2020春

模式识别与深度学习 (13)

多层感知器算法

左旺孟

综合楼309

视觉感知与认知组

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参考教材

- 深度学习， Ian GoodFellow，Yoshua Bengio，Aaron Courville著，张志华 译，人民邮电出版社，2017.8

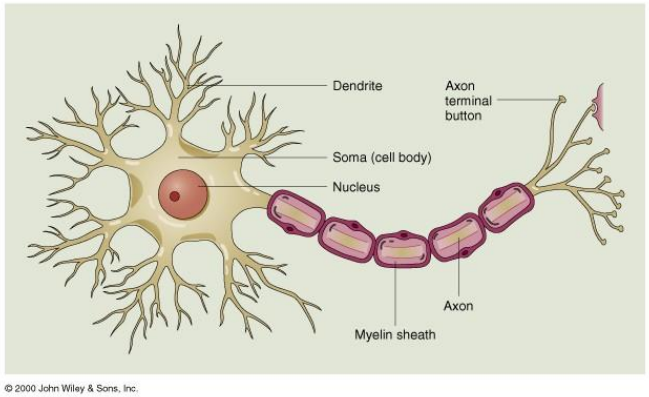
神经网络发展的三个阶段

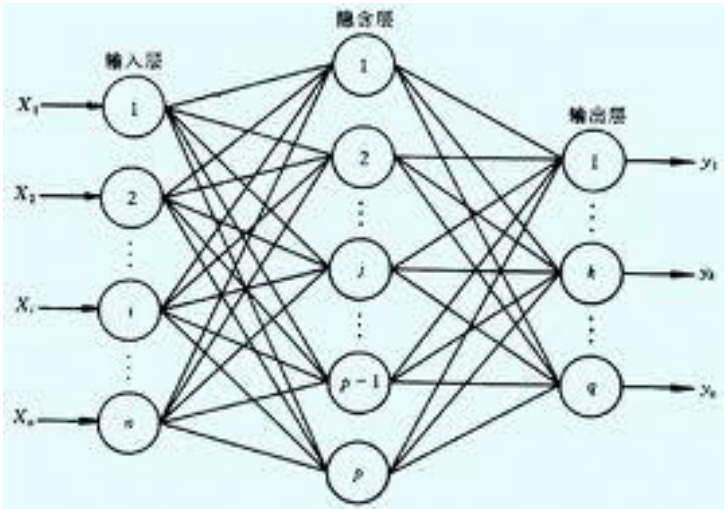
- 一、感知器
  - McCulloch & Pitts / Hebb / Rosenblatt /
  - Minski
- 二、多层感知器感知器
  - Hinton / LeCun
  - Minski
- 三、深度学习（Hinton、LeCun、 Bengio）

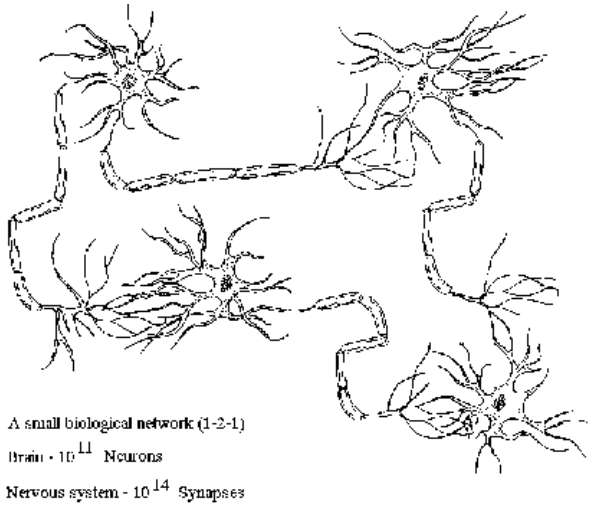
人脑：神经元及其连接

神经网络、感知器、人工神经网络

- 神经元、突触
- 神经网络

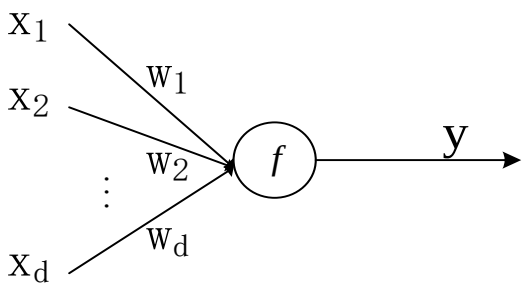


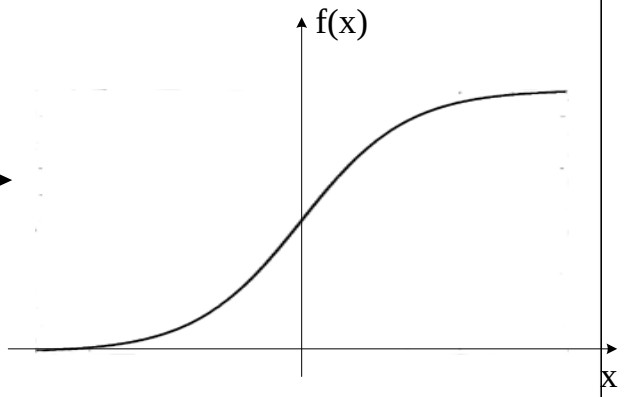


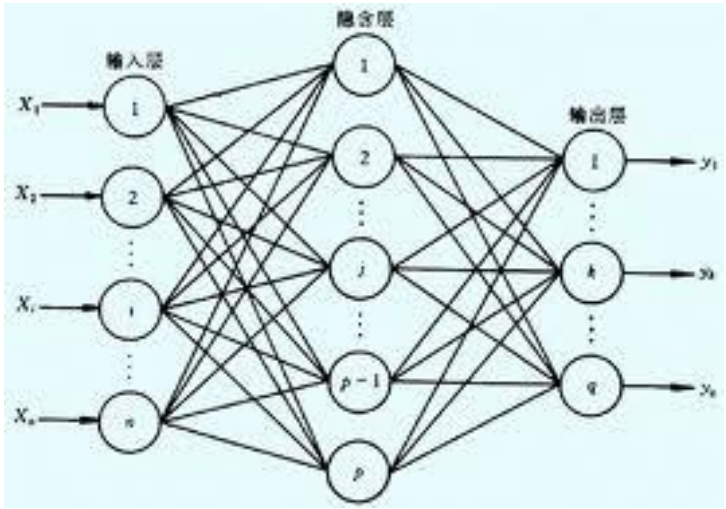


人工神经网络

- 出发点
  - 模拟人类智能
- 建模方法
  - 神经元-突触
  - 网络结构、函数形式
  - 模型参数？
- 学习方法
  - 参数学习 （BP，反向传播）
  - 结构学习（NAS，网络结构搜索）





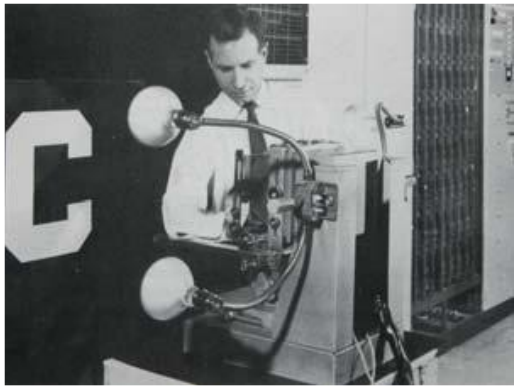


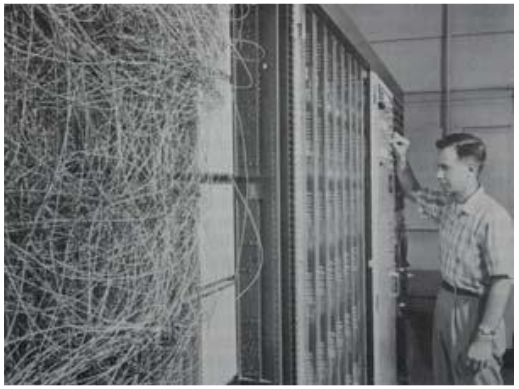
约·冯·诺依曼，《计算机与人脑》，商务出版社（1958, 1965, 2011）

