神经网络

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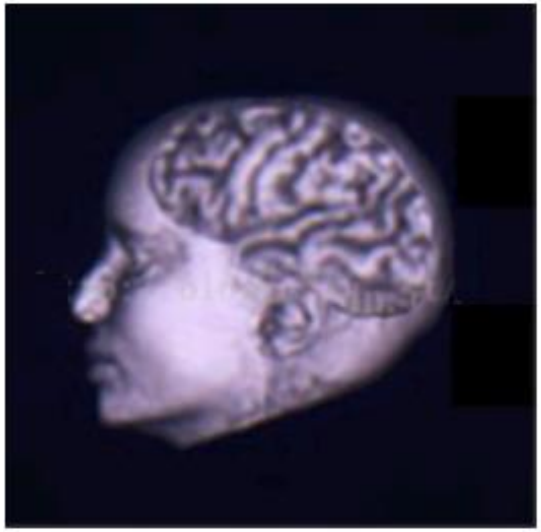
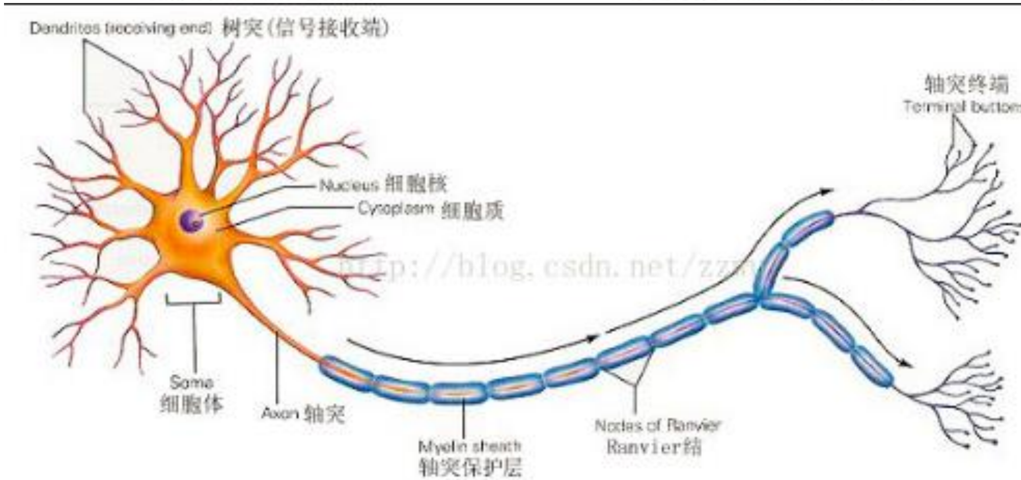
How our brain works?

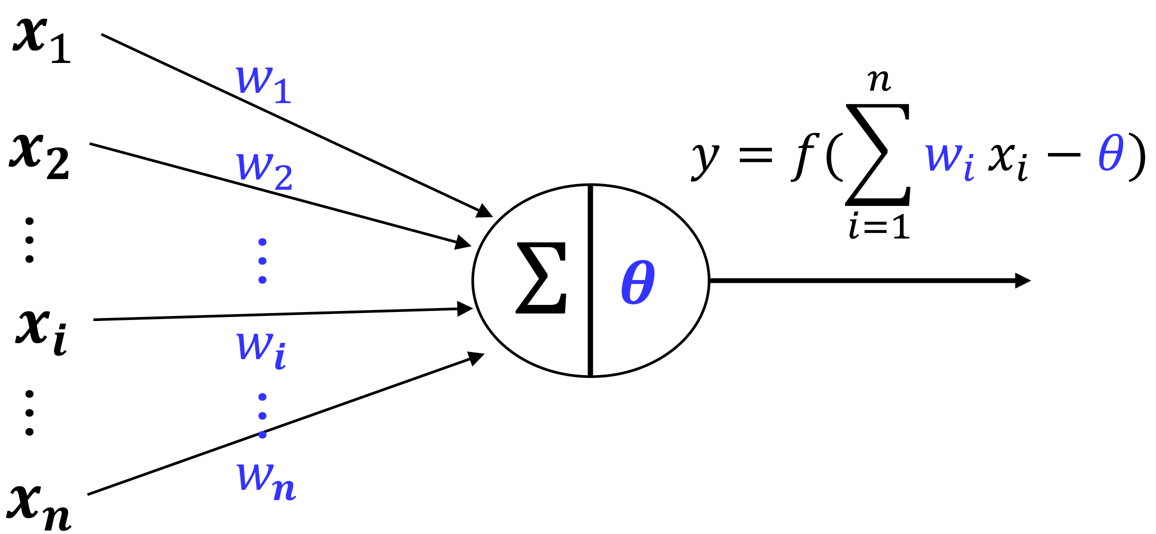


1 大脑半球像半个核桃

2 大脑皮层由灰质白质组成



神经元模型



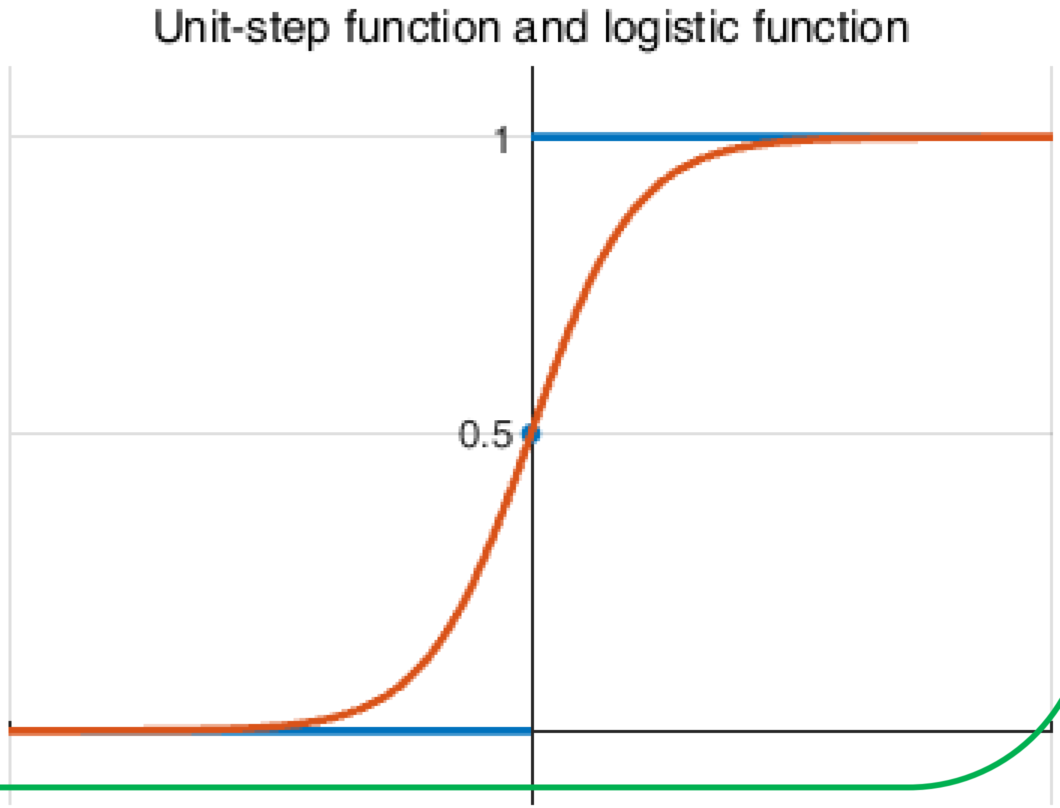
- x_i ： 第 i 个神经元的输入
- w_i ： 第 i 个神经元的权重
- θ ： 阈值(threshold)或称为偏置（bias）
- y ： 神经元状态（兴奋或抑制）

