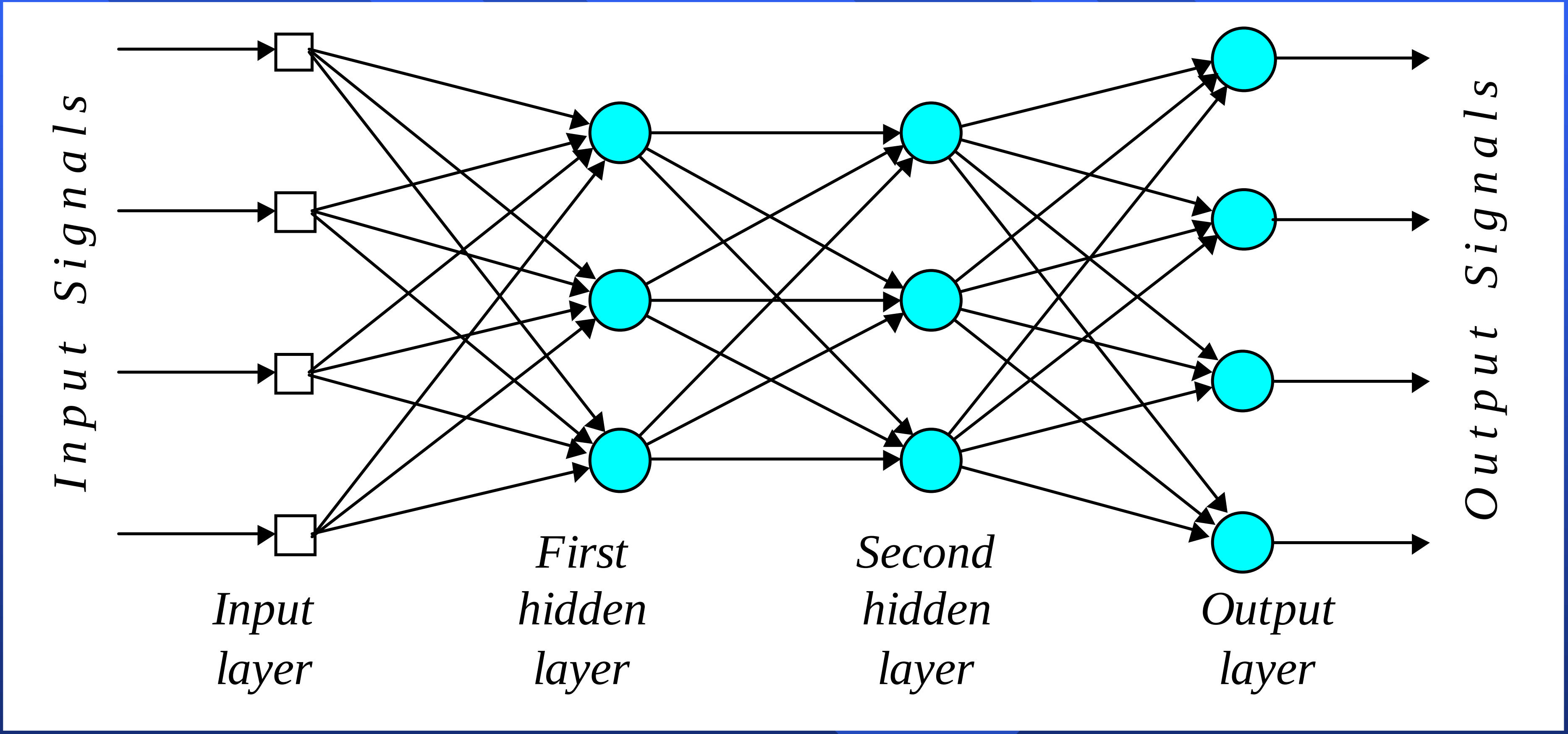
Multilayer neural networks

- A multilayer perceptron is a feedforward neural network with one or more hidden layers.
- The network consists of an **input layer** of source neurons, at least one middle or **hidden layer** of computational neurons, and an **output layer** of computational neurons.
- The input signals are propagated in a forward direction on a layer-by-layer basis.

Multilayer perceptron with two hidden layers



What does the middle layer hide?

