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Artificial Neural Networks

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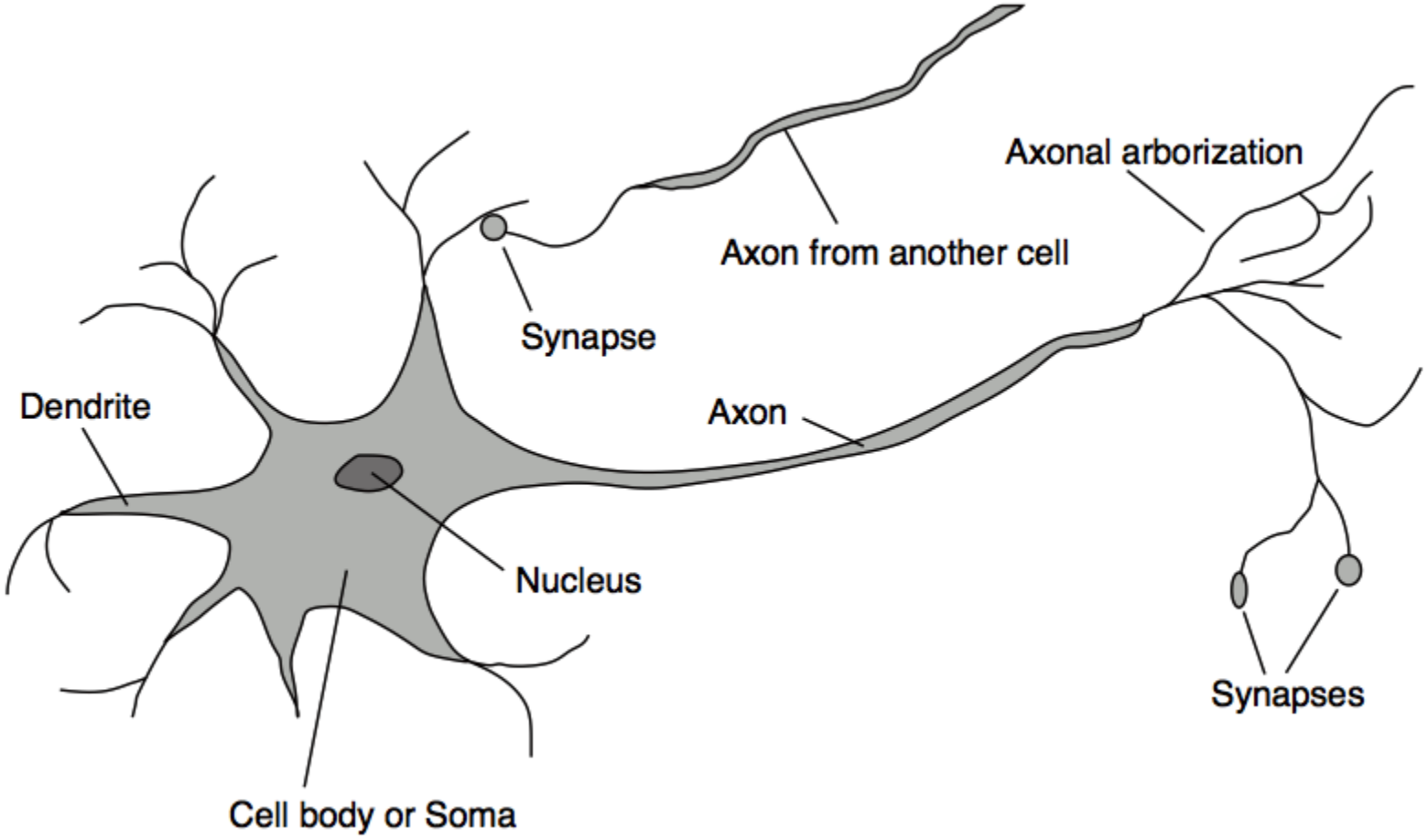
Neurons and Computation



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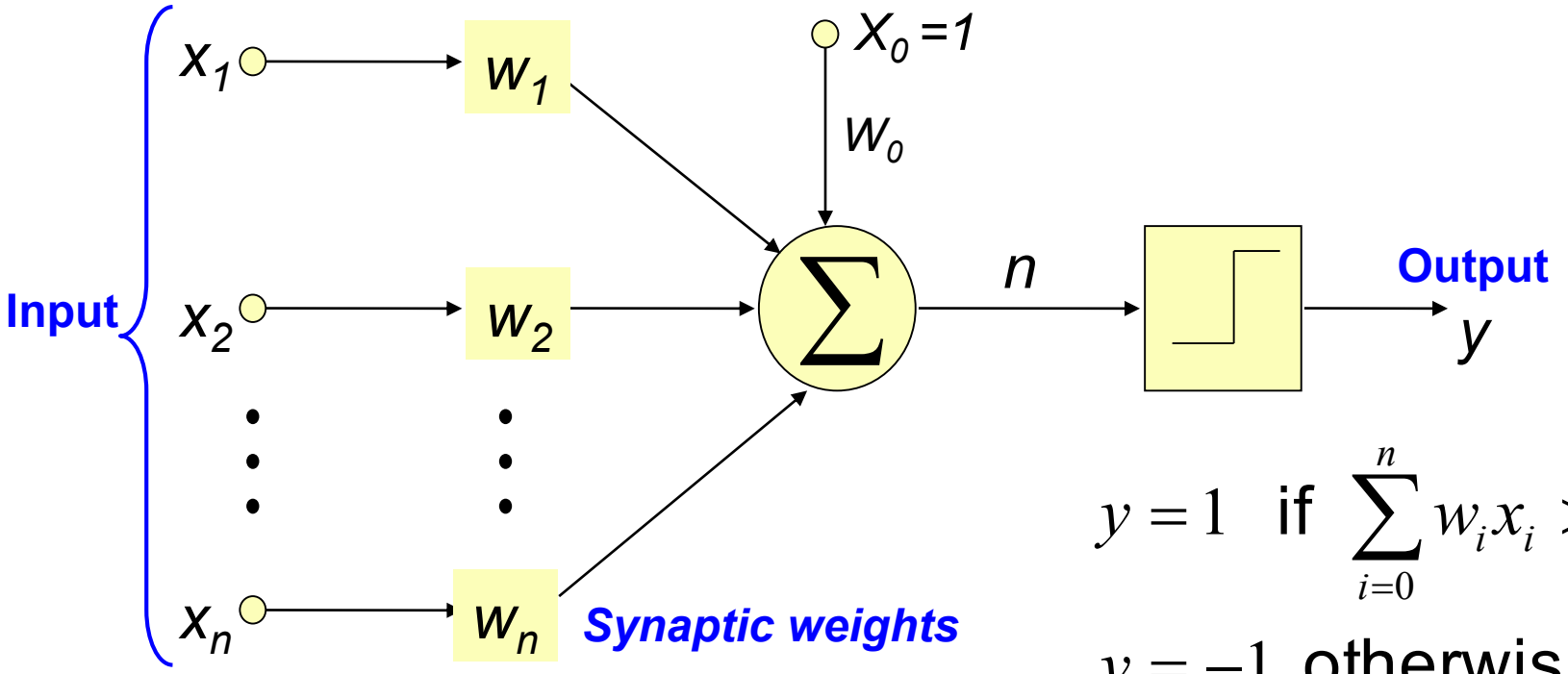
McCulloch-Pitts computational model of a neuron

