Chapter 6: Multilayer Neural Networks

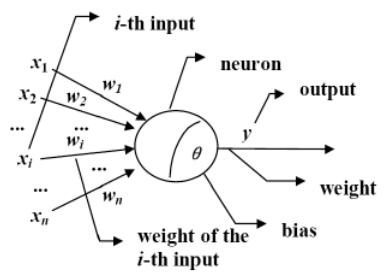
6.1 Artificial Neural Networks (ANN)

Artificial Neural Networks (ANN) are **massively parallel interconnected networks of simple (usually adaptive) elements and their hierarchical organization** which are intended to interact with the objects of the real world in the same way as biological nervous systems do.

6.1.1 The M-P neuron model

The M-P neuron receives input signals from n other neurons and conveys them through weighted connections.

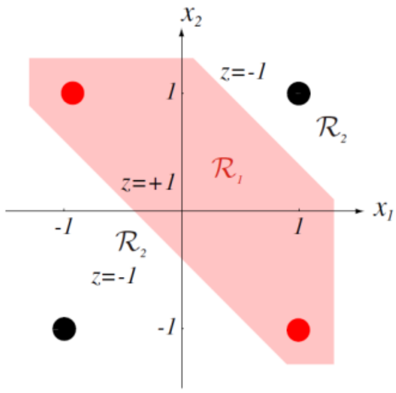
The total input value received by the M-P neuron will be compared with the neuron's threshold, and then processed by the **Activation Function** to produce the neuron's output.



- **Input**: $x_i \; (1 \leq i \leq n)$
- **Weight**: $w_i \; (1 \leq i \leq n)$
- **Bias/Threshold**: θ
- **Activation Function**: $f(\cdot)$
- **Output**: $y = f(\sum_{i=1}^{n} w_i x_i - \theta)$
- **One mathematical understanding**:
  - The output of the M-P neuron is the function of $x_1, x_2, \ldots, x_m$, then we have (**First-order Taylor function approximation**):

$$
\begin{aligned}
y &= f(x_1, x_2, ..., x_m) \\
&\approx f(0,0,...,0) + \sum_{i=1}^{N}[\frac{\partial f}{\partial x_i}|(0,0,...,0)]x_i + ... \\
&= \sum_{i=1}^{m} w_i x_i + b
\end{aligned}
$$

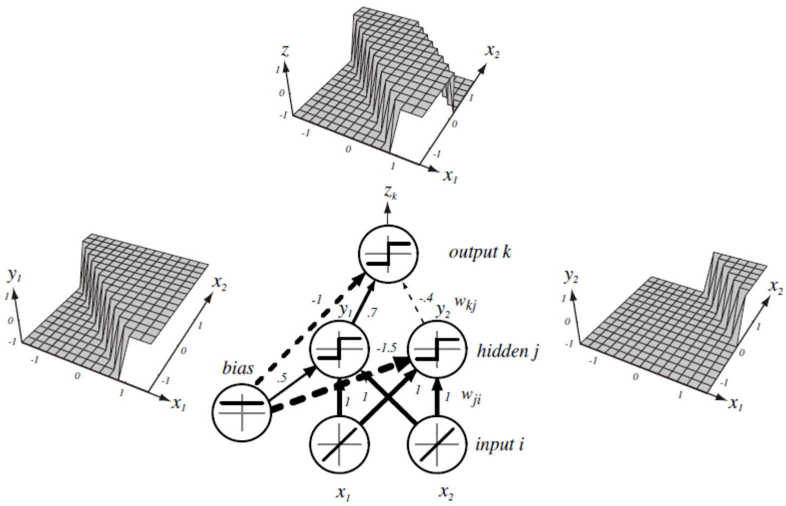
The XOR Problem:



$$
\begin{aligned}
&\text{Decide } +1 \text{ if } x_1 \cdot x_2 = 1 \\
&\text{Decide } -1 \text{ if } x_1 \cdot x_2 = -1
\end{aligned}
\implies \text{Linear Inseparable}
$$

We cannot use a **single** M-P neuron to solve a linear inseparable problem.

