Neural Networks and Learning Systems
TBMI26 / 732A55
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Lecture 2

Supervised learning – Linear classifiers

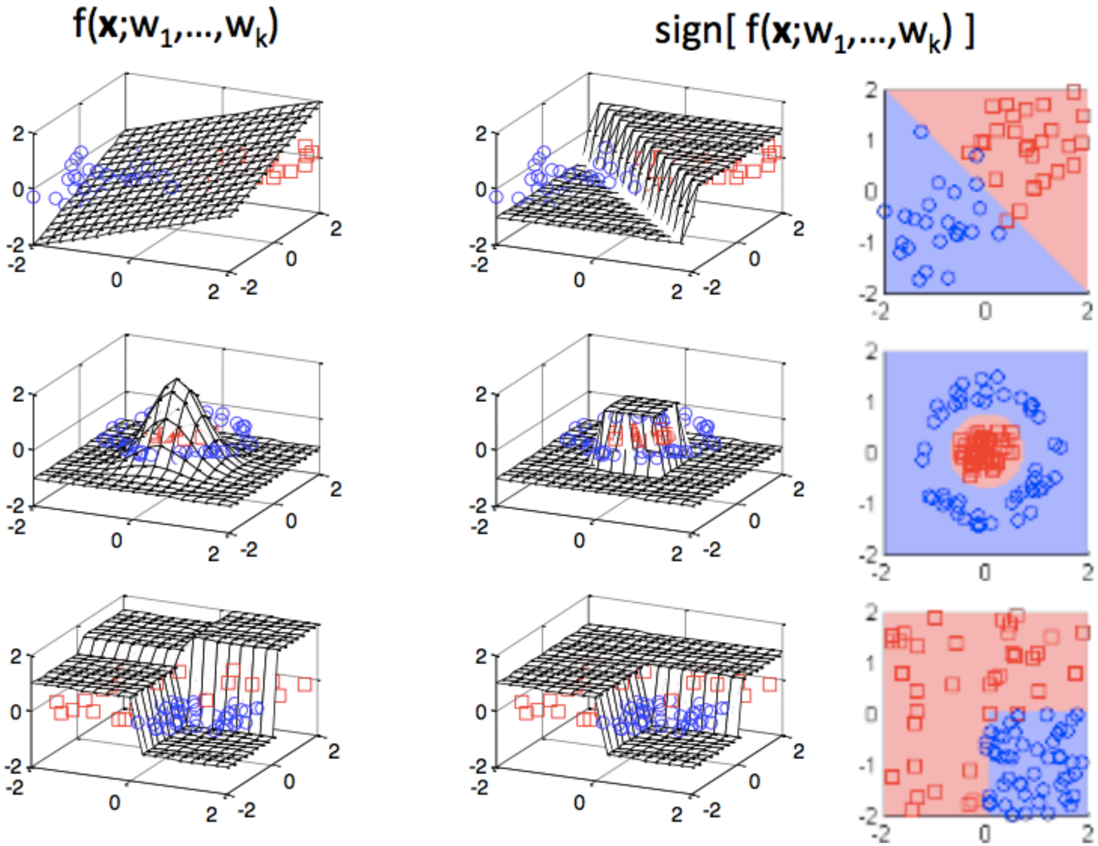
Magnus Borga
magnus.borga@liu.se

Recap - Supervised learning

- **Task:** Learn to predict/classify new data from labelled examples.
- **Input:** Training data examples {$\mathbf{x}_i$, y_i} i=1...N, where $\mathbf{x}_i$ is a feature vector and y_i is a class label in the set Ω. Today we'll assume two classes: $\Omega = \{-1, 1\}$
- **Output:** A discriminant function sign[$f(\mathbf{x}; w_1,\ldots,w_k)$]$\rightarrow \Omega$

Find a function f and adjust the parameters $w_1,\ldots,w_k$ so that new feature vectors are classified correctly. Generalization!

The function f($\mathbf{x}$;w_1,…,w_k)



Advantages of a parametric function $f(\mathbf{x}; w_1, \ldots, w_k)$

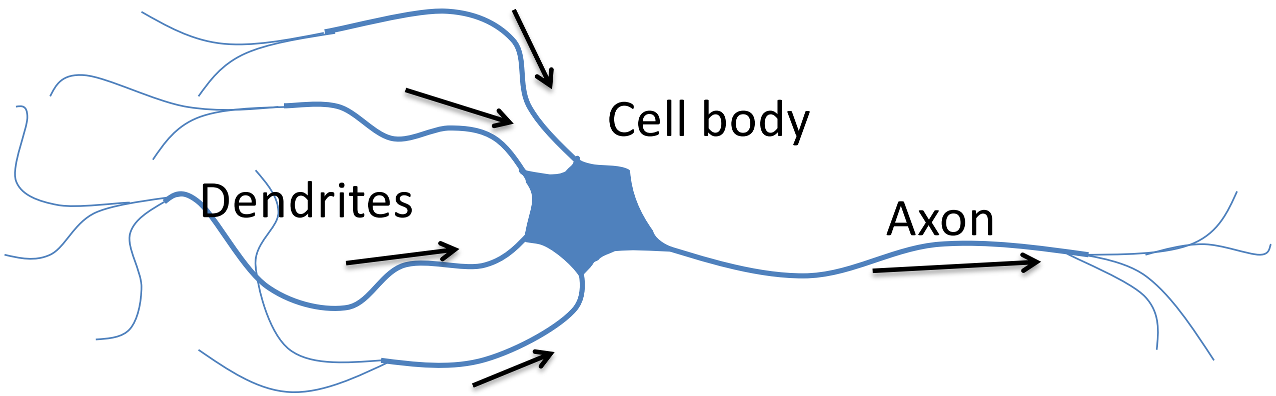
- Only stores a few parameters (w_0, w_1, …, w_n) instead of all the training samples, as in *k*-NN.

- Fast to evaluate on which side of the line a new sample is on, for example $\mathbf{w}^T\mathbf{x} < 0$ or $\mathbf{w}^T\mathbf{x} > 0$ for a linear function.

How does the brain take decisions?

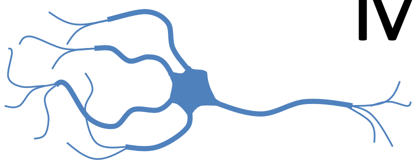
(on the low level!)