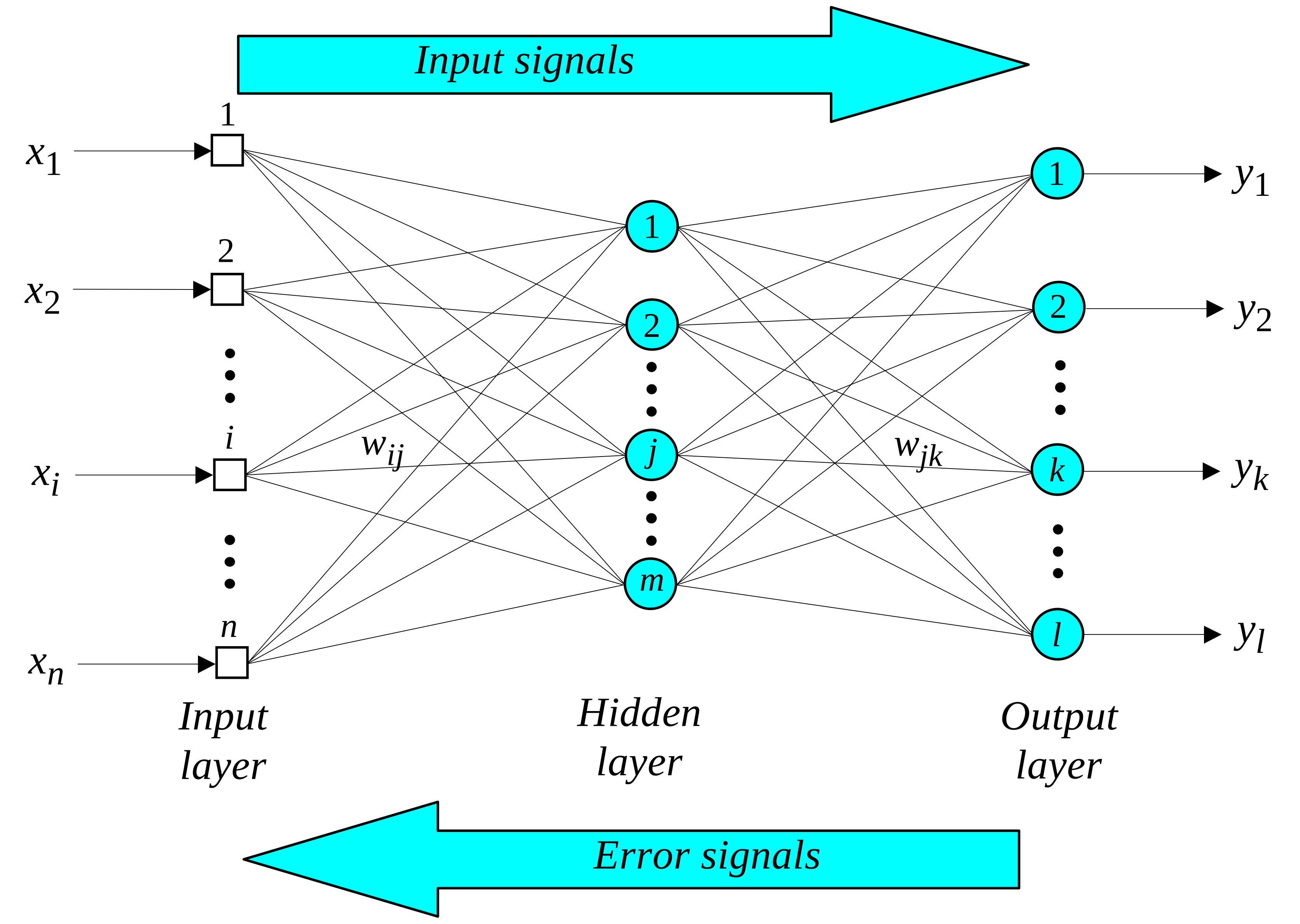
- A hidden layer "hides" its desired output. Neurons in the hidden layer cannot be observed through the input/output behaviour of the network. There is no obvious way to know what the desired output of the hidden layer should be.
- Commercial ANNs incorporate three and sometimes four layers, including one or two hidden layers. Each layer can contain from 10 to 1000 neurons. Experimental neural networks may have five or even six layers, including three or four hidden layers, and utilise millions of neurons.

Back-propagation neural network

- Learning in a multilayer network proceeds the same way as for a perceptron.
- A training set of input patterns is presented to the network.
- The network computes its output pattern, and if there is an error – or in other words a difference between actual and desired output patterns – the weights are adjusted to reduce this error.

- In a back-propagation neural network, the learning algorithm has two phases.
- First, a training input pattern is presented to the network input layer. The network propagates the input pattern from layer to layer until the output pattern is generated by the output layer.
- If this pattern is different from the desired output, an error is calculated and then propagated backwards through the network from the output layer to the input layer. The weights are modified as the error is propagated.

Three-layer back-propagation neural network



The back-propagation training algorithm

Step 1: Initialisation

Set all the weights and threshold levels of the network to random numbers uniformly distributed inside a small range:

$$\left(-\frac{2.4}{F_i}, \; +\frac{2.4}{F_i} \right)$$

where F_i is the total number of inputs of neuron i in the network. The weight initialisation is done on a neuron-by-neuron basis.

Step 2: Activation

Activate the back-propagation neural network by applying inputs $x_1(p)$, $x_2(p)$,…, $x_n(p)$ and desired outputs $y_{d,1}(p)$, $y_{d,2}(p)$,…, $y_{d,n}(p)$.

(*a*) Calculate the actual outputs of the neurons in the hidden layer:

$$y_j(p) = sigmoid\left[\sum_{i=1}^{n} x_i(p) \cdot w_{ij}(p) - \theta_j\right]$$

where *n* is the number of inputs of neuron *j* in the hidden layer, and *sigmoid* is the *sigmoid* activation function.

Step 2: Activation (continued)

(*b*) Calculate the actual outputs of the neurons in the output layer:

$$y_k(p) = sigmoid\left[\sum_{j=1}^{m} x_{jk}(p) \cdot w_{jk}(p) - \theta_k\right]$$

where *m* is the number of inputs of neuron *k* in the output layer.

Step 3: Weight training

Update the weights in the back-propagation network propagating backward the errors associated with output neurons.

(*a*) Calculate the error gradient for the neurons in the output layer:

$$\delta_k(p) = y_k(p) \cdot [1 - y_k(p)] \cdot e_k(p)$$

where $e_k(p) = y_{d,k}(p) - y_k(p)$

Calculate the weight corrections:

$$\Delta w_{jk}(p) = \alpha \cdot y_j(p) \cdot \delta_k(p)$$

Update the weights at the output neurons:

$$w_{jk}(p+1) = w_{jk}(p) + \Delta w_{jk}(p)$$

Step 3: Weight training (continued)

(*b*) Calculate the error gradient for the neurons in the hidden layer:

$$\delta_j(p) = y_j(p) \cdot [1 - y_j(p)] \cdot \sum_{k=1}^{l} \delta_k(p)\, w_{jk}(p)$$

Calculate the weight corrections:

$$\Delta w_{ij}(p) = \alpha \cdot x_i(p) \cdot \delta_j(p)$$

Update the weights at the hidden neurons:

