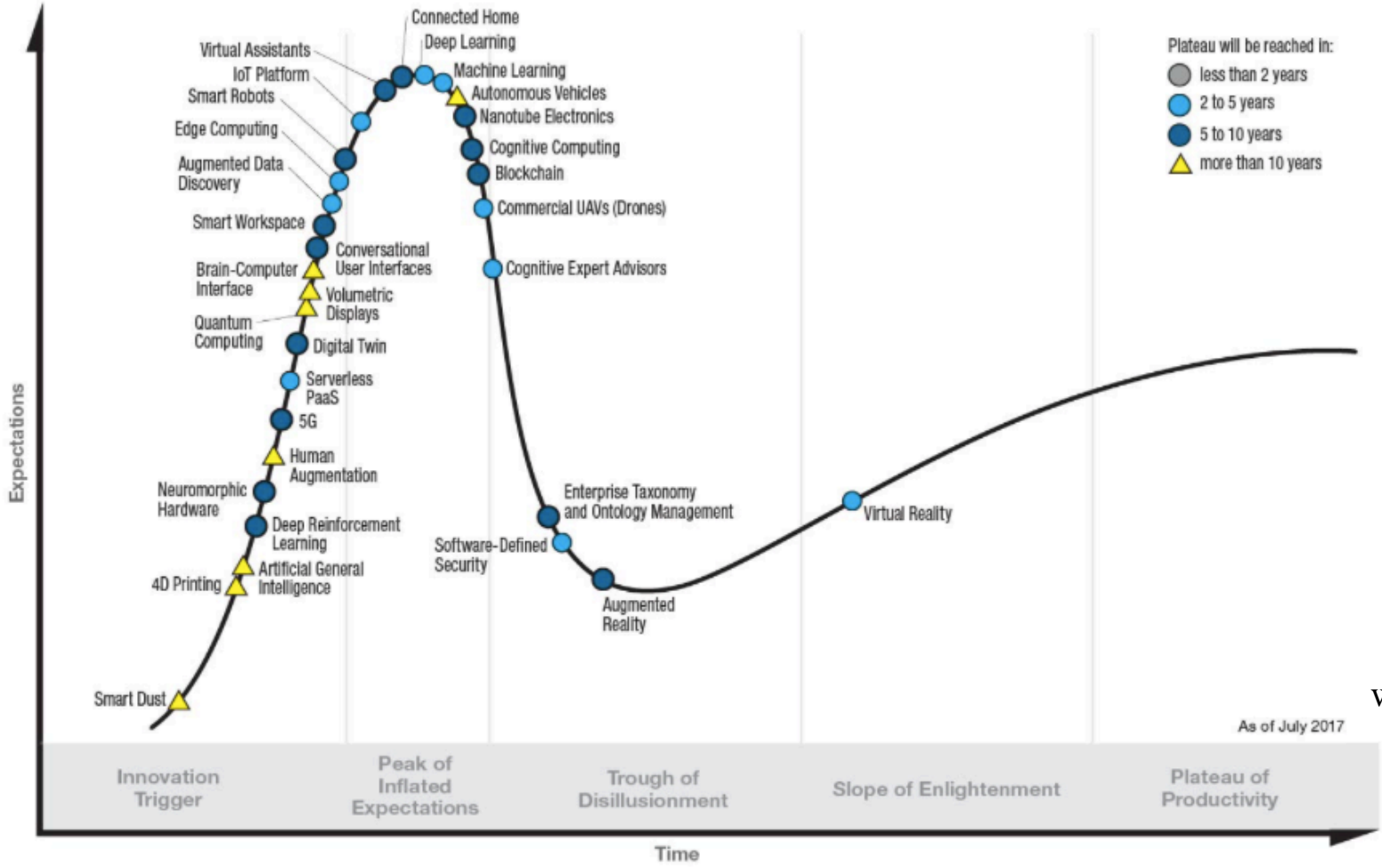
Neural Networks and Learning Systems
TBMI 26, 2018

# Lecture 2

# Supervised learning – Linear classification

*Magnus Borga*
*magnus.borga@liu.se*

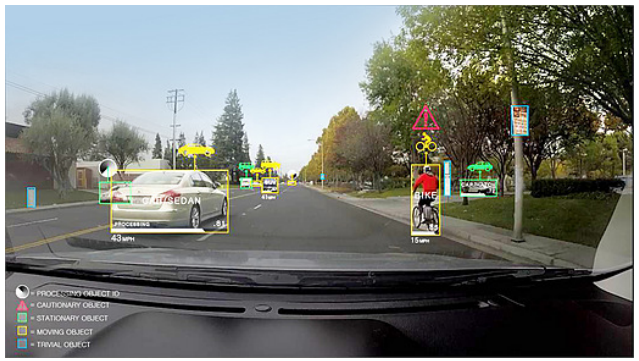
# Gartner Hype Cycle 2017




www.gartner.com

# What is the hype about?

## Autonomous driving



## Automatic image tagging

A person riding a motorcycle on a dirt road.

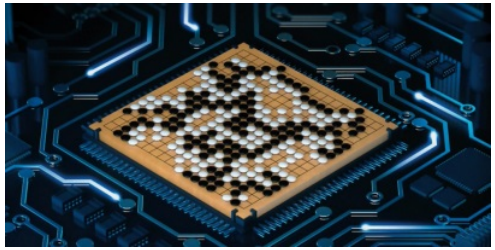
Two dogs play in the grass.

A group of young people playing a game of frisbee.

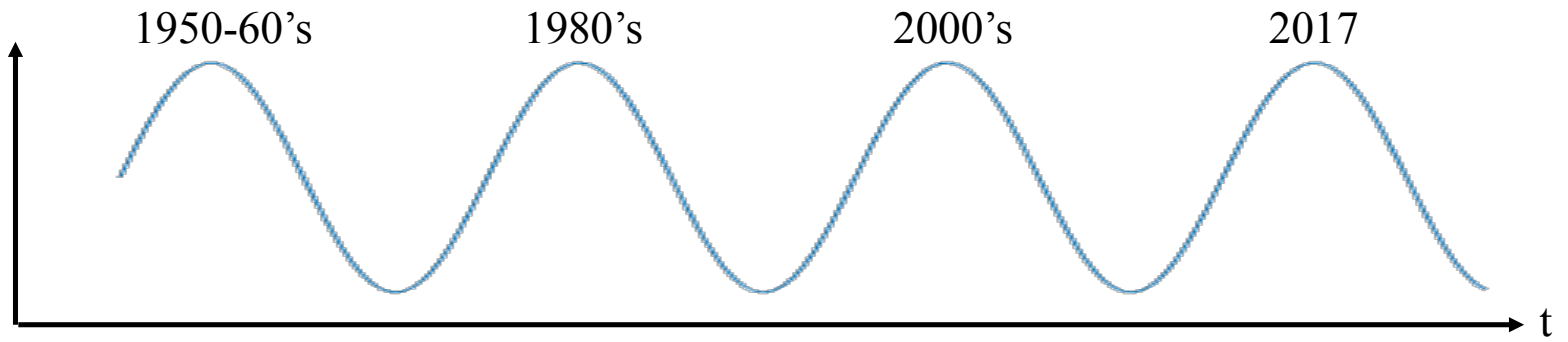
Two hockey players are fighting over the puck.