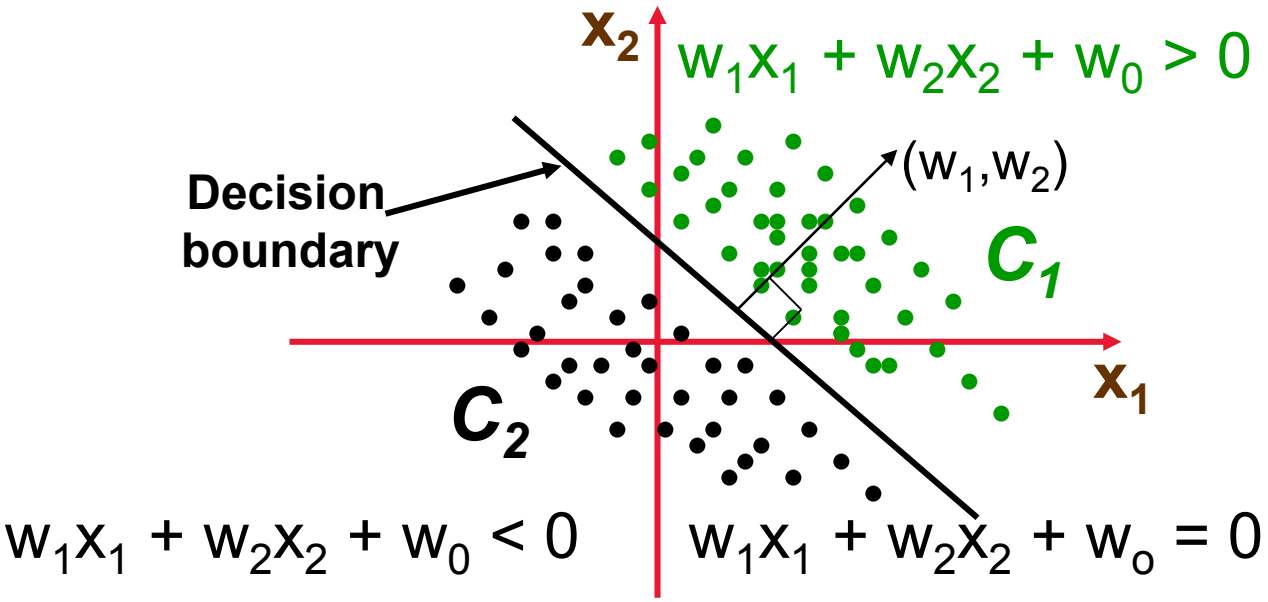


$$y = 1 \quad \text{if} \quad \sum_{i=0}^{n} w_i x_i > 0$$

$$y = -1 \quad \text{otherwise}$$

When a neuron receives input signals from other neurons, its membrane voltage increases. When it exceeds a certain threshold, the neuron "fires" a burst of pulses.

Threshold neuron – Connection with Geometry



$$\sum_{i=1}^{n} w_i x_i + w_0 = 0$$ **describes a hyperplane which divides the instance space $\Re^n$ into two half–spaces**

$$\chi_+ = \left\{ X_p \in \Re^n \middle| W \bullet X_p + w_0 > 0 \right\} \text{ and } \chi_- = \left\{ X_p \in \Re^n \middle| W \bullet X_p + w_0 < 0 \right\}$$

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McCulloch-Pitts neuron or Threshold neuron

$$y = sign\left(\mathrm{W} \bullet \mathrm{X} + w_0\right)$$
$$= sign\left(\sum_{i=0}^{n} w_i x_i\right)$$
$$= sign\left(\mathrm{W}^T \mathrm{X} + w_0\right)$$

$$\mathbf{X} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \qquad \mathbf{W} = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}$$

$$sign\left(v\right) = 1 \text{ if } v > 0$$
$$= 0 \text{ otherwise}$$

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Threshold neuron – Connection with Geometry

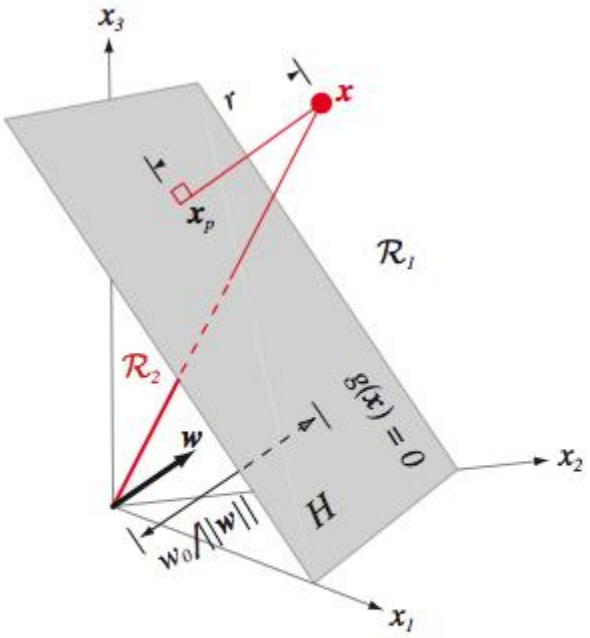

FIGURE 5.2. The linear decision boundary H, where $g(\mathbf{x}) = \mathbf{w}^t\mathbf{x} + w_0 = 0$, separates the feature space into two half-spaces $\mathcal{R}_1$ (where $g(\mathbf{x}) > 0$) and $\mathcal{R}_2$ (where $g(\mathbf{x}) < 0$). From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

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Threshold neuron – Connection with Geometry

- **Instance space** $\Re^n$
- **Hypothesis space is the set of (*n*-1)-dimensional hyperplanes defined in the *n*-dimensional instance space**
- **A hypothesis is defined by** $\sum_{i=0}^{n} w_i x_i = 0$
- **Orientation of the hyperplane is governed by** $(w_1 \ldots w_n)^T$
- ***W* determines the orientation of the hyperplane *H*: given two points *X1* and *X2* on the hyperplane,**

$$W(X_1 - X_2) = 0$$

→ ***W* is normal to any vector lying in *H***

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Threshold neuron as a pattern classifier

- **The threshold neuron can be used to classify a set of instances into one of two classes C_1, C_2**
- **If the output of the neuron for input pattern X_p is +1 then X_p is assigned to class C_1**
- **If the output is -1 then the pattern X_p is assigned to C_2**
- **Example**

$$[w_0 \; w_1 \; w_2]^T = [-1 \; -1 \; 1]^T$$

$$\mathrm{X}_p^T = [1 \; 0]^T \quad \mathrm{W} \bullet \mathrm{X}_p + w_0 = -1 + (-1) = -2$$

$$\mathrm{X}_p \text{ is assigned to class } C_2$$

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Threshold neuron – Connection with Logic

- Suppose the input space is $\{0,1\}^n$
- Then threshold neuron computes a Boolean function
  f: $\{0,1\}^n \rightarrow \{-1,1\}$

- **Example**
  - Let $w_0 = -1.5$; $w_1 = w_2 = 1$
  - In this case, the threshold neuron implements the logical AND function

x_1	x_2	$g(X)$	y
0	0	-1.5	-1
0	1	-0.5	-1
1	0	-0.5	-1
1	1	0.5	1

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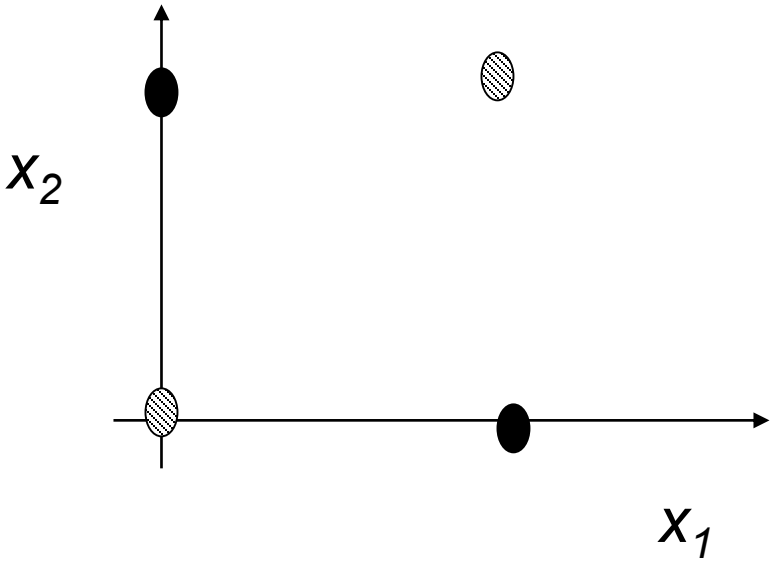
Threshold neuron – Connection with Logic

- **Theorem: There exist functions that cannot be implemented by a *single* threshold neuron**

- **Example: Exclusive OR**



Why?

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Terminology and Notation

- **Synonyms: Threshold function, Linearly separable function, Linear discriminant function**

- **Synonyms: Threshold neuron, McCulloch-Pitts neuron, Perceptron, Threshold Logic Unit (TLU)**

- **We often include w_0 as one of the components of W and incorporate x_0 as the corresponding component of X with the understanding that $x_0 = 1$; Then $y = 1$ if $W \cdot X > 0$ and $y = -1$ otherwise**

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Learning Threshold functions

- **A training example E_k is an ordered pair (X_k, d_k) where**

$X_k = [x_{0k}\ x_{1k}\ ....\ x_{nk}]^T$ **is an (*n+1*) dimensional input pattern, and**

$d_k = f(X_k) \in \{-1, 1\}$ **is the desired output of the classifier and *f* is an unknown target function to be learned**

- **A training set *E* is simply a multi-set of examples**

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Learning Threshold functions

$$S^+ = \left\{ \mathrm{X}_k \middle| \left(\mathrm{X}_k, d_k \right) \in E \text{ and } d_k = 1 \right\}$$
$$S^- = \left\{ \mathrm{X}_k \middle| \left(\mathrm{X}_k, d_k \right) \in E \text{ and } d_k = -1 \right\}$$

- **We say that a training set *E* is linearly separable if and only if**

$$\exists \mathrm{W}^* \text{ such that } \forall \mathrm{X}_p \in S^+, \mathrm{W}^* \bullet \mathrm{X}_p > 0$$
$$\text{and } \forall \mathrm{X}_p \in S^-, \mathrm{W}^* \bullet \mathrm{X}_p < 0$$