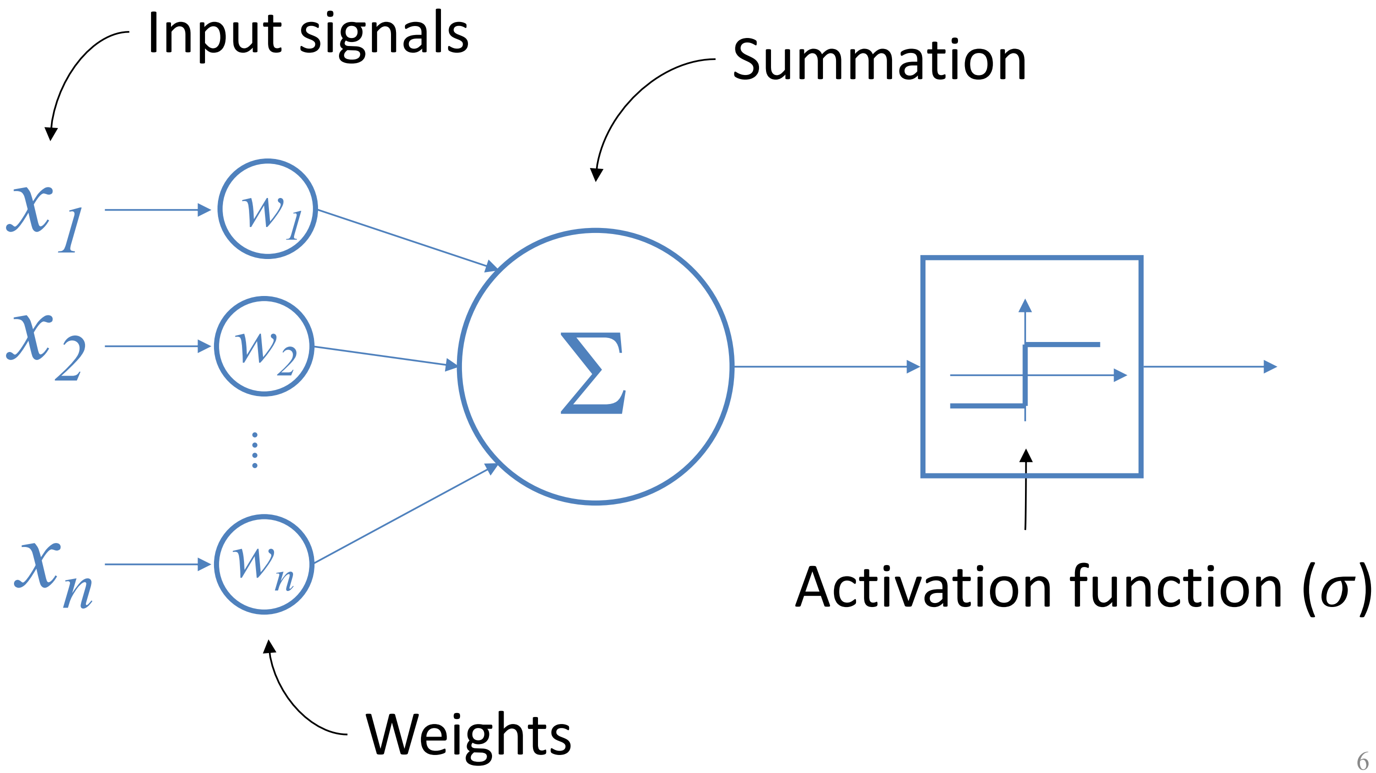
- Basic unit: the neuron



- The human brain has approximately 100 billion (10^{11}) neurons.
- Each neuron connected to about 7000 other neurons.
- Approx. 10^{14} - 10^{15} synapses (connections).

Model of a neuron

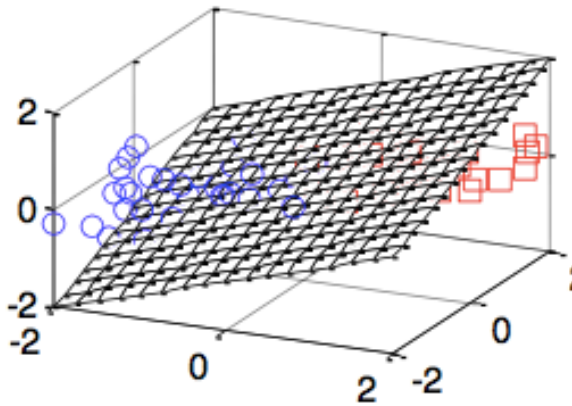


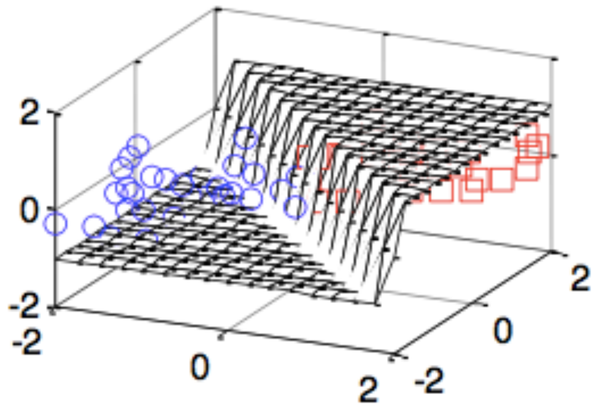


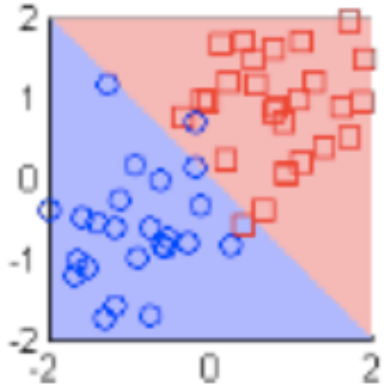
The Perceptron

(McCulloch & Pitts 1943, Rosenblatt 1962)

$$f\left(x_1,\ldots,x_n;w_0,\ldots,w_n\right)=\sigma\left(w_0+\sum_{i=1}^{n}w_i x_i\right)=\sigma\left(w_0+\mathbf{w}^T\mathbf{x}\right)$$







Extra reading on the history of the perceptron:
http://www.csulb.edu/~cwallis/artificialn/History.htm