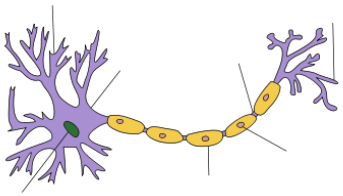
## Speech recognition

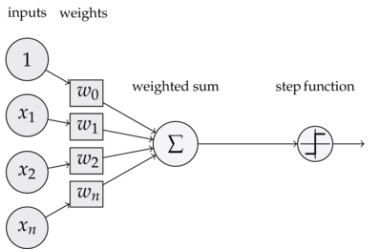
## AlphaGo

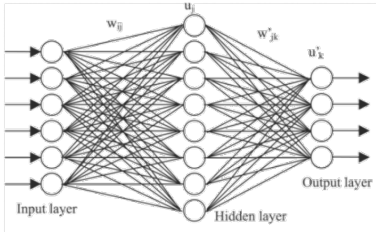


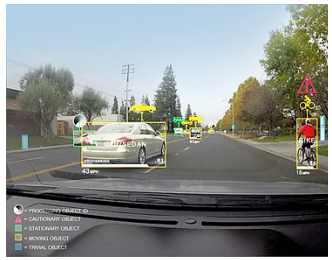
# A history of hypes

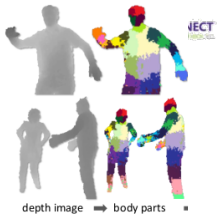




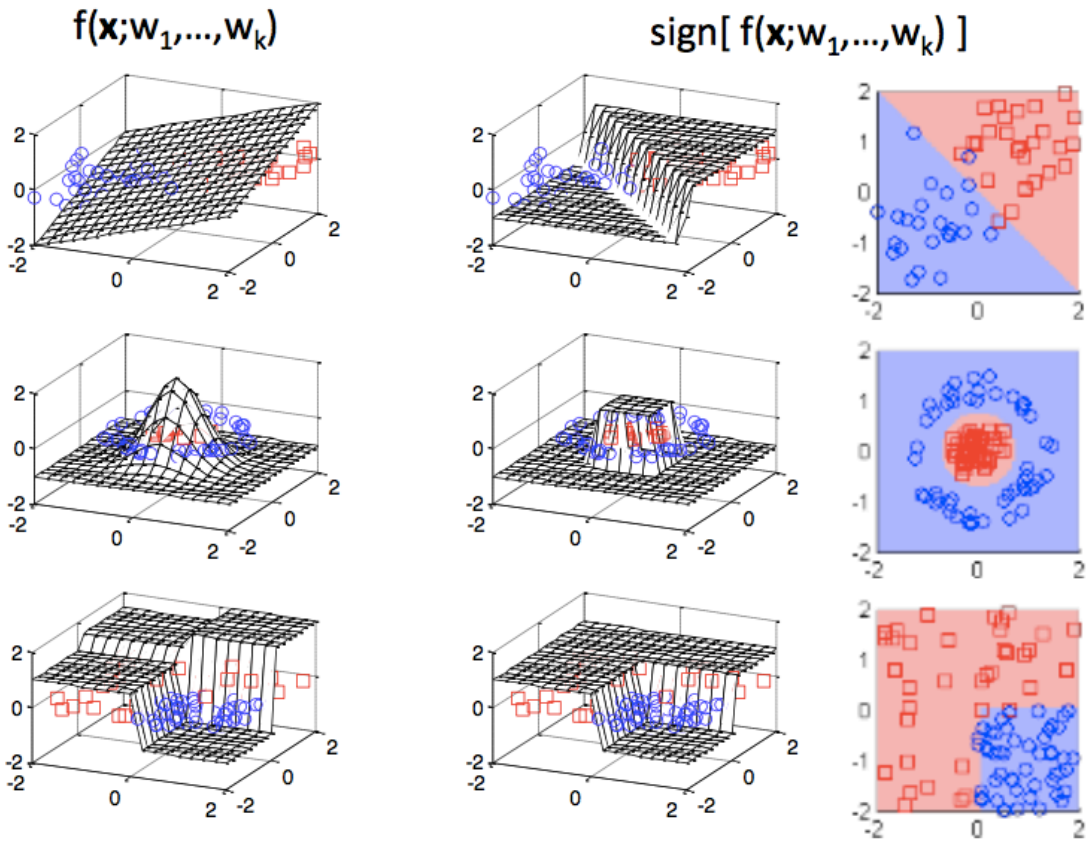



# Recap - Supervised learning

- **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 $\Omega$. Today we'll assume two classes: $\Omega = \{-1, 1\}$
- **Output:** A function $\text{sign}[f(\mathbf{x}; w_1, \ldots, w_k)] \rightarrow \Omega$

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

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



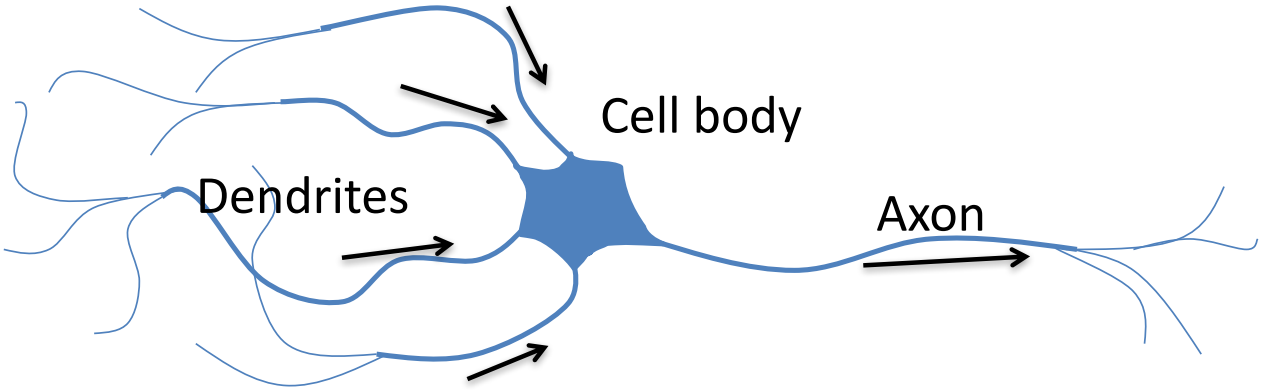
# Advantages of a parametric function $f(\mathbf{x};w_1,\ldots,w_k)$

- 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?

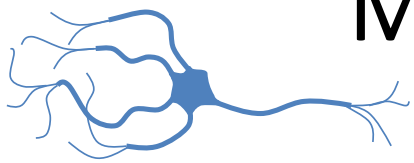
(on the low level!)

