Chapter ML:VI

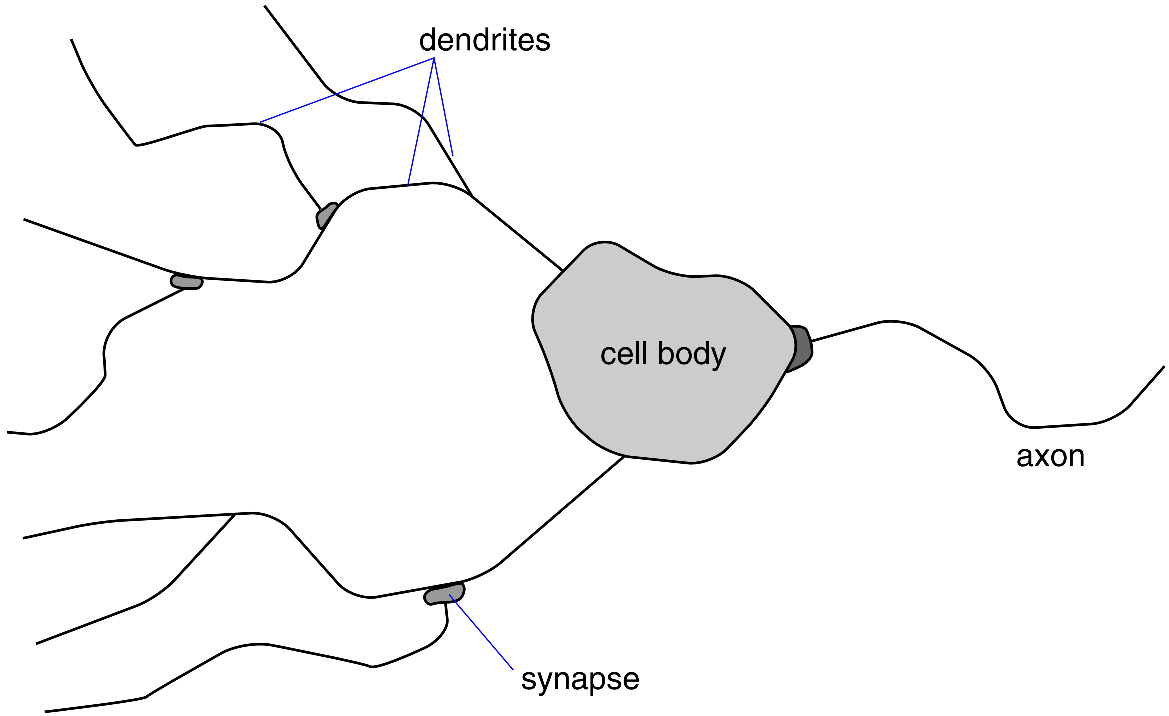
VI. Neural Networks

- Perceptron Learning
- Gradient Descent
- Multilayer Perceptron
- Radial Basis Functions

Perceptron Learning

The Biological Model

Simplified model of a neuron:



Perceptron Learning

The Biological Model (continued)

Neuron characteristics:

- The numerous dendrites of a neuron serve as its input channels for electrical signals.
- At particular contact points between the dendrites, the so-called synapses, electrical signals can be initiated.
- A synapse can initiate signals of different strengths, where the strength is encoded by the frequency of a pulse train.
- The cell body of a neuron accumulates the incoming signals.
- If a particular stimulus threshold is exceeded, the cell body generates a signal, which is output via the axon.
- The processing of the signals is unidirectional. (from left to right in the figure)

Perceptron Learning

History

1943 Warren McCulloch and Walter Pitts present a model of the neuron.

1949 Donald Hebb postulates a new learning paradigm: reinforcement only for active neurons. (those neurons that are involved in a decision process)

1958 Frank Rosenblatt develops the perceptron model.

1962 Rosenblatt proves the perceptron convergence theorem.

1969 Marvin Minsky and Seymour Papert publish a book on the limitations of the perceptron model.

1970

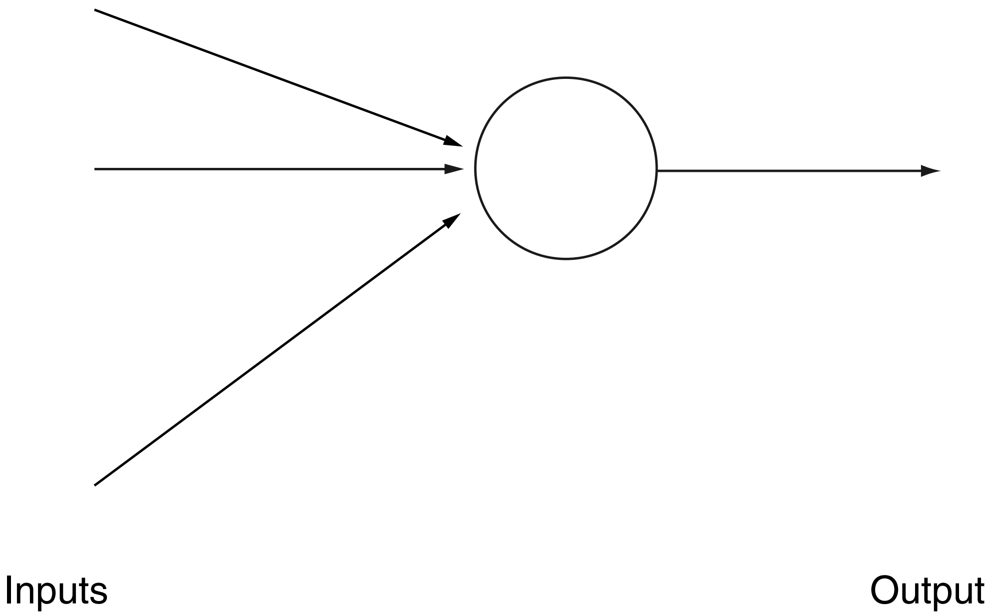
⋮

1985

1986 David Rumelhart and James McClelland present the multilayer perceptron.

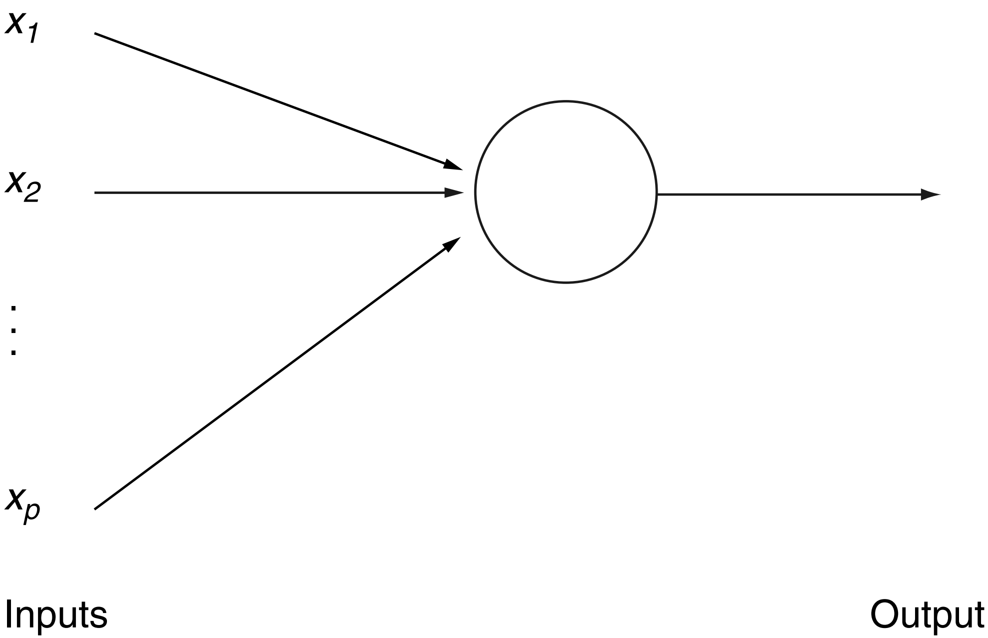
Perceptron Learning

The Perceptron of Rosenblatt [1958]



Perceptron Learning

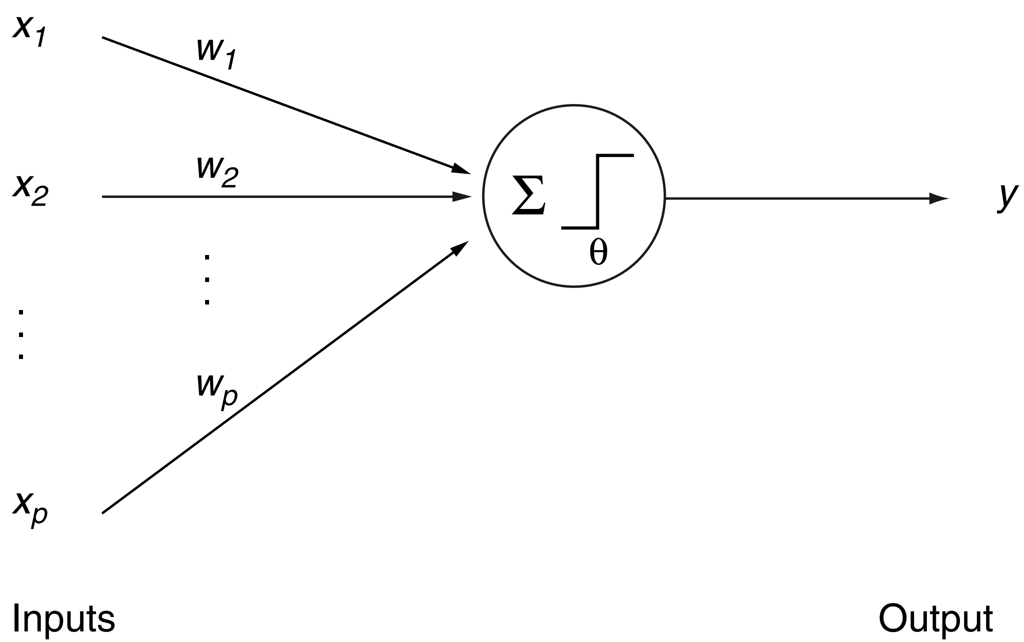
The Perceptron of Rosenblatt [1958]



$$x_j, w_j \in \mathbf{R}, \quad j = 1 \ldots p$$

Perceptron Learning

The Perceptron of Rosenblatt [1958]



$x_j, w_j \in \mathbf{R}, \quad j = 1 \ldots p$

Remarks:

- The perceptron of Rosenblatt is based on the neuron model of McCulloch and Pitts.
- The perceptron is a “feed forward system”.

Perceptron Learning

Specification of Classification Problems [ML Introduction]

Characterization of the model (model world):

- X is a set of feature vectors, also called feature space. $X \subseteq \mathbf{R}^p$
- C is a set of classes. $C = \{0, 1\}$
- $c : X \to C$ is the ideal classifier for X.
- $D = \{(\mathbf{x}_1, c(\mathbf{x}_1)), \ldots, (\mathbf{x}_n, c(\mathbf{x}_n))\} \subseteq X \times C$ is a set of examples.

How could the hypothesis space H look like?

Perceptron Learning

Computation in the Perceptron [Regression]

If $\sum_{j=1}^{p} w_j x_j \geq \theta$ then $y(\mathbf{x}) = 1$, and

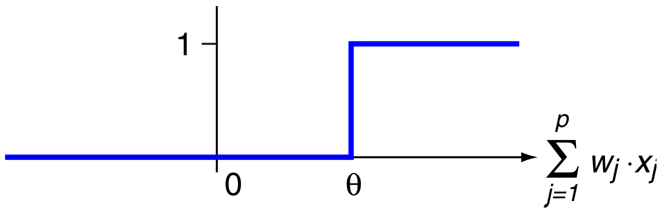
if $\sum_{j=1}^{p} w_j x_j < \theta$ then $y(\mathbf{x}) = 0$.

Perceptron Learning

Computation in the Perceptron [Regression]

If $\sum_{j=1}^{p} w_j x_j \geq \theta$ then $y(\mathbf{x}) = 1$, and

if $\sum_{j=1}^{p} w_j x_j < \theta$ then $y(\mathbf{x}) = 0$.



where $\sum_{j=1}^{p} w_j x_j = \mathbf{w}^T\mathbf{x}$. (or other notations for the scalar product)

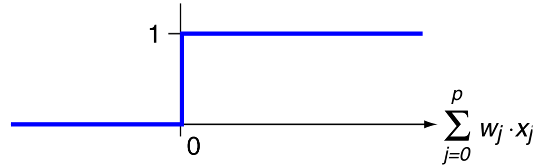
➜ A hypothesis is determined by $\theta, w_1, \ldots, w_p$.

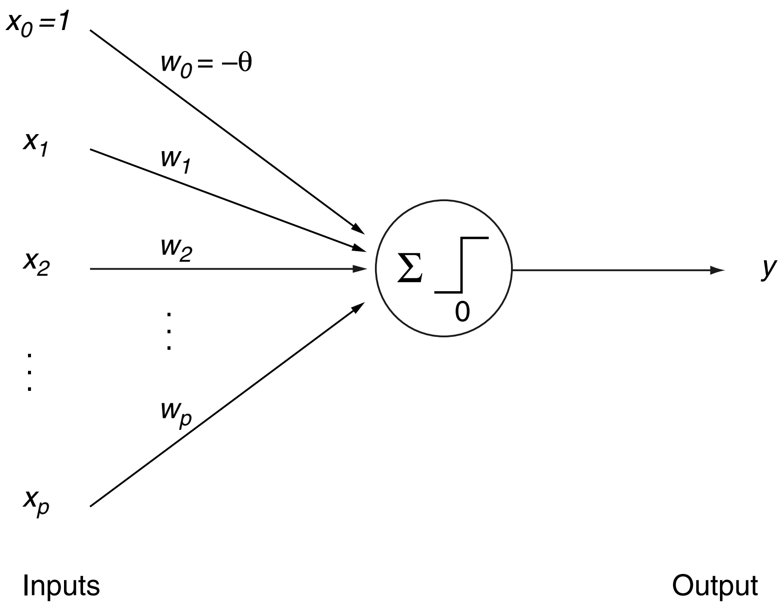
Perceptron Learning

Computation in the Perceptron (continued)

$$y(\mathbf{x}) = \textit{heaviside}(\sum_{j=1}^{p} w_j x_j - \theta)$$

$$= \textit{heaviside}(\sum_{j=0}^{p} w_j x_j) \quad \text{with } w_0 = -\theta,\ x_0 = 1$$





➜ A hypothesis is determined by $w_0, w_1, \ldots, w_p$.