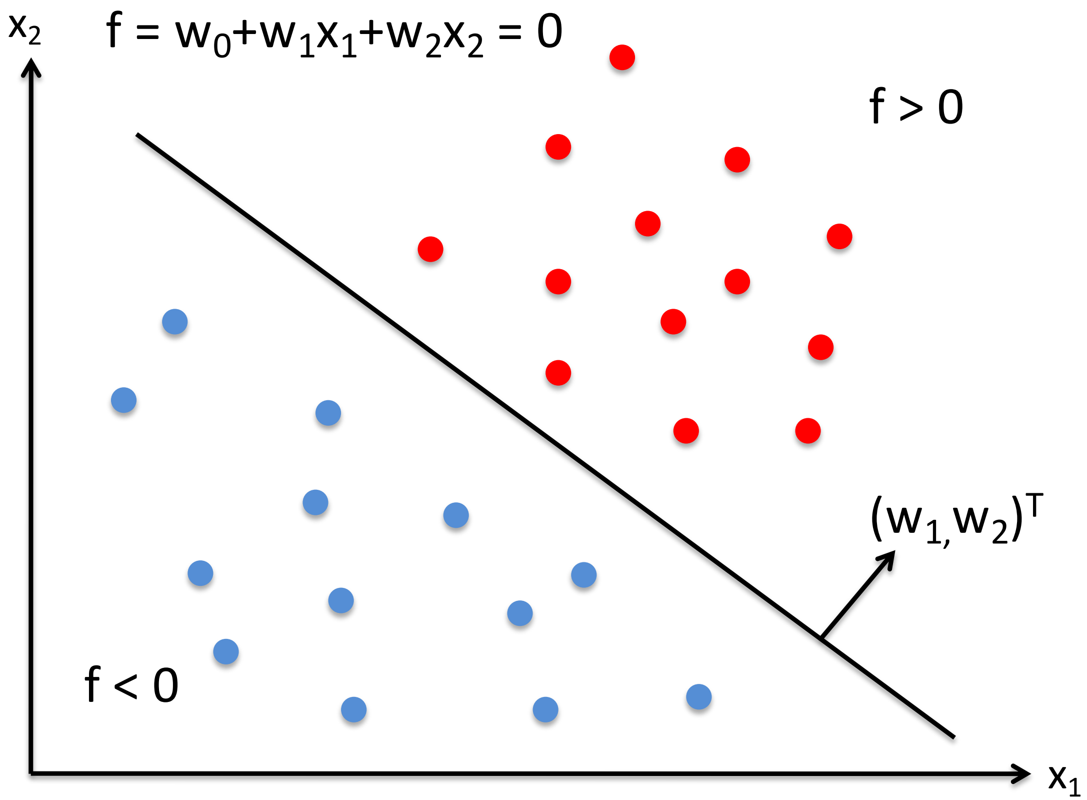
Notational simplification: Bias weight

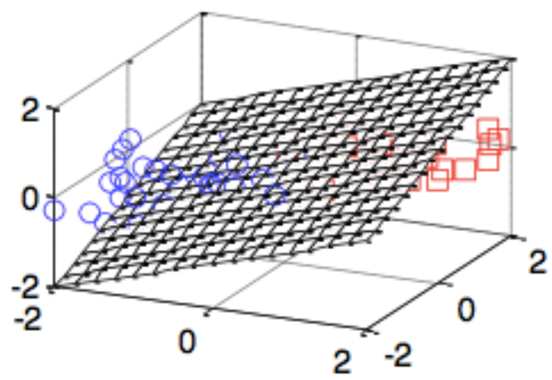
Add a constant 1 to the feature vector so that we don't have to treat w_0 separately.

Instead of $\mathbf{x} = [x_1,\ldots,x_n]^T$, we have $\mathbf{x} = [1, x_1,\ldots,x_n]^T$

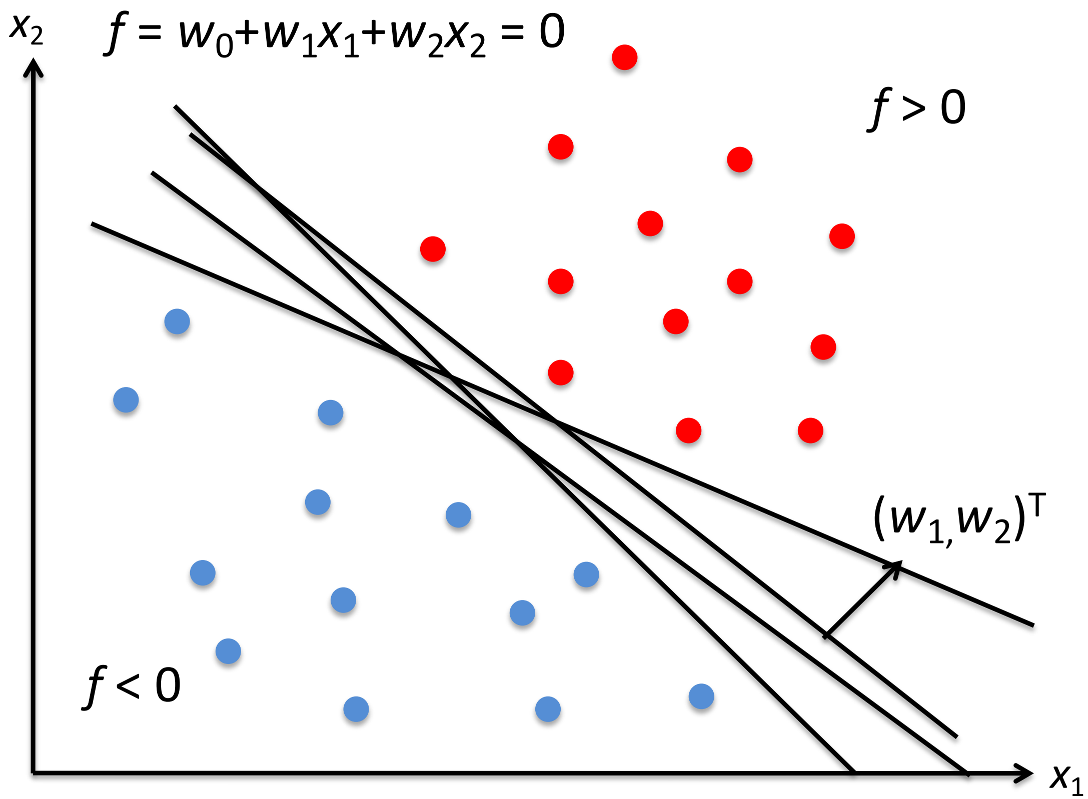
$$\mathrm{f}(x_1,\ldots,x_\mathrm{n}; w_0,\ldots, w_n) = \sigma\left(\sum_{\mathrm{i}=0}^{\mathrm{n}} w_\mathrm{i} x_\mathrm{i}\right) = \sigma(\mathbf{w}^T\mathbf{x})$$

Geometry of linear classifiers



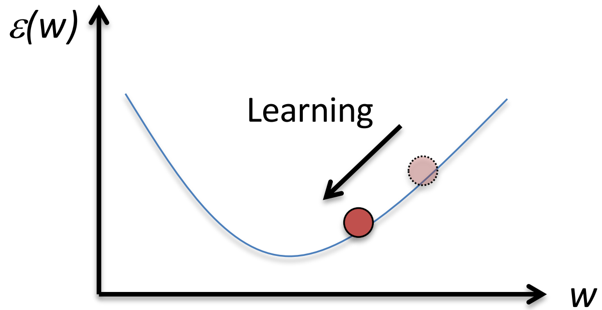


Which linear classifier to choose?



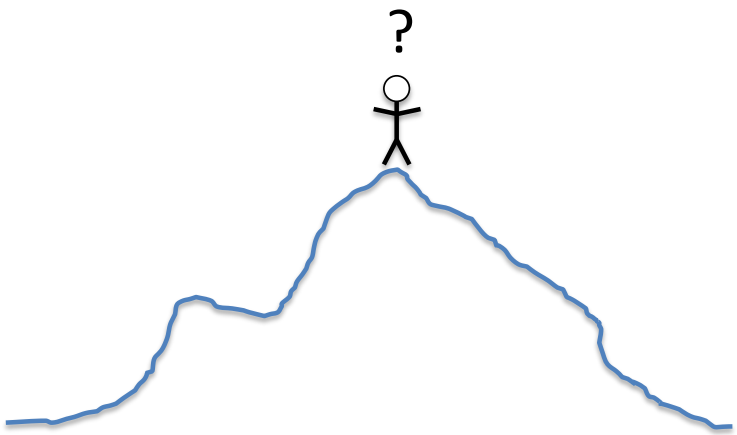
Find the best separator – optimization!

- Min of a loss function $\varepsilon(w_0, w_1, \ldots, w_n)$ with the weights $w_0, w_1, \ldots, w_n$ as parameters.

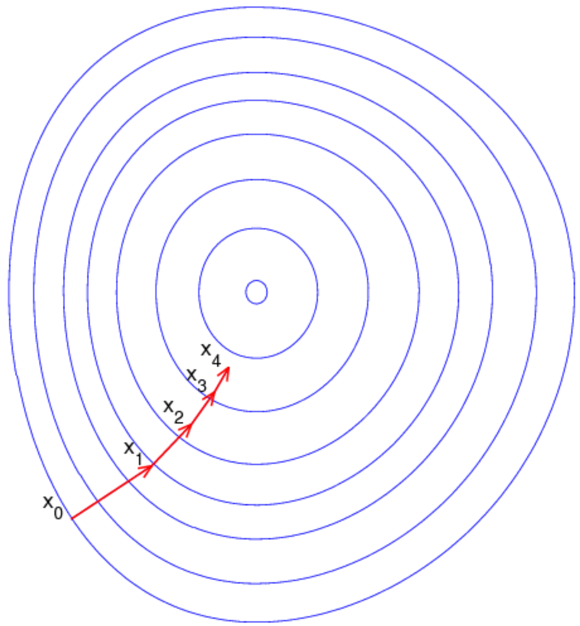


- Ways to optimize:
  - Algebraic: Set derivative $\frac{\partial \varepsilon}{\partial w_i} = 0$ and solve.
  - Brute force: Try many values systematically and choose the best.
  - Iterative: Follow the gradient direction until the minimum of ε is reached.