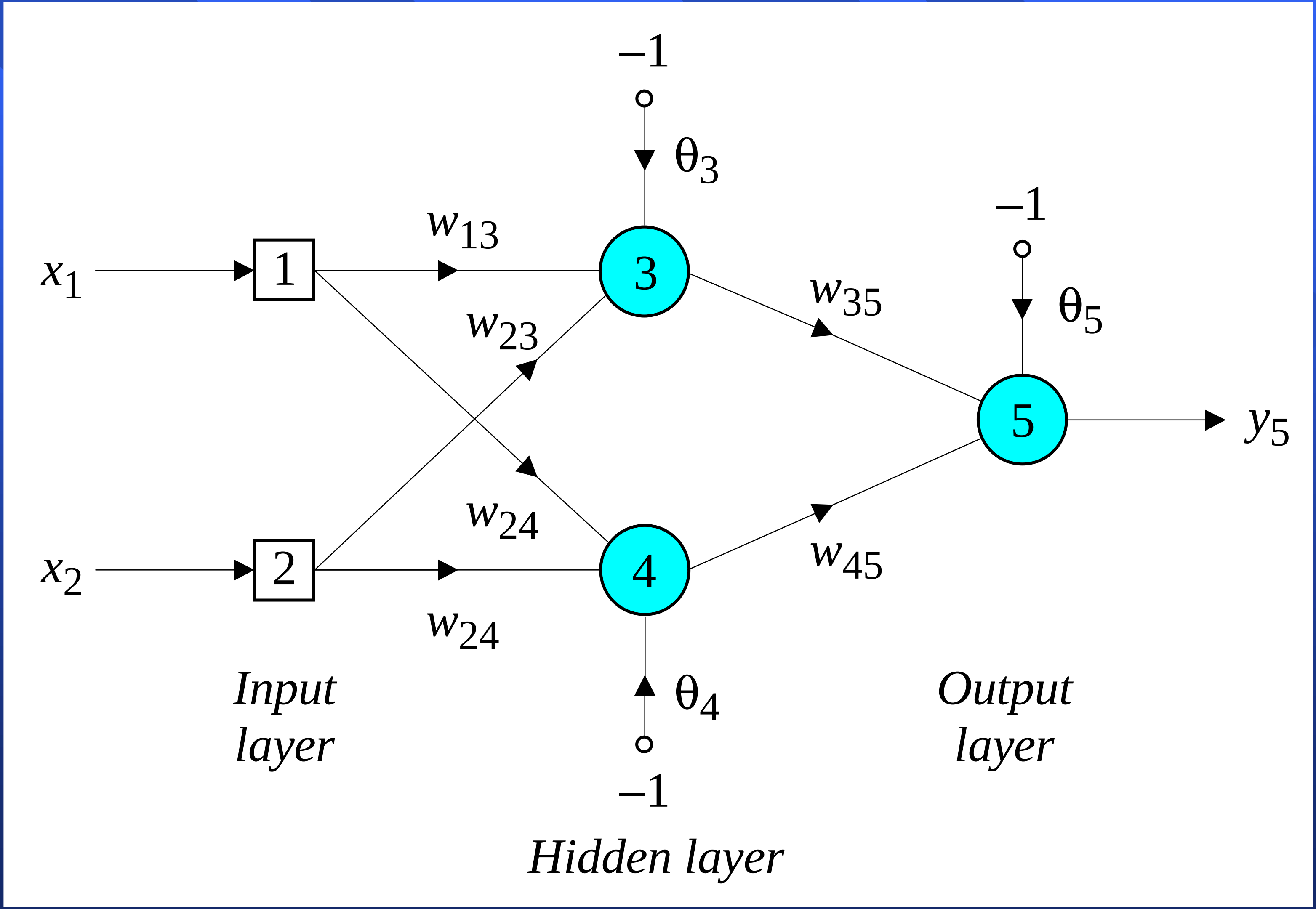
$$w_{ij}(p+1) = w_{ij}(p) + \Delta w_{ij}(p)$$

Step 4: Iteration

Increase iteration p by one, go back to *Step 2* and repeat the process until the selected error criterion is satisfied.

As an example, we may consider the three-layer back-propagation network. Suppose that the network is required to perform logical operation *Exclusive-OR*. Recall that a single-layer perceptron could not do this operation. Now we will apply the three-layer net.

Three-layer network for solving the Exclusive-OR operation



- The effect of the threshold applied to a neuron in the hidden or output layer is represented by its weight, θ, connected to a fixed input equal to –1.
- The initial weights and threshold levels are set randomly as follows:
  $w_{13} = 0.5$, $w_{14} = 0.9$, $w_{23} = 0.4$, $w_{24} = 1.0$, $w_{35} = -1.2$, $w_{45} = 1.1$, $\theta_3 = 0.8$, $\theta_4 = -0.1$ and $\theta_5 = 0.3$.

- We consider a training set where inputs x_1 and x_2 are equal to 1 and desired output $y_{d,5}$ is 0. The actual outputs of neurons 3 and 4 in the hidden layer are calculated as

$$y_3 = sigmoid\,(x_1 w_{13} + x_2 w_{23} - \theta_3) = 1 \Big/ \left[1 + e^{-(1\cdot 0.5 + 1\cdot 0.4 - 1\cdot 0.8)}\right] = 0.5250$$

$$y_4 = sigmoid\,(x_1 w_{14} + x_2 w_{24} - \theta_4) = 1 \Big/ \left[1 + e^{-(1\cdot 0.9 + 1\cdot 1.0 + 1\cdot 0.1)}\right] = 0.8808$$

- Now the actual output of neuron 5 in the output layer is determined as:

$$y_5 = sigmoid(y_3 w_{35} + y_4 w_{45} - \theta_5) = 1 \Big/ \left[1 + e^{-(-0.5250\cdot 1.2 + 0.8808\cdot 1.1 - 1\cdot 0.3)}\right] = 0.5097$$

