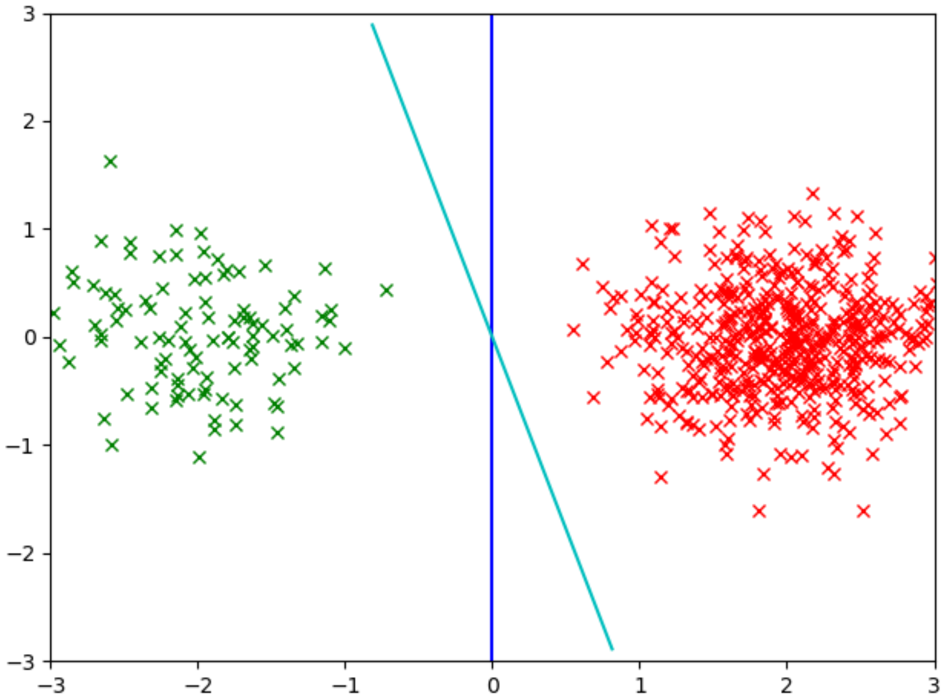
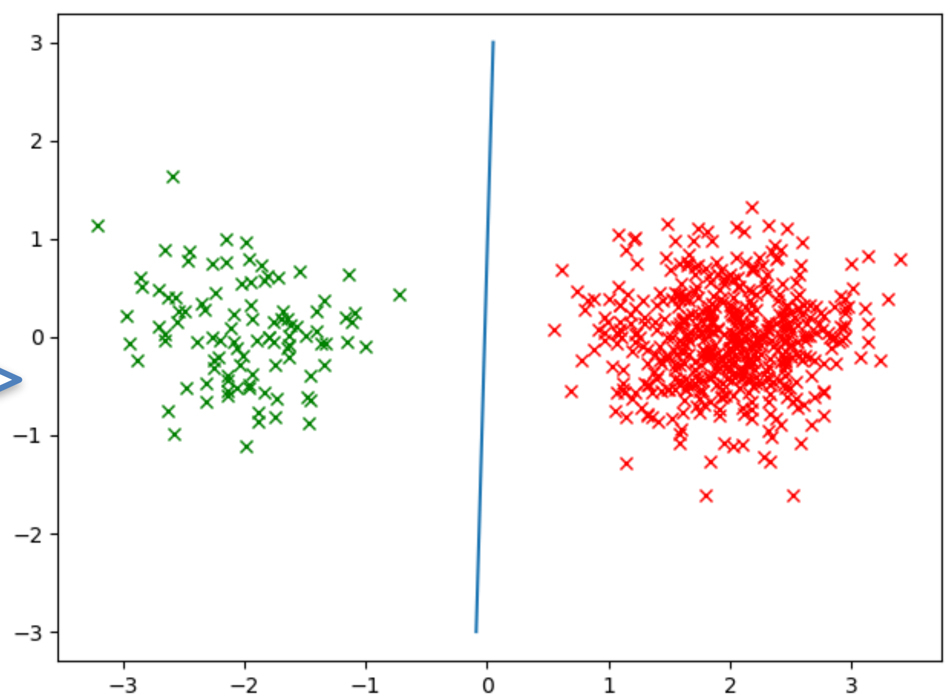
Maximizing the Margin

Pascal Fua
IC-CVLab

Logistic Regression is Better than the Perceptron



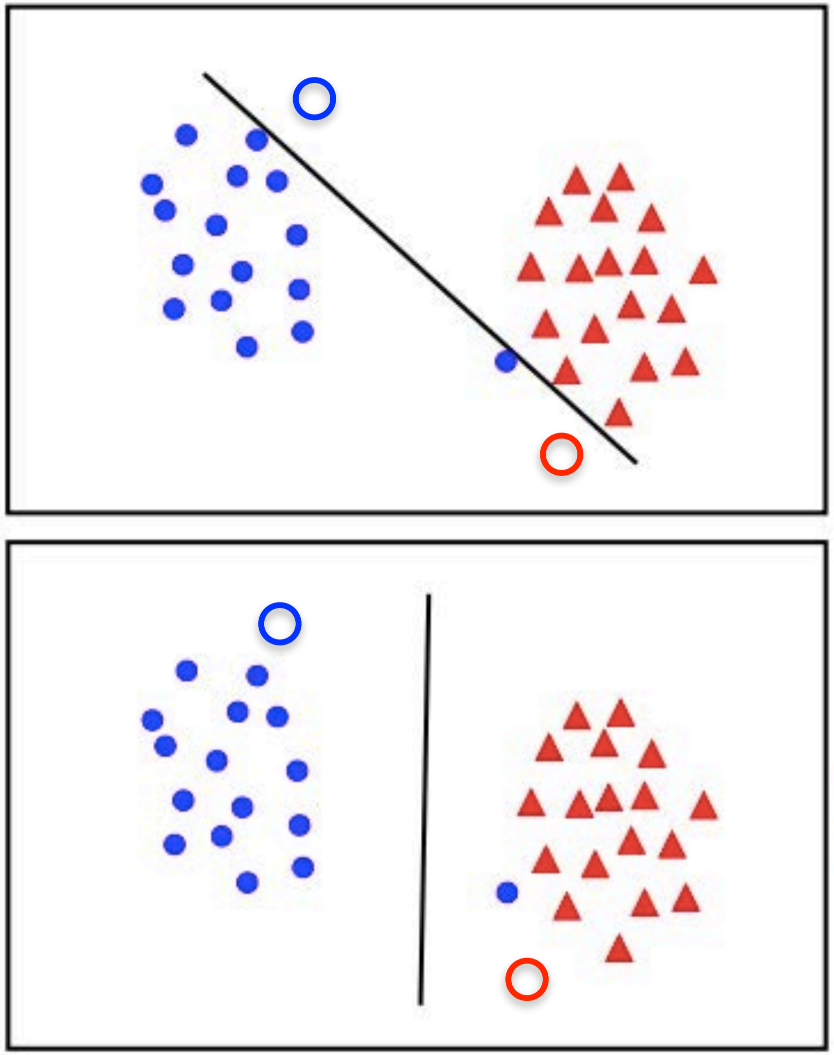
Perceptron



Logistic

But ….