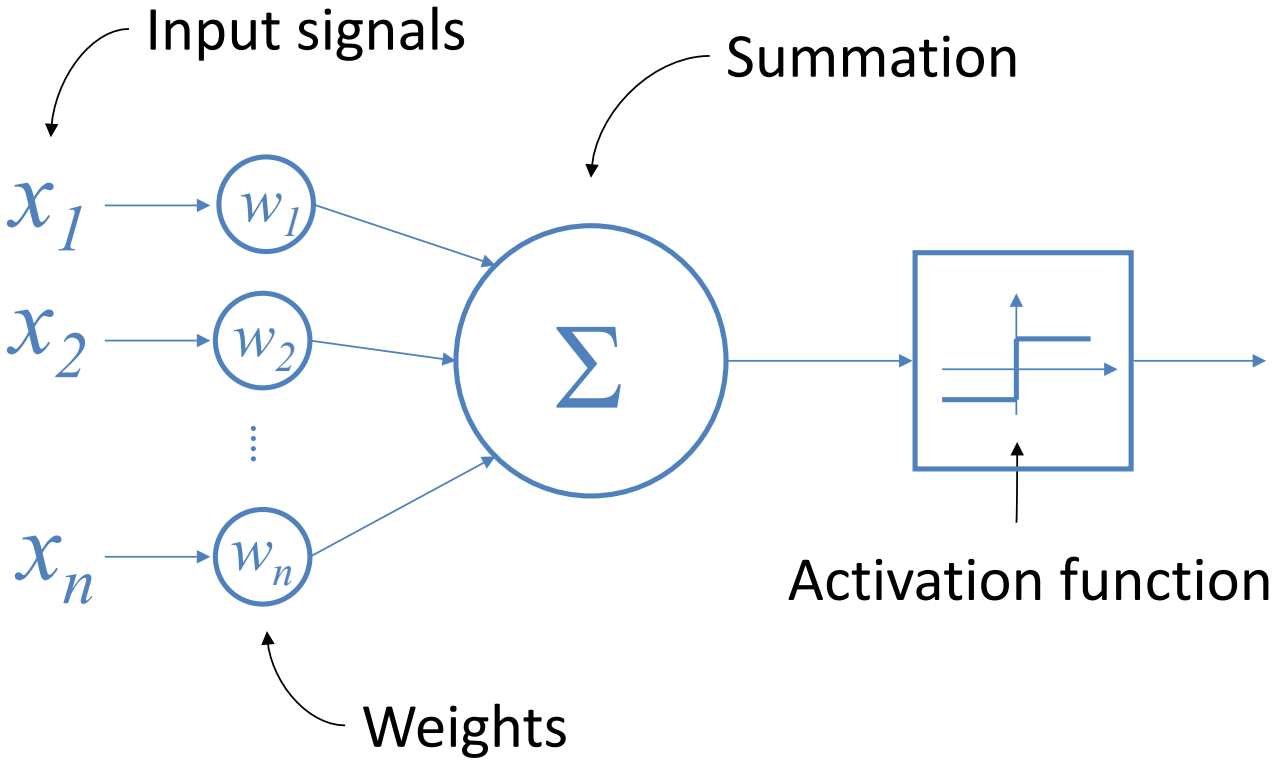
- Basic unit: the neuron




- 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

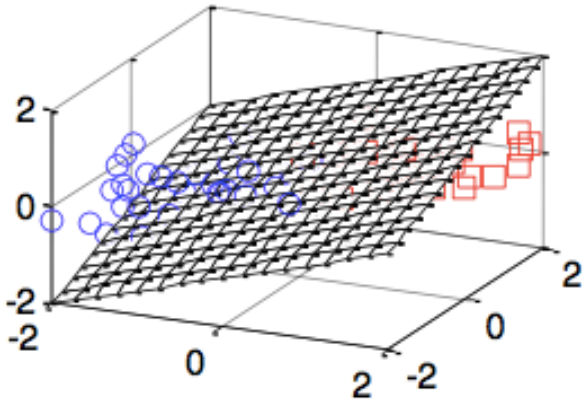


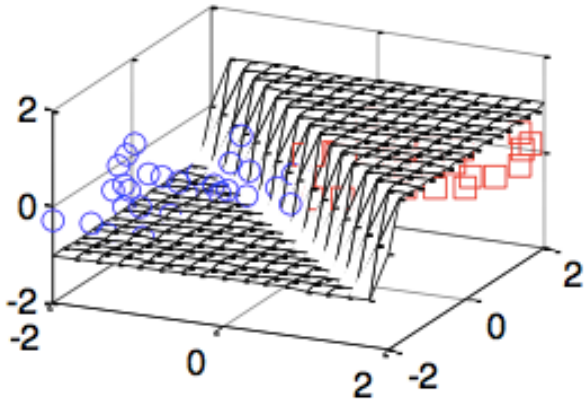


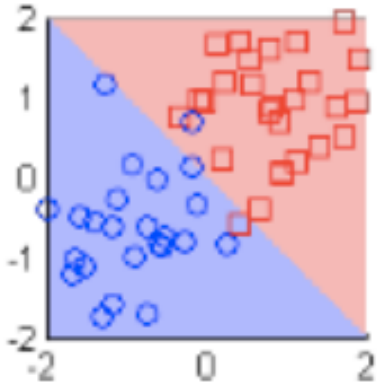
# The Perceptron

(McCulloch & Pitts 1943, Rosenblatt 1962)

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




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

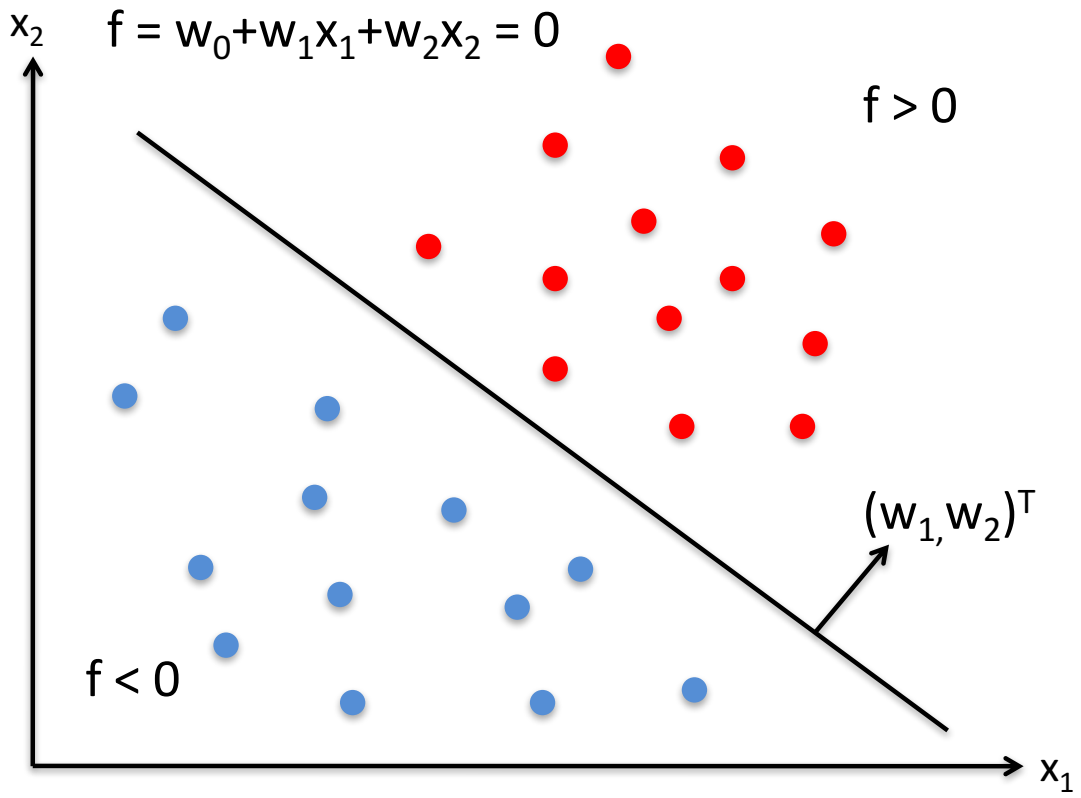
# Notational simplification: Bias weight

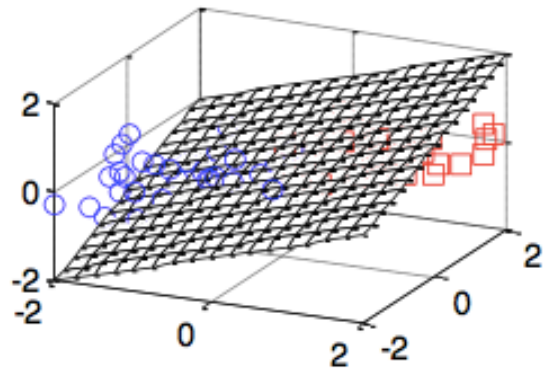
Add a constant 1 to the feature vector so that we don‘t have to treat $w_0$ separately.

