Introduction to

Machine Learning and Data Mining

(Học máy và Khai phá dữ liệu)

Khoat Than

School of Information and Communication Technology

Hanoi University of Science and Technology

2021

Outline

- Introduction to Machine Learning & Data Mining
- Unsupervised learning
- **Supervised learning**
  - **Artificial neural network**
- Practical advice

Artificial neural network: introduction (1)

- Artificial neural network (ANN) (mạng nơron nhân tạo)
  - Simulates the biological neural systems (human brain)
  - ANN is a structure/network made of interconnection of artificial neurons

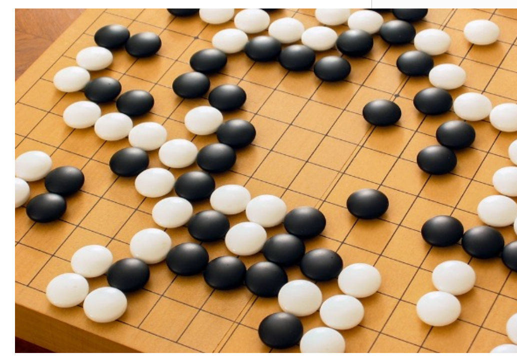
- Neuron
  - Has input/output
  - Executes a local calculation (local function)
- Output of a neuron is charactorized by
  - In/out characteristics
  - Connections between it and other neurons
  - (Possible) other inputs

Artificial neural network: introduction (2)

- ANN can be thought of as a highly decentralized and parallel information processing structure
- ANN has the ability to learn, recall and generalize from the training data
- The ability of an ANN depends on
  - Network architecture
  - Input/output characteristics
  - Learning algorithm
  - Training data

ANN: a huge breakthrough

- AlphaGo of Google the world champion at Go, 3/2016
  - Go is a 2500 year-old game.
  - Go is one of the most complex games
- AlphaGo learns from 30 millions human moves, and plays itself to find new moves



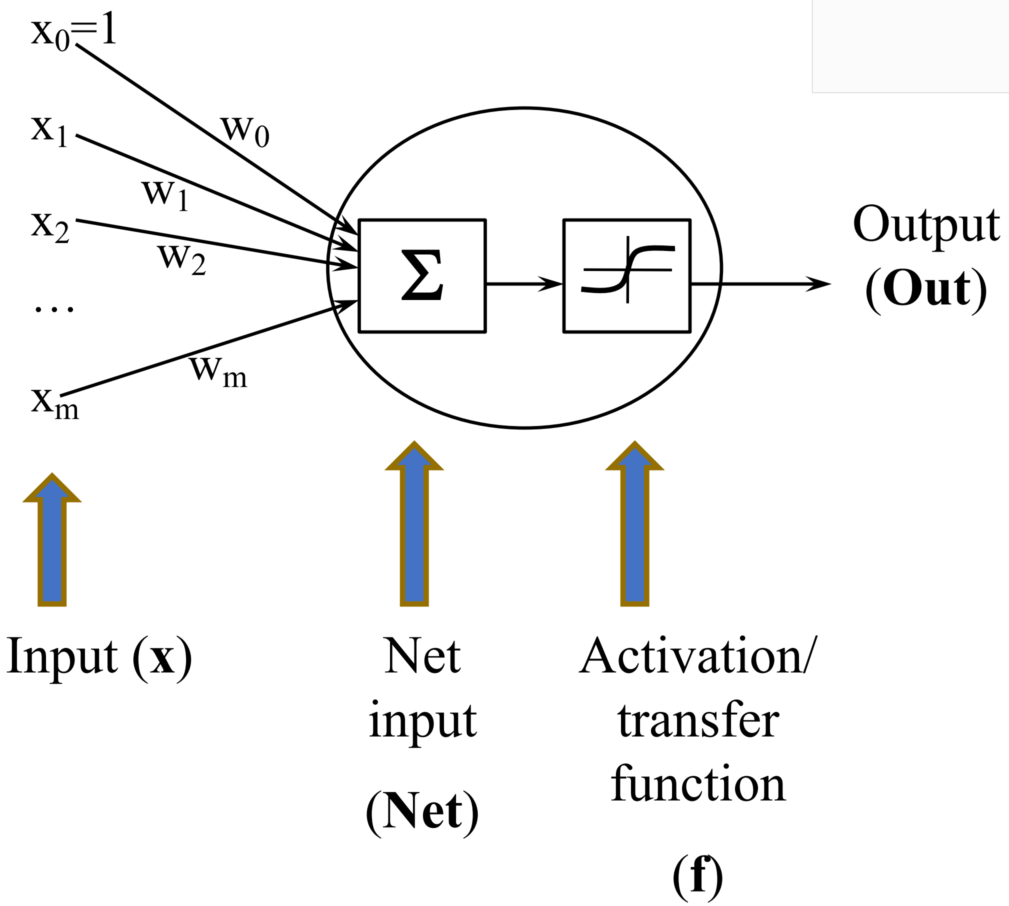
- It beat Lee Sedol (World champion)

  http://www.wired.com/2016/03/two-move
  future/

  http://www.nature.com/news/google-ai-al
  go-1.19234

Structure of a neuron

- Input signals of a neuron
  $\{x_i \,, i = 1 \ldots m\}$
  - Each input signal x_i is associated with a weight w_i
- Bias w_0 (with $x_0 = 1$)
- Net input is a combination of the input signals
  $Net(\boldsymbol{w}, \boldsymbol{x})$
- Activation/transfer function $f(\cdot)$ computes the output of a neuron
- Output
  $Out = f\,(Net\,(\boldsymbol{w}, \boldsymbol{x}))$

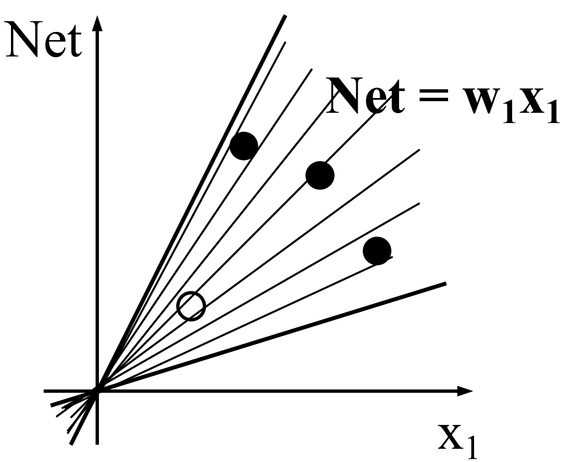


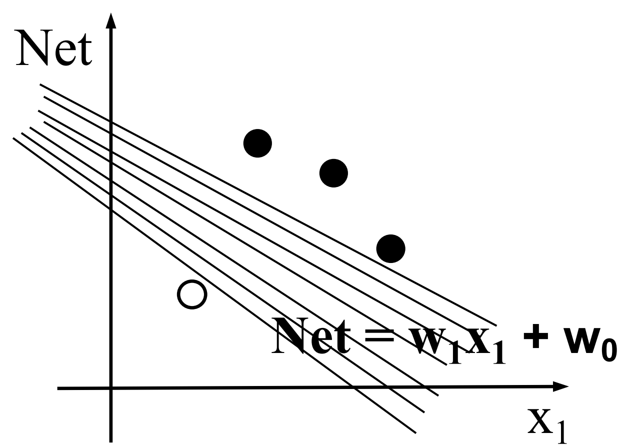
Net Input

- Net input is usually calculated by a function of linear form

$$Net = w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_m x_m = w_0 .1 + \sum_{i=1}^{m} w_i x_i = \sum_{i=0}^{m} w_i x_i$$

- Role of bias:
  - $Net=w_1x_1$ may not separate well the classes
  - $Net=w_1x_1+w_0$ is able to do better





Activation function: hard-limited

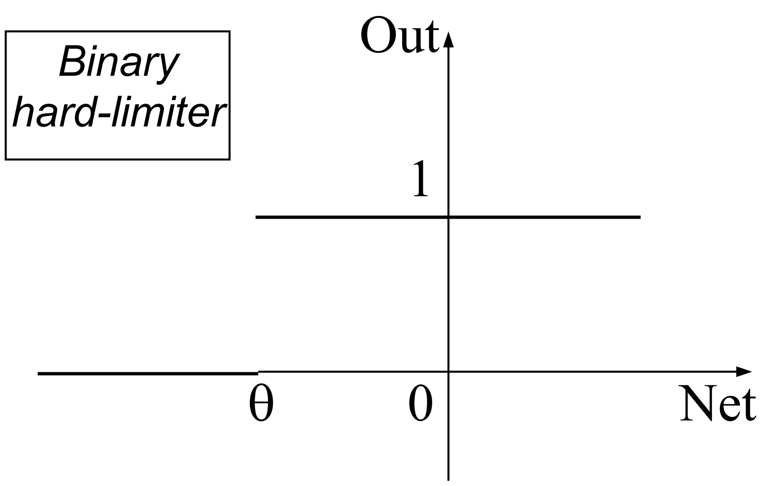
- Also know as a threshold function

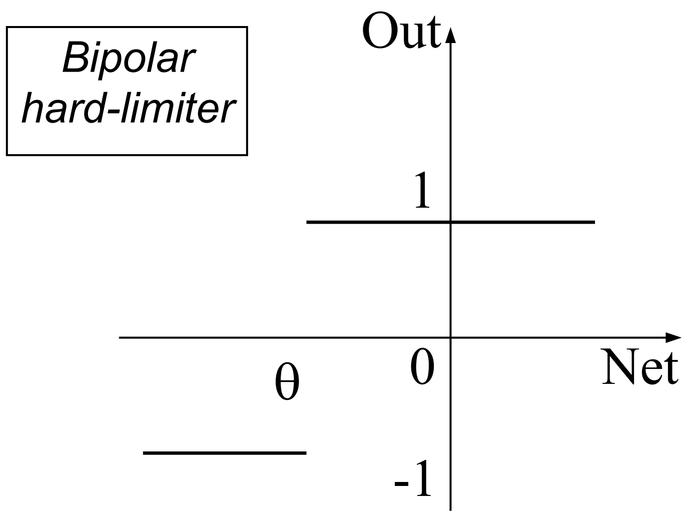
$$Out(Net) = HL(Net, \theta) = \begin{cases} 1, \text{ if } & Net \geq \theta \\ 0, & \text{otherwise} \end{cases}$$

- The output takes one of the two values

$$Out(Net) = HL2(Net, \theta) = sign(Net, \theta)$$

- θ is the threshold value
- **Properties:** discontinuous, non-smoothed (không trơn)



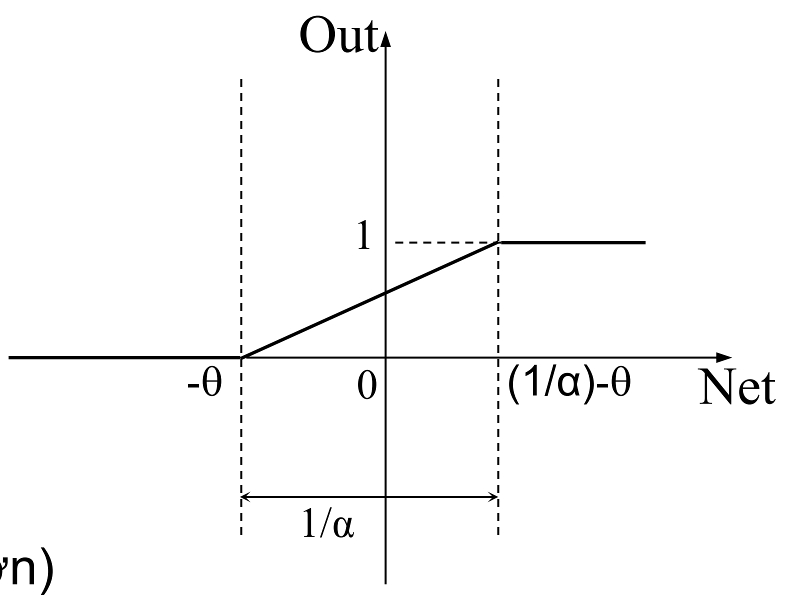


Activation function: threshold logic

$$Out(Net) = tl(Net, \alpha, \theta) = \begin{cases} 0, \ \text{if} & Net < -\theta \\ \alpha(Net+\theta), \text{if} -\theta \le Net \le \dfrac{1}{\alpha} - \theta \\ 1, \ \text{if} & Net > \dfrac{1}{\alpha} - \theta \end{cases} \qquad (\alpha > 0)$$

$$= \max(0, \min(1, \alpha(Net + \theta)))$$

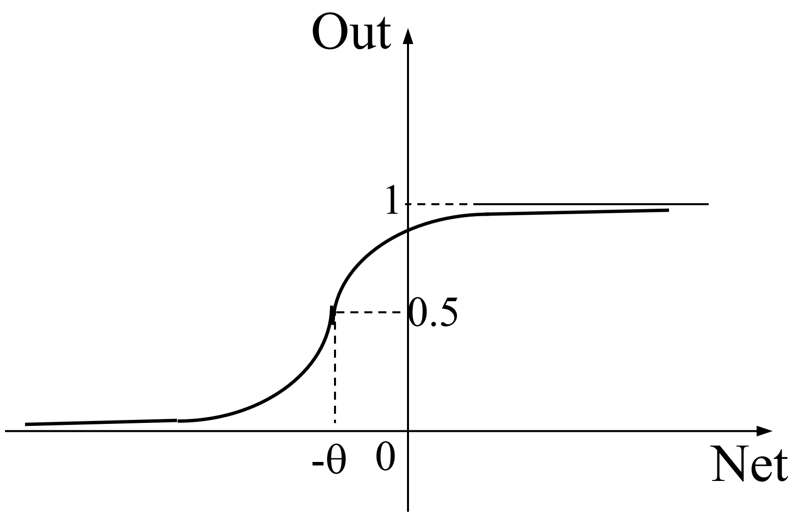
- Also known as a saturating linear function
- Combination of 2 activation functions: linear and tight limits
- α determines the slope of the linear range
- **Properties:** continuous, non-smoothed (liên tục, nhưng không trơn)