Gradient descent



How to get to the lowest point?



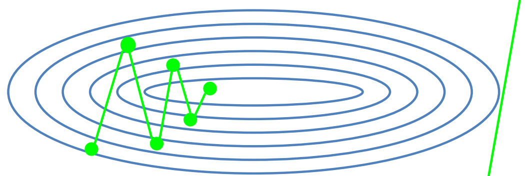
$$\nabla \varepsilon = \frac{\partial \varepsilon}{\partial \mathbf{w}} = \begin{pmatrix} \dfrac{\partial \varepsilon}{\partial w_1} \\ \dfrac{\partial \varepsilon}{\partial w_2} \end{pmatrix}$$

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} - \eta \frac{\partial \varepsilon}{\partial \mathbf{w}}$$

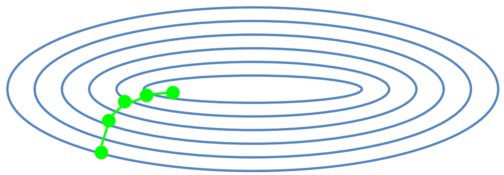
Gradient descent

Choosing the step length

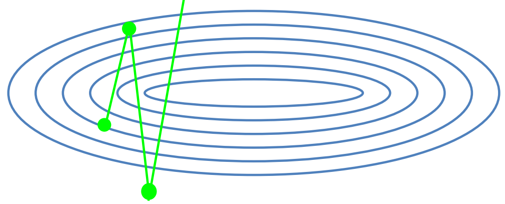
Large η



Small η

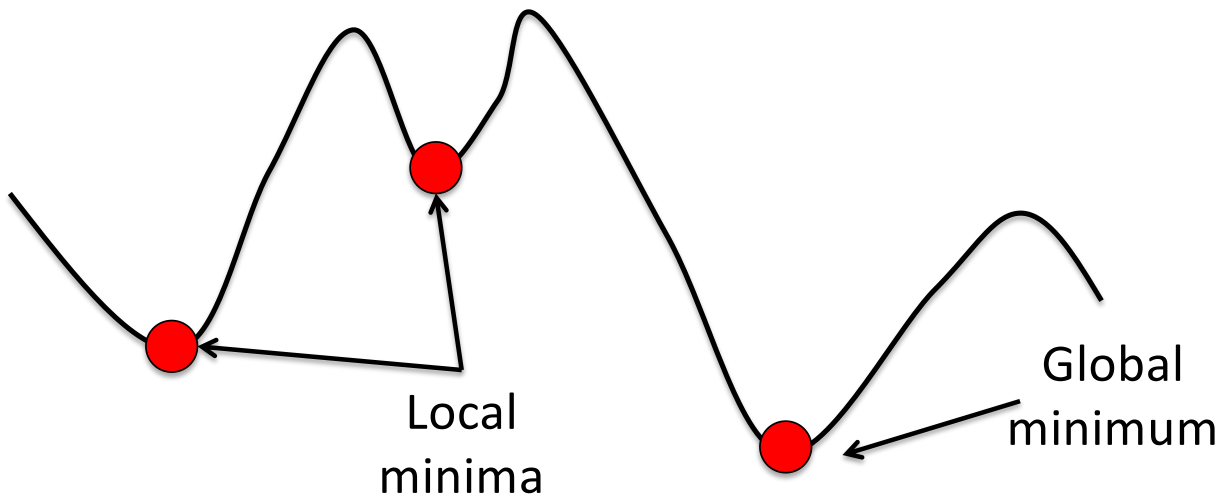


Too large η



Local optima

- Gradient descent is not guaranteed to find the global minimum.
- With a sufficiently small step length, the closest local minimum will be found.



Many different loss functions $\varepsilon(\mathbf{w})$

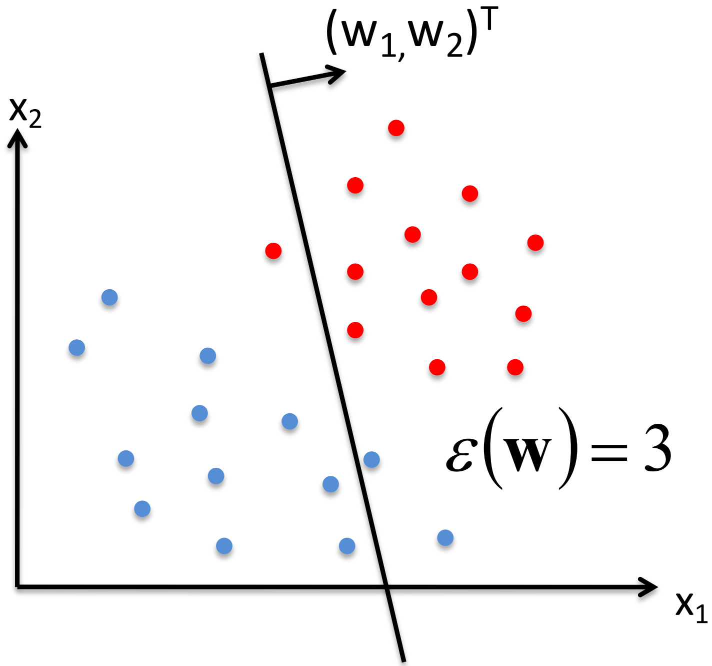
- 0-1 loss function / empirical risk
- Square error → Neural networks
- Maximum margin → Support Vector Machines

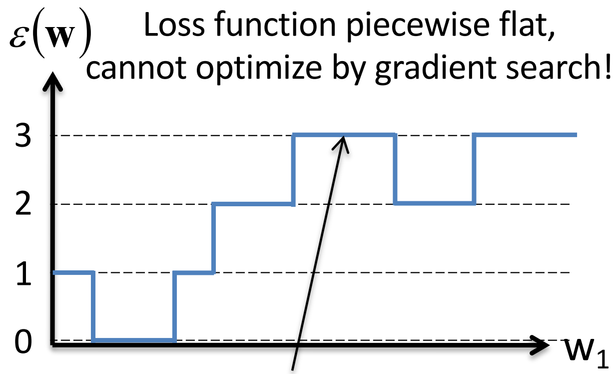
0-1 loss function / empirical risk

"empirical" because it is over the observed training data

$$\varepsilon(\mathbf{w}) = \sum_{i=1}^{N} I\left(f(\mathbf{x}_i;\mathbf{w}) \neq y_i\right)$$ = Number of wrong classifications

0/1 function





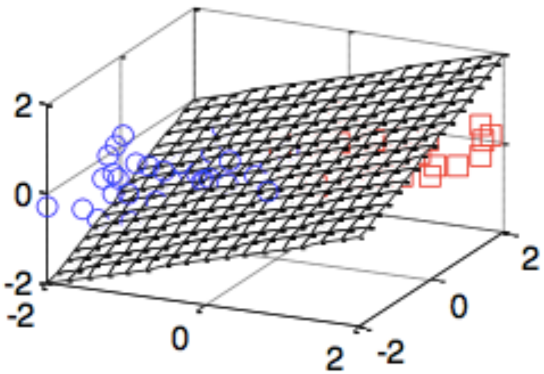
$$\frac{\partial \varepsilon}{\partial w_1} = 0$$, no information!