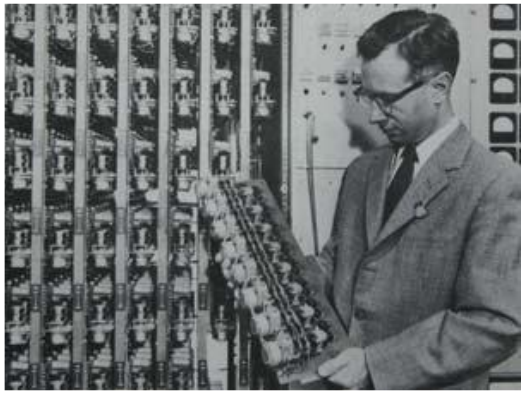
感知器算法: 历史

- 1957年，Rosenblatt提出感知器算法

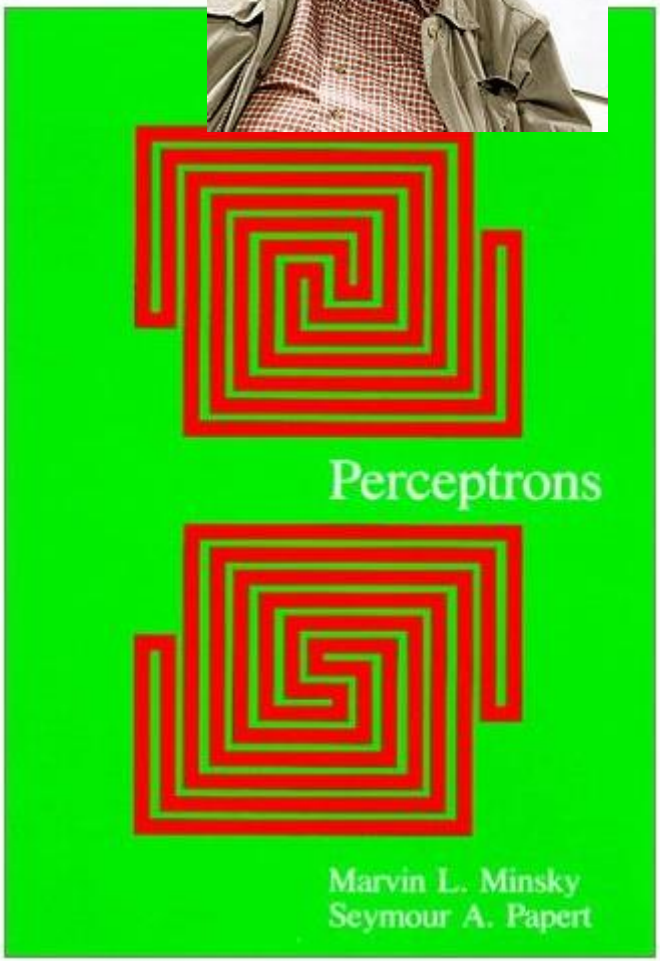
- 线性 vs. 非线性







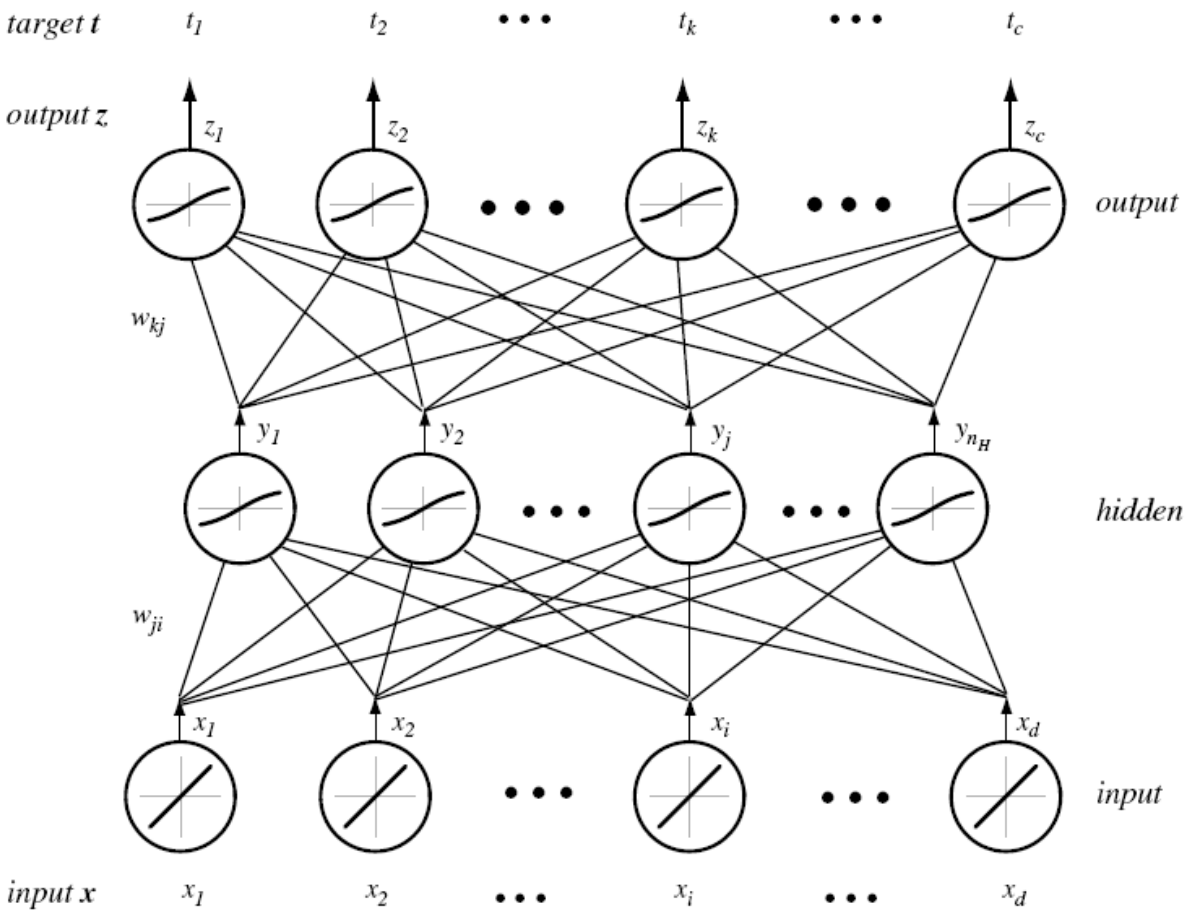
Perceptrons: An Introduction to Computational Geometry



- 1969, 1987
- **AI winter**

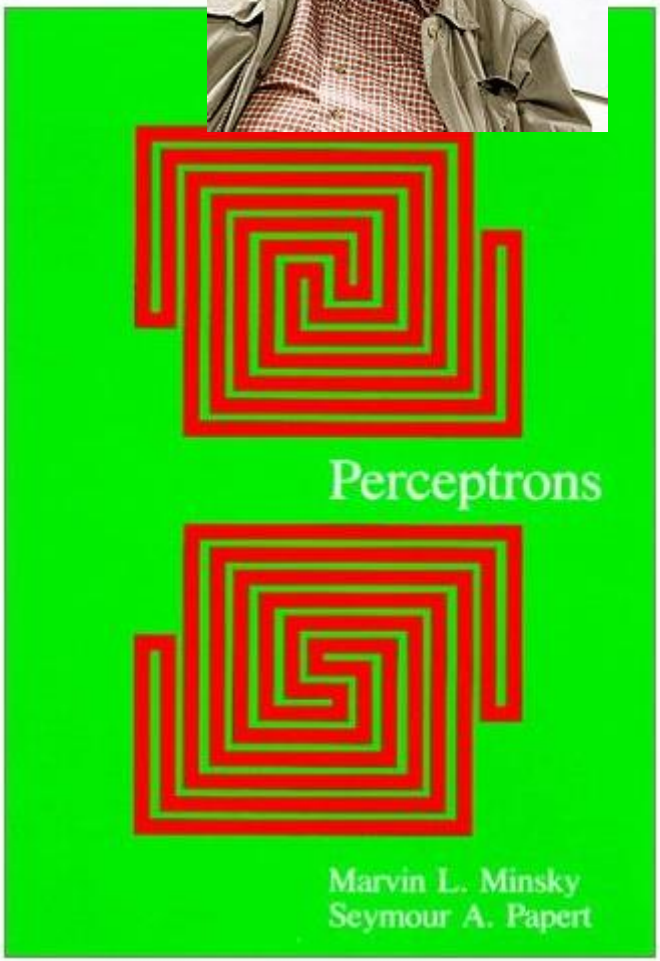
- ***Turing*** Award, the ***Japan*** Prize, the ***IJCAI*** Award for Research Excellence, and the ***Benjamin Franklin Medal***, ***Fellow of the Computer History Museum***.
- An adviser on the movie ***2001: A Space Odyssey*** and is referred to in the movie.

多层感知器



D. E. Rumelhart, G. E. Hinton & R. J. Williams, Learning representations by back-propagating errors, Nature 323, 533 - 536 (09 October 1986)

Perceptrons: An Introduction to Computational Geometry



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Deep Learning

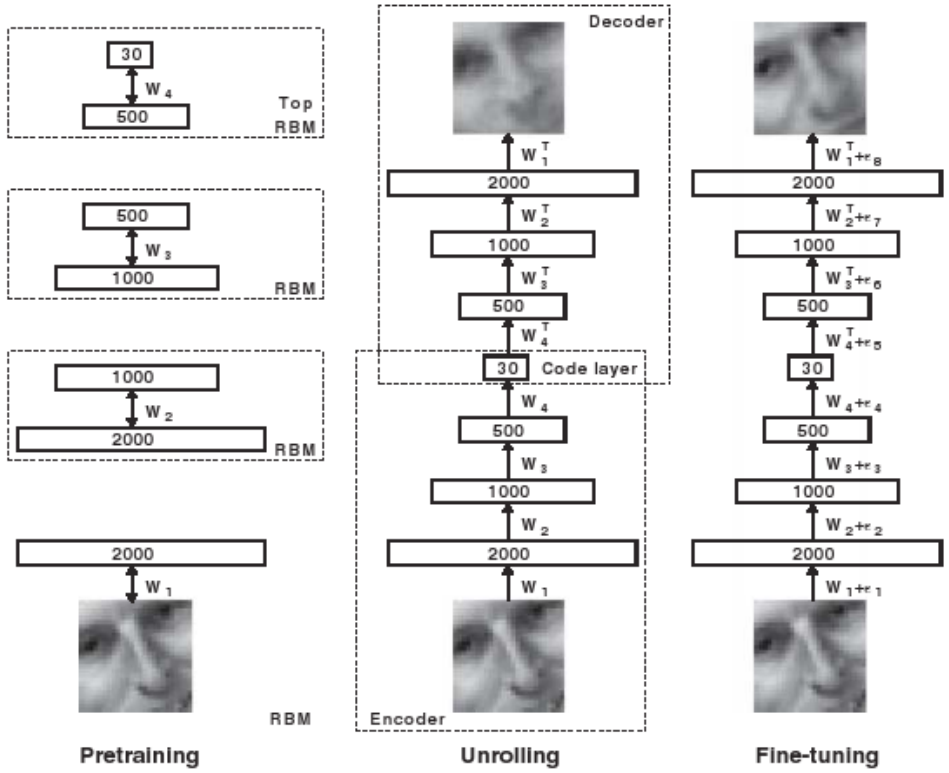
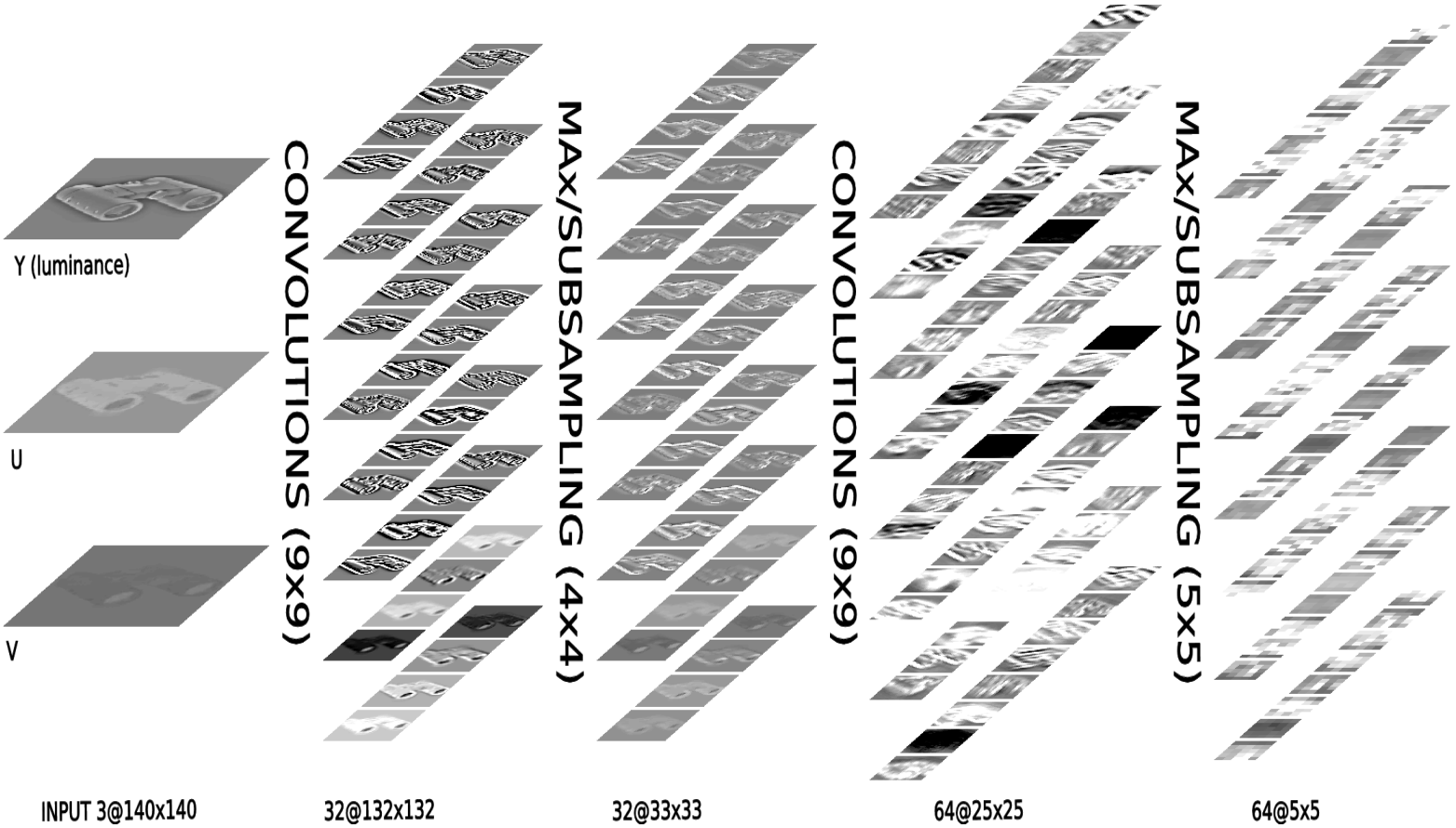