Activation function: Sigmoid

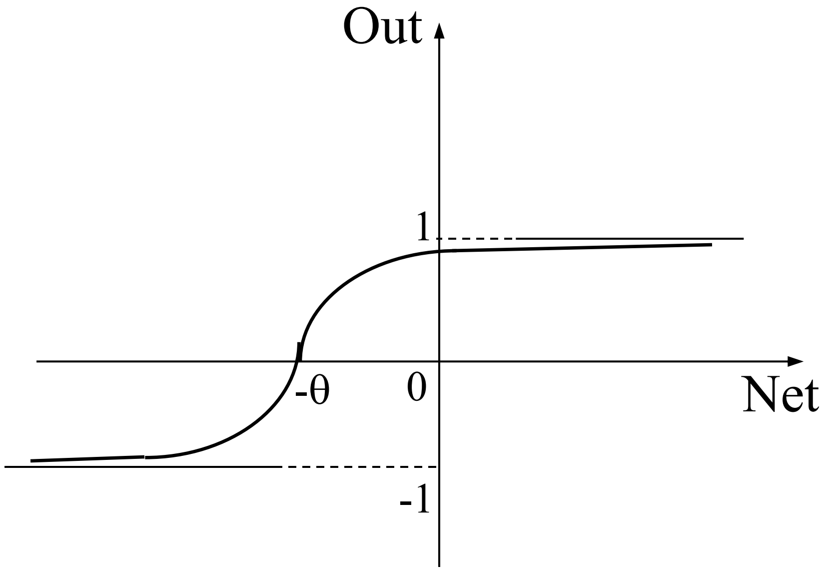
$$Out(Net) = sf(Net, \alpha, \theta) = \frac{1}{1 + e^{-\alpha(Net+\theta)}}$$

- Popular
- The parameter α determines the slope
- Output in the range of 0 and 1
- **Advantages**
  - Continuous, smoothed
  - Gradient of a sigmoid function is represented by a function of itself



Activation function: Hyperbolic tangent

$$Out(Net) = \tanh(Net, \alpha, \theta) = \frac{1 - e^{-\alpha(Net+\theta)}}{1 + e^{-\alpha(Net+\theta)}} = \frac{2}{1 + e^{-\alpha(Net+\theta)}} - 1$$

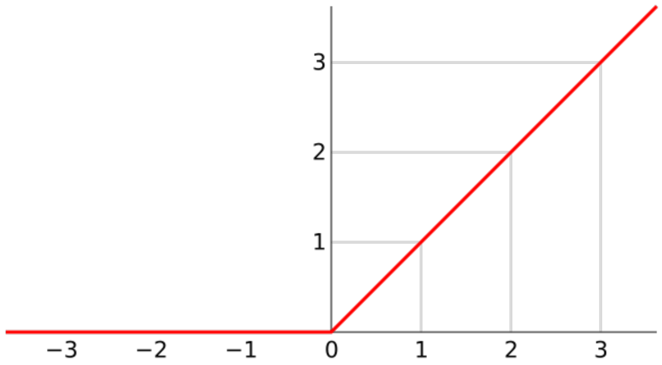


- Popular
- The parameter α determines the slope
- Output in the range of -1 and 1
- Advantages
  - Continuous, continuous derivative
  - Gradient of a tanh function is represented by a function of itself

Act. function: Rectified linear unit (ReLU)

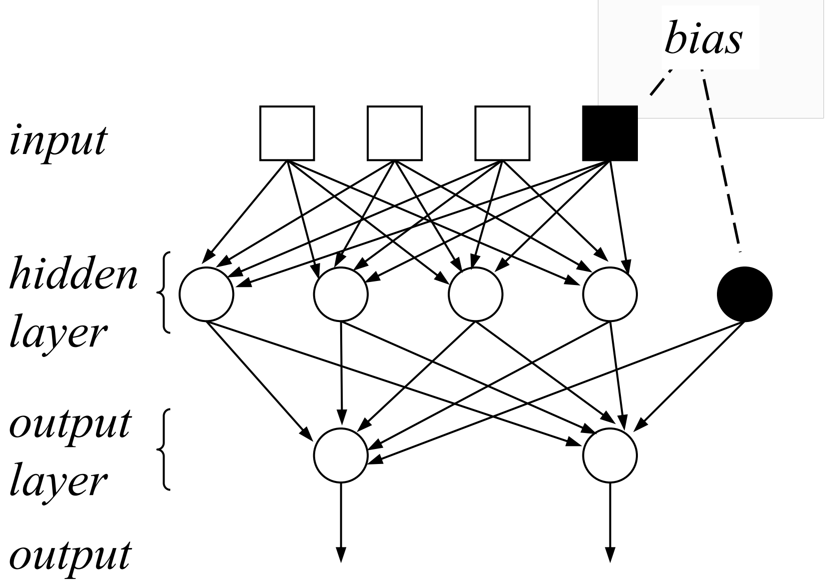
$$Out(net) = \max(0, net)$$

- Most popular
- Output is non-negative
- Advantages
  - Continuous
  - No derivative at point 0
  - Easy to calculate



ANN: Architecture (1)

- ANN's architecture is determined by
  - Number of input and output signals
  - Number of layers
  - Number of neurons in each layer
  - Number of connection for each neuron
  - How neurons (with in a layer, or between layers) are connected
- An ANN must have
  - An input layer
  - An output layer
  - No, single, or multiple hidden layers

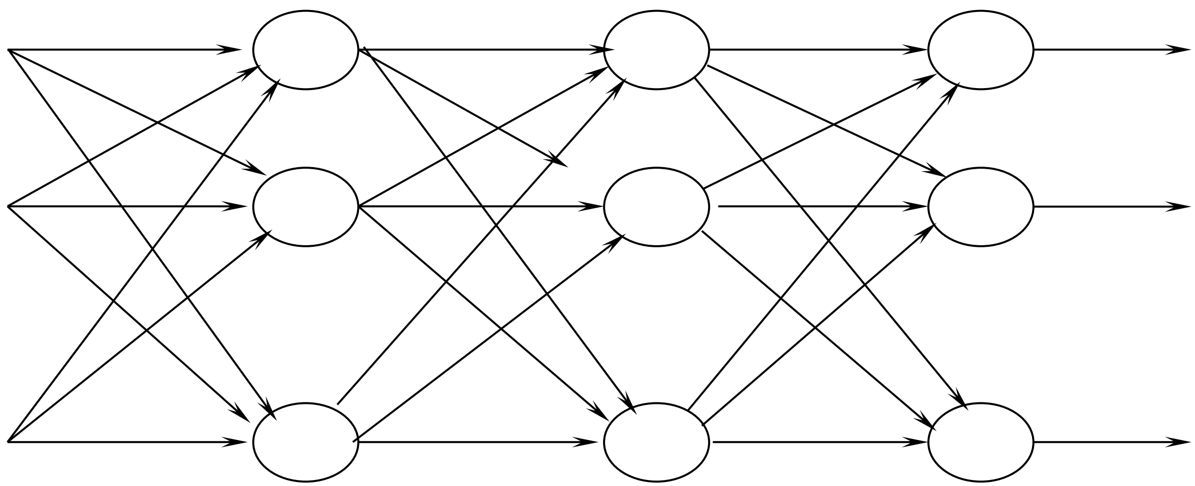


E.g: An ANN with single hidden layer

- Input: 3 signals
- Output: 2 signals
- Total, have 6 neurons
  - 4 neurons at hidden layer
  - 2 neurons at output layer

ANN: Architecture (2)

- A layer (tầng) contains a set of neurons
- Hidden layer (tầng ẩn) is a layer between input layer and output layer
- Hidden nodes do not interact directly with external environment of the neural network
- An ANN is called a **fully connected** if outputs of a layer are connected to all neurons of the next layer

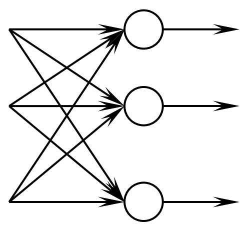


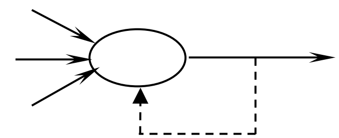
ANN: Architecture (3)

- An ANN is called a **feed-forward network** (mạng lan truyền tiến) if there is not any output of a node being input of another node of the same layer or a previous layer
- When the output of a node is the input of the node the same layer or a previous layer, it is called a **feedback network** (mạng phản hồi)
  - If feedback connects to the input of nodes of the same layer, then it is called a **lateral feedback**.
- Feedback networks with closed loops are called **recurrent networks** (mạng hồi quy)

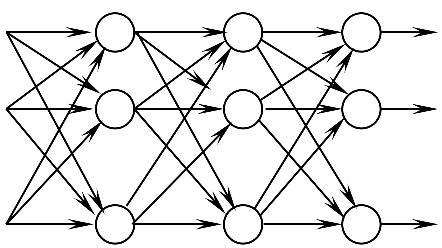
ANN: Architecture (4)

Feed-forward network

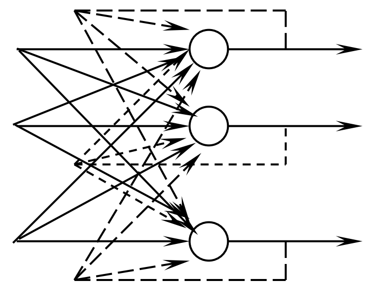




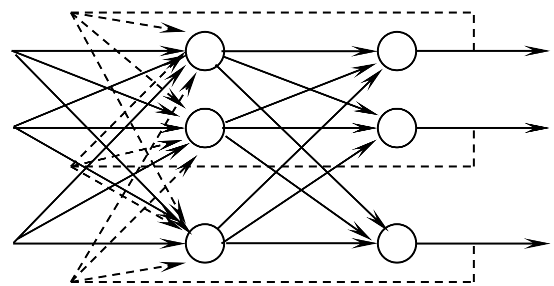
A neuron with feedback to itself



Feed-forward network with multiple layers



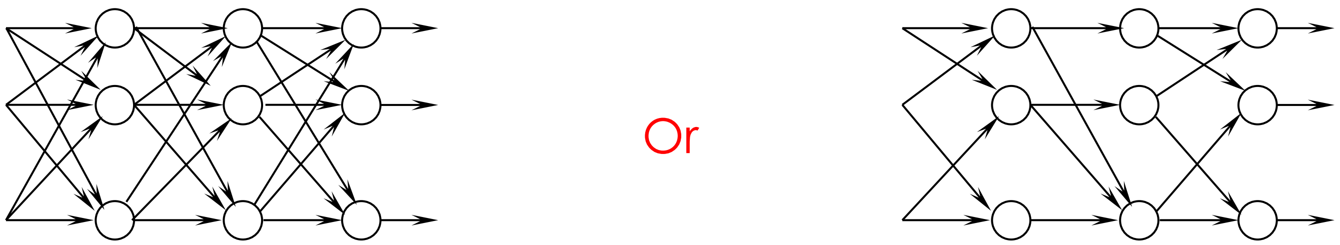
Recurrent network with single layer



Recurrent network with multiple layers

ANN: Training

- 2 types of learning in ANNs
  - ***Parameter learning***: The goal is to adapt the weights of the connections in the ANN, given a fixed network structure
  - ***Structure learning***: The goal is to learn the network structure, including the number of neurons and the types of connections between them, and the weights



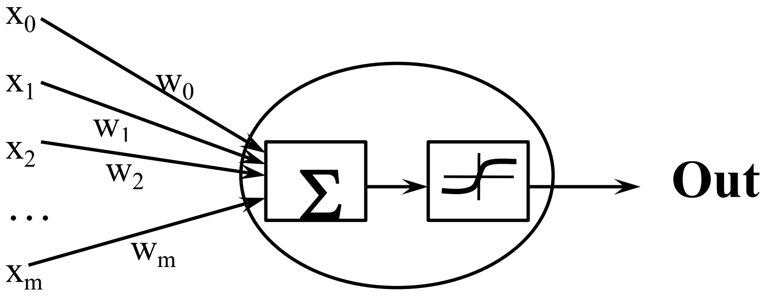
- Those two types can be done simultaneously or separately
- In this lecture, we will only consider parameter learning

ANN: Idea for training

- Training a neural network (when fixing the architecture) is learning the weights **w** of the network from training data **D**
- Learning can be done by minimizing an empirical error function

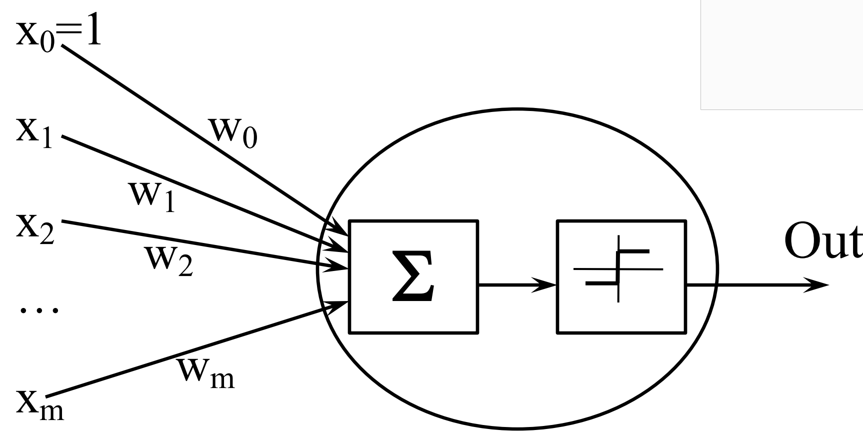
$$\mathrm{L}(\boldsymbol{w}) = \frac{1}{|\boldsymbol{D}|} \sum_{\boldsymbol{x} \in \boldsymbol{D}} loss(d_x, \mathrm{out}(\boldsymbol{x}))$$

  - Where out(**x**) is the output of the network, with the input **x** labeled accordingly as d_x; loss is a function for measuring prediction error
- Many gradient-based methods:
  - Backpropagation
  - Stochastic gradient decent (SGD)
  - Adam
  - AdaGrad



Perceptron

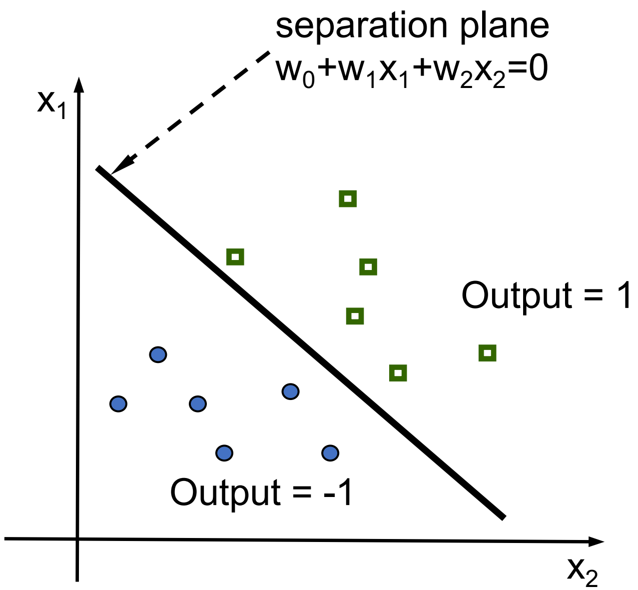
- A perceptron is the simplest type of ANNs (consists of only one neuron).