Remarks:

- If the weight vector is extended by $w_0 = -\theta$, and, if the feature vectors are extended by the constant feature $x_0 = 1$, the learning algorithm gets a canonical form. Implementations of neural networks introduce this extension often implicitly.
- Be careful with regard to the dimensionality of the weight vector: it is always denoted as $\mathbf{w}$ here, irrespective of the fact whether the w_0-dimension, with $w_0 = -\theta$, is included.
- The function *heaviside* is named after the mathematician Oliver Heaviside.
  [Heaviside: step function Oliver]

Perceptron Learning

Weight Adaptation [*IGD* Algorithm]

Algorithm:	*PT*	Perceptron Training
Input:	D	Training examples of the form $(\mathbf{x}, c(\mathbf{x}))$ with $\lvert\mathbf{x}\rvert = p+1,\; c(\mathbf{x}) \in \{0,1\}$.
	η	Learning rate, a small positive constant.
Internal:	$y(D)$	Set of $y(\mathbf{x})$-values computed from the elements $\mathbf{x}$ in D given some $\mathbf{w}$.
Output:	$\mathbf{w}$	Weight vector.

PT(D, η)

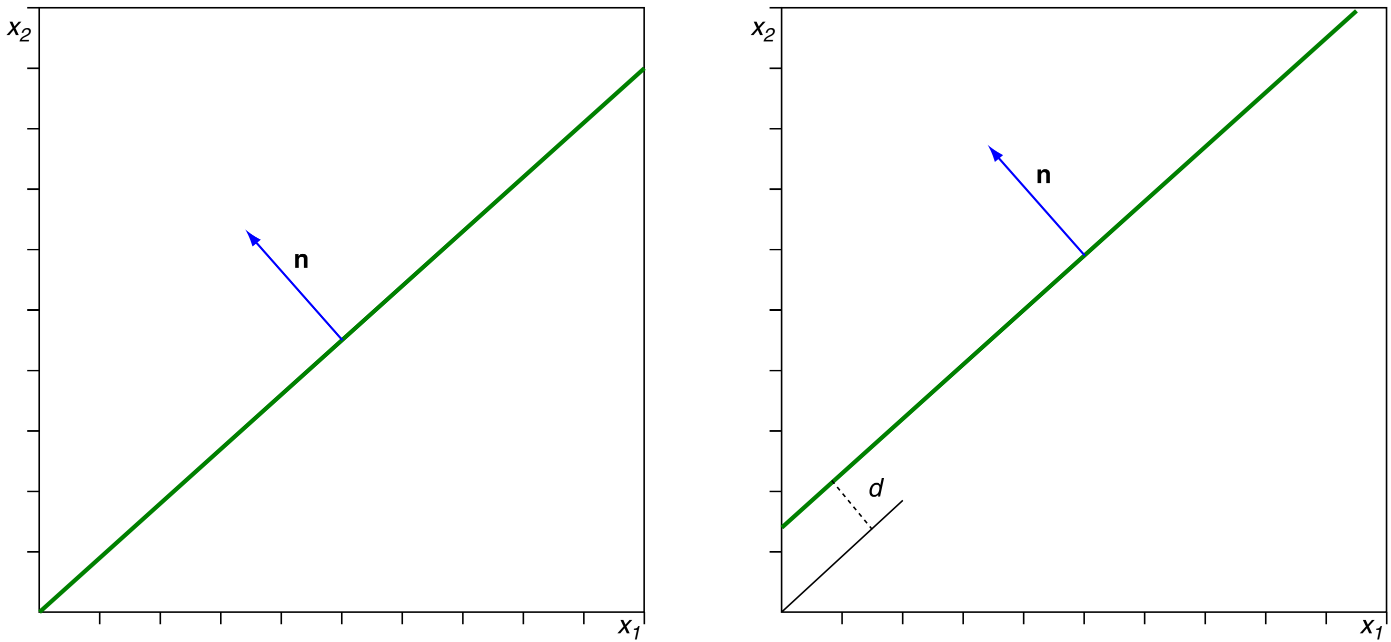
initialize_random_weights$(\mathbf{w})$, $t = 0$
REPEAT
  $t = t + 1$
  $(\mathbf{x}, c(\mathbf{x})) =$ *random_select*(D)
  error $= c(\mathbf{x}) -$ *heaviside*$(\mathbf{w}^T\mathbf{x})$
  FOR $j = 0$ **TO** p **DO**
    $\Delta w_j = \eta \cdot$ *error* $\cdot x_j$
    $w_j = w_j + \Delta w_j$
  ENDDO
UNTIL(*convergence*$(D, y(D))$ **OR** $t > t_{\text{max}}$)
return$(\mathbf{w})$

Remarks:

- The variable t denotes the time. At each point in time the learning algorithm gets an example presented and, as a consequence, may adapt the weight vector.
- The weight adaptation rule compares the true class $c(\mathbf{x})$ (the ground truth) to the class computed by the perceptron. In case of a wrong classification of a feature vector $\mathbf{x}$, *Err* is either -1 or $+1$—independent of the exact numeric difference between $c(\mathbf{x})$ and $\mathbf{w}^T\mathbf{x}$.
- $y(D)$ is the set of $y(\mathbf{x})$-values given $\mathbf{w}$ for the elements $\mathbf{x}$ in D.

Perceptron Learning

Weight Adaptation (continued)

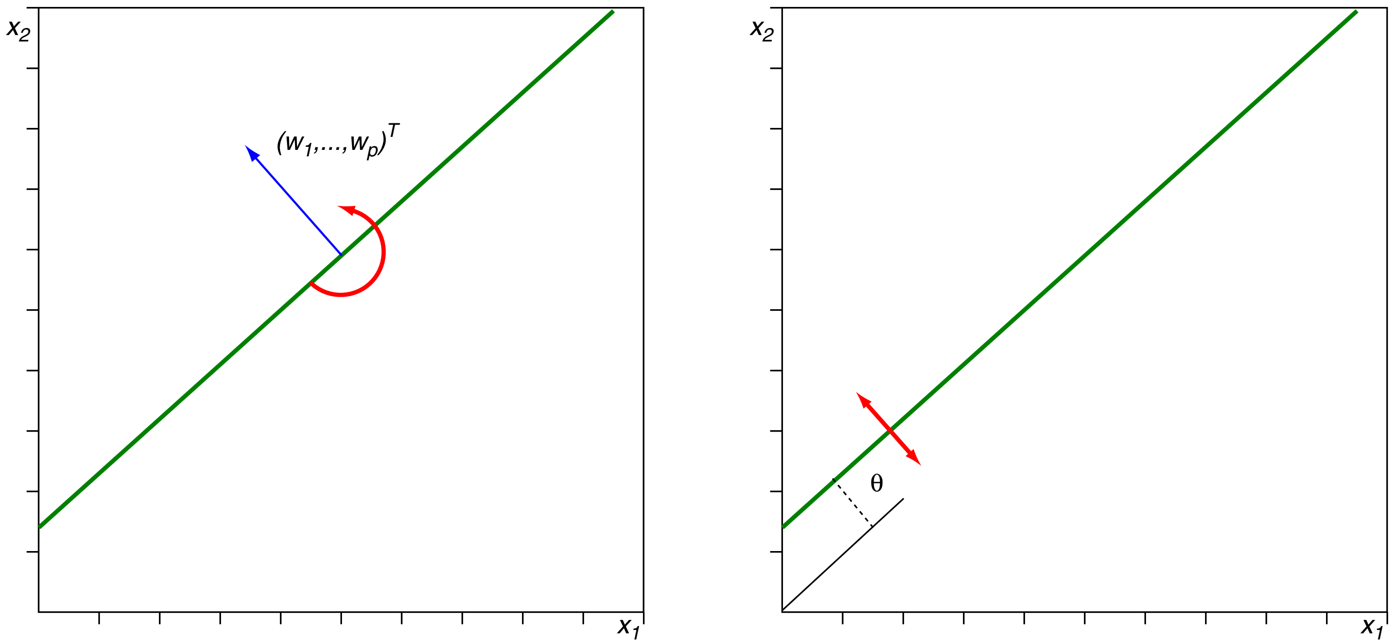


Definition of an (affine) hyperplane: $\mathbf{n}^T\mathbf{x} = d$ [Wikipedia]

- $\mathbf{n}$ denotes a normal vector that is perpendicular to the hyperplane.
- If $||\mathbf{n}|| = 1$ then $|d|$ corresponds to the distance of the origin to the hyperplane.
- If $\mathbf{n}^T\mathbf{x} < d$ and $d \geq 0$ then $\mathbf{x}$ and the origin lie on the same side of the hyperplane.

Perceptron Learning

Weight Adaptation (continued)



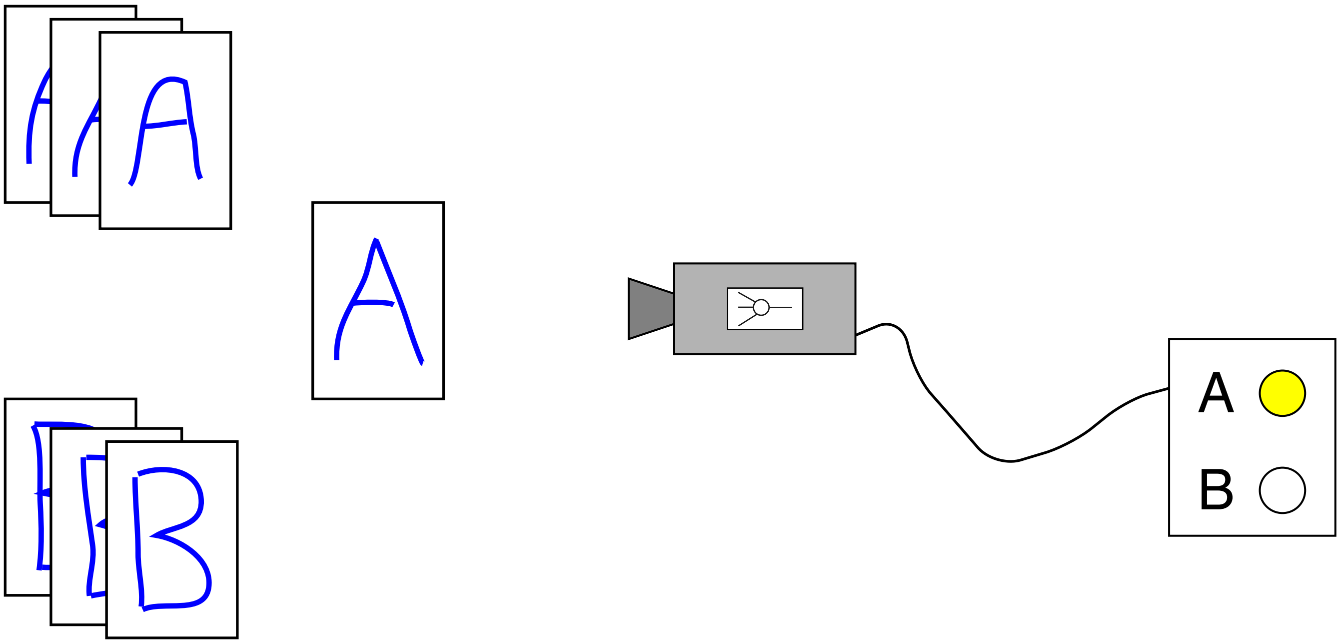
Definition of an (affine) hyperplane: $\mathbf{w}^T\mathbf{x} = 0 \;\Leftrightarrow\; \sum_{j=1}^{p} w_j x_j = \theta = -w_0$

Remarks:

- A perceptron defines a hyperplane that is perpendicular (= normal) to $(w_1, \ldots, w_p)^T$.
- θ or $-w_0$ specify the offset of the hyperplane from the origin, along $(w_1, \ldots, w_p)^T$ and as multiple of $1/||(w_1, \ldots, w_p)^T||$.
- The set of possible weight vectors $\mathbf{w} = (w_0, w_1, \ldots, w_p)^T$ form the hypothesis space H.
- Weight adaptation means learning, and the shown learning paradigm is supervised.
- The computation of the weight difference Δw_j in Line 7 of the *PT* Algorithm considers the feature vector $\mathbf{x}$ componentwise. In particular, if some x_j is zero, Δw_j will be zero as well. Keyword: Hebbian learning [Hebb 1949]

Perceptron Learning

Illustration



- The examples are presented to the perceptron.
- The perceptron computes a value that is interpreted as class label.

Perceptron Learning

Illustration (continued)

Encoding:

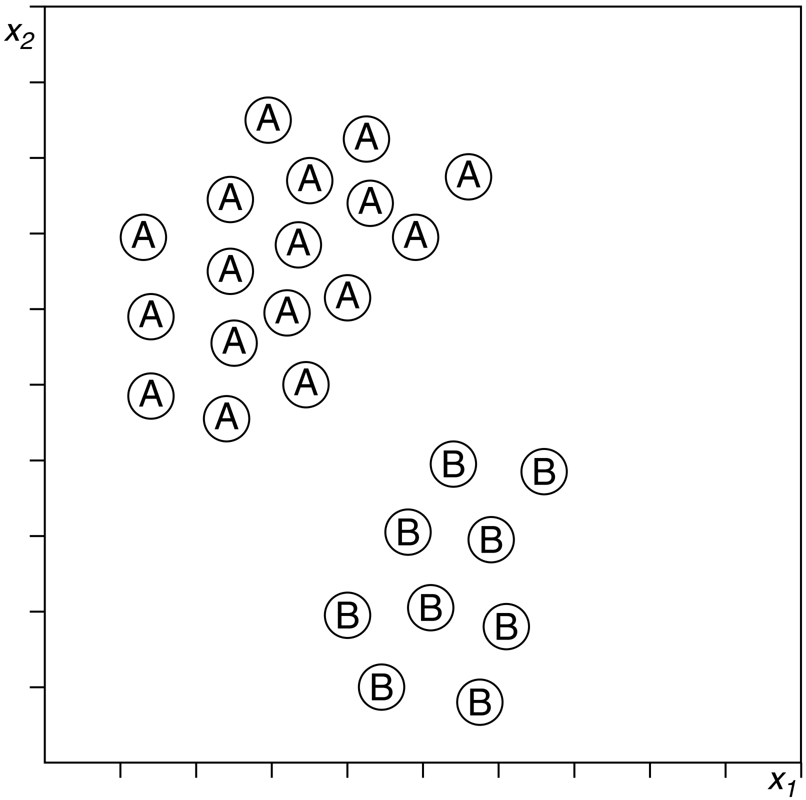
- The encoding of the examples is based on expressive features: number of line crossings, most acute angle, longest line, etc.
- The class label, $c(\mathbf{x})$, is encoded as a number. Examples from A are labeled with 1, examples from B are labeled with 0.