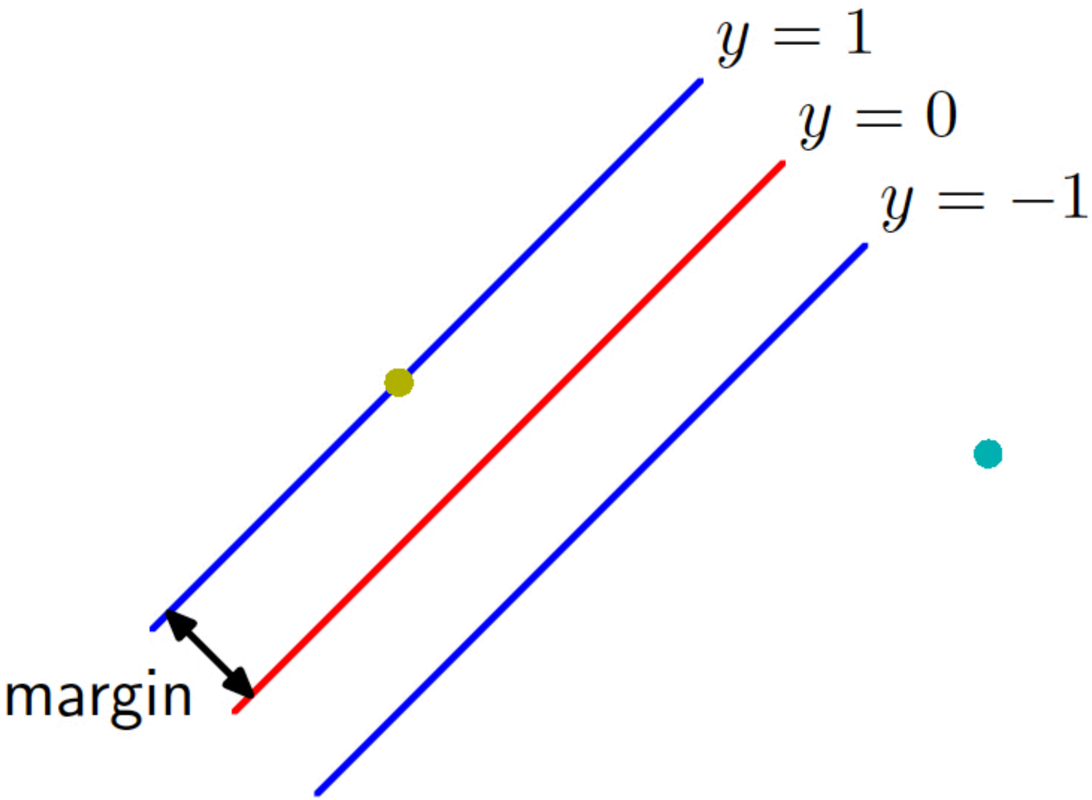
Outliers Can Cause Problems



- Logistic regression tries to minimize the error-rate at training time.
- Can result in poor classification rates at test time.

—> Must sometime accept to misclassify a few training samples.

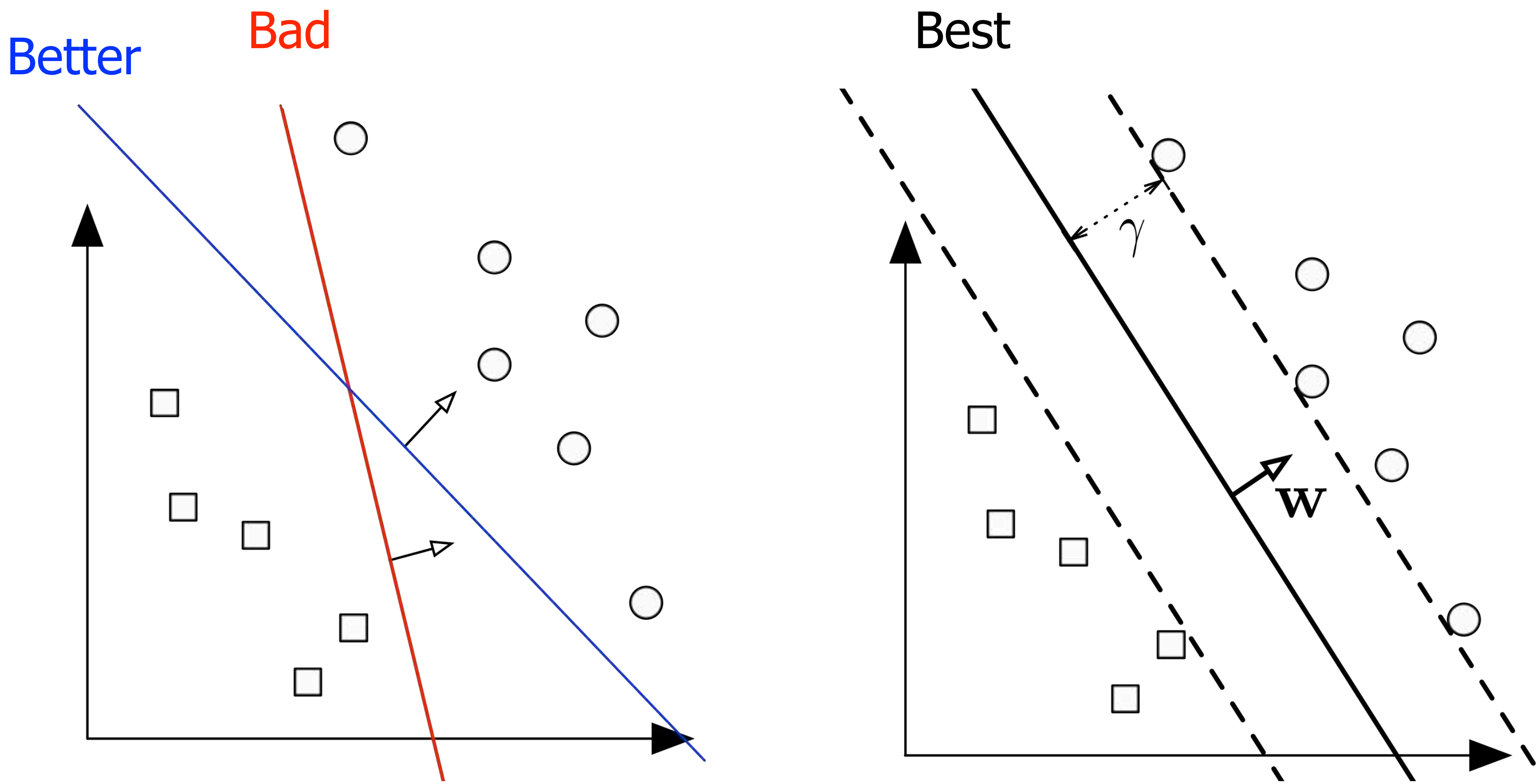
Margin



The orthogonal distance between the decision boundary and the nearest sample is called the **margin**.