- Use the hard-limited activation function

$$Out = sign(Net(w,x)) = sign\left(\sum_{j=0}^{m} w_j x_j\right)$$

- For input **x**, the output value of perceptron
  - 1 if Net(**w**,**x**)>0
  - -1 otherwise



Perceptron: Algorithm

- Training data **D** = **{(x**, d**)}**
  - **x** is input vector
  - d is output (1 or -1)
- The goal of perceptron learning (training) process determines a weight vector that allows the perceptron to produce the correct output value (-1 or 1) for each data point
- For data point **x** correctly classified by perceptron, the weight vector **w** unchanged
- If d = 1 but the perceptron produces -1 (Out = -1), then **w** needs to be changed so that the value of Net (**w, x**) increases
- If d = -1 but the perceptron produces 1 (Out = 1), then **w** needs to be changed so that the value of Net (**w, x**) decreases

Perceptron: Algorithm

Perceptron_batch(**D**, η)

Initialize **w** (w_i ← an initial (small) random value)

do

  Δ**w** ← 0

  for each training instance (**x**,d)∈**D**

    Compute the real output value Out

    if (Out≠d)

      Δ**w** ← Δ**w** + η(d-Out)**x**

  end for

  w ← **w** + Δ**w**

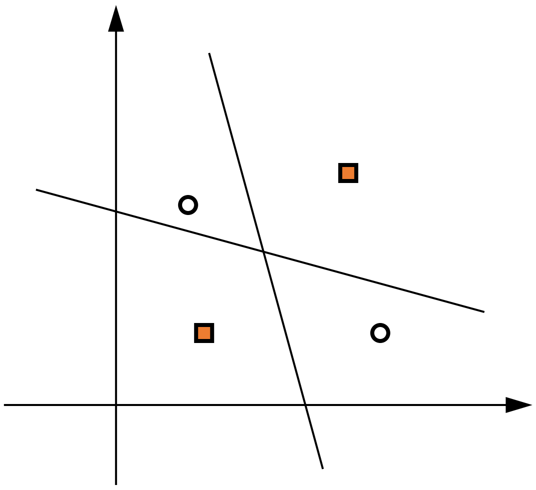
until all the training instances in **D** are correctly classified

return **w**

Perceptron: Limitation

- The training algorithm for perceptron is proved to converge if:
  - Data points are linearly separable
  - Use a learning rate η small enough
- The training algorithm for perceptron may not converge if data points are not linearly separable

A perceptron cannot classify correctly for this case!



Loss function

- Consider an ANN that has n output neurons
- For data point ($\mathbf{x}$, d), the **training error** value caused by the (current) weight vector **w**:

$$E_{\mathbf{x}}(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{n}\left(d_i - Out_i\right)^2$$

- **Training error** for the training data **D** is

$$E_D(\mathbf{w}) = \frac{1}{|D|}\sum_{\mathbf{x}\in D} E_{\mathbf{x}}(\mathbf{w})$$

Minimize errors with gradients

- Gradient of E (denoted by ∇E) is a vector

$$\nabla E(\mathbf{w}) = \left(\frac{\partial E}{\partial w_1}, \frac{\partial E}{\partial w_2}, \ldots, \frac{\partial E}{\partial w_N} \right)$$

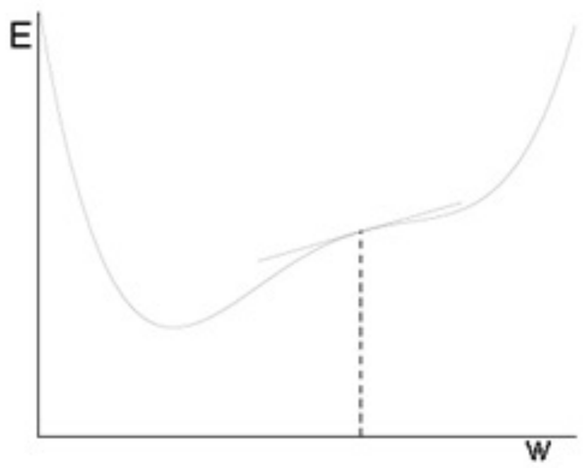
  - where N is the total number of weights (connections) in the ANN
- The gradient ∇E determines the direction that causes the **steepest increase** for the error value E
- Therefore, the direction that causes the **steepest decrease** is opposite to the gradient of E

$$\Delta \boldsymbol{w} = -\eta . \nabla E(\boldsymbol{w}); \quad \Delta w_i = -\eta \frac{\partial E}{\partial w_i} \text{ for } i = 1 \ldots N$$

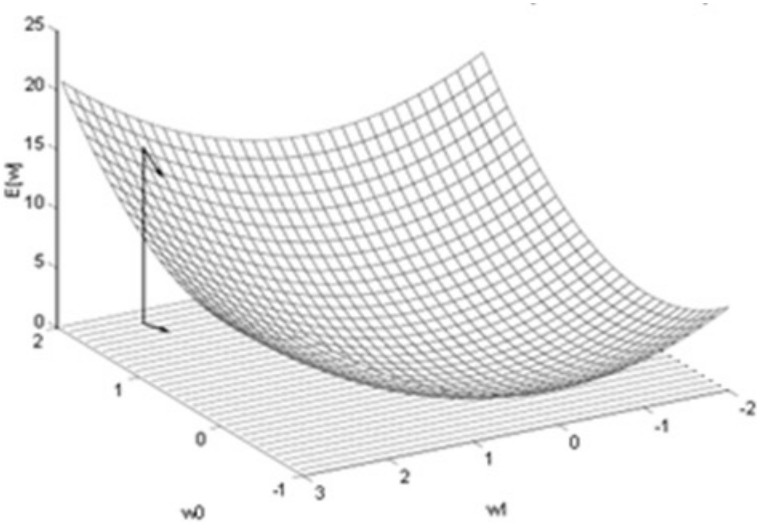
- Requirement: all the activation functions must be smoothed

Gradient descent: Illustration

One-dimensional space
E(w)



2-dimensional space
$E(w_1,w_2)$



Algorithm

Gradient_descent_incremental ($\mathbf{D}$, η)

Initialize $\mathbf{w}$ ($w_i \leftarrow$ an initial (small) random value)

do

for each training instance $(\mathbf{x}, d) \in \mathbf{D}$

Compute the network output

for each weight component w_i

$$w_i \leftarrow w_i - \eta(\partial E_{\mathbf{x}} / \partial w_i)$$

end for

end for

until (stopping criterion satisfied)

return $\mathbf{w}$

Stopping criterion: epochs, threshold error, ...

If we take a small *subset* (mini-batch) *randomly* from **D** to update the weights, we will have mini-batch training.

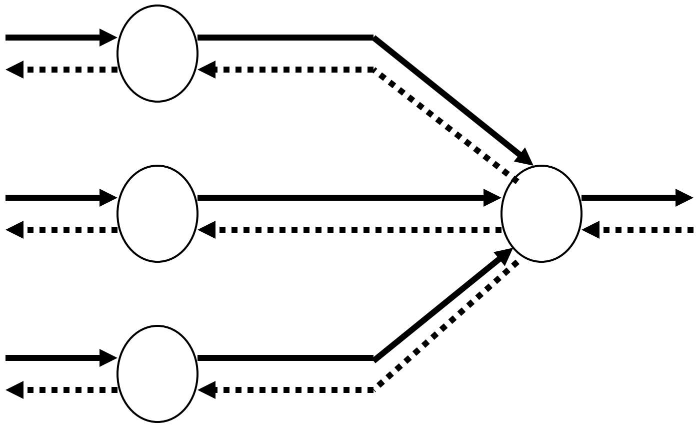
Backpropagation algorithm

- A perceptron can only represent a linear function
- A multi-layer NN learned by the **Backpropagation** (BP) algorithm can represent a highly non-linear function
- The BP algorithm is used to learn the weights of an ANN
  - Fixed network structure (một cấu trúc mạng đã chọn trước)
  - For each neuron, the activation function must be differentiable
- The BP algorithm applies a *gradient descent* strategy to the rules for updating weights
  - To minimize errors between actual output values and desired output values, for training data

Backpropagation algorithm (1)

- Back propagation algorithm seeks a vector of weights that minimizes the net errors on the training data
- The BP algorithm consists of 2 phases:
  - **Forward pass:** The input signals (input vector) are forwarded from the input layer to the output layer (passing through hidden layers).
  - **Error backward:**
    - Based on the desired output value of the input vector, calculate the error value
    - From the output layer, the error value is backward-propagated across the network, from a layer to previous layer, to the input layer.
    - Error back-propagation is executed by calculating (regressively) the local gradient values of each neuron

Backpropagation algorithm (2)



Signal forward phase:

- Forward signals via the network

Error backward phase:

- Calculate the error at the output
- Error back-propagation

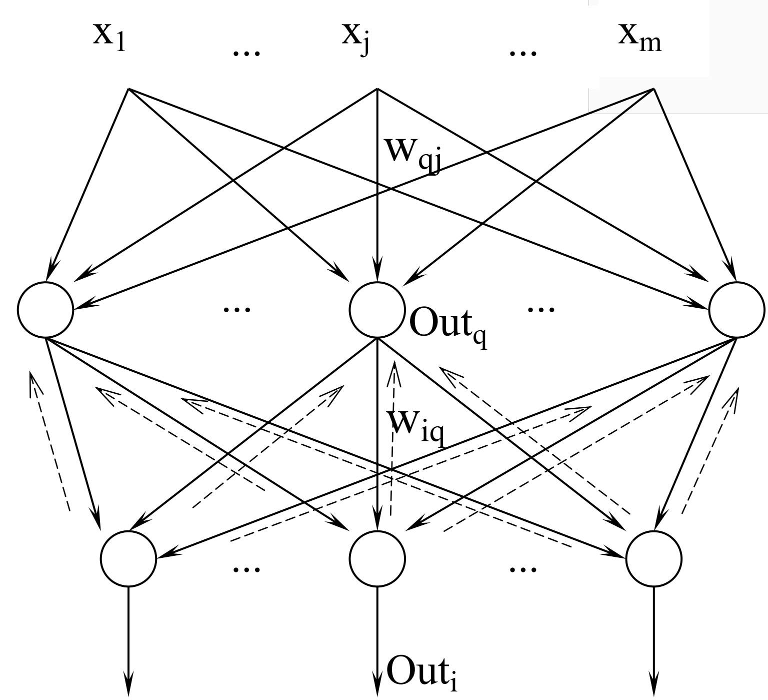
Network structure

- Consider the 3-layer neural network (in the figure) to illustrate the BP algorithm
- m input signals x_j (j=1..m)
- l hidden neurons z_q (q=1..l)
- n output neurons y_i (i=1..n)
- w_{qj} is the weight of the connection from the input signal x_j to the hidden neuron z_q

Input x_j (j=1..m)

Hidden neuron z_q (q=1..l)

Output neuron y_i (i=1..n)



- w_{iq} is the weight of the connection from the hidden neuron z_q to the output y_i
- Out_q is the (local) output value of the hidden neuron z_q
- Out_i is the output value of the network corresponding to the output neuron y_i

BP algorithm: Forward (1)

- For each data point **x**
  - Input vector **x** is forwarded from the input layer to the output layer
  - The network will generate an actual output value **Out** (a vector with value Out_i, i = 1..n)
- For an input vector **x**, a neuron z_q at the hidden layer receives the value of net input:

$$Net_q = \sum_{j=1}^{m} w_{qj} x_j$$

then produces a (local) output value

$$Out_q = f(Net_q) = f\left(\sum_{j=1}^{m} w_{qj} x_j\right)$$

where *f(.)* is a activation function of neuron z_q

BP algorithm: Forward (2)

- Net input value of the neuron y_i at the output layer

$$Net_i = \sum_{q=1}^{l} w_{iq} Out_q = \sum_{q=1}^{l} w_{iq} f\left(\sum_{j=1}^{m} w_{qj} x_j \right)$$

- Neuron y_i produces output value (is an output value of network)

$$Out_i = f(Net_i) = f\left(\sum_{q=1}^{l} w_{iq} Out_q \right) = f\left(\sum_{q=1}^{l} w_{iq} f\left(\sum_{j=1}^{m} w_{qj} x_j \right) \right)$$

- Vector of the output values Out_i (i=1..n) is the actual output value of the network, for the input vector **x**

BP algorithm: Backward (1)

- For each data point **x**
  - Error signals due to the difference between the desired output value d and the actual output value **Out** are calculated
  - These error signals are **back-propagated** from the output layer to the front layers, to update weights
- To consider the error signals and their back-propagated ones, an error function needs to be defined

$$E(w) = \frac{1}{2}\sum_{i=1}^{n}(d_i - Out_i)^2 = \frac{1}{2}\sum_{i=1}^{n}[d_i - f(Net_i)]^2$$

$$= \frac{1}{2}\sum_{i=1}^{n}\left[d_i - f\left(\sum_{q=1}^{l} w_{iq} Out_q\right)\right]^2$$

BP algorithm: Backward (2)

- According to the gradient-descent method, the weights of the connections from the hidden layer to the output layer are updated by

$$\Delta w_{iq} = -\eta \frac{\partial E}{\partial w_{iq}}$$

- Using the derivative chain rule for $\partial E/\partial w_{iq}$, we have

$$\Delta w_{iq} = -\eta \left[\frac{\partial E}{\partial Out_i}\right]\left[\frac{\partial Out_i}{\partial Net_i}\right]\left[\frac{\partial Net_i}{\partial w_{iq}}\right] = \eta [d_i - Out_i][f'(Net_i)][Out_q] = \eta \delta_i Out_q$$

- δ_i is **error signals** of neuron y_i at output layer

$$\delta_i = -\frac{\partial E}{\partial Net_i} = -\left[\frac{\partial E}{\partial Out_i}\right]\left[\frac{\partial Out_i}{\partial Net_i}\right] = [d_i - Out_i][f'(Net_i)]$$

where Net_i is the net input of the neuron y_i at the output layer, and $f'(Net_i)=\partial f(Net_i)/\partial Net_i$

BP algorithm: Backward (3)

- To update the weights of the connections from the input layer to the hidden layer, we also apply the gradient-descent method and the derivative chain rule

$$\Delta w_{qj} = -\eta \frac{\partial E}{\partial w_{qj}} = -\eta \left[\frac{\partial E}{\partial Out_q}\right]\left[\frac{\partial Out_q}{\partial Net_q}\right]\left[\frac{\partial Net_q}{\partial w_{qj}}\right]$$

- From the formula for calculating the error function E(**w**), we see that each error component (d_i-y_i) (i=1..n) is a function of Out_q

$$E(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{n}\left[d_i - f\left(\sum_{q=1}^{l} w_{iq} Out_q\right)\right]^2$$

BP algorithm: Backward (4)

- Apply the derivation chain rule, we have

$$\Delta w_{qj} = \eta \sum_{i=1}^{n} \left[\left(d_i - Out_i\right) f'\left(Net_i\right) w_{iq} \right] f'\left(Net_q\right) x_j$$

$$= \eta \sum_{i=1}^{n} \left[\delta_i w_{iq} \right] f'\left(Net_q\right) x_j = \eta \delta_q x_j$$