- **<u>Learning task</u>: Given a linearly separable training set *E*, find a solution $\mathbf{W}^*$**

$$\text{such that } \forall \mathbf{X}_p \in S^+, \mathbf{W}^* \bullet \mathbf{X}_p > 0 \text{ and } \forall \mathbf{X}_p \in S^-, \mathbf{W}^* \bullet \mathbf{X}_p < 0$$

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Rosenblatt's Perceptron Learning Algorithm

1. **Initialize** $\mathrm{W} = [0\ 0 \ldots\ldots 0]^T$

2. **Set learning rate** $\eta > 0$

3. **<u>Repeat until</u> a complete pass through *E* results in no weight updates**

   For each training example $E_k \in E$

   {

   $$y_k \leftarrow sign\left(\mathrm{W} \bullet \mathrm{X}_k\right)$$

   $$\mathrm{W} \leftarrow \mathrm{W} + \eta\left(d_k - y_k\right)\mathrm{X}_k$$

   }

4. $\mathbf{W}^* \leftarrow \mathbf{W}$; **Return** $\mathbf{W}^*$

Perceptron Learning Algorithm – Example

Let

$S^+ = \{(1, 1, 1), (1, 1, -1), (1, 0, -1)\}$

$S^- = \{(1,-1, -1), (1,-1, 1), (1,0, 1)\}$

$W = (0\ 0\ 0)$

$$\eta = \frac{1}{2}$$

$$w^* = w + \eta (d_n - y_n) x_n$$

X_k	d_k	W	$W.X_k$	y_k	Update?	Updated W
(1, 1, 1)	1	(0, 0, 0)	0	-1	Yes	(1, 1, 1)
(1, 1, -1)	1	(1, 1, 1)	1	1	No	(1, 1, 1)
(1,0, -1)	1	(1, 1, 1)	0	-1	Yes	(2, 1, 0)
(1, -1, -1)	-1	(2, 1, 0)	1	1	Yes	(1, 2, 1)
(1,-1, 1)	-1	(1, 2, 1)	0	-1	No	(1, 2, 1)
(1,0, 1)	-1	(1, 2, 1)	2	1	Yes	(0, 2, 0)
(1, 1, 1)	1	(0, 2, 0)	2	1	No	(0, 2, 0)

Perceptron Convergence Theorem (Novikoff)

Theorem:

Let $E = \{(\mathbf{X}_k, d_k)\}$ **be a training set where** $\mathbf{X}_k \in \{1\} \times \Re^n$ **and** $d_k \in \{-1, 1\}$

Let $S^+ = \{\mathbf{X}_k | (\mathbf{X}_k, d_k) \in E \;\&\; d_k = 1\}$ and $S^- = \{\mathbf{X}_k | (\mathbf{X}_k, d_k) \in E \;\&\; d_k = -1\}$

The perceptron algorithm is guaranteed to terminate after a bounded number *t* of weight updates with a weight vector $\mathbf{W}^*$

such that $\forall \mathbf{X}_k \in S^+, \mathbf{W}^* \bullet \mathbf{X}_k \geq \delta$ and $\forall \mathbf{X}_k \in S^-, \mathbf{W}^* \bullet \mathbf{X}_k \leq -\delta$

for some $\delta > 0$, **whenever such** $\mathbf{W}^* \in \Re^{n+1}$ and $\delta > 0$ **exist – that is,** ***E is linearly separable.***

The bound on the number *t* of weight updates is given by

$$t \leq \left(\frac{\|\mathbf{W}^*\| L}{\delta} \right)^2 \quad \text{where } L = \max_{\mathbf{X}_k \in S} \|\mathbf{X}_k\| \quad \text{and } S = S^+ \cup S^-$$

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Limitations of Perceptrons

- Perceptrons can only represent threshold functions
- Perceptrons can only learn linear decision boundaries
- What if the data are not linearly separable?
  - Modify the learning procedure or the weight update equation?
    (e.g. Pocket algorithm, Thermal perceptron)
  - More complex networks?
  - Non-linear transformations into a feature space where the data become separable?

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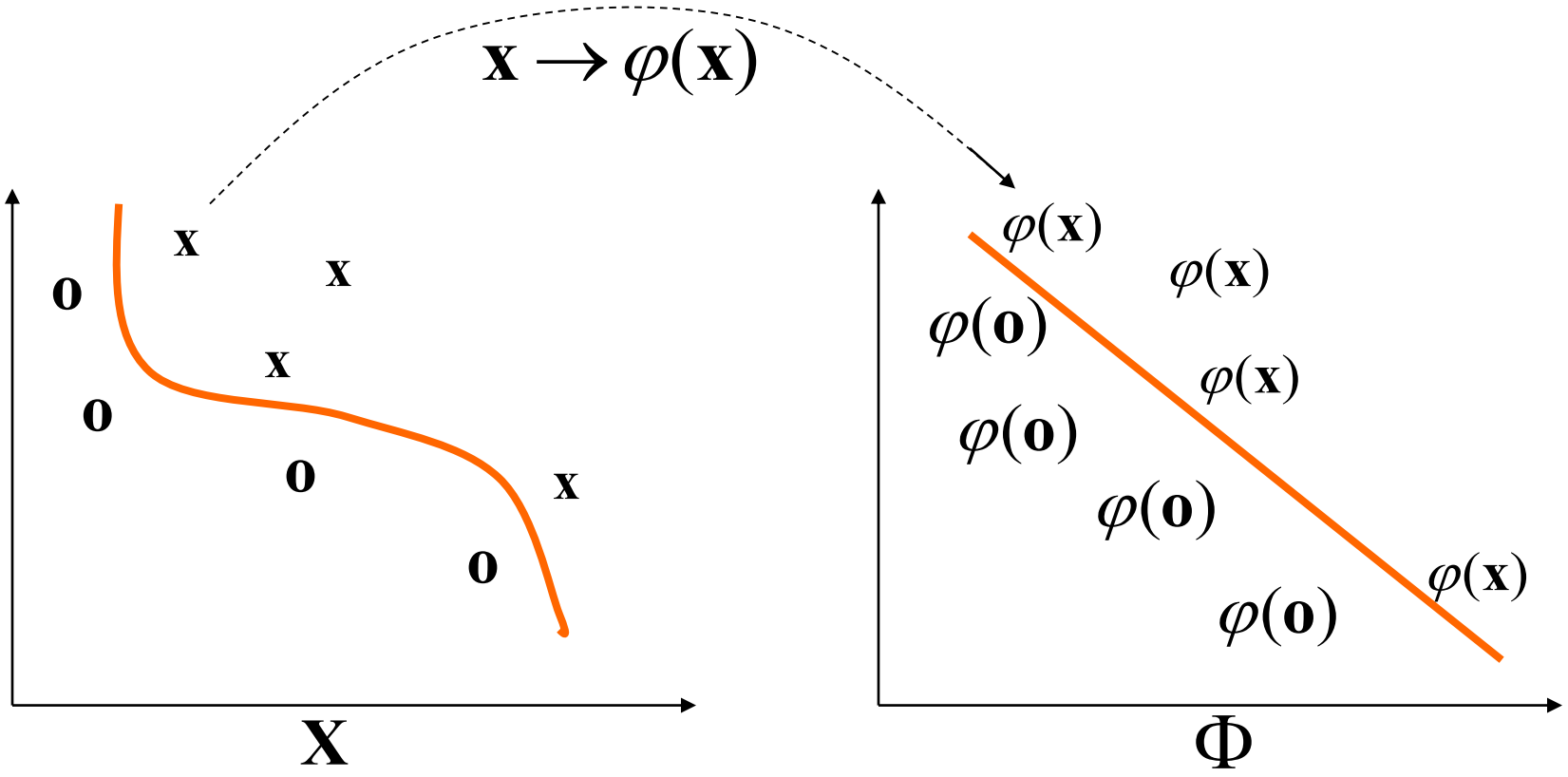
Extending Linear Classifiers: Learning in feature spaces

- Map data into a feature space where they are linearly separable



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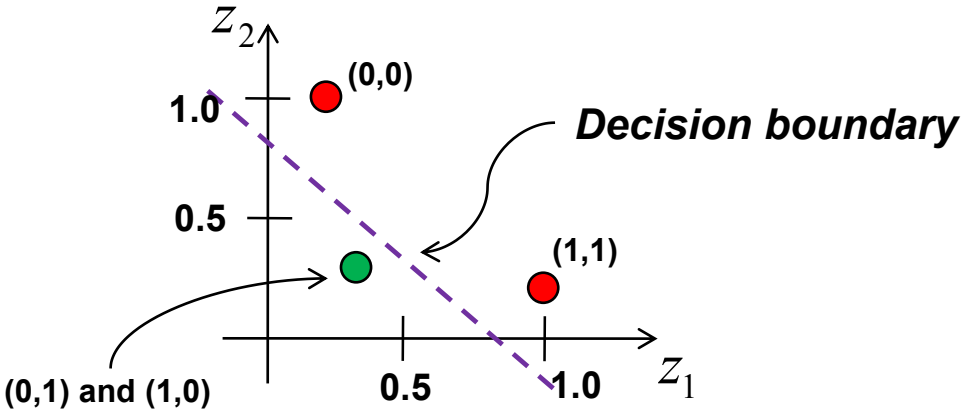
Exclusive OR revisited

