From the Perceptron to SVMs

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  Training stage, test stage.

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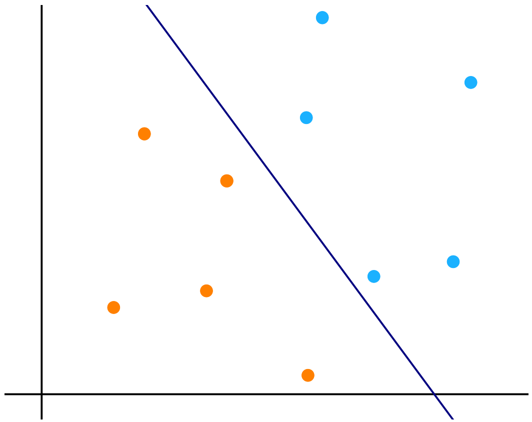

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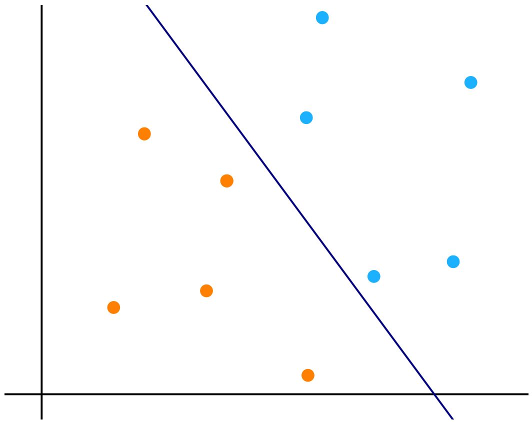

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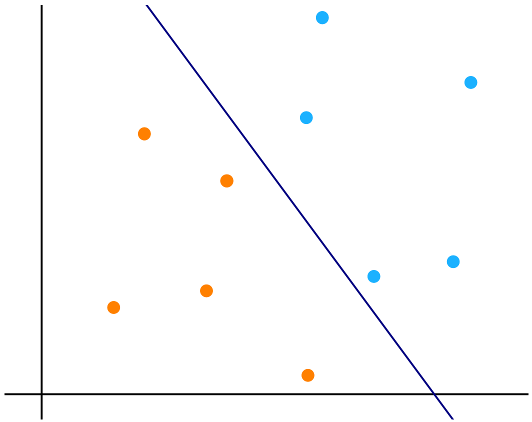

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- Round 4: (Kind of) Non linear classifiers

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  High testing time, poor performance, lots of memory required.

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$$y(\overline{x}) = W^T \overline{x} = \text{“class scores” for datum } \overline{x} \in \mathbb{R}^{D+1}.$$

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- Prediction: $y(x) = Y^\top X^{\dagger^\top} \overline{x}$. Easy but mostly wrong.

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Alternatively:

$$E_{\text{per}}(\overline{w}) = \sum_{i=1}^{N} \max\{0, -y_i\, \overline{w} \cdot \overline{x}_i\}$$

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- **Properties:**
  a) Each step **not** guaranteed to reduce *overall* error.
  b) Convergence guaranteed to *some* solution **if** data linearly separable.
  c) Solution will depend on w_0, b_0.
  d) Doesn't minimise generalisation error $\Rightarrow$ worse generalisation.

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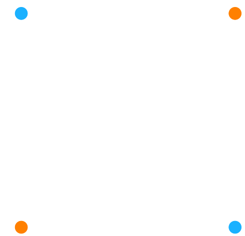

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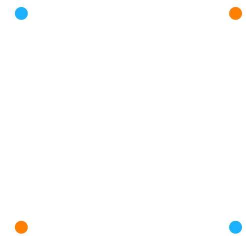

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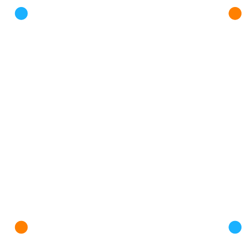