Square error loss

Minimize the following loss function

$$\varepsilon(\mathbf{w}) = \sum_{i=1}^{N} \left(\mathbf{w}^T \mathbf{x}_i - y_i\right)^2$$

N = # training samples
$y_i \in \{-1,1\}$ depending on the class of training sample i



Minimization algorithm

$$\varepsilon(\mathbf{w}) = \sum_{i=1}^{N} \left(\mathbf{w}^T \mathbf{x}_i - y_i\right)^2$$

$$\frac{\partial \varepsilon}{\partial \mathbf{w}} = 2\sum_{i=1}^{N} \left(\mathbf{w}^T \mathbf{x}_i - y_i\right)\mathbf{x}_i$$

Exercise!

Gradient descent:

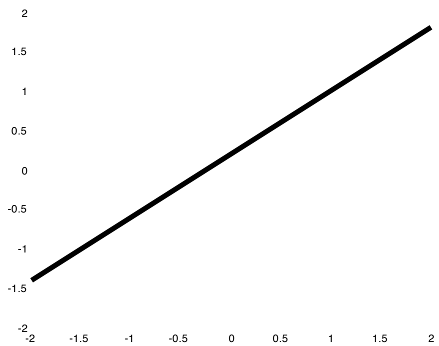
$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \frac{\partial \varepsilon}{\partial \mathbf{w}} = \mathbf{w}_t - \eta \sum_{i=1}^{N} \left(\mathbf{w}_t{}^T \mathbf{x}_i - y_i\right)\mathbf{x}_i \quad (\text{Eq.}1)$$

Algorithm:

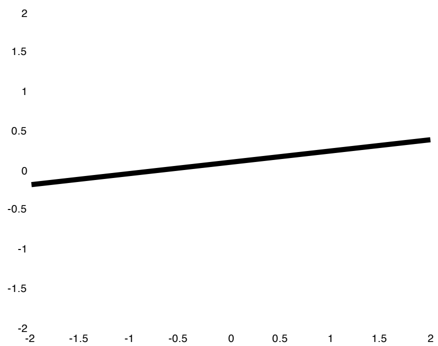
1. Start with a random **w**
2. Iterate Eq. 1 until convergence

Example

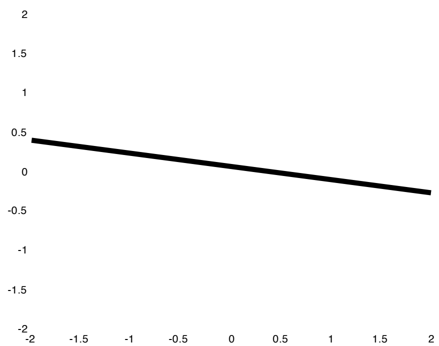
Random init



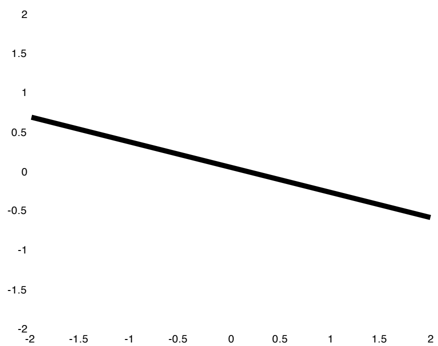
First iteration



Second iteration

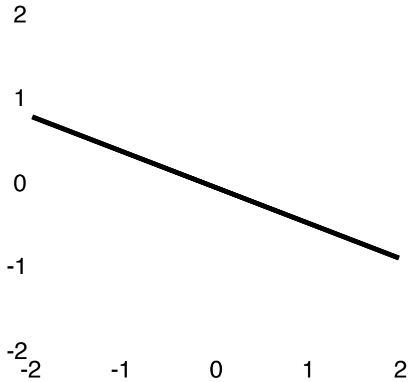


Third iteration

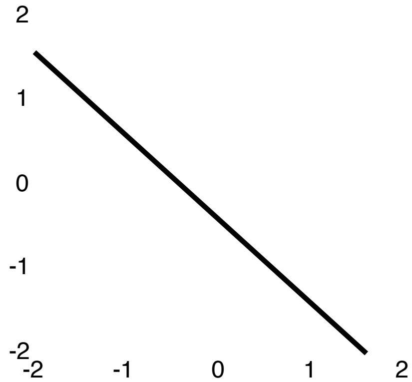


More examples

Unevenly distributed
training data

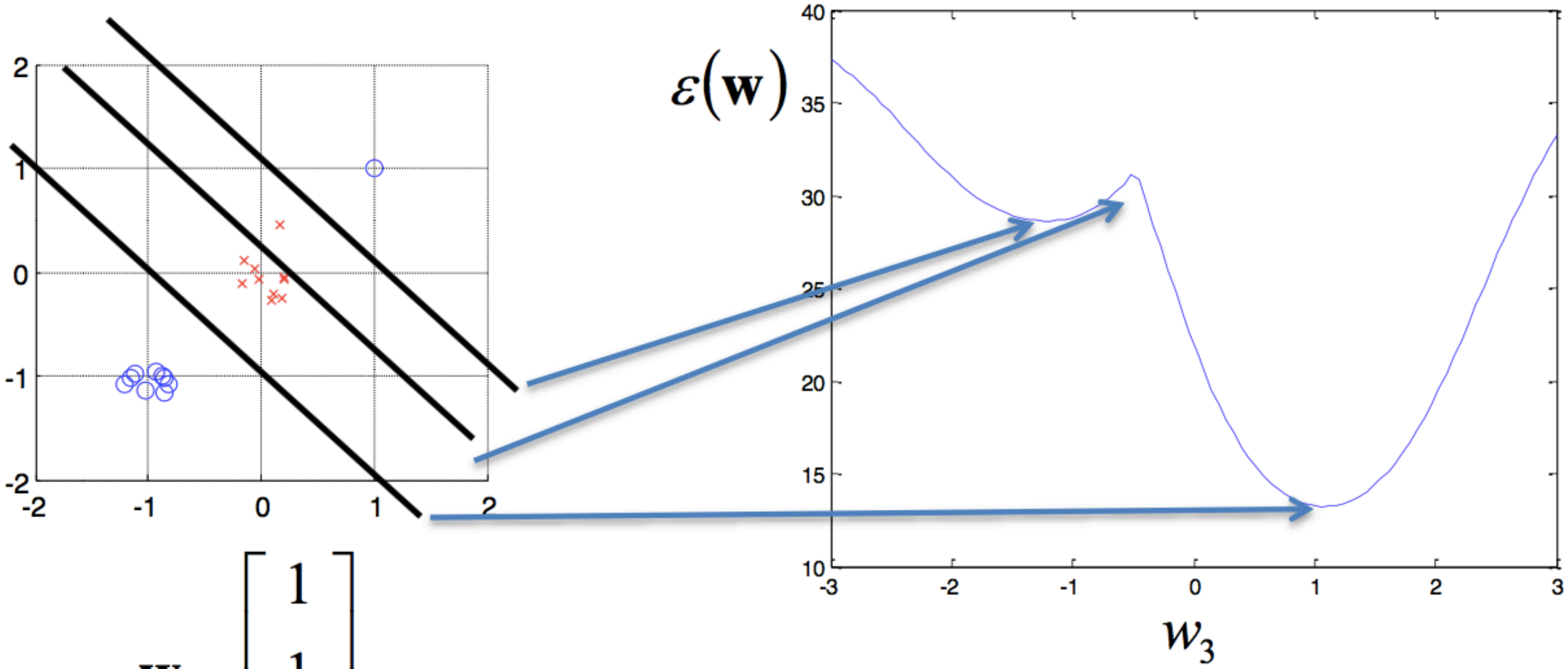


Outlier



$$\varepsilon(\mathbf{w}) = \sum_{i=1}^{N} \left(\mathbf{w}^T \mathbf{x}_i - y_i \right)^2$$

