Cooperating Intelligent Systems

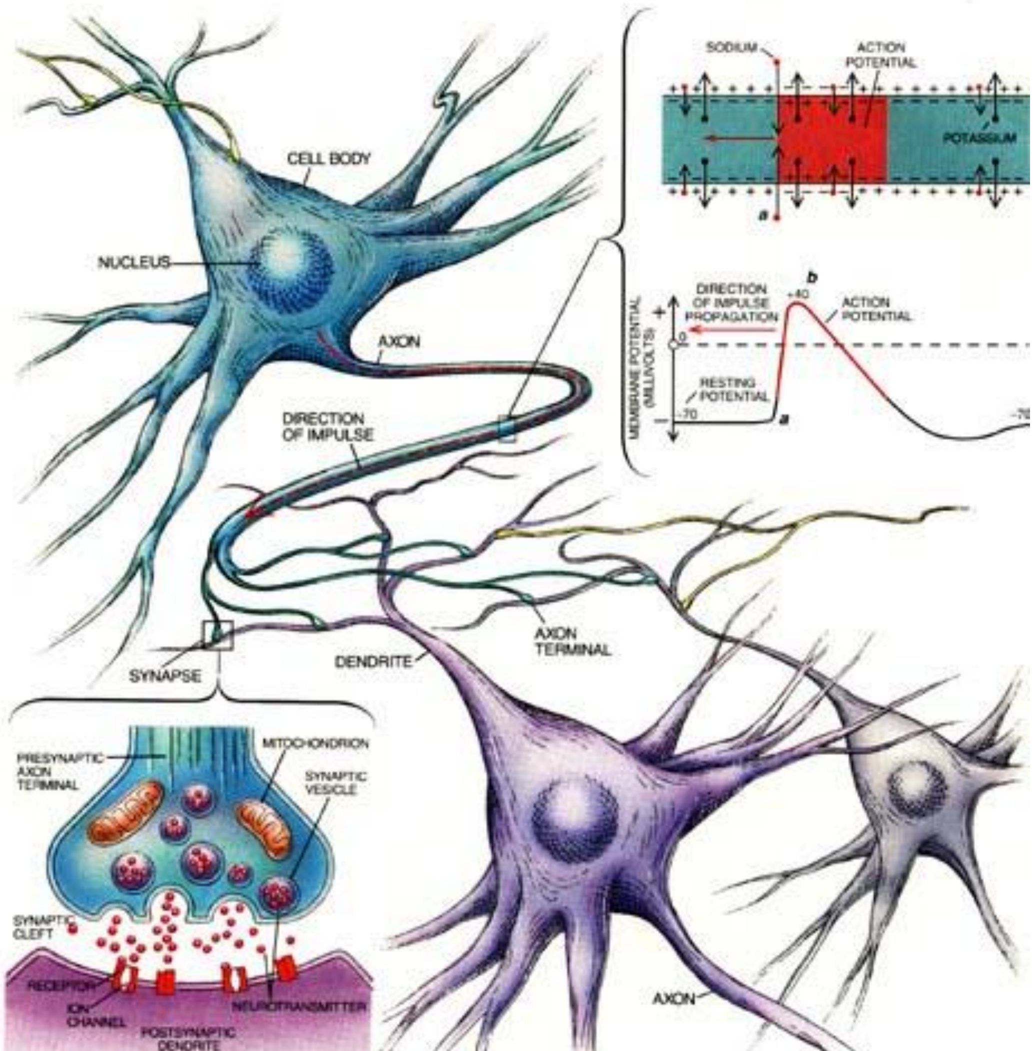
Statistical learning methods

Chapter 20, AIMA 2nd ed.

Chapter 18, AIMA 3rd ed.

(only ANNs & SVMs)

Artificial neural networks



The brain is a pretty intelligent system.

Can we ”copy” it?

There are approx. 10^{11} neurons in the human brain. Elephant brains have twice as many.

The simple model

- The McCulloch-Pitts model (1943)

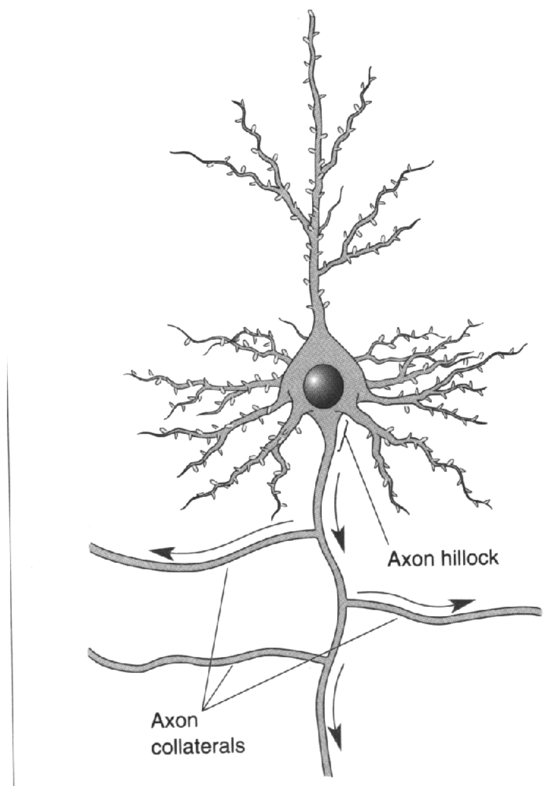
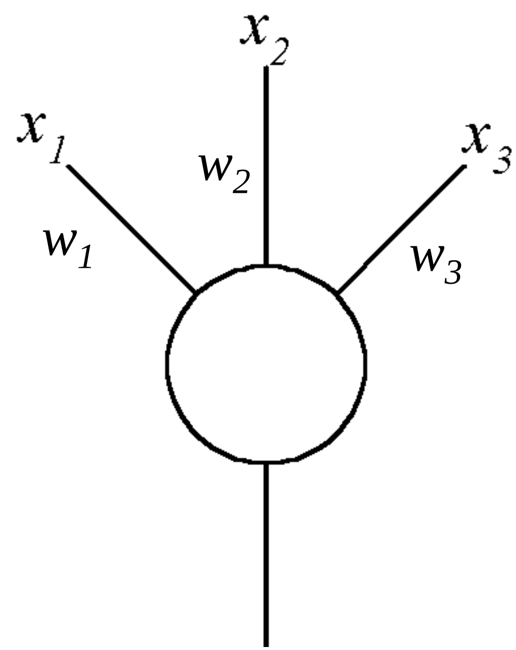
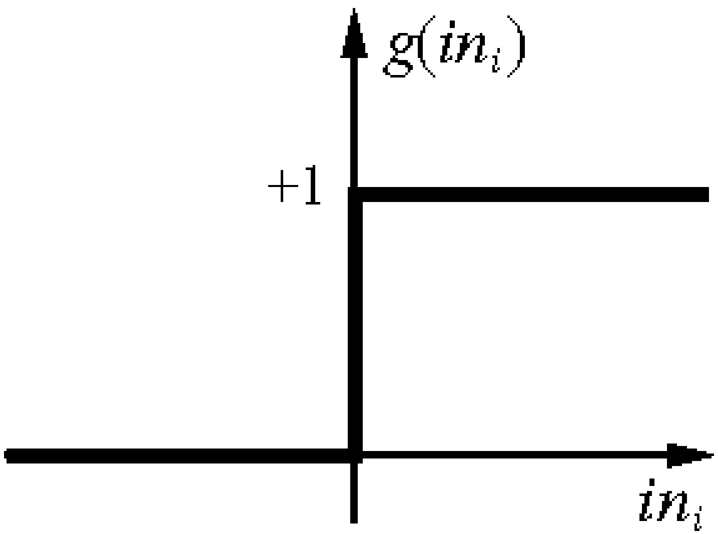


Image from
Neuroscience: Exploring the brain
by Bear, Connors, and Paradiso



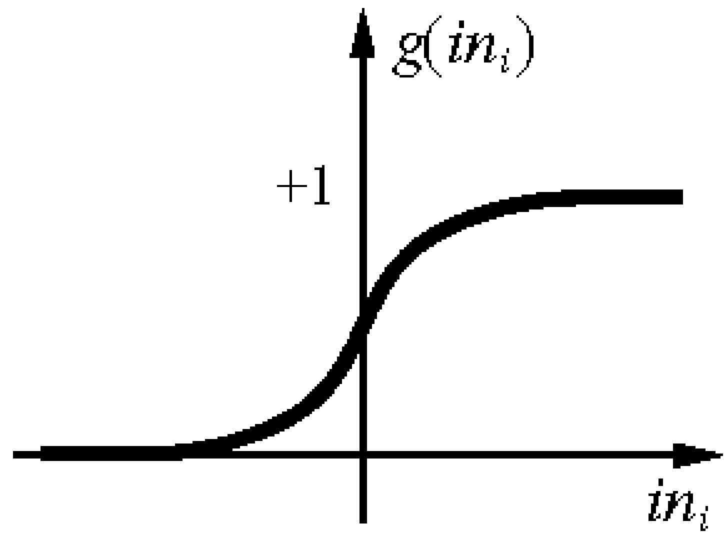
$$y = g(w_0 + w_1 x_1 + w_2 x_2 + w_3 x_3)$$

Transfer functions *g(z)*



(a)

The Heaviside function



(b)

The logistic function

The simple perceptron

With {-1,+1} representation

$$y(\mathbf{x}) = \mathrm{sgn}[\mathbf{w}^T\mathbf{x}] = \begin{cases} +1 & \text{if } \mathbf{w}^T\mathbf{x} > 0 \\ -1 & \text{if } \mathbf{w}^T\mathbf{x} < 0 \end{cases}$$

Traditionally (early 60:s) trained with *Perceptron learning.*

$$\mathbf{w}^T\mathbf{x} = w_0 + w_1 x_1 + w_2 x_2 + \cdots$$

Perceptron learning

Desired output $$f(n) = \begin{cases} +1 & \text{if } \mathbf{x}(n) \text{ belongs to class } A \\ -1 & \text{if } \mathbf{x}(n) \text{ belongs to class } B \end{cases}$$