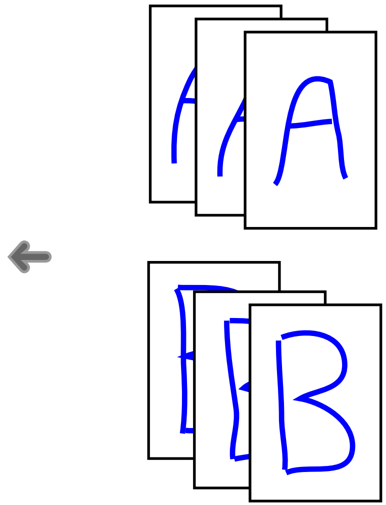
$$\underbrace{\begin{pmatrix} x_{1_1} \\ x_{1_2} \\ \vdots \\ x_{1_p} \end{pmatrix} \quad \cdots \quad \begin{pmatrix} x_{k_1} \\ x_{k_2} \\ \vdots \\ x_{k_p} \end{pmatrix}}_{\text{Class } A \;\simeq\; c(\mathbf{x}) = 1} \qquad \underbrace{\begin{pmatrix} x_{l_1} \\ x_{l_2} \\ \vdots \\ x_{l_p} \end{pmatrix} \quad \cdots \quad \begin{pmatrix} x_{m_1} \\ x_{m_2} \\ \vdots \\ x_{m_p} \end{pmatrix}}_{\text{Class } B \;\simeq\; c(\mathbf{x}) = 0}$$

Perceptron Learning

Illustration (continued)

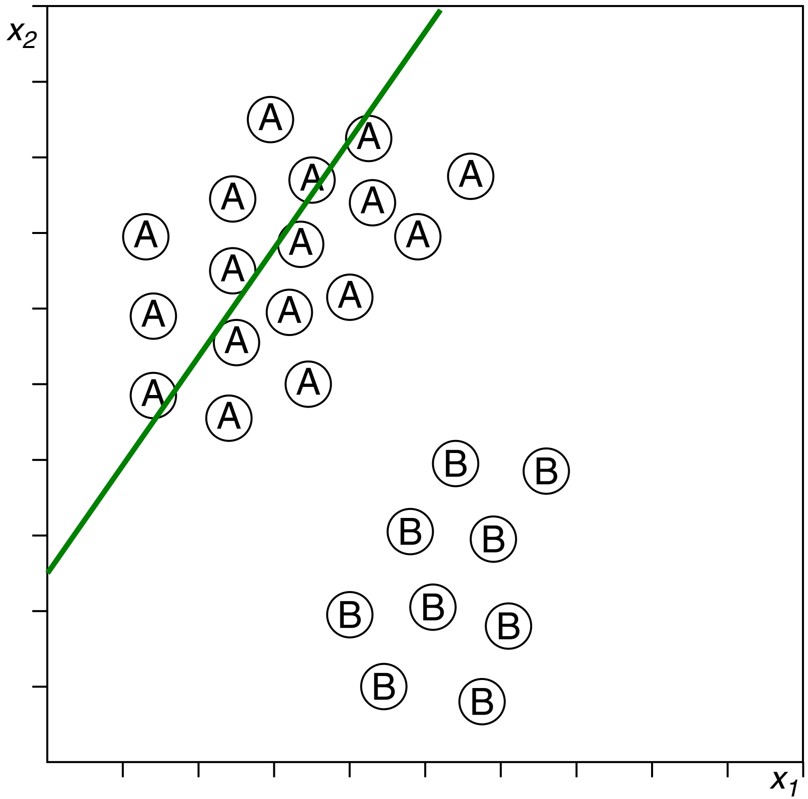
A possible configuration of encoded objects in the feature space X :





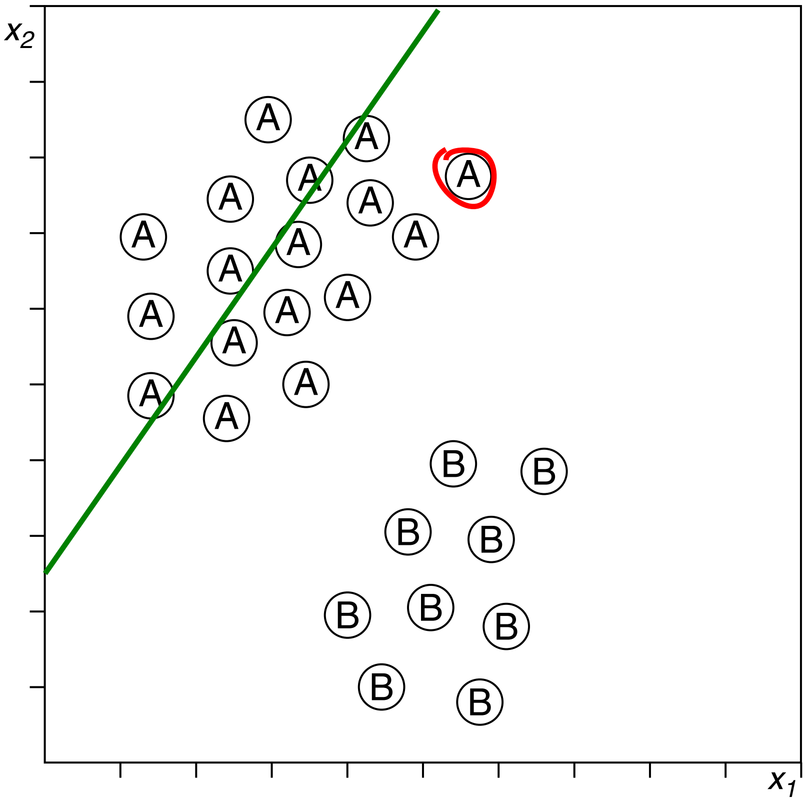
Perceptron Learning

Illustration (continued) [*PT* Algorithm]



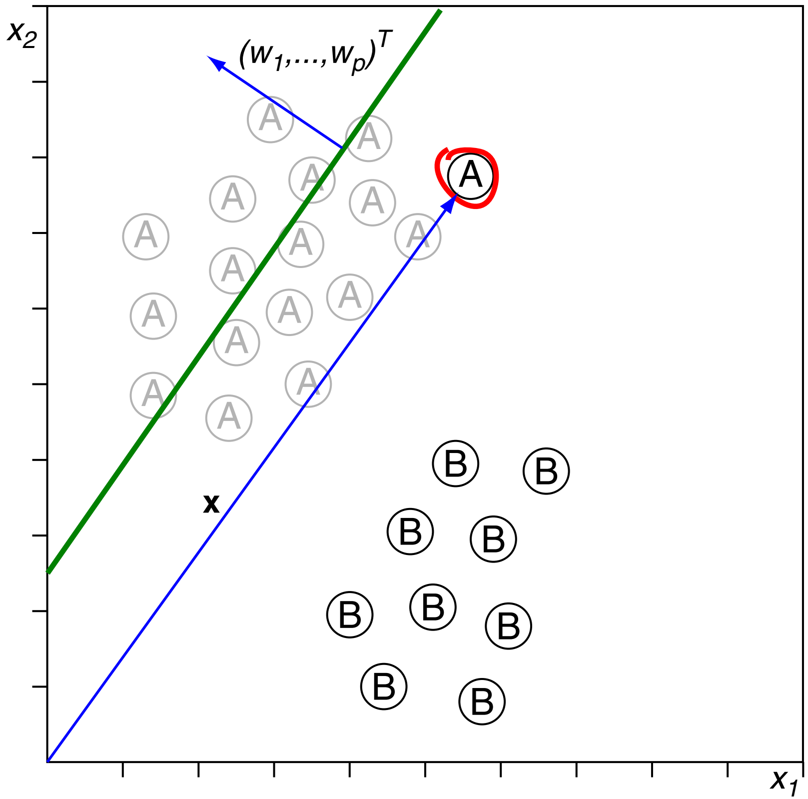
Perceptron Learning

Illustration (continued) [*PT* Algorithm]



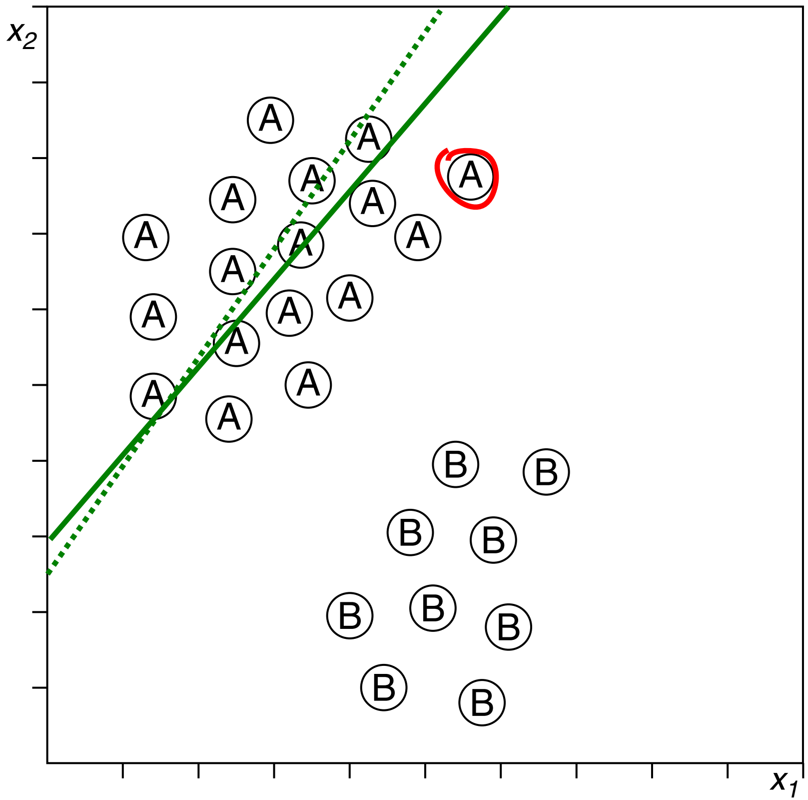
Perceptron Learning

Illustration (continued) [*PT* Algorithm]



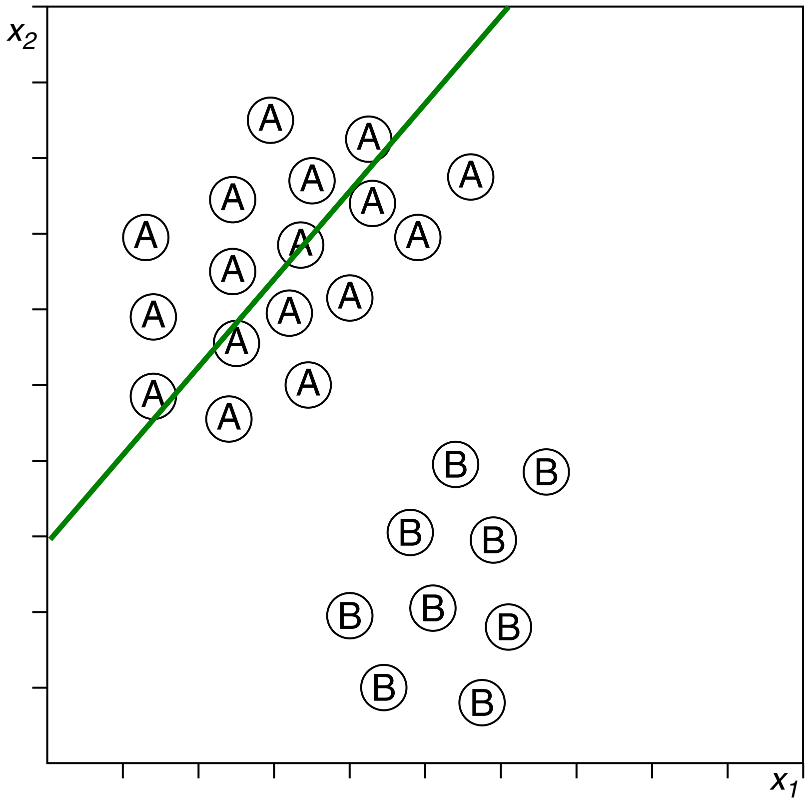
Perceptron Learning

Illustration (continued) [*PT* Algorithm]



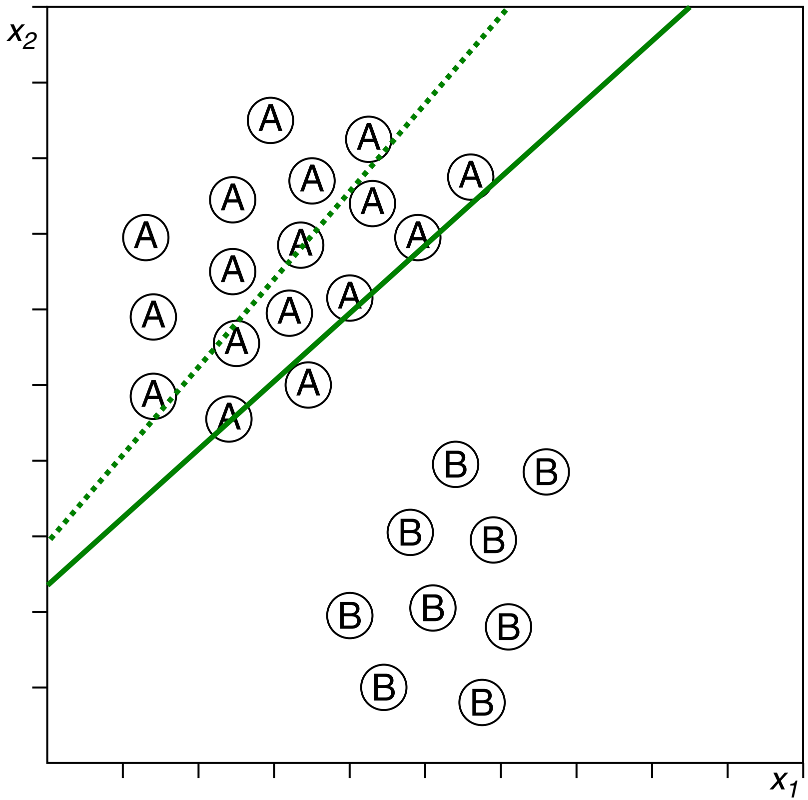
Perceptron Learning

Illustration (continued) [*PT* Algorithm]



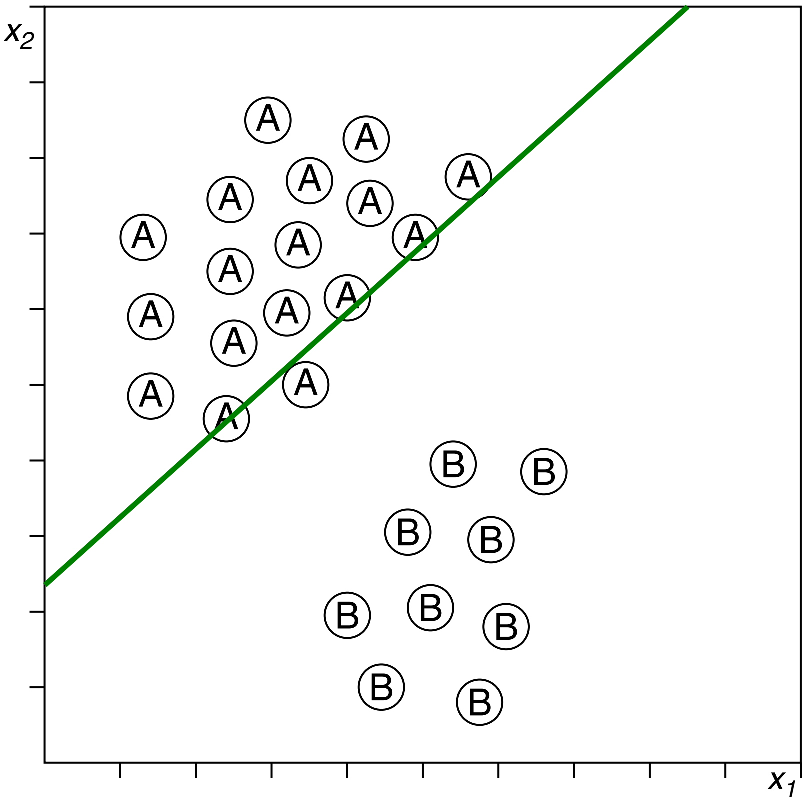
Perceptron Learning

Illustration (continued) [PT Algorithm]