Fig. 1. Pretraining consists of learning a stack of restricted Boltzmann machines (RBMs), each having only one layer of feature detectors. The learned feature activations of one RBM are used as the "data" for training the next RBM in the stack. After the pretraining, the RBMs are "unrolled" to create a deep autoencoder, which is then fine-tuned using backpropagation of error derivatives.

G. E. Hinton, and R. R. Salakhutdinov, (2006) Reducing the dimensionality of data with neural networks. Science, Vol. 313. no. 5786, pp. 504 - 507, 28 July 2006.

Convolutional Net



LeCun et al., NIPS 1989

2. 多层感知器网络

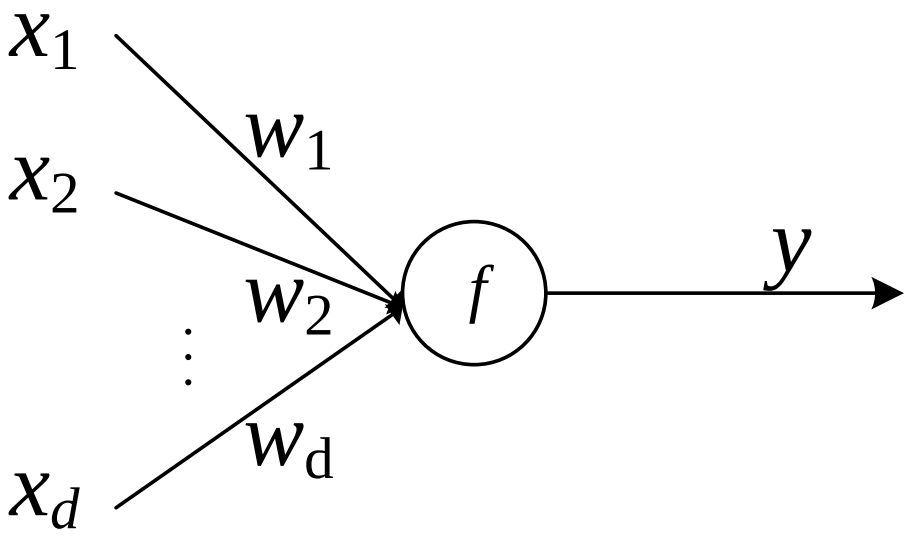
- 多层感知器网络（MLP，Multilayer Perceptron）
  - 多层神经网络
  - BP神经网络
- 主要任务
  - P1: 网络设计
  - P2: 训练

数据的表示

- 单变量: x, y, z, x_1
- 向量: $\mathbf{x}, \mathbf{y}, \mathbf{x}_1$ $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{x}_1$
  - 向量中的组元 $\mathbf{x} = [x_1, \cdots, x_d]^t$
- 矩阵 $\mathbf{A}, \mathbf{X}, \mathbf{M}$ $\boldsymbol{A}, \boldsymbol{X}, \boldsymbol{M}$
  - 矩阵$\mathbf{X}$中的组元(元素): $\mathbf{x}_i$， x_{ij}

2. 多层感知器网络
（MLP，Multilayer Perceptron）

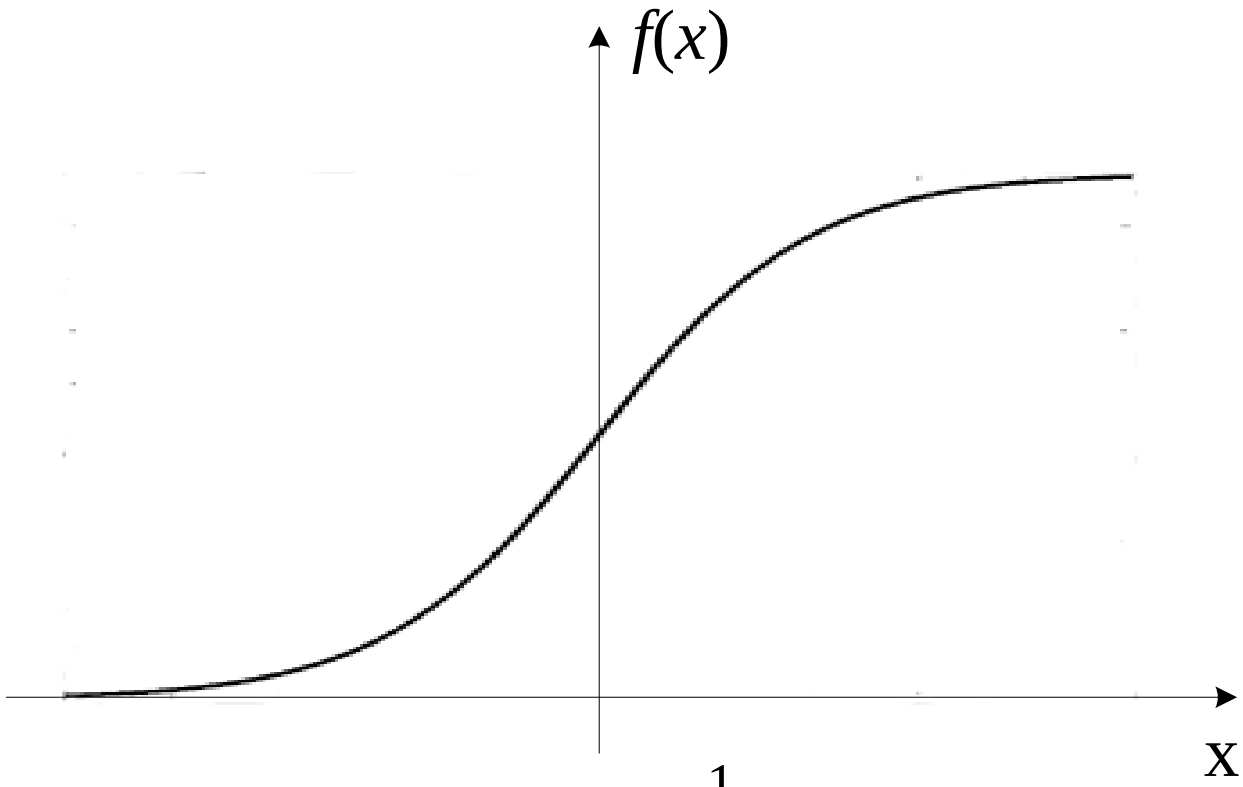
- 神经元模型



$$y = f\left(\mathbf{w}^t\mathbf{x}\right) = f\left(\sum_{i=1}^{d} w_i x_i\right),$$

