

## Lecture 8: Multi Class SVM

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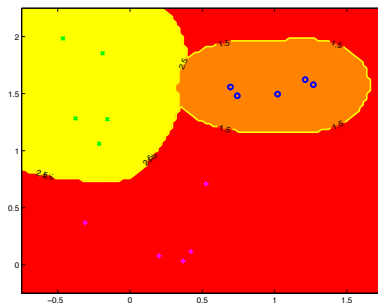
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# Roadmap

## 1 Multi Class SVM

- 3 different strategies for multi class SVM
- Multi Class SVM by decomposition
- Multi class SVM
- Coupling convex hulls



### 3 different strategies for multi class SVM

#### 1 Decomposition approaches

- ▶ one vs all: winner takes all
- ▶ one vs one:
  - ★ max-wins voting
  - ★ pairwise coupling: use probability
- ▶  $c$  SVDD

#### 2 global approach (size $c \times n$ ),

- ▶ formal (different variations)

$$\left\{ \begin{array}{ll} \min_{f \in \mathcal{H}, \alpha_0, \xi \in \mathbb{R}^n} & \frac{1}{2} \sum_{\ell=1}^c \|f_{\ell}\|_{\mathcal{H}}^2 + \frac{C}{p} \sum_{i=1}^n \sum_{\ell=1, \ell \neq y_i}^c \xi_{i\ell}^p \\ \text{with} & f_{y_i}(\mathbf{x}_i) + b_{y_i} \geq f_{\ell}(\mathbf{x}_i) + b_{\ell} + 2 - \xi_{i\ell} \\ \text{and} & \xi_{i\ell} \geq 0 \text{ for } i = 1, \dots, n; \ell = 1, \dots, c; \ell \neq y_i \end{array} \right.$$

non consistent estimator but practically useful

- ▶ structured outputs

#### 3 A coupling formulation using the convex hulls

### 3 different strategies for multi class SVM

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- ▶ one vs all: winner takes all
- ▶ one vs one:
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  - ★ pairwise coupling: use probability – best results
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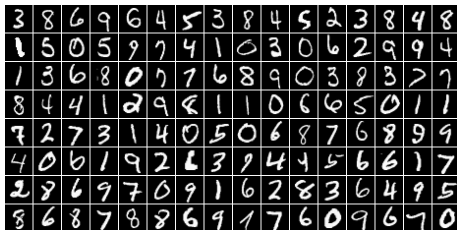
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- ▶ structured outputs

#### 3 A coupling formulation using the convex hulls

## Multiclass SVM: complexity issues

- $n$  training data  
 $n = 60,000$  for MNIST
- $c$  class  
 $c = 10$  for MNIST

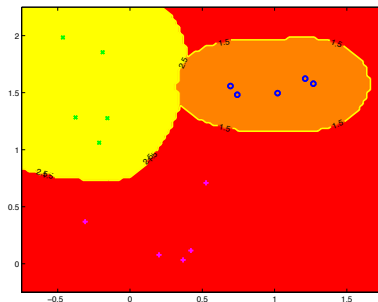


approach	problem size	number of sub problems	discrimination	rejection
<i>1 vs. all</i>	$n$	$c$	++	-
<i>1 vs. 1</i>	$\frac{2n}{c}$	$\frac{c(c-1)}{2}$	++	-
<i>c SVDD</i>	$\frac{n}{c}$	$c$	-	++
<i>all together</i>	$n \times c$	1	++	-
<i>coupling CH</i>	$n$	1	+	+

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# Multi Class SVM by decomposition

## One-Against-All Methods

→ winner-takes-all strategy

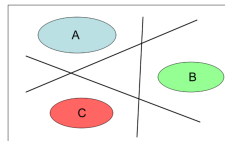


Figure 1: Diagram of binary OAA region boundaries on a basic problem

## One-vs-One: pairwise methods

→ max-wins voting

→ directed acyclic graph (DAG)