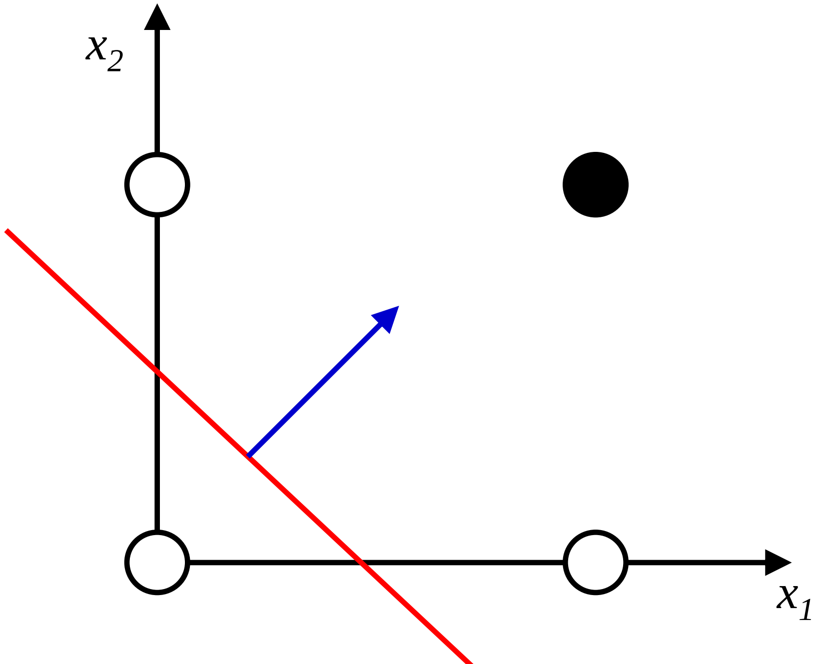
Repeat until no errors are made anymore

1. Pick a random example $[\mathbf{x}(n), f(n)]$
2. If the classification is correct,
   i.e. if $y(\mathbf{x}(n)) = f(n)$, then do nothing
3. If the classification is wrong, then do the following update to the parameters
   (η, the learning rate, is a small positive number)

$$w_i = w_i + \eta f(n) x_i(n)$$

Example: Perceptron learning

x_1	x_2	f
0	0	-1
0	1	-1
1	0	-1
1	1	+1



The AND function

Initial values:

$\eta = 0.3$

$$\mathbf{w} = \begin{pmatrix} -0.5 \\ 1 \\ 1 \end{pmatrix}$$

Example: Perceptron learning

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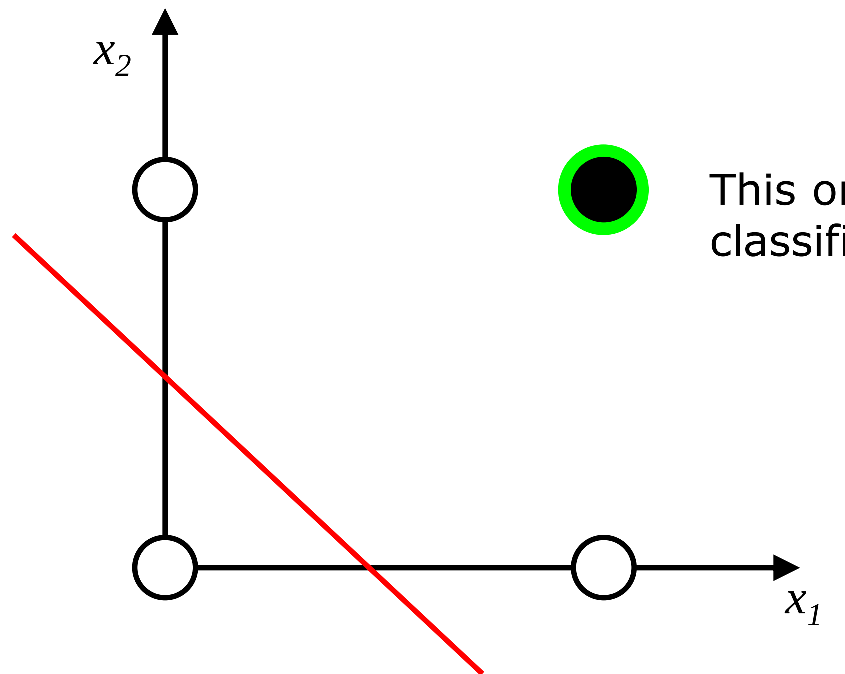

This one is correctly classified, no action.

The AND function

$$\mathbf{w} = \begin{pmatrix} -0.5 \\ 1 \\ 1 \end{pmatrix}$$

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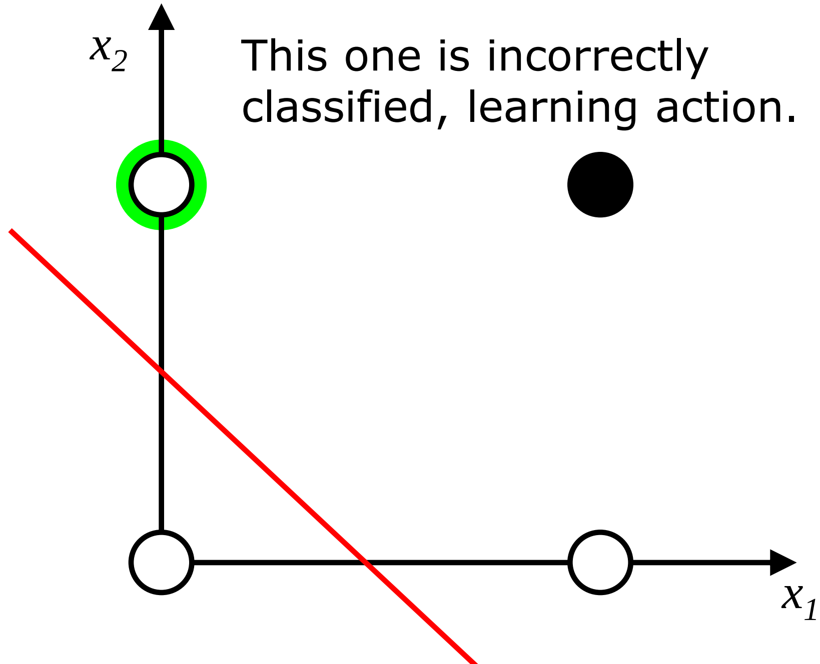

This one is incorrectly classified, learning action.

The AND function

$$\mathbf{w} = \begin{pmatrix} -0.5 \\ 1 \\ 1 \end{pmatrix}$$

$$w_0 = w_0 - \eta \cdot 1 = -0.8$$
$$w_1 = w_1 - \eta \cdot 0 = +1$$
$$w_2 = w_2 - \eta \cdot 1 = 0.7$$

Example: Perceptron learning

x_1	x_2	f
0	0	-1
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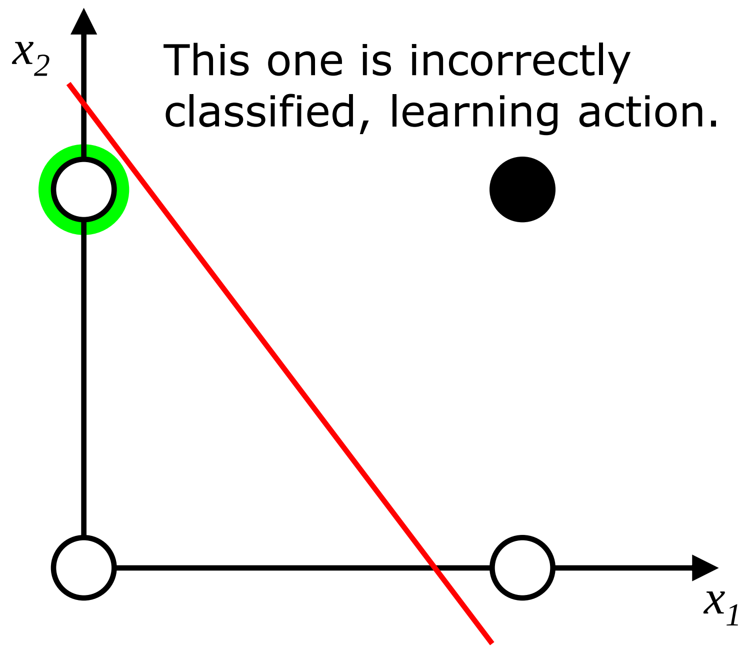

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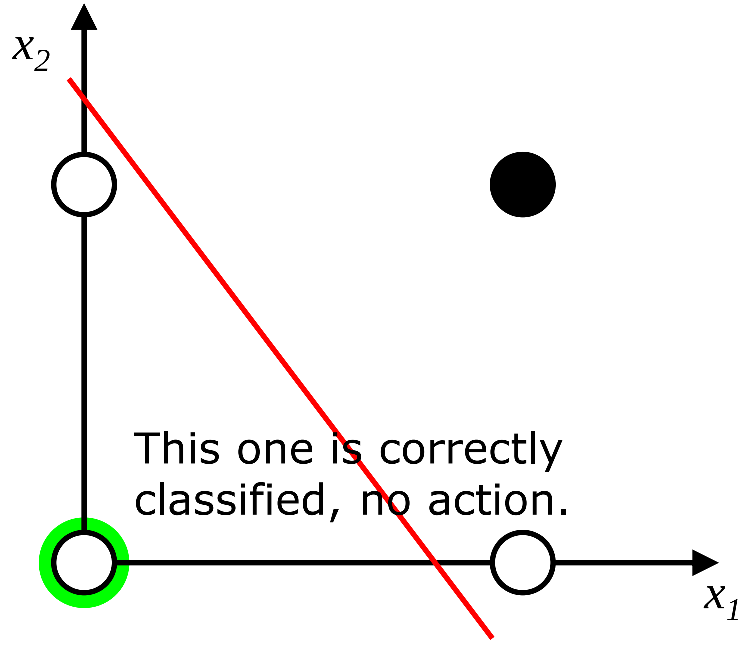

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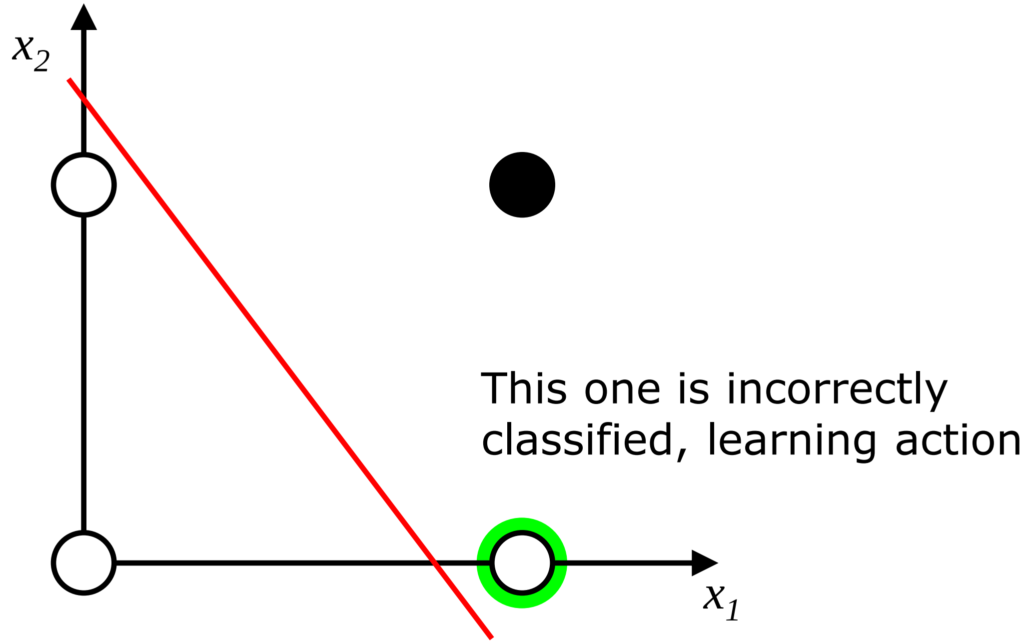