Bishop, Chapter 7.1

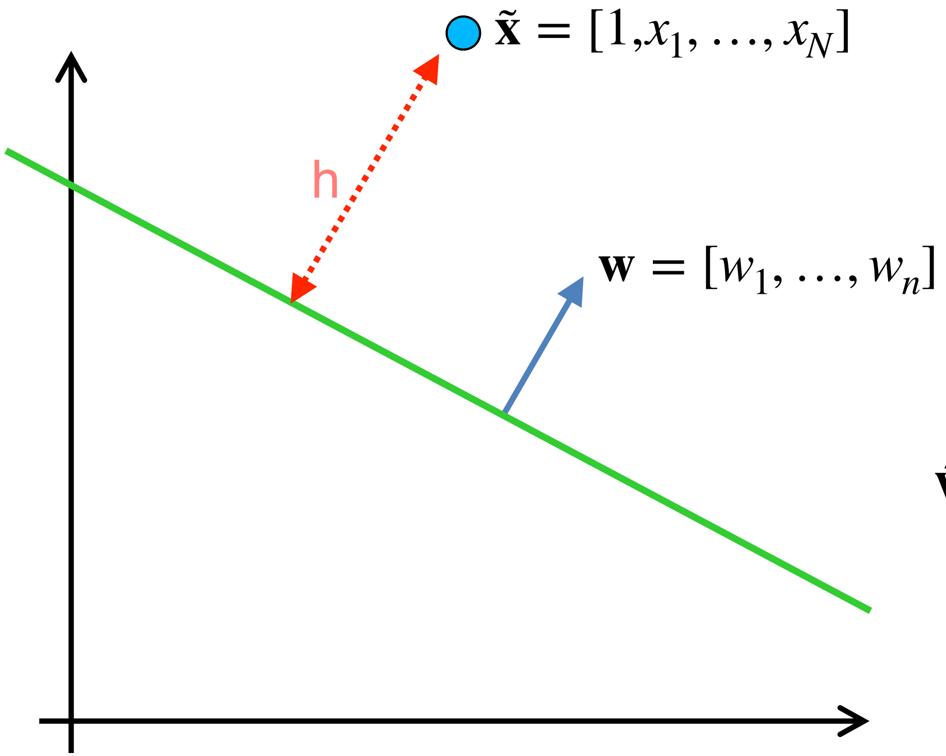
Maximizing the Margin



- The larger the margin, the better!
- The logistic regression does not guarantee a large one.

How do we maximize it?

Reminder: Signed Distance



h=0: Point is on the decision boundary.
h>0: Point on one side.
h<0: Point on the other side.

$\tilde{\mathbf{w}} = [w_0, w_1, \ldots, w_n]$ with $\sum_{i=1}^{N} w_i^2 = 1$

Hyperplane: $\mathbf{x} \in R^N, \tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}} = 0$, with $\tilde{\mathbf{x}} = [1 \,|\, \mathbf{x}]$.

Signed distance: $\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}$, with $\tilde{\mathbf{w}} = [w_0 \,|\, \mathbf{w}]$ and $||\mathbf{w}|| = 1$.

Binary Classification in N Dimensions

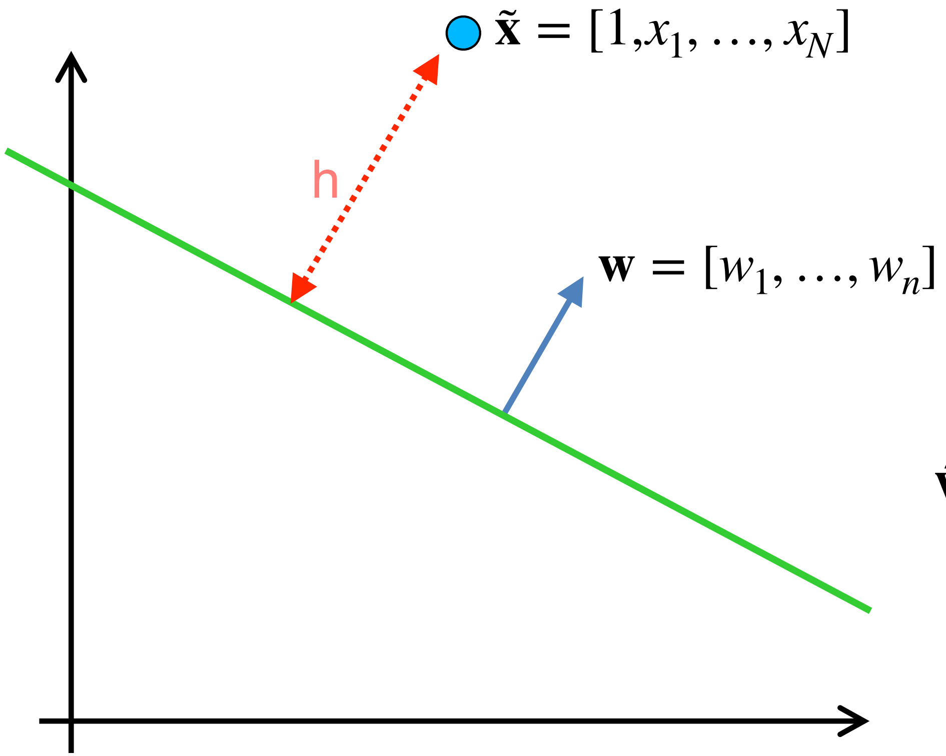
Hyperplane: $\mathbf{x} \in R^N$, $\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}} = 0$, with $\tilde{\mathbf{x}} = [1 \,|\, \mathbf{x}]$.

Signed distance: $\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}$, with $\tilde{\mathbf{w}} = [w_0 \,|\, \mathbf{w}]$ and $||\mathbf{w}|| = 1$.

Problem statement: Find $\tilde{\mathbf{w}}$ such that

- for all or most positive samples $\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}} > 0$,
- for all or most negative samples $\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}} < 0$.