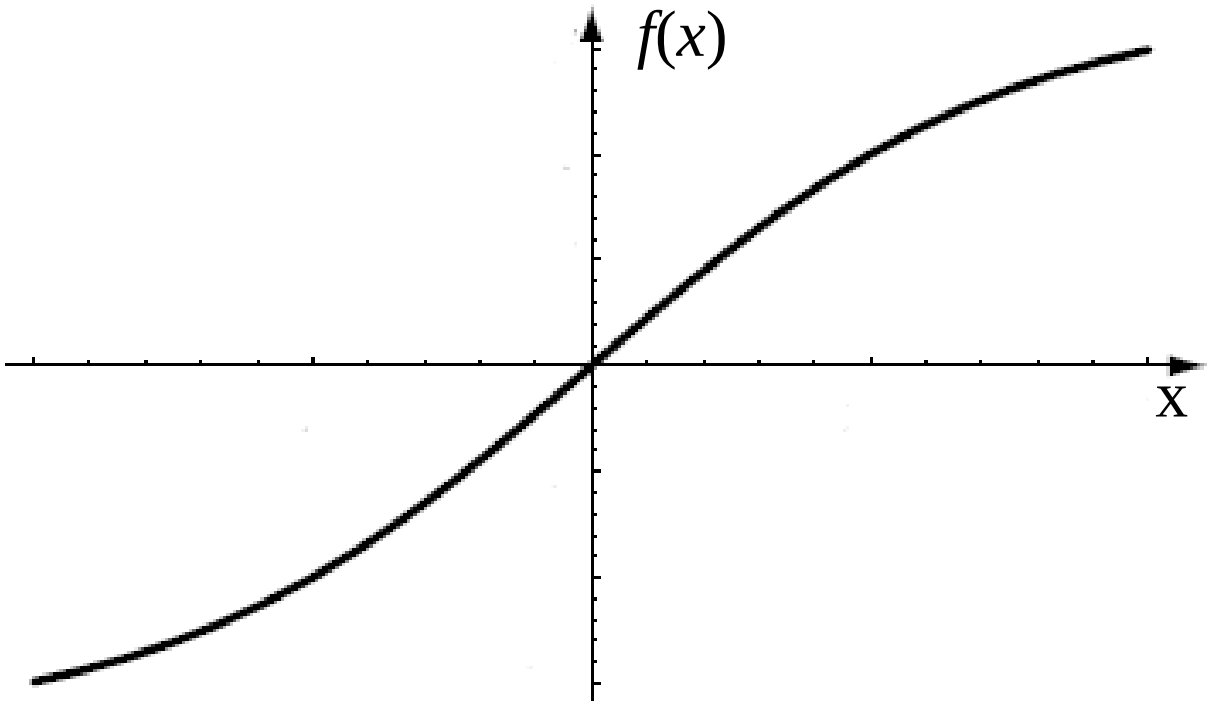
f 称为**激活函数**

激活函数—对数Sigmoid函数



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

激活函数—双曲正切Sigmoid函数

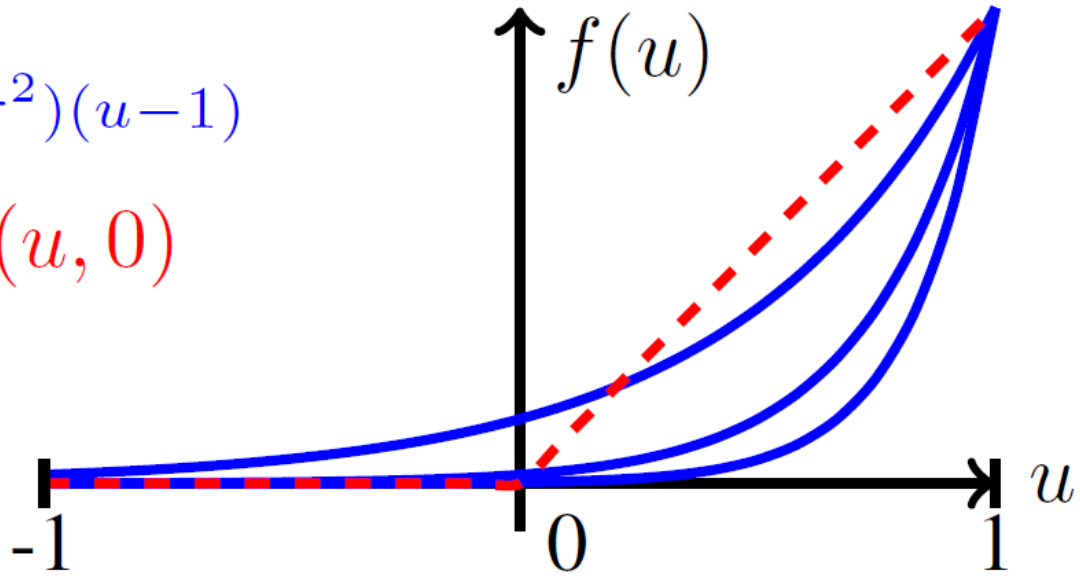


$$f\left(x\right)=\tanh(x)=\frac{e^{x}-e^{-x}}{e^{x}+e^{-x}}$$

激活函数—Rectified linear unit函数

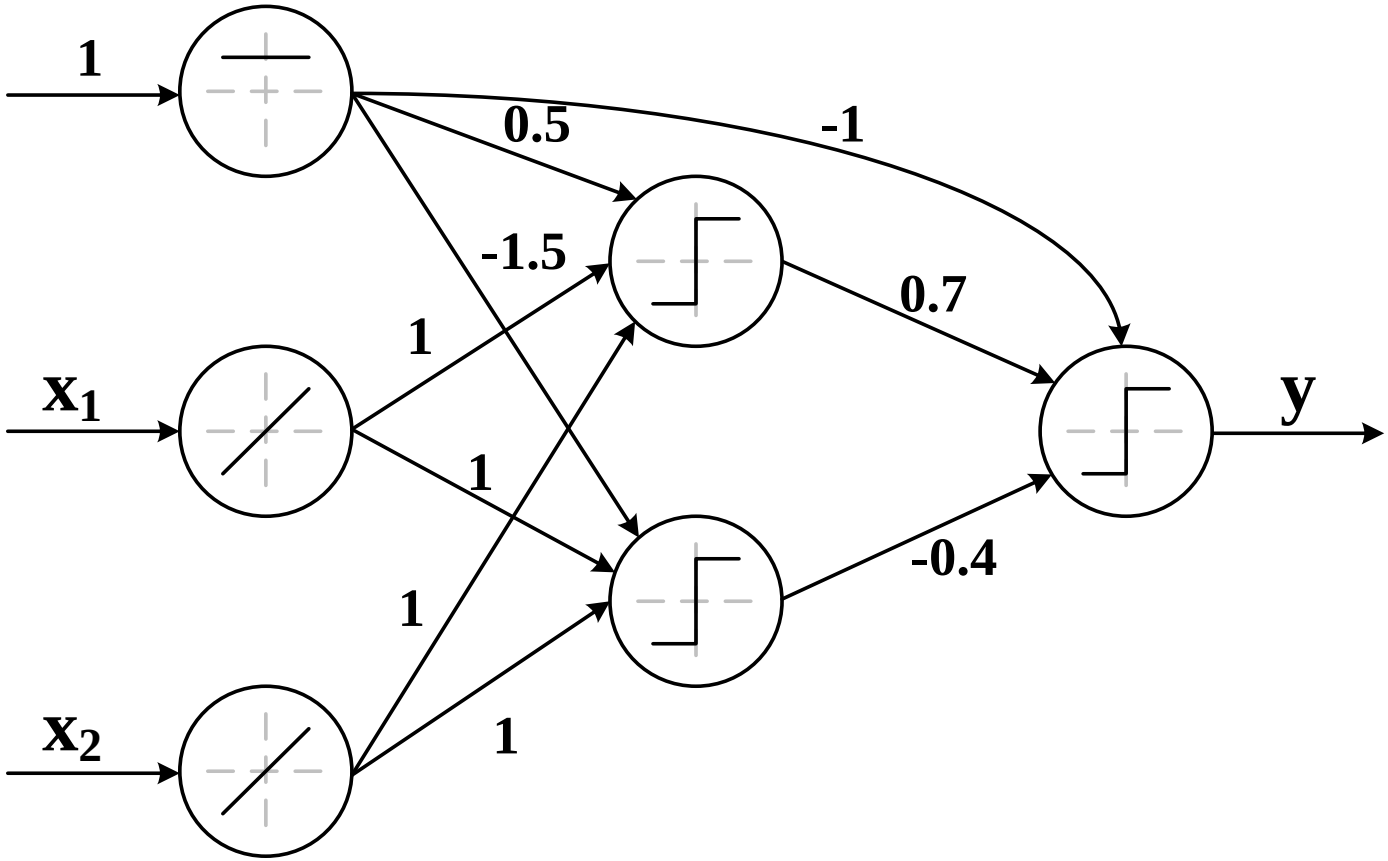
$$f(u) = e^{(2/\sigma^2)(u-1)}$$

$$f(u) = \max(u, 0)$$



Vinod Nair, Geoffrey E. Hinton, Rectified Linear Units Improve Restricted Boltzmann Machines, ICML 2010.