→ error-correcting codes

→ post process probabilities

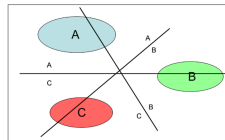
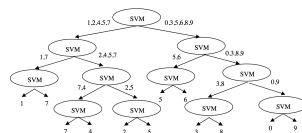


Figure 3: Diagram of pairwise SVM decision boundaries on a basic problem



Hierarchical binary tree for  
multi-class SVM

<http://courses.media.mit.edu/2006fall/mas622j/Projects/aizen-project/>

## SVM and probabilities (Platt, 1999)

The decision function of the SVM is:  $\text{sign}(f(\mathbf{x}) + b)$

$\log \frac{\mathbb{P}(Y = 1|\mathbf{x})}{\mathbb{P}(Y = -1|\mathbf{x})}$  should have (almost) the same sign as  $f(\mathbf{x}) + b$

$$\log \frac{\mathbb{P}(Y = 1|\mathbf{x})}{\mathbb{P}(Y = -1|\mathbf{x})} = a_1(f(\mathbf{x}) + b) + a_2 \quad \mathbb{P}(Y = 1|\mathbf{x}) = 1 - \frac{1}{1 + \exp^{a_1(f(\mathbf{x})+b)+a_2}}$$

$a_1$  et  $a_2$  estimated using maximum likelihood on new data

$$\max_{a_1, a_2} L$$

$$\text{with } L = \prod_{i=1}^n \mathbb{P}(Y = 1|\mathbf{x}_i)^{y_i} + (1 - \mathbb{P}(Y = 1|\mathbf{x}_i))^{(1-y_i)}$$

$$\begin{aligned} \text{and } \log L &= \sum_{i=1}^n y_i \log(\mathbb{P}(Y = 1|\mathbf{x}_i)) + (1 - y_i) \log(1 - \mathbb{P}(Y = 1|\mathbf{x}_i)) \\ &= \sum_{i=1}^n y_i \log\left(\frac{\mathbb{P}(Y=1|\mathbf{x}_i)}{1 - \mathbb{P}(Y=1|\mathbf{x}_i)}\right) + \log(1 - \mathbb{P}(Y = 1|\mathbf{x}_i)) \\ &= \sum_{i=1}^n y_i (a_1(f(\mathbf{x}_i) + b) + a_2) - \log(1 + \exp^{a_1(f(\mathbf{x}_i)+b)+a_2}) \\ &= \sum_{i=1}^n y_i (\mathbf{a}^\top \mathbf{z}_i) - \log(1 + \exp^{\mathbf{a}^\top \mathbf{z}_i}) \end{aligned}$$

Newton iterations:  $\mathbf{a}^{new} \leftarrow \mathbf{a}^{old} - H^{-1} \nabla \log L$



## SVM and probabilities (Platt, 1999)

$$\max_{\mathbf{a} \in \mathbb{R}^2} \log L = \sum_{i=1}^n y_i (\mathbf{a}^\top \mathbf{z}_i) - \log(1 + \exp^{\mathbf{a}^\top \mathbf{z}_i})$$

Newton iterations

$$\mathbf{a}^{new} \leftarrow \mathbf{a}^{old} - H^{-1} \nabla \log L$$

$$\begin{aligned} \nabla \log L &= \sum_{i=1}^n y_i \mathbf{z}_i - \frac{\exp^{\mathbf{a}^\top \mathbf{z}_i}}{1 + \exp^{\mathbf{a}^\top \mathbf{z}_i}} \mathbf{z}_i \\ &= \sum_{i=1}^n (y_i - \mathbb{P}(Y = 1 | \mathbf{x}_i)) \mathbf{z}_i = Z^\top (\mathbf{y} - \mathbf{p}) \end{aligned}$$

$$H = - \sum_{i=1}^n \mathbf{z}_i \mathbf{z}_i^\top \mathbb{P}(Y = 1 | \mathbf{x}_i) (1 - \mathbb{P}(Y = 1 | \mathbf{x}_i)) = -Z^\top W Z$$

