# Chapter ML:VI (continued)

### VI. Neural Networks

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

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### **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,  $w_0, w_1, \ldots, w_p$ , exist such that holds:

1. 
$$\forall \mathbf{x} \in X_0$$
:  $\sum_{j=0}^p w_j x_j < 0$ 

**2.** 
$$\forall \mathbf{x} \in X_1$$
:  $\sum_{j=0}^{p} w_j x_j \ge 0$ 

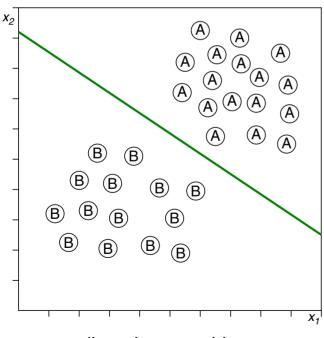
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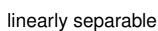
### **Definition 1** (Linear Separability)

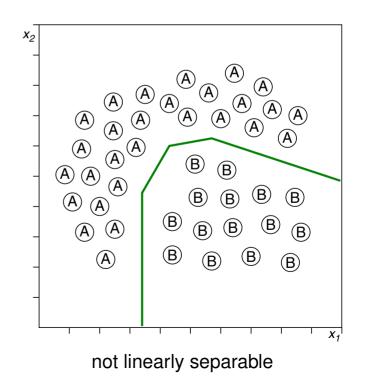
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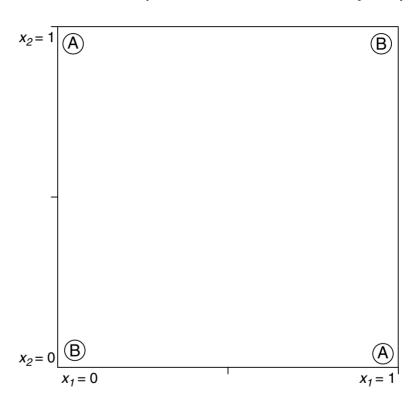


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### Separability

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     |

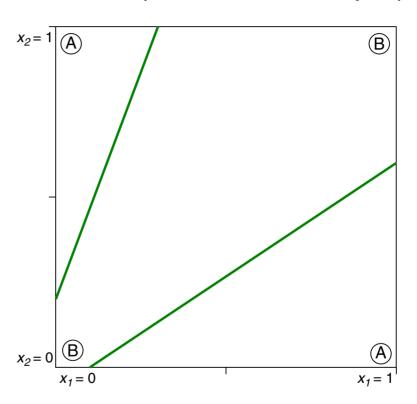


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Separability (continued)

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

| $x_1$ | $x_2$ | XOR | Class          |
|-------|-------|-----|----------------|
| 0     | 0     | 0   | $\overline{B}$ |
| 1     | 0     | 1   | A              |
| 0     | 1     | 1   | A              |
| 1     | 1     | 0   | B              |



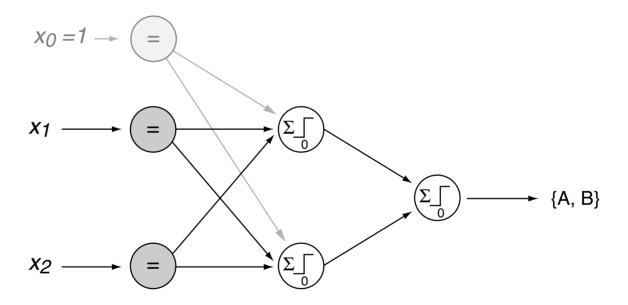
- → specification of several hyperplanes
  - combination of several perceptrons

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Separability (continued)

Layered combination of several perceptrons: the multilayer perceptron.

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



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#### 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 (and non-linear) threshold functions along with 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]

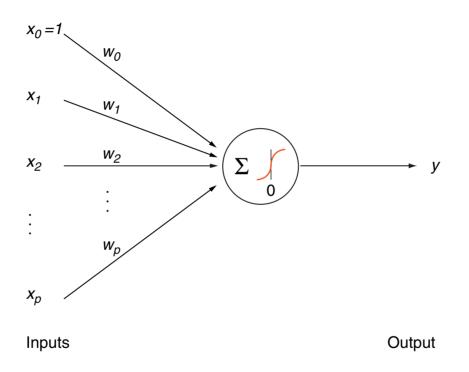


[Marvin Minsky: MIT Media Lab, Wikipedia]

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Computation in the Network [Heaviside]

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



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

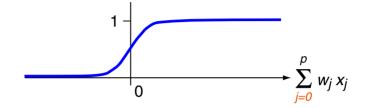
$$\sigma(z) = \frac{1}{1 + e^{-z}} \quad \text{where} \quad \frac{d\sigma(z)}{dz} = \sigma(z) \cdot (1 - \sigma(z))$$

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Computation in the Network (continued)