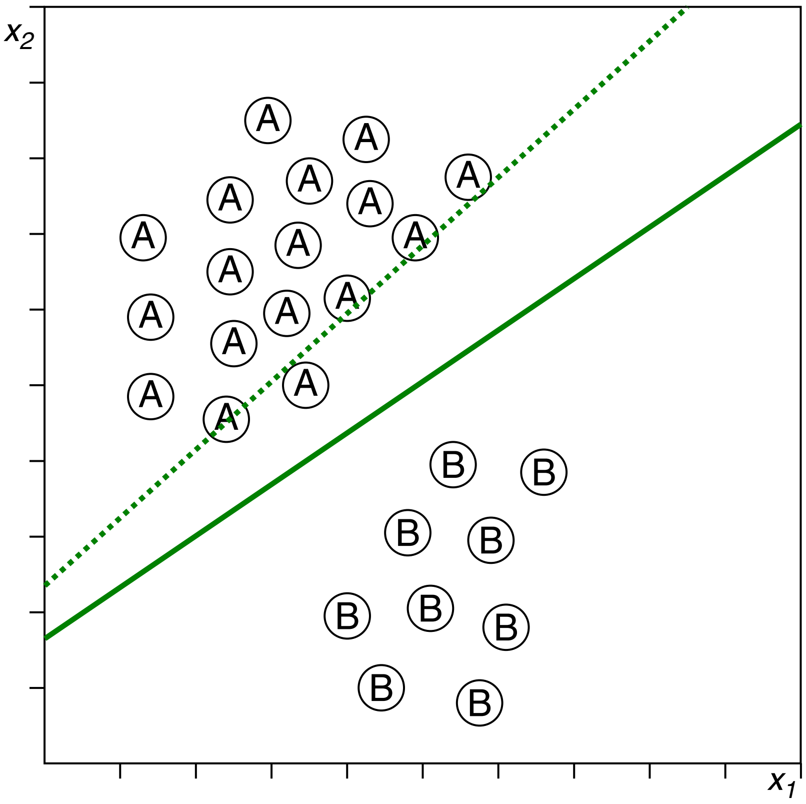
Perceptron Learning

Illustration (continued) [*PT* Algorithm]



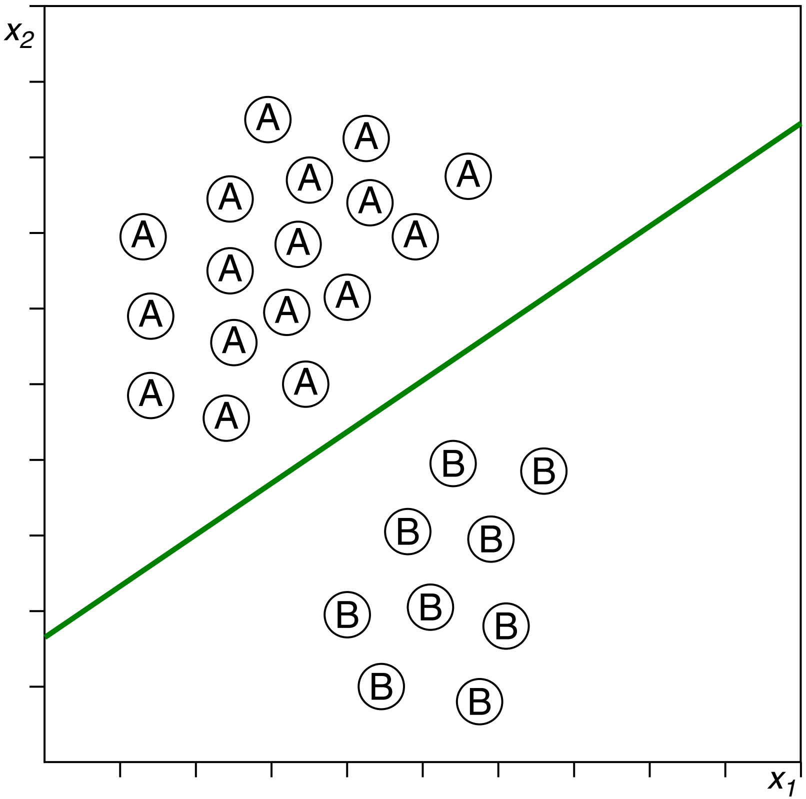
Perceptron Learning

Illustration (continued) [*PT* Algorithm]



Perceptron Learning

Illustration (continued) [*PT* Algorithm]



Perceptron Learning

Perceptron Convergence Theorem

Questions:

1. Which kind of learning tasks can be addressed with the functions of the hypothesis space H?
2. Can the *PT* Algorithm construct such a function for a given task?

Perceptron Learning

Perceptron Convergence Theorem

Questions:

1. Which kind of learning tasks can be addressed with the functions of the hypothesis space H?
2. Can the *PT Algorithm* construct such a function for a given task?

Theorem 1 (Perceptron Convergence [Rosenblatt 1962]**)**

Let X_0 and X_1 be two finite sets with vectors of the form $\mathbf{x} = (1, x_1, \ldots, x_p)^T$, let $X_1 \cap X_0 = \emptyset$, and let $\widehat{\mathbf{w}}$ define a separating hyperplane with respect to X_0 and X_1. Moreover, let D be a set of examples of the form $(\mathbf{x}, 0)$, $\mathbf{x} \in X_0$ and $(\mathbf{x}, 1)$, $\mathbf{x} \in X_1$. Then holds:

If the examples in D are processed with the *PT Algorithm*, the underlying weight vector $\mathbf{w}$ will converge within a finite number of iterations.

Perceptron Learning

Perceptron Convergence Theorem: Proof

Preliminaries:

- The sets X_1 and X_0 are separated by the hyperplane $\widehat{\mathbf{w}}$. The proof requires that for all $\mathbf{x} \in X_1$ the inequality $\widehat{\mathbf{w}}^T\mathbf{x} > 0$ holds. This condition is always fulfilled, as the following consideration shows.

  Let $\mathbf{x}' \in X_1$ with $\widehat{\mathbf{w}}^T\mathbf{x}' = 0$. Since X_0 is finite, the members $\mathbf{x} \in X_0$ have a minimum positive distance δ with regard to the hyperplane $\widehat{\mathbf{w}}$. Hence, $\widehat{\mathbf{w}}$ can be moved by $\frac{\delta}{2}$ towards X_0, resulting in a new hyperplane $\widehat{\mathbf{w}}'$ that still fulfills $(\widehat{\mathbf{w}}')^T\mathbf{x} < 0$ for all $\mathbf{x} \in X_0$, but that now also fulfills $(\widehat{\mathbf{w}}')^T\mathbf{x} > 0$ for all $\mathbf{x} \in X_1$.

Perceptron Learning

Perceptron Convergence Theorem: Proof

Preliminaries:

- The sets X_1 and X_0 are separated by the hyperplane $\widehat{\mathbf{w}}$. The proof requires that for all $\mathbf{x} \in X_1$ the inequality $\widehat{\mathbf{w}}^T\mathbf{x} > 0$ holds. This condition is always fulfilled, as the following consideration shows.
  Let $\mathbf{x}' \in X_1$ with $\widehat{\mathbf{w}}^T\mathbf{x}' = 0$. Since X_0 is finite, the members $\mathbf{x} \in X_0$ have a minimum positive distance δ with regard to the hyperplane $\widehat{\mathbf{w}}$. Hence, $\widehat{\mathbf{w}}$ can be moved by $\frac{\delta}{2}$ towards X_0, resulting in a new hyperplane $\widehat{\mathbf{w}}'$ that still fulfills $(\widehat{\mathbf{w}}')^T\mathbf{x} < 0$ for all $\mathbf{x} \in X_0$, but that now also fulfills $(\widehat{\mathbf{w}}')^T\mathbf{x} > 0$ for all $\mathbf{x} \in X_1$.

- For the weight vector $\mathbf{w}$ that is to be constructed by the *PT* Algorithm, the two inequalities must hold as well: $\mathbf{w}^T\mathbf{x} < 0$ for all $\mathbf{x} \in X_0$, and $\mathbf{w}^T\mathbf{x} > 0$ for all $\mathbf{x} \in X_1$.

- Consider the set $X' = X_1 \cup \{-\mathbf{x} \mid \mathbf{x} \in X_0\}$: the searched $\mathbf{w}$ fulfills $\mathbf{w}^T\mathbf{x} > 0$ for all $\mathbf{x} \in X'$.

Perceptron Learning

Perceptron Convergence Theorem: Proof

Preliminaries:

- The sets X_1 and X_0 are separated by the hyperplane $\widehat{\mathbf{w}}$. The proof requires that for all $\mathbf{x} \in X_1$ the inequality $\widehat{\mathbf{w}}^T\mathbf{x} > 0$ holds. This condition is always fulfilled, as the following consideration shows.
  Let $\mathbf{x}' \in X_1$ with $\widehat{\mathbf{w}}^T\mathbf{x}' = 0$. Since X_0 is finite, the members $\mathbf{x} \in X_0$ have a minimum positive distance δ with regard to the hyperplane $\widehat{\mathbf{w}}$. Hence, $\widehat{\mathbf{w}}$ can be moved by $\frac{\delta}{2}$ towards X_0, resulting in a new hyperplane $\widehat{\mathbf{w}}'$ that still fulfills $(\widehat{\mathbf{w}}')^T\mathbf{x} < 0$ for all $\mathbf{x} \in X_0$, but that now also fulfills $(\widehat{\mathbf{w}}')^T\mathbf{x} > 0$ for all $\mathbf{x} \in X_1$.

- For the weight vector $\mathbf{w}$ that is to be constructed by the *PT* Algorithm, the two inequalities must hold as well: $\mathbf{w}^T\mathbf{x} < 0$ for all $\mathbf{x} \in X_0$, and $\mathbf{w}^T\mathbf{x} > 0$ for all $\mathbf{x} \in X_1$.

- Consider the set $X' = X_1 \cup \{-\mathbf{x} \mid \mathbf{x} \in X_0\}$: the searched $\mathbf{w}$ fulfills $\mathbf{w}^T\mathbf{x} > 0$ for all $\mathbf{x} \in X'$.

- The *PT* Algorithm performs a number of iterations, where $\mathbf{w}(t)$ denotes the weight vector for iteration t, which form the basis for the weight vector $\mathbf{w}(t+1)$. $\mathbf{x}(t) \in X'$ denotes the feature vector chosen in round t, and $c(\mathbf{x}(t))$ denotes the respective class label. The first (and randomly chosen) weight vector is denoted as $\mathbf{w}(0)$.

- Recall the Cauchy-Schwarz inequality: $||\mathbf{a}||^2 \cdot ||\mathbf{b}||^2 \geq (\mathbf{a}^T\mathbf{b})^2$, where $||\mathbf{x}|| := \sqrt{\mathbf{x}^T\mathbf{x}}$ denotes the Euclidean norm.

Perceptron Learning

Perceptron Convergence Theorem: Proof (continued)

Line of argument:

(a) A lower bound for the adapation of $\mathbf{w}$ can be stated. The derivation of this lower bound exploits the presupposed linear separability of X_0 and X_1, which in turn guarantees the existence of a separating hyperplane $\widehat{\mathbf{w}}$.

(b) An upper bound for the adapation of $\mathbf{w}$ can be stated. The derivation of this upper bound exploits the finiteness of X_0 and X_1, which in turn guarantees an upper bound for the norm of the maximum feature vector.

(c) Both bounds can be expressed as functions in the number of iterations n, where the lower bound grows faster than the upper bound. Hence, in order to fulfill the inequality, the number of iterations is finite.

Perceptron Learning

Perceptron Convergence Theorem: Proof (continued)

1. The *PT* Algorithm computes in iteration t the scalar product $\mathbf{w}(t)^T\mathbf{x}(t)$. If classified correctly, $\mathbf{w}(t)^T\mathbf{x}(t) > 0$ and $\mathbf{w}$ is unchanged. Otherwise, $\mathbf{w}(t+1) = \mathbf{w}(t) + \eta \cdot \mathbf{x}(t)$.

Perceptron Learning

Perceptron Convergence Theorem: Proof (continued)

1. The *PT* Algorithm computes in iteration t the scalar product $\mathbf{w}(t)^T\mathbf{x}(t)$. If classified correctly, $\mathbf{w}(t)^T\mathbf{x}(t) > 0$ and $\mathbf{w}$ is unchanged. Otherwise, $\mathbf{w}(t+1) = \mathbf{w}(t) + \eta \cdot \mathbf{x}(t)$.

2. Consider a sequence of n incorrectly classified feature vectors, $(x(t))$, along with the corresponding weight vector adaptation, $\mathbf{w}(t+1) = \mathbf{w}(t) + \eta \cdot \mathbf{x}(t)$:
   - $\mathbf{w}(1) = \mathbf{w}(0) + \eta \cdot \mathbf{x}(0)$
   - $\mathbf{w}(2) = \mathbf{w}(1) + \eta \cdot \mathbf{x}(1) = \mathbf{w}(0) + \eta \cdot \mathbf{x}(0) + \eta \cdot \mathbf{x}(1)$

   $\vdots$
   - $\mathbf{w}(n) = \mathbf{w}(0) + \eta \cdot \mathbf{x}(0) + \ldots + \eta \cdot \mathbf{x}(n-1)$

Perceptron Learning

Perceptron Convergence Theorem: Proof (continued)

1. The *PT* Algorithm computes in iteration t the scalar product $\mathbf{w}(t)^T\mathbf{x}(t)$. If classified correctly, $\mathbf{w}(t)^T\mathbf{x}(t) > 0$ and $\mathbf{w}$ is unchanged. Otherwise, $\mathbf{w}(t+1) = \mathbf{w}(t) + \eta \cdot \mathbf{x}(t)$.

2. Consider a sequence of n incorrectly classified feature vectors, $(x(t))$, along with the corresponding weight vector adaptation, $\mathbf{w}(t+1) = \mathbf{w}(t) + \eta \cdot \mathbf{x}(t)$:
   - $\mathbf{w}(1) = \mathbf{w}(0) + \eta \cdot \mathbf{x}(0)$
   - $\mathbf{w}(2) = \mathbf{w}(1) + \eta \cdot \mathbf{x}(1) = \mathbf{w}(0) + \eta \cdot \mathbf{x}(0) + \eta \cdot \mathbf{x}(1)$

   $\vdots$
   - $\mathbf{w}(n) = \mathbf{w}(0) + \eta \cdot \mathbf{x}(0) + \ldots + \eta \cdot \mathbf{x}(n-1)$

3. The hyperplane defined by $\widehat{\mathbf{w}}$ separates X_1 and X_0 : $\forall \mathbf{x} \in X' : \widehat{\mathbf{w}}^T\mathbf{x} > 0$
   Let $\delta := \min_{\mathbf{x} \in X'} \widehat{\mathbf{w}}^T\mathbf{x}$. Observe that $\delta > 0$ holds.