Newton iterations

$$\mathbf{a}^{new} \leftarrow \mathbf{a}^{old} + (Z^\top W Z)^{-1} Z^\top (\mathbf{y} - \mathbf{p})$$

## SVM and probabilities: practical issues

$$\mathbf{y} \longrightarrow \mathbf{t} = \begin{cases} 1 - \varepsilon_+ = \frac{n_+ + 1}{n_+ + 2} & \text{if } y_i = 1 \\ \varepsilon_- = \frac{1}{n_- + 2} & \text{if } y_i = -1 \end{cases}$$

① in:  $X, \mathbf{y}, f$  / out:  $\mathbf{p}$

②  $\mathbf{t} \leftarrow$

③  $Z \leftarrow$

④ loop until convergence

①  $\mathbf{p} \leftarrow 1 - \frac{1}{1 + \exp^{\mathbf{a}^\top \mathbf{z}}}$

②  $W \leftarrow \text{diag}(\mathbf{p}(1 - \mathbf{p}))$

③  $\mathbf{a}^{\text{new}} \leftarrow \mathbf{a}^{\text{old}} + (Z^\top W Z)^{-1} Z^\top (\mathbf{t} - \mathbf{p})$

## SVM and probabilities: pairwise coupling

From pairwise probabilities  $\mathbb{P}(c_\ell, c_j)$  to class probabilities  $p_\ell = \mathbb{P}(c_\ell|\mathbf{x})$

$$\min_{\mathbf{p}} \sum_{\ell=1}^c \sum_{j=1}^{\ell-1} \mathbb{P}(c_\ell, c_j)^2 (p_\ell - p_j)^2$$

$$\begin{pmatrix} Q & \mathbf{e} \\ \mathbf{e}^\top & 0 \end{pmatrix} \begin{pmatrix} \mathbf{p} \\ \mu \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{with } Q_{\ell j} = \begin{cases} \mathbb{P}(c_\ell, c_j)^2 & \ell \neq j \\ \sum_i \mathbb{P}(c_\ell, c_i)^2 & \ell = j \end{cases}$$

The global procedure :

- ①  $(X_a, y_a, X_t, y_t) \leftarrow \text{split}(X, y)$
- ②  $(X_\ell, y_\ell, X_p, y_p) \leftarrow \text{split}(X_a, y_a)$
- ③ loop for all pairs  $(c_i, c_j)$  of classes
  - ①  $\text{model}_{ij} \leftarrow \text{train\_SVM}(X_\ell, y_\ell, (c_i, c_j))$
  - ②  $\mathbb{P}(c_i, c_j) \leftarrow \text{estimate\_proba}(X_p, y_p, \text{model})$  % Platt estimate
- ④  $\mathbf{p} \leftarrow \text{post\_process}(X_t, y_t, \mathbb{P})$  % Pairwise Coupling

# SVM and probabilities

## Some facts

- SVM is universally consistent (converges towards the Bayes risk)
- SVM asymptotically implements the bayes rule
- but theoretically: **no consistency towards conditional probabilities** (due to the nature of sparsity)
- to estimate conditional probabilities on an interval (typically  $[\frac{1}{2} - \eta, \frac{1}{2} + \eta]$ ) to sparseness in this interval (all data points have to be support vectors)

## SVM and probabilities (2/2)

An alternative approach

$$g(\mathbf{x}) - \varepsilon^-(\mathbf{x}) \leq \mathbb{P}(Y = 1|\mathbf{x}) \leq g(\mathbf{x}) + \varepsilon^+(\mathbf{x})$$

with  $g(\mathbf{x}) = \frac{1}{1+4^{-f(\mathbf{x})-\alpha_0}}$

non parametric functions  $\varepsilon^-$  and  $\varepsilon^+$  have to verify:

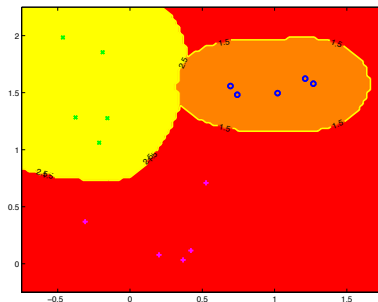
$$\begin{aligned} g(\mathbf{x}) + \varepsilon^+(\mathbf{x}) &= \exp^{-a_1(1-f(\mathbf{x})-\alpha_0)_+ + a_2} \\ 1 - g(\mathbf{x}) - \varepsilon^-(\mathbf{x}) &= \exp^{-a_1(1+f(\mathbf{x})+\alpha_0)_+ + a_2} \end{aligned}$$

with  $a_1 = \log 2$  and  $a_2 = 0$

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# Multi class SVM: the decision function

One hyperplane by class

$$f_{\ell}(\mathbf{x}) = \mathbf{w}_{\ell}^{\top} \mathbf{x} + b_{\ell} \quad \ell = 1, c$$

Winner takes all decision function

$$D(\mathbf{x}) = \underset{\ell=1,c}{\operatorname{Argmax}} \left( \mathbf{w}_1^{\top} \mathbf{x} + b_1, \mathbf{w}_2^{\top} \mathbf{x} + b_2, \dots, \mathbf{w}_{\ell}^{\top} \mathbf{x} + b_{\ell}, \dots, \mathbf{w}_c^{\top} \mathbf{x} + b_c \right)$$

We can revisit the 2 classes case in this setting

$c \times (d + 1)$  unknown variables  $(\mathbf{w}_{\ell}, b_{\ell}); \ell = 1, c$

# Multi class SVM: the optimization problem

The margin in the multidimensional case

$$m = \min_{\ell \neq y_i} (\mathbf{v}_{y_i}^\top \mathbf{x}_i - a_{y_i} - \mathbf{v}_\ell^\top \mathbf{x}_i + a_\ell) = \mathbf{v}_{y_i}^\top \mathbf{x}_i + a_{y_i} - \max_{\ell \neq y_i} (\mathbf{v}_\ell^\top \mathbf{x}_i + a_\ell)$$

The maximal margin multiclass SVM

$$\begin{cases} \max_{\mathbf{v}_\ell, a_\ell} & m \\ \text{with} & \mathbf{v}_{y_i}^\top \mathbf{x}_i + a_{y_i} - \mathbf{v}_\ell^\top \mathbf{x}_i - a_\ell \geq m \quad \text{for } i = 1, n; \quad \ell = 1, c; \quad \ell \neq y_i \\ \text{and} & \frac{1}{2} \sum_{\ell=1}^c \|\mathbf{v}_\ell\|^2 = 1 \end{cases}$$

The multiclass SVM

$$\begin{cases} \min_{\mathbf{w}_\ell, b_\ell} & \frac{1}{2} \sum_{\ell=1}^c \|\mathbf{w}_\ell\|^2 \\ \text{with} & \mathbf{x}_i^\top (\mathbf{w}_{y_i} - \mathbf{w}_\ell) + b_{y_i} - b_\ell \geq 1 \quad \text{for } i = 1, n; \quad \ell = 1, c; \quad \ell \neq y_i \end{cases}$$