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

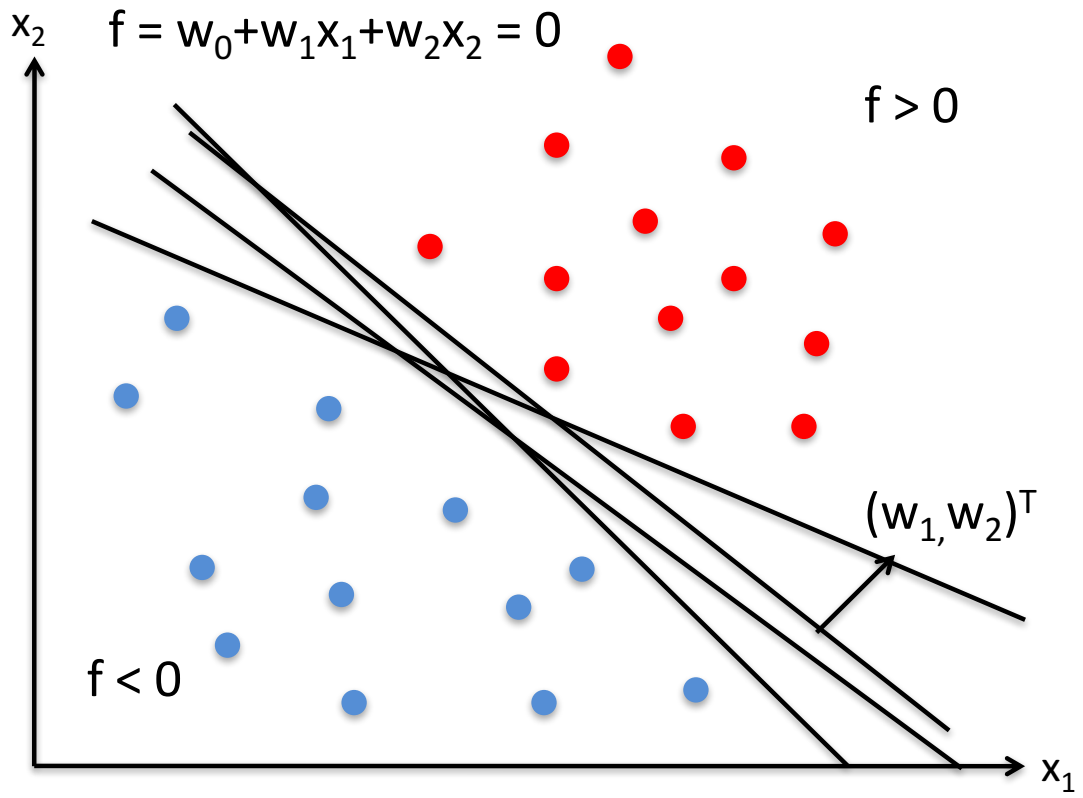
$$f(x_1,...,x_n; w_0,...,w_n) = \sigma\left(\sum_{i=0}^{n} w_i x_i\right) = \sigma\left(\mathbf{w}^T \mathbf{x}\right)$$

# Geometry of linear classifiers



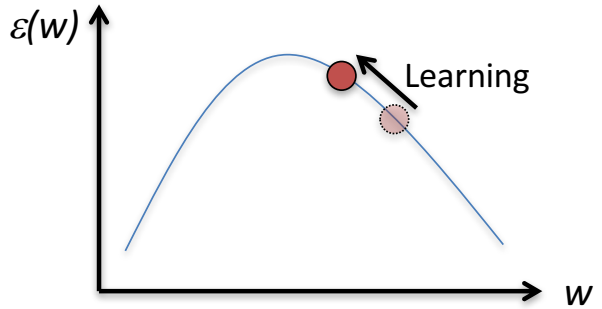



# Which linear classifier to choose?



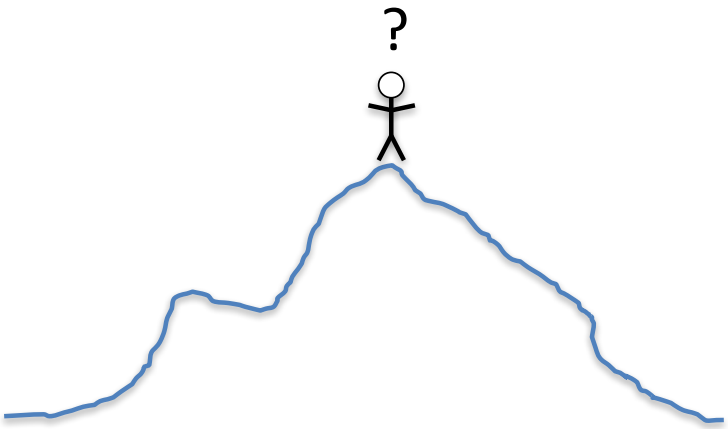
# Find the best separator – optimization!

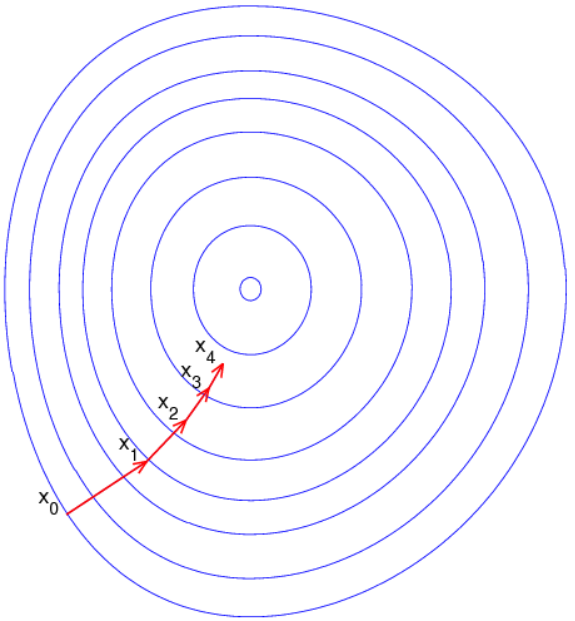
- Min/max of a cost function $\varepsilon(w_0, w_1, \ldots, w_n)$ with the weights $w_0, w_1, \ldots, w_n$ as parameters.




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

# Gradient descent/ascent



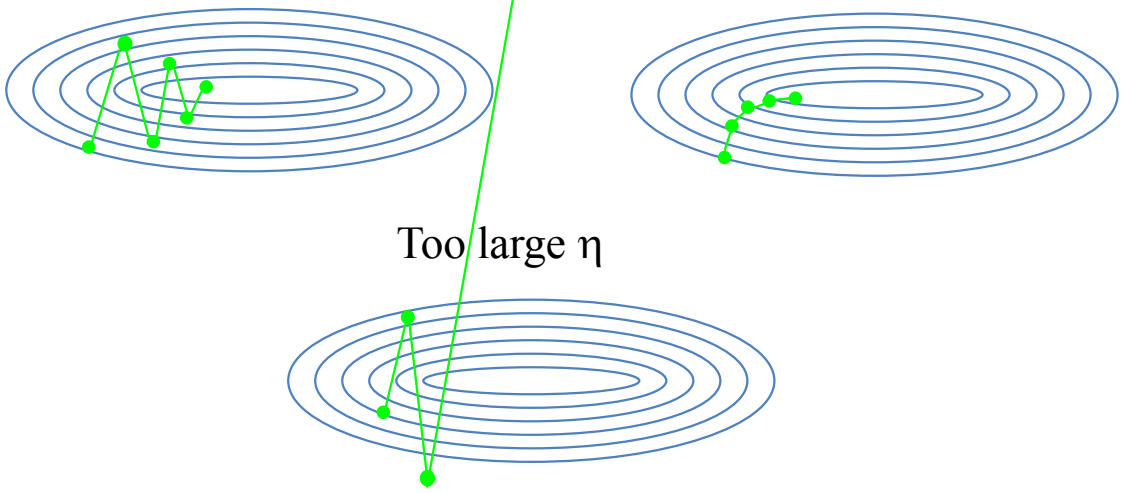

How to get to the lowest point?