激活函数（ Activation function ）

由于单位阶跃函数不是一个连续函数，我们通常选择一些性质好的函数作为替代函数。

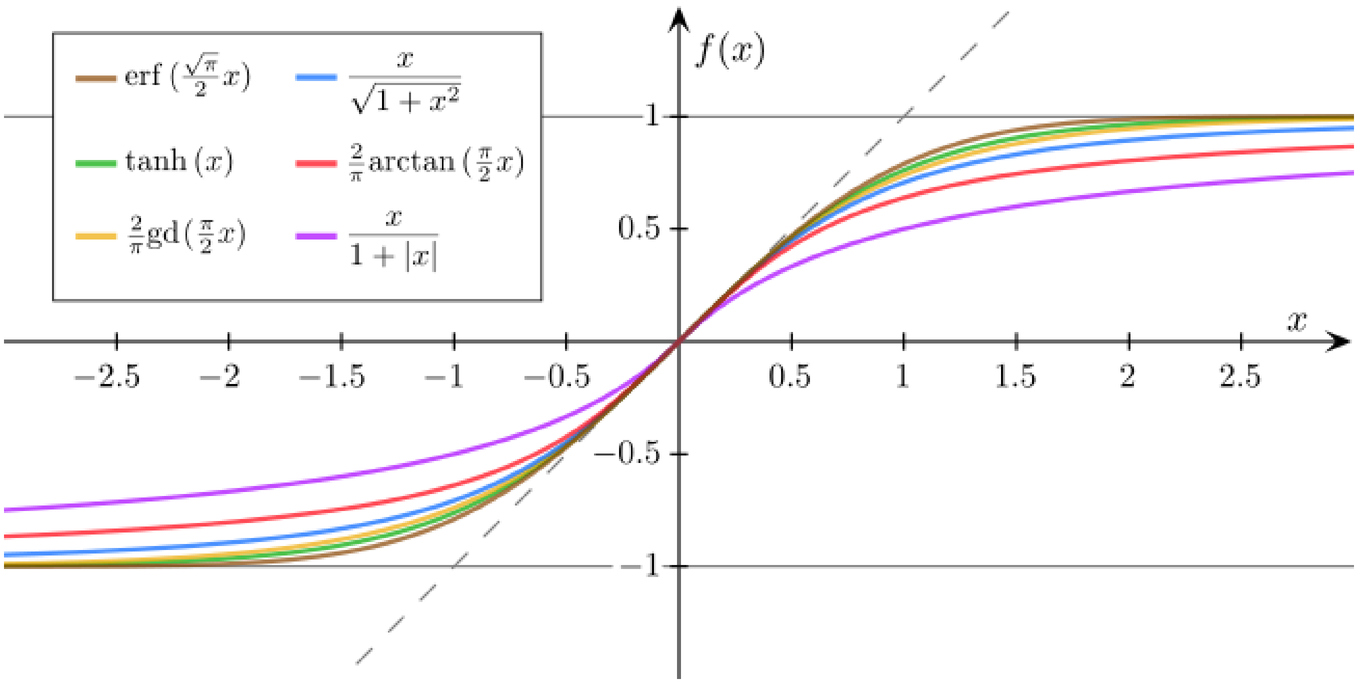
Logistic function:

$$y = \frac{1}{1 + e^{-z}}$$



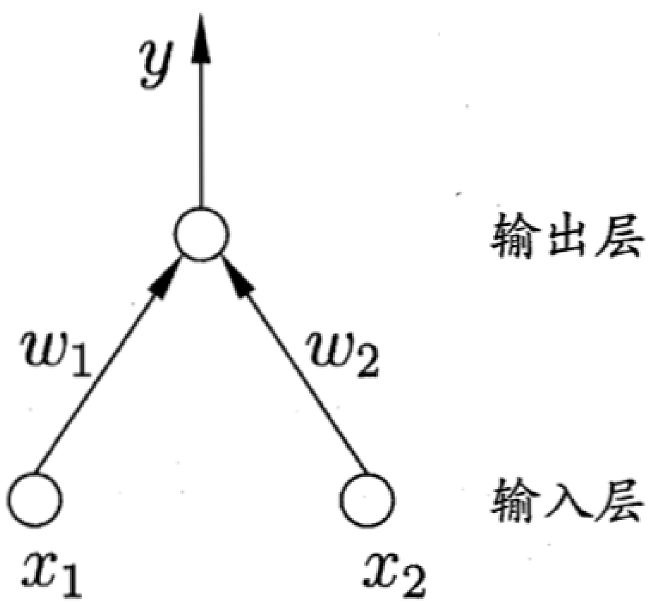
激活函数（ Activation function ）

$f(\cdot)$函数称为激活函数(activation function)或挤压函数（Squashing function）.



感知机（Perceptron）

感知机（Perceptron）由两层神经元组成，是最简单的神经网络。



感知机（Perceptron）

对于上述感知机模型，给定训练点(x, y), 令$\boldsymbol{w_0} = \boldsymbol{\theta}, \boldsymbol{x_0} = -\mathbf{1}$(哑结点), 则$\widehat{\boldsymbol{w}}^{\mathbf{T}}\widehat{\boldsymbol{x}} = w_1x_1 + w_2x_2 + w_0x_0$。

感知机模型为：

$$\min_{\widehat{\boldsymbol{w}}} \ (\widehat{\boldsymbol{y}} - \boldsymbol{y})\widehat{\boldsymbol{w}}^{\mathbf{T}}\widehat{\boldsymbol{x}}$$

其中 $\hat{y} = f\left(\widehat{\boldsymbol{w}}^{\mathbf{T}}\widehat{\boldsymbol{x}}\right)$为感知机当前的输出结果。

感知机参数$\widehat{\boldsymbol{w}}$的更新公式：

$$\widehat{\boldsymbol{w}} \leftarrow \widehat{\boldsymbol{w}} - \boldsymbol{\eta}\frac{\boldsymbol{\partial}((\widehat{\boldsymbol{y}} - \boldsymbol{y})\widehat{\boldsymbol{w}}^{\mathbf{T}}\widehat{\boldsymbol{x}})}{\boldsymbol{\partial}\widehat{\boldsymbol{w}}} \leftarrow \widehat{\boldsymbol{w}} - \boldsymbol{\eta}(\widehat{\boldsymbol{y}} - \boldsymbol{y})\widehat{\boldsymbol{x}}$$

若样例(x, y)预测正确 $\Rightarrow$ $\widehat{\boldsymbol{y}} = \boldsymbol{y}$ $\Rightarrow$ $\widehat{\boldsymbol{w}}$ 不再更新

若样例(x, y)预测错误 $\Rightarrow$ $\widehat{\boldsymbol{y}} \neq \boldsymbol{y}$ $\Rightarrow$ $\widehat{\boldsymbol{w}}$ 继续更新