## Multi class SVM: KKT and dual form: The 3 classes case

$$\left\{ \begin{array}{ll} \min_{\mathbf{w}_\ell, b_\ell} & \frac{1}{2} \sum_{\ell=1}^3 \|\mathbf{w}_\ell\|^2 \\ \text{with} & \mathbf{w}_{y_i}^\top \mathbf{x}_i + b_{y_i} \geq \mathbf{w}_\ell^\top \mathbf{x}_i + b_\ell + 1 \quad \text{for } i = 1, n; \quad \ell = 1, 3; \quad \ell \neq y_i \end{array} \right.$$

$$\left\{ \begin{array}{ll} \min_{\mathbf{w}_\ell, b_\ell} & \frac{1}{2} \|\mathbf{w}_1\|^2 + \frac{1}{2} \|\mathbf{w}_2\|^2 + \frac{1}{2} \|\mathbf{w}_3\|^2 \\ \text{with} & \begin{array}{ll} \mathbf{w}_1^\top \mathbf{x}_i + b_1 \geq \mathbf{w}_2^\top \mathbf{x}_i + b_2 + 1 & \text{for } i \text{ such that } y_i = 1 \\ \mathbf{w}_1^\top \mathbf{x}_i + b_1 \geq \mathbf{w}_3^\top \mathbf{x}_i + b_3 + 1 & \text{for } i \text{ such that } y_i = 1 \\ \mathbf{w}_2^\top \mathbf{x}_i + b_2 \geq \mathbf{w}_1^\top \mathbf{x}_i + b_1 + 1 & \text{for } i \text{ such that } y_i = 2 \\ \mathbf{w}_2^\top \mathbf{x}_i + b_2 \geq \mathbf{w}_3^\top \mathbf{x}_i + b_3 + 1 & \text{for } i \text{ such that } y_i = 2 \\ \mathbf{w}_3^\top \mathbf{x}_i + b_3 \geq \mathbf{w}_1^\top \mathbf{x}_i + b_1 + 1 & \text{for } i \text{ such that } y_i = 3 \\ \mathbf{w}_3^\top \mathbf{x}_i + b_3 \geq \mathbf{w}_2^\top \mathbf{x}_i + b_2 + 1 & \text{for } i \text{ such that } y_i = 3 \end{array} \end{array} \right.$$

$$L = \frac{1}{2} (\|\mathbf{w}_1\|^2 + \|\mathbf{w}_2\|^2 + \|\mathbf{w}_3\|^2) - \alpha_{12}^\top (X_1(\mathbf{w}_1 - \mathbf{w}_2) + b_1 - b_2 - 1) - \alpha_{13}^\top (X_1(\mathbf{w}_1 - \mathbf{w}_3) + b_1 - b_3 - 1) - \alpha_{21}^\top (X_2(\mathbf{w}_2 - \mathbf{w}_1) + b_2 - b_1 - 1) - \alpha_{23}^\top (X_2(\mathbf{w}_2 - \mathbf{w}_3) + b_2 - b_3 - 1) - \alpha_{31}^\top (X_3(\mathbf{w}_3 - \mathbf{w}_1) + b_3 - b_1 - 1) - \alpha_{32}^\top (X_3(\mathbf{w}_3 - \mathbf{w}_2) + b_3 - b_2 - 1)$$

## Multi class SVM: KKT and dual form: The 3 classes case

$$L = \frac{1}{2} \|\mathbf{w}\|^2 - \alpha^\top (\mathcal{X} \mathcal{M} \mathbf{w} + A \mathbf{b} - 1)$$

with

$$\mathbf{w} = \begin{pmatrix} \mathbf{w}_1 \\ \mathbf{w}_2 \\ \mathbf{w}_3 \end{pmatrix} \in \mathbb{R}^{3d} \quad \mathcal{M} = M \otimes I = \begin{pmatrix} I & -I & 0 \\ I & 0 & -I \\ -I & I & 0 \\ 0 & I & -I \\ -I & 0 & I \\ 0 & -I & I \end{pmatrix} \quad \begin{array}{l} \text{a } 6d \times 3d \text{ matrix} \\ \text{where} \\ I \text{ the identity matrix} \end{array}$$

and

$$\mathcal{X} = \begin{pmatrix} X_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & X_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & X_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & X_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & X_3 & 0 \\ 0 & 0 & 0 & 0 & 0 & X_3 \end{pmatrix} \quad \begin{array}{l} \text{a } 2n \times 6d \text{ matrix} \\ \text{with input data} \end{array}$$
$$X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} \quad n \times d$$