The AND function

$$\mathbf{w} = \begin{pmatrix} -0.8 \\ 1 \\ 0.7 \end{pmatrix}$$

$$w_0 = w_0 - \eta \cdot 1 = -1.1$$
$$w_1 = w_1 - \eta \cdot 1 = 0.7$$
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Example: Perceptron learning

x_1	x_2	f
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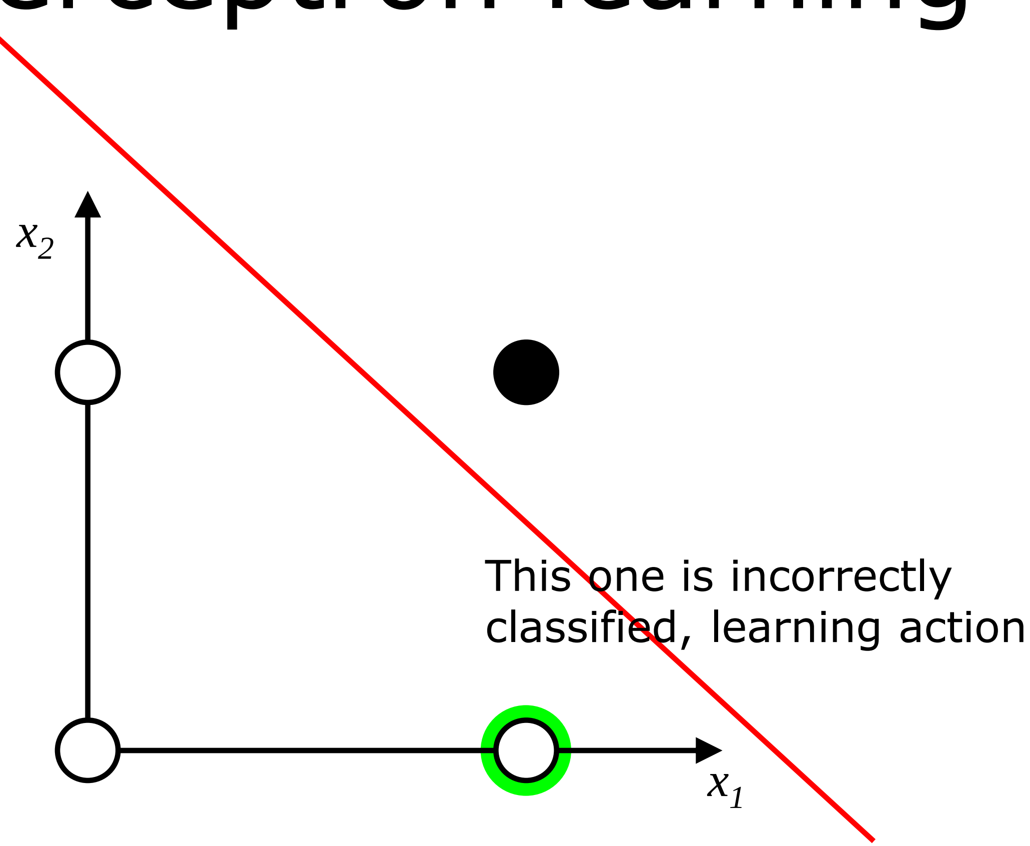

The AND function

$$\mathbf{w} = \begin{pmatrix} -1.1 \\ 0.7 \\ 0.7 \end{pmatrix}$$

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Example: Perceptron learning

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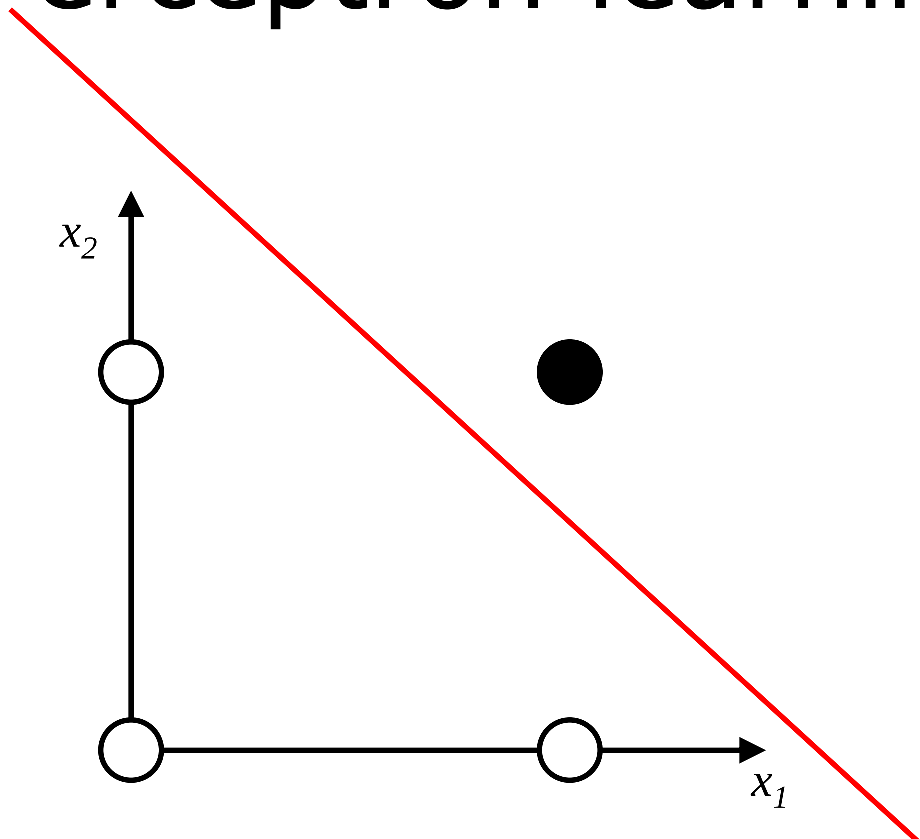


The AND function

$$\mathbf{w} = \begin{pmatrix} -1.1 \\ 0.7 \\ 0.7 \end{pmatrix}$$

Final solution

Perceptron learning

- Perceptron learning is guaranteed to find a solution in finite time, if a solution exists.
- Perceptron learning cannot be generalized to more complex networks.

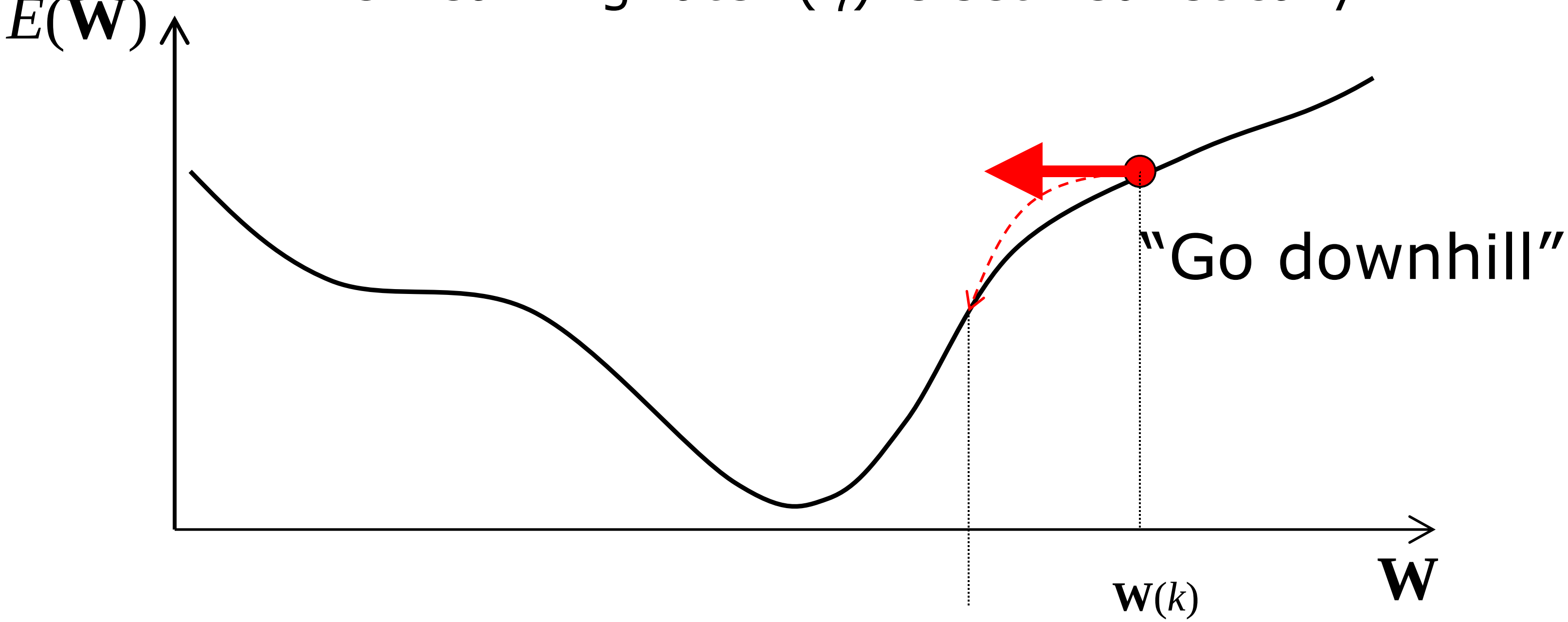
- Better to use gradient descent – based on formulating an error and differentiable functions

$$E(\mathbf{W}) = \sum_{n=1}^{N} \left[f(n) - y(\mathbf{W}, n) \right]^2$$

Gradient search

$$\Delta \mathbf{W} = -\eta \nabla_W E(\mathbf{W})$$

The "learning rate" (η) is set heuristically



$\mathbf{W}(k+1) = \mathbf{W}(k) + \Delta\mathbf{W}(k)$

The Multilayer Perceptron (MLP)