Reformulating the Signed Distance Again



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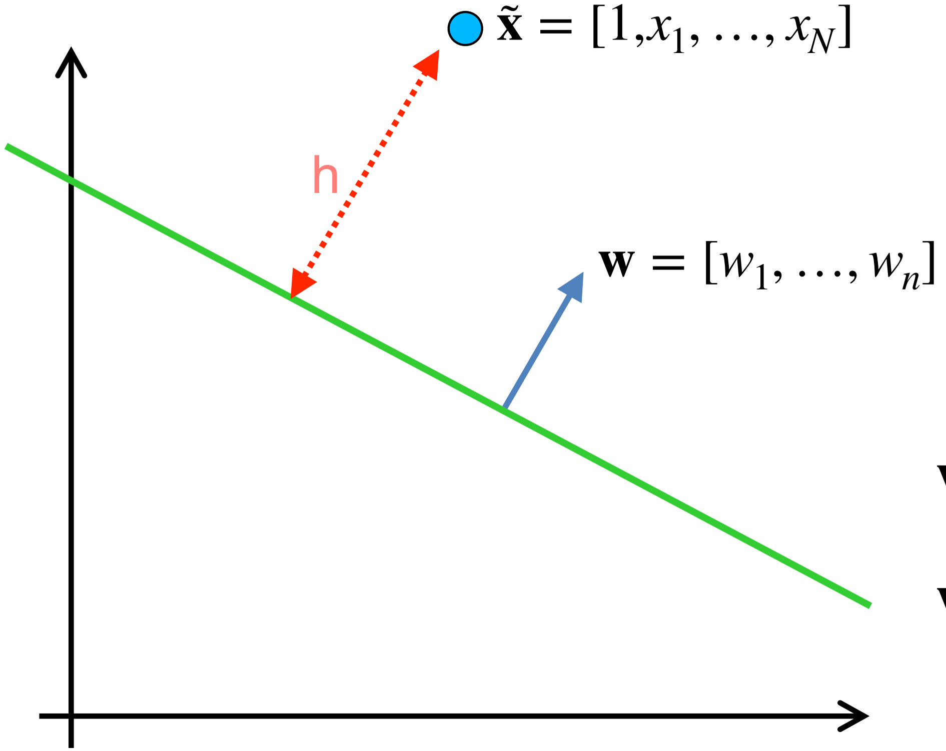
$\tilde{\mathbf{w}} = [w_0, w_1, \ldots, w_n]$ with $\cancel{\sum_{i=1}^{N} w_i^2 = 1}$

Hyperplane: $\mathbf{x} \in R^N, \tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}} = 0$, with $\tilde{\mathbf{x}} = [1 \,|\, \mathbf{x}]$.

Signed distance: $\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}$, with $\tilde{\mathbf{w}} = [1 \,|\, \mathbf{w}]$ and $||\mathbf{w}|| = 1$.

Reformulated Signed Distance



h=0: Point is on the decision boundary.
h>0: Point on one side.
h<0: Point on the other side.

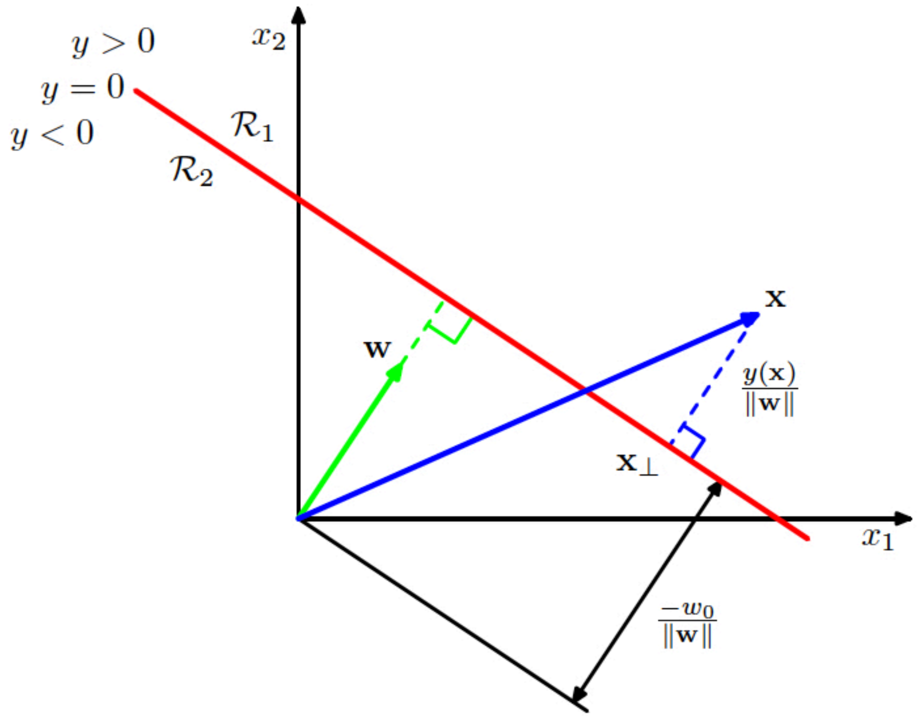
$$\tilde{\mathbf{w}} = [w_0 | \mathbf{w}] \in R^{N+1}$$

$$\tilde{\mathbf{w}}' = \frac{\tilde{\mathbf{w}}}{||\mathbf{w}||} = [\frac{w_0}{||\mathbf{w}||} | \frac{\mathbf{w}}{||\mathbf{w}||}]$$

Hyperplane: $\mathbf{x} \in R^N, \tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}} = 0$, with $\tilde{\mathbf{x}} = [1 | \mathbf{x}]$.

Signed distance: $\tilde{\mathbf{w}}' \cdot \tilde{\mathbf{x}} = \boxed{\frac{\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}}{||\mathbf{w}||}, \forall \tilde{\mathbf{w}} \in R^{N+1}.}$

Geometric Interpretation



$$\frac{\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}}{||\mathbf{w}||} = \frac{y(\mathbf{x})}{||\mathbf{w}||}$$

We are going to use this to find a classifier whose decision boundary is as far as possible from all the points.

Maximum Margin Classifier

- Given a training set $\{(\mathbf{x}_n, t_n)_{1\leq n\leq N}\}$ with $t_n \in \{-1,1\}$ and solution such that all the points are correctly classified, we have

$$\forall n, \quad t_n(\tilde{\mathbf{w}}_n \cdot \tilde{\mathbf{x}}_n) >= 0 \, .$$

- We can write the **unsigned** distance to the decision boundary as

$$d_n = t_n \frac{(\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}_n)}{||\mathbf{w}||}$$

—> A maximum margin classifier aims to maximize this distance for the point closest to the boundary, that, is maximize the minimum such distance.

$$\tilde{\mathbf{w}}^* = \text{argmax}_{\tilde{\mathbf{w}}} \min_n \left(\frac{t_n \cdot (\tilde{\mathbf{w}} \cdot \mathbf{x}_n)}{\|\mathbf{w}\|} \right)$$

Maximum Margin Classifier

$$\tilde{\mathbf{w}}^* = \text{argmax}_{\tilde{\mathbf{w}}} \min_n \left(\frac{t_n \cdot (\tilde{\mathbf{w}} \cdot \mathbf{x}_n)}{||\mathbf{w}||} \right)$$

- Unfortunately, this is a difficult optimization problem to solve.
- We will convert it into an equivalent, but easier to solve, problem.

Maximum Margin Classifier

- The signed distance is invariant to a scaling of $\tilde{\mathbf{w}}$:

$$\tilde{\mathbf{w}} \rightarrow \lambda\tilde{\mathbf{w}} : d_n = t_n \frac{(\lambda\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}_n)}{||\lambda\mathbf{w}||} = \frac{(\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}_n)}{||\mathbf{w}||} \ .$$

- We can choose λ so that for the point m closest to the boundary, we have

$$t_m \cdot (\tilde{\mathbf{w}} \cdot \mathbf{x}_m) = 1 \ .$$

- For all points we therefore have

$$t_n \cdot (\tilde{\mathbf{w}} \cdot \mathbf{x}_n) \geq 1 \ ,$$

and the equality holds for at least one point.