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

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} \pm \eta \left. \frac{\partial \varepsilon}{\partial \mathbf{w}} \right|_{\mathbf{w}^{(t)}}$$

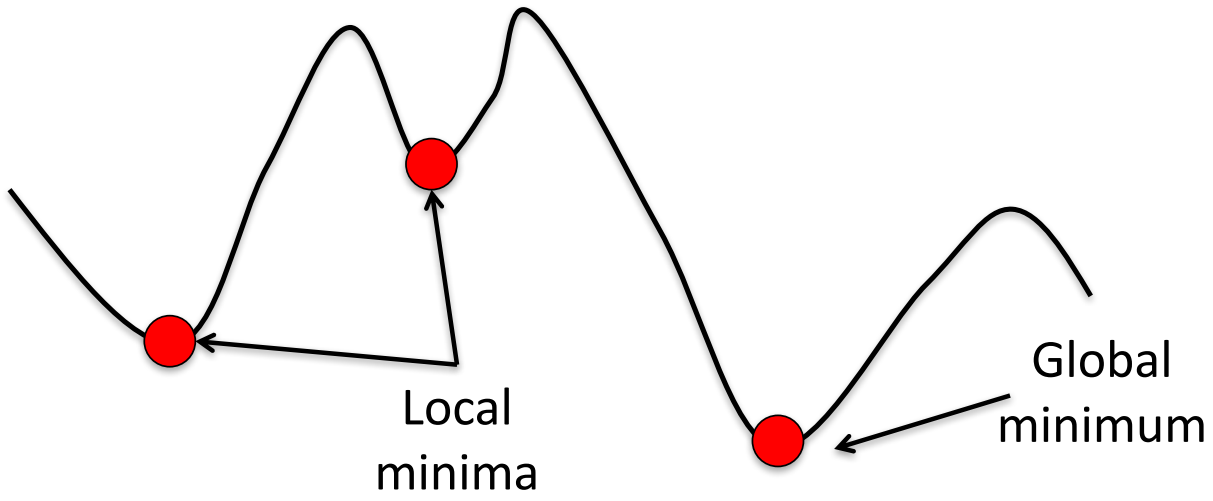
# Gradient escent

Choosing the step length



# Local optima

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

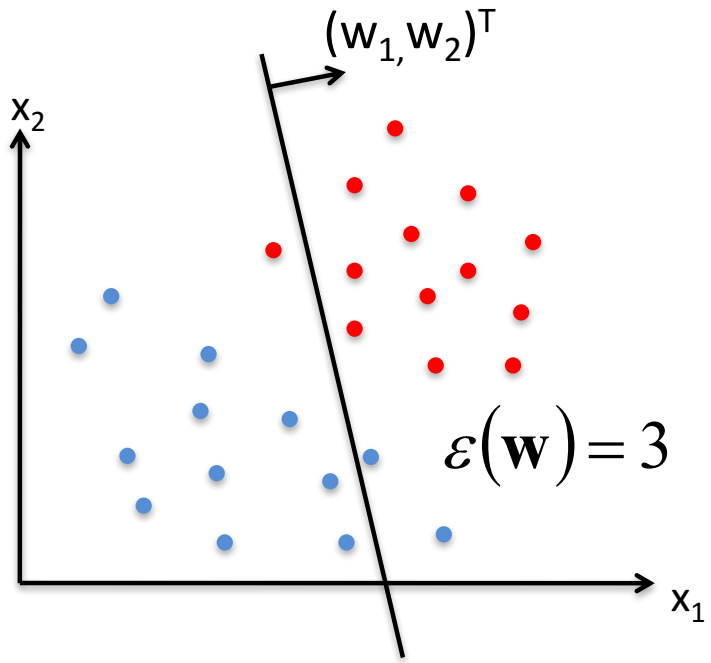


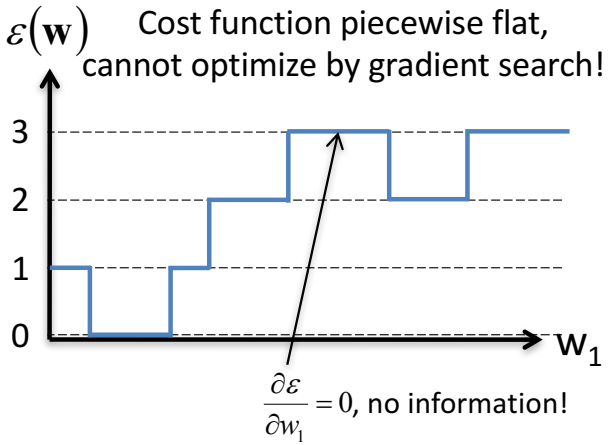
# 0-1 loss function / empirical risk

"empirical" because it is over the observed training data

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

0 or 1 function



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

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

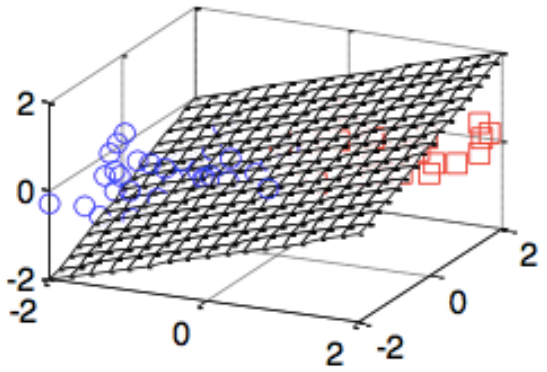
# Square error cost

*Minimize* the following cost 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:

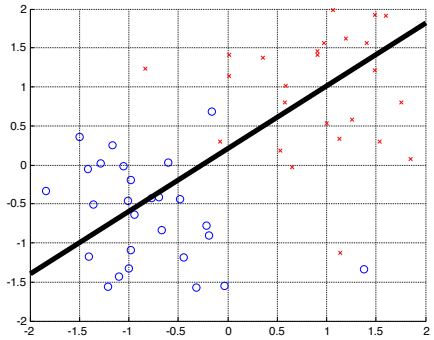
$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \frac{\partial \varepsilon}{\partial \mathbf{w}} = \mathbf{w}_t - \eta \sum_{i=1}^{N} \left(\mathbf{w}_t{}^T \mathbf{x}_i - y_i\right)\mathbf{x}_i \quad (\text{Eq.1})$$

**Algorithm:**

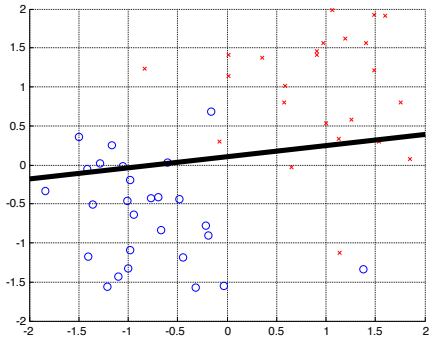
1. Start with a random **w**
2. Iterate Eq. 1 until convergence