- δ_q is **error signals** of neuron z_q at hidden layer

$$\delta_q = -\frac{\partial E}{\partial Net_q} = -\left[\frac{\partial E}{\partial Out_q}\right]\left[\frac{\partial Out_q}{\partial Net_q}\right] = f'\left(Net_q\right) \sum_{i=1}^{n} \delta_i w_{iq}$$

where Net_g is the net input of the neuron z_q at the hidden layer, and $f'(Net_q)=\partial f(Net_q)/\partial Net_q$

BP algorithm: Backward (5)

- According to the formulas for calculating the error signals δ_i and δ_q, the error signal of a neuron in the hidden layer is different from the error signal of a neuron in the output layer
- Because of this difference, the weight update procedure in BP algorithm is also known as general **delta learning rule**
- Error signals δ_q of neuron z_q at hidden layer determined by:
  - Error signals δ_i of neuron y_i at output layer (to which neuron z_q are connected)
  - The weights w_{iq}

BP algorithm: Backward (6)

- The process of calculating the error signals as above can be extended (generalized) easily for neural networks with more than 1 hidden layer
- The general form of the weighting update rule in BP algorithm

$$\Delta w_{ab} = \eta \delta_a x_b$$

  - b and a are 2 indices corresponding to the two ends of the connection (b → a) (from a neuron (or input signal) b to neuron a)
  - $\boldsymbol{x}_b$ is the output value of the neuron at the hidden layer (or input signal) b
  - δ_a is error signal of neuron a

BP algorithm

Back_propagation_incremental(D, η)

Neural network consists of Q layer, $q = 1,2,...,Q$

$^{q}Net_i$ and $^{q}Out_i$ are net input and output value of neuron i at the layer q

Network has m input signals and n output neuron

$^{q}w_{ij}$ is the weight of the connection from neuron j at the layer $(q-1)$ to the neuron i at the layer q

Step 0 (Initialization)

Select the error threshold $E_{threshold}$ (the error value is acceptable)

Initialize the initial value of the weights with random small values

Assign E=0

Step 1 (Start a training cycle)

Apply the input vector of the data point k to the input layer (q=1)

$^{q}Out_i = {}^{1}Out_i = x_i^{(k)}, \forall i$

Step 2 (Forward)

Forward the input signals over the network, until the network output values (at the output layer) are received $^{Q}Out_i$

$$^{q}Out_i = f\left(^{q}Net_i\right) = f\left(\sum_j {}^{q}w_{ij}\, {}^{q-1}Out_j\right)$$

BP algorithm

Step 3 (Calculate the output error)

Calculate network output error and error signal ${}^{Q}\delta_i$ of each neuron at output layer

$$E = E + \frac{1}{2}\sum_{i=1}^{n}(d_i^{(k)} - {}^{Q}Out_i)^2$$

$${}^{Q}\delta_i = (d_i^{(k)} - {}^{Q}Out_i)f'({}^{Q}Net_i)$$

Step 4 (Error backward)

Backpropagation the error to update the weights and calculate the error signals ${}^{q-1}\delta_i$ for the front layers

$$\Delta^{q}w_{ij} = \eta.({}^{q}\delta_i).({}^{q-1}Out_j); \qquad {}^{q}w_{ij} = {}^{q}w_{ij} + \Delta^{q}w_{ij}$$

$${}^{q-1}\delta_i = f'({}^{q-1}Net_i)\sum_j {}^{q}w_{ji}\,{}^{q}\delta_j; \quad \text{for all } q = Q, Q-1, \ldots, 2$$

Step 5 (Check stopping criterion satisfied)

Check if the entire training data has been used yet

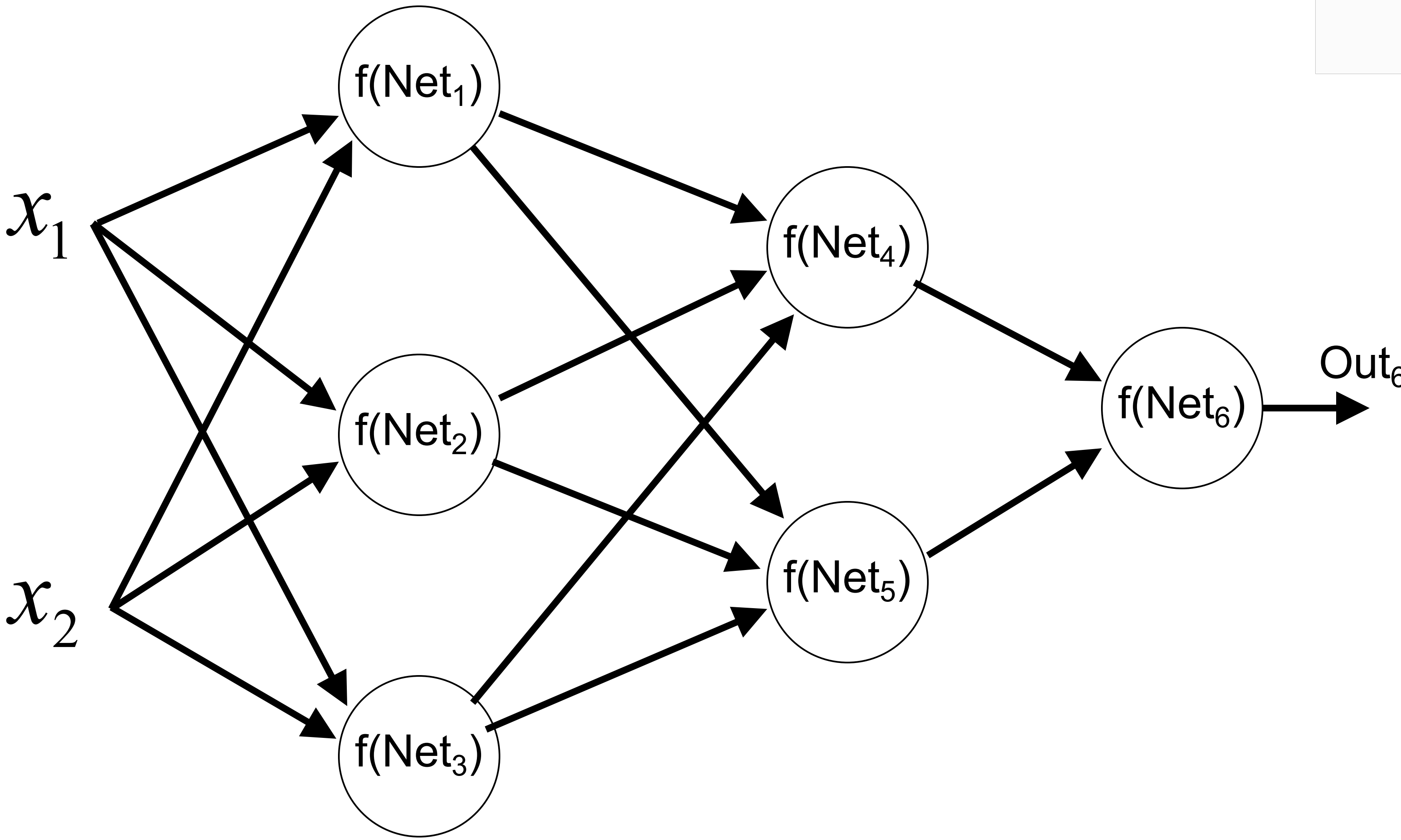
If the entire training data has used, go to Step 6, otherwise go to Step 1

Step 6 (Check net error)

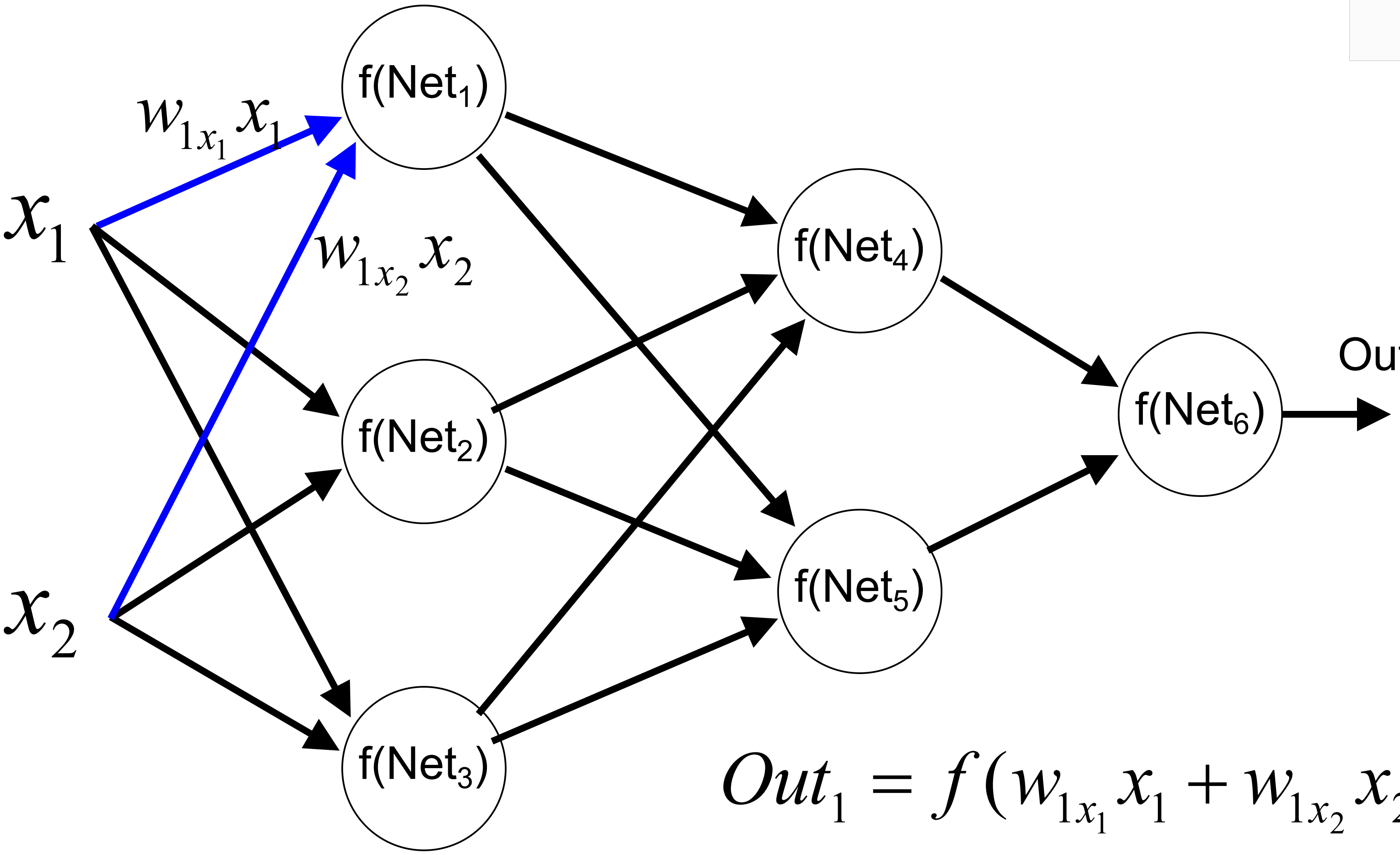
If net error E is less than the acceptable threshold ($<E_{threshold}$), then training is completed and returns the learned weights;

otherwise, assign E=0, and start new training cycle (go back to Step 1)

BP algorithm: Forward (1)

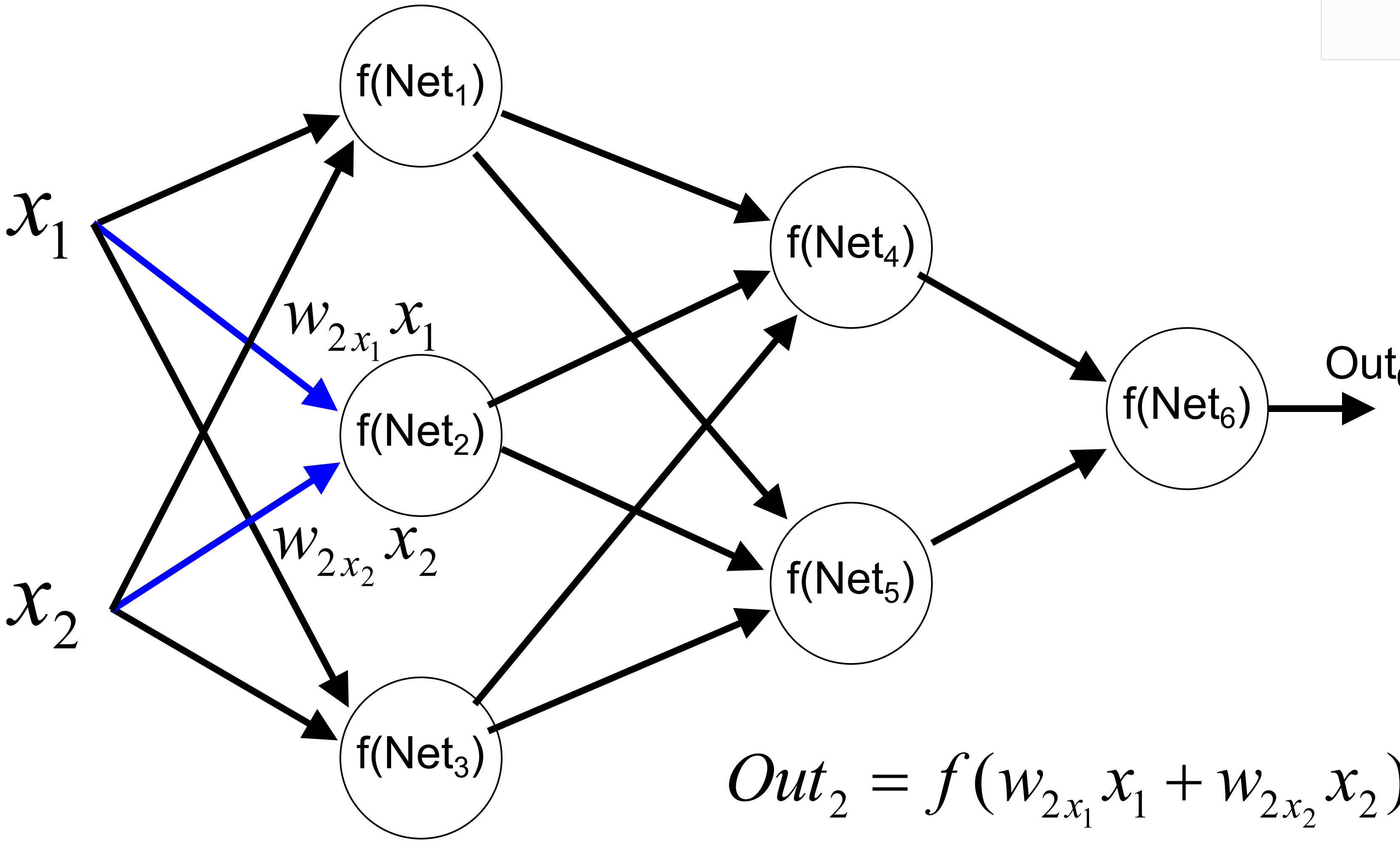


BP algorithm: Forward (2)