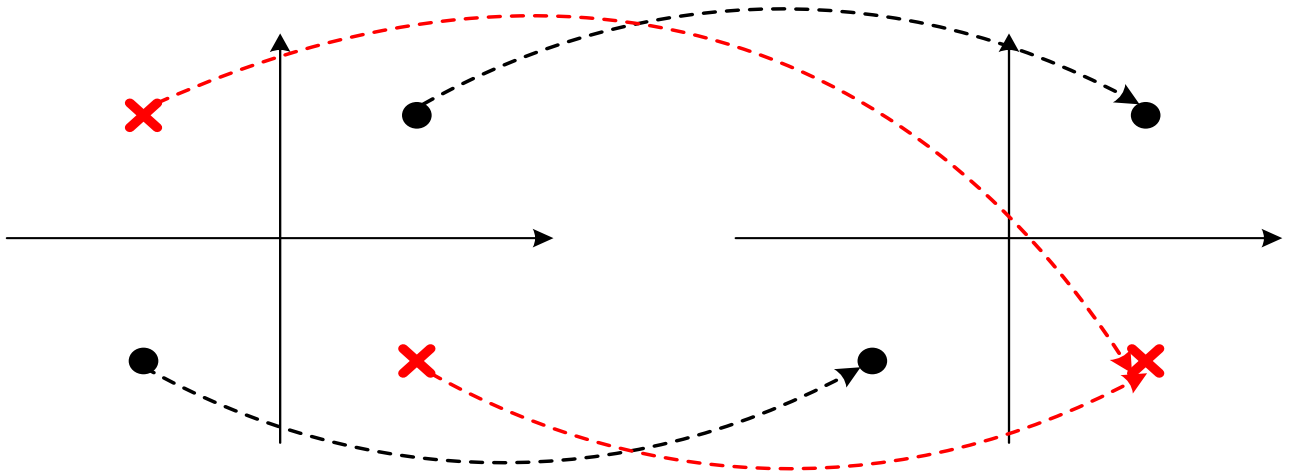
解决异或（±1）问题的多层感知器



输入层　　隐含层　　输出层

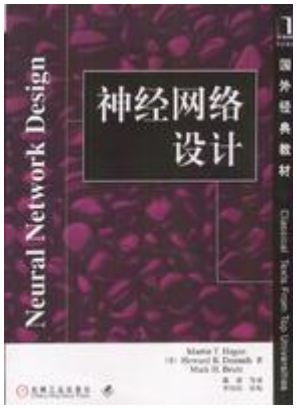
多层感知器的分类原理

- 隐含层实现对输入空间的非线性映射，输出层实现线性分类；
- 非线性映射方式和线性判别函数可以同时学习。

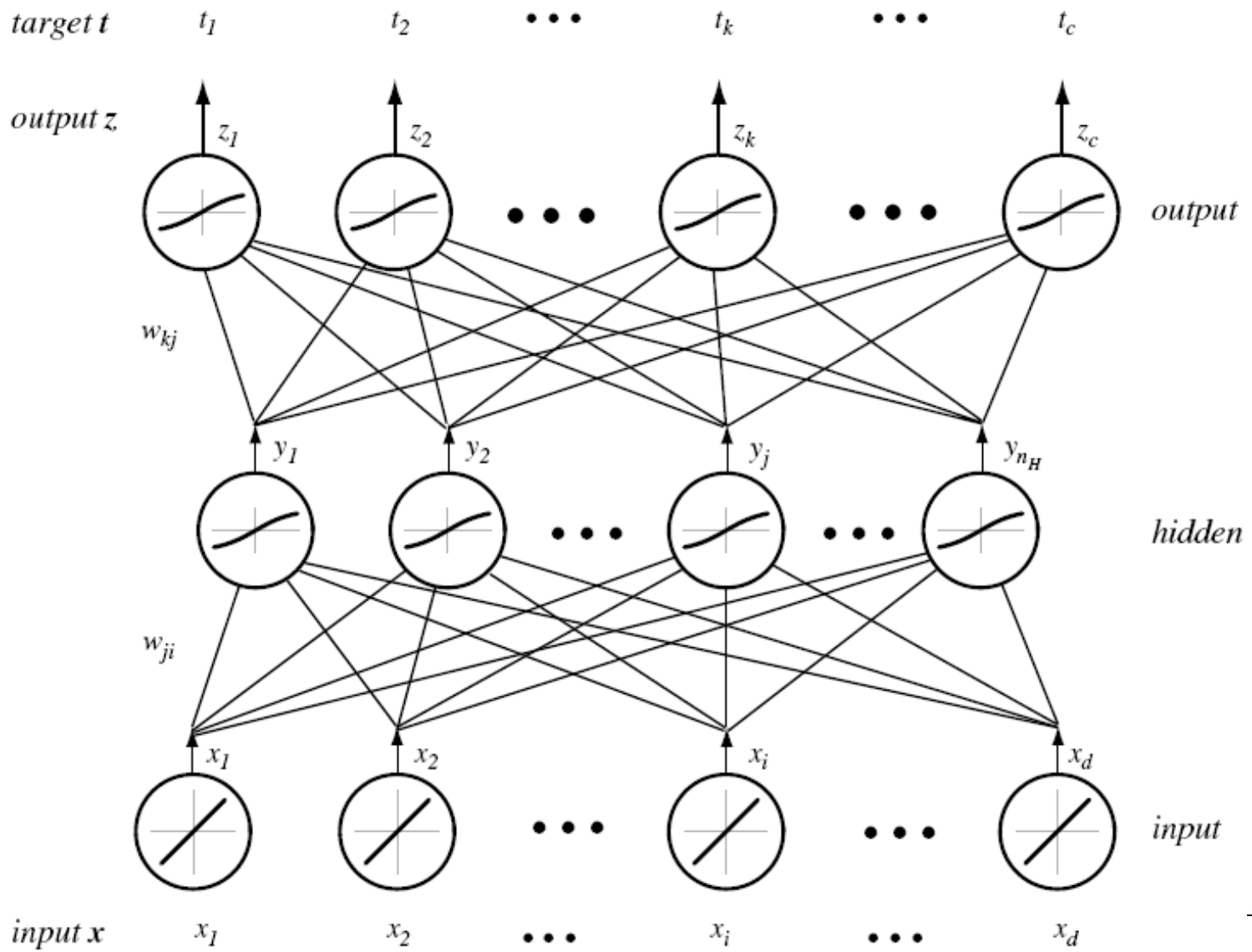


参考书

- **《神经网络设计》**，[美]哈根等 著，戴葵等 译，机械工业出版社，2002-9-1



标准的三层感知器网络


target t
t_1
t_2
t_k
t_c
output z
z_1
z_2
z_k
z_c
output
w_{kj}
y_1
y_2
y_j
y_{n_H}
hidden
w_{ji}
x_1
x_2
x_i
x_d
input
input x
x_1
x_2
x_i
x_d

多层感知器网络

- 主要任务
  - P1: 网络设计
  - P2: 训练

多层感知器网络的设计

- 选定层数：三层网络 -> 深层网络
  - 增加网络层数并不能提高网络的分类能力？
- 输入层：输入层**节点数**为输入特征的维数d，**映射函数**采用线性函数；
- 隐含层：隐含层**节点数**需要设定，一般来说，隐层节点数越多，网络的分类能力越强，**映射函数**一般采用Sigmoid函数；
- 输出层：输出层**节点数**可以等于类别数C，也可以采用编码输出的方式，少于类别数C，**输出函数**可以采用线性函数或Sigmoid函数。

三层网络的判别函数形式

$$g_k(\mathbf{x}) = f_2\left(\sum_{j=1}^{n_H} w_{kj} f_1\left(\sum_{i=1}^{d} w_{ji} x_i + w_{j0}\right) + w_{k0}\right)$$

第k个输出层神经元的输出，其中d为特征维数，n_H为隐层节点数。

2.2 学习机制

- 大脑神经网络的学习过程
  - 环境
  - 网络结构/参数调整
  - 响应、反馈

- 神经网络学习机制
  - 错误校正
  - 记忆学习
  - Hebbian学习
  - 竞争学习

Who Invented Backpropagation

- http://people.idsia.ch/~juergen/who-invented-backpropagation.html

- The first NN-specific application of efficient BP as above was described in 1981 (Werbos, 1981).
- Related work was published several years later (Parker, 1985; LeCun, 1985).
- A paper of 1986 significantly contributed to the popularisation of BP for NNs (Rumelhart et al., 1986).

2.2 MLP的训练--误差反向传播算法

（BP，Backpropagation algorithm）

$$z_k = f_2\left(\sum_{j=1}^{n_H} w_{kj} f_1\left(\sum_{i=1}^{d} w_{ji} x_i + w_{j0}\right) + w_{k0}\right)$$

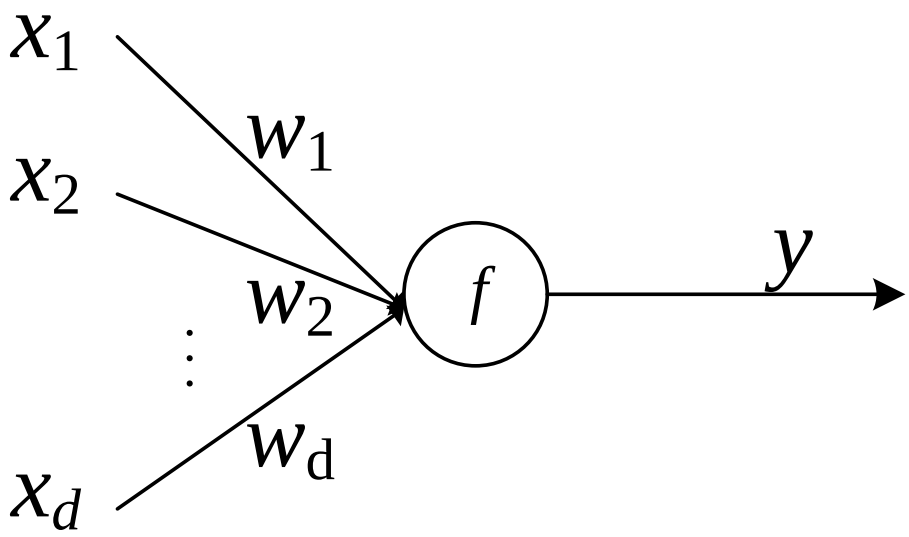
- BP算法的实质是一个**均方误差最小算法** (LMS)

- 符号定义：训练样本**x**，期望输出$\mathbf{t} = (t_1,\ldots, t_c)$，网络实际输出$z = (z_1,\ldots, z_c)$，隐层输出$\mathbf{y} = (y_1,\ldots, y_{n_H})$，第$k$个神经元的净输出$\text{net}_k$。

- 目标函数：$$J(\mathbf{w}) = \frac{1}{2}\|\mathbf{t}-\mathbf{z}\|^2 = \frac{1}{2}\sum_{i=1}^{c}(t_i - z_i)^2$$

迭代公式： $$\mathbf{w}(m+1) = \mathbf{w}(m) + \Delta\mathbf{w}(m) = \mathbf{w}(m) - \eta\frac{\partial J}{\partial \mathbf{w}}$$