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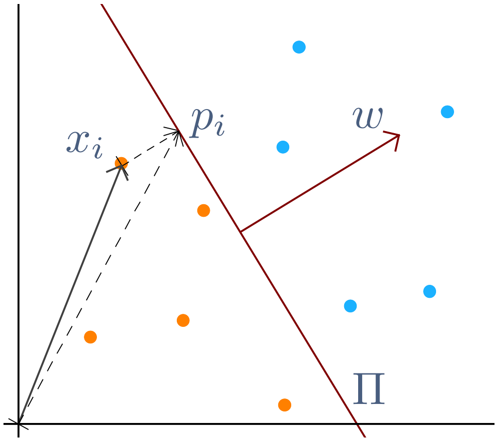
- Let's try to fix it.

Let's compute the distance to a hyperplane $\Pi := \{x \in \mathbb{R}^D : w \cdot x + b = 0\}$.



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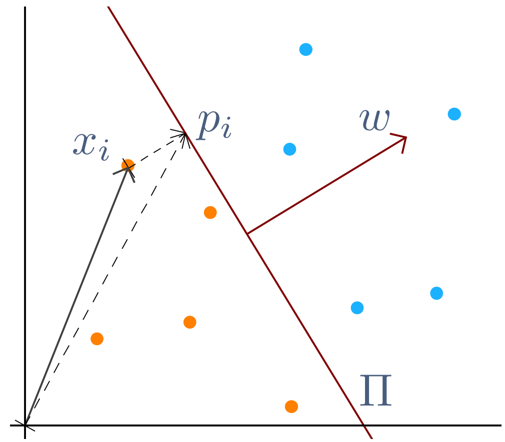

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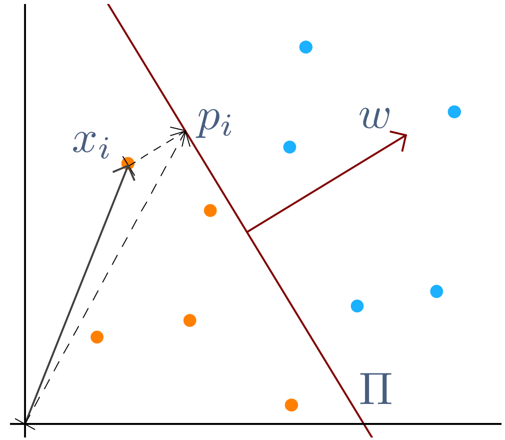

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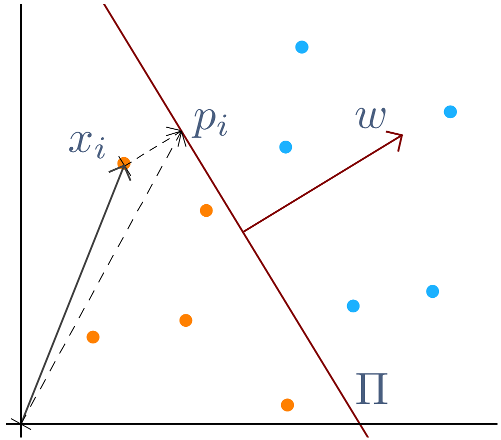

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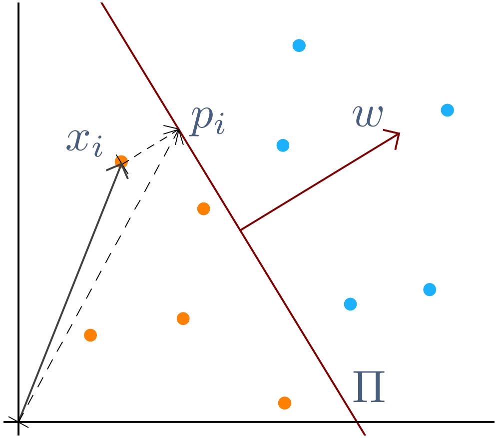