# Example

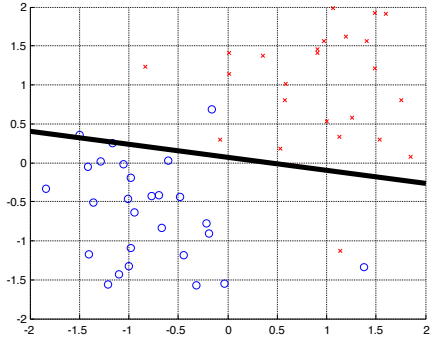
Random init



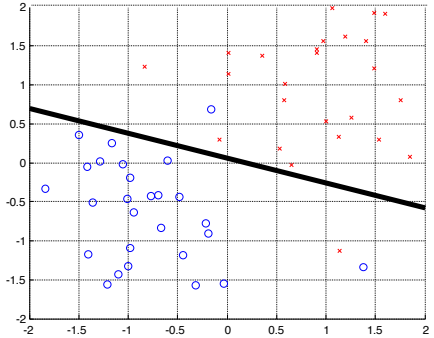

First iteration




Second iteration

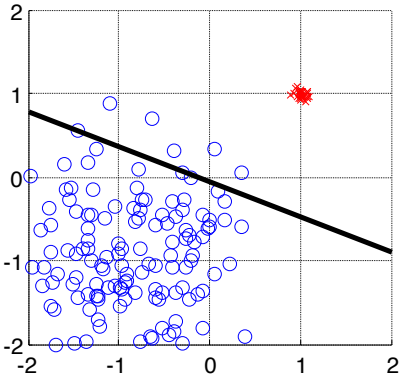



Third iteration

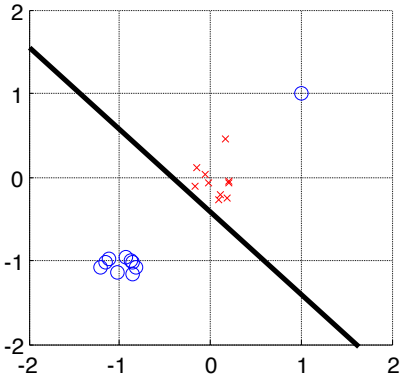


# More examples

Unevenly distributed training data

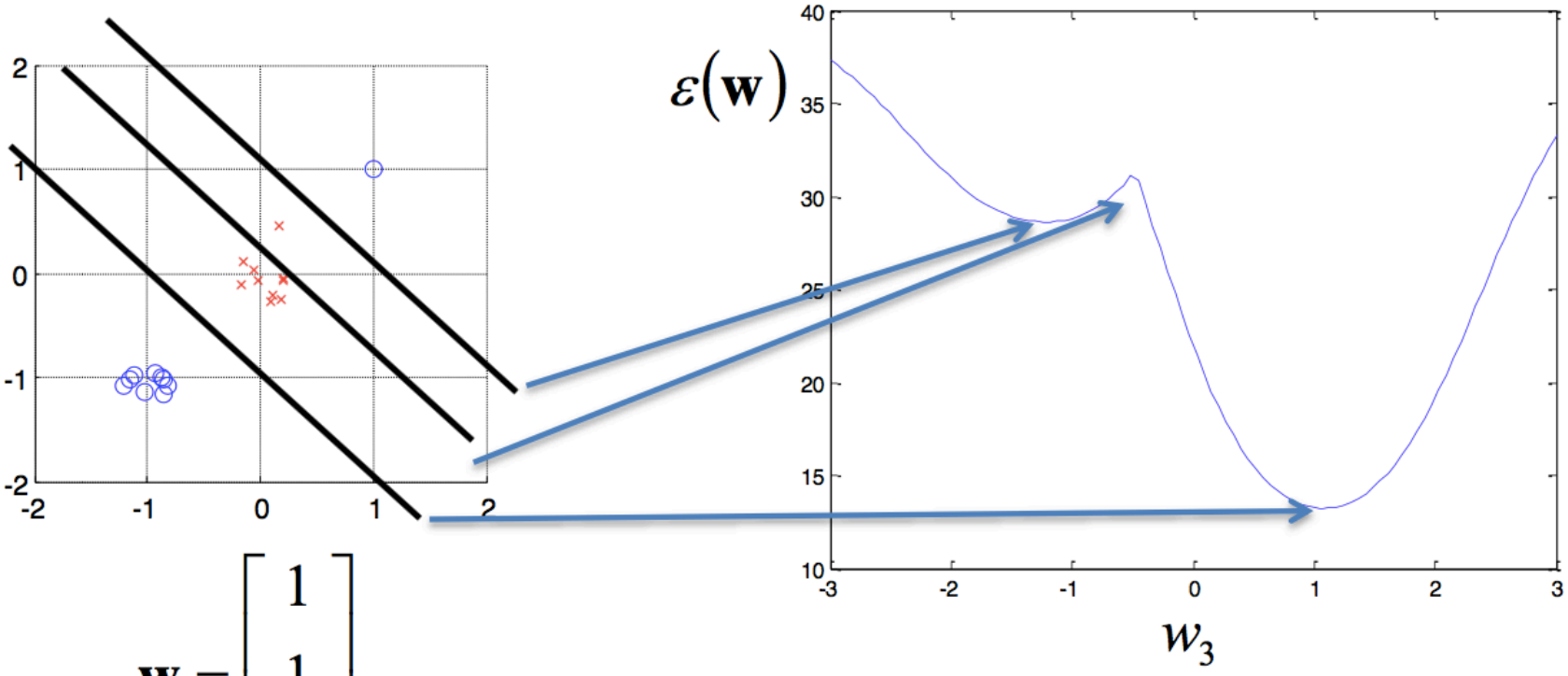



Outlier




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

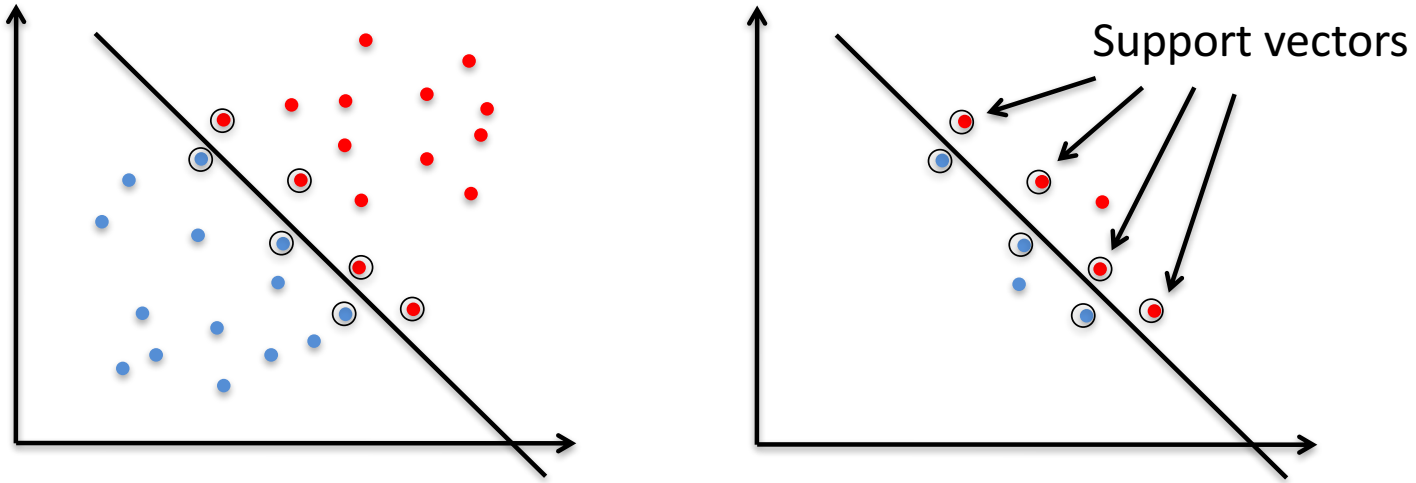
# Example of local minimum




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

# Support Vector Machines (SVM)

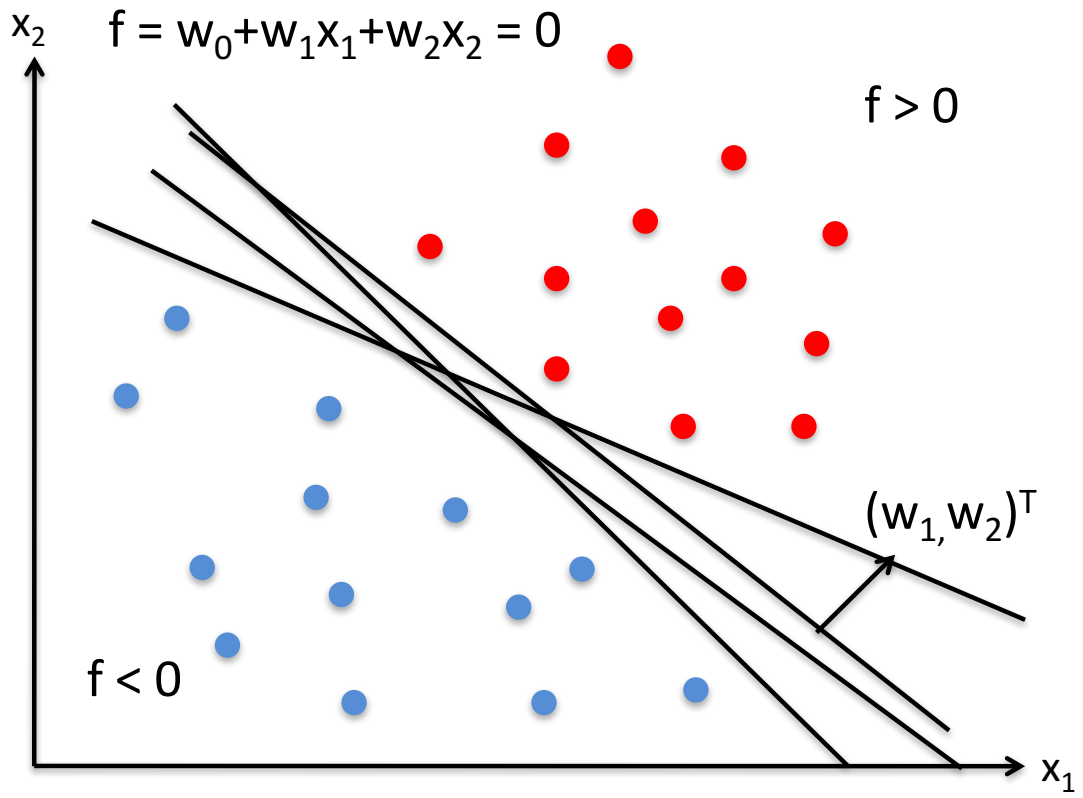
Idea!