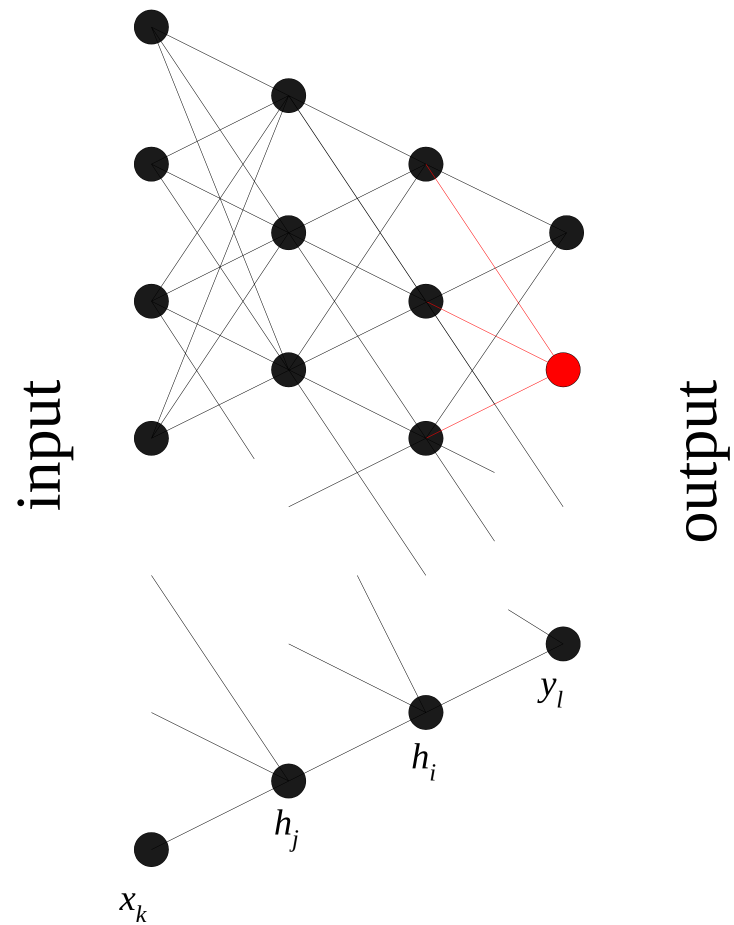
- Combine several single layer perceptrons.
- Each single layer perceptron uses a sigmoid function

E.g.

$$\phi(z) = \tanh(z)$$

$$\phi(z) = \left[1 + \exp(-z)\right]^{-1}$$

Can be trained using gradient descent



Example: One hidden layer

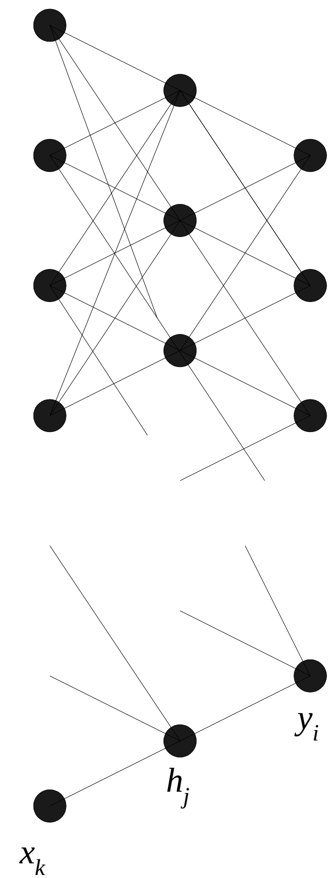
- Can approximate <u>any</u> continuous function

$$y_i(\mathbf{x}) = \theta\left[v_{i0} + \sum_{j=1}^{J} v_{ij} h_j(\mathbf{x}) \right]$$

$$h_j(\mathbf{x}) = \phi\left[w_{j0} + \sum_{k=1}^{D} w_{jk} x_k \right]$$

$\theta(z)$ = sigmoid or linear,

$\phi(z)$ = sigmoid.



Example of computing the gradient

$$\Delta W = -\eta \nabla_W E(W)$$

$$E(W) = MSE = \frac{1}{N}\sum_{n=1}^{N}(\hat{y}(W, x(n)) - y(n))^2 = \frac{1}{N}\sum_{n=1}^{N} e^2$$

$$\nabla_W E(W) = \nabla_W \left(\frac{1}{N}\sum_{n=1}^{N} e^2(n) \right) = \frac{2}{N}\sum_{n=1}^{N} e(n)(\nabla_W e(n)) = \frac{2}{N}\sum_{n=1}^{N} e(n)(\nabla_W \hat{y})$$

What we need to do is to compute $\nabla_W \hat{y}$

Equation for a single output, one hidden layer network:

$$\hat{y} = \theta(v_0 + \sum_{j=1}^{J} v_j h_j (w_{j0} + \sum_{k=1}^{K} x_k w_{jk}))$$

Example of computing the gradient

$$\hat{y} = \theta(v_0 + \sum_{j=1}^{J} v_j h_j (w_{j0} + \sum_{k=1}^{K} x_k w_{jk})) \qquad \theta(z) = z$$

$$\nabla_W \hat{y} = \begin{bmatrix} \boxed{\nabla_{w_{j0}} \hat{y}} \\ \boxed{\nabla_{w_{jk}} \hat{y}} \\ \nabla_{v_0} \hat{y} \\ \nabla_{v_j} \hat{y} \end{bmatrix}$$

$$\nabla_{w_{j0}} \hat{y} = v_j h_j' (w_{j0} + \sum_k x_k w_{jk})$$

$$\nabla_{w_{jk}} \hat{y} = \frac{\partial \hat{y}}{\partial w_{jk}} = \frac{\partial}{\partial w_{jk}} \left(\sum_j v_j h_j (w_{j0} + \sum_k x_k w_{jk}) \right) =$$

$$= v_j h_j' (w_{j0} + \sum_k x_k w_{jk}) x_k$$

$$h(z) = \tanh(z) \quad \Rightarrow \quad h'(z) = 1 - h^2(z)$$

Gradient descent (Backpropagation)

$$\Delta W = -\eta \nabla_W E(W)$$

RPROP (Resilient PROPagation)

Parameter update rule:

$$\boxed{\Delta W_i = -\eta_i(t) sign(\nabla_{W_i} E(W_i))}$$

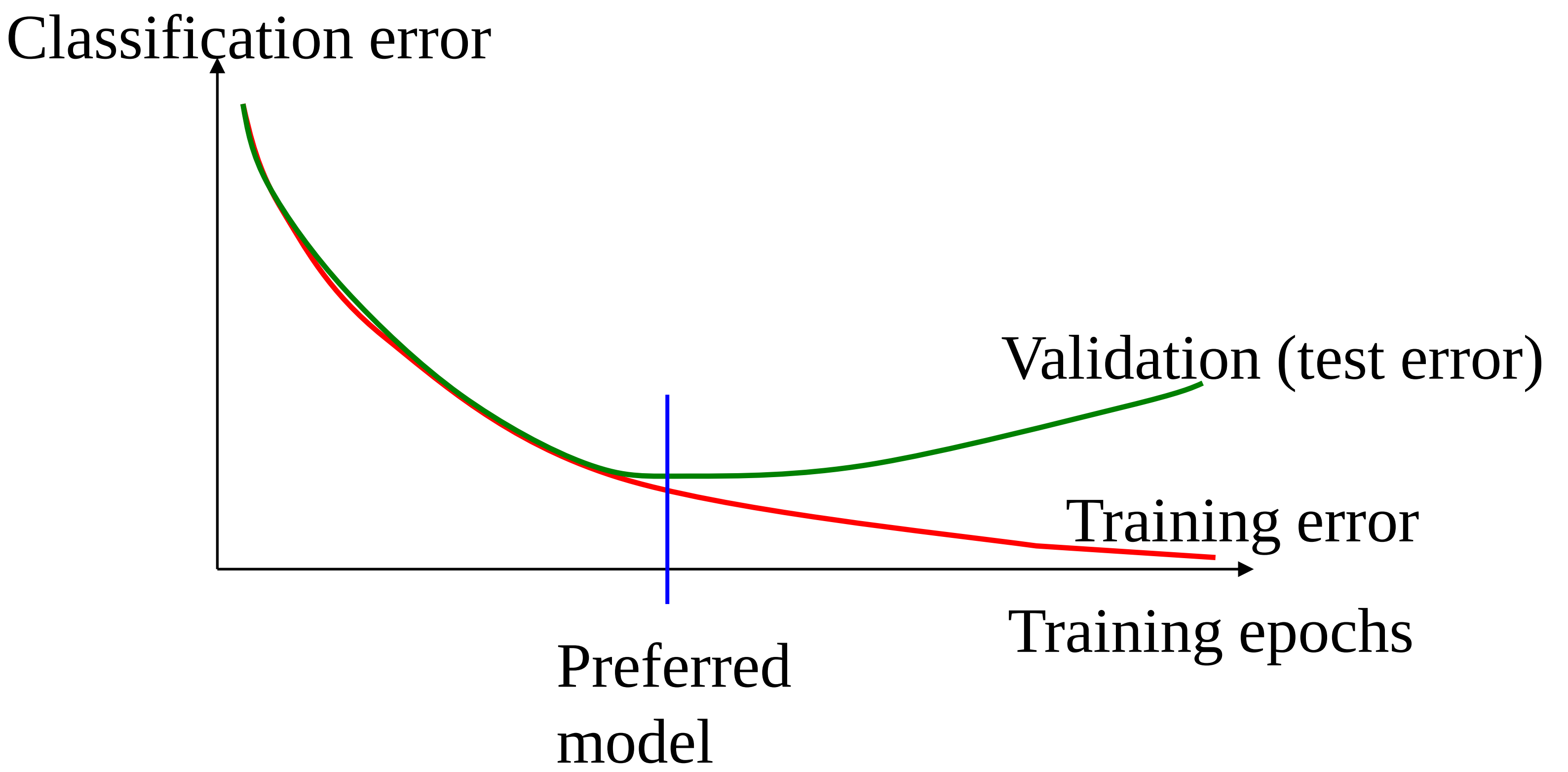
Learning rate update rule:

$$\boxed{\eta_i(t) = \begin{cases} 1.2\eta_i(t-1) & if \quad \nabla_{W_i} E_t(W_i) \cdot \nabla_{W_i} E_{t-1}(W_i) > 0 \\ 0.5\eta_i(t-1) & if \quad \nabla_{W_i} E_t(W_i) \cdot \nabla_{W_i} E_{t-1}(W_i) < 0 \end{cases}}$$