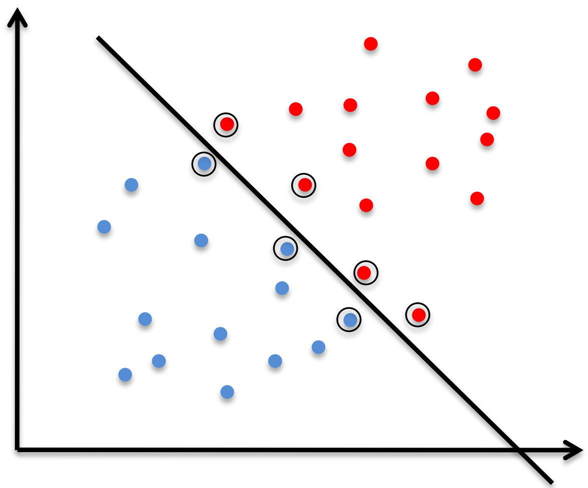
Example of local minimum

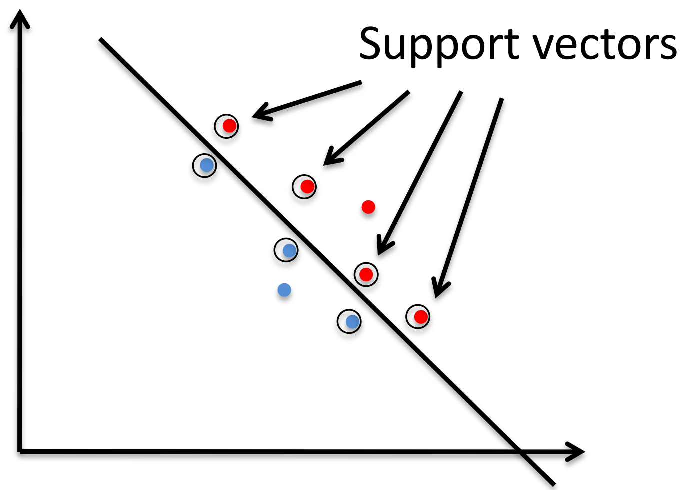


$$\mathbf{w} = \begin{bmatrix} 1 \\ 1 \\ w_3 \end{bmatrix}$$

Support Vector Machines (SVM)

Idea!

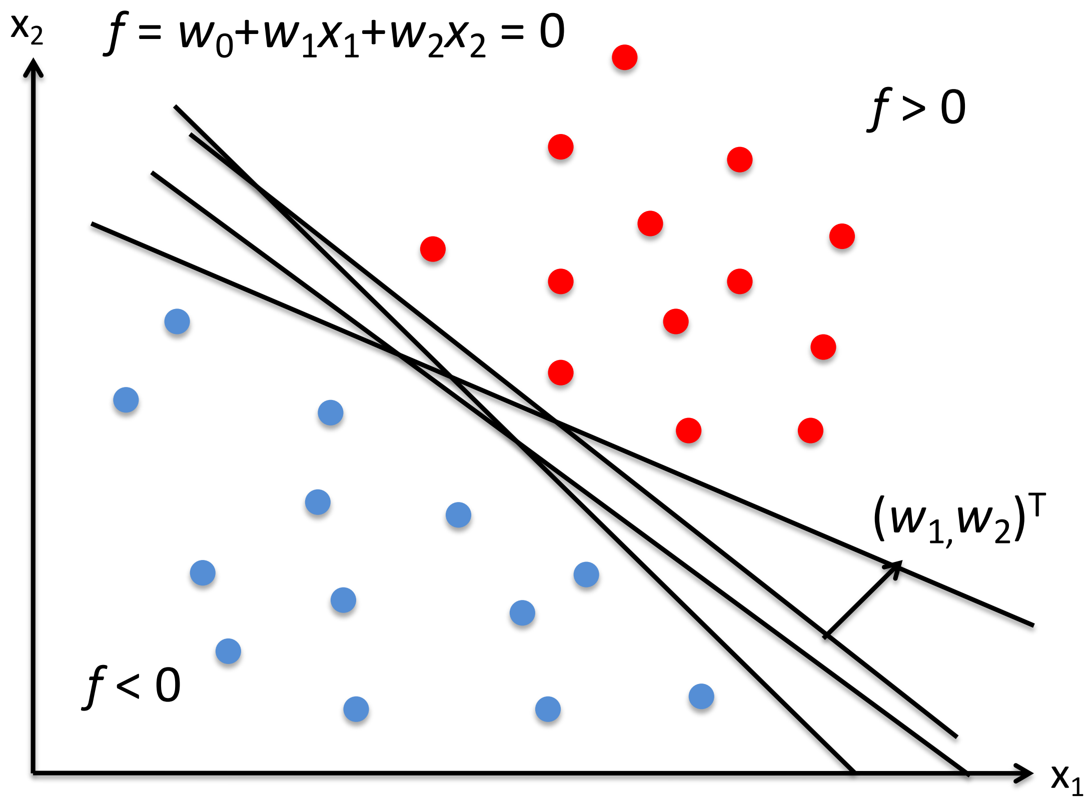




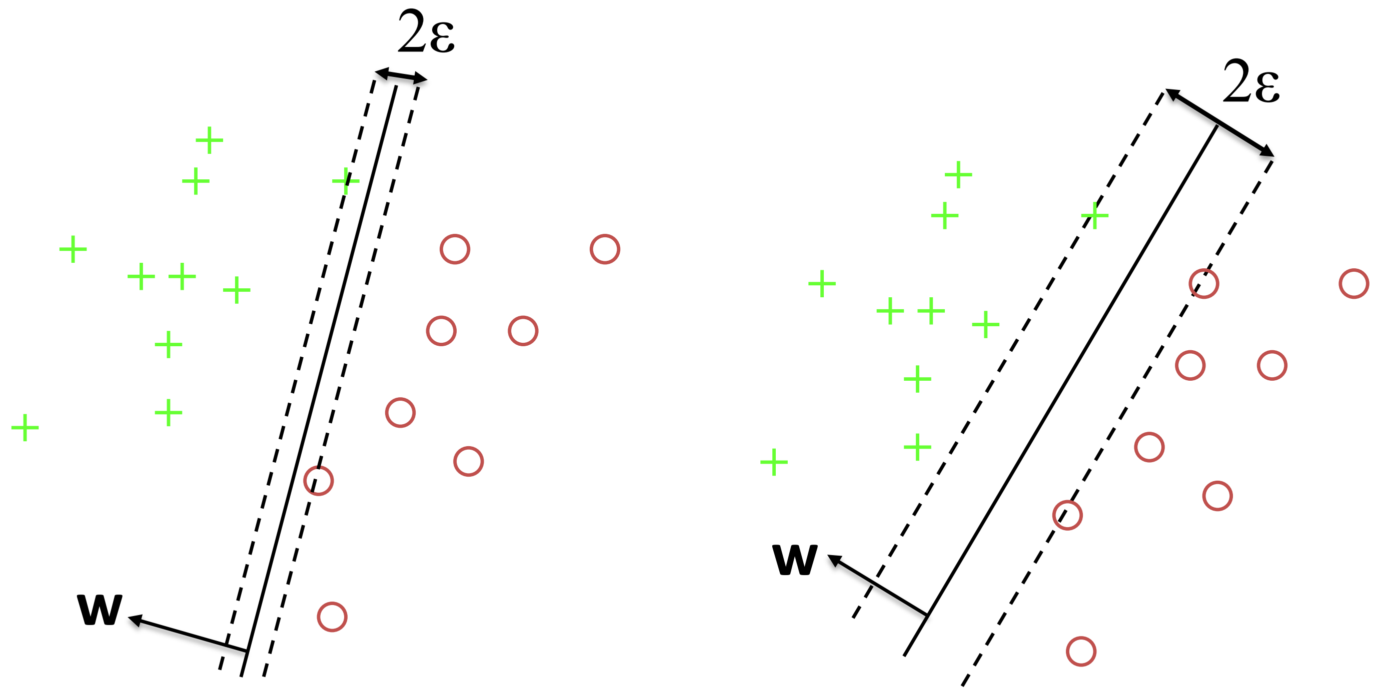
Optimal separation line remains the same, feature points close to the class limits are more important!