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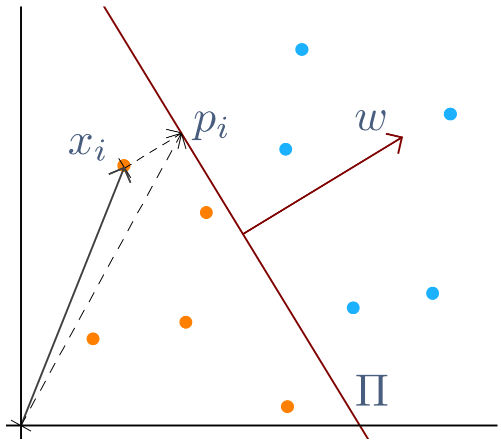

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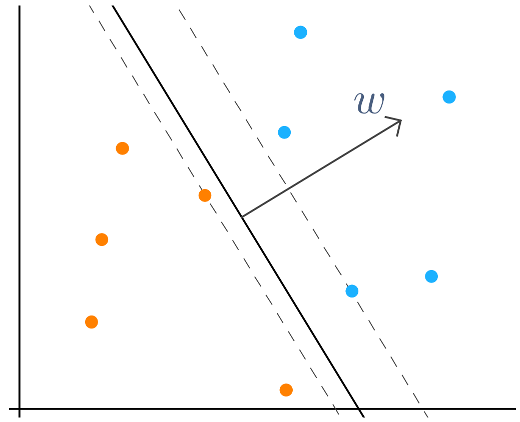
- Define the **geometric margin of x_i** as $\gamma_i := y_i\left(\frac{w}{|w|} \cdot x_i + \frac{b}{|w|}\right)$.

We want to maximize the margin to all points in the training set:

$$\underset{w,b}{\operatorname{argmax}} \min_{i=1,\dots,N} \gamma_i(x_i, w, b) = \underset{w,b}{\operatorname{argmax}} \min_{i=1,\dots,N} y_i\left(\frac{w}{|w|} \cdot x_i + \frac{b}{|w|}\right).$$



Maximal margins and two closest points

The maximal margin is attained at:

$$
\begin{aligned}
(w^\star, b^\star) &= \operatorname*{argmax}_{w,b} \min_{i=1,\ldots,N} \gamma_i(x_i, w, b) \\
&= \operatorname*{argmax}_{w,b} \left\{ \gamma \in \mathbb{R}_+ \colon \gamma_i = y_i \left(\frac{w}{|w|} \cdot x_i + \frac{b}{|w|} \right) \geqslant \gamma, i = 1, \ldots, N \right\} \\
&= \operatorname*{argmax}_{w,b} \left\{ \frac{\hat{\gamma}}{|w|} \in \mathbb{R}_+ \colon y_i \left(w \cdot x_i + b \right) \geqslant \hat{\gamma}, i = 1, \ldots, N, \hat{\gamma} = \gamma \, |w| \right\} \\
&= \operatorname*{argmax}_{w,b} \left\{ \frac{1}{|w|} \in \mathbb{R}_+ \colon y_i \left(w \cdot x_i + b \right) \geqslant 1, i = 1, \ldots, N \right\} \\
&= \operatorname*{argmin}_{w,b} \left\{ \frac{1}{2} |w|^2 \colon y_i \, \overline{w} \cdot \overline{x}_i \geqslant 1, i = 1, \ldots, N \right\}.
\end{aligned}
$$

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- Optimisation (possible) using off-the-shelf Quadratic Programming routines / software.
- But... Infamous XOR! (Later: in the dual formulation, target function $-\infty$).

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- Better generalisation performance.

What *are* these slack variables?

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- Therefore:

$$\begin{cases} \xi_i = 1 & \text{if } x_i \text{ is on the decision boundary } (y(x_i) = \overline{w}\cdot\overline{x}_i = 0), \\ \xi_i > 1 & \text{if } x_i \text{ is misclassified.} \end{cases}$$

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$$\underset{w,b}{\operatorname{argmin}} \frac{1}{2}|w|^2 + C\sum_{i=1}^{N} \max\{0, 1 - y_i\,\overline{w}\cdot\overline{x}_i\}. \qquad (\mathcal{P})$$

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- First compute the gradient of ($\mathcal{P}$)