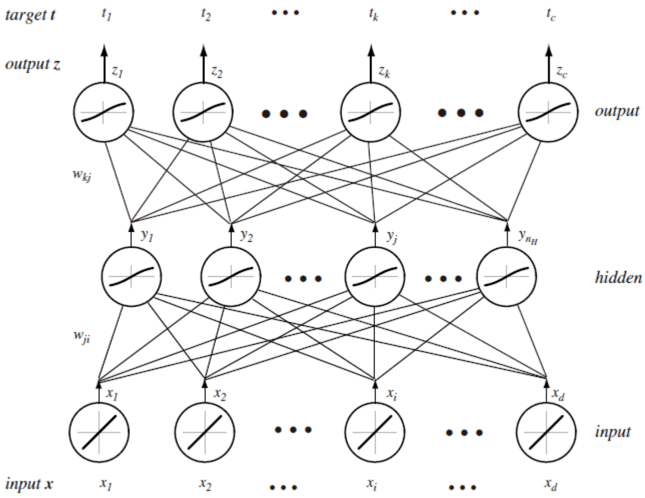
One possible solution:



This is a 2-2-1 three-layer ANN ($d = 2, n_H = 2$):

- **Inpute to the hidden unit**: $\text{net}_j = \sum_{i=1}^{d} w_{ji}x_i + w_{j0} = w_j^t x$
- **Activation of the hidden unit**: $y_j = f(\text{net}_j); f(\text{net}) = \text{Sgn}(net) = \begin{cases} 1 & \text{if net} \geq 0 \\ -1 & \text{if net} \leq 0 \end{cases}$
- **Input to the output unit**: $\text{net}_k = \sum_{j=1}^{n_H} w_{kj}y_j + w_{k0} = w_k^t y$
- **Activation of the output unit**: $z_k = f(\text{net}_k)$

6.1.2 Feedforward Neural Network



Settings (A d-n_H-c fully connected three-layer network)

- **Featurs**: d
- **Hidden neurons**: n_H
- **Output neurons**: c
- **Training pattern**: $x = (x_1, x_2, \ldots, x_d)^t$
- **Desired output**: $t = (t_1, t_2, \ldots, t_c)^t$

Parameters to be learned:

- **Input-to-hidden** layer weight (i-th feature to j-th hidden unit): w_{ji}
- **Hidden-to-output** layer weight (j-th hidden unit to k-th output unit): $w_{kj} \quad (1 \leq i \leq d); (1 \leq j \leq n_H); (1 \leq k \leq c);$
- total $n_H \cdot (d + c)$ parameters in w: $w = (w_{11}, \ldots, w_{n_H d}, \ldots, w_{cn_H})^t$

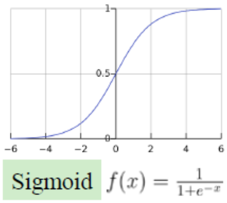
Feedforward procedure:

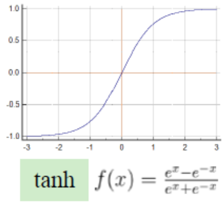
- $\text{net}_j = \sum_{i=1}^{d} w_{ji} x_i \quad (1 \leq j \leq n_H)$
- $y_j = f(\text{net}_j) \quad (1 \leq j \leq n_H)$
- $\text{net}_k = \sum_{j=1}^{n_H} w_{kj} y_j \quad (1 \leq k \leq c)$
- $z_k = f(\text{net}_k) \quad (1 \leq k \leq c)$
- **Discriminant function**: $g_k = z_k = f(\sum_{j=1}^{n_H} w_{kj} f(\sum_{i=1}^{d} w_{ji} x_i))$

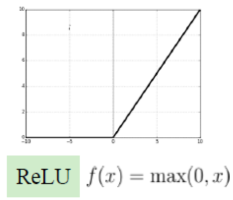
6.1.3 Expressive power of ANN

One layer of hidden units with **sigmoid activation function (a step function)** is sufficient for approximating any function with finitely many discontinuities to arbitrary precision

6.1.4 Activation function

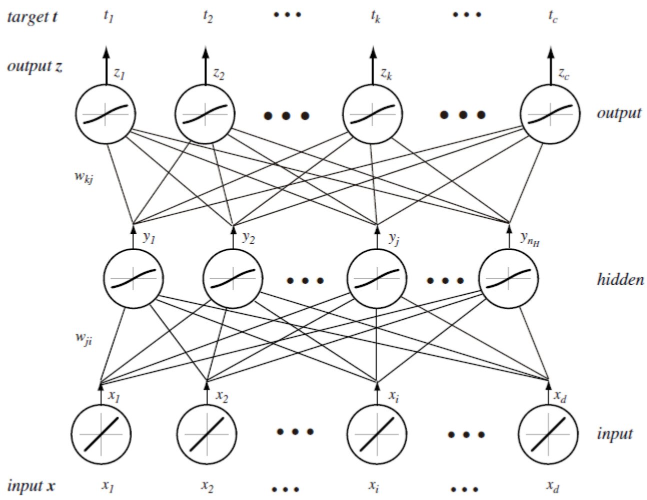






1. **Sigmoid**: $f(x) = \frac{1}{1+e^{-x}}$
2. **tanh**: $f(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$
3. **ReLU**: $f(x) = \max(0, x)$