Perceptron Learning

Perceptron Convergence Theorem: Proof (continued)

1. The *PT* Algorithm computes in iteration t the scalar product $\mathbf{w}(t)^T\mathbf{x}(t)$. If classified correctly, $\mathbf{w}(t)^T\mathbf{x}(t) > 0$ and $\mathbf{w}$ is unchanged. Otherwise, $\mathbf{w}(t+1) = \mathbf{w}(t) + \eta \cdot \mathbf{x}(t)$.

2. Consider a sequence of n incorrectly classified feature vectors, $(x(t))$, along with the corresponding weight vector adaptation, $\mathbf{w}(t+1) = \mathbf{w}(t) + \eta \cdot \mathbf{x}(t)$:
   - $\mathbf{w}(1) = \mathbf{w}(0) + \eta \cdot \mathbf{x}(0)$
   - $\mathbf{w}(2) = \mathbf{w}(1) + \eta \cdot \mathbf{x}(1) = \mathbf{w}(0) + \eta \cdot \mathbf{x}(0) + \eta \cdot \mathbf{x}(1)$

   $\vdots$
   - $\mathbf{w}(n) = \mathbf{w}(0) + \ \eta \cdot \mathbf{x}(0) + \ldots + \eta \cdot \mathbf{x}(n-1)$

3. The hyperplane defined by $\widehat{\mathbf{w}}$ separates X_1 and X_0 : $\forall \mathbf{x} \in X' : \widehat{\mathbf{w}}^T\mathbf{x} > 0$
   Let $\delta := \min\limits_{\mathbf{x} \in X'} \widehat{\mathbf{w}}^T\mathbf{x}$. Observe that $\delta > 0$ holds.

4. Analyze the scalar product between $\mathbf{w}(n)$ and $\widehat{\mathbf{w}}$:

$$\begin{aligned}
& \widehat{\mathbf{w}}^T\mathbf{w}(n) = \widehat{\mathbf{w}}^T\mathbf{w}(0) + \eta \cdot \widehat{\mathbf{w}}^T\mathbf{x}(0) + \ldots + \eta \cdot \widehat{\mathbf{w}}^T\mathbf{x}(n-1) \\
\Rightarrow \quad & \widehat{\mathbf{w}}^T\mathbf{w}(n) \geq \widehat{\mathbf{w}}^T\mathbf{w}(0) + n\eta\delta \geq 0 \\
\Rightarrow \quad & (\widehat{\mathbf{w}}^T\mathbf{w}(n))^2 \geq (\widehat{\mathbf{w}}^T\mathbf{w}(0) + n\eta\delta)^2
\end{aligned}$$

5. Apply the Cauchy-Schwarz inequality:

$$||\widehat{\mathbf{w}}||^2 \cdot ||\mathbf{w}(n)||^2 \ \geq \ (\widehat{\mathbf{w}}^T\mathbf{w}(0) + n\eta\delta)^2 \quad \Rightarrow \quad ||\mathbf{w}(n)||^2 \ \geq \ \frac{(\widehat{\mathbf{w}}^T\mathbf{w}(0) + n\eta\delta)^2}{||\widehat{\mathbf{w}}||^2}$$

Perceptron Learning

Perceptron Convergence Theorem: Proof (continued)

6. Consider again the weight adaptation $\mathbf{w}(t+1) = \mathbf{w}(t) + \eta \cdot \mathbf{x}(t)$:

$$\begin{aligned}
||\mathbf{w}(t+1)||^2 &= ||\mathbf{w}(t) + \eta \cdot \mathbf{x}(t)||^2 \\
&= (\mathbf{w}(t) + \eta \cdot \mathbf{x}(t))^T (\mathbf{w}(t) + \eta \cdot \mathbf{x}(t)) \\
&= \mathbf{w}(t)^T \mathbf{w}(t) + \eta^2 \cdot \mathbf{x}(t)^T \mathbf{x}(t) + 2\eta \cdot \mathbf{w}(t)^T \mathbf{x}(t) \\
&\leq ||\mathbf{w}(t)||^2 + ||\eta \cdot \mathbf{x}(t)||^2, \quad \text{since} \ \ \mathbf{w}(t)^T \mathbf{x}(t) < 0
\end{aligned}$$

Perceptron Learning

Perceptron Convergence Theorem: Proof (continued)

6. Consider again the weight adaptation $\mathbf{w}(t+1) = \mathbf{w}(t) + \eta \cdot \mathbf{x}(t)$:

$$\begin{aligned}
||\mathbf{w}(t+1)||^2 &= ||\mathbf{w}(t) + \eta \cdot \mathbf{x}(t)||^2 \\
&= (\mathbf{w}(t) + \eta \cdot \mathbf{x}(t))^T(\mathbf{w}(t) + \eta \cdot \mathbf{x}(t)) \\
&= \mathbf{w}(t)^T\mathbf{w}(t) + \eta^2 \cdot \mathbf{x}(t)^T\mathbf{x}(t) + 2\eta \cdot \mathbf{w}(t)^T\mathbf{x}(t) \\
&\leq ||\mathbf{w}(t)||^2 + ||\eta \cdot \mathbf{x}(t)||^2, \quad \text{since } \mathbf{w}(t)^T\mathbf{x}(t) < 0
\end{aligned}$$

7. Consider a sequence of n weight adaptations:

$$\begin{aligned}
||\mathbf{w}(n)||^2 &\leq ||\mathbf{w}(n-1)||^2 + ||\eta \cdot \mathbf{x}(n-1)||^2 \\
&\leq ||\mathbf{w}(n-2)||^2 + ||\eta \cdot \mathbf{x}(n-2)||^2 + ||\eta \cdot \mathbf{x}(n-1)||^2 \\
&\leq ||\mathbf{w}(0)||^2 + ||\eta \cdot \mathbf{x}(0)||^2 + \ldots + ||\eta \cdot \mathbf{x}(n-1)||^2 \\
&= ||\mathbf{w}(0)||^2 + \sum_{j=0}^{n-1} ||\eta \cdot \mathbf{x}(i)||^2
\end{aligned}$$

8. With $\varepsilon := \max_{\mathbf{x} \in X'} ||\mathbf{x}||^2$ follows $||\mathbf{w}(n)||^2 \leq ||\mathbf{w}(0)||^2 + n\eta^2\varepsilon$

9. Both inequalities must be fulfilled:

$$||\mathbf{w}(n)||^2 \geq \frac{(\widehat{\mathbf{w}}^T\mathbf{w}(0) + n\eta\delta)^2}{||\widehat{\mathbf{w}}||^2} \quad \text{and} \quad ||\mathbf{w}(n)||^2 \leq ||\mathbf{w}(0)||^2 + n\eta^2\varepsilon, \text{ hence}$$

$$\frac{(\widehat{\mathbf{w}}^T\mathbf{w}(0) + n\eta\delta)^2}{||\widehat{\mathbf{w}}||^2} \leq ||\mathbf{w}(n)||^2 \leq ||\mathbf{w}(0)||^2 + n\eta^2\varepsilon$$

10. Observe:

$$\frac{(\widehat{\mathbf{w}}^T\mathbf{w}(0) + n\eta\delta)^2}{||\widehat{\mathbf{w}}||^2} \in \Theta(n^2) \quad \text{and} \quad ||\mathbf{w}(0)||^2 + n\eta^2\varepsilon \in \Theta(n)$$

Perceptron Learning

Perceptron Convergence Theorem: Proof (continued)

9. Both inequalities must be fulfilled:

$$||\mathbf{w}(n)||^2 \geq \frac{(\widehat{\mathbf{w}}^T\mathbf{w}(0) + n\eta\delta)^2}{||\widehat{\mathbf{w}}||^2} \quad \text{and} \quad ||\mathbf{w}(n)||^2 \leq ||\mathbf{w}(0)||^2 + n\eta^2\varepsilon, \text{ hence}$$

$$\frac{(\widehat{\mathbf{w}}^T\mathbf{w}(0) + n\eta\delta)^2}{||\widehat{\mathbf{w}}||^2} \leq ||\mathbf{w}(n)||^2 \leq ||\mathbf{w}(0)||^2 + n\eta^2\varepsilon$$

10. Observe:

$$\frac{(\widehat{\mathbf{w}}^T\mathbf{w}(0) + n\eta\delta)^2}{||\widehat{\mathbf{w}}||^2} \in \Theta(n^2) \quad \text{and} \quad ||\mathbf{w}(0)||^2 + n\eta^2\varepsilon \in \Theta(n)$$

11. An upper bound for n:

$$\frac{(\widehat{\mathbf{w}}^T\mathbf{w}(0) + n\eta\delta)^2}{||\widehat{\mathbf{w}}||^2} \leq ||\mathbf{w}(0)||^2 + n\eta^2\varepsilon$$

For $\mathbf{w}(0) = \mathbf{0}$ (set all initial weights to zero) follows:

$$0 < n \leq \frac{\varepsilon}{\delta^2}||\widehat{\mathbf{w}}||^2$$

➜ The *PT Algorithm* terminates within a finite number of iterations.

Perceptron Learning

Perceptron Convergence Theorem: Discussion

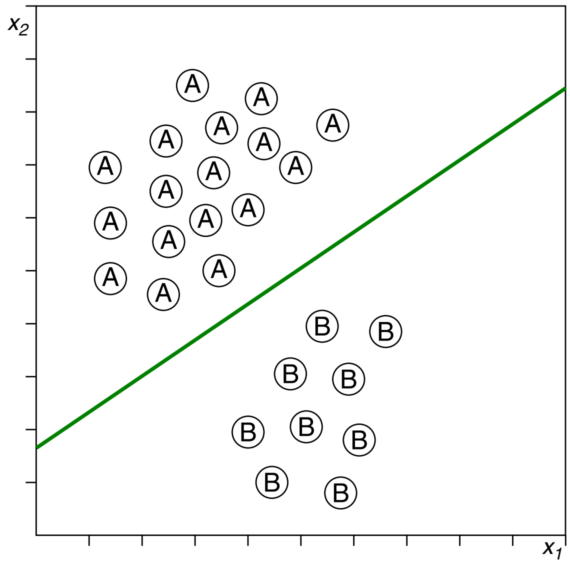
- If a separating hyperplane between X_0 and X_1 exists, the *PT* Algorithm will converge. If no such hyperplane exists, convergence cannot be guaranteed.
- A separating hyperplane can be found in polynomial time with linear programming. The *PT* Algorithm, however, may require an exponential number of iterations.

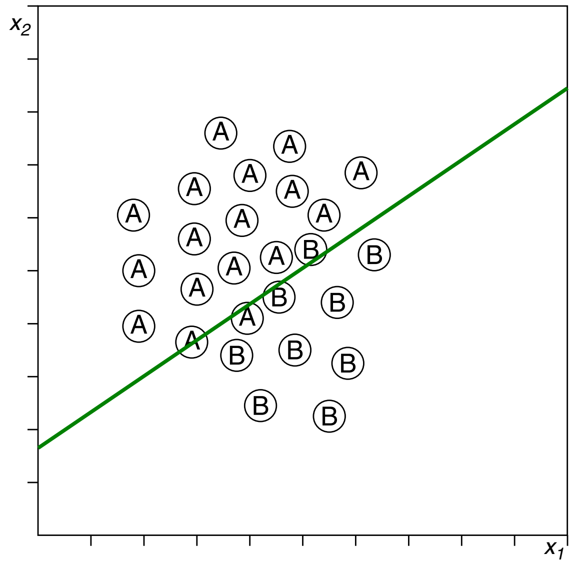
Perceptron Learning

Perceptron Convergence Theorem: Discussion

- If a separating hyperplane between X_0 and X_1 exists, the *PT* Algorithm will converge. If no such hyperplane exists, convergence cannot be guaranteed.
- A separating hyperplane can be found in polynomial time with linear programming. The *PT* Algorithm, however, may require an exponential number of iterations.

- Classification problems with noise (right-hand side) are problematic:





Gradient Descent

Classification Error

Gradient descent considers the true error (better: the hyperplane distance) and will converge even if X_1 and X_0 cannot be separated by a hyperplane. However, this convergence process is of an asymptotic nature and no finite iteration bound can be stated.

Gradient descent applies the so-called *delta rule*, which will be derived in the following. The delta rule forms the basis of the backpropagation algorithm.

Gradient Descent

Classification Error

Gradient descent considers the true error (better: the hyperplane distance) and will converge even if X_1 and X_0 cannot be separated by a hyperplane. However, this convergence process is of an asymptotic nature and no finite iteration bound can be stated.

Gradient descent applies the so-called *delta rule*, which will be derived in the following. The delta rule forms the basis of the backpropagation algorithm.

Consider the linear perceptron *without* a threshold function:

$$y(\mathbf{x}) = \mathbf{w}^T\mathbf{x} = \sum_{j=0}^{p} w_j x_j$$

[Heaviside]

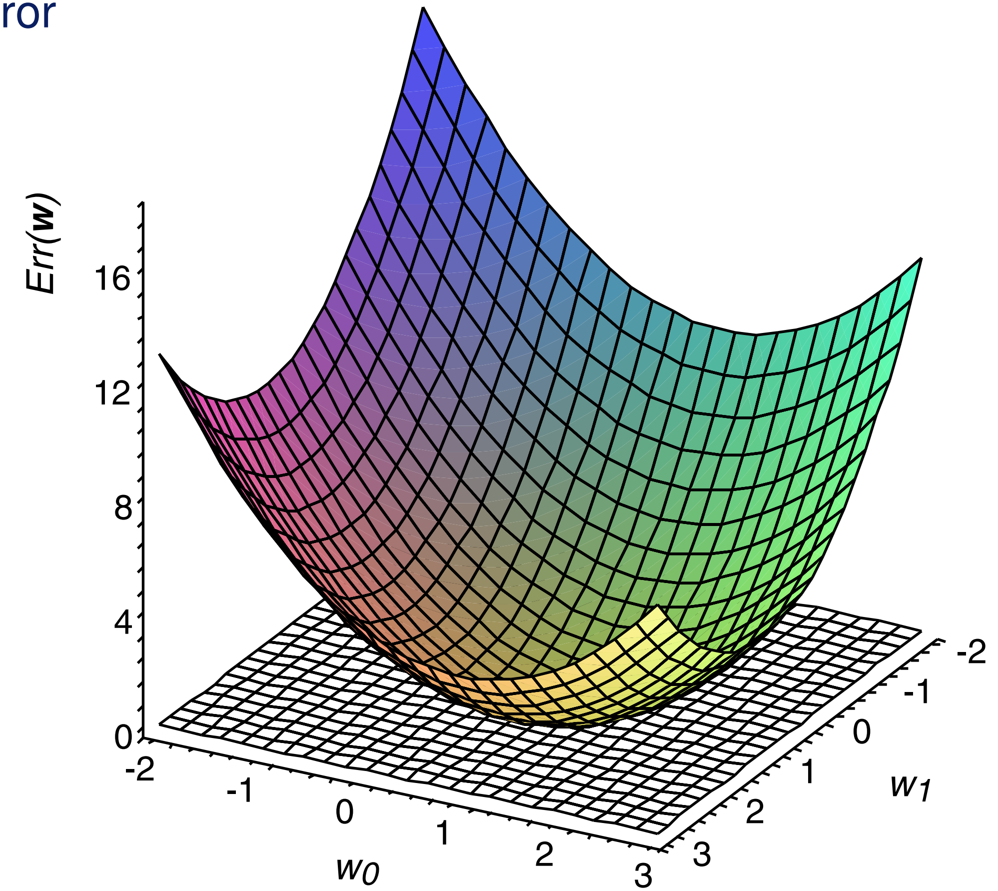
The classification error *Err*$(\mathbf{w})$ of a weight vector (= hypothesis) $\mathbf{w}$ with regard to D can be defined as follows:

$$\textit{Err}(\mathbf{w}) = \frac{1}{2} \sum_{(\mathbf{x}, c(\mathbf{x})) \in D} (c(\mathbf{x}) - y(\mathbf{x}))^2$$