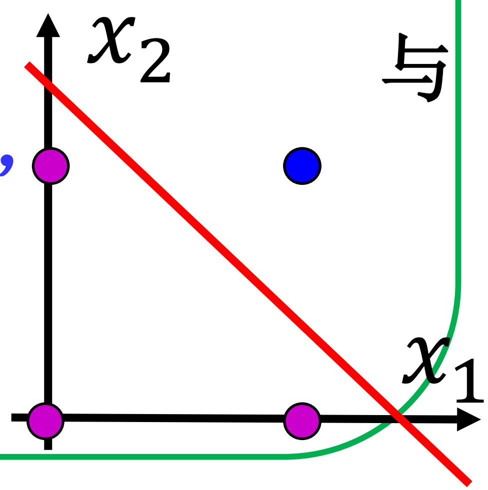
逻辑运算 I

"与" 运算$(\boldsymbol{x_1} \wedge \boldsymbol{x_2} \wedge \cdots \wedge \boldsymbol{x_n})$，其中$\boldsymbol{x_i} \in \{\boldsymbol{0}, \boldsymbol{1}\}$。

令权重 $w_1 = w_2 = \cdots = w_n = 1$, 阈值 $\theta = n$.

则输出 $y = f(\sum_{\boldsymbol{i=1}}^{\boldsymbol{n}} \boldsymbol{w_i}\, \boldsymbol{x_i} - \boldsymbol{\theta}) = f(\sum_{\boldsymbol{i=1}}^{\boldsymbol{n}} \boldsymbol{x_i} - n)$

当且仅当 $\boldsymbol{x}_1 = \boldsymbol{x}_2 = \cdots = \boldsymbol{x}_n = 1$ 时，
$y = 1$。



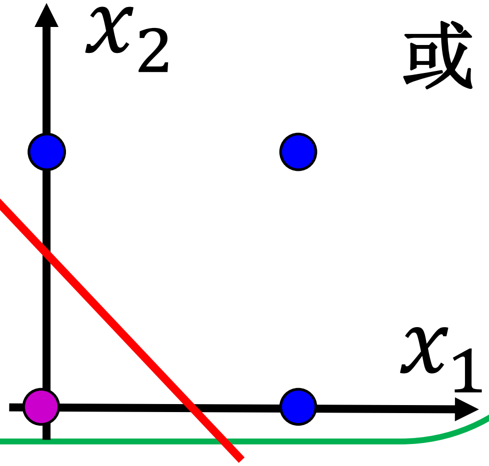
逻辑运算 II

"或" 运算$(\boldsymbol{x_1} \vee \boldsymbol{x_2} \vee \cdots \vee \boldsymbol{x_n})$，其中$\boldsymbol{x_i} \in \{\mathbf{0}, \mathbf{1}\}$。

令权重 $w_1 = w_2 = \cdots = w_n = 1$, 阈值 $\theta = \mathbf{1/2}$.

输出 $y = f(\sum_{i=1}^{n} \boldsymbol{w_i}\,\boldsymbol{x_i} - \boldsymbol{\theta}) = f(\sum_{i=1}^{n} \boldsymbol{x_i} - \mathbf{1/2})$

当且仅当至少有一个$\boldsymbol{x_i} = 1$时，$y = 1$。



逻辑运算 III

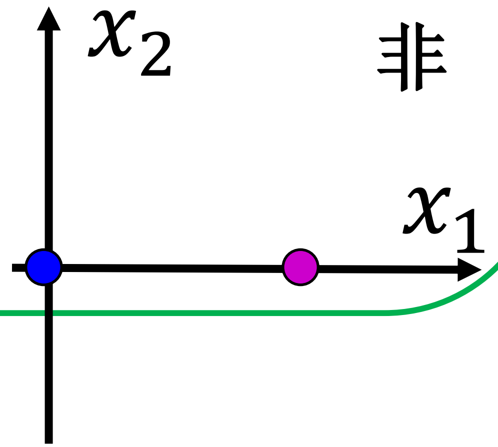
"非" 运算($\sim \boldsymbol{x_i}$)，其中$\boldsymbol{x_i} \in \{\mathbf{0}, \mathbf{1}\}$。

令 $w_i = -\mathbf{2}$, 其他 $w_j = \mathbf{0}$，阈值 $\theta = -\mathbf{1}$.

输出 $y = f(\sum_{i=1}^{n} \boldsymbol{w_i}\, \boldsymbol{x_i} - \boldsymbol{\theta}) = f(-\mathbf{2}\boldsymbol{x_i} + \mathbf{1})$

当 $\boldsymbol{x_i} = \mathbf{1}$ 时，$y = f(-\mathbf{1}) = \mathbf{0}$;

当 $\boldsymbol{x_i} = \mathbf{0}$ 时，$y = f(\mathbf{1}) = \mathbf{1}$。



逻辑运算 IV

"异或" 运算$(x_i \oplus x_j)$，其中$x_i \in \{0,1\}$。

若感知机可以解决异或运算，则

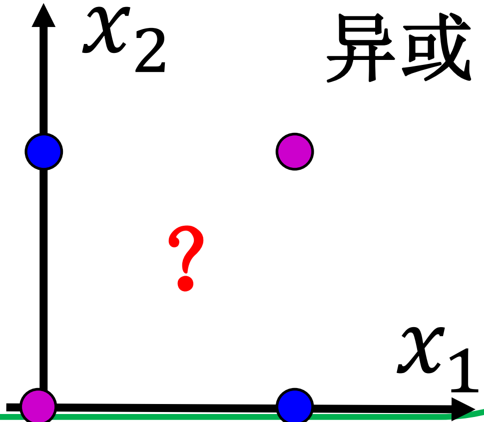
当 $x_i = x_j$ 时，$y = f(\sum_{i=1}^{n} w_i x_i - \theta) = 0$