## Multi class SVM: KKT and dual form: The 3 classes case

KKT Stationality conditions =

$$\begin{aligned}\nabla_{\mathbf{w}} L &= \mathbf{w} - \mathcal{M}^T \mathcal{X}^T \alpha \\ \nabla_{\mathbf{b}} L &= A^T \alpha\end{aligned}$$

The dual

$$\begin{aligned}\min_{\alpha \in \mathbb{R}^{2n}} \quad & \frac{1}{2} \alpha^T G \alpha - \mathbf{e}^T \alpha \\ \text{with} \quad & A \mathbf{b} = 0 \\ \text{and} \quad & 0 \leq \alpha\end{aligned}$$

With

$$\begin{aligned}G &= \mathcal{X} \mathcal{M} \mathcal{M}^T \mathcal{X}^T \\ &= \mathcal{X} (M \otimes I) (M \otimes I)^T \mathcal{X}^T \\ &= \mathcal{X} (M M^T \otimes I) \mathcal{X}^T \\ &= (M M^T \otimes I) \cdot \times X X^T \\ &= (M M^T \otimes I) \cdot \times \mathbb{I} K \mathbb{I}^T\end{aligned} \quad \text{and} \quad M = \begin{pmatrix} 1 & -1 & 0 \\ 1 & 0 & -1 \\ -1 & 1 & 0 \\ 0 & 1 & -1 \\ -1 & 0 & 1 \\ 0 & -1 & 1 \end{pmatrix}$$

# Multi class SVM and slack variables (2 variants)

- A slack for all (Vapnik & Blanz, Weston & Watkins 1998)

$$\left\{ \begin{array}{ll} \min_{\mathbf{w}_\ell, b_\ell, \xi \in \mathbb{R}^{cn}} & \frac{1}{2} \sum_{\ell=1}^c \|\mathbf{w}_\ell\|^2 + C \sum_{i=1}^n \sum_{\ell=1, \ell \neq y_i}^c \xi_{i\ell} \\ \text{with} & \mathbf{w}_{y_i}^\top \mathbf{x}_i + b_{y_i} - \mathbf{w}_\ell^\top \mathbf{x}_i - b_\ell \geq 1 - \xi_{i\ell} \\ \text{and} & \xi_{i\ell} \geq 0 \end{array} \right. \quad \text{for } i = 1, n; \ell = 1, c; \ell \neq y_i$$

The dual

$$\begin{array}{ll} \min_{\alpha \in \mathbb{R}^{2n}} & \frac{1}{2} \alpha^\top G \alpha - \mathbf{e}^\top \alpha \\ \text{with} & A\mathbf{b} = 0 \\ \text{and} & 0 \leq \alpha \leq C \end{array}$$

- Max error, a slack per training data (Cramer and Singer, 2001)

$$\left\{ \begin{array}{ll} \min_{\mathbf{w}_\ell, b_\ell, \xi \in \mathbb{R}^n} & \frac{1}{2} \sum_{\ell=1}^c \|\mathbf{w}_\ell\|^2 + C \sum_{i=1}^n \xi_i \\ \text{with} & (\mathbf{w}_{y_i} - \mathbf{w}_\ell)^\top \mathbf{x}_i \geq 1 - \xi_i \quad \text{for } i = 1, n; \ell = 1, c; \ell \neq y_i \\ \text{and} & \xi_i \geq 0 \quad \text{for } i = 1, n \end{array} \right.$$