6.2 Backpropagation algorithm



Settings (A d-n_H-c fully connected three-layer network)

- **Featurs**: d
- **Hidden neurons**: n_H
- **Output neurons**: c
- **Weights**: w
- **Training pattern**: $x = (x_1, x_2, \dots, x_d)^t$
- **Desired output**: $t = (t_1, t_2, \dots, t_c)^t$

6.2.1 Criterion function

We set the **Criterion function** as

$$J(w) = \frac{1}{2} \sum_{k=1}^{c} (t_k - z_k)^2 = \frac{1}{2} ||t - z||^2$$

Gradient descent:

$$w \leftarrow w + \Delta w$$
$$\Delta w = -\eta \frac{\partial J}{\partial w} \ (\Delta w_{pq} = -\eta \frac{\partial J}{\partial w_{pq}})$$

- for **hidden-to-output** layer weight (j-th hidden unit to k-th output unit): w_{kj}
  - **Activation function**:
    - **Sigmoid**: $f^{'} = f \cdot (1 - f)$

- **tanh**: $f^{'} = 1 - f^2$

$$\frac{\partial J}{\partial w_{kj}} = \frac{\partial J}{\partial \text{net}_k}\frac{\partial \text{net}_k}{\partial w_{kj}} = \frac{\partial J}{\partial \text{net}_k}\frac{\sum_{j=1}^{n_H} w_{kj}y_j}{\partial w_{ki}} = -\delta_k y_j$$

$$\delta_k = -\frac{\partial J}{\partial \text{net}_k} = -\frac{\partial J}{\partial z_k}\cdot\frac{\partial z_k}{\partial \text{net}_k}$$

$$= -\frac{\partial(\frac{1}{2}\sum_{k=1}^{c}(t_k - z_k)^2)}{\partial z_k}\frac{f(\text{net}_k)}{\partial \text{net}_k} = (t_k - z_k)f^{'}(\text{net}_k)$$

$$\Delta w_{kj} = -\eta\frac{\partial J}{\partial w_{kj}} = \eta\delta_k y_j = \eta(t_k - z_k)f^{'}(\text{net}_k)y_j$$

- for **input-to-hidden** layer weight (i-th feature to j-th hidden unit): w_{ji}

$$\frac{\partial J}{\partial w_{ji}} = \frac{\partial J}{\partial y_j}\frac{\partial y_j}{\partial \text{net}_j}\frac{\partial \text{net}_j}{\partial w_{ji}} = \frac{\partial J}{\partial y_j}\frac{\partial y_j}{\partial \text{net}_j}\frac{\partial(\sum_{i=1}^{d} w_{ji}x_i)}{\partial w_{ji}}$$

$$= \frac{\partial J}{\partial y_j}f'(\text{net}_j)x_i = -\delta_j x_i$$

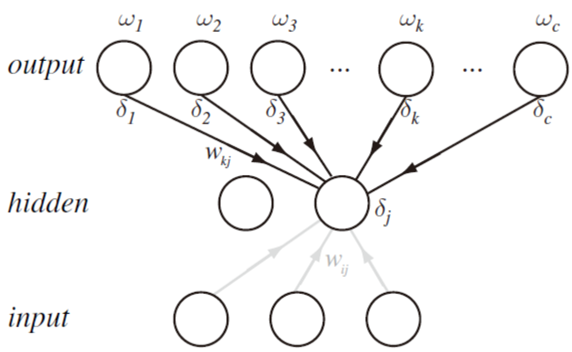
$$\frac{\partial J}{\partial y_j} = \frac{\partial}{\partial y_j}\left[\frac{1}{2}\sum_{k=1}^{c}(t_k - z_k)^2\right] = -\sum_{k=1}^{c}(t_k - z_k)\frac{\partial z_k}{\partial y_j}$$

$$= -\sum_{k=1}^{c}(t_k - z_k)\frac{\partial z_k}{\partial \text{net}_j}\frac{\partial \text{net}_j}{\partial y_j}$$

$$= -\sum_{k=1}^{c}(t_k - z_k)f'(\text{net}_k)w_{kj} = -\sum_{k=1}^{c} w_{kj}\delta_k,$$

$$\Delta w_{ji} = -\eta\frac{\partial J}{\partial w_{ji}} = \eta\delta_j x_i = -\eta\frac{\partial J}{\partial y_j}f'(\text{net}_j)x_i = \eta\left[\sum_{k=1}^{c} w_{kj}\delta_k\right]f'(\text{net}_j)x_i$$