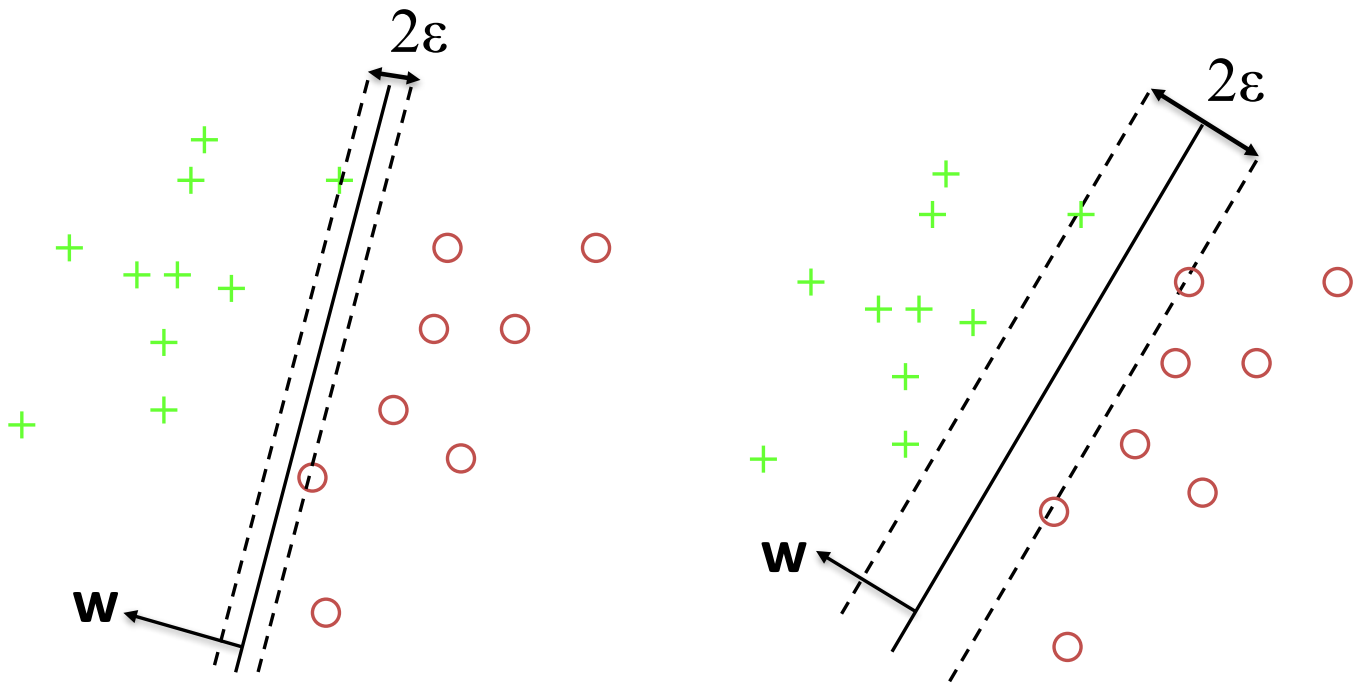

Optimal separation line remains the same, feature points close to the class limits are more important!

These are called *support vectors*!

# Which linear classifier to choose?



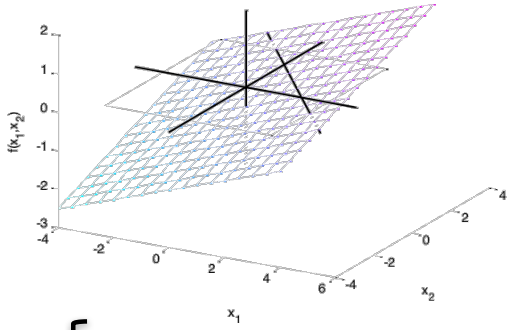
# SVM – Maximum margin




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

# SVM – Cost function

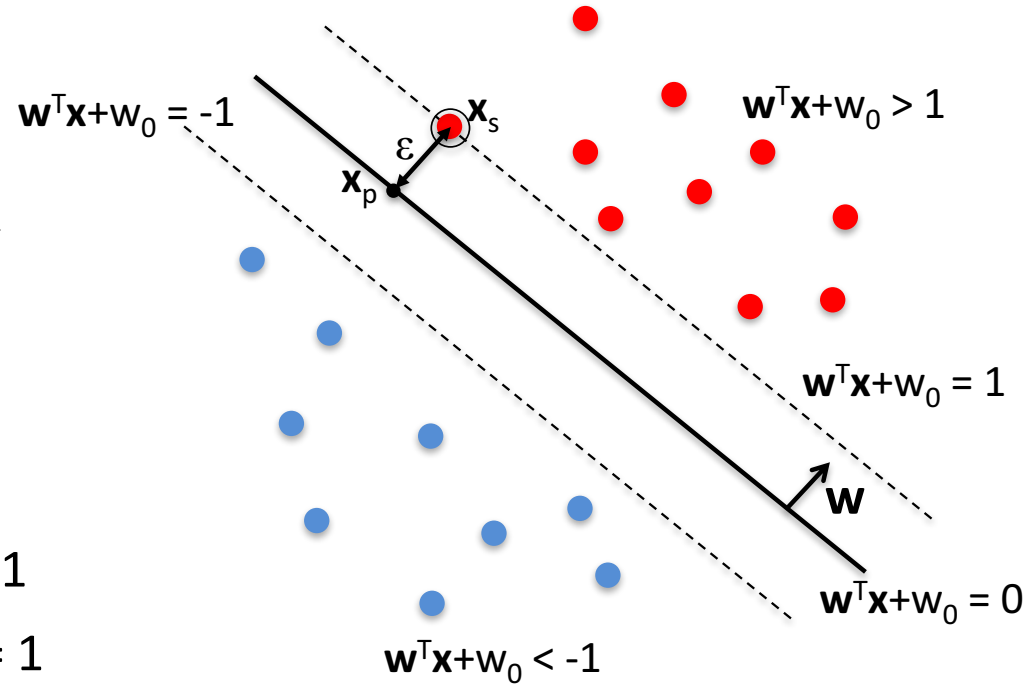
Scaling of **w** is free – Pick arbitrary sample $\mathbf{x}_s$ as support vector and choose scaling so that $\mathbf{w}^T\mathbf{x}_s + w_0 = 1$!



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

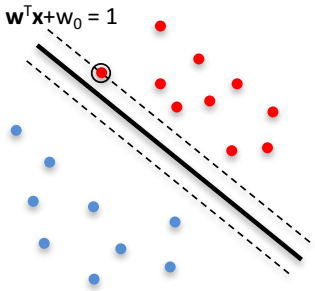
$$\mathbf{w}^T(\mathbf{x}_p + \varepsilon\hat{\mathbf{w}}) + w_0 = 1$$

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

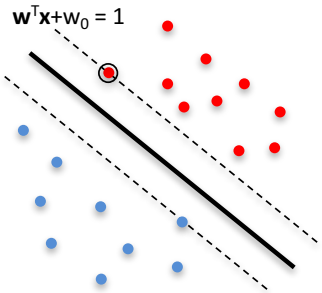



For the chosen support vector, $\varepsilon(\mathbf{w}) = 1 / \|\mathbf{w}\|$

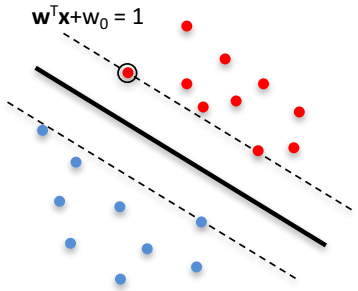
# SVM cost function examples




**Example 1:**
Boundary not in middle →
Large ||w|| (steep function) →
Low 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 – Cost function, cont.