- Thus, the following error is obtained:

$$e = y_{d,5} - y_5 = 0 - 0.5097 = -0.5097$$

- The next step is weight training. To update the weights and threshold levels in our network, we propagate the error, *e*, from the output layer backward to the input layer.
- First, we calculate the error gradient for neuron 5 in the output layer:

$$\delta_5 = y_5\,(1 - y_5)\,e = 0.5097 \cdot (1 - 0.5097) \cdot (-0.5097) = -0.1274$$

- Then we determine the weight corrections assuming that the learning rate parameter, α, is equal to 0.1:

$$\Delta w_{35} = \alpha \cdot y_3 \cdot \delta_5 = 0.1 \cdot 0.5250 \cdot (-0.1274) = -0.0067$$
$$\Delta w_{45} = \alpha \cdot y_4 \cdot \delta_5 = 0.1 \cdot 0.8808 \cdot (-0.1274) = -0.0112$$
$$\Delta \theta_5 = \alpha \cdot (-1) \cdot \delta_5 = 0.1 \cdot (-1) \cdot (-0.1274) = -0.0127$$

- Next we calculate the error gradients for neurons 3 and 4 in the hidden layer:

$$\delta_3 = y_3(1-y_3)\cdot\delta_5\cdot w_{35} = 0.5250\cdot(1-0.5250)\cdot(-0.1274)\cdot(-1.2) = 0.0381$$

$$\delta_4 = y_4(1-y_4)\cdot\delta_5\cdot w_{45} = 0.8808\cdot(1-0.8808)\cdot(-0.1274)\cdot 1.1 = -0.0147$$

- We then determine the weight corrections:

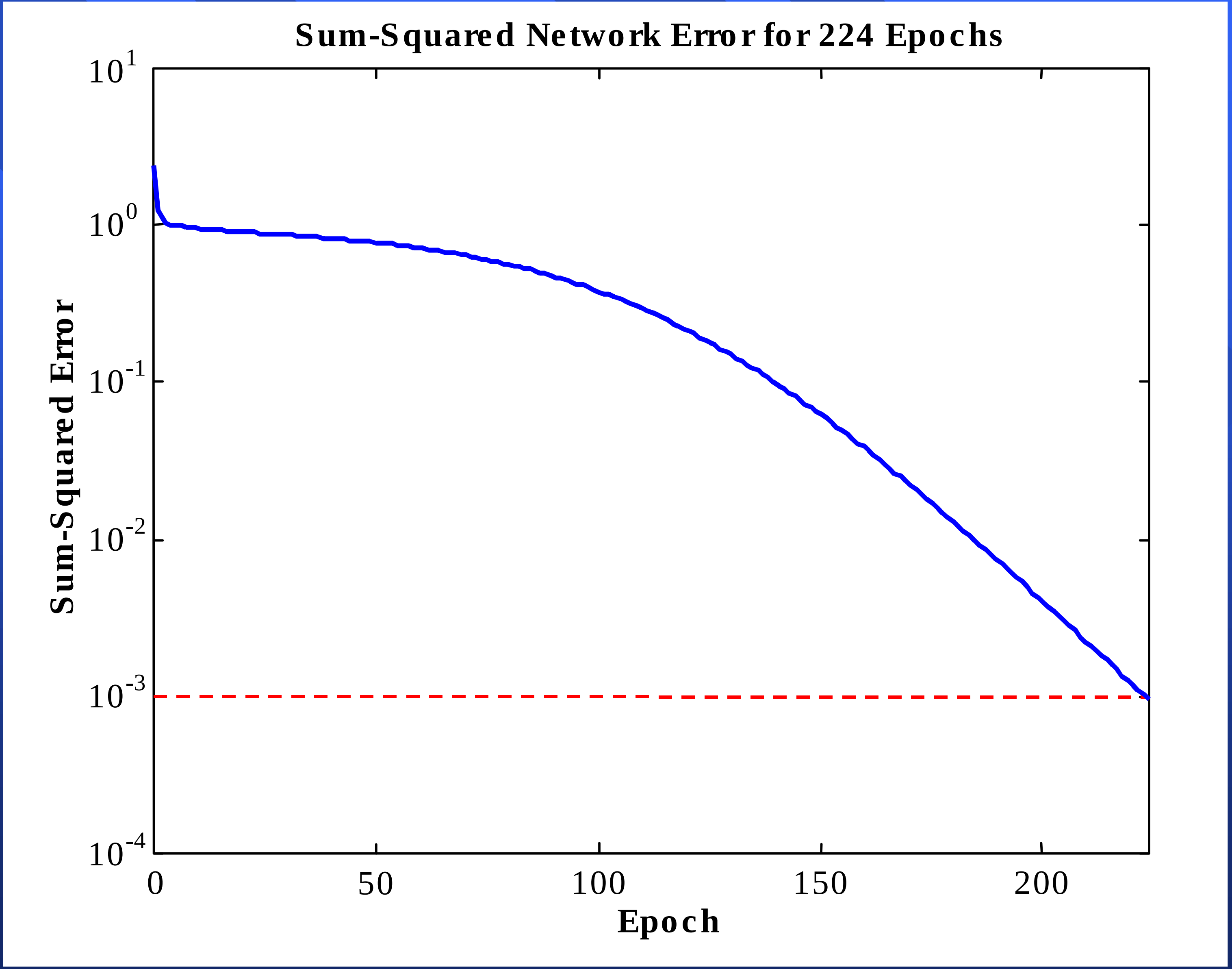
$$\Delta w_{13} = \alpha\cdot x_1\cdot\delta_3 = 0.1\cdot 1\cdot 0.0381 = 0.0038$$
$$\Delta w_{23} = \alpha\cdot x_2\cdot\delta_3 = 0.1\cdot 1\cdot 0.0381 = 0.0038$$
$$\Delta \theta_3 = \alpha\cdot(-1)\cdot\delta_3 = 0.1\cdot(-1)\cdot 0.0381 = -0.0038$$
$$\Delta w_{14} = \alpha\cdot x_1\cdot\delta_4 = 0.1\cdot 1\cdot(-0.0147) = -0.0015$$
$$\Delta w_{24} = \alpha\cdot x_2\cdot\delta_4 = 0.1\cdot 1\cdot(-0.0147) = -0.0015$$
$$\Delta \theta_4 = \alpha\cdot(-1)\cdot\delta_4 = 0.1\cdot(-1)\cdot(-0.0147) = 0.0015$$