$w_i + w_j - \theta < 0, -\theta < 0$

当 $x_i \neq x_j$ 时，$y = f(\sum_{i=1}^{n} w_i x_i - \theta) = 1$

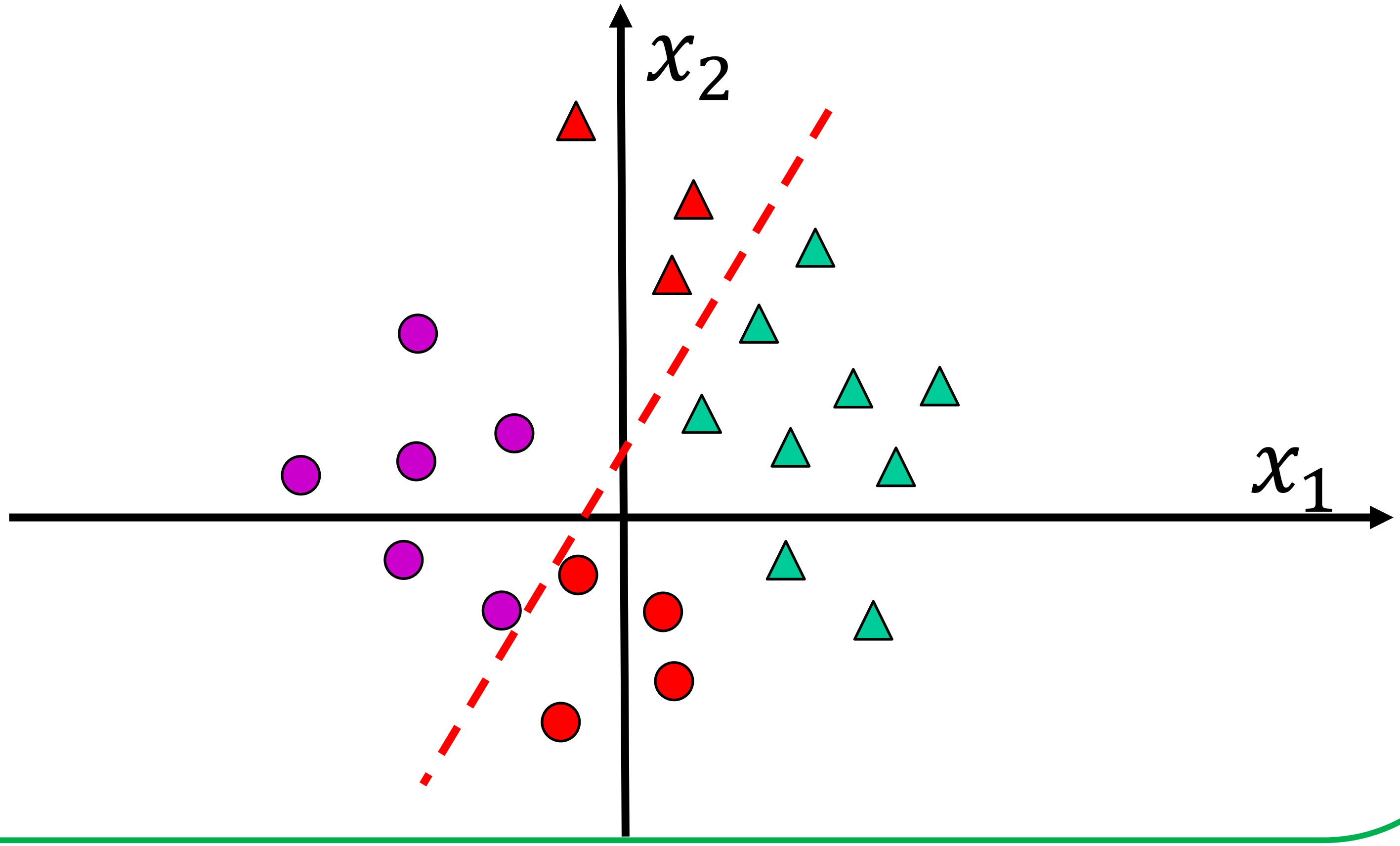
$w_i - \theta \geq 0, w_j - \theta \geq 0$

不存在这样的 w_i和w_j！！！



感知机原理

考虑二分类问题，红色点代表着误分类点。



误分类点

考虑输出变量 $y_i \in \{0,1\}$，定义

$$\gamma_i = (\hat{y}_i - y_i)\frac{w^{\mathrm{T}}x_i - \theta}{\|w\|} \geq 0$$

其中 $\hat{y}_i = f(w^{\mathrm{T}}x_i - \theta)$。

若 $\hat{y}_i = y_i$，则 $\gamma_i = 0$；若 $\hat{y}_i \neq y_i$，则 $\gamma_i = \frac{|w^{\mathrm{T}}x_i - \theta|}{\|w\|}$

因此$(\hat{y}_i - y_i)(w^{\mathrm{T}}x_i - \theta)$衡量着误分类点$x_i$到分类超平面的距离。

感知机模型

令 $\boldsymbol{w}_0 = \boldsymbol{\theta}, \boldsymbol{x}_0 = -\mathbf{1}$, 即将阈值 $\boldsymbol{\theta}$ 看作是“哑结点” $\boldsymbol{x}_0$ 所对应的权重, 则感知机最小化误分类点到分类平面的距离和：

$$\min_{\hat{\boldsymbol{w}}} \sum_{i=1}^{n} (\hat{\boldsymbol{y}}_i - \boldsymbol{y}_i)\hat{\boldsymbol{w}}^{\mathrm{T}}\hat{\boldsymbol{x}}_i$$

$\hat{\boldsymbol{w}} = [\boldsymbol{w}_0; \boldsymbol{w}_1; \cdots; \boldsymbol{w}_d]$， $\hat{\boldsymbol{x}}_i = [\boldsymbol{x}_0; \boldsymbol{x}_{i1}; \cdots; \boldsymbol{x}_{id}]$。

注意，上述求和仅当$\hat{\boldsymbol{y}}_i \neq \boldsymbol{y}_i$时起作用！

感知机模型

感知机模型：

$$\min_{\hat{\boldsymbol{w}}} \sum_{i=1}^{n} (\hat{y}_i - y_i)\hat{\boldsymbol{w}}^{\mathrm{T}}\hat{\boldsymbol{x}}_i$$