Linear Support Vector Machine

$$\forall n, \quad t_n(\tilde{\mathbf{w}} \cdot \mathbf{x}_n) \geq 1$$

$$\exists n \quad t_n(\tilde{\mathbf{w}} \cdot \mathbf{x}_n) = 1$$

$$\Rightarrow min_n d_n = min_n \frac{t_n(\tilde{\mathbf{w}} \cdot \mathbf{x}_n)}{||\mathbf{w}||} = \frac{1}{||\mathbf{w}||}$$

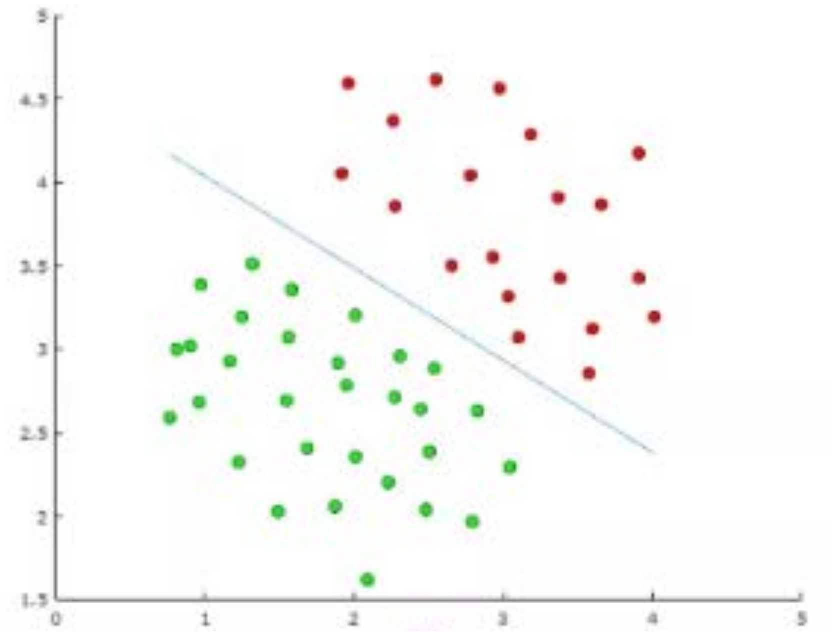
- To maximize the margin, we only need to maximize $1/||\mathbf{w}||$.
- This is equivalent to minimizing $\frac{1}{2}||\mathbf{w}||^2$.
- We can find max margin classifier as

$$\mathbf{w}^* = min_{\mathbf{w}} \frac{1}{2}||\mathbf{w}||^2 \text{subject to } \forall n, \quad t_n \cdot (\tilde{\mathbf{w}} \cdot \mathbf{x}_n) \geq 1$$

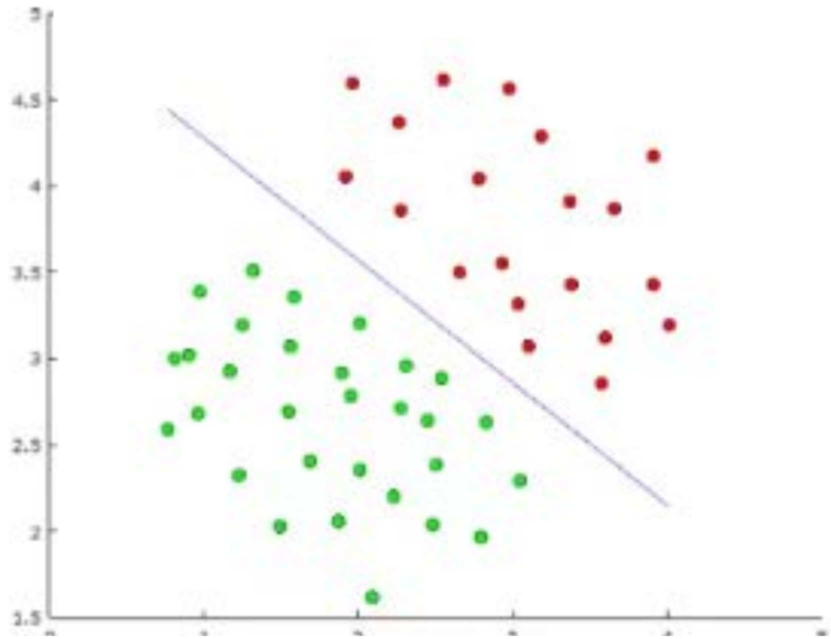
- This is a quadratic program, which is a **convex** problem.

—> It can be solved to optimality.

LR vs Linear SVM



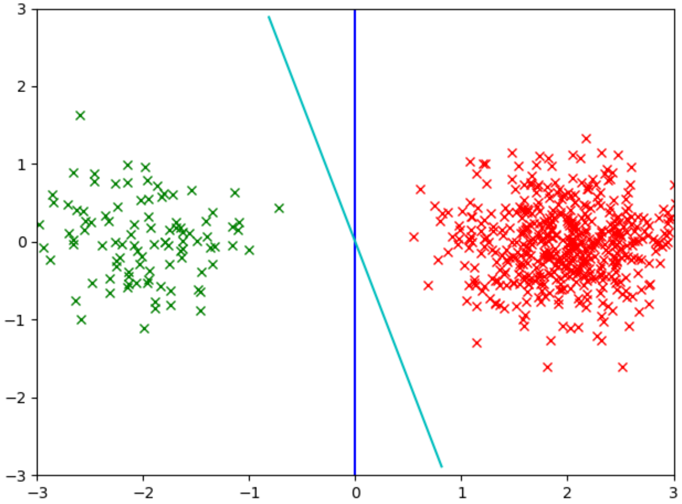
Logistic regression



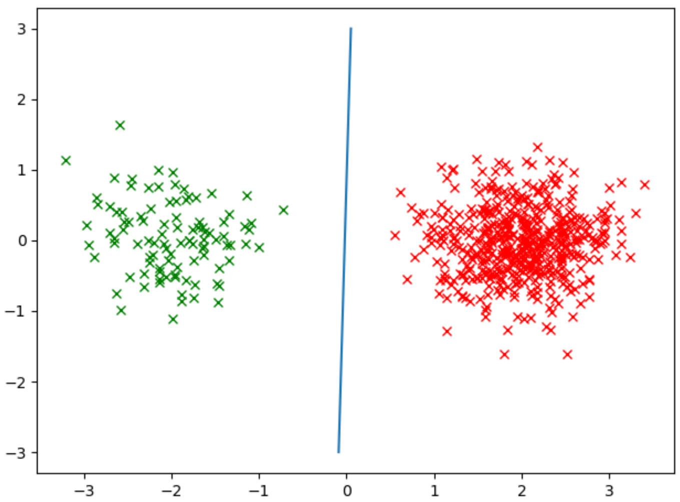
Linear SVM

- The LR decision boundary can come close to some of the training examples.
- The SVM tries to prevent that.