- At last, we update all weights and threshold:

$$w_{13} = w_{13} + \Delta w_{13} = 0.5 + 0.0038 = 0.5038$$
$$w_{14} = w_{14} + \Delta w_{14} = 0.9 - 0.0015 = 0.8985$$
$$w_{23} = w_{23} + \Delta w_{23} = 0.4 + 0.0038 = 0.4038$$
$$w_{24} = w_{24} + \Delta w_{24} = 1.0 - 0.0015 = 0.9985$$
$$w_{35} = w_{35} + \Delta w_{35} = -1.2 - 0.0067 = -1.2067$$
$$w_{45} = w_{45} + \Delta w_{45} = 1.1 - 0.0112 = 1.0888$$
$$\theta_3 = \theta_3 + \Delta\theta_3 = 0.8 - 0.0038 = 0.7962$$
$$\theta_4 = \theta_4 + \Delta\theta_4 = -0.1 + 0.0015 = -0.0985$$
$$\theta_5 = \theta_5 + \Delta\theta_5 = 0.3 + 0.0127 = 0.3127$$

- The training process is repeated until the sum of squared errors is less than 0.001.

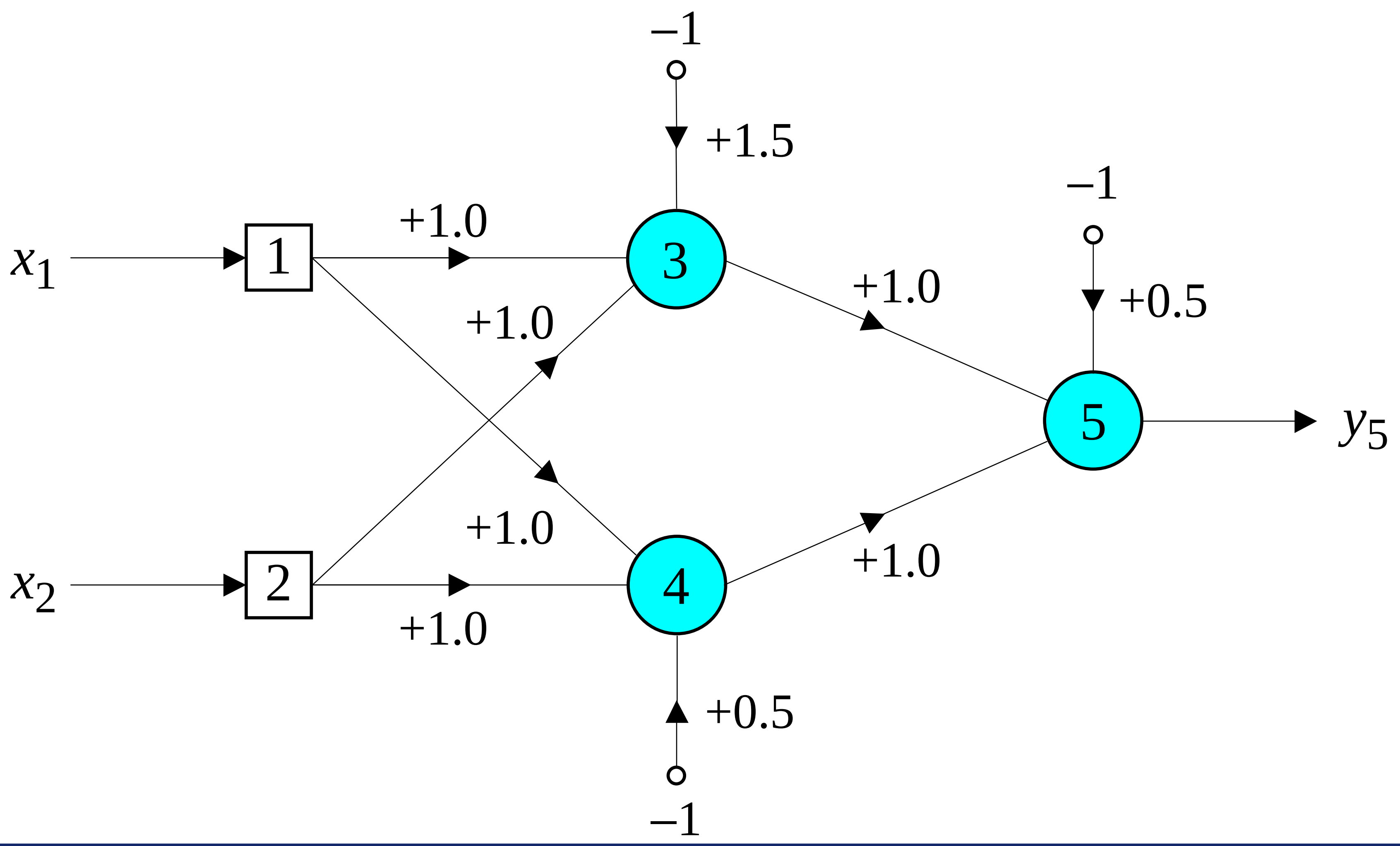
Learning curve for operation *Exclusive-OR*



