s}(x)_r(\omega_r^t x+\omega_{r0}) & \text{if } x \text{ is wrong classified with respect to } \mathscr{H}\\ 0 & \text{otherwise}\end{cases}$$

Error functions



Continuous variables

$$\omega_r \in \mathbb{R}^p, \;\; \omega_{r0} \in \mathbb{R}, \qquad r = 1, \ldots m$$

$$e_{ir} \geq 0, \qquad i = 1, \ldots, n, \;\; r = 1, \ldots, m$$

$$d_{ir} \geq 0, \qquad i = 1, \ldots, n, \;\; r = 1, \ldots, m$$

Binary variables

- $t_{ir} = \begin{cases} 1 & \text{if } \omega_r^t x_i + \omega_{r0} \geq 0 \\ 0 & \text{otherwise} \end{cases}, \; i = 1, \ldots, n, \; r = 1, \ldots, m$

- $z_{is} = \begin{cases} 1 & \text{if } i \text{ is assigned to class } s \\ 0 & \text{otherwise} \end{cases}, \; i = 1, \ldots, n, \; s = 1, \ldots, k$

Binary variables

- $$\xi_i = \begin{cases} 0 & \text{if the class assigned to } i \\ & \text{coincides with } y_i \\ 1 & \text{otherwise} \end{cases}, \ i = 1, \ldots, n$$

- $$h_{ij} = \begin{cases} 1 & \text{if } x_j \text{ is well classified and} \\ & \text{is the representative of } x_i \\ 0 & \text{otherwise} \end{cases}, \ i,j = 1, \ldots, n \ (y_i = y_j)$$

MCSVM formulation

$$\min \quad \frac{1}{2}\|\omega_1\|_2^2 + C_1 \sum_{i=1}^{n}\sum_{r=1}^{m} e_{ir} + C_2 \sum_{i=1}^{n}\sum_{r=1}^{m} d_{ir}$$

$$\begin{aligned}
\text{s.a:} \quad & \frac{1}{2}\|\omega_1\|_2^2 \geq \frac{1}{2}\|\omega_r\|_2^2 && \forall r = 2,\ldots,m && (1)\\
& \omega_{ir}^t x_i + w_{r_0} \geq -T(1 - t_{ir}) && \forall i \in N, r \in M && (2)\\
& \omega_{ir}^t x_i + w_{r_0} \leq T t_{ir} && \forall i \in N, r \in M && (3)\\
& \sum_{s=1}^{k} z_{is} = 1 && \forall i \in N && (4)
\end{aligned}$$

MCSVM formulation

$$\|z_i - z_j\|_1 \leq 2\|t_i - t_j\|_1 \qquad \forall i,j \in N \qquad (5)$$

$$\xi_i = \|z_i - \delta_i\|_1 \qquad \forall i \in N \qquad (6)$$

$$\sum_{\substack{j \in N: \\ y_i = y_j}} h_{ij} = 1 \qquad \forall i \in N \qquad (7)$$

$$\xi_j + h_{ij} \leq 1 \qquad \forall i,j \in N(y_i = y_j) \qquad (8)$$

$$h_{ii} = 1 - \xi_i \qquad \forall i \in N \qquad (9)$$

MCSVM formulation

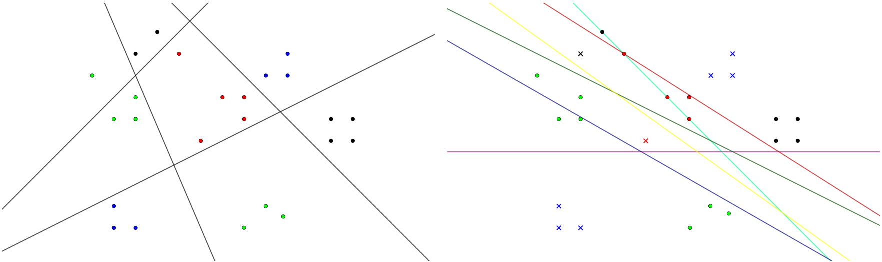
$$\omega_r^t x_i + \omega_{r0} \geq 1 - e_{ir} - T\left(3 - t_{ir} - t_{jr} - h_{ij}\right) \quad \forall i,j \in N, r \in M \tag{10}$$

$$\omega_r^t x_i + \omega_{r0} \leq -1 + e_{ir} + T\left(1 + t_{ir} + t_{jr} - h_{ij}\right) \quad \forall i,j \in N, r \in M \tag{11}$$