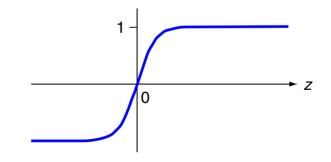
Computation of the perceptron output  $y(\mathbf{x})$  via the sigmoid function  $\sigma$ :

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



An alternative to the sigmoid function is the tanh function:

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

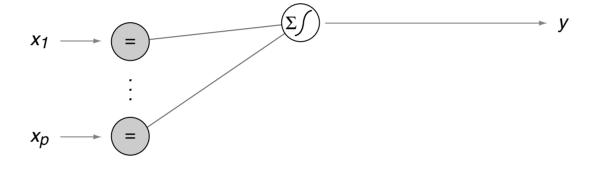


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Computation in the Network (continued)

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

Uı

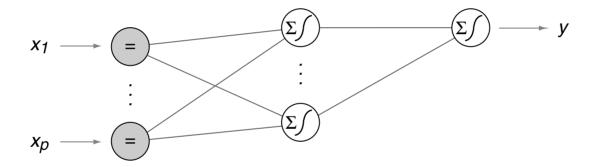


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Computation in the Network (continued)

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

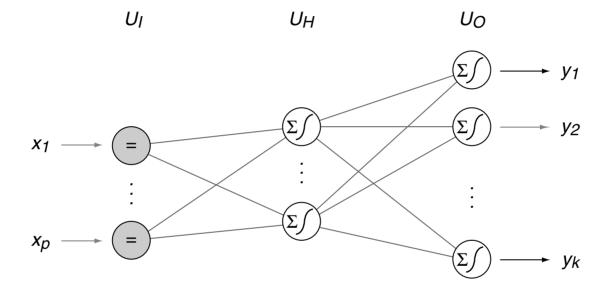
U<sub>I</sub> U<sub>H</sub>



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Computation in the Network (continued)

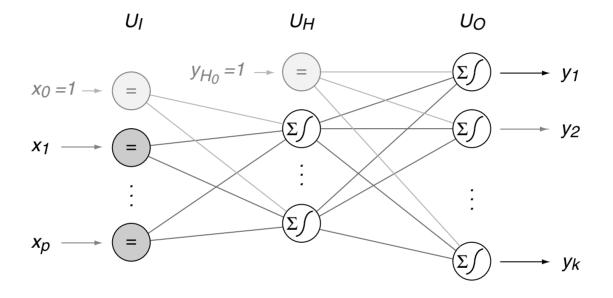
Distinguish units (nodes, perceptrons) of type input, hidden, and output:



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Computation in the Network (continued)

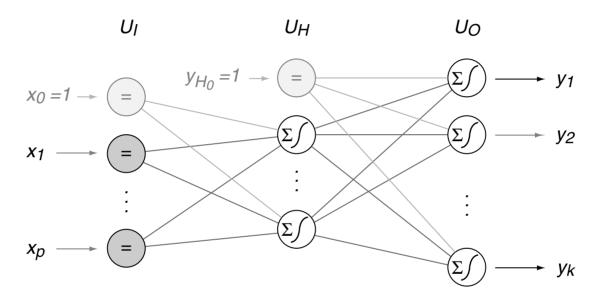
Distinguish units (nodes, perceptrons) of type input, hidden, and output:



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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  $w_{jk}, \ \Delta w_{jk}$  Weight and weight adaptation for the edge connecting the units j and k Input value (single incoming edge) for unit k, provided at the output of unit j  $y_k, \ \delta_k$  Output value and classification error of unit k Weight vector (all incoming edges) of unit k Input vector for a unit of the hidden layer  $y_H, \ y_O$  Output vector of the hidden layer and the output layer respectively

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#### Remarks:

- $\Box$  The units of the input layer,  $U_I$ , perform no computations at all. They distribute the input values to the next layer.
- $\Box$  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 allows for networks that approximate every (computable) function. For this capability 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.

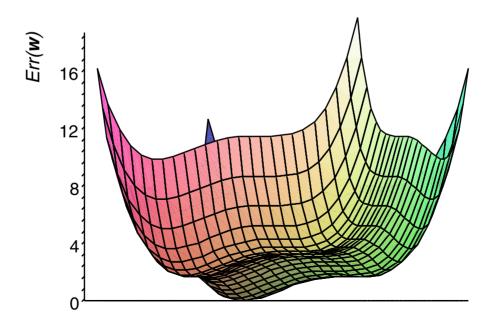
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### Classification Error

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

$$Err(\mathbf{w}) = \frac{1}{2} \sum_{(\mathbf{x}, \mathbf{c}(\mathbf{x})) \in D} \sum_{v \in U_O} (\mathbf{c}(\mathbf{x})|_v - \mathbf{y}_O(\mathbf{x})|_v)^2$$