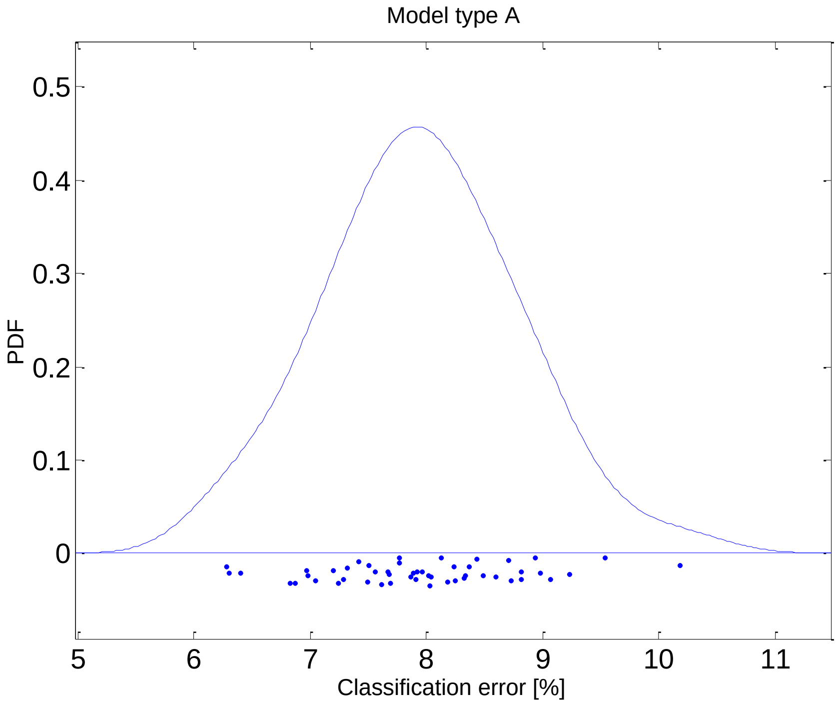
No parameter tuning unlike standard backpropagation!

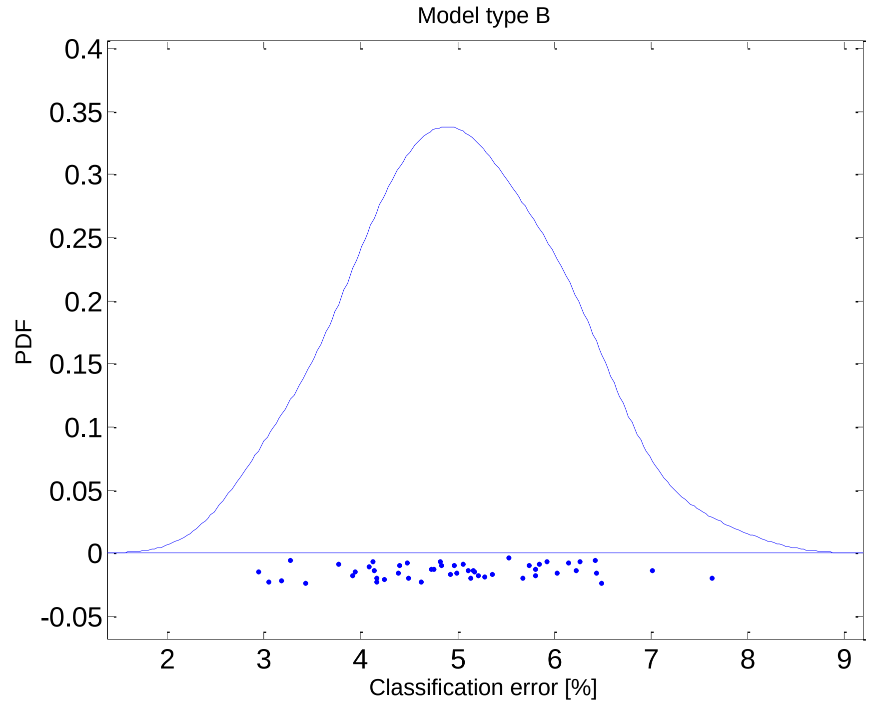
When should you stop learning?

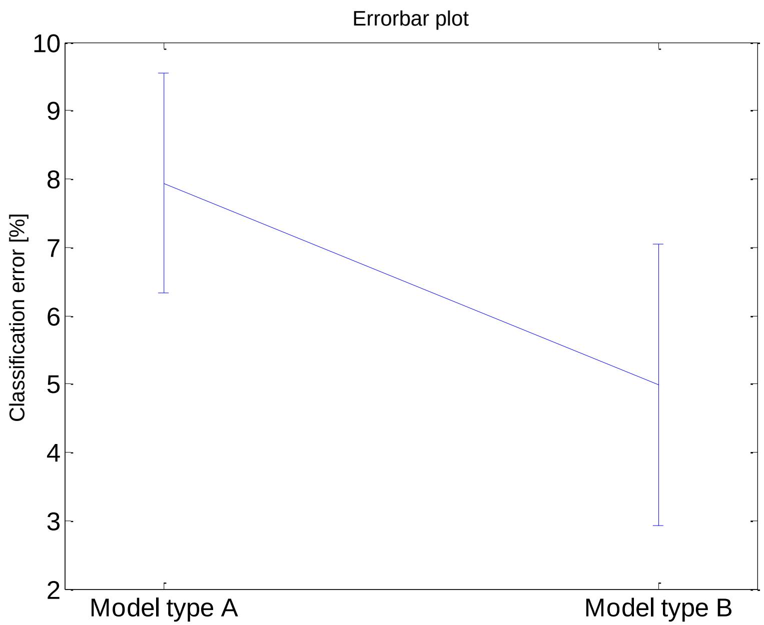
- After a set number of learning epochs
- When the change in the gradient becomes smaller than a certain number
- Validation data - “early stopping”



Model selection







Can use to determine:

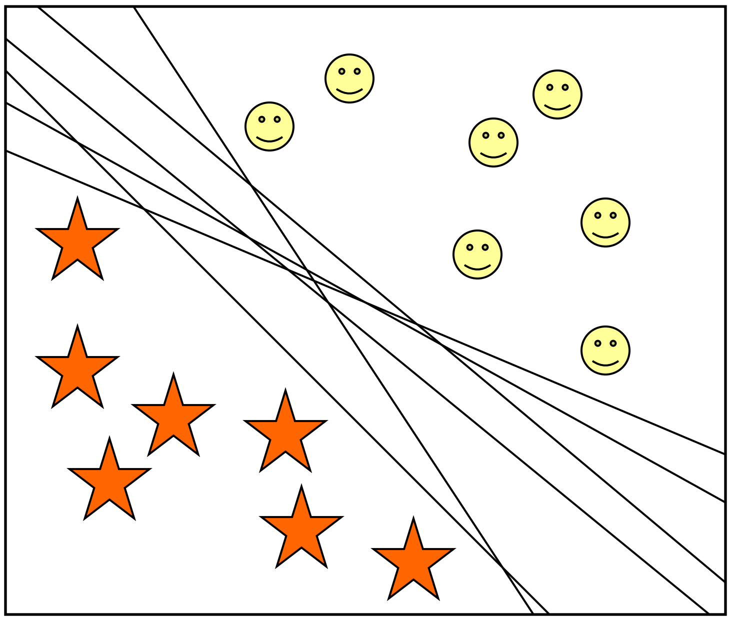
- Number of hidden nodes
- Which input signals to use
- If a pre-processing strategy is good or not
- Etc...

Variability typically induced by:

- Varying training and test data sets
- Random initial model parameters

Support vector machines

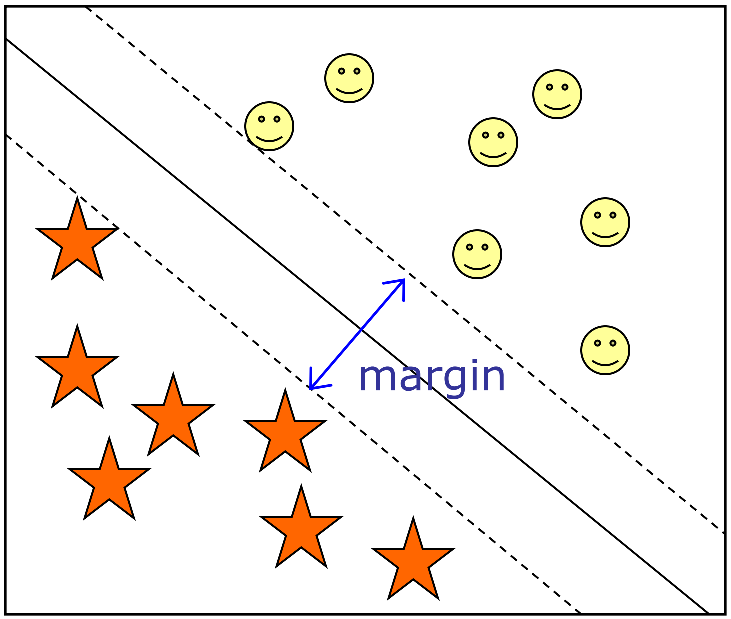
Linear classifier on a linearly separable problem



There are infinitely many lines that have zero training error.

Which line should we choose?

Linear classifier on a linearly separable problem



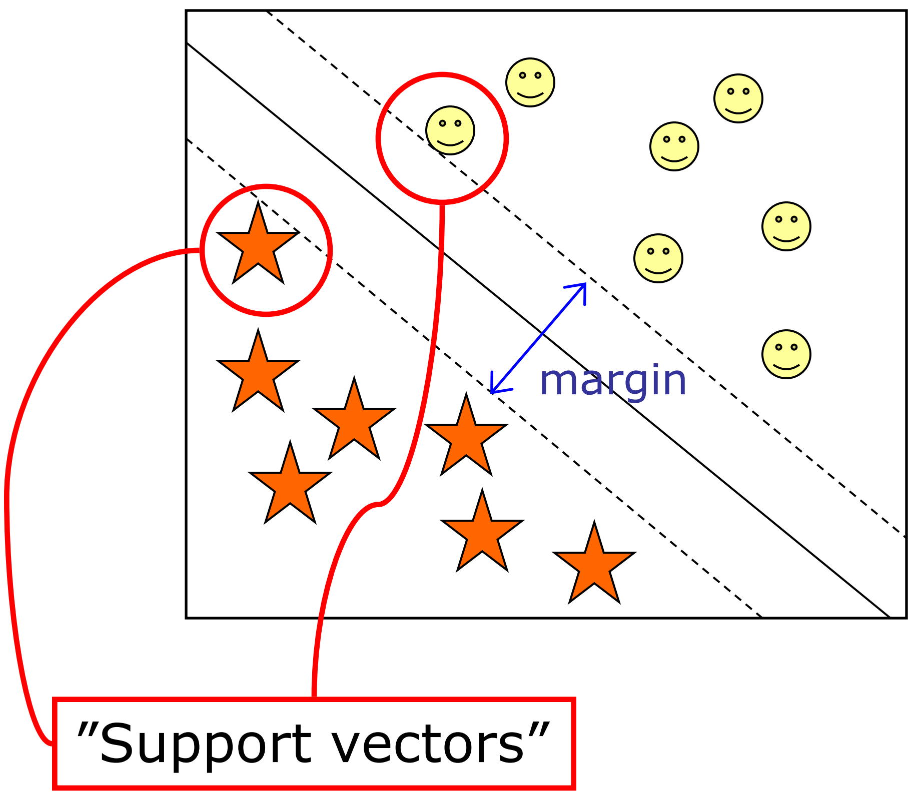
There are infinitely many lines that have zero training error.