These are called *support vectors*!

Which linear classifier to choose?



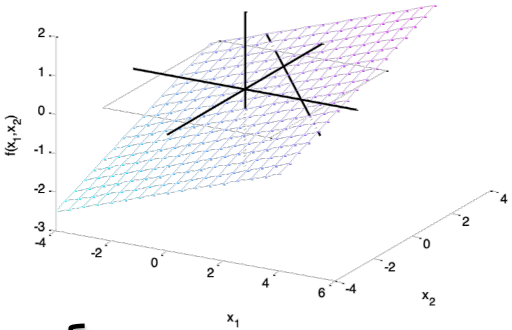
SVM – Maximum margin



Choose **w** that gives maximum margin ε!

SVM – Loss function

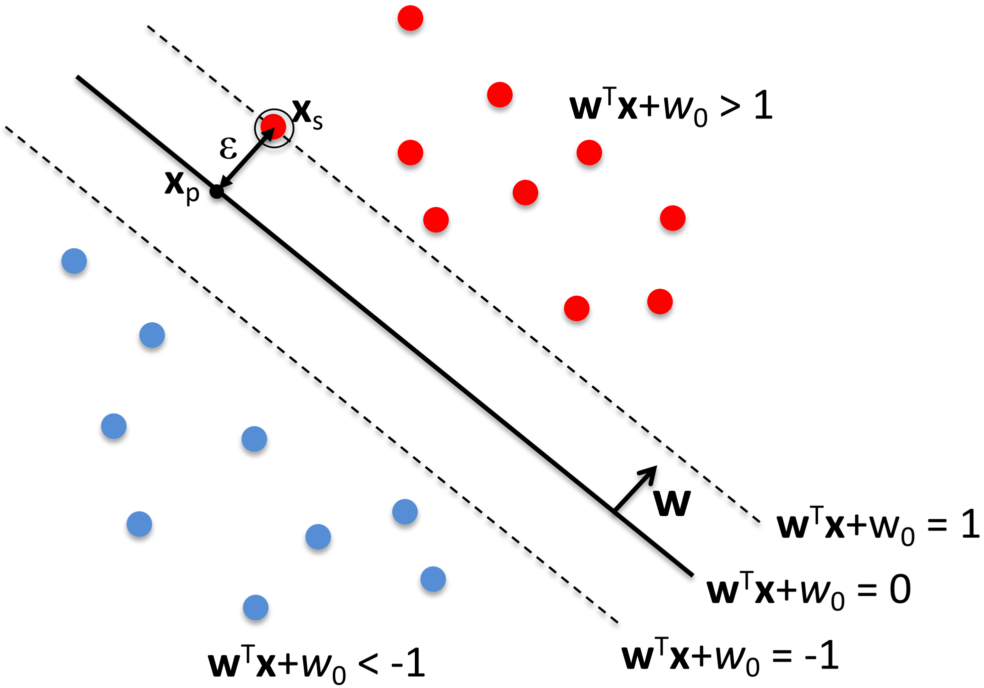
Scaling of **w** is free – Pick arbitrary sample $\mathbf{x}_s$ as support vector and choose scaling so that $\mathbf{w}^T\mathbf{x}_s+w_0 = 1$!



$$\begin{cases} \mathbf{w}^T\mathbf{x}_s + w_0 = 1 \\ \mathbf{x}_s = \mathbf{x}_p + \varepsilon\hat{\mathbf{w}} \end{cases}$$

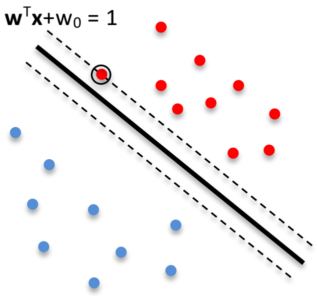
$$\mathbf{w}^T(\mathbf{x}_p + \varepsilon\,\hat{\mathbf{w}}) + w_0 = 1$$

$$\varepsilon\,\underbrace{\mathbf{w}^T\hat{\mathbf{w}}}_{\|\mathbf{w}\|\,\hat{\mathbf{w}}^T\hat{\mathbf{w}} = \|\mathbf{w}\|} + \underbrace{\mathbf{w}^T\mathbf{x}_p + w_0}_{0} = 1$$

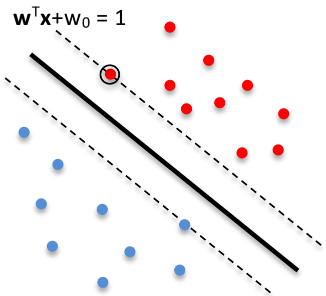


For the chosen support vector, $\varepsilon(\mathbf{w}) = 1 / \|\mathbf{w}\|$

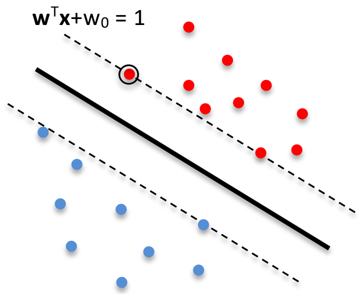
SVM loss function examples



Example 1:
Boundary not in middle →
Large ||w|| (steep function) →
Small margin ε(**w**) = 1 / ||**w**||



Example 2:
Boundary more in middle →
Smaller ||w|| (flatter function) →
Larger margin ε(**w**) = 1 / ||**w**||



Example 3:
Tilt boundary somewhat→
Smallest possible ||w|| →
Largest margin ε(**w**) = 1 / ||**w**||

Choosing another training sample as reference support vector can give an even larger margin!

SVM – Loss function, cont.

Maximizing $\varepsilon = 1 / ||\mathbf{w}||$ is the same as minimizing $||\mathbf{w}||^2$!