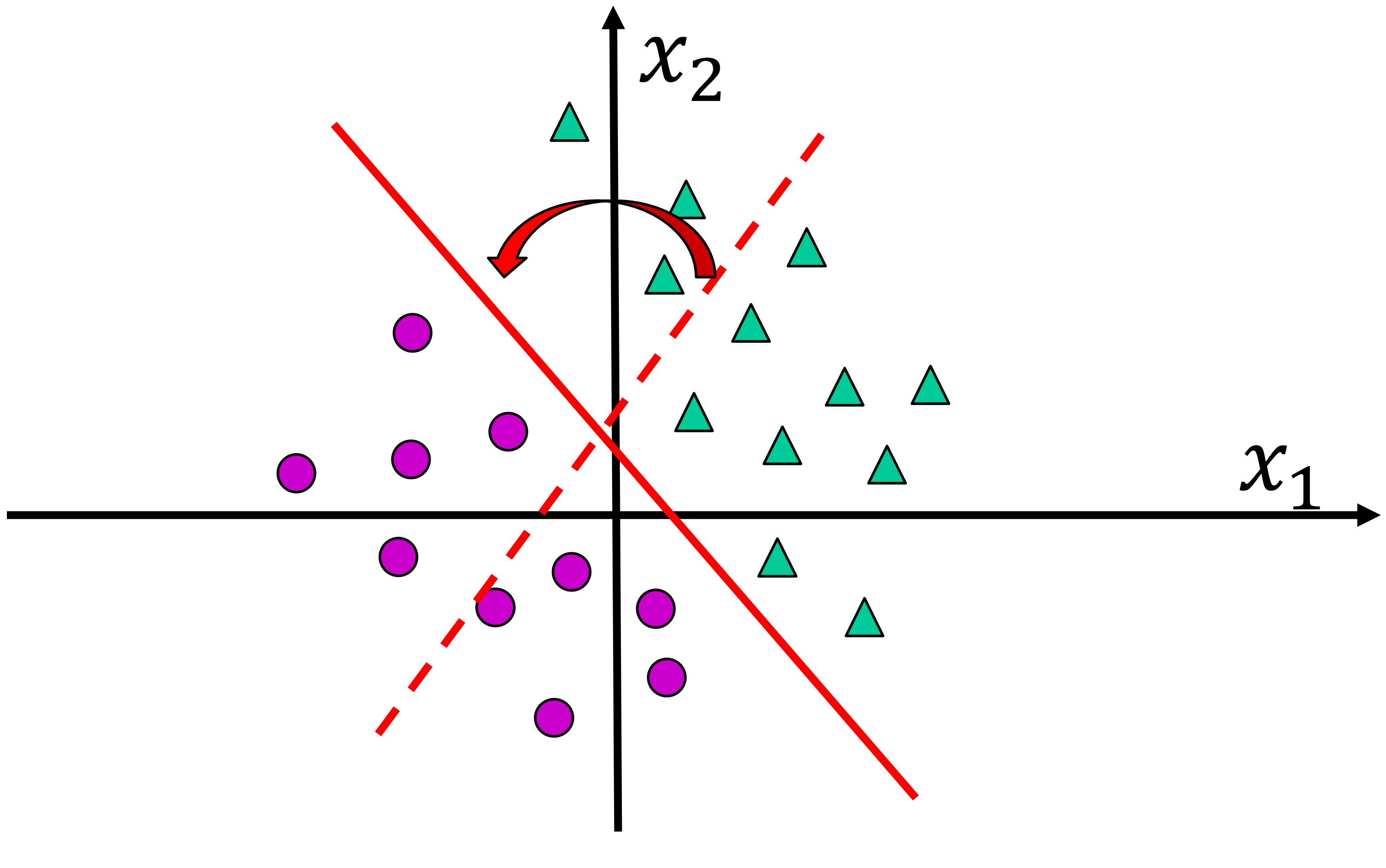
梯度下降法：

$$\hat{\boldsymbol{w}} \leftarrow \hat{\boldsymbol{w}} - \eta\Delta\hat{\boldsymbol{w}}$$

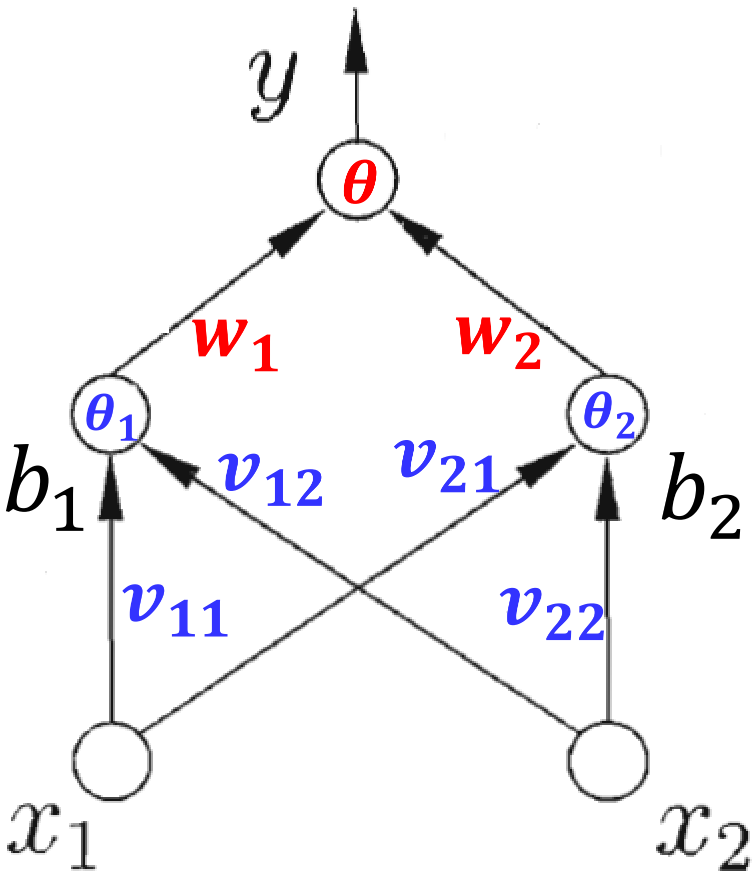
其中

$$\Delta\hat{\boldsymbol{w}} = \frac{\partial\left(\sum_{i=1}^{n}(\hat{y}_i - y_i)\hat{\boldsymbol{w}}^{\mathrm{T}}\hat{\boldsymbol{x}}_i\right)}{\partial\hat{\boldsymbol{w}}} = \sum_{i=1}^{n}(\hat{y}_i - y_i)\hat{\boldsymbol{x}}_i = \boldsymbol{X}^{\mathrm{T}}(\hat{\boldsymbol{y}} - \boldsymbol{y})$$

感知机原理



单隐层神经网络



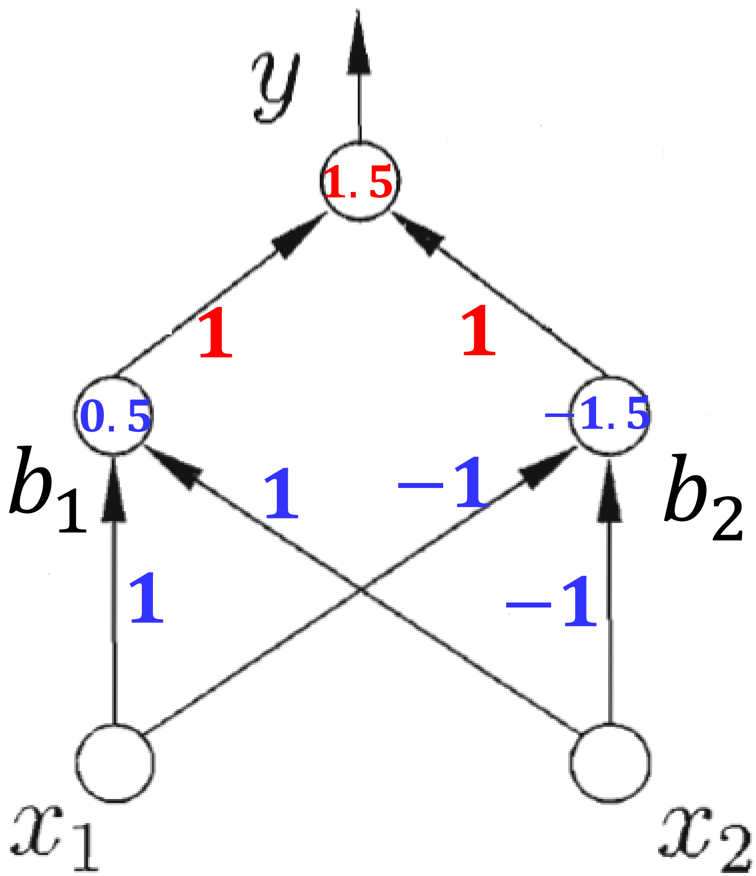
第一层：

$$b_1 = f(v_{11}x_1 + v_{12}x_2 - \theta_1)$$
$$b_2 = f(v_{21}x_1 + v_{22}x_2 - \theta_2)$$