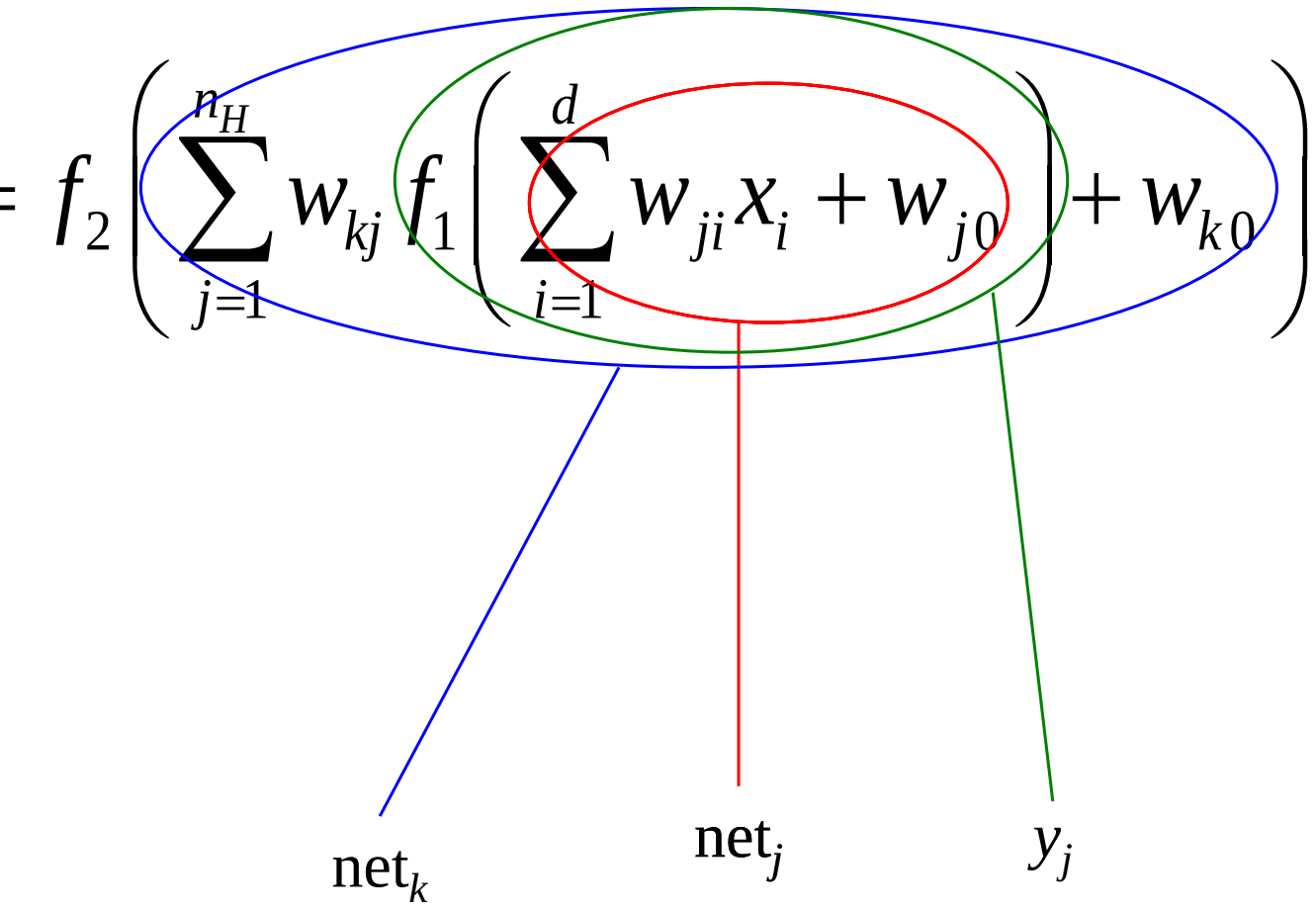
神经元

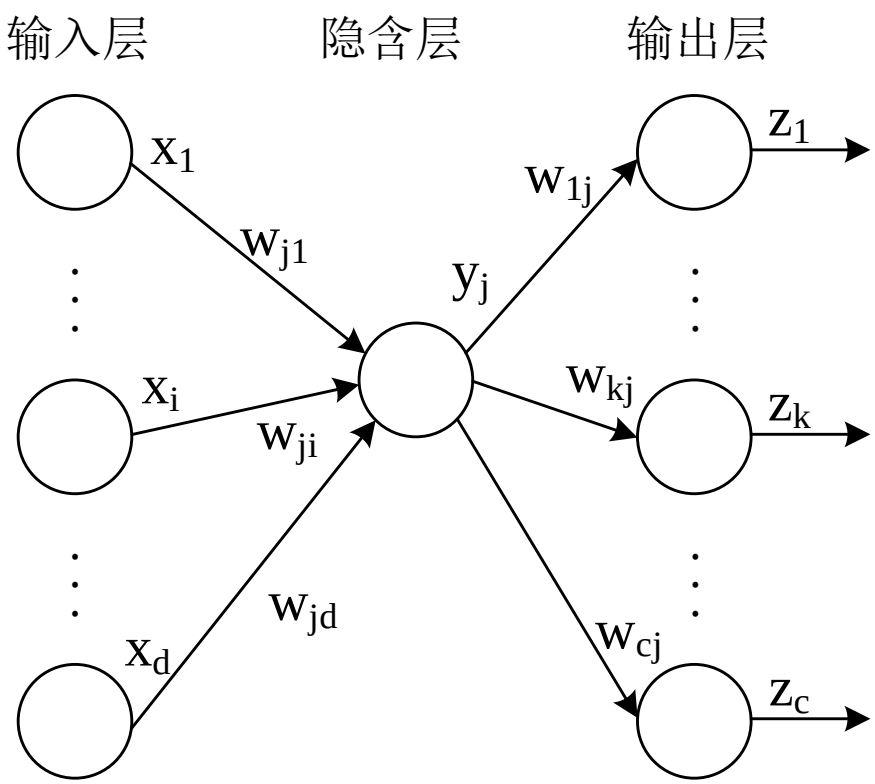


$$y = f\left(\mathbf{w}^t\mathbf{x}\right) = f\left(\sum_{i=1}^{d} w_i x_i\right),$$

f称为激活函数

$$g_k(\mathbf{x}) = f_2\left(\sum_{j=1}^{n_H} w_{kj} f_1\left(\sum_{i=1}^{d} w_{ji} x_i + w_{j0}\right) + w_{k0}\right)$$




输入层
隐含层
输出层
x_1
x_i
x_d
w_{j1}
w_{ji}
w_{jd}
y_j
w_{1j}
w_{kj}
w_{cj}
z_1
z_k
z_c

输出层

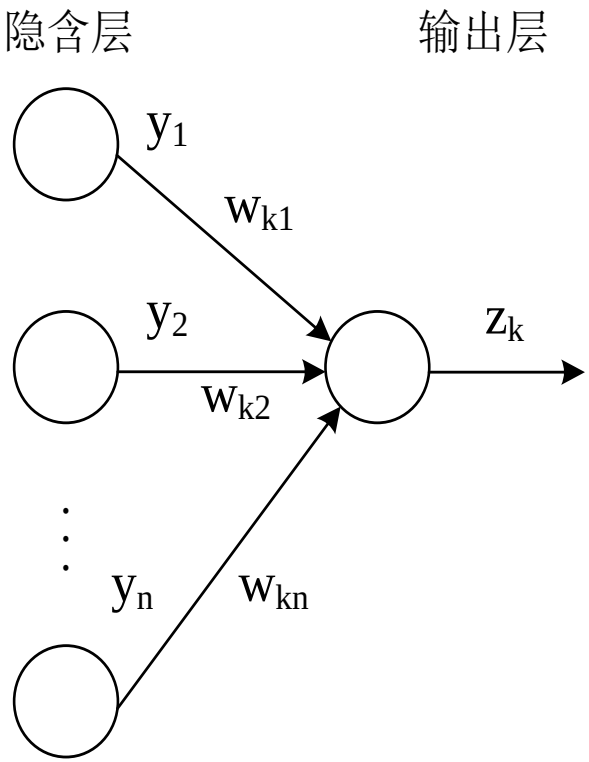
$$\frac{\partial J}{\partial w_{kj}} = \frac{\partial J}{\partial net_k}\frac{\partial net_k}{\partial w_{kj}} = \frac{\partial J}{\partial z_k}\frac{\partial z_k}{\partial net_k}\frac{\partial net_k}{\partial w_{kj}}$$

$$net_k = \sum_{j=0}^{n_H} w_{kj} y_j, \qquad \frac{\partial net_k}{\partial w_{kj}} = y_j$$

$$\frac{\partial J}{\partial net_k} = \frac{\partial J}{\partial z_k}\frac{\partial z_k}{\partial net_k} = -\left(t_k - z_k\right) f'\left(net_k\right)$$

$$\frac{\partial J}{\partial w_{kj}} = -\left(t_k - z_k\right) f'\left(net_k\right) y_j = -\delta_k y_j$$

$$\delta_k = \left(t_k - z_k\right) f'\left(net_k\right)$$

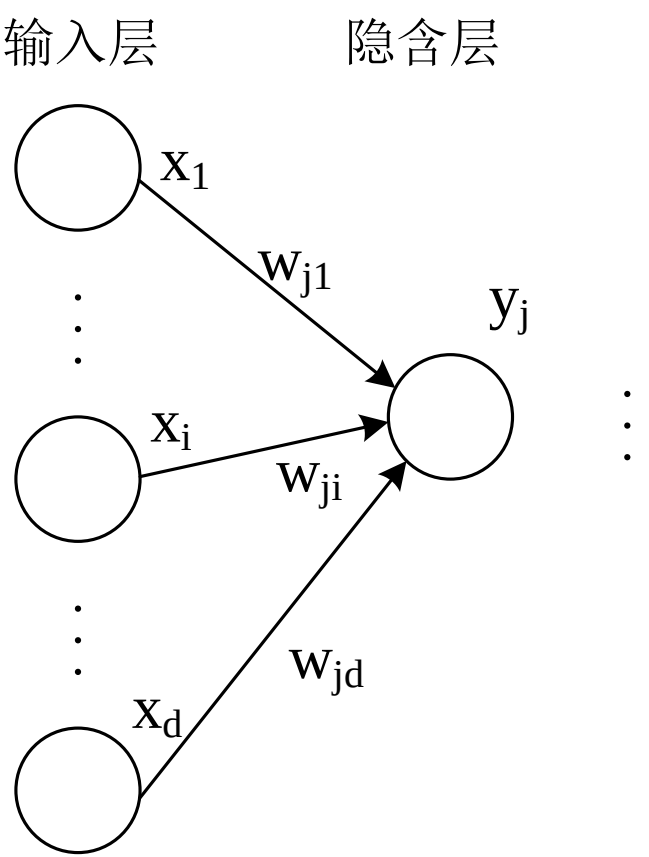


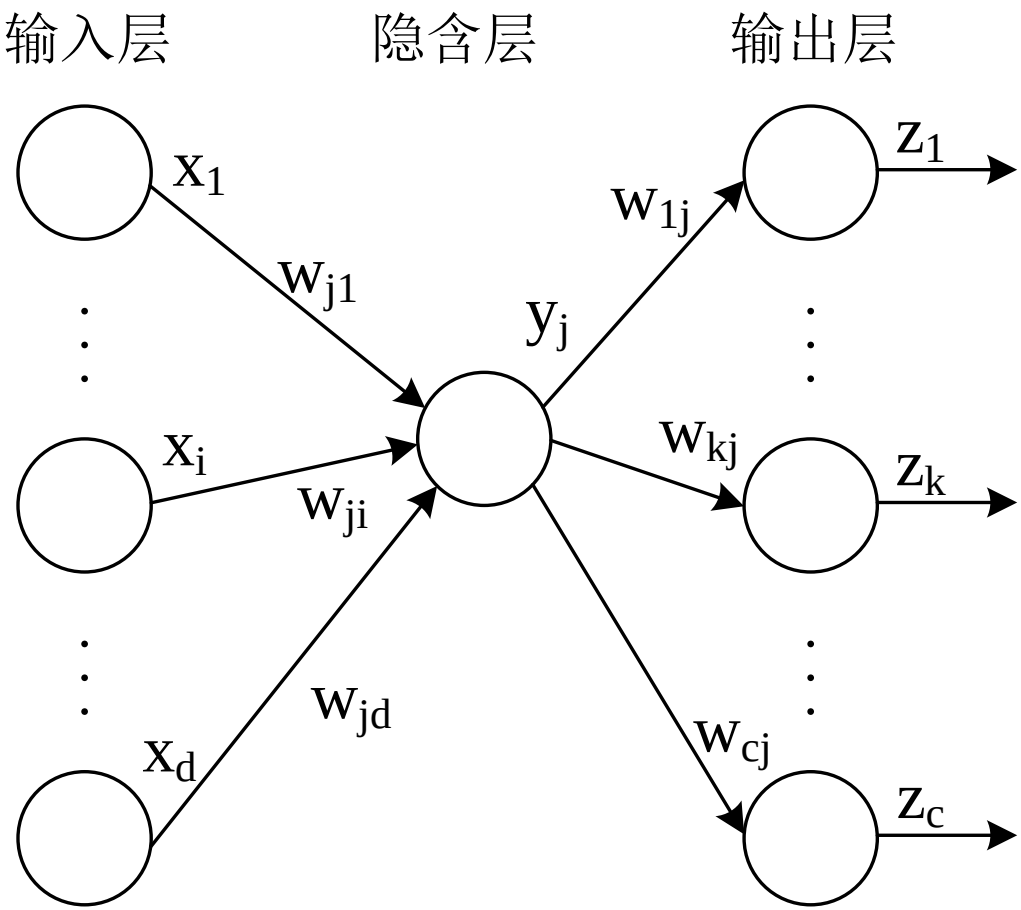
隐含层

$$\frac{\partial J}{\partial w_{ji}} = \frac{\partial J}{\partial y_j}\frac{\partial y_j}{\partial net_j}\frac{\partial net_j}{\partial w_{ji}}$$

$$\frac{\partial y_j}{\partial net_j} = f'\left(net_j\right)$$

$$\frac{\partial net_j}{\partial w_{ji}} = \frac{\partial}{\partial w_{ji}}\left(\sum_{m=0}^{d} w_{jm}x_m\right) = x_i$$




输入层
隐含层
输出层
x_1
x_i
x_d
w_{j1}
w_{ji}
w_{jd}
y_j
w_{1j}
w_{kj}
w_{cj}
z_1
z_k
z_c

隐含层

$$\frac{\partial J}{\partial y_j}=\frac{\partial}{\partial y_j}\left[\frac{1}{2}\sum_{k=1}^{c}\left(t_k-z_k\right)^2\right]=-\sum_{k=1}^{c}\left(t_k-z_k\right)\frac{\partial z_k}{\partial y_j}$$

$$=-\sum_{k=1}^{c}\left(t_k-z_k\right)\frac{\partial z_k}{\partial net_k}\frac{\partial net_k}{\partial y_j}=-\sum_{k=1}^{c}\left(t_k-z_k\right)f'\left(net_k\right)w_{kj}$$

$$\frac{\partial J}{\partial w_{ji}}=-\left[\sum_{k=1}^{c}\left(t_k-z_k\right)f'\left(net_k\right)w_{kj}\right]f'\left(net_j\right)x_i$$

$$\frac{\partial J}{\partial w_{ji}}=-\delta_j x_i,\qquad \delta_j=f'\left(net_j\right)\sum_{k=1}^{c}\delta_k w_{kj}$$