Which line should we choose?

⇒ Choose the line with the largest margin.

The "large margin classifier"

Linear classifier on a linearly separable problem



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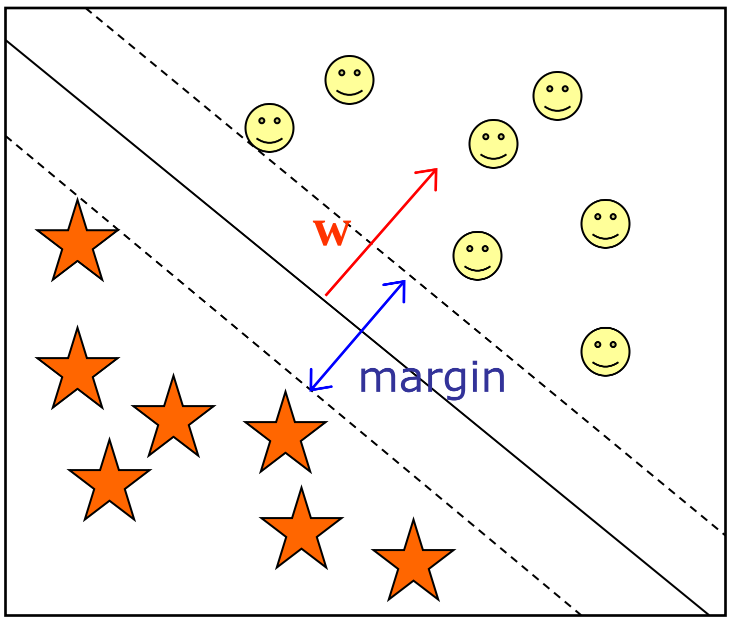
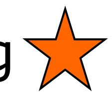
Computing the margin



The plane separating  and  is defined by

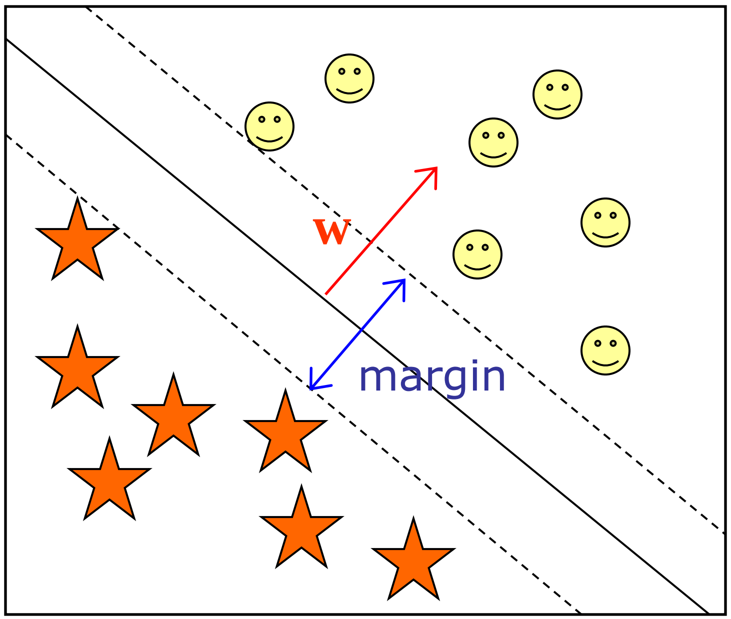
$$\mathbf{w}^T\mathbf{x} = a$$

The dashed planes are given by

$$\mathbf{w}^T\mathbf{x} = a + b$$

$$\mathbf{w}^T\mathbf{x} = a - b$$

Computing the margin



Divide by b

$$\mathbf{w}^T\mathbf{x}/b = a/b + 1$$

$$\mathbf{w}^T\mathbf{x}/b = a/b - 1$$

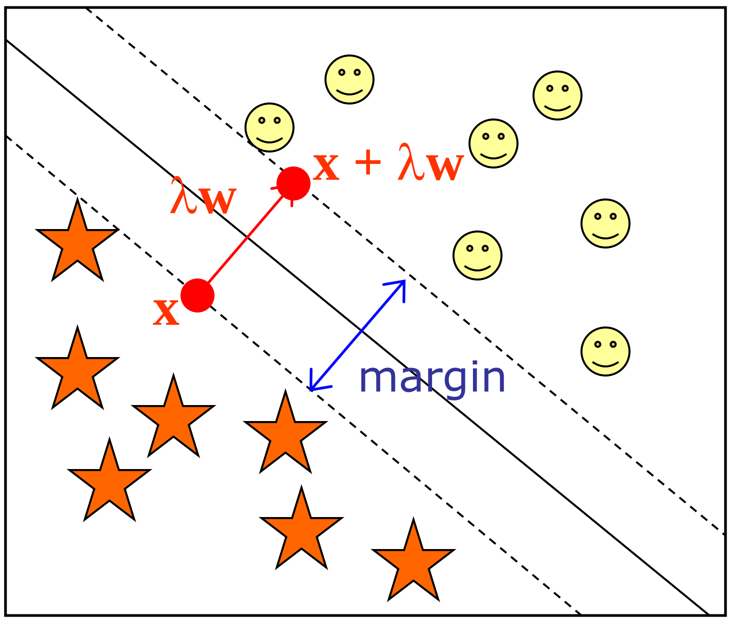
Define new $\mathbf{w}$ = $\mathbf{w}/b$ and α = a/b

$$\mathbf{w}^T\mathbf{x} = \alpha + 1$$

$$\mathbf{w}^T\mathbf{x} = \alpha - 1$$

We have defined a scale for $\mathbf{w}$ and b

Computing the margin



We have

$$\mathbf{w}^T\mathbf{x} = \alpha - 1$$

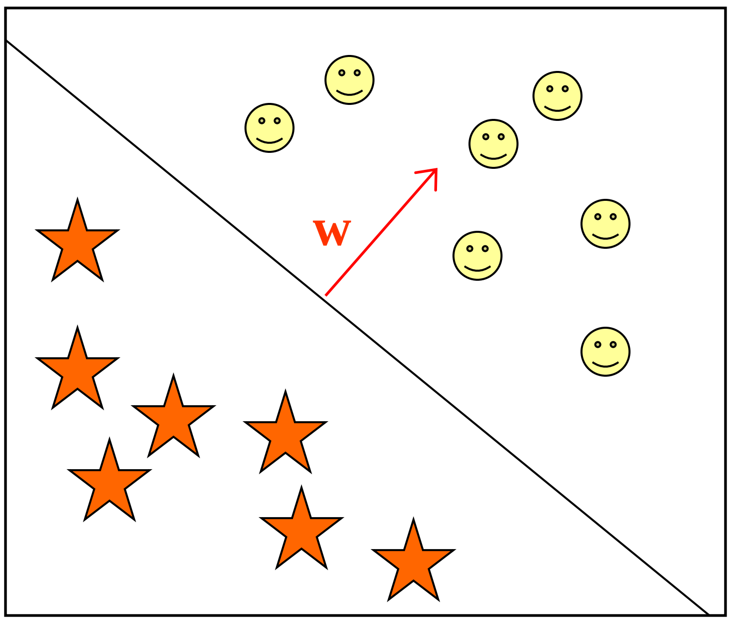
$$\mathbf{w}^T(\mathbf{x} + \lambda\mathbf{w}) = \alpha + 1$$

$$\|\lambda\mathbf{w}\| = \text{margin}$$

which gives

$$\text{margin} = \frac{2}{\|\mathbf{w}\|}$$

Linear classifier on a linearly separable problem

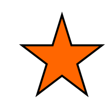


Maximizing the margin is equal to minimizing

$$||\mathbf{w}||$$

subject to the constraints

$\mathbf{w}^{\mathrm{T}}\mathbf{x}(n) - \alpha \geq +1$ for all 

$\mathbf{w}^{\mathrm{T}}\mathbf{x}(n) - \alpha \leq -1$ for all 

Quadratic programming problem,
constraints can be included with Lagrange multipliers.

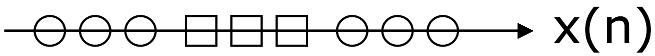
Linear Support Vector Machine

Test phase, the predicted output

$$\hat{y}(\mathbf{x}) = \operatorname{sgn}\left[\mathbf{w}^T\mathbf{x} - \alpha\right] = \operatorname{sgn}\left[\sum_{n \in \Omega_s} \lambda_n y(n)\mathbf{x}(n)^T\mathbf{x} - \alpha\right]$$

Only scalar products in the expression.

How deal with nonlinear case?