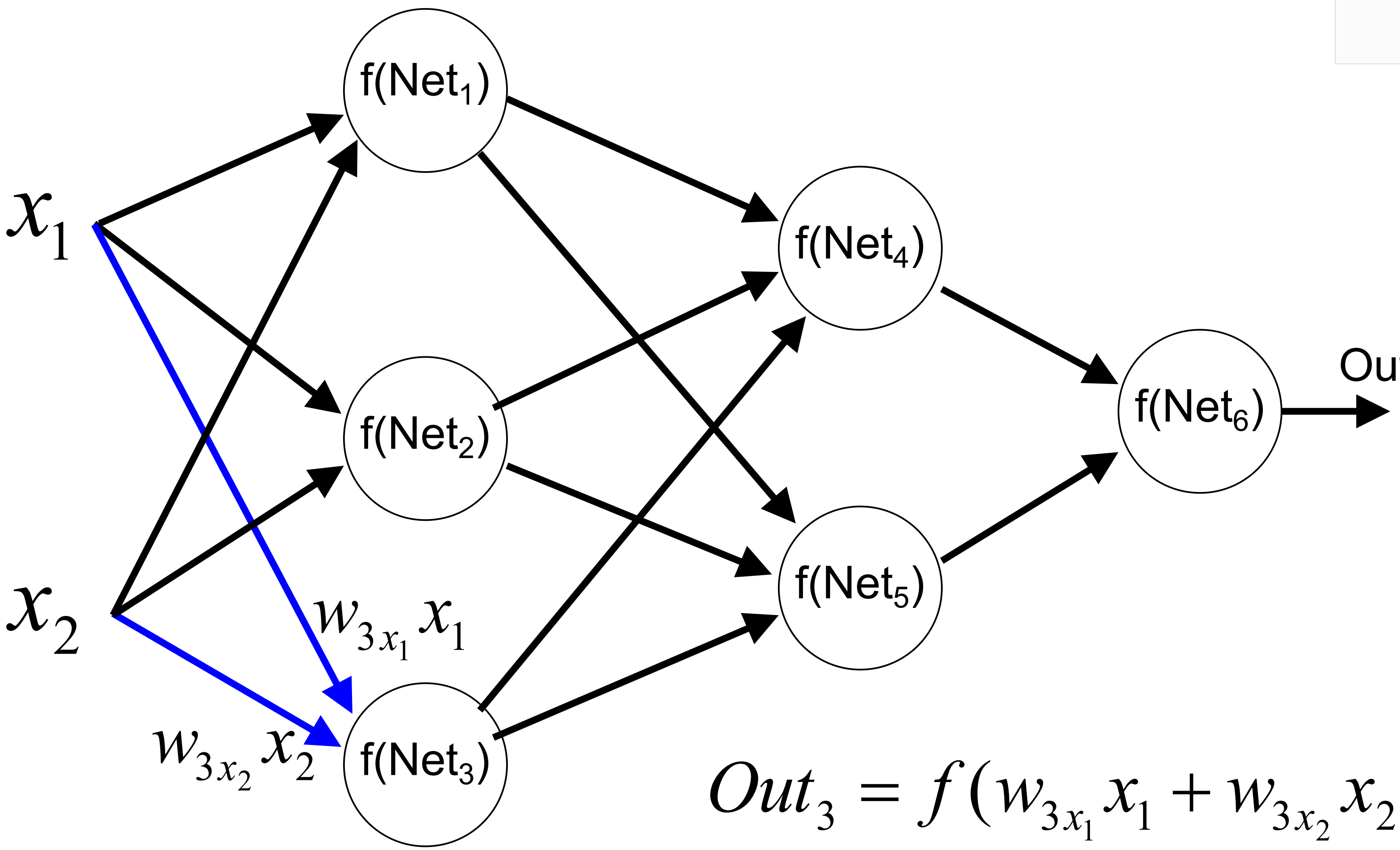
$$Out_1 = f(w_{1x_1}x_1 + w_{1x_2}x_2)$$

BP algorithm: Forward (3)



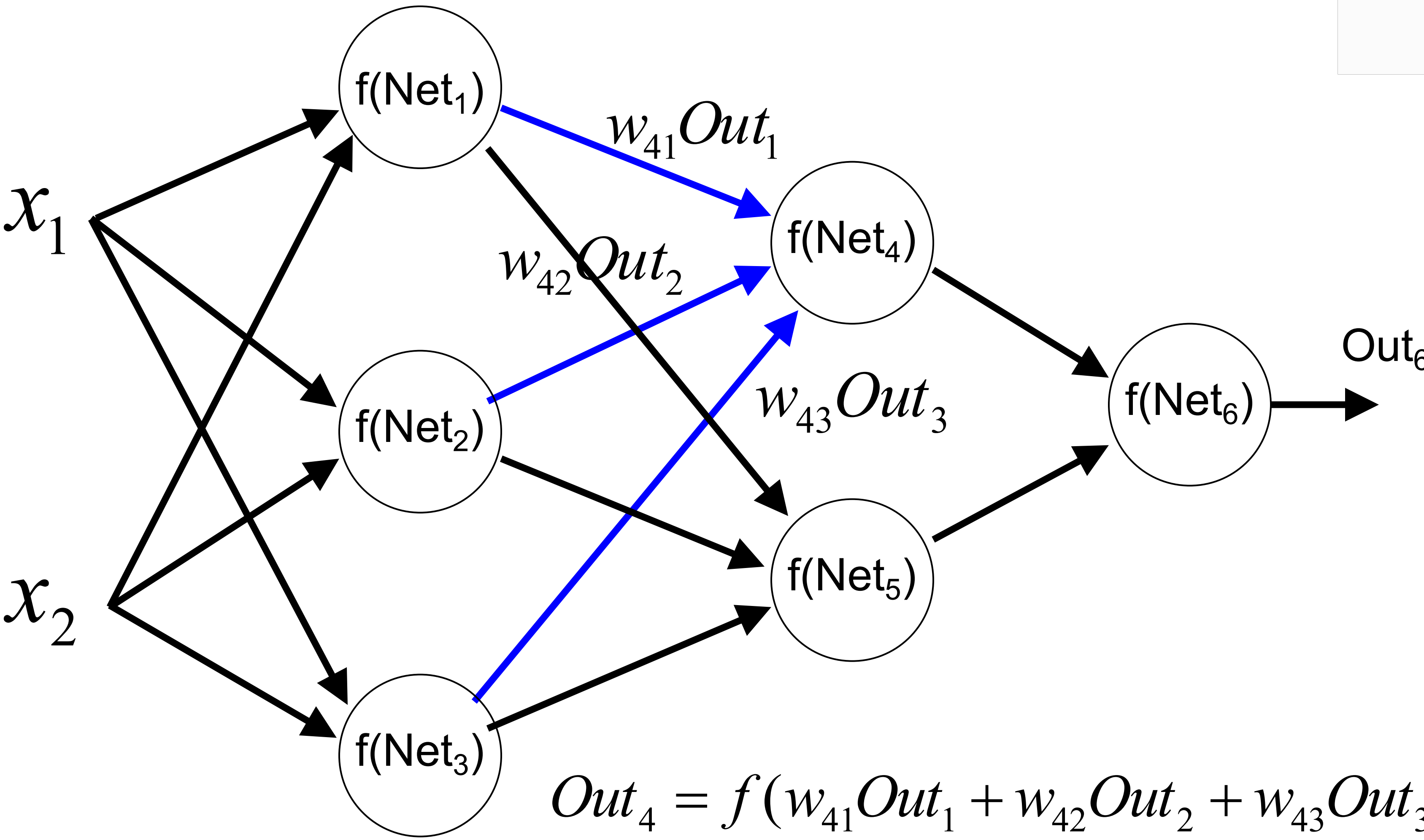
$$Out_2 = f(w_{2x_1}x_1 + w_{2x_2}x_2)$$

BP algorithm: Forward (4)



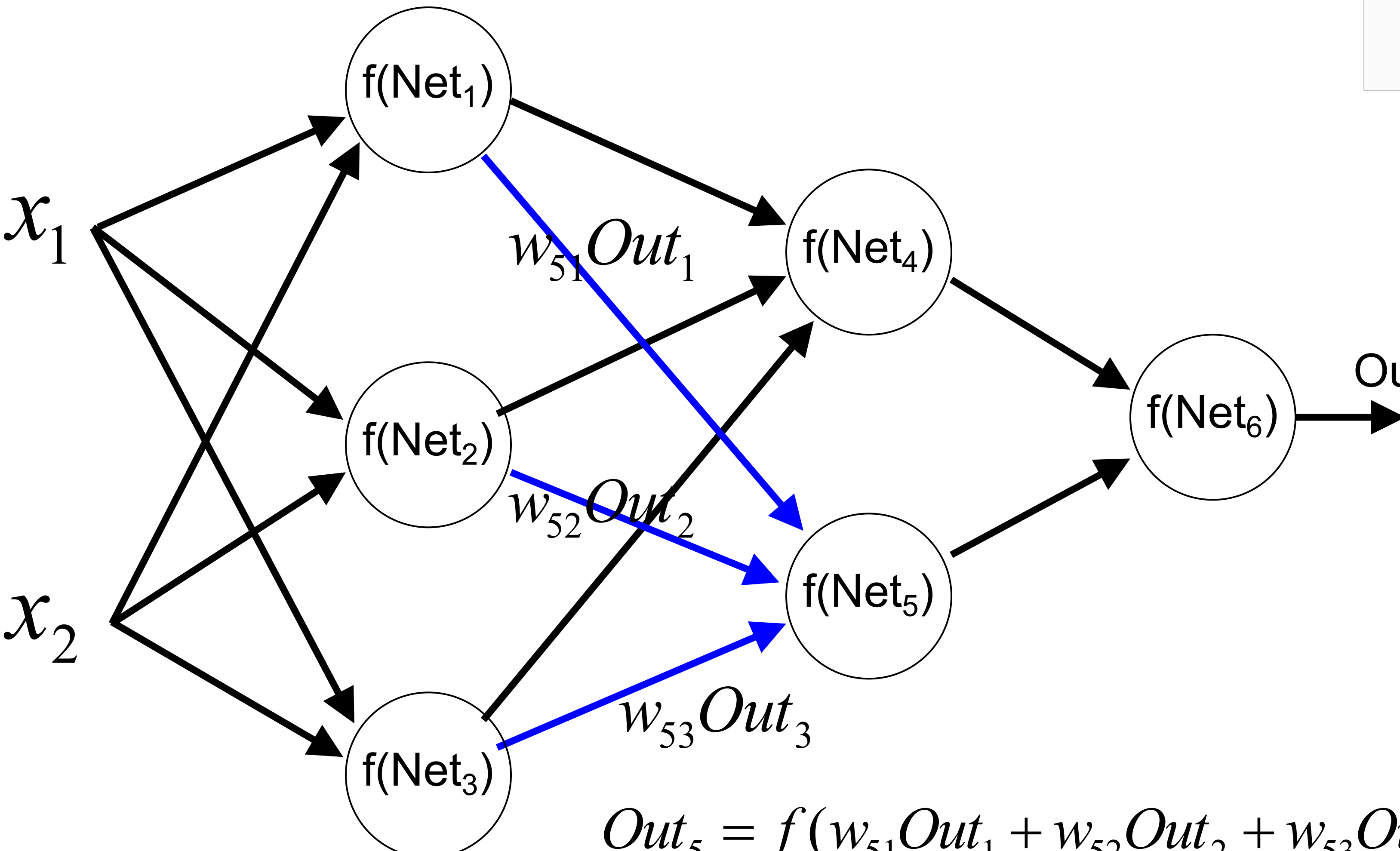
$$Out_3 = f(w_{3x_1}x_1 + w_{3x_2}x_2)$$

BP algorithm: Forward (5)



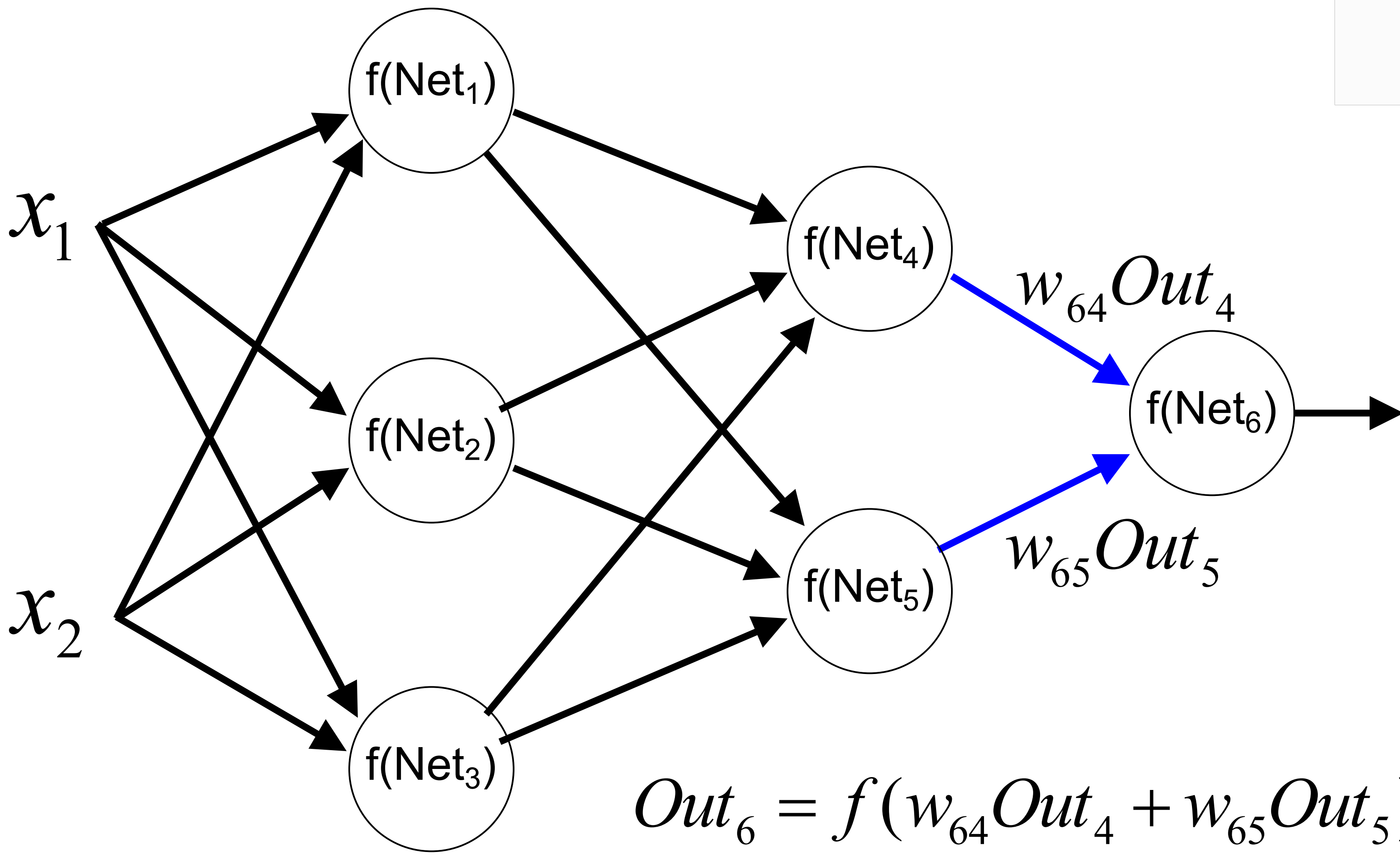
$$Out_4 = f(w_{41}Out_1 + w_{42}Out_2 + w_{43}Out_3)$$