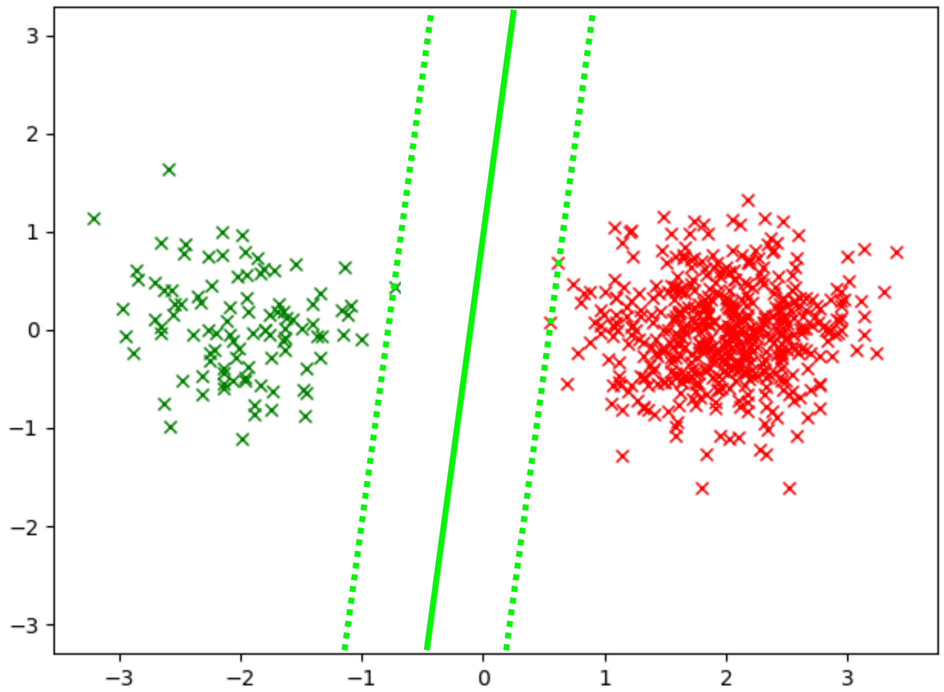
From Perceptron and LR to Linear SVM



Perceptron



Logistic Regression



Linear SVM

Are we done yet?

No!

EPFL

Maximum Margin Classifier

Rarely achievable in practice.

- Given a training set $\{(\mathbf{x}_n, t_n)_{1 \leq n \leq N}\}$ with $t_n \in \{-1, 1\}$ and solution such that all the points are correctly classified, we have

$$\boxed{\forall n, \quad t_n(\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}_n) >= 1 \,.}$$

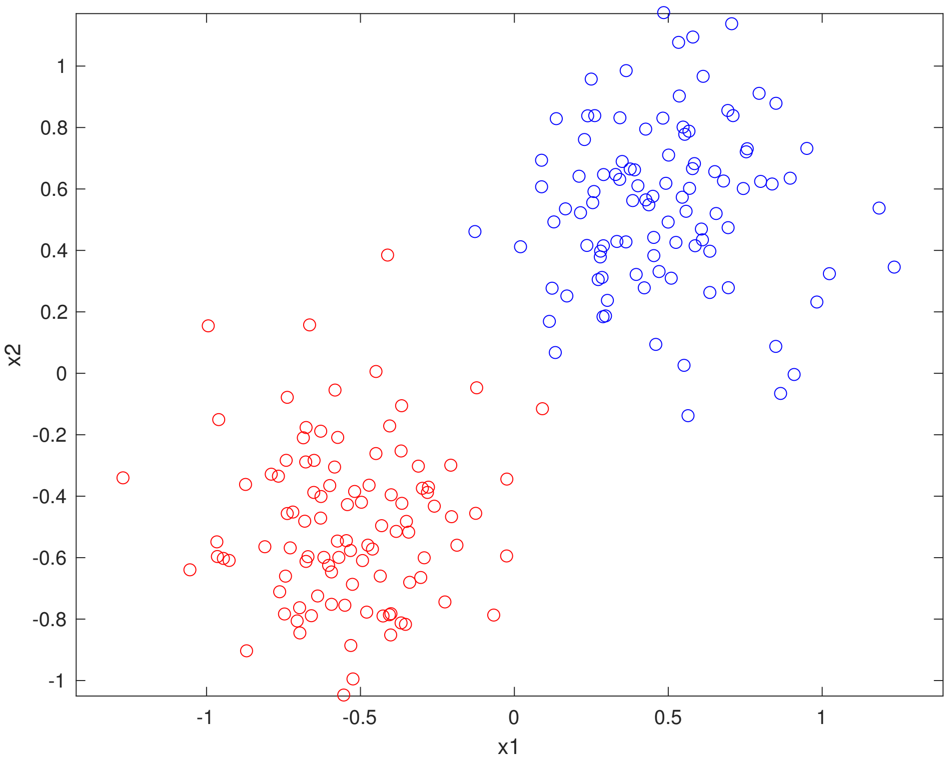
- We can write the **unsigned** distance to the decision boundary as

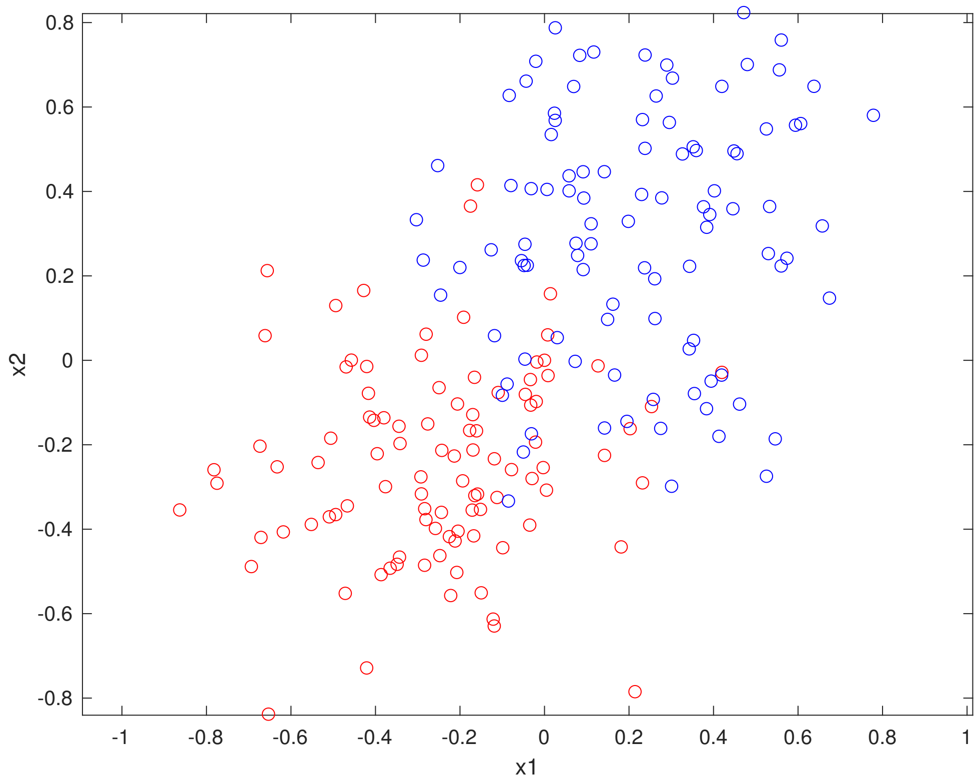
$$d_n = t_n \frac{(\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}_n)}{||\mathbf{w}||}$$

—> A maximum margin classifier aims to maximize this distance for the point closest to the boundary, that, is maximize the minimum such distance.

$$\tilde{\mathbf{w}}^* = \operatorname{argmax}_{\tilde{\mathbf{w}}} \min_n \left(\frac{t_n \cdot (\tilde{\mathbf{w}} \cdot \mathbf{x}_n)}{\|\mathbf{w}\|} \right)$$

Overlapping Classes





The data rarely looks like this.

