Neural Networks and Learning Systems
TBMI 26, 2017

Lecture 2

Supervised learning – Linear classification

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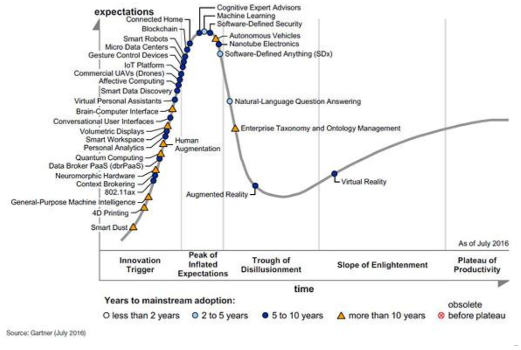
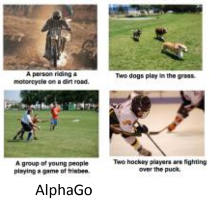
Gartner Hype Cycle 2016



What is the hype about?

Autonomous driving

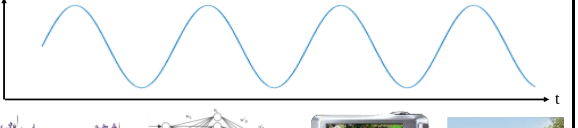
Automatic image tagging

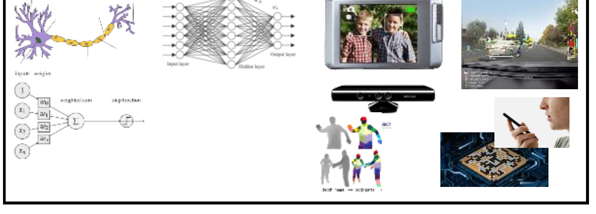


Speech recognition

AlphaGo

A history of hypes





Recap - Supervised learning

- **Task:** Learn to predict/classify new data from labeled 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. <u>Today we'll assume two classes: $\Omega = \{-1,1\}$</u>
- **Output:** A function sign[f($\mathbf{x}$;w_1,…,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!

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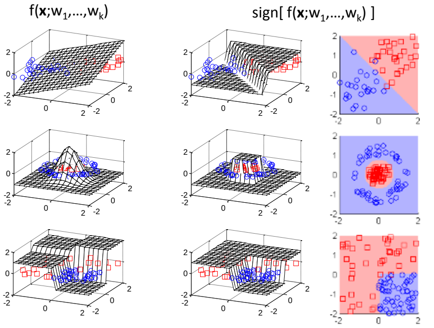
The function f($\mathbf{x}$;w_1,…,w_k)



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Advantages of a parametric function f($\mathbf{x}$;w_1,…,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.

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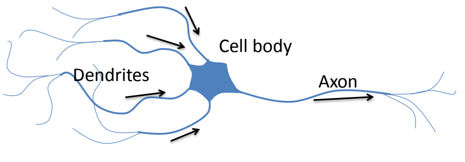
How does the brain take decisions?

(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).

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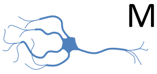
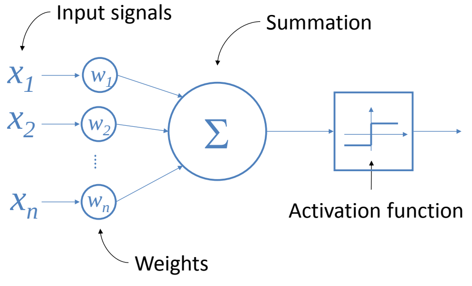
Model of a neuron





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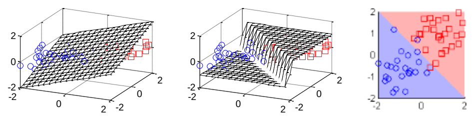
The Perceptron

(McCulloch & Pitts 1943, Rosenblatt 1962)

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



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

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

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

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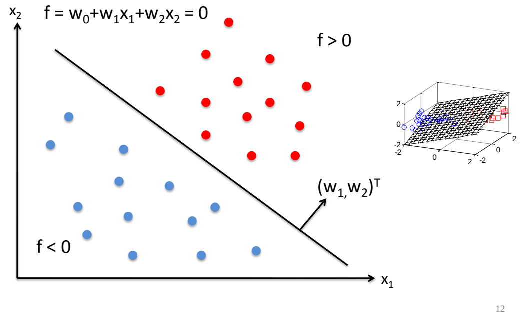
Geometry of linear classifiers