迭代公式

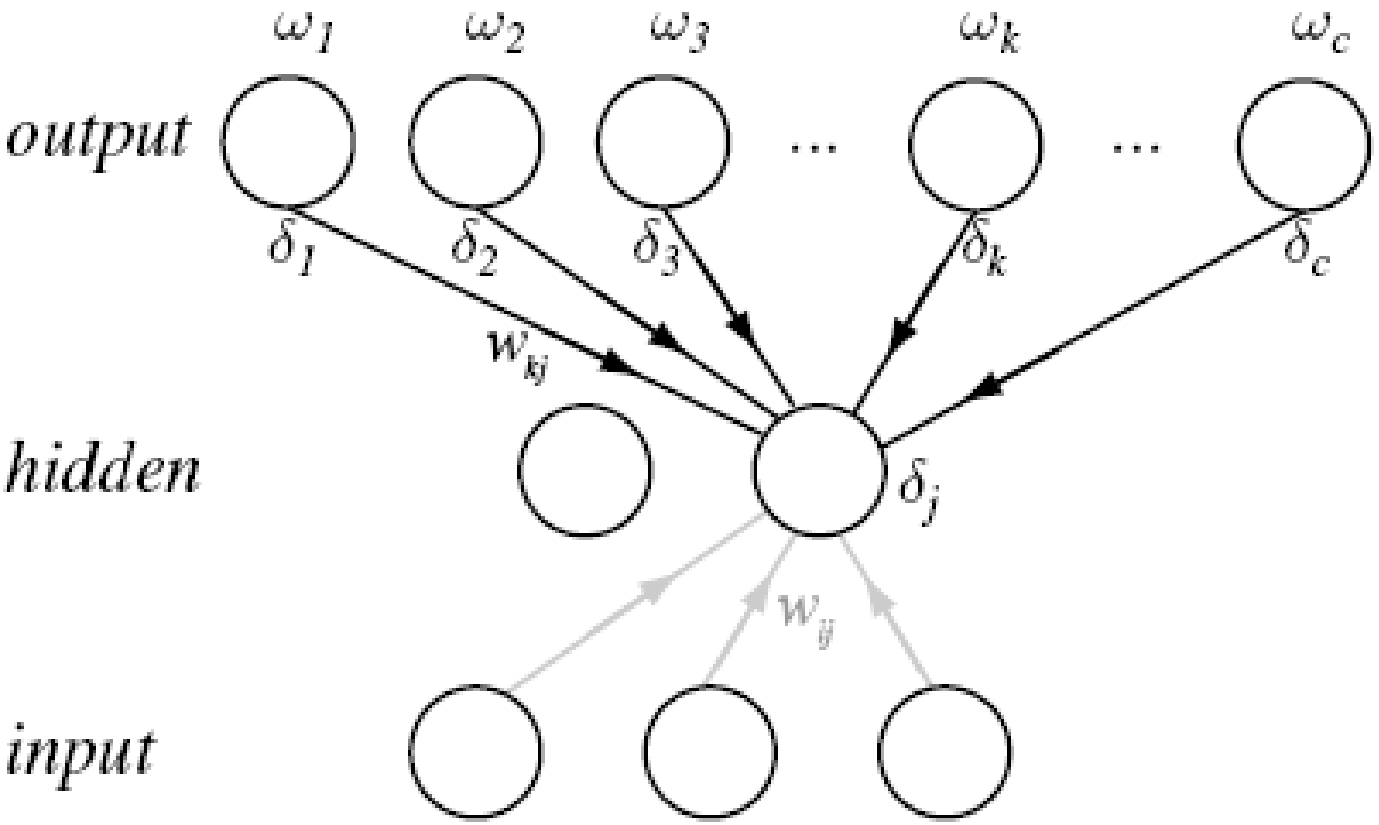
- 输出层：

$$\frac{\partial J}{\partial w_{kj}} = -\delta_k y_j, \qquad \delta_k = \left(t_k - z_k\right) f'\left(net_k\right)$$

- 隐含层：

$$\frac{\partial J}{\partial w_{ji}} = -\delta_j x_i, \qquad \delta_j = f'\left(net_j\right)\sum_{k=1}^{c}\delta_k w_{kj}$$

误差反向传播


ω_1
ω_2
ω_3
ω_k
ω_c
output
δ_1
δ_2
δ_3
δ_k
δ_c
w_{kj}
hidden
δ_j
w_{ij}
input

P2: BP算法—批量修改

1. begin initialize n，w，θ，η，r←0
2. do r←r+1
3. m←0;Δw_{ji}←0;Δw_{kj}←0
4. do m←m+1
5. x_m←select pattern
6. Δw_{kj}←$\Delta w_{kj}+\eta\delta_k y_j$ Δw_{ji}←$\Delta w_{ji}+\eta\delta_j x_i$;
7. until m = n
8. w_{ji}← $w_{ji}+\Delta w_{ji}$; w_{kj}← $w_{kj}+\Delta w_{kj}$
9. until $\|\nabla J(w)\|<\theta$
10. return w
11. end

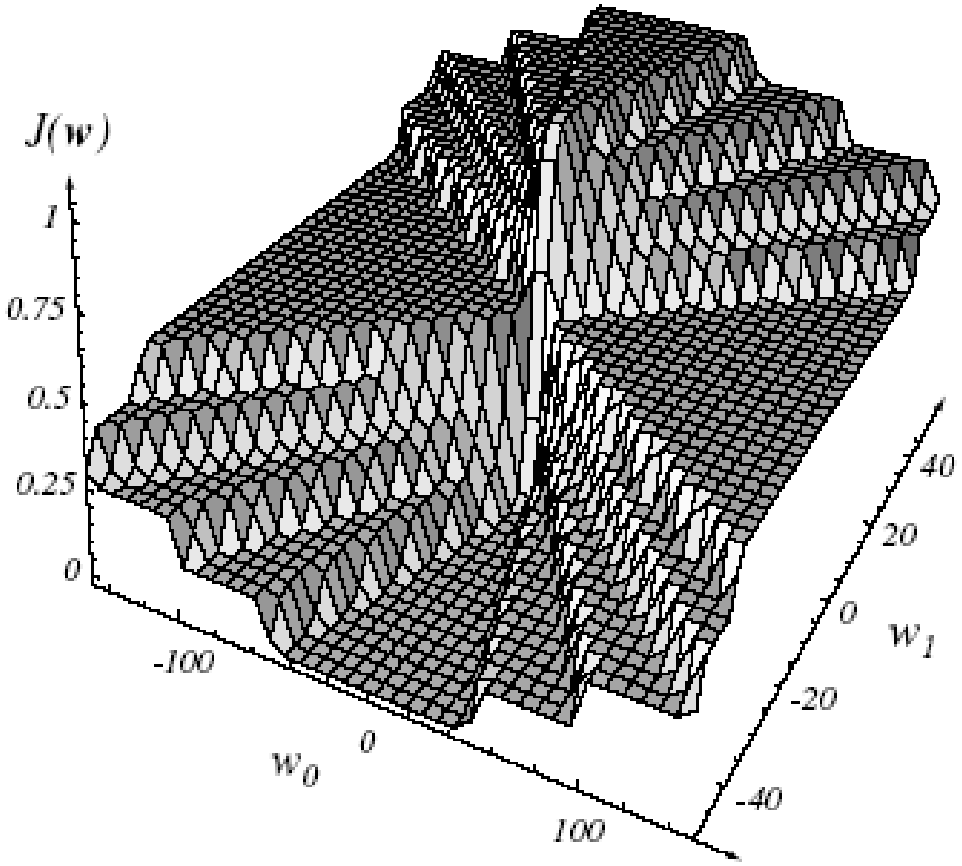
BP算法的一些实用技术

- **激活函数的选择**：一般可以选择双曲型的Sigmoid函数，最近倾向于使用ReLU激活函数；
- **目标值**：期望输出一般选择**(-1, +1)**或**(0, 1)**；
- **规格化**：训练样本每个特征一般要规格化为**0均值和标准差**；
- **权值初始化**：期望每个神经元的-1<net<+1，因此权值一般初始化为 $-1/\sqrt{d} < w < 1/\sqrt{d}$ ；
- **学习率的选择**：太大容易发散，太小则收敛较慢；
- **冲量项**：有助于提高收敛速度。

$$\mathbf{w}(m+1) = \mathbf{w}(m) + (1-\alpha)\Delta\mathbf{w}_{bp}(m) + \alpha\Delta\mathbf{w}(m-1)$$