第二层：

$$y = g(w_1 b_1 + w_2 b_2 - \theta)$$

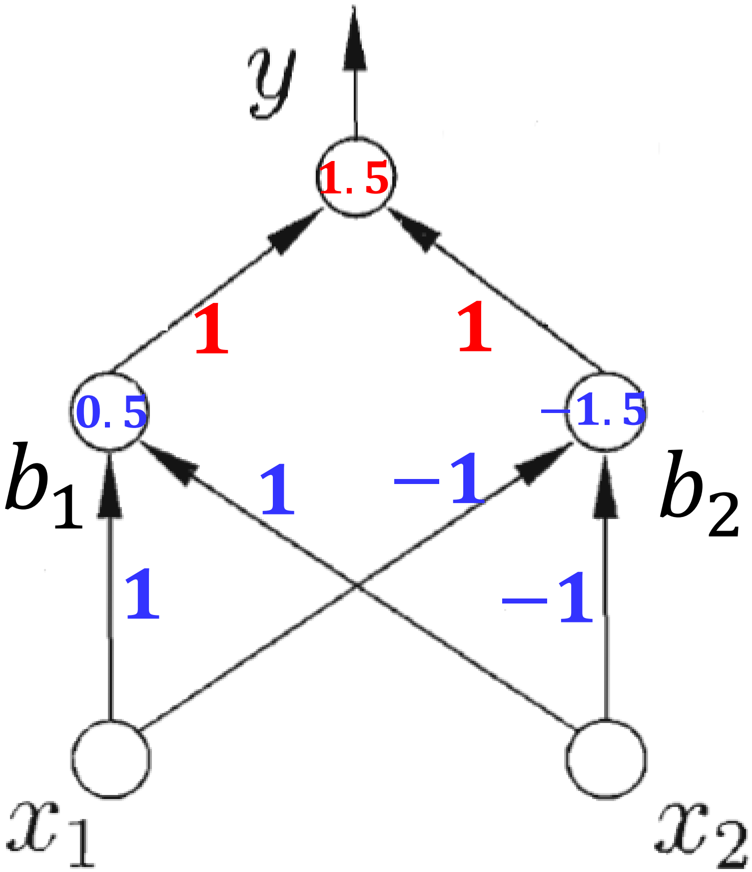
异或问题



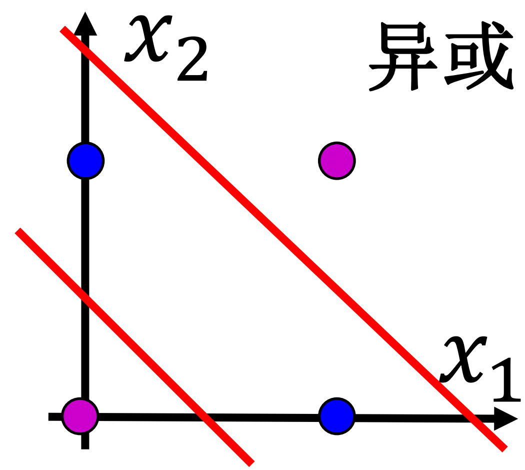
$$b_1 = f(\ \ x_1 + x_2 - 0.5)$$
$$b_2 = f(-x_1 - x_2 + 1.5)$$
$$y = g(b_1 + b_2 - 1.5)$$

$x_1 = 0$， $x_2 = 0$;
$b_1 = 0, b_2 = 1, y = 0$
$x_1 = 0$， $x_2 = 1$;
$b_1 = 1, b_2 = 1, y = 1$
$x_1 = 1$， $x_2 = 0$;
$b_1 = 1, b_2 = 1, y = 1$
$x_1 = 1$， $x_2 = 1$;
$b_1 = 1, b_2 = 0, y = 0$

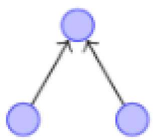
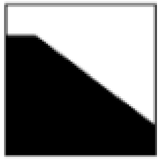
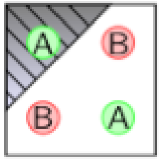
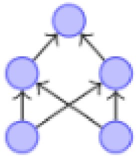
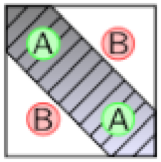
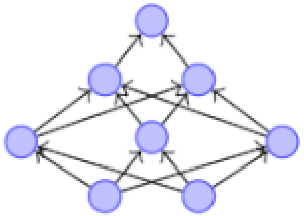
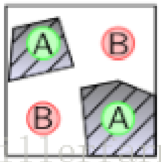
异或问题



$x_1 = 0$， $x_2 = 0, y = 0$
$x_1 = 0$， $x_2 = 1, y = 1$
$x_1 = 1$， $x_2 = 0, y = 1$
$x_1 = 1$， $x_2 = 1, y = 0$