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- We actually have a **Subgradient Method**, with update rule

$$\overline{w}_{t+1} = ((1 - \lambda_t)\, w_t, b_t) + \lambda_t\, C \sum_{i=1}^{N} \chi_{(0,\infty)}(1 - y_i\, \overline{w}_t \cdot \overline{x}_i)\, y_i\, \overline{x}_i.$$

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Algorithm SGD

1. Pick x_i at random.
2. Update the parameters according to

$$w_{t+1} = w_t - \lambda_t \nabla_w l(x_i, w_t, b_t) \quad \text{and} \quad b_{t+1} = b_t - \lambda_t \partial_b l(x_i, w_t, b_t).$$

   where $\lambda_t \to 0$ for $t \to \infty$ and $\sum \lambda_t^2 < \infty, \sum \lambda_t = \infty$. [because...]
3. Go to 1. until ...? (ε-acc. sol, validation)

Alternatively:

2'. *Mini-batch update:* for some $r \in \mathbb{N}$, pick $x_i, ..., x_{i_r}$ at random and do

$$w_{t+1} = w_t - \lambda_t \sum_{j=1}^{r} \nabla_w l(x_{i_j}, w_t).$$

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- Finale: Handling multiple classes. Examples.

- Use Lagrange multipliers α_i, β_i to incorporate the constraints $(\mathcal{P}_c)$ into the cost $(\mathcal{P}_f)$

$$\mathcal{L}(w, b, \xi, \alpha, \beta) := \frac{1}{2}|w|^2 + C\sum_{i=1}^{N}\xi_i - \sum_{i=1}^{N}\alpha_i\left(y_i\,\overline{w}\cdot\overline{x}_i - 1 + \xi_i\right) - \sum_{i=1}^{N}\beta_i\,\xi_i.$$

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- Optimisation later...

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- What did we win? Enter Messrs. **Karush-Kuhn-Tucker**:

$$\begin{cases} \alpha_i^\star = 0 & \Leftrightarrow \quad y_i \, \overline{w}^\star \cdot \overline{x}_i > 1 \quad \Leftrightarrow \quad x_i \text{ is “away”}, \\ 0 < \alpha_i^\star < C & \Leftrightarrow \quad y_i \, \overline{w}^\star \cdot \overline{x}_i = 1 \quad \Leftrightarrow \quad x_i \text{ is on the margin}, \\ \alpha_i^\star = C & \Leftrightarrow \quad y_i \, \overline{w}^\star \cdot \overline{x}_i < 1 \quad \Leftrightarrow \quad x_i \text{ is inside the margin}. \end{cases}$$

Most samples will be away. The others (by design few) are the **support vectors**.

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- This **kernel trick** “embeds” the problem in a high(er) dimensional feature space (but as a lower dimensional set, no magic).

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  In the example:

  $$k(x, y) = \left(x_1^2, \sqrt{2}\, x_1\, x_2, x_2^2\right) \cdot \left(y_1^2, \sqrt{2}\, y_1\, y_2, y_2^2\right) = (x \cdot y)^2.$$

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  The **decision boundary** will be a conic.

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$$w \cdot \phi(x) + b = \sum_{i \in I} \alpha_i \underbrace{\phi(x_i)\ \phi(x)}_{=k(x_i, x)} + b.$$

  In the example:

$$k(x, y) = \left(x_1^2, \sqrt{2}\, x_1\, x_2, x_2^2\right) \cdot \left(y_1^2, \sqrt{2}\, y_1\, y_2, y_2^2\right) = (x \cdot y)^2.$$

- Two typical kernels:

$$k(x, y) = (x \cdot y + 1)^n, \quad k(x, y) = \mathrm{e}^{-c\,|x-y|^2}.$$

- Optimising the quadratic form $\sum_{i,j=1}^{N} \alpha_i \alpha_j y_i k(\overline{x}_i, \overline{x}_j)$ involves an $\mathcal{O}(N^2)$ matrix!

The dual problem

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  - Clear stopping criterion.