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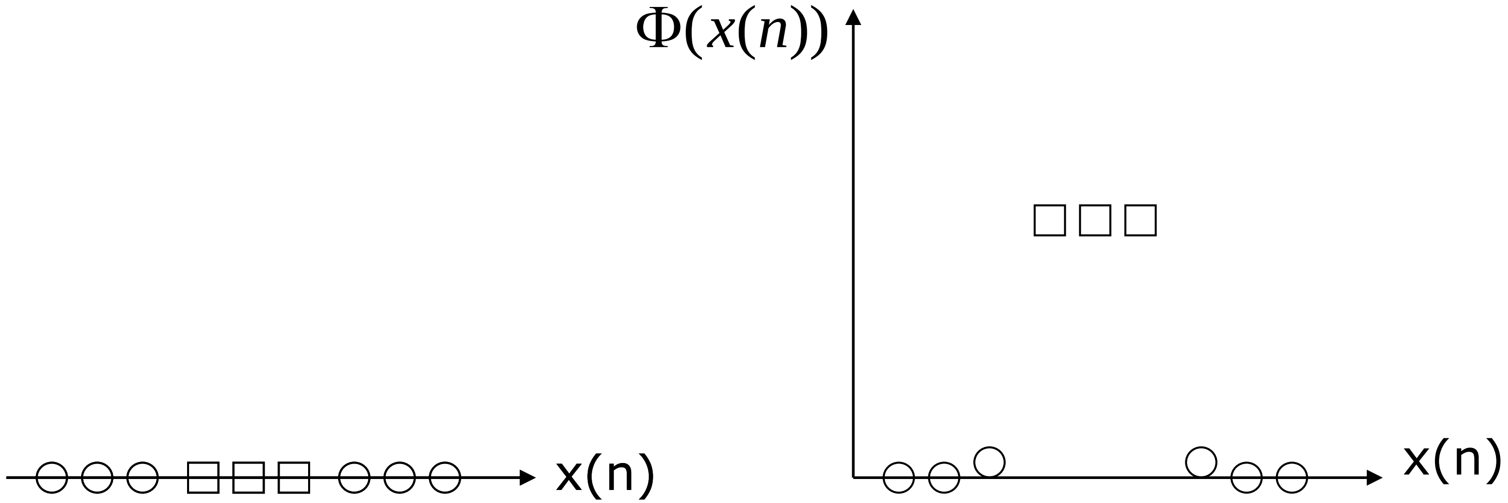
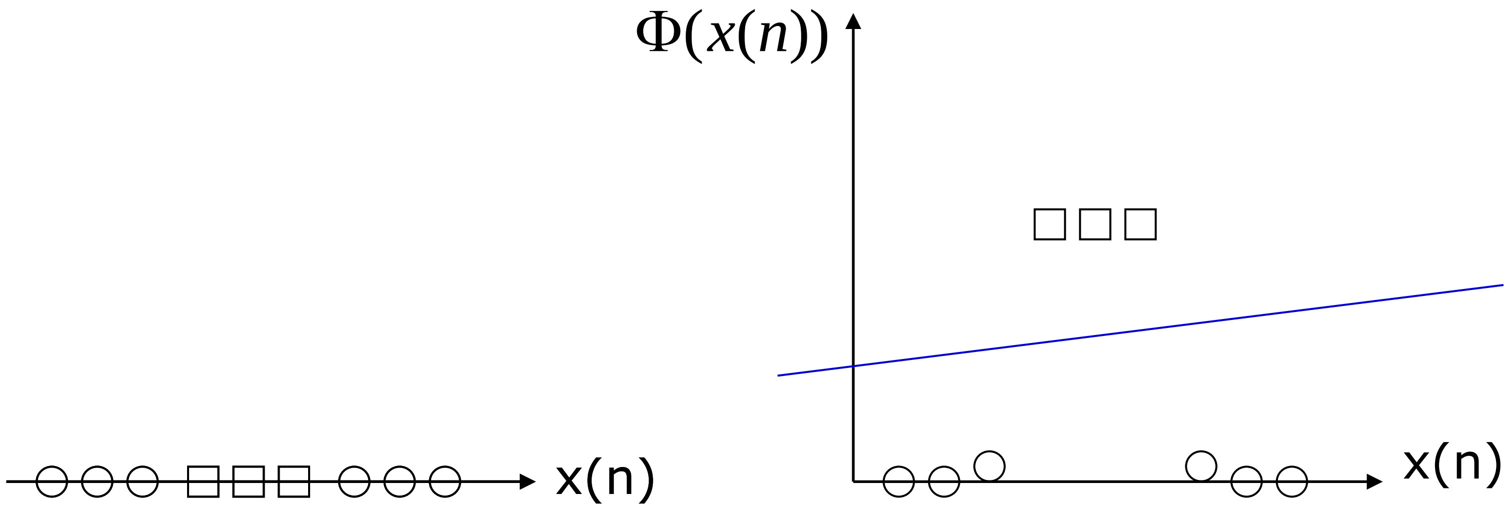


How deal with nonlinear case?



How deal with nonlinear case?

- Project data into high-dimensional space $\mathbf{Z}$.

$$\mathbf{z}(n) = \boldsymbol{\varphi}[\mathbf{x}(n)]$$

- We don’t even have to know the projection...!

Scalar product kernel trick

If we can find kernel such that

$$K(\mathbf{x}(n), \mathbf{x}(m)) = \boldsymbol{\varphi}(\mathbf{x}(n))^T \boldsymbol{\varphi}(\mathbf{x}(m))$$

Then we don't even have to know the mapping
to solve the problem...

Kernel trick – computation example

$$K(x,z) = (x^T z)^2 = (\sum_{i=1}^{N} x_i z_i)(\sum_{j=1}^{N} x_j z_j) = \sum_{i=1}^{N}\sum_{j=1}^{N} (x_i x_j)(z_i z_j) = \varphi(x)^T \varphi(z)$$

Kernel trick – computation example

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For N=3

$$\varphi(x) = \begin{bmatrix} x_1 x_1 \\ x_1 x_2 \\ x_1 x_3 \\ x_2 x_1 \\ x_2 x_2 \\ \vdots \\ x_3 x_3 \end{bmatrix}$$

Need O(N^2) to compute $\varphi(x)$

Kernel trick – computation example

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For N=3

$$\varphi(x) = \begin{bmatrix} x_1 x_1 \\ x_1 x_2 \\ x_1 x_3 \\ x_2 x_1 \\ x_2 x_2 \\ \vdots \\ x_3 x_3 \end{bmatrix}$$

Need $O(N^2)$ to compute $\varphi(x)$

$\boxed{\text{Need only } O(N) \text{ to compute } K(x,z)}$

Valid kernels (Mercer's theorem)

Define the matrix

$$\mathbf{K} = \begin{pmatrix} K[\mathbf{x}(1),\mathbf{x}(1)] & K[\mathbf{x}(1),\mathbf{x}(2)] & \cdots & K[\mathbf{x}(1),\mathbf{x}(N)] \\ K[\mathbf{x}(2),\mathbf{x}(1)] & K[\mathbf{x}(2),\mathbf{x}(2)] & \cdots & K[\mathbf{x}(2),\mathbf{x}(N)] \\ \vdots & \vdots & \ddots & \vdots \\ K[\mathbf{x}(N),\mathbf{x}(1)] & K[\mathbf{x}(N),\mathbf{x}(2)] & \cdots & K[\mathbf{x}(N),\mathbf{x}(N)] \end{pmatrix}$$

If $\mathbf{K}$ is symmetric, $\mathbf{K} = \mathbf{K}^T$, and positive semi-definite, then $K[\mathbf{x}(i),\mathbf{x}(j)]$ is a valid kernel.

Examples of kernels

$$K[\mathbf{x}(i), \mathbf{x}(j)] = \exp\left[-\left\|\mathbf{x}(i) - \mathbf{x}(j)\right\|^2 / 2\sigma\right]$$

$$K[\mathbf{x}(i), \mathbf{x}(j)] = \left[\mathbf{x}(i)^T \mathbf{x}(j)\right]^d$$

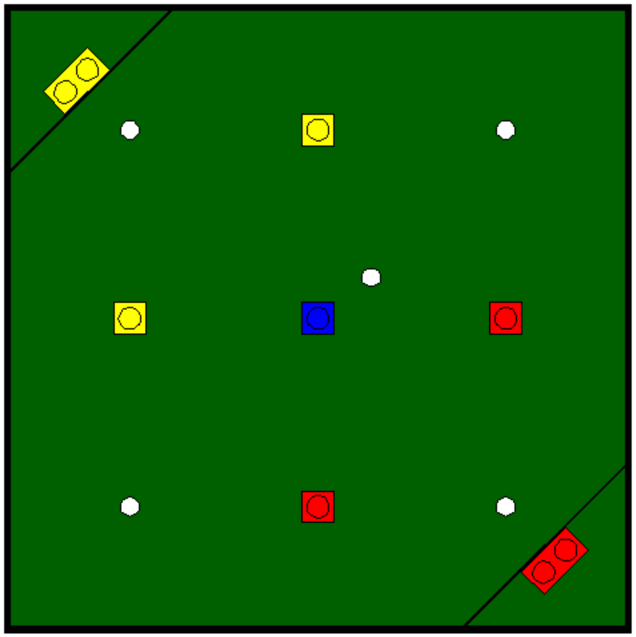
First, Gaussian kernel.

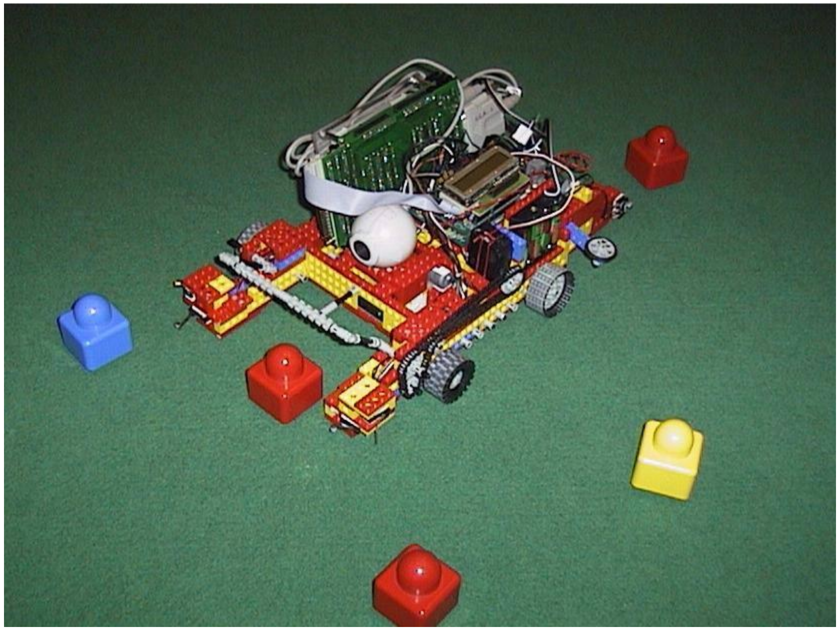
Second, polynomial kernel. With $d=1$ we have linear SVM.

Linear SVM often used with good success on high dimensional data (e.g. text classification).