- **In the feature (hidden) space:**

$$\varphi_1(x_1, x_2) = e^{-\|X - W_1\|^2} = z_1 \qquad W_1 = [1,1]^T$$

$$\varphi_2(x_1, x_2) = e^{-\|X - W_2\|^2} = z_2 \qquad W_2 = [0,0]^T$$



- **When mapped into the feature space <z_1, z_2>, C_1 and C_2 become *linearly separable*. So a linear classifier with $\varphi_1(X)$ and $\varphi_2(X)$ as inputs can be used to solve the XOR problem.**

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Learning in the Feature Space

- **High dimensional feature spaces**

$$X = (x_1, x_2, \cdots, x_n) \rightarrow \varphi(X) = (\varphi_1(X), \varphi_2(X), \cdots, \varphi_d(X))$$

where typically *d* >> *n* solve the problem of expressing complex functions

- **But this introduces**
  - **Computational problem (working with very large vectors)**
    - **→ Solved using the kernel trick – implicit feature spaces**
  - **Generalization problem (curse of dimensionality)**
    - **→ Solved by maximizing the margin of separation – first implemented in SVM (Vapnik)**

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Margin Based Bounds on Error of Classification

- **The error ε of classification function h for separable data sets is**

$$\varepsilon = O\left(\frac{d}{l}\right)$$

- **Can prove margin based bound:**

$$\varepsilon = O\left(\frac{1}{l}\left(\frac{L}{\bar{\gamma}}\right)^2\right) \qquad L = \max_p \left\|\mathbf{X}_p\right\|$$

$$\bar{\gamma} = \min_i \frac{y_i f(\mathbf{x}_i)}{\|\mathbf{w}\|} \qquad f(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle + b$$

- **Important insight:**

  Error of the classifier trained on a separable data set is inversely proportional to its margin, and is independent of the dimensionality of the input space!

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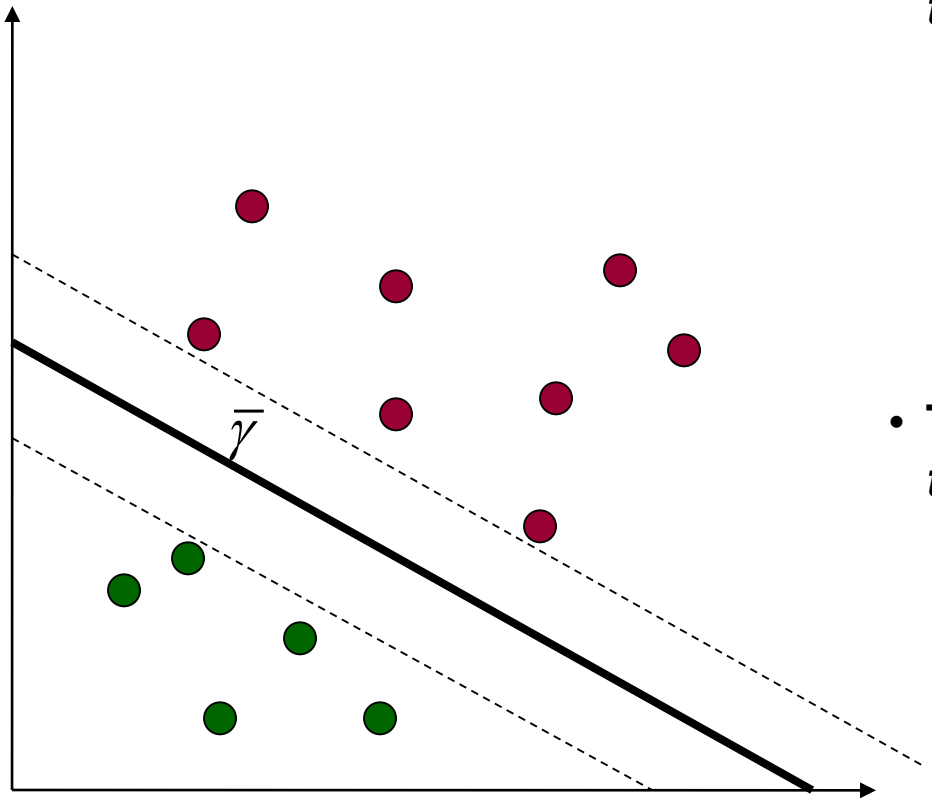
Margin of a Training Set



- **The functional margin of a *training set***

$$\gamma = \min_i \gamma_i$$

- **The geometric margin of a *training set***

$$\bar{\gamma} = \min_i \bar{\gamma}_i$$

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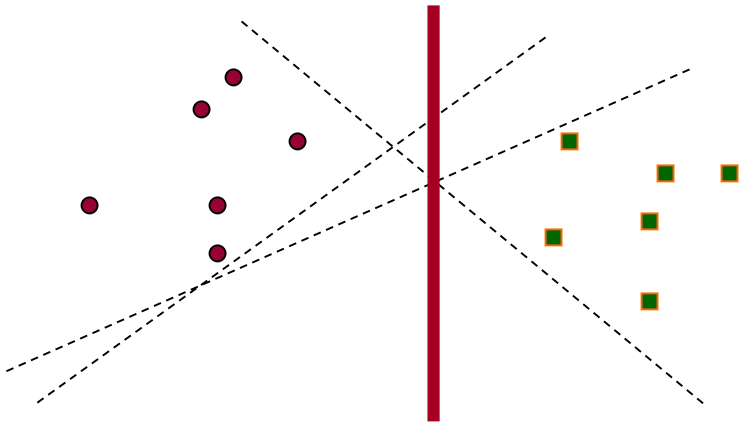
Maximum Margin Separating Hyperplane

- $\gamma = \min_i \gamma_i$ **is called the (functional) margin of (*W,b*) w.r.t. the data set *S*={(*Xi,yi*)}**

- **The margin of a training set *S* is the maximum geometric margin over all hyperplanes; A hyperplane realizing this maximum is a maximal margin hyperplane**



Maximal Margin Hyperplane

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Maximizing Margin → Minimizing ||*W*||

- **Definition of hyperplane (*W,b*) does not change if we rescale it to (σ*W*, σ*b*), for σ>*0*.**
- **Functional margin depends on scaling, but geometric margin $\bar{\gamma}$ does not**
- **If we fix (by rescaling) the functional margin to 1, the geometric margin will be equal 1/||*W*||**
- **Then, we can maximize the margin by minimizing the norm ||*W*||**

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Learning as Optimization

- **Minimize**

$$\langle \mathbf{W}, \mathbf{W} \rangle$$

Subject to:

$$y_i \left(\langle \mathbf{W}, \mathbf{X}_i \rangle + b \right) \geq 1$$

- **The problem of finding the maximal margin hyperplane: constrained optimization (quadratic programming) problem**

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Taylor Series Approximation of Functions

Taylor series approximation of $f(x)$

If $f(x)$ is differentiable i.e., its derivatives

$$\frac{df}{dx},\ \frac{d^2 f}{dx^2} = \frac{d}{dx}\left(\frac{df}{dx}\right),\ \ldots \frac{d^n f}{dx^n} \text{ exist at } x = X_0 \text{ and}$$

$f(x)$ is continuous in the neighborhood of $x = X_0$, then

$$f(x) = f(X_0) + \left(\frac{df}{dx}\bigg|_{x=X_0}\right)(x - X_0) + \ldots.. + \frac{1}{n!}\left(\frac{df^n}{dx^n}\bigg|_{x=X_0}\right)(x - X_0)^n$$

$$f(x) \approx f(X_0) + \left(\frac{df}{dx}\bigg|_{x=X_0}\right)(x - X_0)$$

Minimizing/Maximizing Multivariate Functions

To find $\mathbf{X}^*$ that minimizes $f(\mathbf{X})$, we change current guess $\mathbf{X}^C$ in the direction of the negative gradient of $f(\mathbf{X})$ evaluated at $\mathbf{X}^C$

$$\mathbf{X}^C \leftarrow \mathbf{X}^C - \eta \left(\frac{\partial f}{\partial x_0}, \frac{\partial f}{\partial x_1} \ldots\ldots\ldots \ldots \frac{\partial f}{\partial x_n} \right) \Bigg|_{\mathbf{X}=\mathbf{X}^C} \quad \text{(why?)}$$

for small (ideally infinitesimally small)

Minimizing/Maximizing Multivariate Functions

Suppose we more from Z_0 to Z_1. We want to ensure $f(Z_1) \leq f(Z_0)$.