BP algorithm: Forward (6)



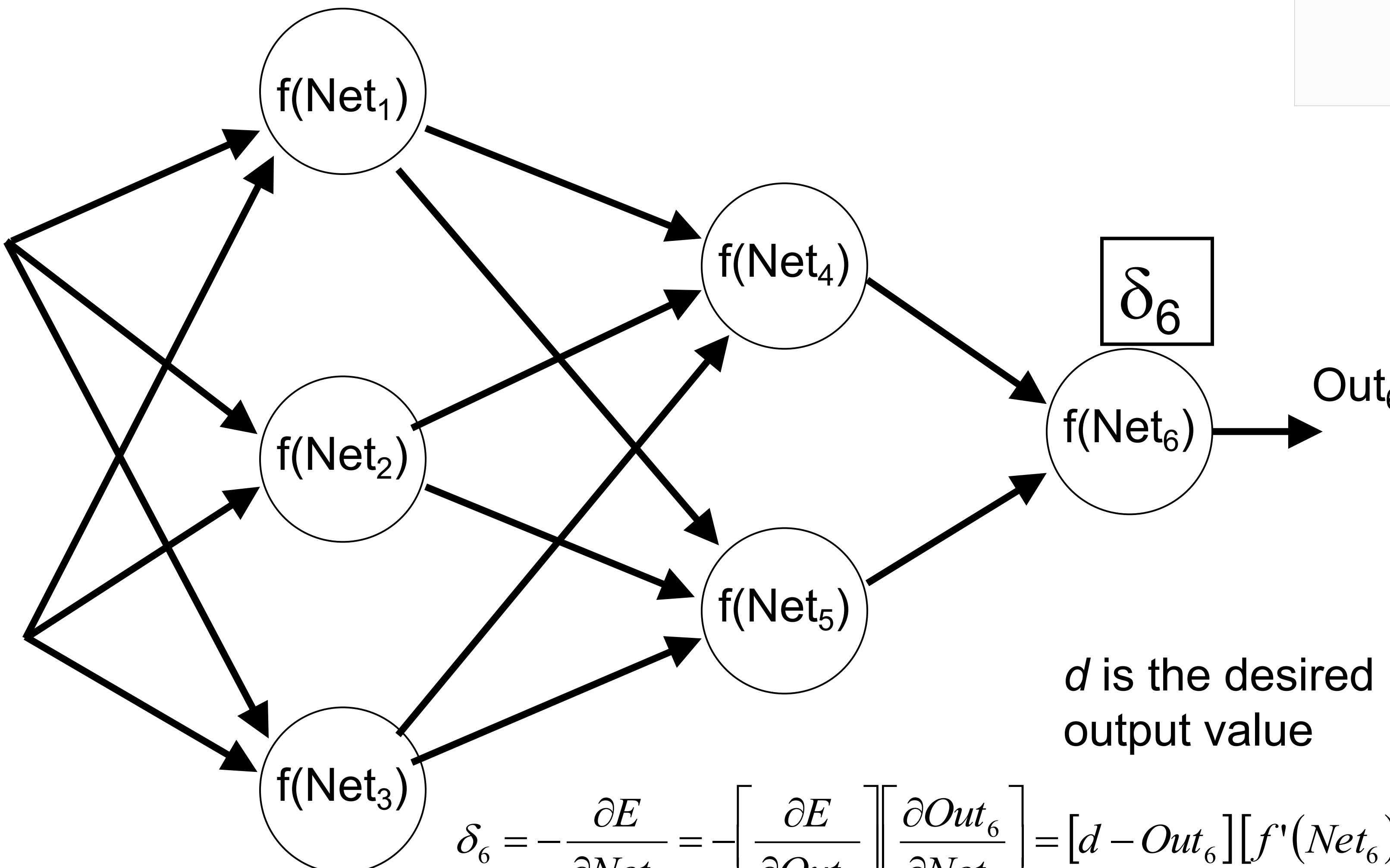
$$Out_5 = f(w_{51}Out_1 + w_{52}Out_2 + w_{53}Out_3)$$

BP algorithm: Forward (7)



$$Out_6 = f(w_{64}Out_4 + w_{65}Out_5)$$

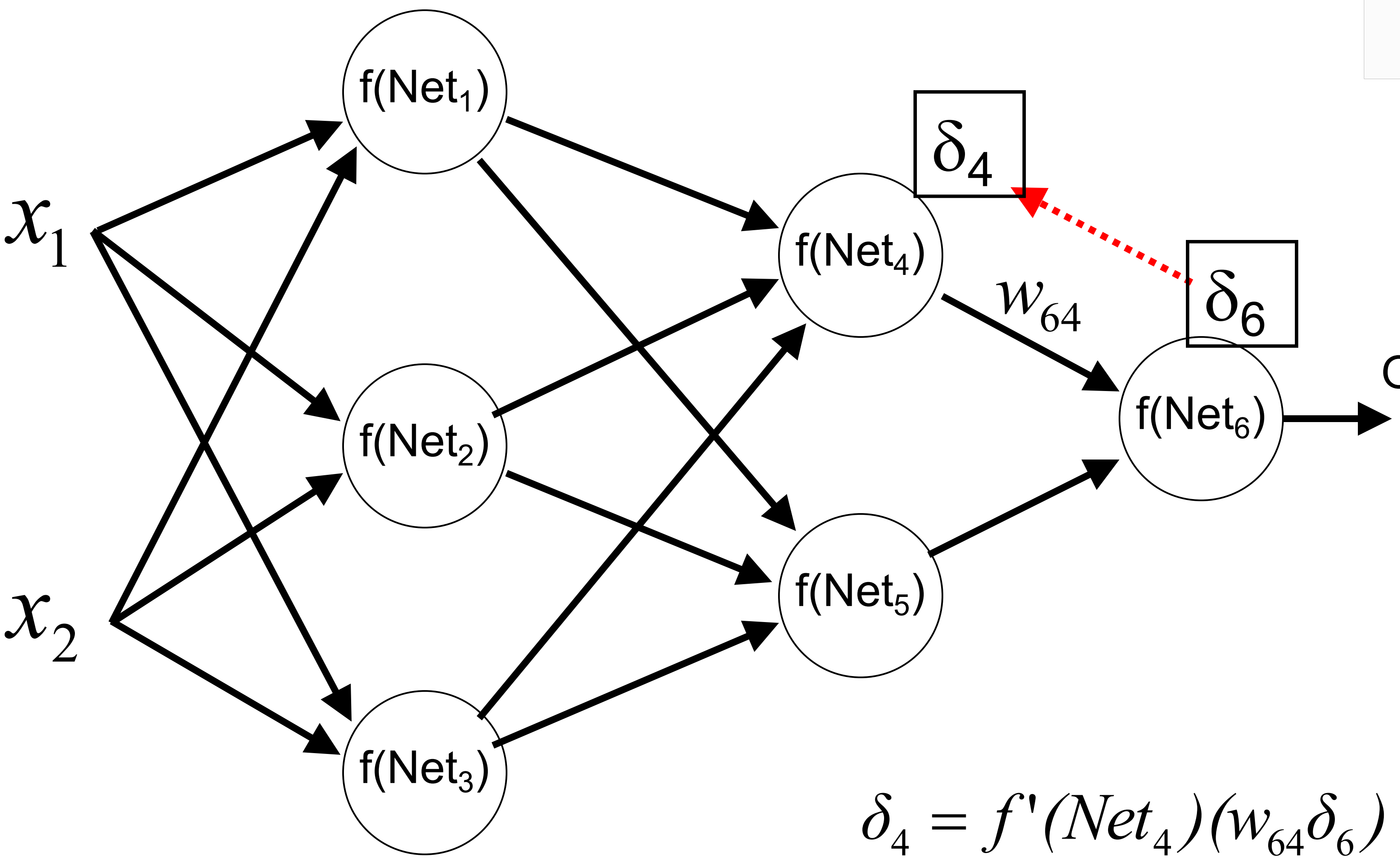
BP algorithm: Calculate error



d is the desired output value

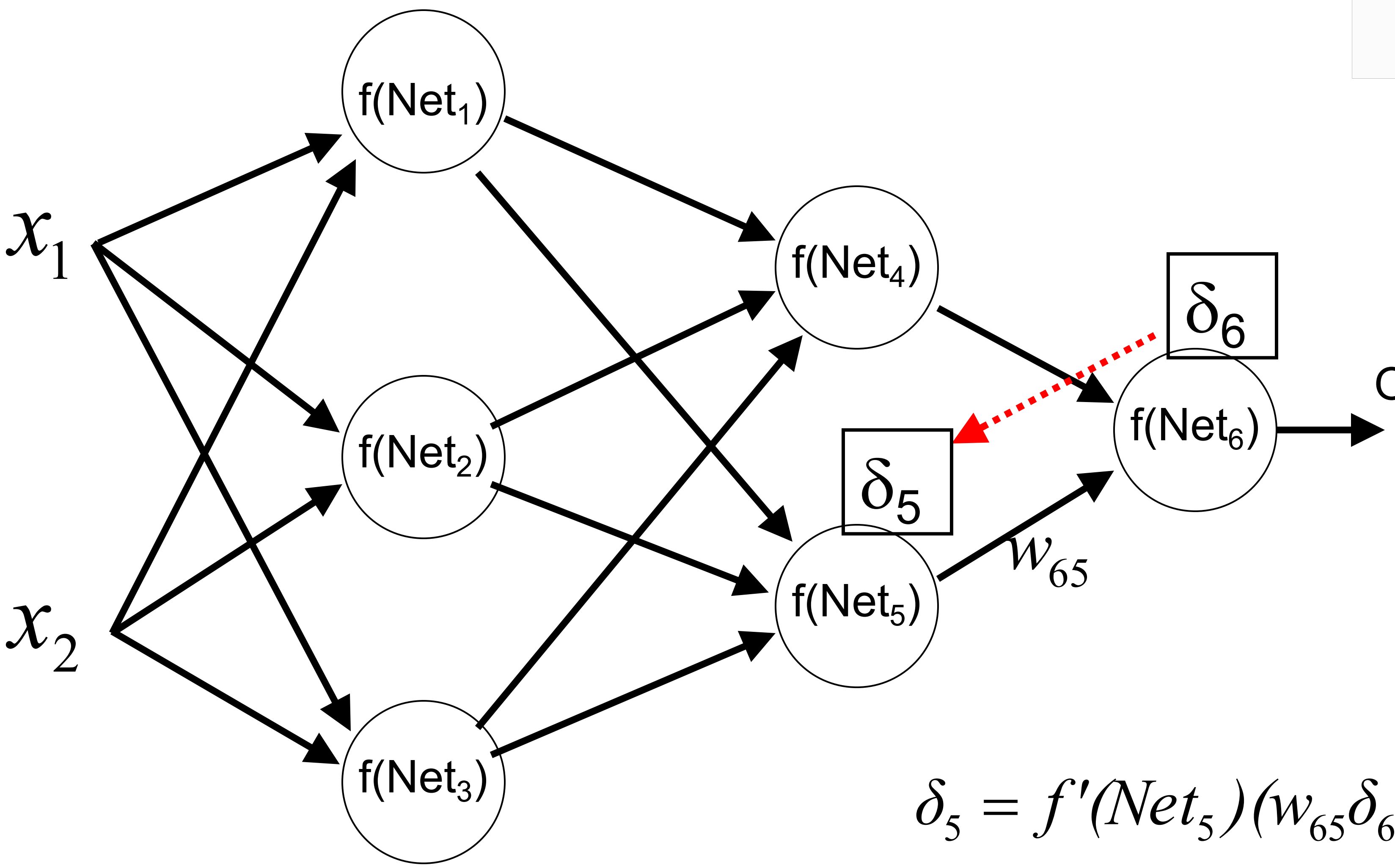
$$\delta_6 = -\frac{\partial E}{\partial Net_6} = -\left[\frac{\partial E}{\partial Out_6}\right]\left[\frac{\partial Out_6}{\partial Net_6}\right] = [d - Out_6][f'(Net_6)]$$

BP algorithm: Backward(1)



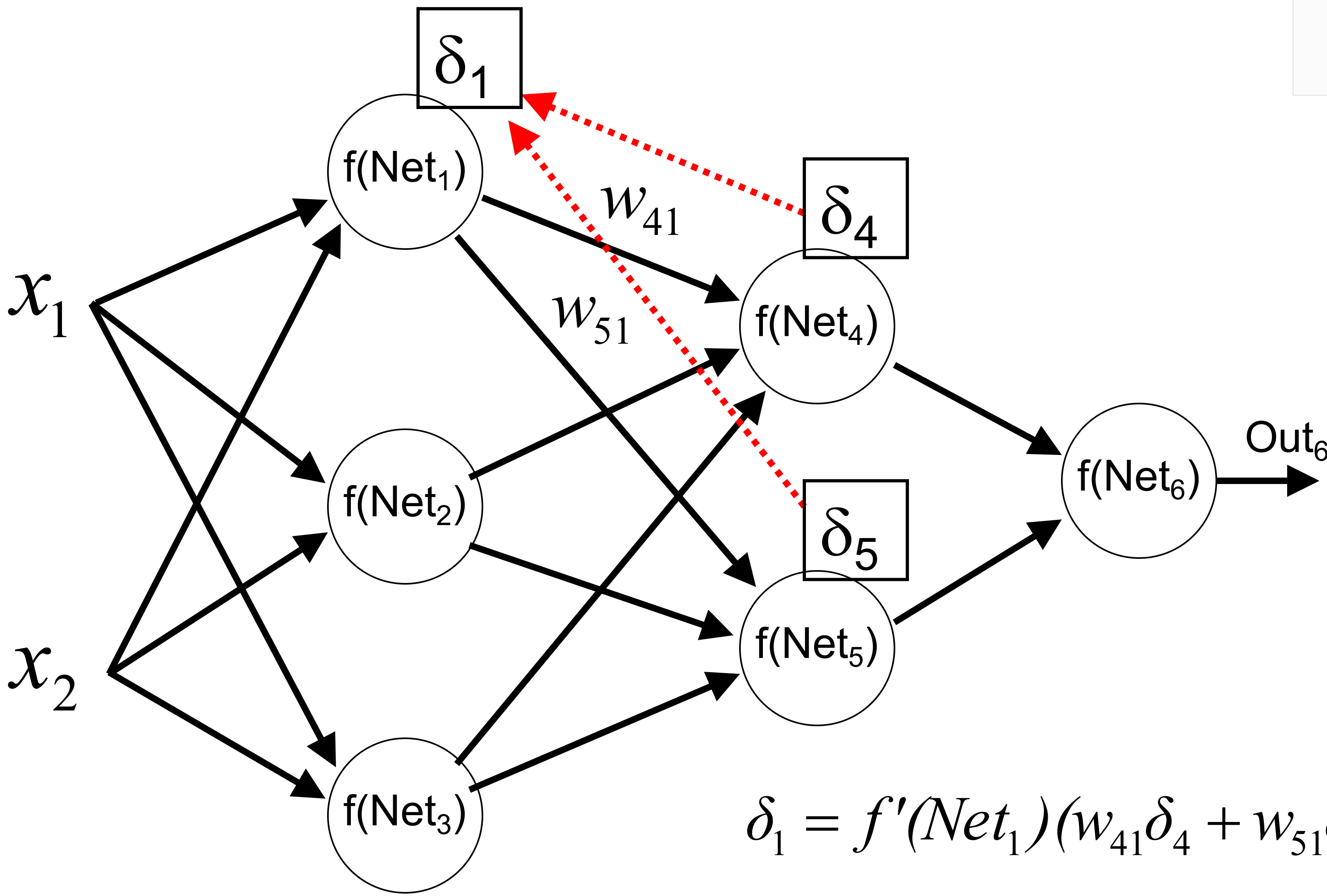
$$\delta_4 = f'(Net_4)(w_{64}\delta_6)$$