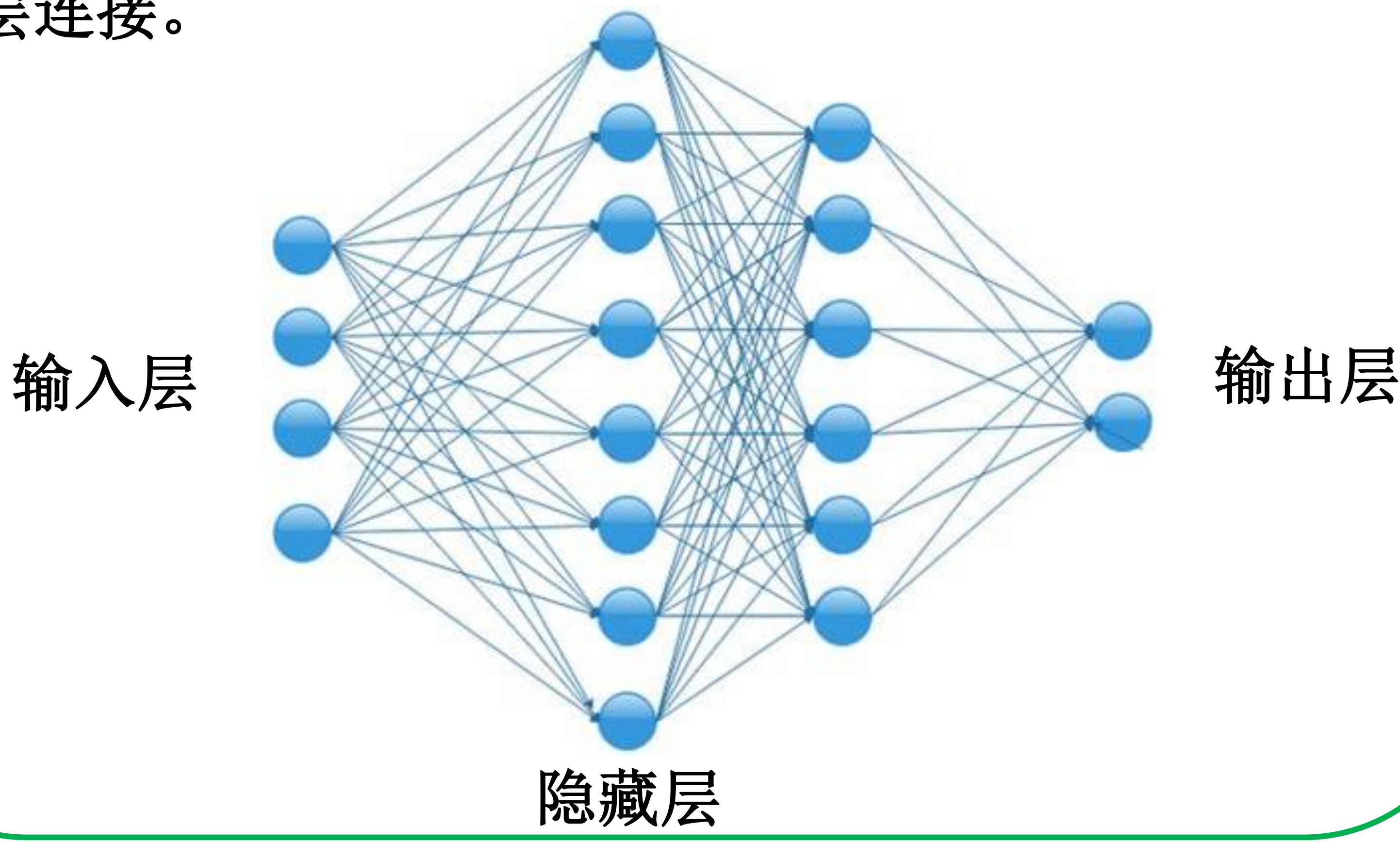


多层神经网络

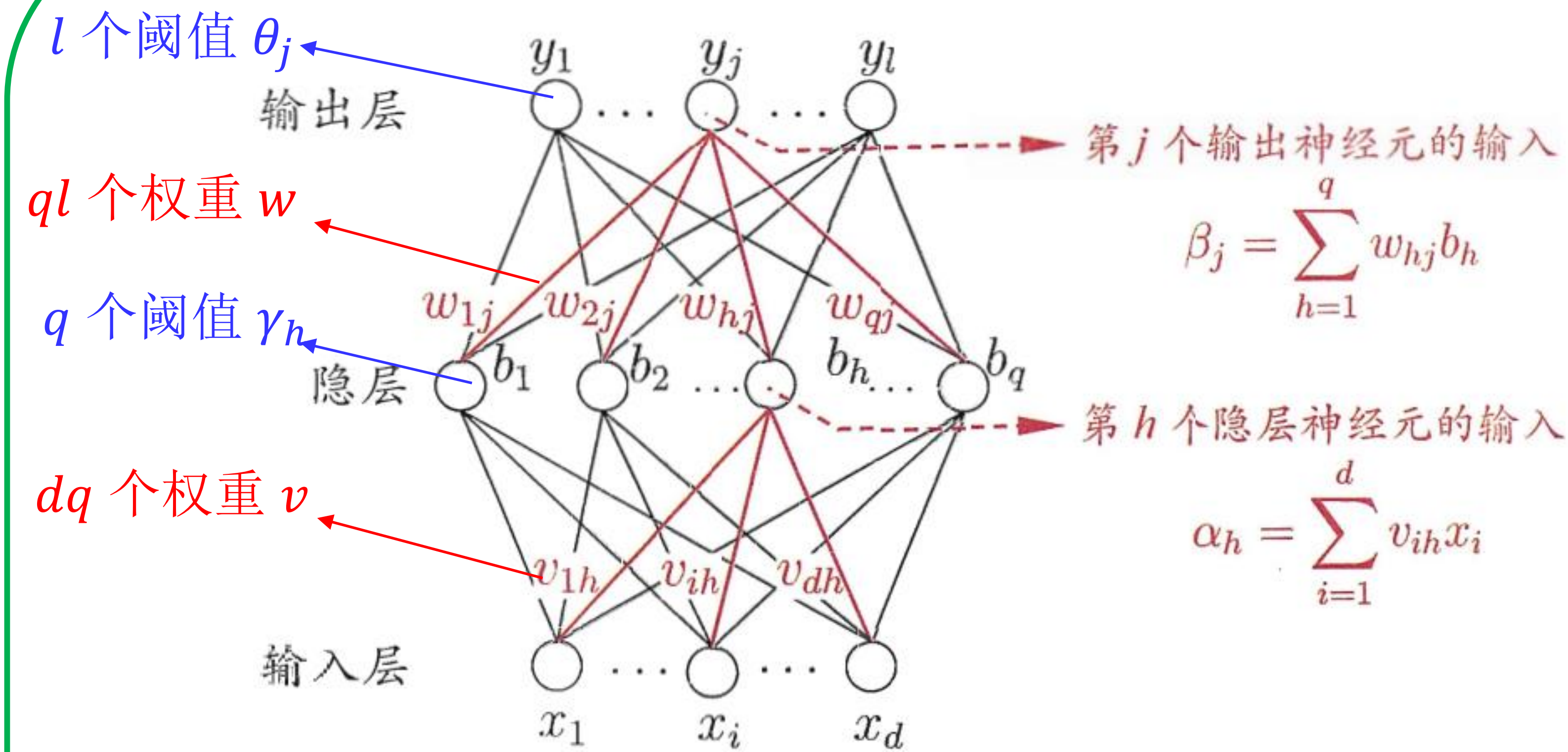
结构	决策区域类型	区域形状	异或问题
无隐层 	由一超平面分成两个		
单隐层 	开凸区域或闭凸区域		
双隐层 	任意形状（其复杂度由单元数目确定）		

多层前馈神经网络

多层前馈神经网络: 每层神经元与下一层神经元完全相连，神经元之间不存在同层连接，也不存在跨层连接。



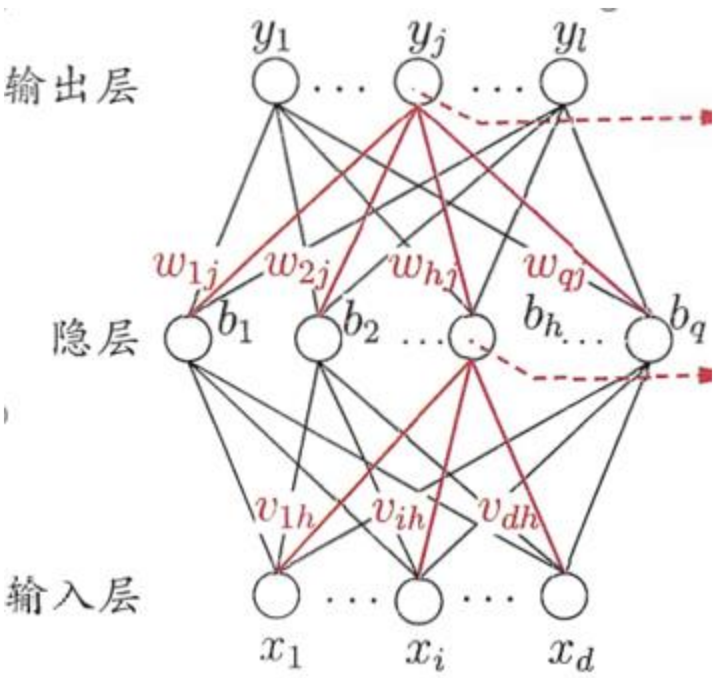
误差逆传播算法



总参数：$l + ql + q + dq$

图 5.7 BP 网络及算法中的变量符号

误差逆传播算法



$$\hat{y}_j^k = f(\beta_j - \theta_j);$$

$$\beta_j = \sum_{h=1}^{q} \omega_{hj} b_h$$

$$b_h = f(\alpha_h - \gamma_h)$$

$$\alpha_h = \sum_{i=1}^{d} v_{ih} x_i$$

其中f是对数几率函数。

$$f' = f(1-f)$$

BP网络均方误差： $E_k = \frac{1}{2}\sum_{j=1}^{l}(\hat{y}_j^k - y_j^k)^2$

误差逆传播算法

$$\hat{y}_j^k = f(\beta_j - \theta_j);$$

$$\beta_j = \sum_{h=1}^{q} \omega_{hj} b_h$$

$$b_h = f(\alpha_h - \gamma_h)$$

$$\alpha_h = \sum_{i=1}^{d} v_{ih} x_i$$

其中f是对数几率函数。

$$f' = f(1-f)$$

$$\frac{\partial E_k}{\partial \omega_{hj}} = \frac{\partial E_k}{\partial \hat{y}_j^k} \frac{\partial \hat{y}_j^k}{\partial \beta_j} \frac{\partial \beta_j}{\partial \omega_{hj}}$$