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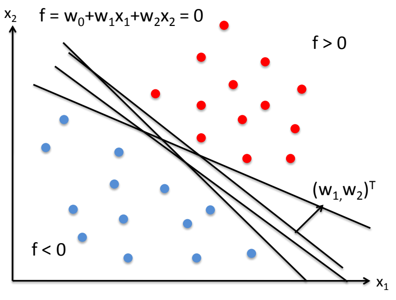
Which linear classifier to choose?



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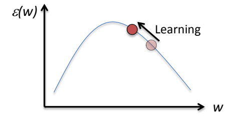
Find the best separator – optimization!

- 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 ε is reached.
  – Brute force: Try many values systematically and choose the best.

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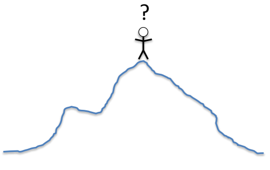
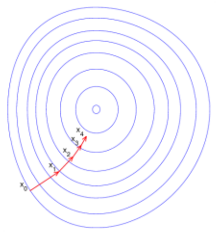
Gradient descent/ascent



How to get to the lowest point?



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

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

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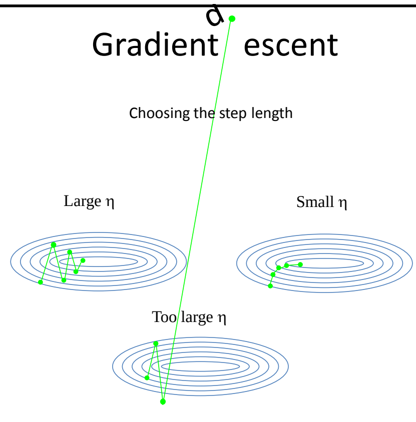
Gradient descent

Choosing the step length



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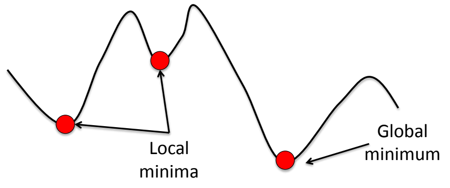
Local optima

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

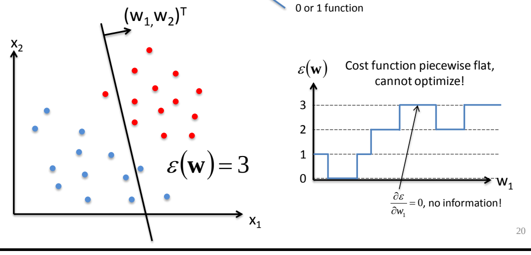


0-1 loss function / empirical risk

„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 $\varepsilon(\mathbf{w})$

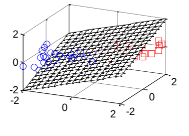
- 0-1 loss function / empirical risk
- Square error → Neural networks
- Maximum margin → Support Vector Machines

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

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

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

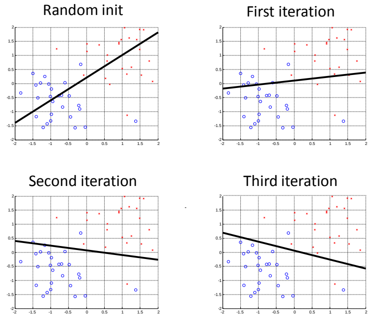
Gradient descent:

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

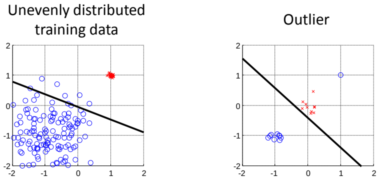
Algorithm:

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

Example

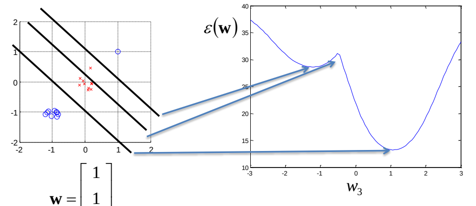


More examples



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

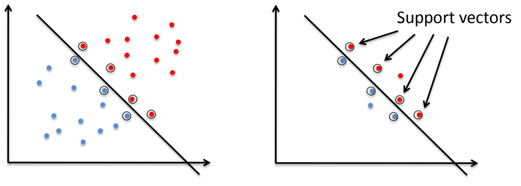
Example of local minima



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

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*!