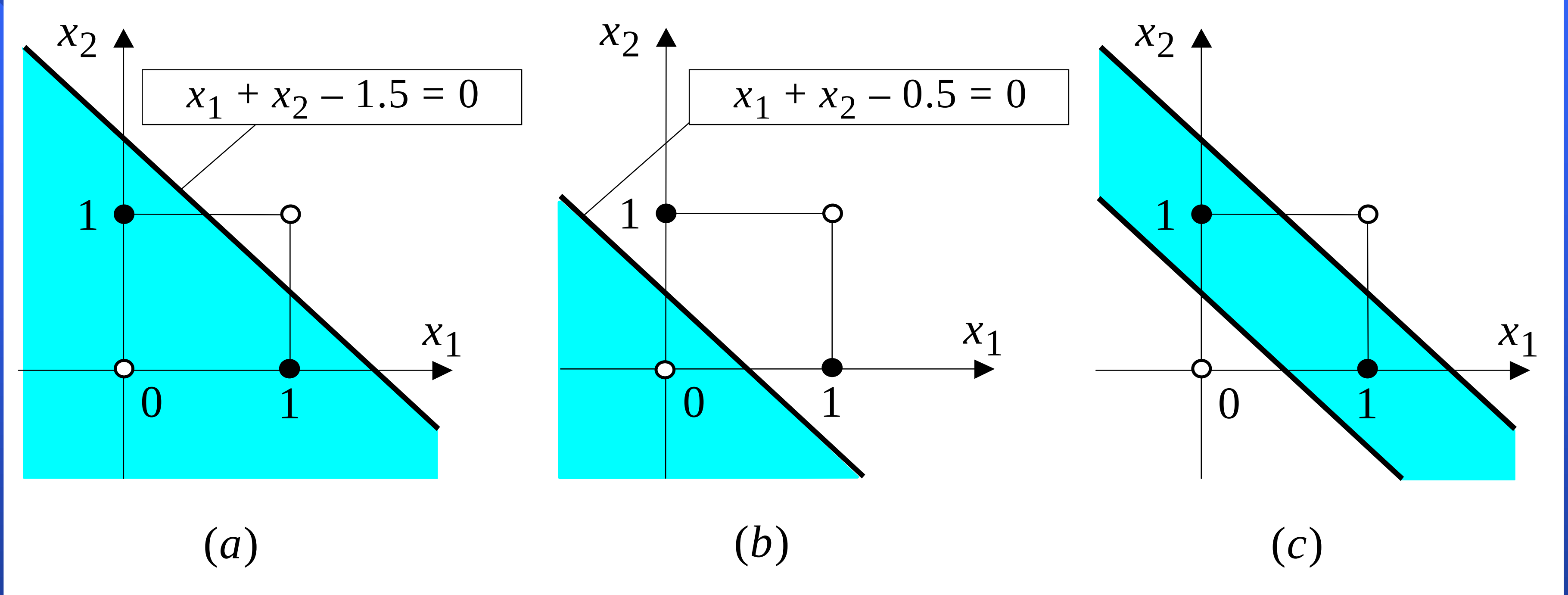
Final results of three-layer network learning

Inputs		Desired output	Actual output	Error	Sum of squared errors
x_1	x_2	y_d	y_5	e	
1	1	0	0.0155	–0.0155	0.0010
0	1	1	0.9849	0.0151	
1	0	1	0.9849	0.0151	
0	0	0	0.0175	–0.0175	

Network represented by McCulloch-Pitts model for solving the *Exclusive-OR* operation



Decision boundaries



(*a*) Decision boundary constructed by hidden neuron 3;
(*b*) Decision boundary constructed by hidden neuron 4;
(*c*) Decision boundaries constructed by the complete three-layer network

Accelerated learning in multilayer neural networks

- A multilayer network learns much faster when the sigmoidal activation function is represented by a **hyperbolic tangent**:

$$Y^{tanh} = \frac{2a}{1 + e^{-bX}} - a$$

where *a* and *b* are constants.