# Multi class SVM and Kernels

$$\left\{ \begin{array}{ll} \min_{f \in \mathcal{H}, \alpha_0, \xi \in \mathbb{R}^{cn}} & \frac{1}{2} \sum_{\ell=1}^c \|f_{\ell}\|_{\mathcal{H}}^2 + C \sum_{i=1}^n \sum_{\ell=1, \ell \neq y_i}^c \xi_{i\ell} \\ \text{with} & f_{y_i}(\mathbf{x}_i) + b_{y_i} - f_{\ell}(\mathbf{x}_i) - b_{\ell} \geq 1 - \xi_{i\ell} \\ \text{and} & \xi_{i\ell} \geq 0 \quad \text{for } i = 1, n; \ell = 1, c; \ell \neq y_i \end{array} \right.$$

The dual

$$\begin{array}{ll} \min_{\alpha \in \mathbb{R}^{2n}} & \frac{1}{2} \alpha^{\top} G \alpha - \mathbf{e}^{\top} \alpha \\ \text{with} & A \mathbf{b} = 0 \\ \text{and} & 0 \leq \alpha \leq C \end{array}$$

where  $G$  is the **multi class** kernel matrix

# Other Multi class SVM

Lee, Lin & Wahba, 2004

$$\left\{ \begin{array}{l} \min_{f \in \mathcal{H}} \quad \frac{\lambda}{2} \sum_{\ell=1}^c \|f_{\ell}\|_{\mathcal{H}}^2 + \frac{1}{n} \sum_{i=1}^n \sum_{\ell=1, \ell \neq y_i}^c (f_{\ell}(\mathbf{x}_i) + \frac{1}{c-1})_+ \\ \text{with} \quad \sum_{\ell=1}^c f_{\ell}(\mathbf{x}) = 0 \quad \forall \mathbf{x} \end{array} \right.$$

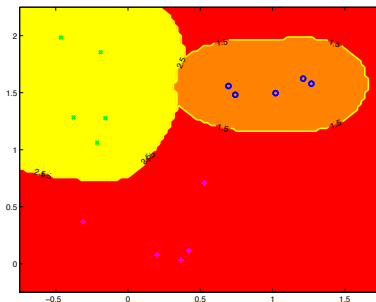
Structured outputs = Cramer and Singer, 2001

MSVMpack : A Multi-Class Support Vector Machine Package Fabien Lauer  
& Yann Guermeur

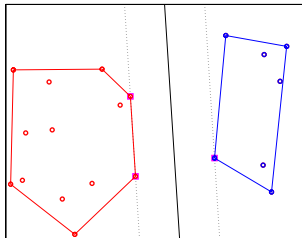
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## One more way to derivate SVM



Minimizing the distance between the convex hulls

$$\left\{ \begin{array}{l} \min_{\alpha} \quad \|u - v\|^2 \\ \text{with} \quad u(\mathbf{x}) = \sum_{\{i|y_i=1\}} \alpha_i (\mathbf{x}_i^\top \mathbf{x}), \quad v(\mathbf{x}) = \sum_{\{i|y_i=-1\}} \alpha_i (\mathbf{x}_i^\top \mathbf{x}) \\ \text{and} \quad \sum_{\{i|y_i=1\}} \alpha_i = 1, \quad \sum_{\{i|y_i=-1\}} \alpha_i = 1, \quad 0 \leq \alpha_i \quad i = 1, n \end{array} \right.$$



## The multi class case

$$\left\{ \begin{array}{ll} \min_{\alpha} & \sum_{\ell=1}^c \sum_{\ell'=1}^c \|u_{\ell} - u_{\ell'}\|^2 \\ \text{with} & u_{\ell}(\mathbf{x}) = \sum_{\{i|y_i=\ell\}} \alpha_{i,\ell}(\mathbf{x}_i^{\top} \mathbf{x}), \quad \ell = 1, c \\ \text{and} & \sum_{\{i|y_i=\ell\}} \alpha_{i,\ell} = 1, \quad 0 \leq \alpha_{i,\ell} \quad i = 1, n; \ell = 1, c \end{array} \right.$$

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