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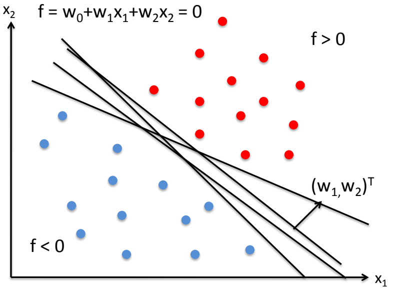
Which linear classifier to choose?



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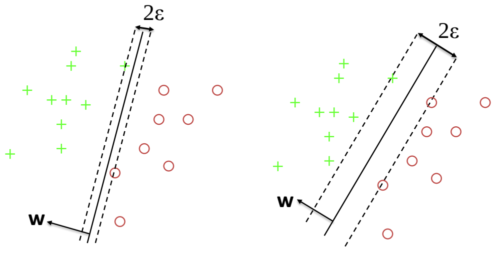
SVM – Maximum margin



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

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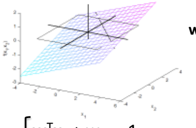
SVM – Cost function

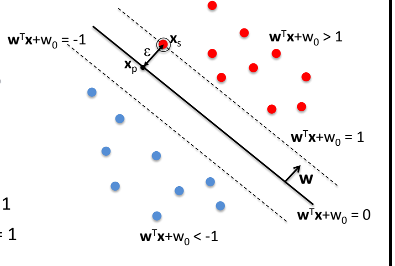
Scaling of **w** is free – Pick arbitrary sample $\mathbf{x}_s$ as support vector and choose scaling so that $\mathbf{w}^T\mathbf{x}_s+w_0 = 1$!



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

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

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



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

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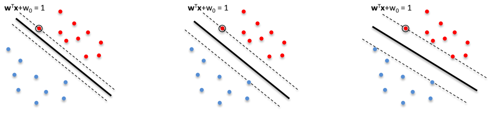
SVM cost function examples



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!

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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…

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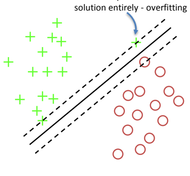
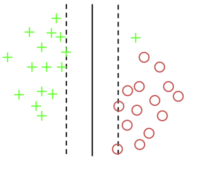
SVM – Soft margin

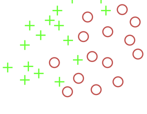
This sample controls the solution entirely - overfitting



Would this be a better boundary?



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



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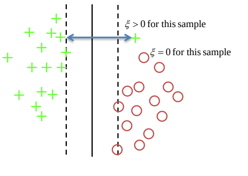
SVM – Soft margin, cont.

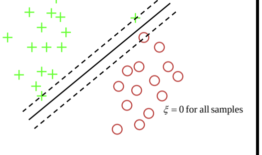
user-defined trade-off parameter

$$\min \|\mathbf{w}\|^2 + C\sum \xi_i$$
$$\text{subject to } y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq 1 - \xi_i$$

slack variable



Solution for small *C*



Solution for large *C*

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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	Test data
Training data	Test data	Training data
Test data	Training data	Training data

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

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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 7).
  - Many software packages exist on the internet.
  - No local minima.
- **Fisher Linear Discriminant (Lecture 6)**
  - Simple to implement, very useful as a first classifier to try

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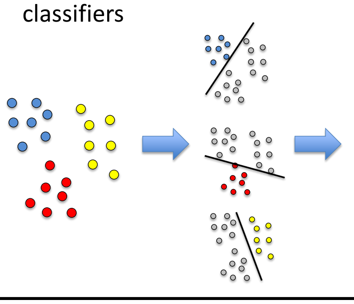
What about more than 2 classes?

- Common solution: Combine several binary classifiers



Evaluate most likely class

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