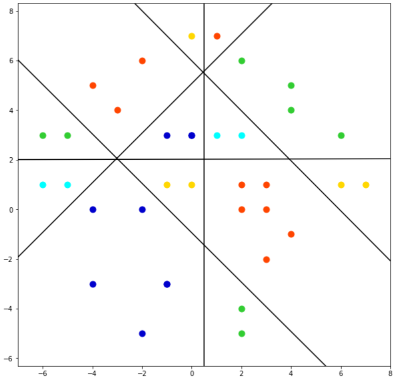
$$d_{ir} \geq 1 - \omega_r^t x_i - \omega_{r0} - T\left(2 + t_{ir} - t_{jr} - h_{ij}\right) \quad \forall i,j \in N, r \in M \tag{12}$$

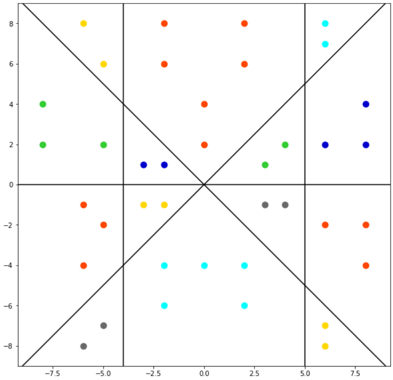
$$d_{ir} \geq 1 + \omega_r^t x_i + \omega_{r0} - T\left(2 - t_{ir} + t_{jr} - h_{ij}\right) \quad \forall i,j \in N, r \in M \tag{13}$$

MCSVM (left) and OVO (right)



Some MCSVM examples





Computational experiments

Description

Dataset	n_{Tr}	n_{Te}	p	k	m	m_{OVO}
Forest	75	448	28	4	3	6
Glass	75	139	10	6	6	15
Iris	75	75	4	3	2	3
Seeds	75	135	7	3	2	3
Wine	75	103	13	3	2	3
Zoo	75	26	17	7	4	21

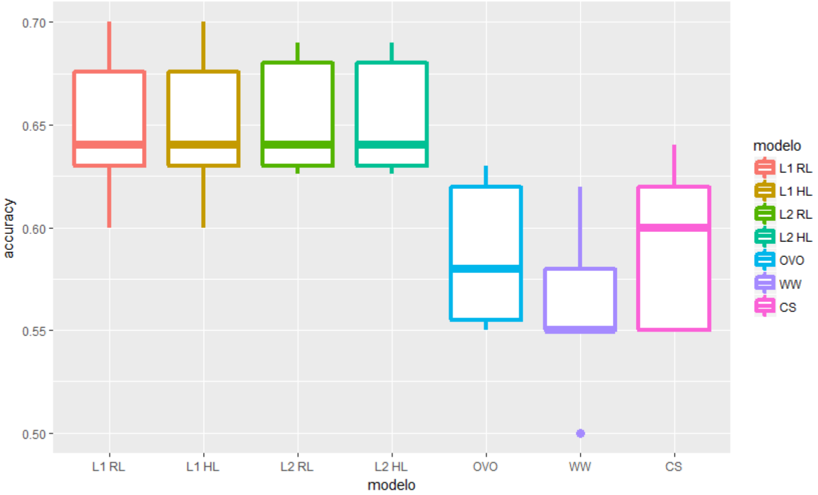
Computational experiments

Average accuracy results

Dataset	ℓ_1 RL	ℓ_1 HL	ℓ_2 RL	ℓ_2 HL	OVO	WW	CS
Forest	80.66	80.12	**82.30**	81.62	82.10	78.40	78.60
Glass	64.92	64.92	**65.32**	**65.32**	58.76	56.25	59.26
Iris	95.08	95.40	96.44	**96.66**	93.80	96.44	96.44
Seeds	**93.66**	**93.66**	93.52	93.52	91.02	93.52	93.52
Wine	95.20	95.20	**96.82**	**96.82**	96.34	96.09	96.17
Zoo	**89.75**	**89.75**	**89.75**	**89.75**	87.44	87.68	87.68

Computational experiments

Glass detailed experiment



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2. Weston, J., Watkins, C.: Support vector machines for multi-class pattern recognition. In: European Symposium on Artificial Neural Networks, pp. 219–224 (1999)
3. Crammer, K., Singer, Y.: On the algorithmic implementation of multiclass kernel-based vector machines. Journal of Machine Learning Research **2**, 265–292 (2001)
4. Blanco, V., Japón, A. and Puerto, J. (2018). Optimal arrangements of hyperplanes for multiclass classification. Preprint available at https://arxiv.org/abs/1810.09167.

Conclusions

- We have developed a multiclass model that extends the idea of binary SVM.
- Our model obtains better or compared results on accuracy with respect to traditional SVM multiclass methods.
- We have proven that kernel tools are compatible with our model.