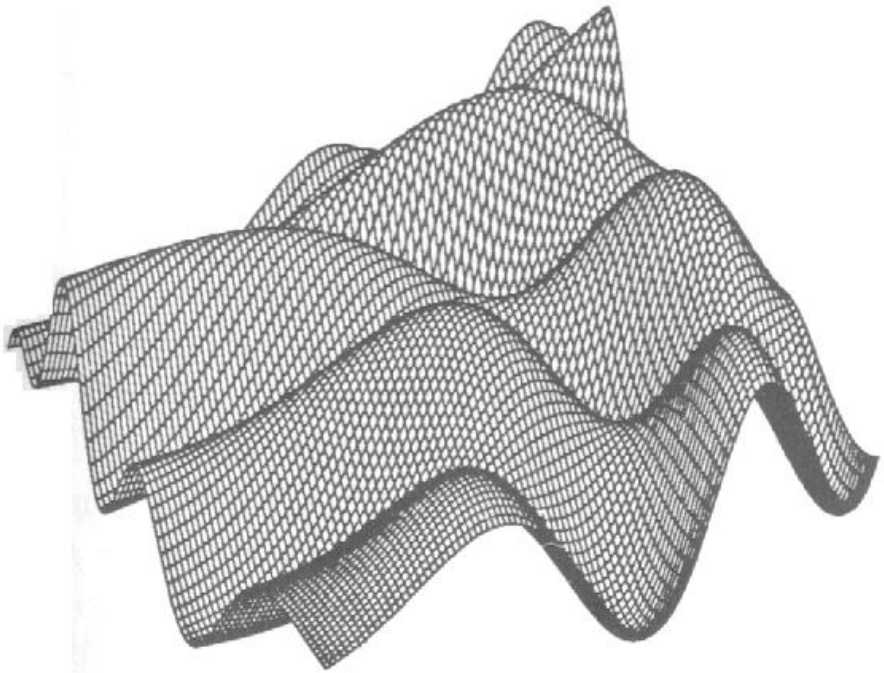
2.3 多层感知器网络存在的问题

1. BP算法的***收敛速度***一般来说比较慢；



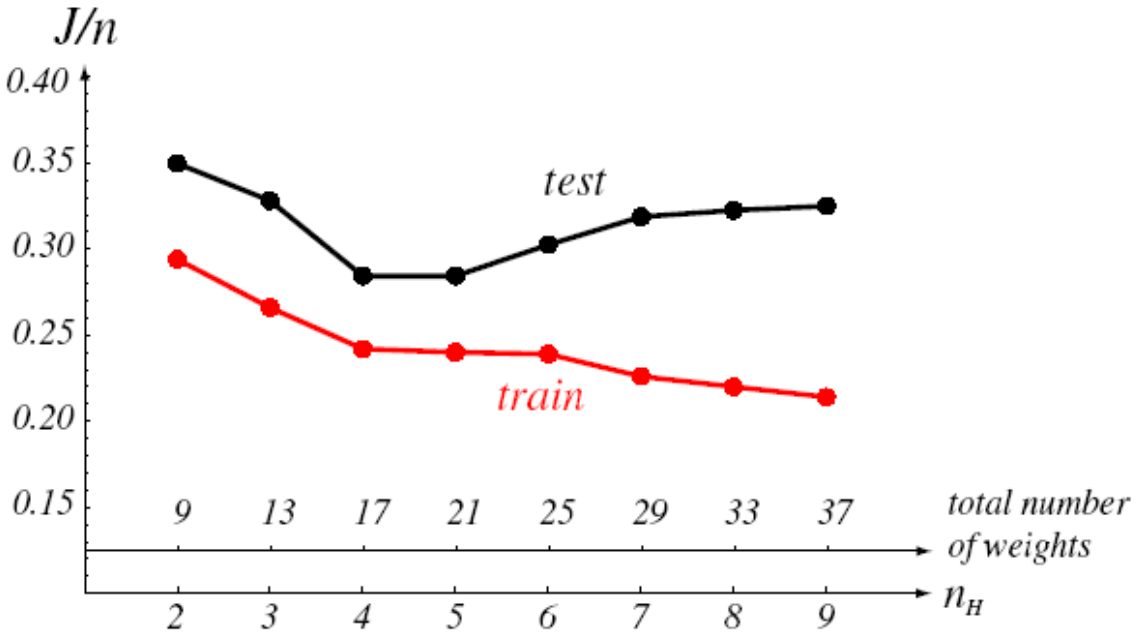
多层感知器网络存在的问题

2. BP算法只能收敛于***局部最优解***，不能保证收敛于全局最优解；



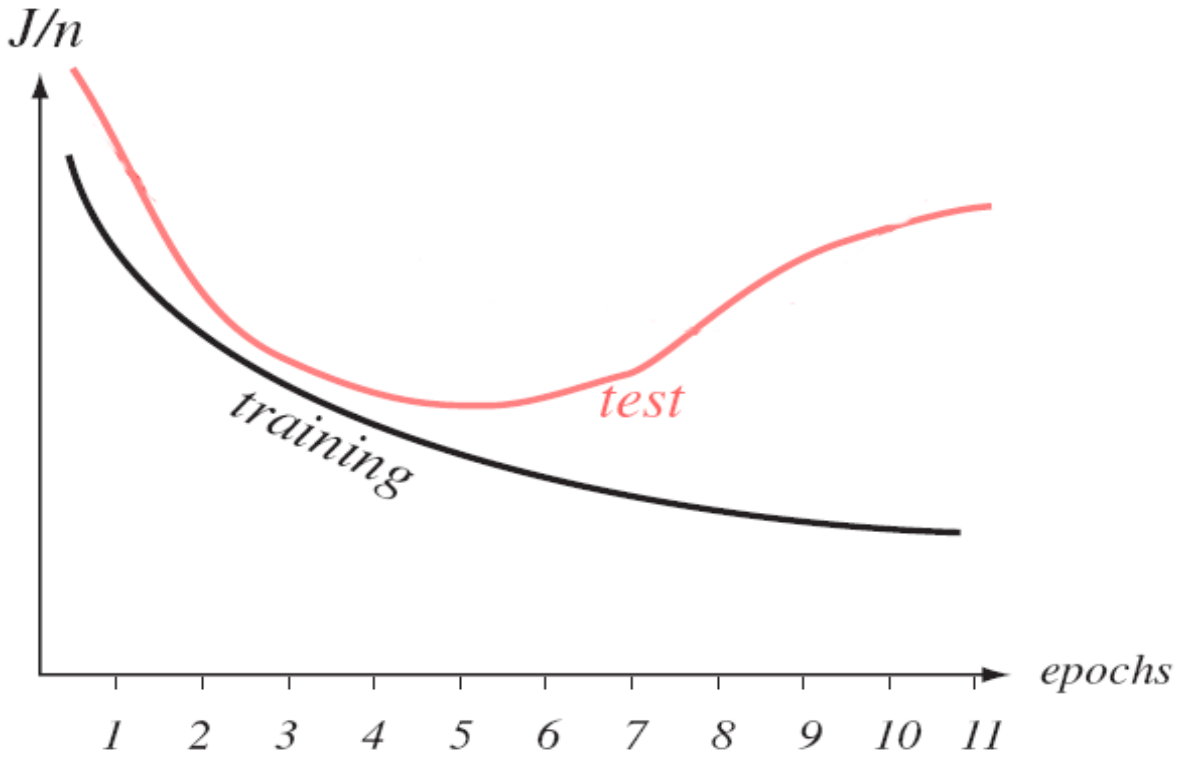
多层感知器网络存在的问题

3. 当**隐层元的数量**足够多时，网络对训练样本的识别率很高，但对测试样本的识别率有可能很差，即网络的***推广能力***有可能较差。(Overfitting)



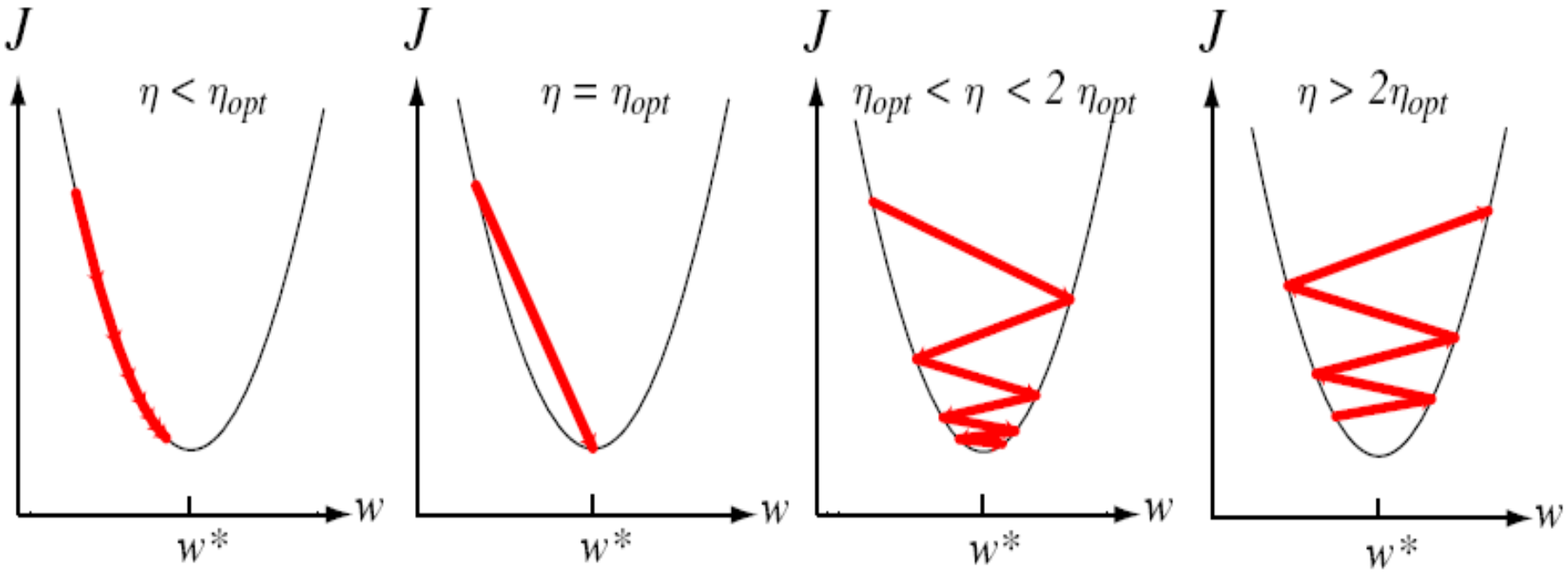
多层感知器网络存在的问题

4. 随着训练周期的增加，在训练样本集上目标函数不断下降，而在测试样本集上反而会上升。**(Bias-Variance 理论)**



2.4 提高收敛速度的方法

- 一个比较直观的想法是通过增大**学习率**来提高收敛速度，但这样有可能造成算法发散。



梯度下降法

- 目标函数的一阶泰勒级数展开：

$$J\left(\mathbf{w}_{k+1}\right)=J\left(\mathbf{w}_k+\Delta\mathbf{w}_k\right)\approx J\left(\mathbf{w}_k\right)+\left(\left.\frac{\partial J\left(\mathbf{w}\right)}{\partial\mathbf{w}}\right|_{\mathbf{w}=\mathbf{w}_k}\right)^t\Delta\mathbf{w}_k$$

目标函数增量：

$$\Delta J\left(\mathbf{w}_k\right)=\left(\left.\frac{\partial J\left(\mathbf{w}\right)}{\partial\mathbf{w}}\right|_{\mathbf{w}=\mathbf{w}_k}\right)^t\Delta\mathbf{w}_k\le 0$$

使目标函数下降最大：

$$\Delta\mathbf{w}_k=-\eta\left(\left.\frac{\partial J\left(\mathbf{w}\right)}{\partial\mathbf{w}}\right|_{\mathbf{w}=\mathbf{w}_k}\right)^t$$

牛顿法

- 目标函数的二阶泰勒级数展开：

$$\Delta J(\mathbf{w}_k)=\left(\left.\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}}\right|_{\mathbf{w}=\mathbf{w}_k}\right)^t \Delta\mathbf{w}_k+\frac{1}{2}\Delta\mathbf{w}_k^t\mathbf{H}\Delta\mathbf{w}_k$$

H是Hessian矩阵，求取目标函数增量的极大值：

$$\frac{d\Delta J(\mathbf{w}_k)}{d\Delta\mathbf{w}_k}=\left(\left.\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}}\right|_{\mathbf{w}=\mathbf{w}_k}\right)+\mathbf{H}\Delta\mathbf{w}_k=0$$

$$\Delta\mathbf{w}_k=-\mathbf{H}^{-1}\left(\left.\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}}\right|_{\mathbf{w}=\mathbf{w}_k}\right)$$

重新思考多层神经网络

- 网络模型：3层 -> 多层
  - 激活函数：ReLU / PReLU, …
  - 网络参数：Dropout
  - 特征规格化：Batch Normalization
  - 网络结构搜索
- 学习算法（Mini-batch）
  - AdaGrad
  - RMSProp
  - Adam，…
- 泛化能力
  - Mini-batch
  - Over-fitting