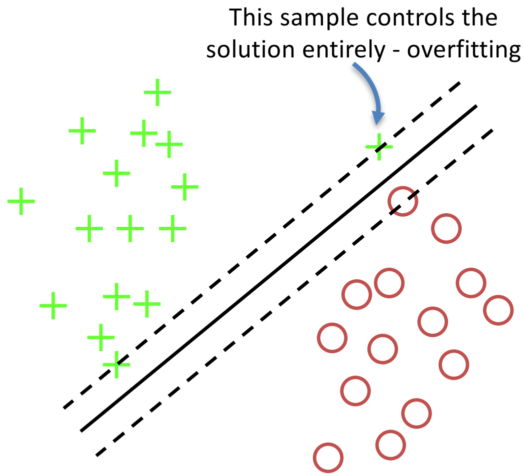
$$\min \|\mathbf{w}\|^2$$

$$\text{subject to } y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq 1$$

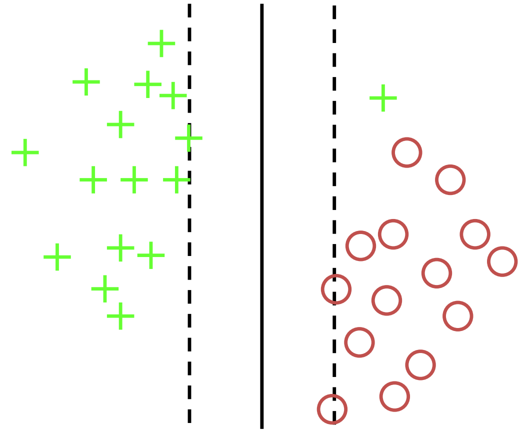
No training samples must reside in the margin region!

Optimization procedure outside the scope of this course…

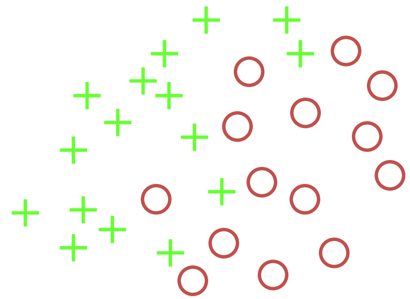
SVM – Soft margin



Would this be a better boundary?



What if the training data is not separable with a line?



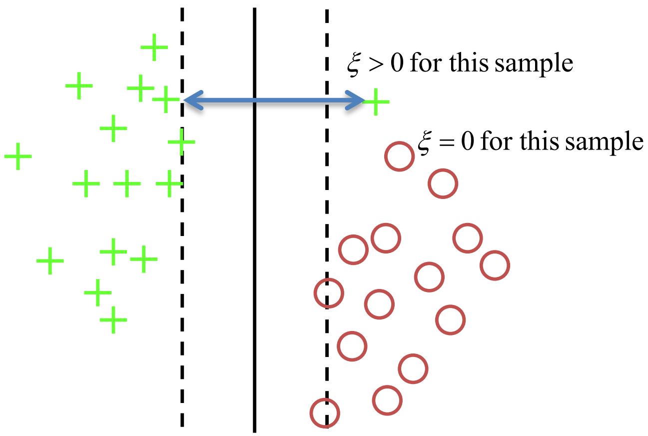
SVM – Soft margin, cont.

user-defined trade-off parameter

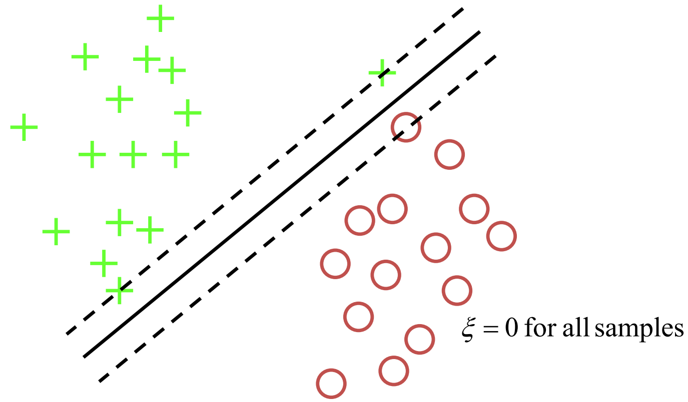
$$\min_{\mathbf{w},w_0,\xi_i} \left\{ \|\mathbf{w}\|^2 + C \sum_{i=1}^{N} \xi_i \right\}$$

slack variable

$$\text{subject to } y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq 1 - \xi_i$$



Solution for small C



Solution for large C

SVM – Choosing *C*

Solve the optimization problem with different *C*:s and choose the solution with highest accuracy according to cross-validation procedure.

$$C = 2^{-5}, 2^{-3}, \ldots, 2^{15}$$

Training data	Training data	Validation data
Training data	Validation data	Training data
Validation data	Training data	Training data

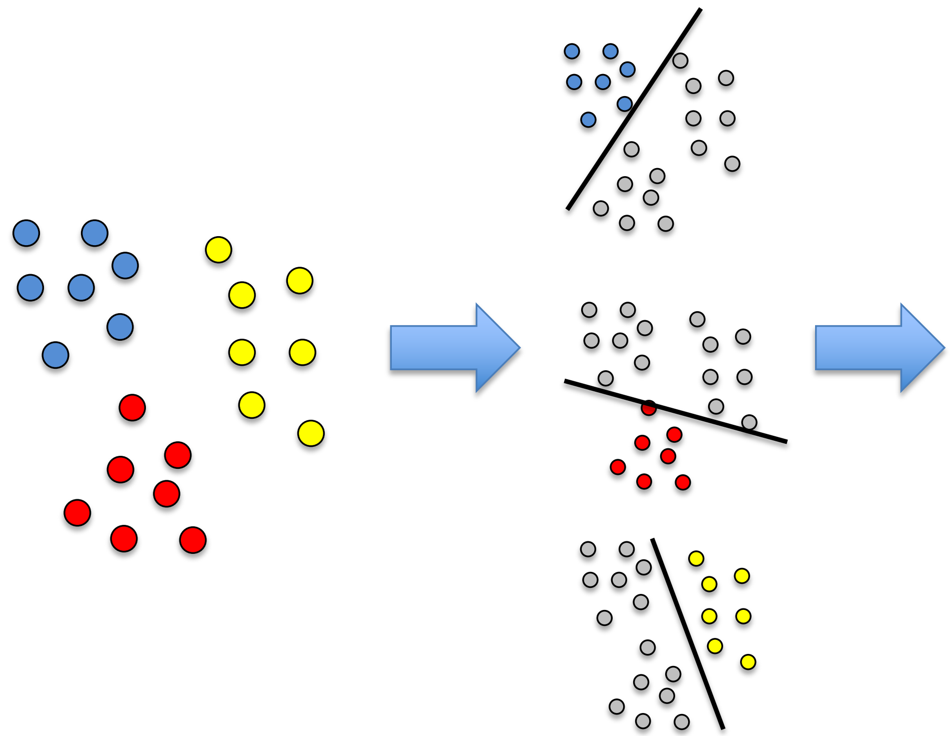
Practical guide:
http://www.csie.ntu.edu.tw/~cjlin/papers/guide/guide.pdf

Summary – Linear classifiers

- **Different loss functions give different algorithms**
- **Square error loss**
  - Sensitive to outliers and training data distribution when applied as in this lecture.
  - Improvements possible (lecture 3).
  - Local minima.
- **Support Vector Machines (maximum margin loss)**
  - By many considered as the state-of-the-art classifier.
  - Non-linear extension possible (lecture 9).
  - No local minima.
- **Linear Discriminant Analysis (Lecture 8)**
  - Simple to implement, very useful as a first classifier to try

What about more than 2 classes?

Combine several binary classifiers



Evaluate most likely class

What about more than 2 classes?

Multiple outputs each representing likelihood for a certain class