In the neighborhood of Z_0, using Taylor series expansion, we can write

$$f(Z_1) = f(Z_0 + \Delta Z) = f(Z_0) + \left(\left. \frac{df}{dZ} \right|_{Z=Z_0} \right)(\Delta Z) + \ldots$$

$$\Delta f = f(Z_1) - f(Z_0) \approx \left(\left. \frac{df}{dZ} \right|_{Z=Z_0} \right)(\Delta Z)$$

We want to make sure $\Delta f \leq 0$.

If we choose

$$\Delta Z = -\eta \left(\left. \frac{df}{dZ} \right|_{Z=Z_0} \right) \rightarrow \Delta f = -\eta \left(\left. \frac{df}{dZ} \right|_{Z=Z_0} \right)^2 \leq 0$$

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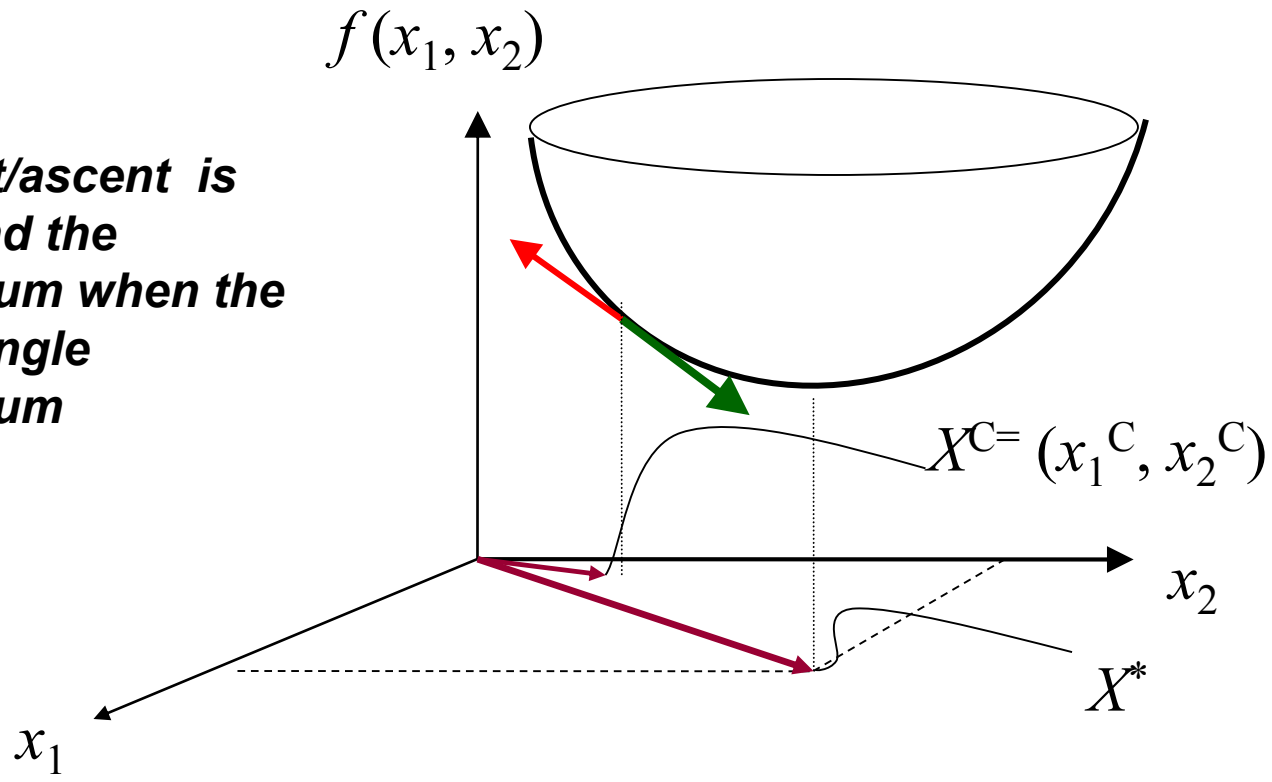
Minimizing/Maximizing Functions

Gradient descent/ascent is guaranteed to find the minimum/maximum when the function has a single minimum/maximum



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Maximum Margin Hyperplane

- The problem of finding the maximal margin hyperplane is a constrained optimization problem

- Use Lagrange theory (extended by Karush, Kuhn, and Tucker – KKT)

- Minimize $\langle \mathbf{W}, \mathbf{W} \rangle$

  subject to

$$y_i\left(\langle \mathbf{W}, \mathbf{X}_i \rangle + b\right) \geq 1$$

- Lagrangian:

$$L_p(\mathbf{w}) = \frac{1}{2}\langle \mathbf{w}, \mathbf{w} \rangle - \sum \alpha_i [y_i(\langle \mathbf{w}, x_i \rangle + b) - 1] \qquad (4)$$

$$\alpha \geq 0$$

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From Primal to Dual

- **Minimize *Lp*(*w*) with respect to (*w,b*) requiring that derivatives of *Lp*(*w*) with respect to (*w,b*) all vanish, subject to the constraints $\alpha_i \geq 0$**

- **Differentiating *Lp*(*w*):**

$$\frac{\partial L_p}{\partial \mathbf{w}} = 0, \quad (5)$$

$$\frac{\partial L_p}{\partial b} = 0 \quad (6)$$

$$\mathbf{w} = \sum_i \alpha_i y_i x_i \quad (7)$$

$$\sum_i \alpha_i y_i = 0 \quad (8)$$

- **Substituting this equality constraints back into *Lp*(*w*) we obtain a dual problem**

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The Dual Problem

- **Maximize:**

$$L_D(\mathbf{w}) = \frac{1}{2}\left\langle \left(\sum_i \alpha_i y_i \mathbf{x}_i\right)\left(\sum_j \alpha_j y_j \mathbf{x}_j\right)\right\rangle$$

$$-\sum_i \alpha_i \left[y_i \left(\left\langle \left(\sum_j \alpha_j y_j \mathbf{x}_j\right), \mathbf{x}_i \right\rangle + b \right) - 1 \right]$$

$$= \frac{1}{2}\sum_{ij} \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle - \sum_{ij} \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle - b\sum_i \alpha_i y_i + \sum_i \alpha_i$$

$$= -\frac{1}{2}\sum_{ij} \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle + \sum_i \alpha_i$$

subject to $\sum_i \alpha_i y_i = 0$ **and** $\alpha_i \geq 0$

- **Duality permits the use of kernels!**
- **This is a quadratic optimization problem: convex, no local minima**
- **Solvable in polynomial time**

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Karush-Kuhn-Tucker Conditions for SVM

- The KKT conditions state that optimal solutions $\alpha_i(\mathbf{w}, b)$ must satisfy

$$\alpha_i\left[y_i\left(\langle \mathbf{w}, \mathbf{x}_i \rangle + b\right) - 1\right] = 0$$

- Only the training samples X_i for which the functional margin = 1 can have nonzero α_i; They are called Support Vectors

- The optimal hyperplane can be expressed in the dual representation in terms of this subset of training samples – the support vectors

$$f(\mathbf{x}, \boldsymbol{\alpha}, b) = \sum_{i=1}^{l} y_i \alpha_i \left\langle \mathbf{x}_i \cdot \mathbf{x} \right\rangle + b = \sum_{i \in \mathrm{SV}} y_i \alpha_i \left\langle \mathbf{x}_i \cdot \mathbf{x} \right\rangle + b$$