BP algorithm: Backward(2)



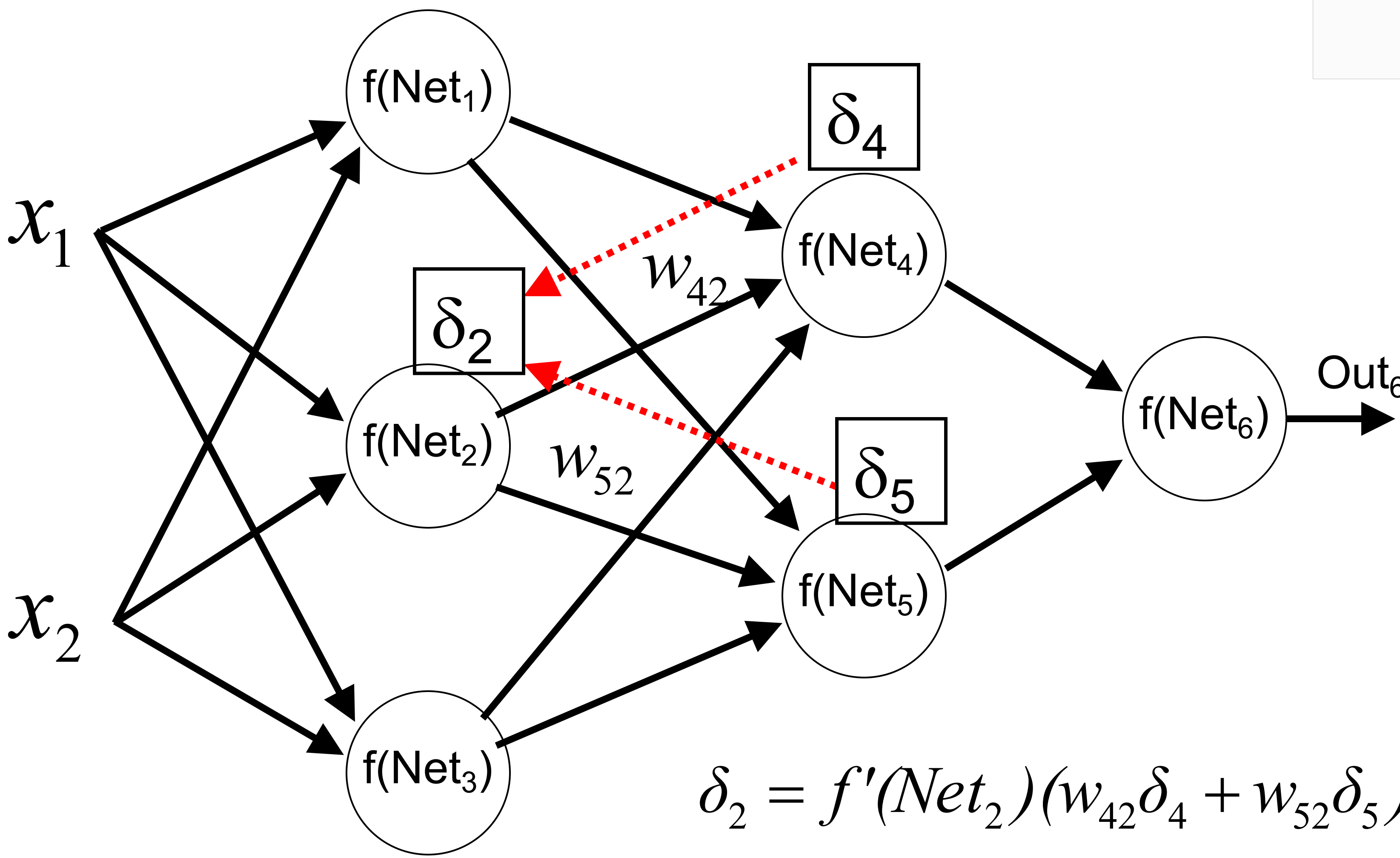
$$\delta_5 = f'(Net_5)(w_{65}\delta_6)$$

BP algorithm: Backward(3)



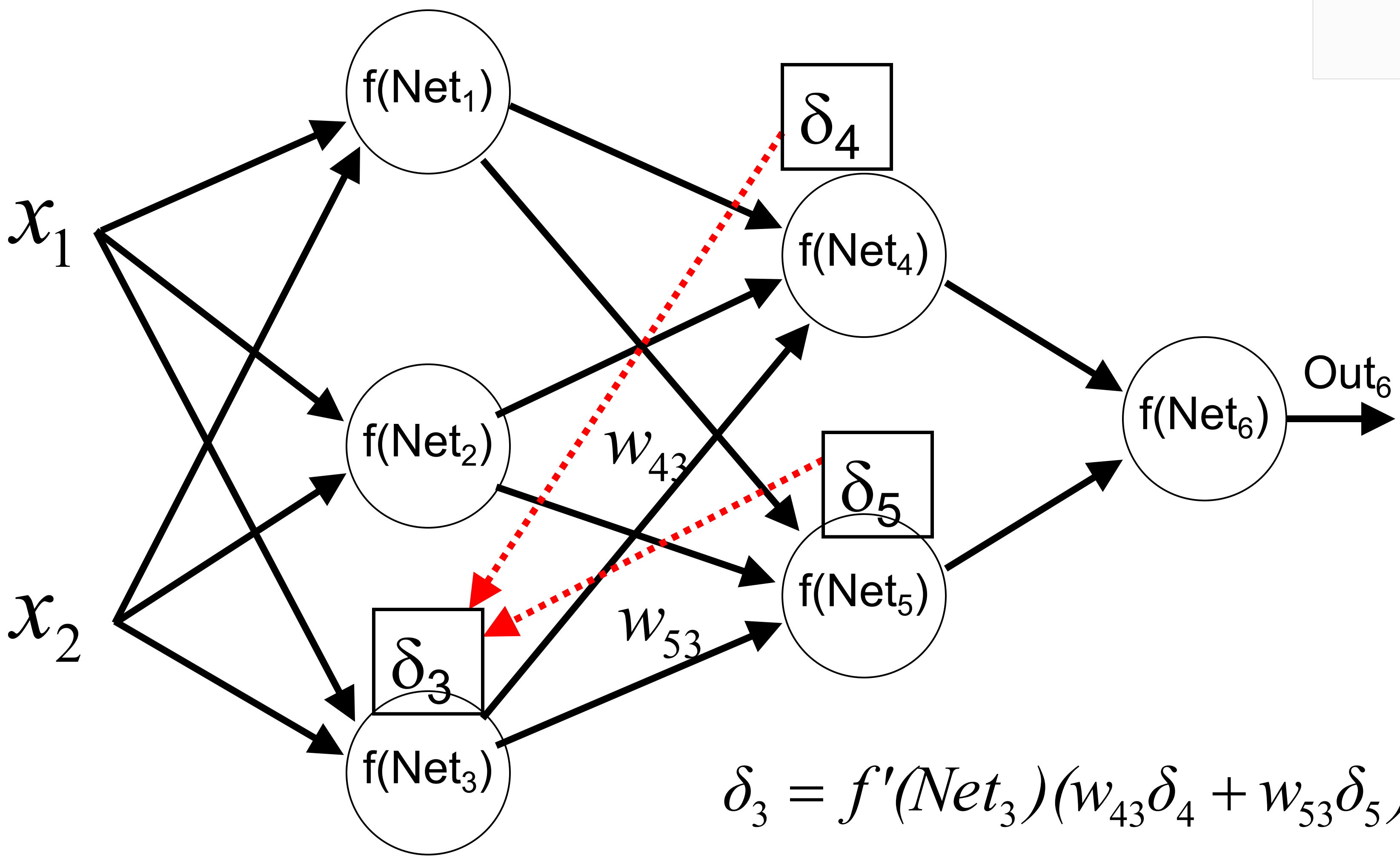
$$\delta_1 = f'(Net_1)(w_{41}\delta_4 + w_{51}\delta_5)$$

BP algorithm: Backward(4)



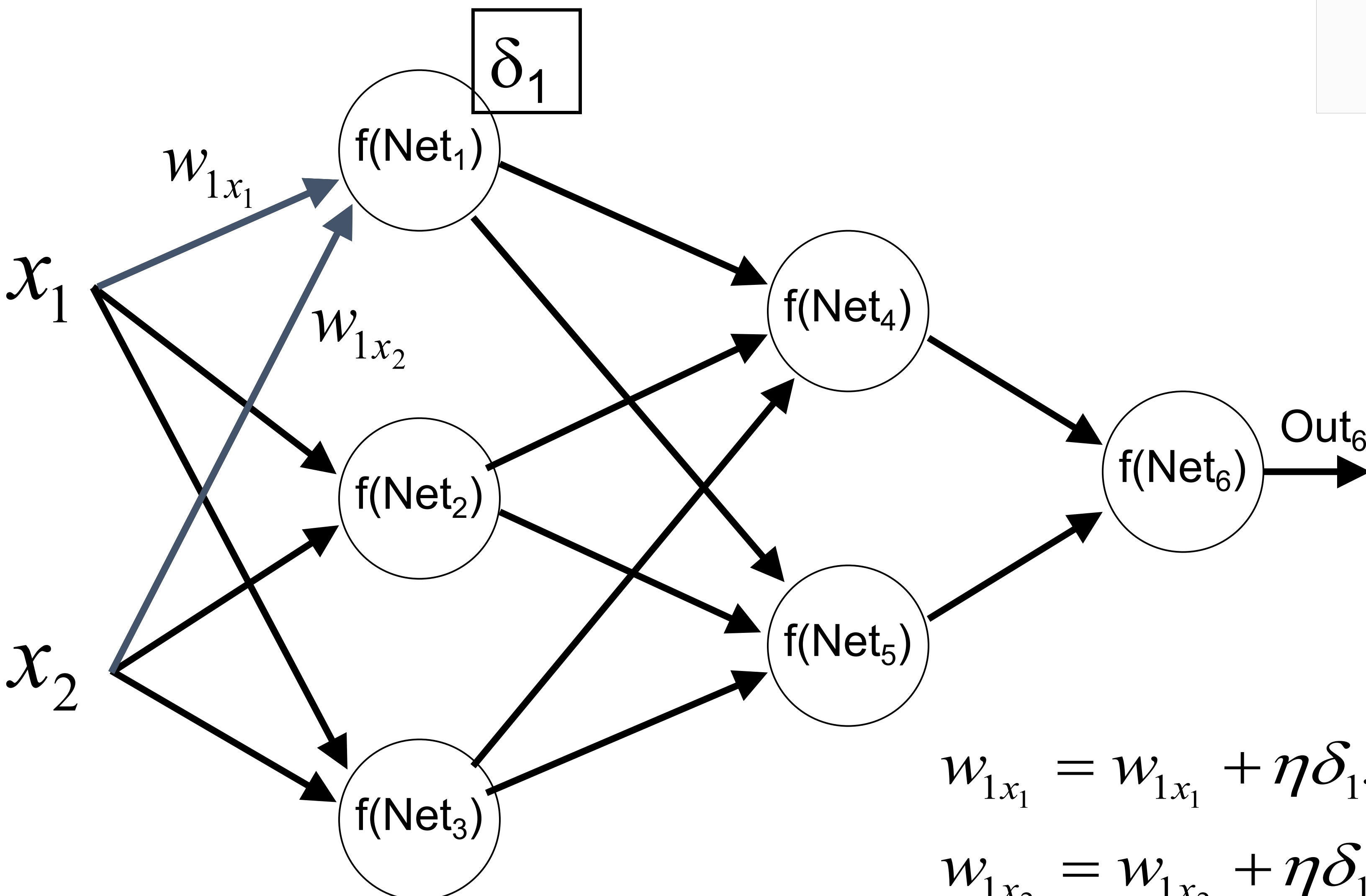
$$\delta_2 = f'(Net_2)(w_{42}\delta_4 + w_{52}\delta_5)$$