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

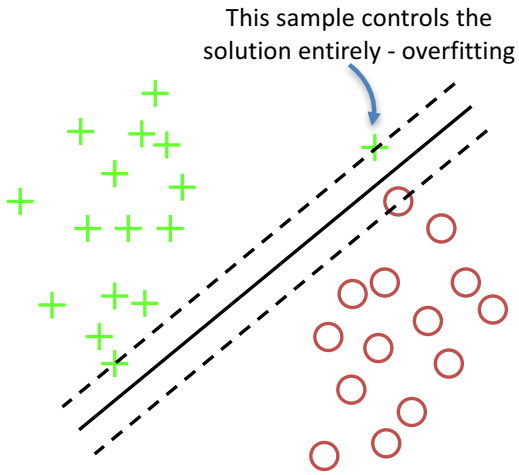
$$\min \|\mathbf{w}\|^2$$

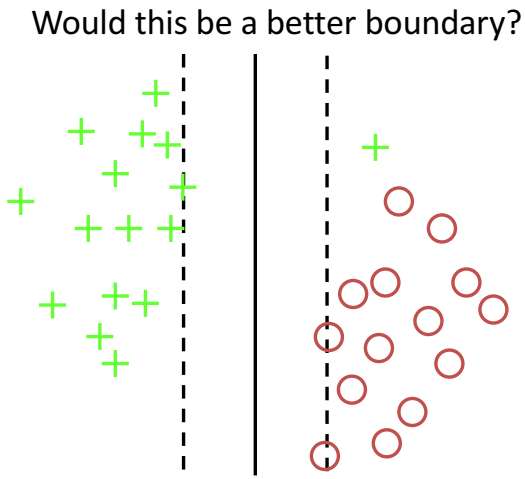
$$\text{subject to } y_i(\mathbf{w}^T \mathbf{x}_i + w_0) \geq 1$$

No training samples must reside in the margin region!

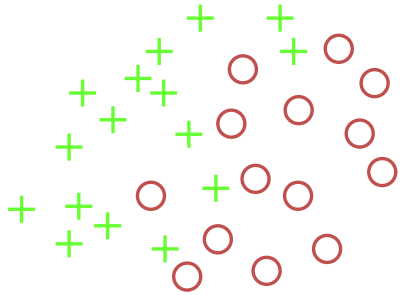
Optimization procedure outside the scope of this course…

# SVM – Soft margin




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



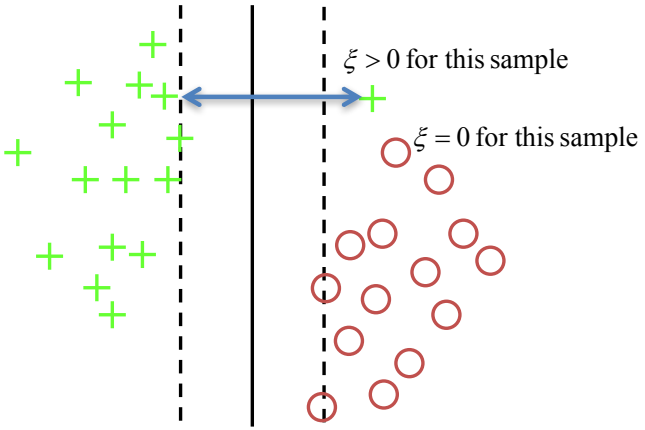
# SVM – Soft margin, cont.

user-defined trade-off parameter

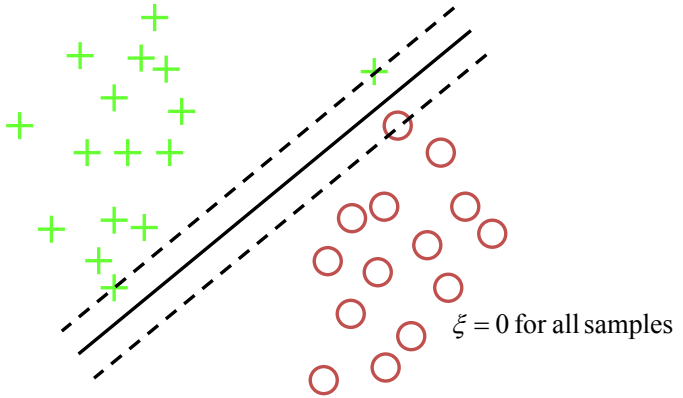
$$\min \|\mathbf{w}\|^2 + C\sum \xi_i$$

slack variable

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




Solution for small *C*

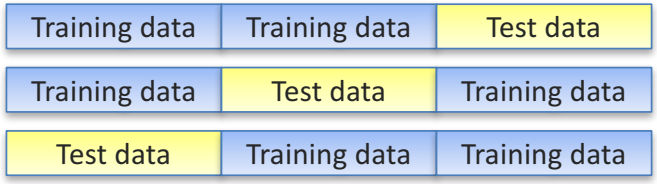



Solution for large *C*

# SVM – Choosing *C*

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

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



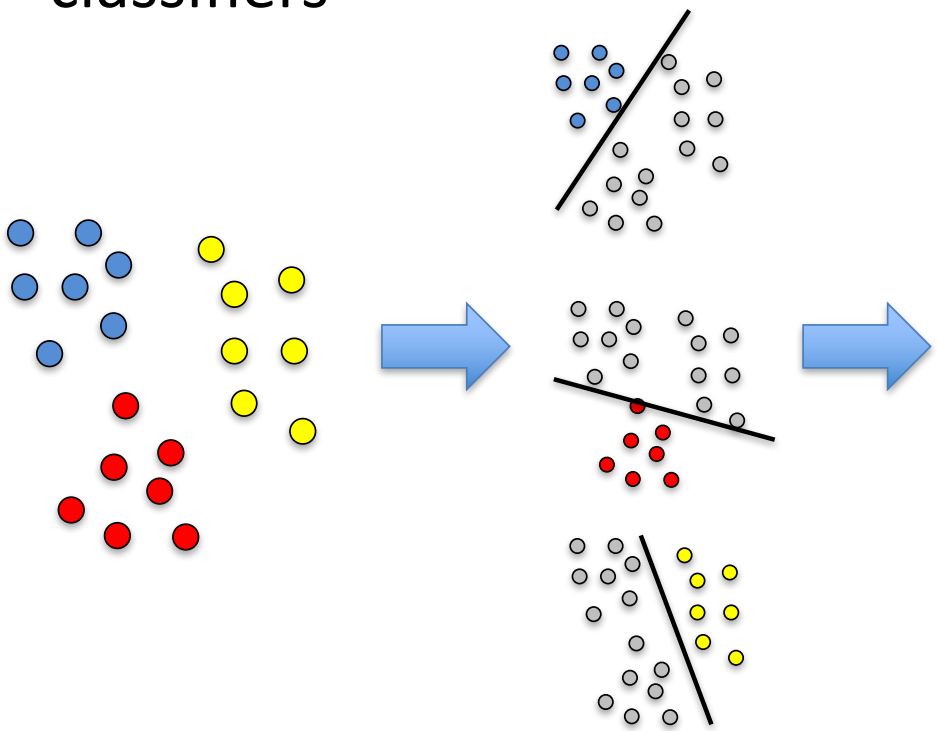

Practical guide:
http://www.csie.ntu.edu.tw/~cjlin/papers/guide/guide.pdf

# Summary – Linear classifiers

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

# What about more than 2 classes?

- Common solution: Combine several binary classifiers



Evaluate most likely class