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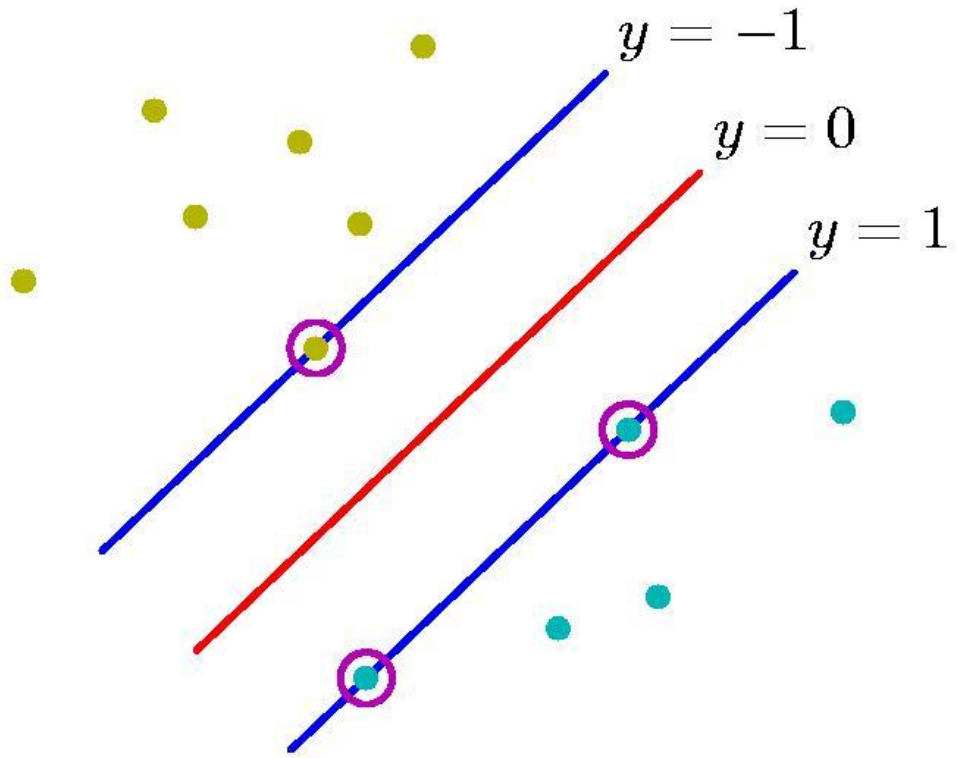
Support Vectors



Implementation Techniques

- **Maximizing a quadratic function, subject to a linear equality and inequality constraints**

$$W(\alpha) = \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j K(x_i, x_j)$$

$$0 \le \alpha_i \le C$$

$$\sum_i \alpha_i y_i = 0$$

$$\frac{\partial W(\boldsymbol{\alpha})}{\partial \alpha_i} = 1 - y_i \sum_j \alpha_j y_j K(x_i, x_j)$$

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Strengths and Weaknesses of SVM

- Strengths
  - Training is relatively easy
    - No local optima
  - It scales relatively well to high dimensional data
  - Tradeoff between classifier complexity and error can be controlled explicitly
  - Non-traditional data like strings and trees can be used as input to SVM, instead of feature vectors

- Weaknesses
  - Need to choose a “good” kernel function

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Learning Linear Functions

- One approach to regression: directly construct an appropriate function $y(\vec{x})$
- *Linear regression* (linear neuron)

$$y(\vec{x}, \vec{w}) = w_0 + \sum_{i=1}^{d} w_i x_i = \vec{w}^t \vec{x}$$

- We want to find a weight vector $\vec{w}$ such that the linear function is a *good* approximation of unknown $f(\vec{x})$ based on training examples.

Learning Linear Functions

- Define a criterion/error function $J(\vec{w})$, and the learning problem reduces to looking for a weight vector that minimizes $J(\vec{w})$.
- Let the output for input $\vec{x}_k = (x_0^k, x_1^k, \ldots, x_d^k)^t$ be

$$o_k = y(\vec{x}_k, \vec{w}) = \sum_{i=0}^{d} w_i x_i^k = \vec{w}^t \vec{x}_k$$

- The error for the labeled input $(\vec{x}_k, t_k)$: $e_k = o_k - t_k$
- We wish to minimize the magnitude of this error irrespective of the sign. We will use the squared error, and we are interested in the error over all training samples

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Learning Linear Functions

- The sum-of-squared-error (*Mean Squared Error*) function

$$J_s(\vec{w}) = \frac{1}{2}\sum_{k=1}^{n}(o_k - t_k)^2 = \frac{1}{2}\sum_{k=1}^{n}(\vec{w}^t\vec{x}_k - t_k)^2$$

  where n: number of samples

- The learning problem reduces to looking for a weight vector that minimizes $J_s(\vec{w})$
  — a minimum-squared-error (MSE) solution.

Learning Linear Functions:
Computing Gradient

$$\frac{\partial J}{\partial w_i} = \frac{\partial}{\partial w_i}\frac{1}{2}\sum_k (o_k - t_k)^2 = \frac{1}{2}\sum_k \frac{\partial}{\partial w_i}(o_k - t_k)^2$$

$$= \frac{1}{2}\sum_k 2(o_k - t_k)\frac{\partial}{\partial w_i}(o_k - t_k)$$

$$= \sum_k (o_k - t_k)\frac{\partial o_k}{\partial w_i}$$

$$\frac{\partial o_k}{\partial w_i} = x_i^k$$

Learning Linear Functions:
Computing Gradient

$$\frac{\partial J}{\partial w_i} = \sum_{k=1}^{n} (o_k - t_k) x_i^k$$

$$\nabla J[\vec{w}] = \sum_{k=1}^{n} (o_k - t_k) \vec{x}_k$$

Necessary condition for minimization

$$\frac{\partial J}{\partial w_i} = 0, \qquad i = 0, \ldots, d$$

Equivalently $\nabla J[\vec{w}] = 0$

- This defines a set of linear equations in w_i's. Can be solved explicitly using linear algebra technique.

Learning Linear Functions:
Linear Algebra Solution

- The weight values that minimize the sum-of-squared-error function can be found explicitly by solving the set of linear equations.

$$\sum_{k=1}^{n}\sum_{j=0}^{d} w_j x_j^k x_i^k = \sum_{k=1}^{n} x_i^k t_k$$

$$\mathbf{Y} = \begin{pmatrix} x_0^1 & \cdots & x_d^1 \\ \vdots & \ddots & \vdots \\ x_0^n & \cdots & x_d^n \end{pmatrix} \quad \mathbf{w} = \begin{pmatrix} w_0 \\ \vdots \\ w_d \end{pmatrix} \quad \mathbf{t} = \begin{pmatrix} t_1 \\ \vdots \\ t_n \end{pmatrix}$$

$$(\mathbf{Y}^t\mathbf{Y})\mathbf{w} = \mathbf{Y}^t\mathbf{t}$$

- *Pseudo-inverse* of Y: $\mathbf{Y}^\dagger = (\mathbf{Y}^t\mathbf{Y})^{-1}\mathbf{Y}^t$
- $\vec{w} = \mathbf{Y}^\dagger\mathbf{t}$
- In practice, this solution can lead to numerical difficulties due to the possibility of $\mathbf{Y}^t\mathbf{Y}$ being singular or nearly singular.
- Use the techniques of *singular value decomposition* (SVD)

Learning Linear Functions:
Delta/Adaline/Widrow-Hoff/LMS(Least-Mean-Squared) Rule

$$w_i \leftarrow w_i - \eta \frac{\partial E_S}{\partial w_i}$$

$$\frac{\partial E_S}{\partial w_i} = \frac{1}{2}\frac{\partial}{\partial w_i}\left\{\sum_p e_p^2\right\} = \frac{1}{2}\left(\sum_p \frac{\partial}{\partial w_i}\left(e_p^2\right)\right)$$

$$= \frac{1}{2}\left(\sum_p \left(2e_p\right)\frac{\partial e_p}{\partial w_i}\right) = \sum_p e_p\left(\frac{\partial e_p}{\partial y_p}\right)\left(\frac{\partial y_p}{\partial w_i}\right) = \sum_p e_p\left(-1\right)\left(\frac{\partial}{\partial w_i}\left(\sum_{j=0}^{n} w_j x_{jp}\right)\right)$$

$$= -\sum_p \left(d_p - y_p\right)\left(\frac{\partial}{\partial w_i}\left(w_i x_{ip} + \sum_{j\neq i} w_j x_{jp}\right)\right)$$

$$= -\sum_p \left(d_p - y_p\right)\left(\frac{\partial}{\partial w_i}\left(w_i x_{ip}\right) + \frac{\partial}{\partial w_i}\left(\sum_{j\neq i} w_j x_{jp}\right)\right)$$

$$= -\sum_p \left(d_p - y_p\right)x_{ip}$$

$$w_i \leftarrow w_i + \eta\sum_p \left(d_p - y_p\right)x_{ip}$$

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Learning Real-Valued Functions

- Universal function approximation theorem
- Learning nonlinear functions using gradient descent in weight space
- Practical considerations and examples

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Universal function approximation theorem (Cybenko, 1989)

- Let $\varphi : \Re \rightarrow \Re$ be a non-constant, bounded (hence non-linear), monotone, continuous function. Let I_N be the N-dimensional unit hypercube in $\Re^N$.