Sequential Minimal Optimization

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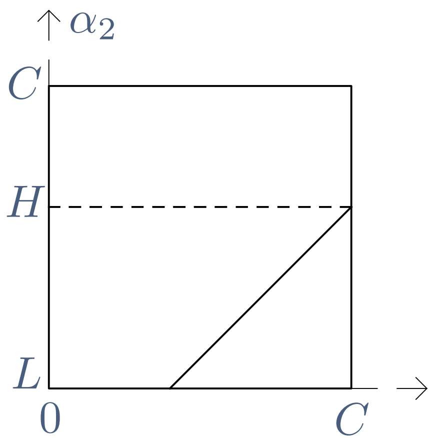
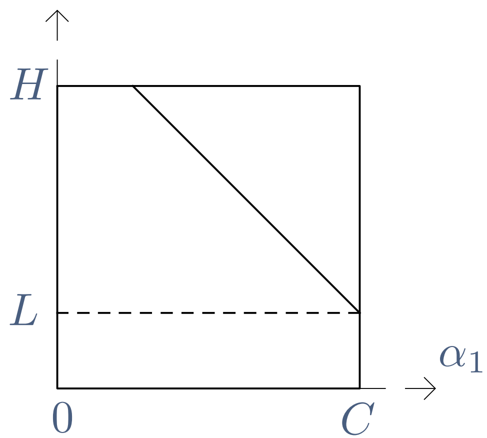


$y_1 \neq y_2 \Rightarrow \alpha_2 = a + \alpha_1$



$y_1 = y_2 \Rightarrow \alpha_2 = a - \alpha_1$

- Write $g(\alpha)$ as a function of α_1, differentiate, equate to 0, plug $\tilde{\alpha}_1, \tilde{\alpha}_2$ from previous step:

$$\alpha_1^\star = \tilde{\alpha}_1 - \frac{y_1 \left[(\tilde{w} \cdot x_1 - y_1) - (\tilde{w} \cdot x_2 - y_2)\right]}{\eta}.$$

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- **Problem**: how to choose which α_i (i.e. which indexes) to optimise?

- **Heuristics** for choosing the next best α_i, α_j to optimise:

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  - Outer loop: go through all α_i violating KKT.
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    - → Until all satisfy KKT within ε (most CPU time in non-clipped samples).
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- Profit!

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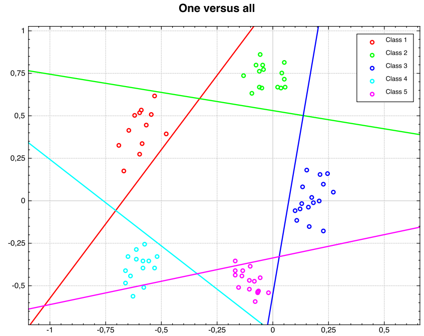

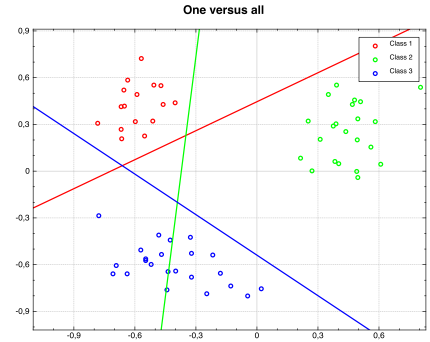

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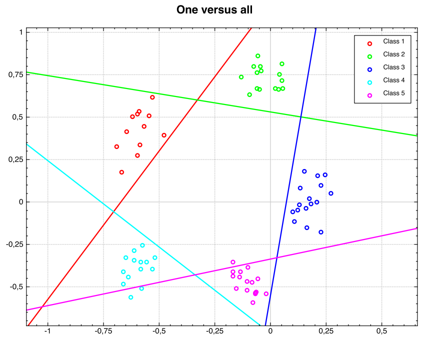