[Singleton error]

Gradient Descent

Classification Error



The gradient $\nabla \mathit{Err}(\mathbf{w})$ of $\mathit{Err}(\mathbf{w})$ defines the steepest ascent or descent:

$$\nabla \mathit{Err}(\mathbf{w}) = \left(\frac{\partial \mathit{Err}(\mathbf{w})}{\partial w_0}, \frac{\partial \mathit{Err}(\mathbf{w})}{\partial w_1}, \ldots, \frac{\partial \mathit{Err}(\mathbf{w})}{\partial w_p} \right)$$

Gradient Descent

Weight Adaptation

$$\mathbf{w} \;\leftarrow\; \mathbf{w} + \Delta\mathbf{w} \quad \text{where} \quad \Delta\mathbf{w} = -\eta \nabla \mathit{Err}(\mathbf{w})$$

Componentwise (dimension-wise) weight adaptation:

$$w_j \;\leftarrow\; w_j + \Delta w_j \quad \text{where} \quad \Delta w_j \;=\; -\eta \, \frac{\partial}{\partial w_j} \mathit{Err}(\mathbf{w})$$

Gradient Descent

Weight Adaptation

$$\mathbf{w} \;\leftarrow\; \mathbf{w} + \Delta\mathbf{w} \quad \text{where} \quad \Delta\mathbf{w} = -\eta \nabla \mathit{Err}(\mathbf{w})$$

Componentwise (dimension-wise) weight adaptation:

$$w_j \;\leftarrow\; w_j + \Delta w_j \quad \text{where} \quad \Delta w_j \;=\; -\eta \, \frac{\partial}{\partial w_j} \mathit{Err}(\mathbf{w})$$

$$\frac{\partial}{\partial w_j} \mathit{Err}(\mathbf{w}) \;=\; \frac{\partial}{\partial w_j} \frac{1}{2} \sum_{(\mathbf{x}, c(\mathbf{x})) \in D} (c(\mathbf{x}) - y(\mathbf{x}))^2 = \frac{1}{2} \sum_{(\mathbf{x}, c(\mathbf{x})) \in D} \frac{\partial}{\partial w_j} (c(\mathbf{x}) - y(\mathbf{x}))^2$$

Gradient Descent

Weight Adaptation

$$\mathbf{w} \leftarrow \mathbf{w} + \Delta\mathbf{w} \quad \text{where} \quad \Delta\mathbf{w} = -\eta \nabla \mathit{Err}(\mathbf{w})$$

Componentwise (dimension-wise) weight adaptation:

$$w_j \leftarrow w_j + \Delta w_j \quad \text{where} \quad \Delta w_j = -\eta \frac{\partial}{\partial w_j} \mathit{Err}(\mathbf{w})$$

$$\frac{\partial}{\partial w_j} \mathit{Err}(\mathbf{w}) = \frac{\partial}{\partial w_j} \frac{1}{2} \sum_{(\mathbf{x}, c(\mathbf{x})) \in D} (c(\mathbf{x}) - y(\mathbf{x}))^2 = \frac{1}{2} \sum_{(\mathbf{x}, c(\mathbf{x})) \in D} \frac{\partial}{\partial w_j} (c(\mathbf{x}) - y(\mathbf{x}))^2$$

$$= \frac{1}{2} \sum_{(\mathbf{x}, c(\mathbf{x})) \in D} 2(c(\mathbf{x}) - y(\mathbf{x})) \cdot \frac{\partial}{\partial w_j} (c(\mathbf{x}) - y(\mathbf{x}))$$

Gradient Descent

Weight Adaptation

$$\mathbf{w} \;\leftarrow\; \mathbf{w} + \Delta\mathbf{w} \quad \text{where} \quad \Delta\mathbf{w} = -\eta \nabla \mathit{Err}(\mathbf{w})$$

Componentwise (dimension-wise) weight adaptation:

$$w_j \;\leftarrow\; w_j + \Delta w_j \quad \text{where} \quad \Delta w_j \;=\; -\eta \, \frac{\partial}{\partial w_j} \mathit{Err}(\mathbf{w})$$

$$\frac{\partial}{\partial w_j} \mathit{Err}(\mathbf{w}) \;=\; \frac{\partial}{\partial w_j} \frac{1}{2} \sum_{(\mathbf{x}, c(\mathbf{x})) \in D} (c(\mathbf{x}) - y(\mathbf{x}))^2 = \frac{1}{2} \sum_{(\mathbf{x}, c(\mathbf{x})) \in D} \frac{\partial}{\partial w_j} (c(\mathbf{x}) - y(\mathbf{x}))^2$$

$$= \frac{1}{2} \sum_{(\mathbf{x}, c(\mathbf{x})) \in D} 2(c(\mathbf{x}) - y(\mathbf{x})) \cdot \frac{\partial}{\partial w_j} (c(\mathbf{x}) - y(\mathbf{x}))$$

$$= \sum_{(\mathbf{x}, c(\mathbf{x})) \in D} (c(\mathbf{x}) - \mathbf{w}^T\mathbf{x}) \cdot \frac{\partial}{\partial w_j} (c(\mathbf{x}) - \mathbf{w}^T\mathbf{x})$$

Gradient Descent

Weight Adaptation

$$\mathbf{w} \leftarrow \mathbf{w} + \Delta\mathbf{w} \quad \text{where} \quad \Delta\mathbf{w} = -\eta \nabla \mathit{Err}(\mathbf{w})$$

Componentwise (dimension-wise) weight adaptation:

$$w_j \leftarrow w_j + \Delta w_j \quad \text{where} \quad \Delta w_j = -\eta \frac{\partial}{\partial w_j} \mathit{Err}(\mathbf{w}) = \eta \sum_{(\mathbf{x},c(\mathbf{x}))\in D} (c(\mathbf{x}) - \mathbf{w}^T\mathbf{x}) \cdot x_j$$

$$\frac{\partial}{\partial w_j} \mathit{Err}(\mathbf{w}) = \frac{\partial}{\partial w_j} \frac{1}{2} \sum_{(\mathbf{x},c(\mathbf{x}))\in D} (c(\mathbf{x}) - y(\mathbf{x}))^2 = \frac{1}{2} \sum_{(\mathbf{x},c(\mathbf{x}))\in D} \frac{\partial}{\partial w_j} (c(\mathbf{x}) - y(\mathbf{x}))^2$$

$$= \frac{1}{2} \sum_{(\mathbf{x},c(\mathbf{x}))\in D} 2(c(\mathbf{x}) - y(\mathbf{x})) \cdot \frac{\partial}{\partial w_j} (c(\mathbf{x}) - y(\mathbf{x}))$$

$$= \sum_{(\mathbf{x},c(\mathbf{x}))\in D} (c(\mathbf{x}) - \mathbf{w}^T\mathbf{x}) \cdot \frac{\partial}{\partial w_j} (c(\mathbf{x}) - \mathbf{w}^T\mathbf{x})$$

$$= \sum_{(\mathbf{x},c(\mathbf{x}))\in D} (c(\mathbf{x}) - \mathbf{w}^T\mathbf{x})(-x_j)$$

Gradient Descent

Weight Adaptation: Batch Gradient Descent [*IGD* Algorithm]

Algorithm:	*BGD*	Batch Gradient Descent
Input:	D	Training examples of the form $(\mathbf{x}, c(\mathbf{x}))$ with $\vert\mathbf{x}\vert = p+1$, $c(\mathbf{x}) \in \{0, 1\}$.
	η	Learning rate, a small positive constant.
Internal:	$y(D)$	Set of $y(\mathbf{x})$-values computed from the elements $\mathbf{x}$ in D given some $\mathbf{w}$.
Output:	$\mathbf{w}$	Weight vector.

BGD(D, η)

initialize_random_weights$(\mathbf{w})$, $t = 0$
REPEAT
  $t = t + 1$
  FOR $j = 0$ **TO** p **DO** $\Delta w_j = 0$
  FOREACH $(\mathbf{x}, c(\mathbf{x})) \in D$ DO
    error $= c(\mathbf{x}) - \mathbf{w}^T\mathbf{x}$
    FOR $j = 0$ **TO** p **DO** $\Delta w_j = \Delta w_j + \eta \cdot$ *error* $\cdot\, x_j$
  ENDDO
  FOR $j = 0$ **TO** p **DO** $w_j = w_j + \Delta w_j$
UNTIL(*convergence*$(D, y(D))$ **OR** $t > t_{\text{max}}$)
return$(\mathbf{w})$

Gradient Descent

Weight Adaptation: Delta Rule

The weight adaptation in the *BGD* Algorithm is set-based: before modifying a weight component in $\mathbf{w}$, the total error of *all* examples (the "batch") is computed.

Weight adaptation with regard to a *single* example $(\mathbf{x}, c(\mathbf{x})) \in D$:

$$\Delta w_j = \eta \cdot (c(\mathbf{x}) - \mathbf{w}^T\mathbf{x}) \cdot x_j$$

This adaptation rule is known under different names:

- delta rule
- Widrow-Hoff rule
- adaline rule
- least mean squares (LMS) rule

The classification error $Err_d(\mathbf{w})$ of a weight vector (= hypothesis) $\mathbf{w}$ with regard to a single example $d \in D$, $d = (\mathbf{x}, c(\mathbf{x}))$, is given as:

$$Err_d(\mathbf{w}) = \frac{1}{2}(c(\mathbf{x}) - \mathbf{w}^T\mathbf{x})^2$$

[Batch error]

Gradient Descent

Weight Adaptation: Incremental Gradient Descent [Algorithms *LMS* *BGD* *PT*]

Algorithm:	*IGD*	Incremental Gradient Descent
Input:	D	Training examples of the form $(\mathbf{x}, c(\mathbf{x}))$ with $\lvert\mathbf{x}\rvert = p+1$, $c(\mathbf{x}) \in \{0, 1\}$.
	η	Learning rate, a small positive constant.
Internal:	$y(D)$	Set of $y(\mathbf{x})$-values computed from the elements $\mathbf{x}$ in D given some $\mathbf{w}$.
Output:	$\mathbf{w}$	Weight vector.

IGD(D, η)

1. *initialize_random_weights*$(\mathbf{w})$, $t = 0$
2. **REPEAT**
3. $\quad t = t + 1$
4. $\quad$ FOREACH $(\mathbf{x}, c(\mathbf{x})) \in D$ DO
5. $\qquad$ *error* $= c(\mathbf{x}) - \mathbf{w}^T\mathbf{x}$
6. $\qquad$ **FOR** $j = 0$ **TO** p **DO**
7. $\qquad\quad \Delta w_j = \eta \cdot$ *error* $\cdot\, x_j$
$\qquad\quad w_j = w_j + \Delta w_j$
8. $\qquad$ **ENDDO**
9. $\quad$ ENDDO
10. **UNTIL**(*convergence*$(D, y(D))$ **OR** $t > t_{\max}$)
11. *return*$(\mathbf{w})$

Remarks:

- The classification error *Err* of incremental gradient descent is specific for each training example $d \in D$, $d = (\mathbf{x}, c(\mathbf{x}))$: $Err_d(\mathbf{w}) = \frac{1}{2}(c(\mathbf{x}) - \mathbf{w}^T\mathbf{x})^2$

- The sequence of incremental weight adaptations approximates the gradient descent of the batch approach. If η is chosen sufficiently small, this approximation can happen at arbitrary accuracy.

- The computation of the total error of batch gradient descent enables larger weight adaptation increments.

- Compared to batch gradient descent, the example-based weight adaptation of incremental gradient descent can better avoid getting stuck in a local minimum of the error function.

Remarks (continued):

- The incremental gradient descend algorithm corresponds to the least mean squares (LMS) algorithm.
- The incremental gradient descend algorithm is similar to the perceptron training (PT) algorithm except for the fact that the latter applies the Heaviside function within the error computation. Consequences:
  - Gradient descend will converge even if the data is not linear separable.
  - Provided linear separability, the PT algorithm converges within a finite number of iterations, which, however, cannot be guaranteed for gradient descend.
  - The error function of the PT algorithm is not differentiable, which prohibits an effective exploitation of the resdiua.
- Incremental gradient descent is also called *stochastic* gradient descent.