- Let $C(I_N) = \{f: I_N \rightarrow \Re\}$ be the set of all continuous functions with domain I_N and range $\Re$. Then for any function $f \in C(I_N)$ and any $\varepsilon > 0$, $\exists$ an integer L and a set of real values $\theta, \alpha_j, \theta_j, w_{ji}$ $(1 \le j \le L; 1 \le i \le N)$ such that

$$F(x_1, x_2 \ldots x_n) = \sum_{j=1}^{L} \alpha_j \varphi\left(\sum_{i=1}^{N} w_{ji} x_i - \theta_j \right) - \theta$$

  is a uniform approximation of f – that is,

$$\forall (x_1, \ldots x_N) \in I_N, \quad \left| F(x_1, \ldots x_N) - f(x_1, \ldots x_N) \right| < \varepsilon$$

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Universal function approximation theorem (UFAT)

$$F(x_1, x_2 \ldots x_n) = \sum_{j=1}^{L} \alpha_j \varphi\left(\sum_{i=1}^{N} w_{ji} x_i - \theta_j \right) - \theta$$

- **Unlike Kolmogorov's theorem, UFAT requires only one kind of nonlinearity to approximate any arbitrary nonlinear function to any desired accuracy**

- **The sigmoid function satisfies the UFAT requirements**

$$\varphi(z) = \frac{1}{1 + e^{-az}}; a > 0 \qquad \lim_{z \to -\infty} \varphi(z) = 0; \lim_{z \to +\infty} \varphi(z) = 1$$

- **Similar universal approximation properties can be guaranteed for other functions (e.g. radial basis functions)**

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Feed-forward neural networks

- A feed-forward 3-layer network consists of 3 layers of nodes
  - *Input* nodes
  - *Hidden* nodes
  - *Output* nodes

- Interconnected by *modifiable weights* from input nodes to the hidden nodes and the hidden nodes to the output nodes

- More general topologies (with more than 3 layers of nodes, or connections that skip layers – e.g., direct connections between input and output nodes) are also possible

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Three-layer feed-forward neural network

- **A single *bias* unit is connected to each unit other than the input units**

- **Net *input***

$$n_j = \sum_{i=1}^{N} x_i w_{ji} + w_{j0} = \sum_{i=0}^{N} x_i w_{ji} \equiv \mathbf{W}_j \bullet \mathbf{X},$$

where the subscript i indexes units in the input layer, j in the hidden; w_{ji} denotes the input-to-hidden layer weights at the hidden unit j.

- **The output of a hidden unit is a nonlinear function of its net input. That is, $y_j = f(n_j)$ e.g.,**

$$y_j = \frac{1}{1 + e^{-n_j}}$$

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Three-layer feed-forward neural network

- **Each output unit similarly computes its net activation based on the hidden unit signals as:**

$$n_k = \sum_{j=1}^{n_H} y_j w_{kj} + w_{k0} = \sum_{j=0}^{n_H} y_j w_{kj} = \mathbf{W}_k \bullet \mathbf{Y},$$

where the subscript k indexes units in the ouput layer and n_H denotes the number of hidden units

- **The output can be a linear or nonlinear function of the net input e.g.,**

$$y_k = n_k$$

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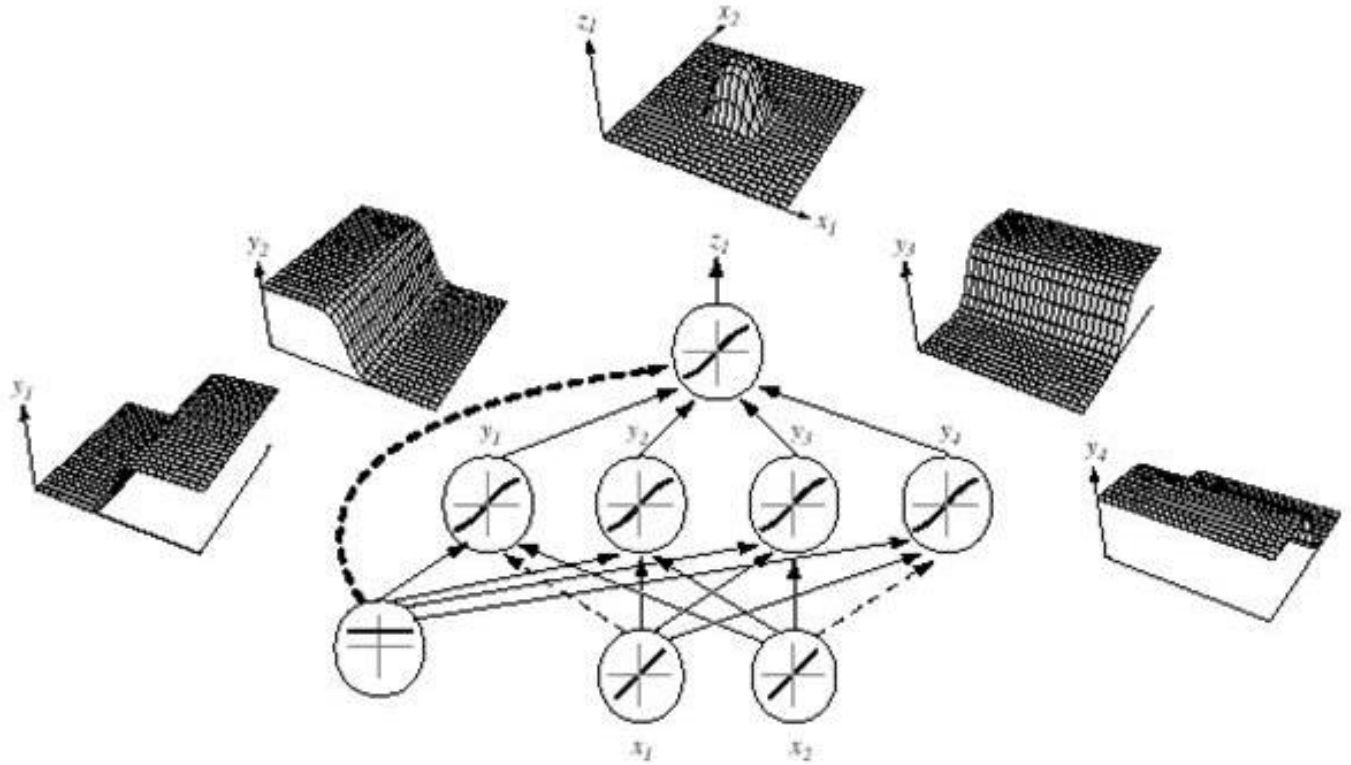
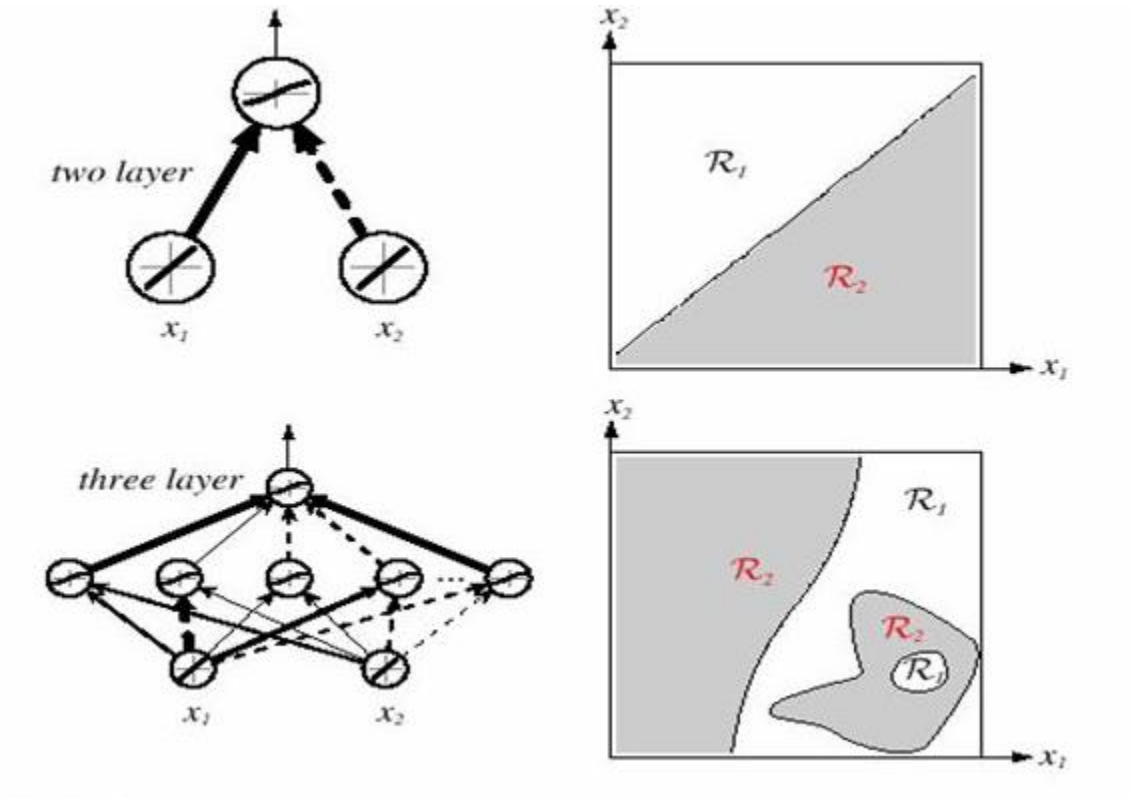
Computing nonlinear functions using a feed-forward neural network