It generally looks like that.

—> Must account for the fact that not all training samples can be correctly classified!

Relaxing the Constraints

- The original problem

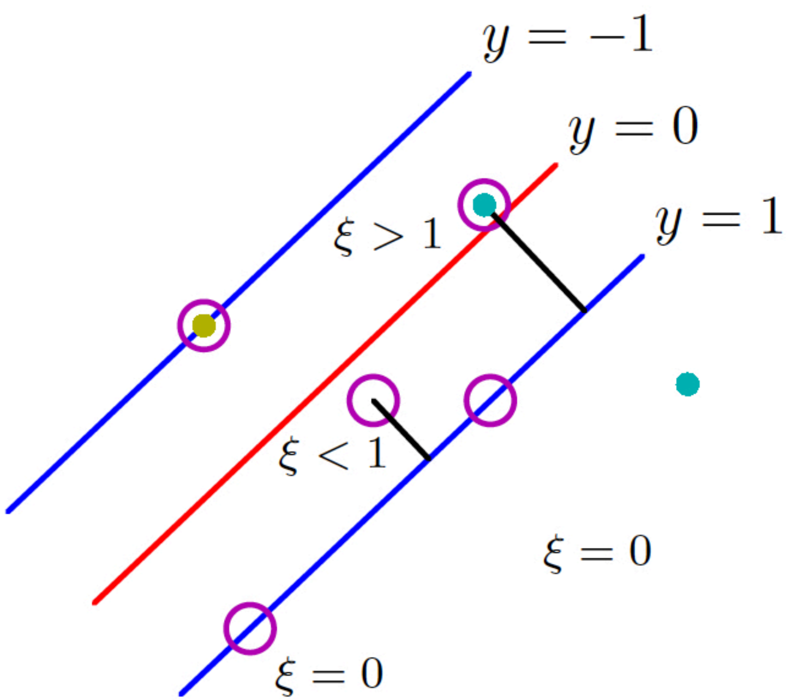
$$\mathbf{w}^* = min_{\mathbf{w}} \frac{1}{2} ||\mathbf{w}||^2 \text{subject to} \forall n, \quad t_n \cdot (\tilde{\mathbf{w}} \cdot \mathbf{x}_n) \geq 1,$$

cannot be satisfied.

- We must allow some of the constraints to violated, but as few as possible.

Slack Variables

- We introduce an additional slack variable ξ_n for each sample.
- We rewrite the constraints as $t_n \cdot (\tilde{\mathbf{w}} \cdot \mathbf{x}_n) \geq 1 - \xi_n$.
- $\xi_i \geq 0$ weakens the original constraints.



- If $0 < \xi_n \leq 1$, sample n lies inside the margin, but is still correctly classified
- If $\xi_n \geq 1$, then sample i is misclassified

Naive Formulation

$$\mathbf{w}^* = min_{\mathbf{w}} \frac{1}{2} ||\mathbf{w}||^2$$

$$\text{subject to } \forall n, \quad t_n \cdot (\tilde{\mathbf{w}} \cdot \mathbf{x}_n) \geq 1 - \xi_n \text{ and } \xi_n \geq 0$$

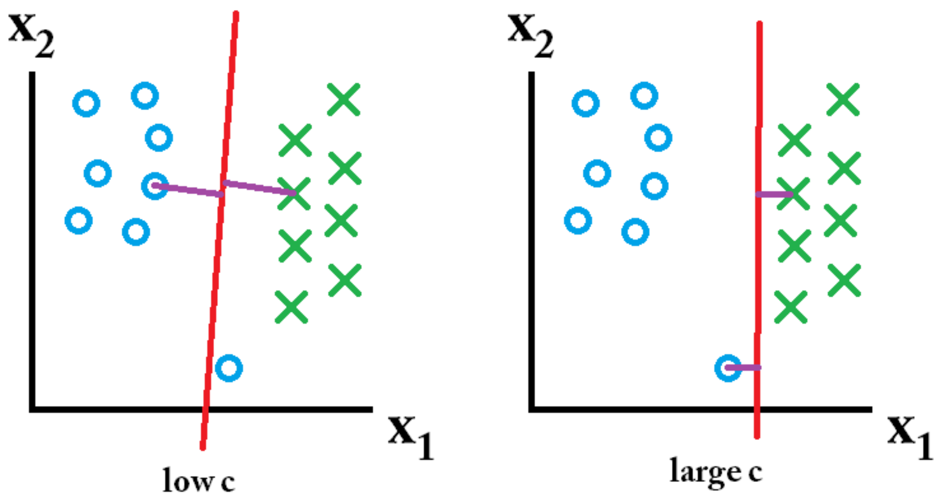
- This would simply allow the model to violate all the original constraints at no cost.
- This would result in a useless classifier.

Improved Formulation

$$\mathbf{w}^* = min_{(\mathbf{w},\{\xi_\mathbf{n}\})} \frac{1}{2} ||\mathbf{w}||^2 + C \sum_{n=1}^{N} \xi_n,$$

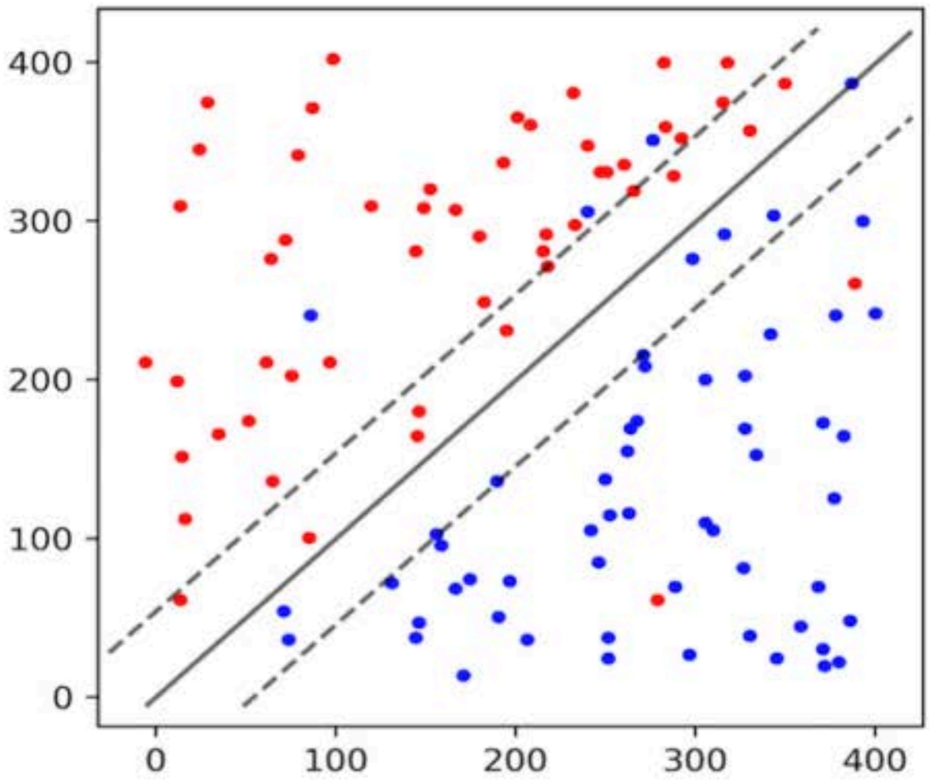
$$\text{subject to } \forall n, \quad t_n \cdot (\tilde{\mathbf{w}} \cdot \mathbf{x}_n) \geq 1 - \xi_n \text{ and } \xi_n \geq 0.$$