Chapter ML:VI (continued)

VI. Neural Networks

- Perceptron Learning
- Gradient Descent
- Multilayer Perceptron
- Radial Basis Functions

Multilayer Perceptron

Definition 1 (Linear Separability)

Two sets of feature vectors, X_0, X_1, of a p-dimensional feature space are called linearly separable, if $p+1$ real numbers, $\theta, w_1, \ldots, w_p$, exist such that holds:

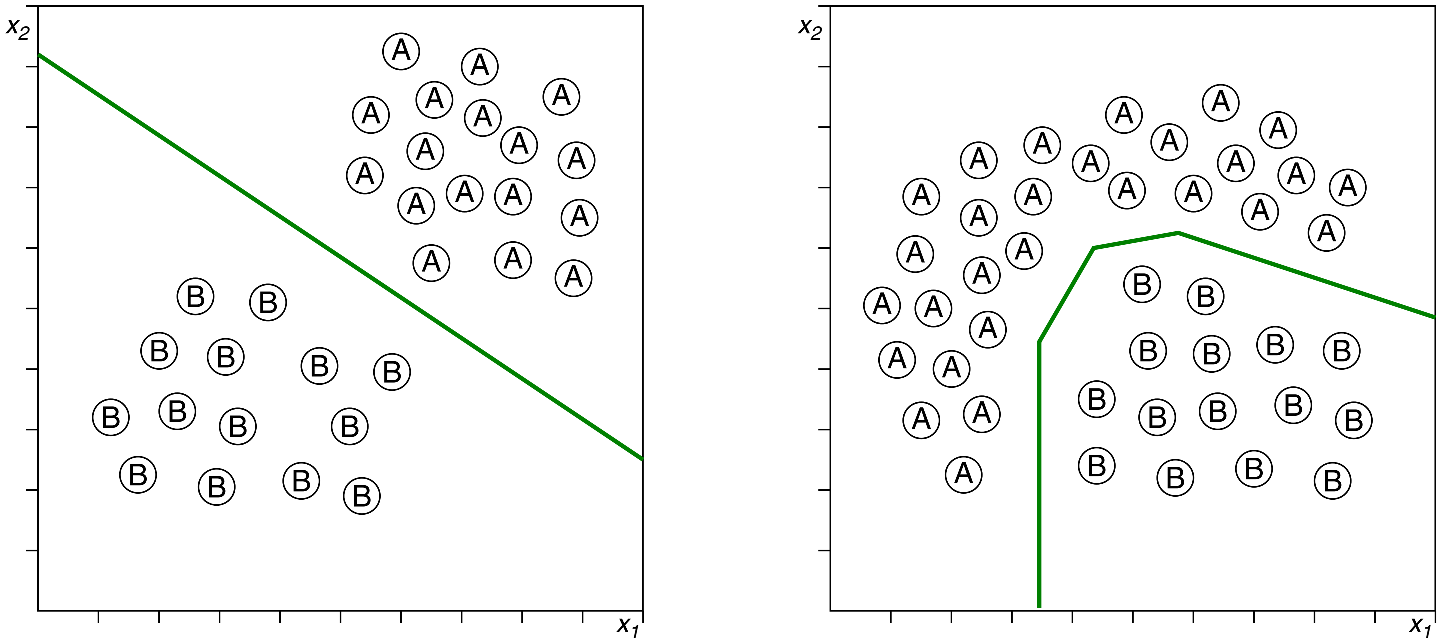
1. $\forall \mathbf{x} \in X_0$: $\sum_{j=1}^{p} w_j x_j < \theta$
2. $\forall \mathbf{x} \in X_1$: $\sum_{j=1}^{p} w_j x_j \geq \theta$

Multilayer Perceptron

Definition 1 (Linear Separability)

Two sets of feature vectors, X_0, X_1, of a p-dimensional feature space are called linearly separable, if $p+1$ real numbers, $\theta, w_1, \ldots, w_p$, exist such that holds:

1. $\forall \mathbf{x} \in X_0$: $\sum_{j=1}^{p} w_j x_j < \theta$
2. $\forall \mathbf{x} \in X_1$: $\sum_{j=1}^{p} w_j x_j \geq \theta$



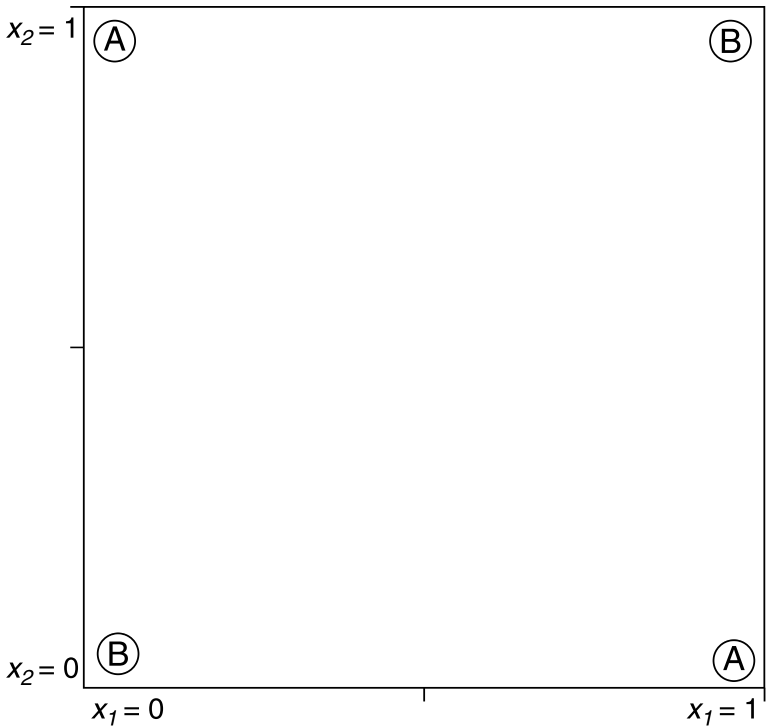
linearly separable   not linearly separable

Multilayer Perceptron

Separability

The *XOR* function defines the smallest example for two not linearly separable sets:

x_1	x_2	XOR	Class
0	0	0	B
1	0	1	A
0	1	1	A
1	1	0	B

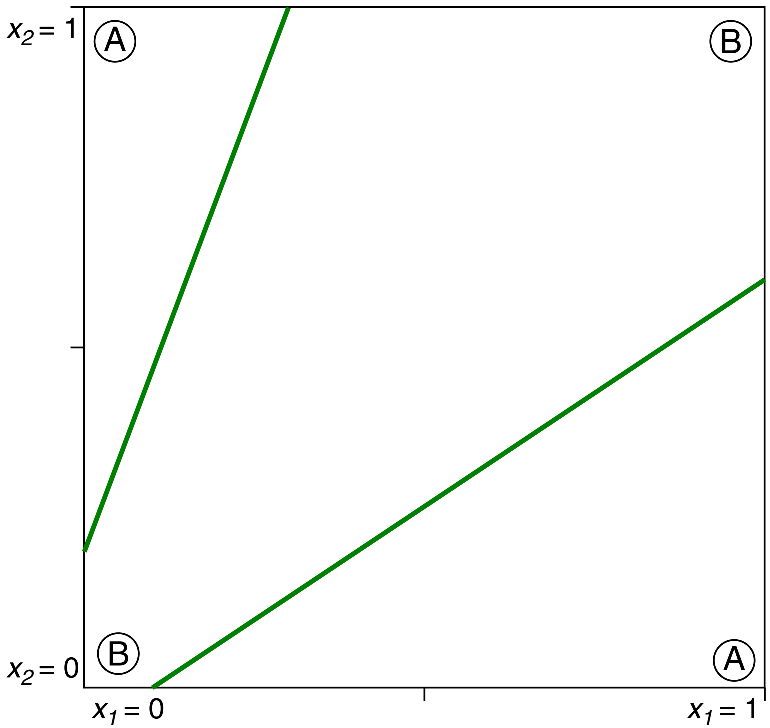


Multilayer Perceptron

Separability (continued)

The *XOR* function defines the smallest example for two not linearly separable sets:

x_1	x_2	XOR	Class
0	0	0	B
1	0	1	A
0	1	1	A
1	1	0	B



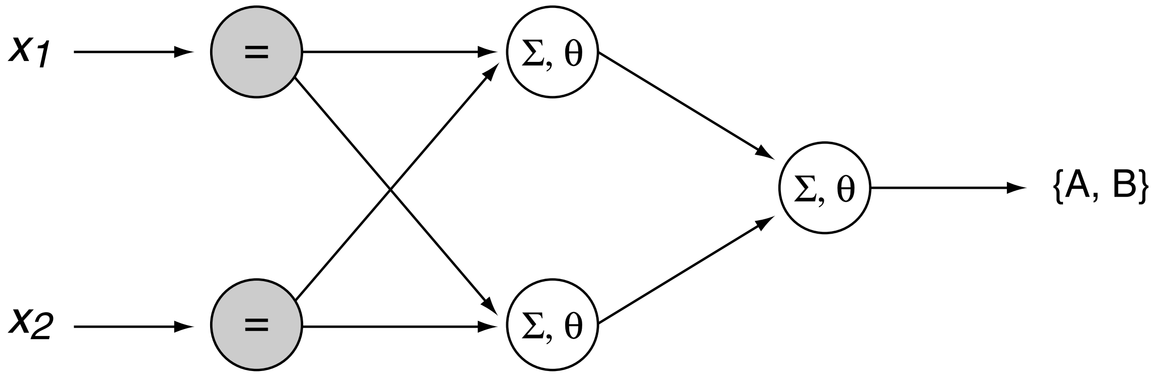
- ➜ specification of several hyperplanes
- ➜ combination of several perceptrons

Multilayer Perceptron

Separability (continued)

Layered combination of several perceptrons: the multilayer perceptron.

Minimum multilayer perceptron that is able to handle the *XOR* problem:



Remarks:

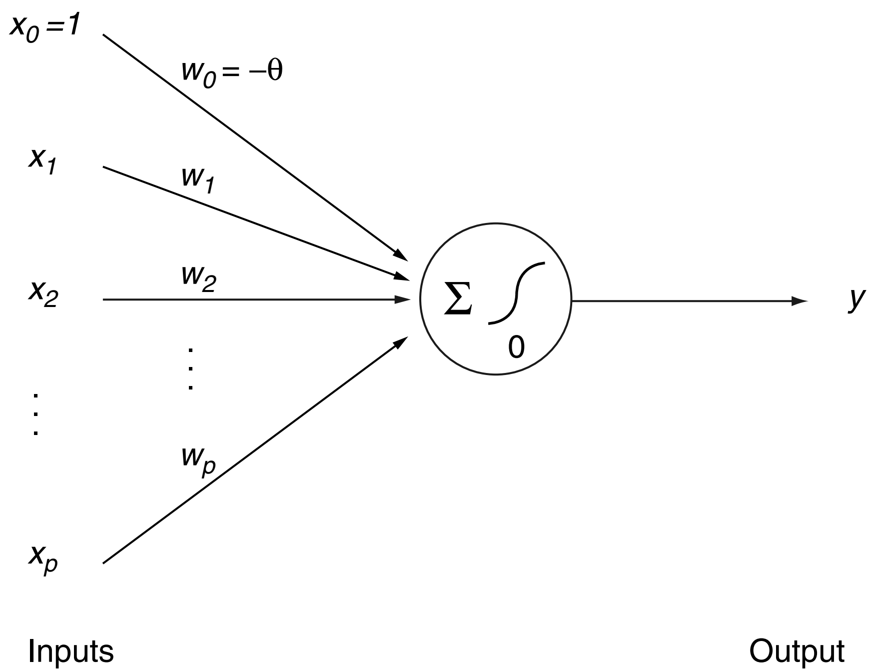
- The multilayer perceptron was presented by Rumelhart and McClelland in 1986. Earlier, but unnoticed, was a similar research work of Werbos and Parker [1974, 1982].
- Compared to a single perceptron the multilayer perceptron poses a significantly more challenging training (= learning) problem, which requires continuous threshold functions and sophisticated learning strategies.
- Marvin Minsky and Seymour Papert showed 1969 with the *XOR* problem the limitations of single perceptrons. Moreover, they assumed that extensions of the perceptron architecture (such as the multilayer perceptron) would be similarly limited as a single perceptron. A fatal mistake. In fact, they brought the research in this field to a halt that lasted 17 years. [Berkeley]

[Marvin Minsky]

Multilayer Perceptron

Computation in the Network [Heaviside]

A perceptron with a continuous, non-linear threshold function:



The sigmoid function $\sigma(z)$ as threshold function:

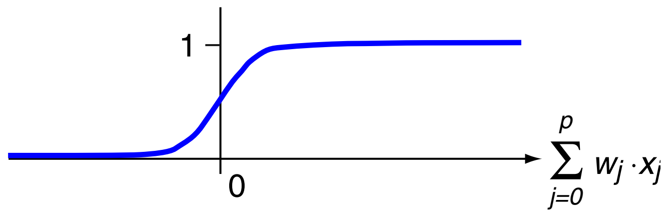
$$\sigma(z) = \frac{1}{1 + e^{-z}} \quad \text{where} \quad \frac{d\sigma(z)}{dz} = \sigma(z) \cdot (1 - \sigma(z))$$

Multilayer Perceptron

Computation in the Network (continued)

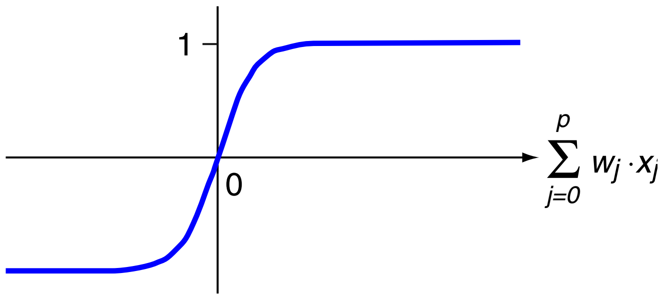
Computation of the perceptron output $y(\mathbf{x})$ via the sigmoid function σ:

$$y(\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w}^T\mathbf{x}}}$$



An alternative to the sigmoid function is the $\tanh$ function:

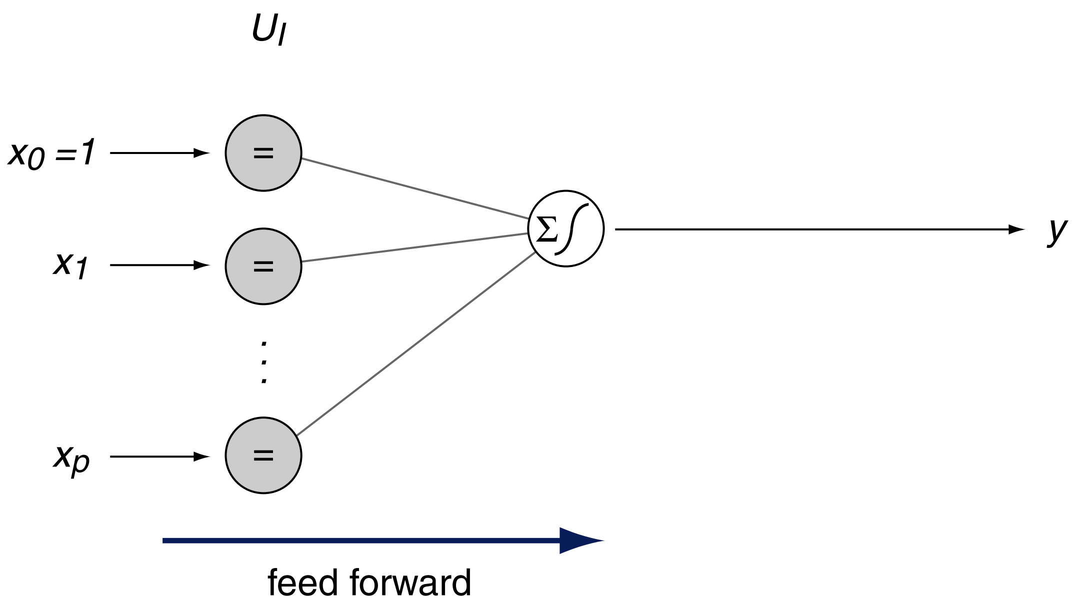
$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = \frac{e^{2x} - 1}{e^{2x} + 1}$$



Multilayer Perceptron

Computation in the Network (continued)