$$\frac{\partial E_k}{\partial \theta_j} = -\frac{\partial E_k}{\partial \hat{y}_j^k} \frac{\partial \hat{y}_j^k}{\partial \beta_j}$$

$$\frac{\partial E_k}{\partial v_{ih}} = \sum_{j=1}^{l} \frac{\partial E_k}{\partial \hat{y}_j^k} \frac{\partial \hat{y}_j^k}{\partial \beta_j} \frac{\partial \beta_j}{\partial b_h} \frac{\partial b_h}{\partial \alpha_h} \frac{\partial \alpha_h}{\partial v_{ih}}$$

$$\frac{\partial E_k}{\partial \gamma_h} = -\sum_{j=1}^{l} \frac{\partial E_k}{\partial \hat{y}_j^k} \frac{\partial \hat{y}_j^k}{\partial \beta_j} \frac{\partial \beta_j}{\partial b_h} \frac{\partial b_h}{\partial \alpha_h}$$

$$\frac{\partial E_k}{\partial \hat{y}_j^k}\,\frac{\partial \hat{y}_j^k}{\partial \beta_j}$$

$$E_k = \frac{1}{2}\sum_{j=1}^{l}(\hat{y}_j^k - y_j^k)^2;$$

$$\hat{y}_j^k = f(\beta_j - \theta_j);\quad \beta_j = \sum_{h=1}^{q} \omega_{hj} b_h$$

$$\frac{\partial E_k}{\partial \hat{y}_j^k} = \frac{\partial(\frac{1}{2}\sum_{j=1}^{l}(\hat{y}_j^k - y_j^k)^2)}{\partial \hat{y}_j^k} = \hat{y}_j^k - y_j^k$$

$$\frac{\partial \hat{y}_j^k}{\partial \beta_j} = \frac{\partial f(\beta_j - \theta_j)}{\partial \beta_j} = f\,(1-f) = \hat{y}_j^k(1-\hat{y}_j^k)$$

$$-g_j = \frac{\partial E_k}{\partial \hat{y}_j^k}\,\frac{\partial \hat{y}_j^k}{\partial \beta_j} = \hat{y}_j^k(1-\hat{y}_j^k)(\hat{y}_j^k - y_j^k)$$

$$\sum_{j=1}^{l} \frac{\partial E_k}{\partial \hat{y}_j^k} \frac{\partial \hat{y}_j^k}{\partial \beta_j} \frac{\partial \beta_j}{\partial b_h} \frac{\partial b_h}{\partial \alpha_h}$$

$$\beta_j = \sum_{h=1}^{q} \omega_{hj} b_h; \quad b_h = f(\alpha_h - \gamma_h)$$

$$\frac{\partial \beta_j}{\partial b_h} = \omega_{hj}$$

$$\frac{\partial b_h}{\partial \alpha_h} = \frac{\partial f(\alpha_h - \gamma_h)}{\partial \alpha_h} = f\,(1 - f) = b_h(1 - b_h)$$

$$\frac{\partial \beta_j}{\partial b_h} \frac{\partial b_h}{\partial \alpha_h} = b_h(1 - b_h)\omega_{hj}$$

$$e_h = \sum_{j=1}^{l} \frac{\partial E_k}{\partial \hat{y}_j^k} \frac{\partial \hat{y}_j^k}{\partial \beta_j} \frac{\partial \beta_j}{\partial b_h} \frac{\partial b_h}{\partial \alpha_h} = b_h(1 - b_h) \sum_{j=1}^{l} \omega_{hj} g_j$$

误差逆传播算法

$$\frac{\partial E_k}{\partial \omega_{hj}} = \frac{\partial E_k}{\partial \hat{y}_j^k} \frac{\partial \hat{y}_j^k}{\partial \beta_j} \frac{\partial \beta_j}{\partial \omega_{hj}} = -g_j b_h$$

$$\frac{\partial E_k}{\partial \theta_j} = -\frac{\partial E_k}{\partial \hat{y}_j^k} \frac{\partial \hat{y}_j^k}{\partial \beta_j} = g_j$$

$$\frac{\partial E_k}{\partial v_{ih}} = \sum_{j=1}^{l} \frac{\partial E_k}{\partial \hat{y}_j^k} \frac{\partial \hat{y}_j^k}{\partial \beta_j} \frac{\partial \beta_j}{\partial b_h} \frac{\partial b_h}{\partial \alpha_h} \frac{\partial \alpha_h}{\partial v_{ih}} = -e_h x_i$$

$$\frac{\partial E_k}{\partial \gamma_h} = -\sum_{j=1}^{l} \frac{\partial E_k}{\partial \hat{y}_j^k} \frac{\partial \hat{y}_j^k}{\partial \beta_j} \frac{\partial \beta_j}{\partial b_h} \frac{\partial b_h}{\partial \alpha_h} = e_h$$

迭代公式：

$$\boldsymbol{\omega_{hj} \leftarrow \omega_{hj} + \eta_\omega g_j b_h}$$

$$\boldsymbol{\theta_j \leftarrow \theta_j - \eta_\theta g_j}$$

$$\boldsymbol{v_{ih} \leftarrow v_{ih} + \eta_v e_h x_i}$$

$$\boldsymbol{\gamma_h \leftarrow \gamma_h - \eta_\gamma e_h}$$

其中$\boldsymbol{\eta} \in (\mathbf{0}, \mathbf{1})$为学习率。

误差逆传播算法

BP算法优化准则：

$$\min_{\theta,\omega,\gamma,\nu} \quad E_k = \frac{1}{2}\sum_{j=1}(\hat{y}_j^k - y_j^k)^2$$

其中预测值$\hat{y}_j^k$与权重$\theta, \omega, \gamma, \nu$相关。

梯度下降法：

$$\frac{\partial E_k}{\partial \theta}, \quad \frac{\partial E_k}{\partial \omega}, \quad \frac{\partial E_k}{\partial \gamma}, \quad \frac{\partial E_k}{\partial \nu}$$

BP算法小结

核心思想：利用前向传播，计算第 n 层输出值

优化目标：输出值和实际值的残差。

计算方法：将残差按影响逐步传递回第 $n-1, n-2, \cdots, 2$层，以修正各层参数。（即所谓的误差逆传播）

主要工具：链式法则（复合函数求偏导）。

BP算法局限性

- 容易过拟合！

  早停、正则化

- 容易陷入局部最优！

  选取多次初值、随机梯度下降法

- 难以设置隐层个数！

  试错法