Example: Robot color vision

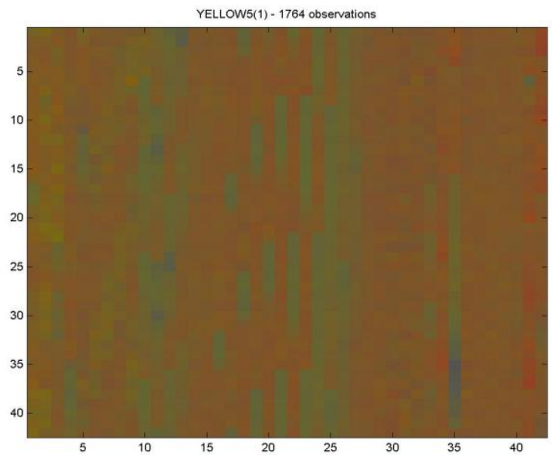
(Competition 1999)

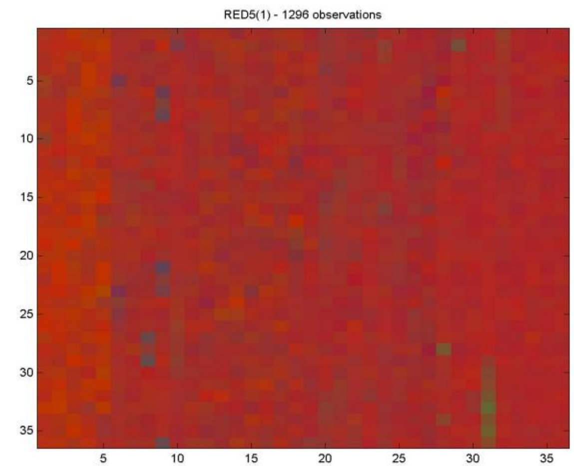




Classify the Lego pieces into *red*, *blue*, and *yellow.*
Classify *white* balls, *black* sideboard, and *green* carpet.

What the camera sees
(RGB space)

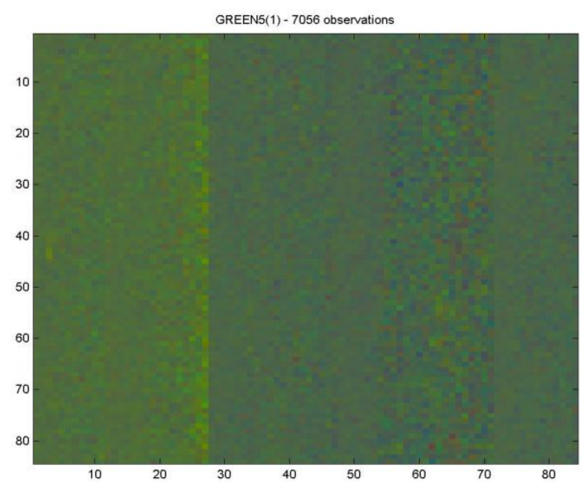




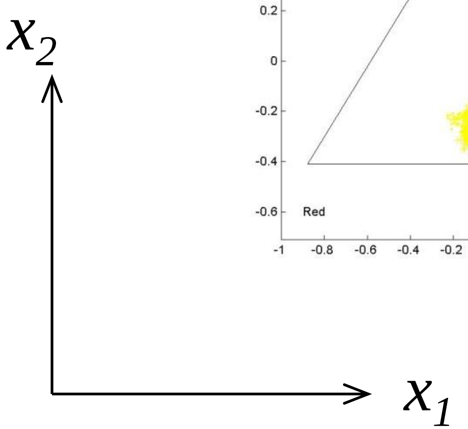
Yellow

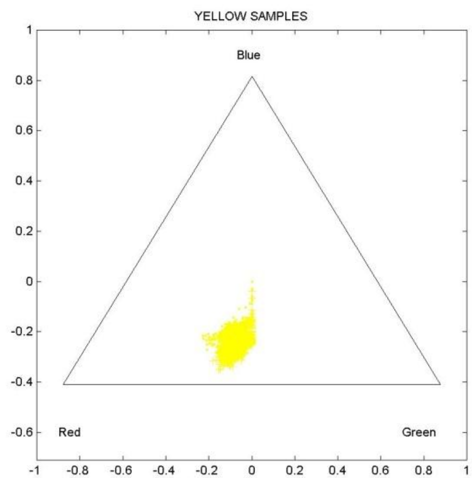
Red

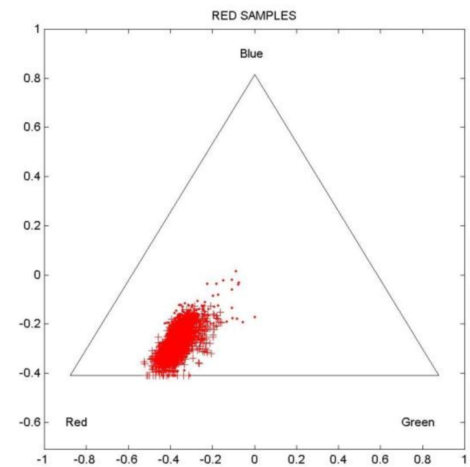
Green



Lego in normalized *rgb* space

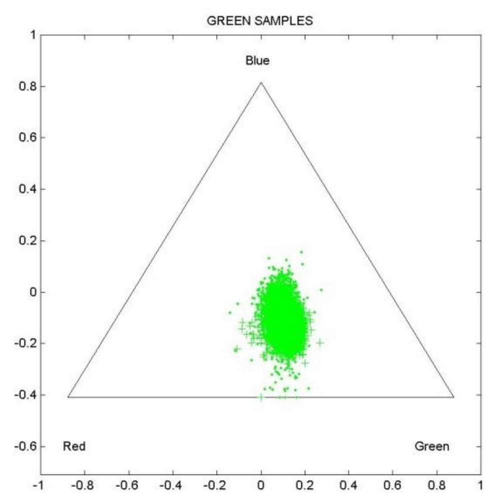






Input is 2D

$$\mathbf{x} \in X^2$$

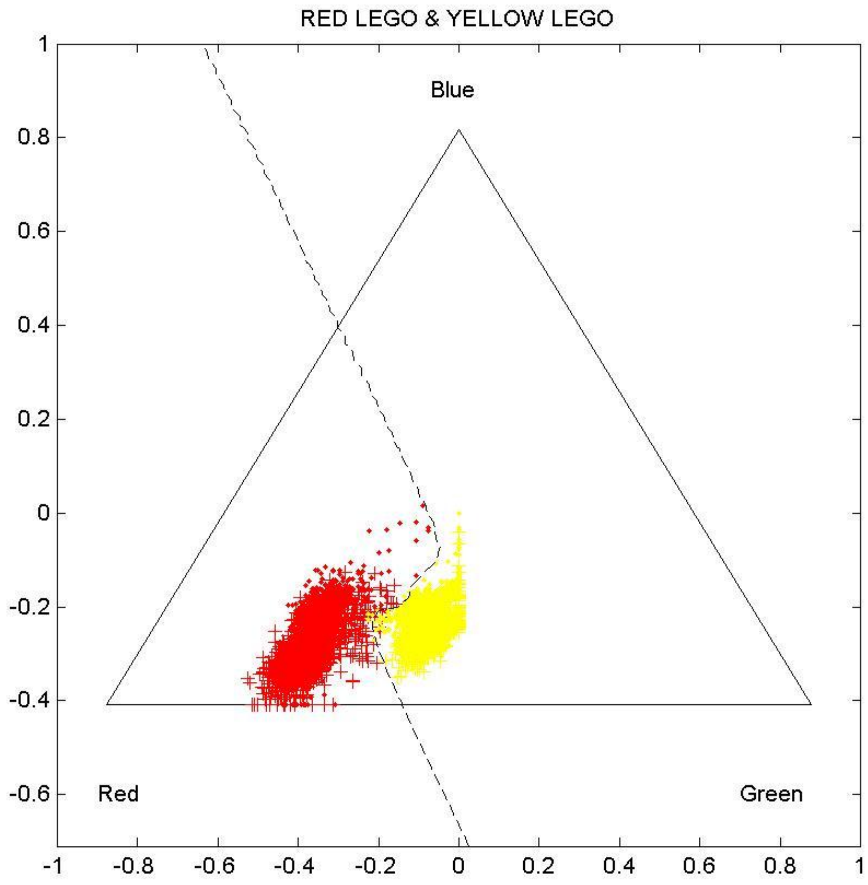


Output is 6D:
{red, blue, yellow, green, black, white}

$$\mathbf{c} \in C^6$$

MLP classifier

2-3-1 MLP
Levenberg-
Marquardt

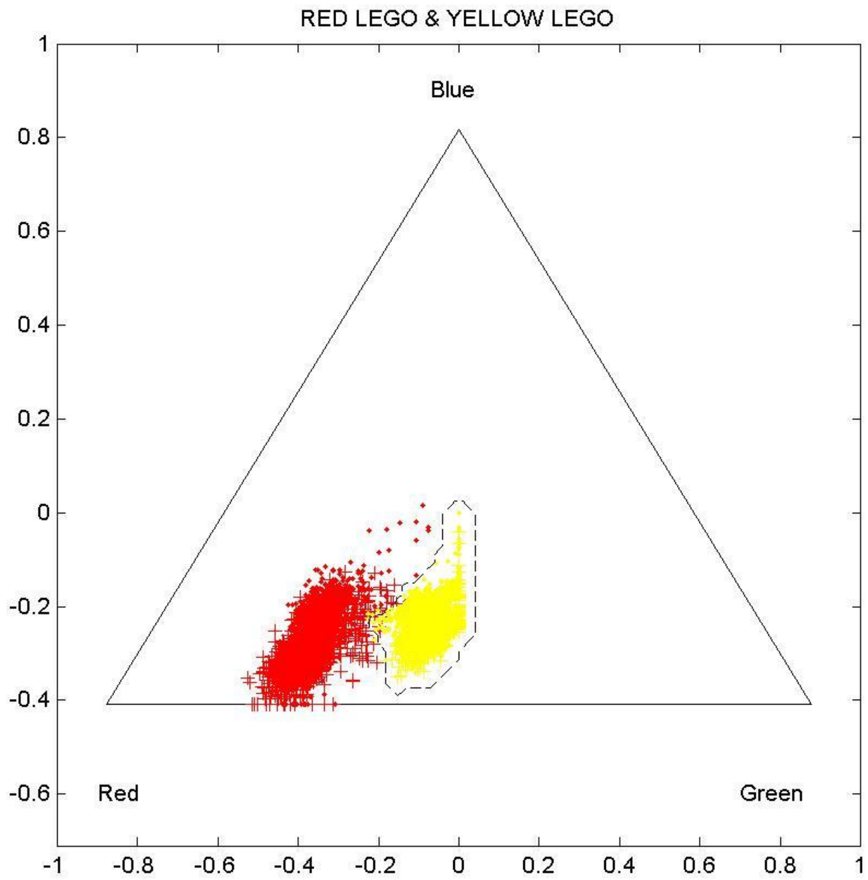


E_train = 0.21%
E_test = 0.24%

Training time
(150 epochs):
51 seconds

SVM classifier

SVM with
γ = 1000



E_train = 0.19%
E_test = 0.20%

Training time:
22 seconds

$$K(\mathbf{x},\mathbf{y}) = \exp\left[-\gamma(\mathbf{x}-\mathbf{y})^2\right]$$

Machine Learning

- Machine learning (multilayer perceptrons, support vector machines, clustering) is covered in great detail in the course ”Learning Systems”.