Suitable values for *a* and *b* are:
a = 1.716 and b = 0.667

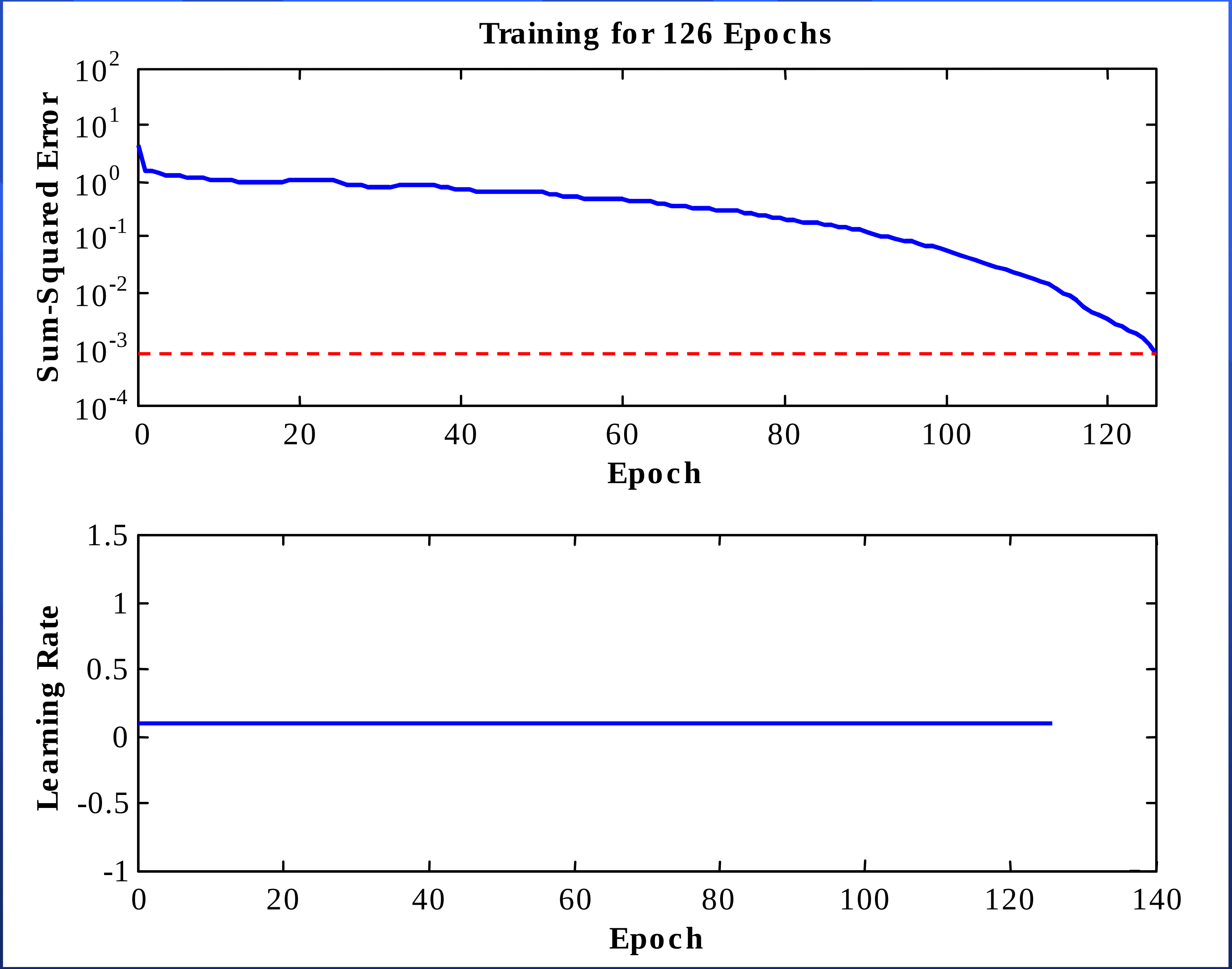
- We also can accelerate training by including a **momentum term** in the delta rule:

$$\boxed{\Delta w_{jk}(p) = \beta \cdot \Delta w_{jk}(p-1) + \alpha \cdot y_j(p) \cdot \delta_k(p)}$$

where β is a positive number ($0 \leq \beta < 1$) called the **momentum constant**. Typically, the momentum constant is set to 0.95.

This equation is called the **generalised delta rule**.

Learning with momentum for operation *Exclusive-OR*



Learning with adaptive learning rate

To accelerate the convergence and yet avoid the danger of instability, we can apply two heuristics:

Heuristic 1

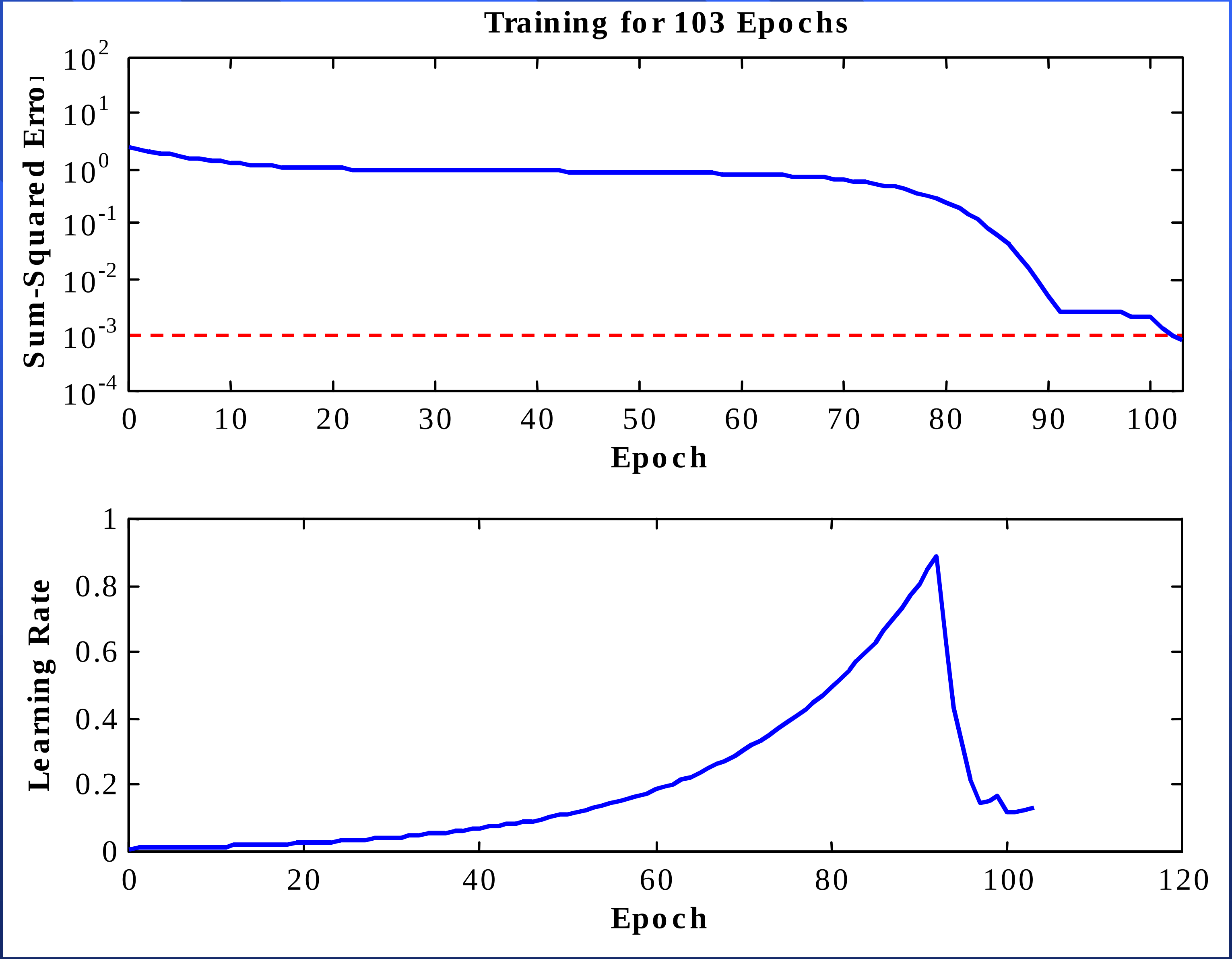
If the change of the sum of squared errors has the same algebraic sign for several consequent epochs, then the learning rate parameter, α, should be increased.