- C is constant that controls how costly constraint violations are.
- The problem is still convex.

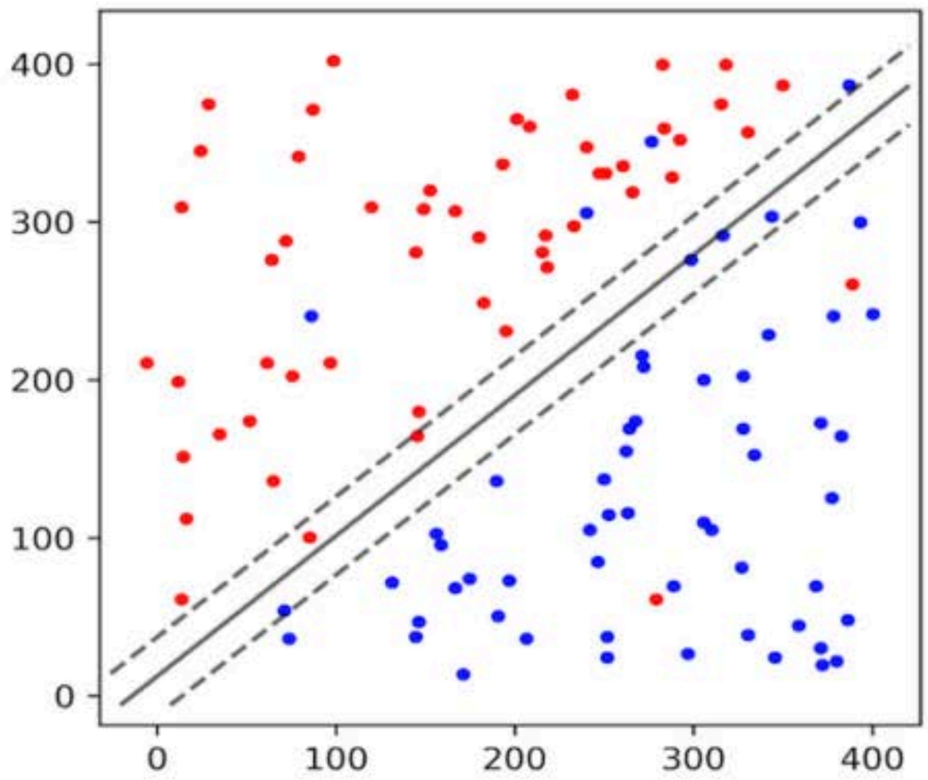


http://www.cristiandima.com/basics-of-support-vector-machines/

Choosing the C Parameter



C=1:
- Large margin.
- Many training samples misclassified.

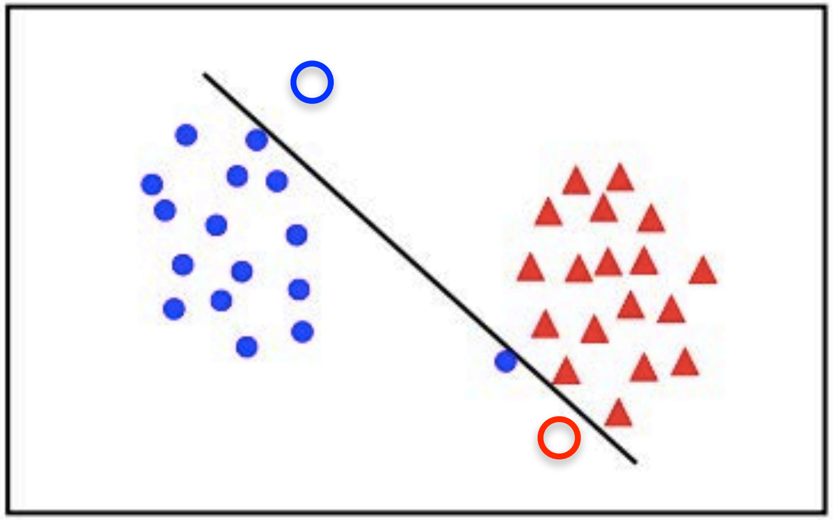


C=100:
- Small margin.
- Few training samples misclassified.

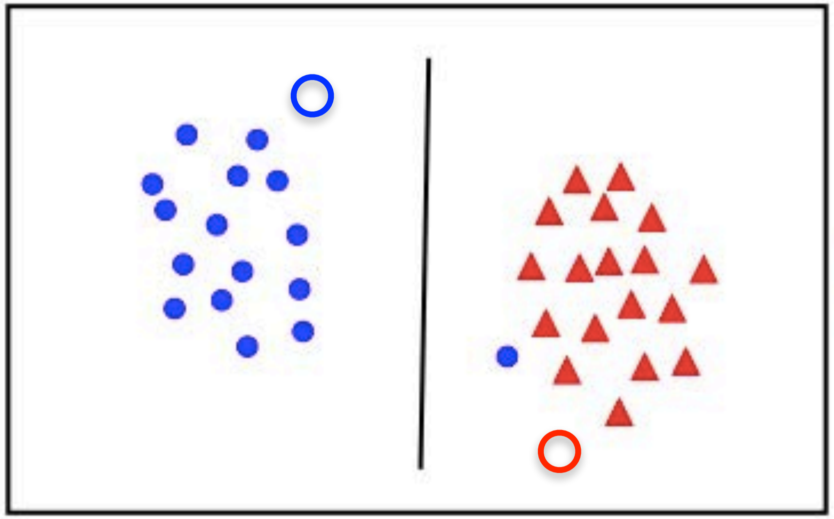
Which is best?
- It depends.
- Must use cross-validation, as we did for k-Means.

EPFL

Optimal vs Best



- The points can be linearly separated but the margin is still very small.
- At test time the two circles will be misclassified.



- The margin is much larger but one training example is misclassified.
- At test time the two circles will be classified correctly.

—> Tradeoff between the number of mistakes on the training data and the margin.

Support Vector Machines