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



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Weight Adaptation: Incremental Gradient Descent [network]

```
Algorithm: MPT Multilayer Perceptron Training
Input:
                        Training examples (\mathbf{x}, \mathbf{c}(\mathbf{x})) with |\mathbf{x}| = p + 1, \mathbf{c}(\mathbf{x}) \in \{0, 1\}^k. // \mathbf{c}(\mathbf{x}) \in \{-1, 1\}^k
               D
                         Learning rate, a small positive constant.
               \eta
                         Weights of the units in U_I, U_H, U_O.
Output:
               \mathbf{W}
        initialize_random_weights(U_I, U_H, U_O), t=0
   2.
        REPEAT
   3. t = t + 1
        FOREACH (\mathbf{x}, \mathbf{c}(\mathbf{x})) \in D DO
   4.
             FOREACH u \in U_H DO y_u = \sigma(\mathbf{w}_u^T \mathbf{x}) // compute output of layer 1
   5.
              FOREACH v \in U_O DO y_v = \sigma(\mathbf{w}_v^T \mathbf{y}_H) // compute output of layer 2
   6.
   7.
   8.
   9.
 10.
 11.
 12.
```

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ENDDO

 $return(\mathbf{w})$ 

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

13.

14.

15.

 $return(\mathbf{w})$ 

15.

Weight Adaptation: Incremental Gradient Descent [network]

```
Algorithm: MPT Multilayer Perceptron Training
                        Training examples (\mathbf{x}, \mathbf{c}(\mathbf{x})) with |\mathbf{x}| = p + 1, \mathbf{c}(\mathbf{x}) \in \{0, 1\}^k. // \mathbf{c}(\mathbf{x}) \in \{-1, 1\}^k
Input:
               D
                        Learning rate, a small positive constant.
               \eta
                        Weights of the units in U_I, U_H, U_O.
Output:
               \mathbf{W}
        initialize_random_weights(U_I, U_H, U_O), t=0
  2.
        REPEAT
  3.
        t = t + 1
  4.
         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 layer1
  5.
              FOREACH v \in U_O DO y_v = \sigma(\mathbf{w}_v^T \mathbf{y}_H) // compute output of layer 2
  6.
  7.
             FOREACH v \in U_O DO \delta_v = y_v \cdot (1 - y_v) \cdot (\mathbf{c}(\mathbf{x})|_v - y_v) // backpropagate layer 2
            FOREACH u \in U_H DO \delta_u = y_u \cdot (1-y_u) \cdot \sum w_{uv} \cdot \delta_v // backpropagate layer1
  8.
  9.
 10.
 11.
 12.
 13.
           ENDDO
 14.
        UNTIL(convergence(D, y_O(D)) OR t > t_{max})
```

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Weight Adaptation: Incremental Gradient Descent [network]

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

14.

15.

 $return(\mathbf{w})$ 

```
Algorithm: MPT Multilayer Perceptron Training
Input:
                D
                         Training examples (\mathbf{x}, \mathbf{c}(\mathbf{x})) with |\mathbf{x}| = p + 1, \mathbf{c}(\mathbf{x}) \in \{0, 1\}^k. // \mathbf{c}(\mathbf{x}) \in \{-1, 1\}^k
                         Learning rate, a small positive constant.
                \eta
                         Weights of the units in U_I, U_H, U_O.
Output:
                \mathbf{W}
        initialize_random_weights(U_I, U_H, U_O), t=0
   2.
        REPEAT
   3. t = t + 1
   4.
        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 layer1
   5.
              FOREACH v \in U_O DO y_v = \sigma(\mathbf{w}_v^T \mathbf{y}_H) // compute output of layer 2
   6.
  7.
             FOREACH v \in U_O DO \delta_v = y_v \cdot (1 - y_v) \cdot (\mathbf{c}(\mathbf{x})|_v - y_v) // backpropagate layer 2
             FOREACH u \in U_H DO \delta_u = y_u \cdot (1-y_u) \cdot \sum w_{uv} \cdot \delta_v // backpropagate layer1
   8.
              FOREACH w_{jk}, (j,k) \in (U_I \times U_H) \cup (U_H \times U_O) DO
   9.
 10.
                 \Delta w_{ik} = \eta \cdot \delta_k \cdot x_{i \to k}
                 w_{ik} = w_{ik} + \Delta w_{ik}
 11.
 12.
              ENDDO
 13.
           ENDDO
```

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#### 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.

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Weight Adaptation: Momentum Term

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

$$\Delta w_{jk}(t) = \eta \cdot \delta_k \cdot x_{j \to k} + \alpha \cdot \Delta w_{jk}(t-1)$$

The term  $\alpha$ ,  $0 \le \alpha < 1$ , is called "momentum".

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Weight Adaptation: Momentum Term

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

$$\Delta w_{jk}(t) = \eta \cdot \delta_k \cdot x_{j \to k} + \alpha \cdot \Delta w_{jk}(t-1)$$

The term  $\alpha$ ,  $0 \le \alpha < 1$ , 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.

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