Heuristic 2

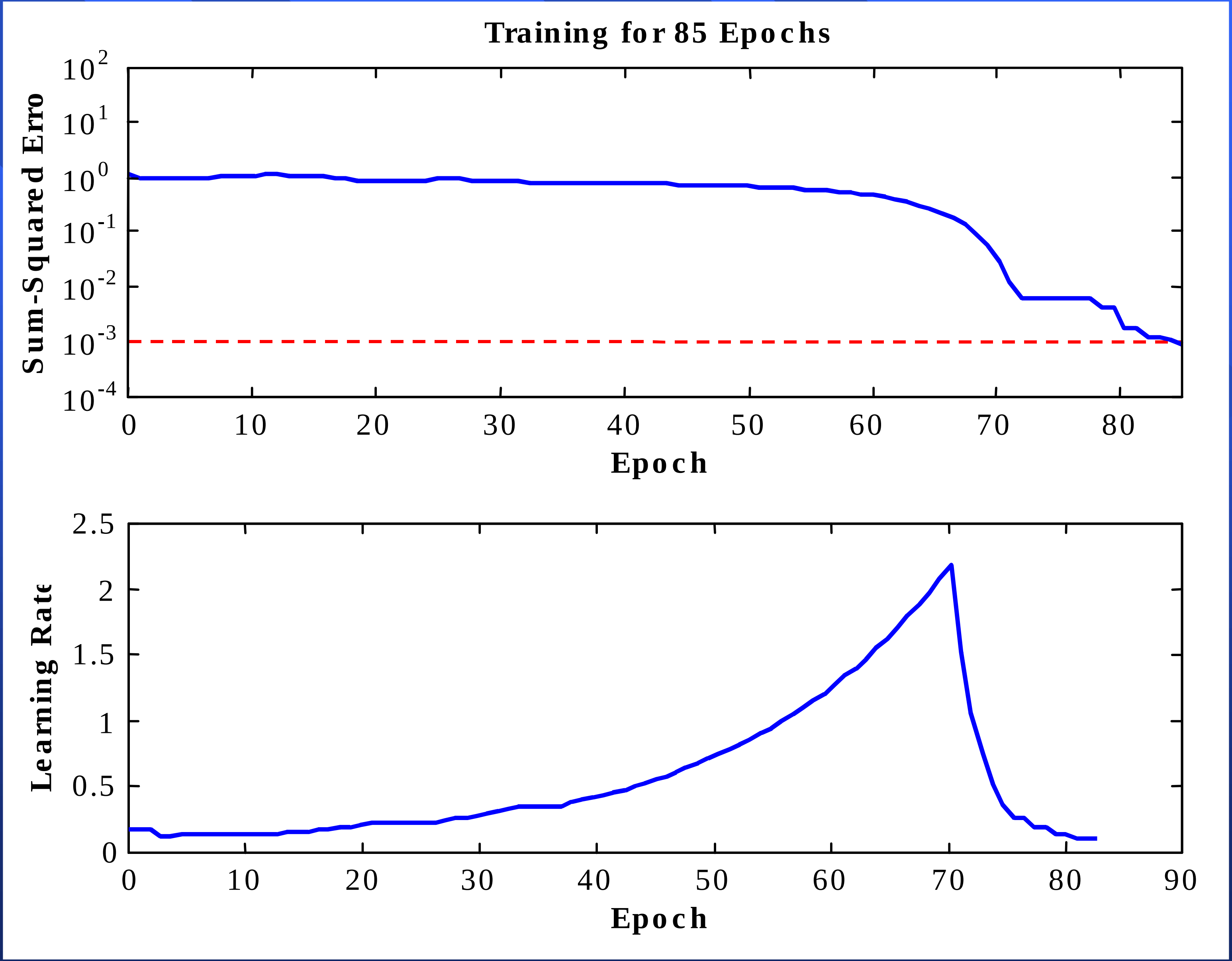
If the algebraic sign of the change of the sum of squared errors alternates for several consequent epochs, then the learning rate parameter, α, should be decreased.

- Adapting the learning rate requires some changes in the back-propagation algorithm.
- If the sum of squared errors at the current epoch exceeds the previous value by more than a predefined ratio (typically 1.04), the learning rate parameter is decreased (typically by multiplying by 0.7) and new weights and thresholds are calculated.
- If the error is less than the previous one, the learning rate is increased (typically by multiplying by 1.05).

Learning with adaptive learning rate



Learning with momentum and adaptive learning rate


Training for 85 Epochs
Sum-Squared Erro
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
Epoch
Learning Rate
Epoch