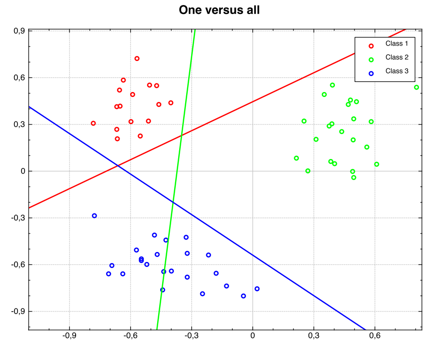

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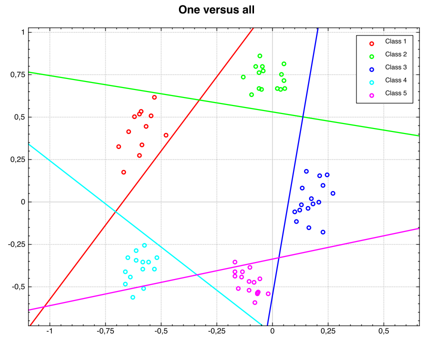

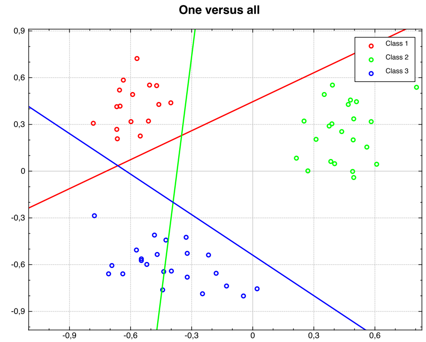

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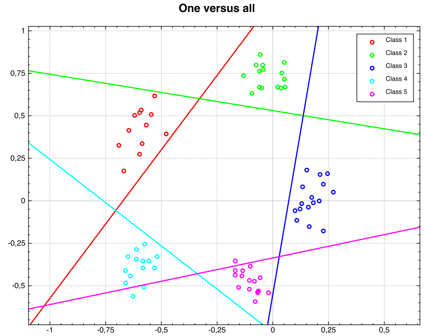

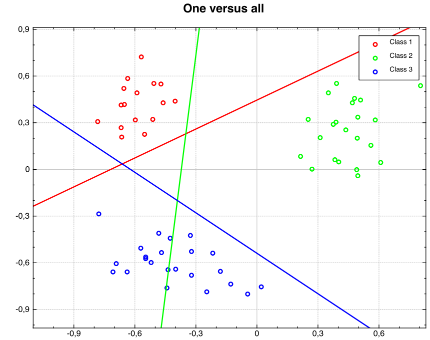

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  Again, caution.

Afterword: Multiple classes

- Why not train for all classes simultaneously? **Multiclass** classifier.

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  Find $W = (w_1, ..., w_K) \in \mathbb{R}^{K\times D}, b \in \mathbb{R}^K, \xi \in \mathbb{R}_+^{N\times K}$ minimising

$$C(W, b, \xi) := \frac{1}{2} W : W + C \sum_{i=1}^{N} \sum_{k \neq y_i} \xi_{ik},$$

  subject to (y_i is the correct class for sample x_i)

$$\overline{w}_{y_i} \cdot \overline{x}_i - \overline{w}_k \cdot \overline{x}_i \geqslant 2 - \xi_{ik}, \text{ and } \xi_{ik} \geqslant 0.$$

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  Equivalently, compute

$$\operatorname*{argmin}_{W, b} \frac{1}{2} W : W + C \sum_{i=1}^{N} \sum_{k \neq y_i} \max\{0, \overline{w}_{y_i} \cdot \overline{x}_i - \overline{w}_k \cdot \overline{x}_i + 2\}.$$

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What next?

- SVMs for regression problems.
- Paralellization techniques.
- Bayesian SVMs: the **Relevance Vector Machine**.
- Go to the beach.

Available on request: the internet remembers everything! You'll need:

- A C++11 compiler. Any recent version of GCC or CLANG should do.
- CMake version $\geqslant 3.0.2$.
- The Qt4 libraries if you want to try the examples with a graphical interface.
- The Armadillo linear algebra library, version $\geqslant 5.200$. OpenBLAS is recommended.
- Optionally some datasets: I've used CIFAR-10 and MNIST.

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End

Happy TeXmacs-ing!