Realizing non linearly separable class boundaries using a 3-layer feed-forward neural network



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Learning nonlinear functions

Given a training set determine:

- **Network structure – number of hidden nodes or more generally, network topology**
  - **Start small and grow the network**
  - **Start with a sufficiently large network and prune away the unnecessary connections**
- **For a given structure, determine the parameters (weights) that minimize the error on the training samples (e.g., the mean squared error)**
- **For now, we focus on the *latter***

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Generalized delta rule – error back-propagation

- Challenge – we know the desired outputs for nodes in the output layer, but not the hidden layer
- Need to solve the credit assignment problem – dividing the credit or blame for the performance of the output nodes among hidden nodes
- Generalized delta rule offers an elegant solution to the credit assignment problem in feed-forward neural networks in which each neuron computes a differentiable function of its inputs
- Solution can be generalized to other kinds of networks, including networks with cycles

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Feed-forward networks

- **Forward operation** (computing output for a given input based on the current weights)
- **Learning –** modification of the network parameters (weights) to minimize an appropriate error measure
- Because each neuron computes a differentiable function of its inputs if error is a differentiable function of the network outputs, the error is a differentiable function of the weights in the network – so we can perform gradient descent!

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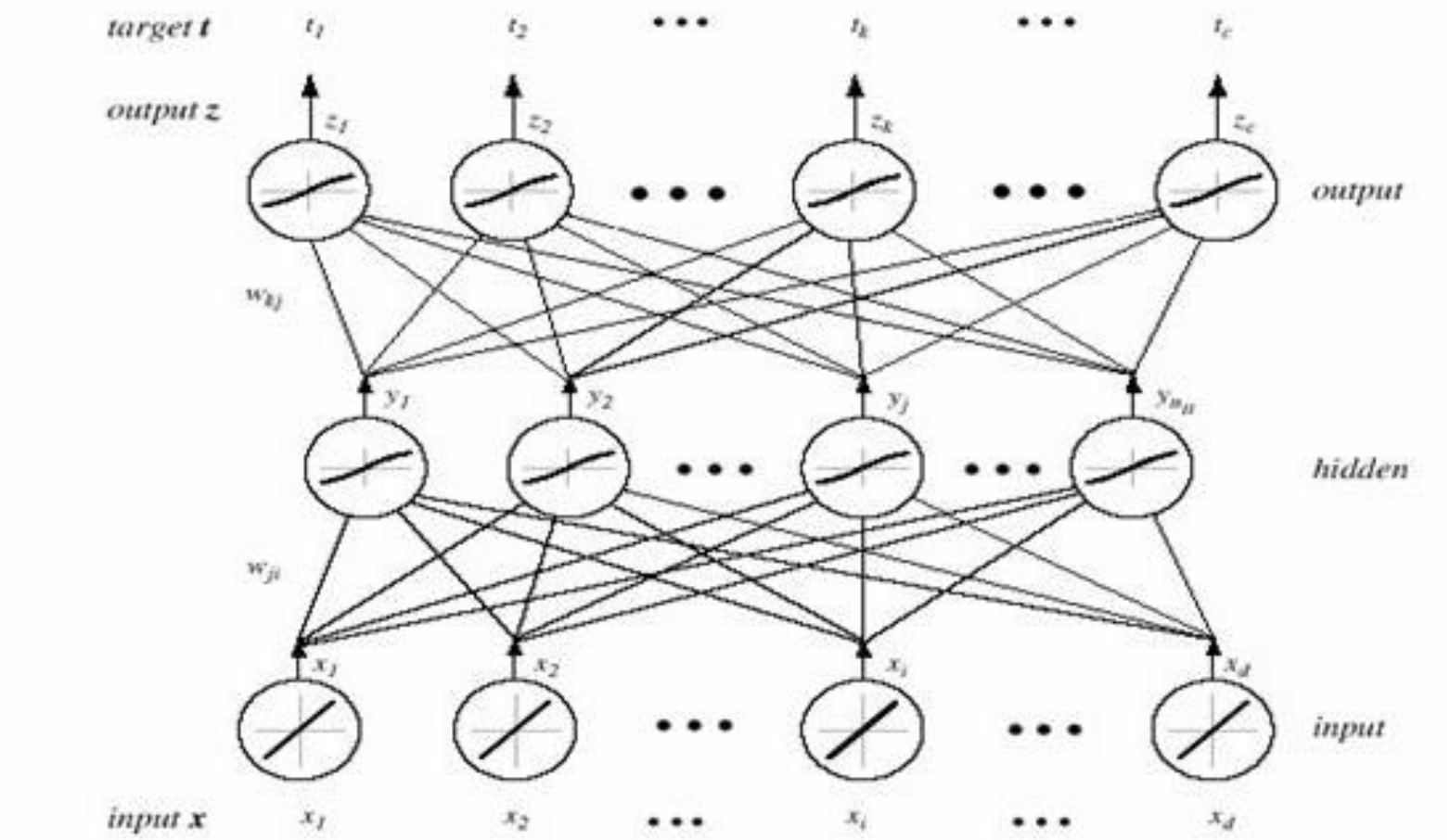
A fully connected 3-layer network



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Generalized delta rule

- Let t_{kp} be the k-th target (or desired) output for input pattern $\mathbf{X}_p$ and z_{kp} be the output produced by k-th output node and let $\mathbf{W}$ represent all the weights in the network

- Training error:

$$E_S(\mathbf{W}) = \frac{1}{2}\sum_p \sum_{k=1}^{M}(t_{kp} - z_{kp})^2 = \sum_p E_p(\mathbf{W})$$

- The weights are initialized with pseudo-random values and are changed in a direction that will reduce the error:

$$\Delta w_{ji} = -\eta \frac{\partial E_S}{\partial w_{ji}} \qquad \Delta w_{kj} = -\eta \frac{\partial E_S}{\partial w_{kj}}$$

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Generalized delta rule

$\eta>0$ is a suitable the learning rate $W \leftarrow W + \Delta W$

Hidden–to-output weights

$$\frac{\partial E_p}{\partial w_{kj}} = \frac{\partial E_p}{\partial n_{kp}} \cdot \frac{\partial n_{kp}}{\partial w_{kj}}$$

$$\frac{\partial n_{kp}}{\partial w_{kj}} = y_{jp}$$

$$\frac{\partial E_p}{\partial n_{kp}} = \frac{\partial E_p}{\partial z_{kp}} \cdot \frac{\partial z_{kp}}{\partial n_{kp}} = -(t_{kp} - z_{kp})(1)$$

$$w_{kj} \leftarrow w_{kj} - \eta \frac{\partial E_p}{\partial w_{kj}} = w_{kj} + (t_{kp} - z_{kp}) y_{jp} = w_{kj} + \delta_{kp} y_{jp}$$

Generalized delta rule

Weights from input to hidden units

$$\frac{\partial E_p}{\partial w_{ji}} = \sum_{k=1}^{M} \frac{\partial E_p}{\partial z_{kp}} \frac{\partial z_{kp}}{\partial w_{ji}} = \sum_{k=1}^{M} \frac{\partial E_p}{\partial z_{kp}} \frac{\partial z_{kp}}{\partial y_{jp}} \cdot \frac{\partial y_{jp}}{\partial n_{jp}} \cdot \frac{\partial n_{jp}}{\partial w_{ji}}$$

$$= \sum_{k=1}^{M} \frac{\partial}{\partial z_{kp}} \left[\frac{1}{2} \sum_{l=1}^{M} (t_{lp} - z_{lp})^2 \right] (w_{kj})(y_{jp})(1 - y_{jp})(x_{ip})$$

$$= -\sum_{k=1}^{M} (t_{kp} - z_{kp})(w_{kj})(y_{jp})(1 - y_{jp})(x_{ip})$$

$$= -\underbrace{\left(\sum_{k=1}^{M} \delta_{kp} (w_{kj})(y_{jp})(1 - y_{jp}) \right)}_{\delta_{jp}} (x_{ip}) = -\delta_{jp} x_{ip}$$

$$w_{ji} \leftarrow w_{ji} + \eta \delta_{jp} x_{ip}$$

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Back propagation algorithm

Start with small random initial weights

Until desired stopping criterion is satisfied do

- Select a training sample from S
- Compute the outputs of all nodes based on current weights and the input sample
- Compute the weight updates for output nodes
- Compute the weight updates for hidden nodes
- Update the weights

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Using neural networks for classification

Network outputs are real valued.

How can we use the networks for classification?

$$F(\mathbf{X}_p) = \underset{k}{\operatorname{argmax}} z_{kp}$$

Classify a pattern by assigning it to the class that corresponds to the index of the output node with the largest output for the pattern