6.2.2 Backpropagation procedure



- δ_k, δ_j: neuron unit's **sensitivity**

Forward procedure

$$\text{net}_j = \sum_{i=1}^{d} w_{ji} x_i \quad (1 \le j \le n_H)$$
$$y_j = f(\text{net}_j) \quad (1 \le j \le n_H)$$
$$\text{net}_k = \sum_{j=1}^{n_H} w_{kj} y_j \quad (1 \le k \le c)$$
$$z_k = f(\text{net}_k) \quad (1 \le k \le c)$$

$$\Longrightarrow$$

Backpropagation procedure

$$\delta_k = (t_k - z_k) f'(\text{net}_k) \quad (1 \le k \le c)$$
$$\delta_j = f'(\text{net}_j) \sum_{k=1}^{c} w_{kj} \delta_k \quad (1 \le j \le n_H)$$

6.2.3 training protocol

6.2.3.1 Stochastic training

- **Stochastic training**:
  - One pattern is randomly selected from the training set, and the weights are updated by presenting the chosen pattern to the network.
- **Stochastic backpropagation**:

$$
\begin{array}{ll}
(1) & \textbf{Begin initialize } n_H, \mathbf{w}, \text{criterion } \theta, \eta, m \leftarrow 0 \\
(2) & \quad \textbf{do } m \leftarrow m + 1 \\
(3) & \qquad \mathbf{x}^m \leftarrow \text{randomly chosen training pattern} \\
(4) & \qquad \text{Invoke the forward and backpropagation procedures on } \mathbf{x}^m \\
 & \qquad \ \text{to obtain } \delta_k \ (1 \le k \le c), y_j \text{ and } \delta_j \ (1 \le j \le n_H) \\
(5) & \qquad w_{ji} \leftarrow w_{ji} + \eta \delta_j x_i; \ w_{kj} \leftarrow w_{kj} + \eta \delta_k y_j \\
(6) & \qquad \textbf{until } \|\nabla J(\mathbf{w})\| \le \theta \\
(7) & \quad \textbf{return w} \\
(8) & \textbf{end}
\end{array}
$$

6.2.3.2 Batch training

- **Batch training**:
  - All patterns in the training set are presented to the network at once, and the weights are updated in **one epoch**
- **Settings** (A d-n_H-c fully connected three-layer network)
  - **Featurs**: d
  - **Hidden neurons**: n_H
  - **Output neurons**: c
  - **Weights**: w
  - **Training set consisting** n **patterns**: $\mathcal{D} = \{(x^m, t^m) | 1 \le m \le n\}$
  - **Training pattern**: $x^m = (x_1, x_2, \ldots, x_d)^t$
  - **Desired output**: $t^m = (t_1, t_2, \ldots, t_c)^t$
    - WLOG (Without Loss of Generality), the superscript m is ignored for elements of x^m and t^m
  - **Criterion function**: $J(w) = \frac{1}{2}||t - z||^2 \implies J(w) = \frac{1}{2} \sum_{m=1}^{n} ||t^m - z^m||^2$

- **Batch backpropagation**

Begin initialize $n_H, \mathbf{w}$, criterion $\theta, \eta, r \leftarrow 0$
    do $r \leftarrow r + 1$ (increment epoch)
        $m \leftarrow 0;\ \Delta w_{ji} \leftarrow 0; \Delta w_{kj} \leftarrow 0$
        do $m \leftarrow m + 1$
            $\mathbf{x}^m \leftarrow$ the m-th pattern in the training set
            Invoke the forward and backpropagation procedures on $\mathbf{x}^m$
              to obtain $\delta_k\ (1 \le k \le c), y_j$ and $\delta_j\ (1 \le j \le n_H)$
            $\Delta w_{ji} \leftarrow \Delta w_{ji} + \eta \delta_j x_i;\ \Delta w_{kj} \leftarrow \Delta w_{kj} + \eta \delta_k y_j$
        until $m = n$
        $w_{ji} \leftarrow w_{ji} + \Delta w_{ji};\ w_{kj} \leftarrow w_{kj} + \Delta w_{kj}$
    until $\|\nabla J(\mathbf{w})\| \le \theta$
    return w
end