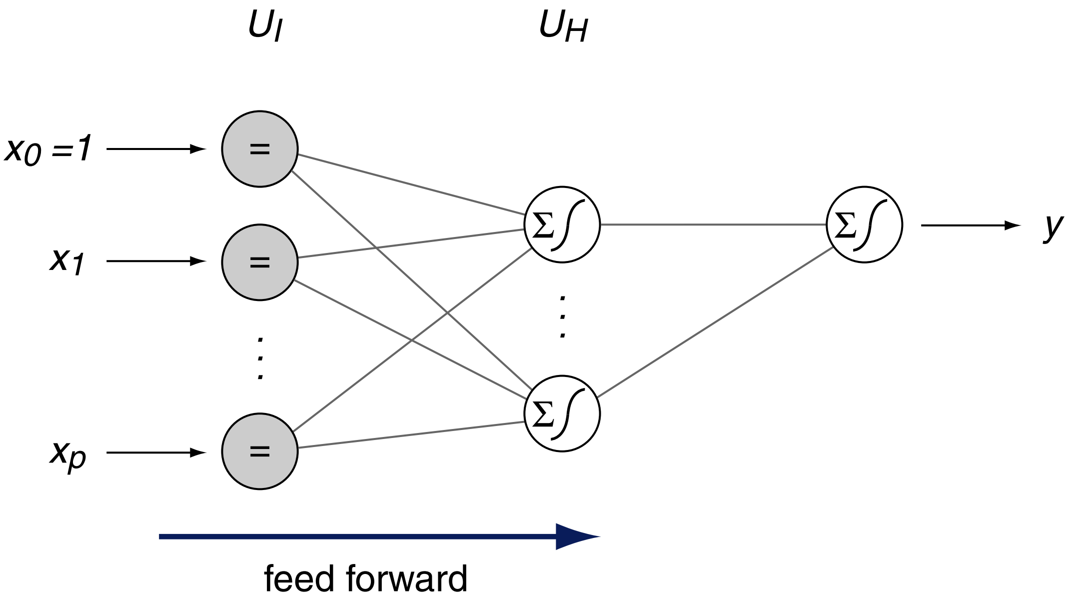
Distinguish units (nodes, perceptrons) of type input, hidden, and output:



Multilayer Perceptron

Computation in the Network (continued)

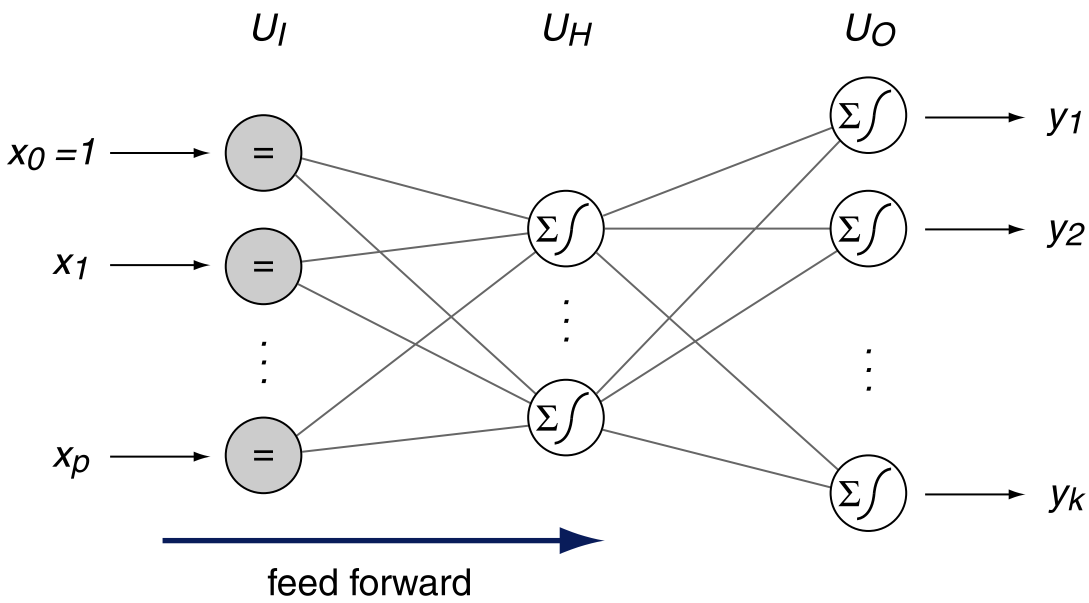
Distinguish units (nodes, perceptrons) of type input, hidden, and output:



Multilayer Perceptron

Computation in the Network (continued)

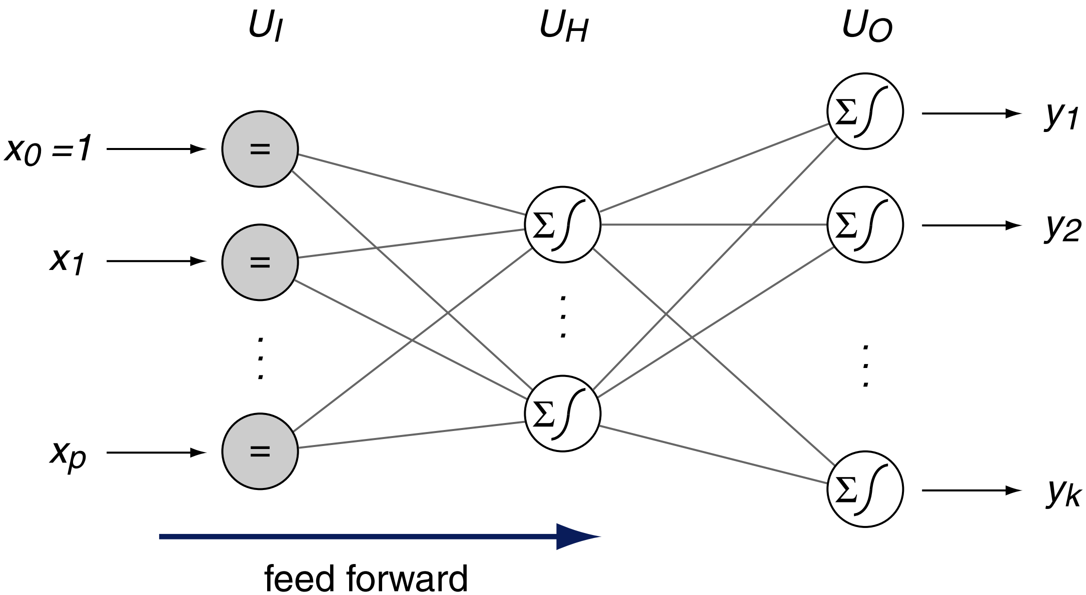
Distinguish units (nodes, perceptrons) of type input, hidden, and output:



Multilayer Perceptron

Computation in the Network (continued)

Distinguish units (nodes, perceptrons) of type input, hidden, and output:



U_I, U_H, U_O	Sets with units of type input, hidden, and output
w_{jk}, Δw_{jk}	Weight and weight adaptation for the edge connecting the units j and k
$x_{j \to k}$	Input value (single incoming edge) for unit k, provided at the output of unit j
y_k, δ_k	Output value and classification error of unit k
$\mathbf{w}_k$	Weight vector (all incoming edges) of unit k
$\mathbf{x}$	Input vector for a unit of the hidden layer
$\mathbf{y}_H$, $\mathbf{y}_O$	Output vector of the hidden layer and the output layer respectively

Remarks:

- The units of the input layer, U_I, perform no computations at all. They distribute the input values to the next layer.
- The network topology corresponds to a complete, bipartite graph between the units in U_I and U_H as well as between the units in U_H and U_O.
- The non-linear characteristic of the sigmoid function makes networks possible that approximate every function. To achieve this flexibility, only three active layers are required, i.e., two layers with hidden units and one layer with output units. Keyword: universal approximator [Kolmogorov Theorem, 1957]
- Multilayer perceptrons are also called multilayer networks or (artificial) neural networks, ANN for short.

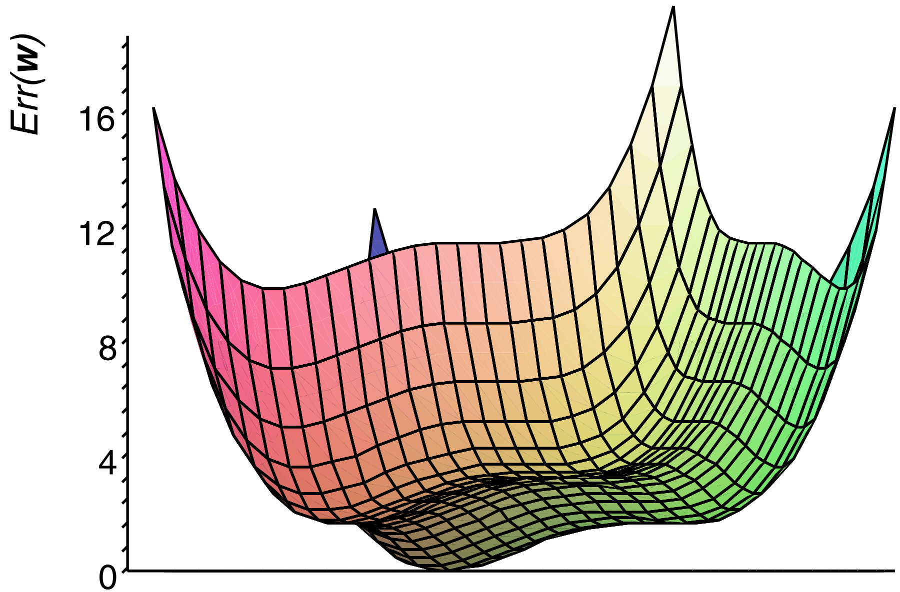
Multilayer Perceptron

Classification Error

The classification error *Err*$(\mathbf{w})$ is computed as sum over the $|U_O| = k$ network outputs:

$$Err(\mathbf{w}) = \frac{1}{2} \sum_{(\mathbf{x},\mathbf{c}(\mathbf{x}))\in D} \sum_{v\in U_O} (c_v(\mathbf{x}) - y_v(\mathbf{x}))^2$$

Due its complex form, *Err*$(\mathbf{w})$ may contain various local minima:



Multilayer Perceptron

Weight Adaptation: Incremental Gradient Descent [network]

Algorithm: *MPT* Multilayer Perceptron Training

Input: D Training examples of the form $(\mathbf{x}, c(\mathbf{x}))$ with $|\mathbf{x}| = p+1,\ c(\mathbf{x}) \in \{0,1\}^k$.

η Learning rate, a small positive constant.

Output: $\mathbf{w}$ Weights of the units in U_I, U_H, U_O.

```
initialize_random_weights(U_I, U_H, U_O),  t = 0
REPEAT
  t = t + 1
  FOREACH (x, c(x)) ∈ D DO
    FOREACH u ∈ U_H DO y_u = σ(w_u^T x)  // compute output of layer 1
    FOREACH v ∈ U_O DO y_v = σ(w_v^T y_H)  // compute output of layer 2
  ENDDO
UNTIL(convergence(D, y_O(D)) OR t > t_max)
return(w)
```

Multilayer Perceptron

Weight Adaptation: Incremental Gradient Descent [network]

Algorithm: *MPT* Multilayer Perceptron Training

Input: D Training examples of the form $(\mathbf{x}, c(\mathbf{x}))$ with $|\mathbf{x}| = p + 1,\ c(\mathbf{x}) \in \{0, 1\}^k$.

η Learning rate, a small positive constant.

Output: $\mathbf{w}$ Weights of the units in U_I, U_H, U_O.

initialize_random_weights(U_I, U_H, U_O), $t = 0$

REPEAT

  $t = t + 1$

  FOREACH $(\mathbf{x}, \mathbf{c}(\mathbf{x})) \in D$ DO

    FOREACH $u \in U_H$ **DO** $y_u = \sigma(\mathbf{w}_u^T \mathbf{x})$ // compute output of layer 1

    FOREACH $v \in U_O$ **DO** $y_v = \sigma(\mathbf{w}_v^T \mathbf{y}_H)$ // compute output of layer 2

    FOREACH $v \in U_O$ DO $\delta_v = y_v \cdot (1 - y_v) \cdot (\mathbf{c}_v(\mathbf{x}) - y_v)$ // backpropagate layer 2

    FOREACH $u \in U_H$ DO $\delta_u = y_u \cdot (1 - y_u) \cdot \sum_{v \in U_o} w_{uv} \cdot \delta_v$ // backpropagate layer 1

  ENDDO

UNTIL(*convergence*$(D, y_O(D))$ **OR** $t > t_{\text{max}}$)

return$(\mathbf{w})$

Multilayer Perceptron

Weight Adaptation: Incremental Gradient Descent [network]

Algorithm: *MPT* Multilayer Perceptron Training

Input: D Training examples of the form $(\mathbf{x}, c(\mathbf{x}))$ with $|\mathbf{x}| = p+1,\ c(\mathbf{x}) \in \{0,1\}^k$.

η Learning rate, a small positive constant.

Output: $\mathbf{w}$ Weights of the units in U_I, U_H, U_O.

initialize_random_weights(U_I, U_H, U_O), $t = 0$

REPEAT

  $t = t + 1$

  FOREACH $(\mathbf{x}, \mathbf{c}(\mathbf{x})) \in D$ DO

    FOREACH $u \in U_H$ **DO** $y_u = \sigma(\mathbf{w}_u^T \mathbf{x})$ // compute output of layer 1

    FOREACH $v \in U_O$ **DO** $y_v = \sigma(\mathbf{w}_v^T \mathbf{y}_H)$ // compute output of layer 2

    FOREACH $v \in U_O$ DO $\delta_v = y_v \cdot (1 - y_v) \cdot (\mathbf{c}_v(\mathbf{x}) - y_v)$ // backpropagate layer 2

    FOREACH $u \in U_H$ DO $\delta_u = y_u \cdot (1 - y_u) \cdot \sum_{v \in U_o} w_{uv} \cdot \delta_v$ // backpropagate layer 1

    FOREACH w_{jk}, $(j,k) \in (U_I \times U_H) \cup (U_H \times U_O)$ **DO**

      $\Delta w_{jk} = \eta \cdot \delta_k \cdot x_{j \to k}$

      $w_{jk} = w_{jk} + \Delta w_{jk}$

    ENDDO

  ENDDO

UNTIL(*convergence*$(D, y_O(D))$ **OR** $t > t_{\text{max}}$)

return$(\mathbf{w})$

Remarks:

- The generic delta rule (Lines 7 and 8 of the *MPT* algorithm) allows for a backpropagation of the classification error and hence the training of multi-layered networks.
- Gradient descent is based on the classification error of the entire network and hence considers the entire network weight vector.

Multilayer Perceptron

Weight Adaptation: Momentum Term

Momentum idea: a weight adaptation in iteration t considers the adaptation in iteration $t{-}1$:

$$\Delta w_{uv}(t) = \eta \cdot \delta_v \cdot x_{u \to v} + \alpha \cdot \Delta w_{uv}(t-1)$$

The term α, $0 \leq \alpha < 1$, is called “momentum”.

Multilayer Perceptron

Weight Adaptation: Momentum Term

Momentum idea: a weight adaptation in iteration t considers the adaptation in iteration $t{-}1$:

$$\Delta w_{uv}(t) = \eta \cdot \delta_v \cdot x_{u \to v} + \alpha \cdot \Delta w_{uv}(t-1)$$

The term α, $0 \leq \alpha < 1$, is called “momentum”.

Effects:

- due the “adaptation inertia” local minima can be overcome
- if the direction of the descent does not change, the adaptation increment and, as a consequence, the speed of convergence is increased.

Neural Networks

Additional Sources on the Web

Application and implementation:

- JNNS. Java Neural Network Simulator.
  http://www-ra.informatik.uni-tuebingen.de/software/JavaNNS
- SNNS. Stuttgart Neural Network Simulator.
  http://www-ra.informatik.uni-tuebingen.de/software/snns