BP algorithm: Backward(5)



$$\delta_3 = f'(Net_3)(w_{43}\delta_4 + w_{53}\delta_5)$$

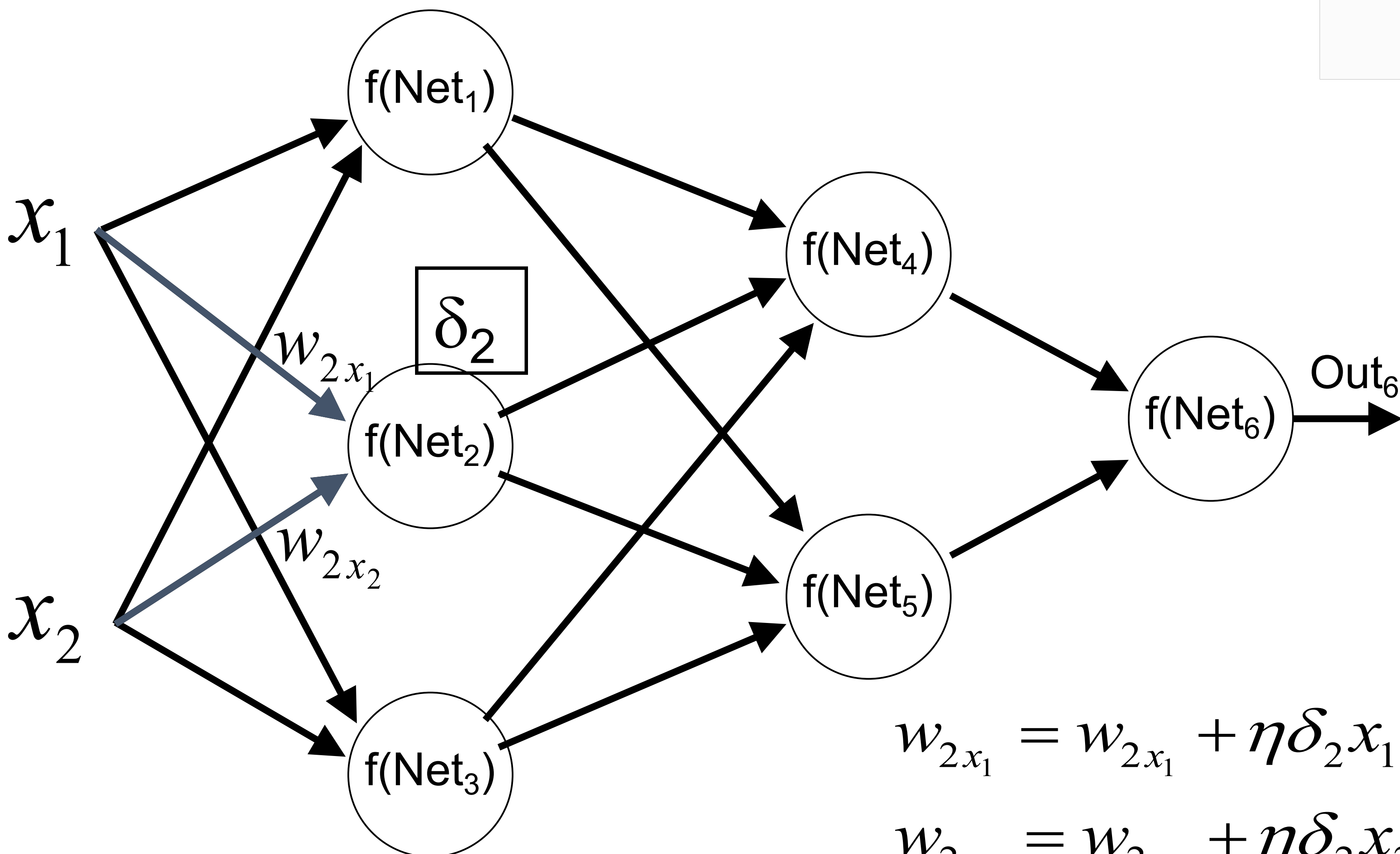
BP algorithm: Update weight(1)



$$w_{1x_1} = w_{1x_1} + \eta\delta_1 x_1$$

$$w_{1x_2} = w_{1x_2} + \eta\delta_1 x_2$$

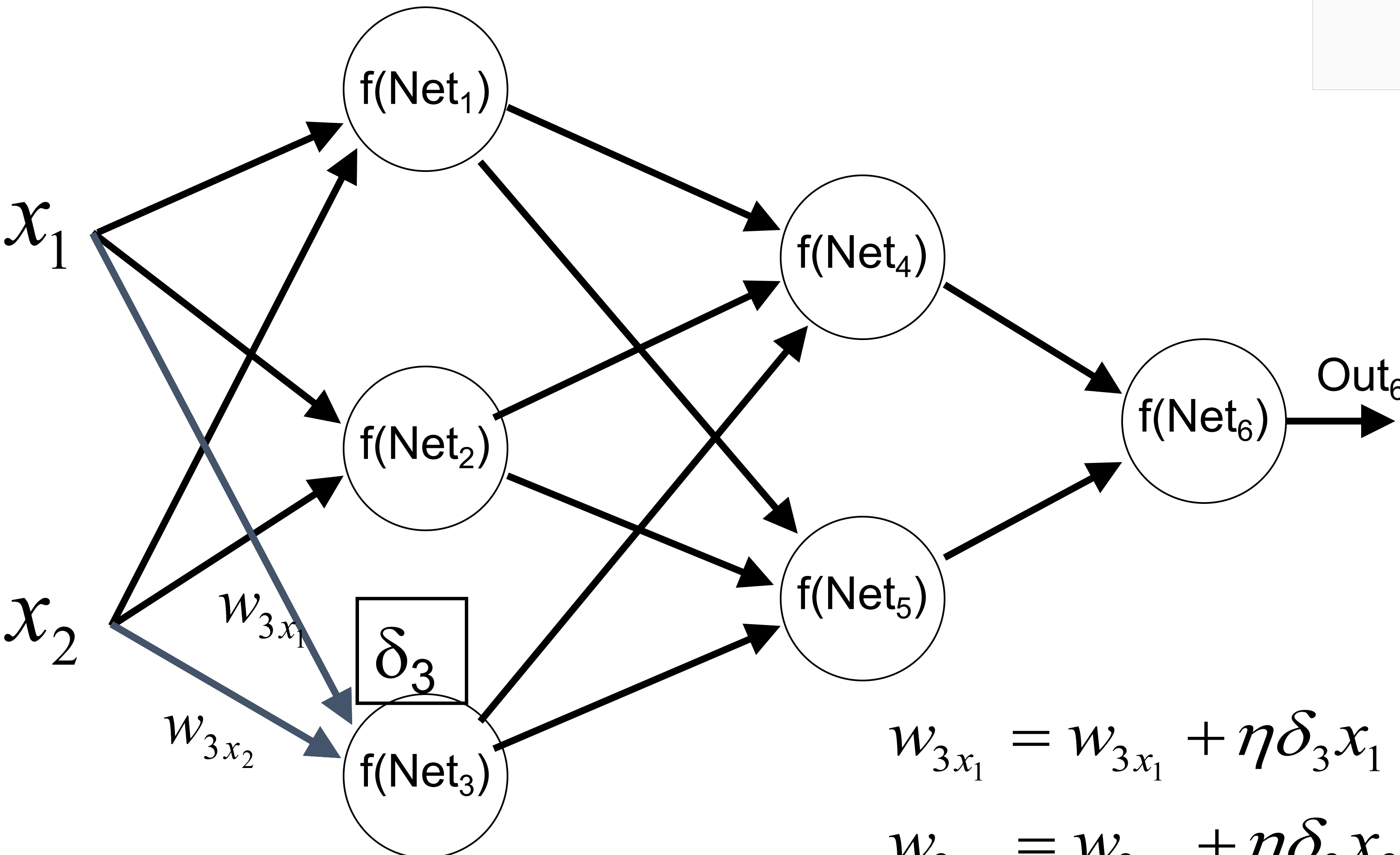
BP algorithm: Update weight(2)



$$w_{2x_1} = w_{2x_1} + \eta\delta_2 x_1$$

$$w_{2x_2} = w_{2x_2} + \eta\delta_2 x_2$$

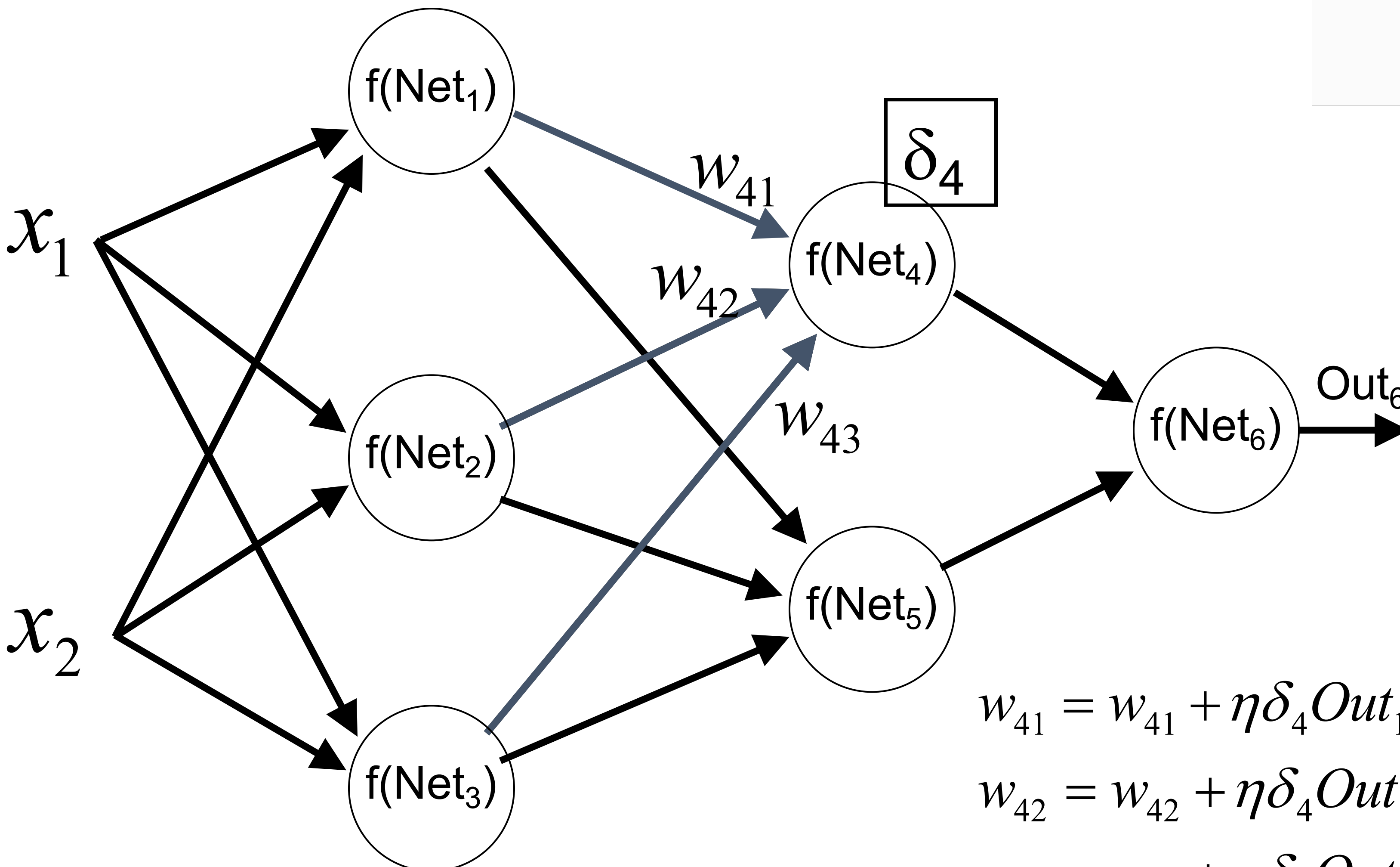
BP algorithm: Update weight(3)



$$w_{3x_1} = w_{3x_1} + \eta \delta_3 x_1$$

$$w_{3x_2} = w_{3x_2} + \eta \delta_3 x_2$$

BP algorithm: Update weight(4)

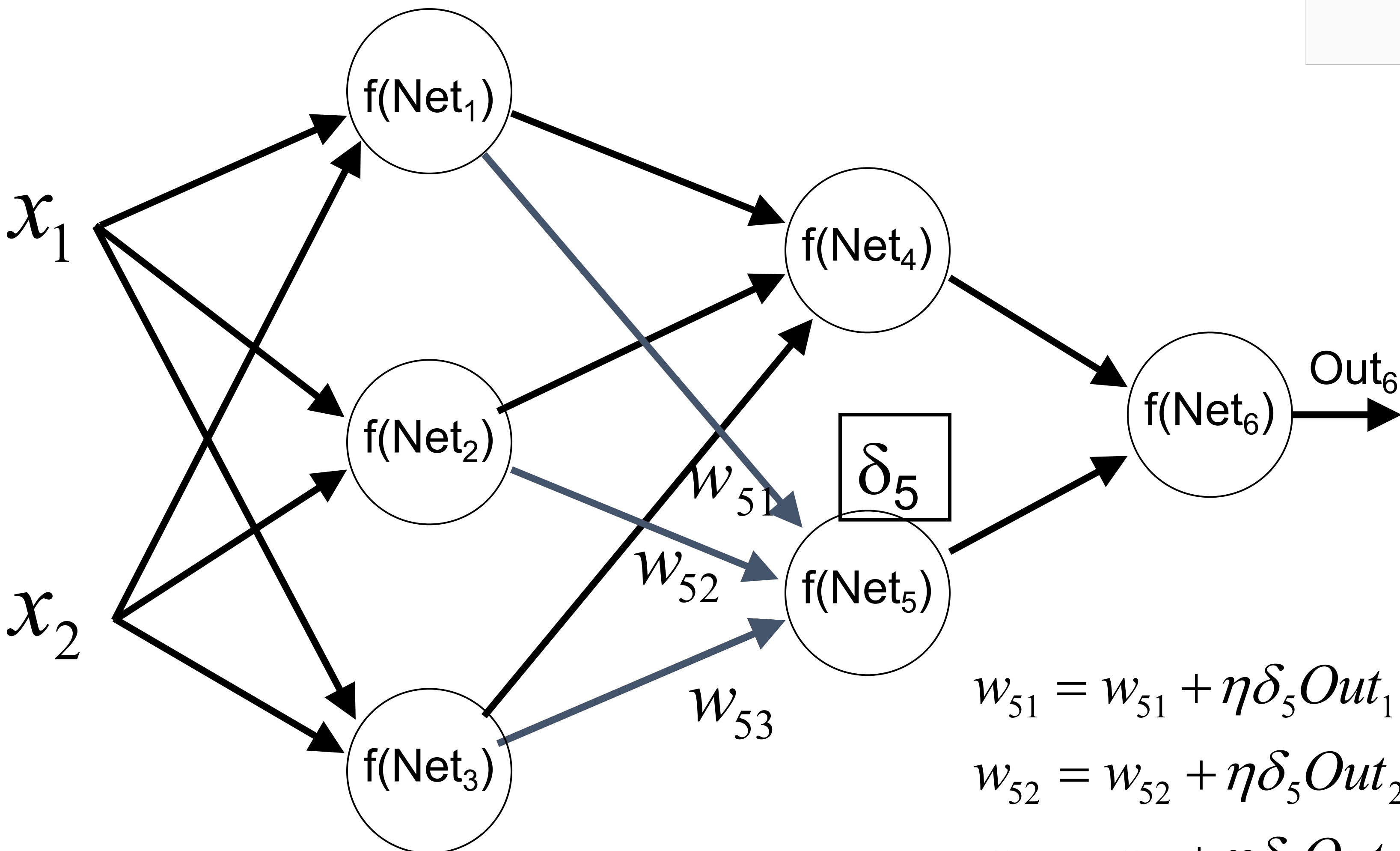


$$w_{41} = w_{41} + \eta\delta_4 Out_1$$

$$w_{42} = w_{42} + \eta\delta_4 Out_2$$

$$w_{43} = w_{43} + \eta\delta_4 Out_3$$

BP algorithm: Update weight(5)

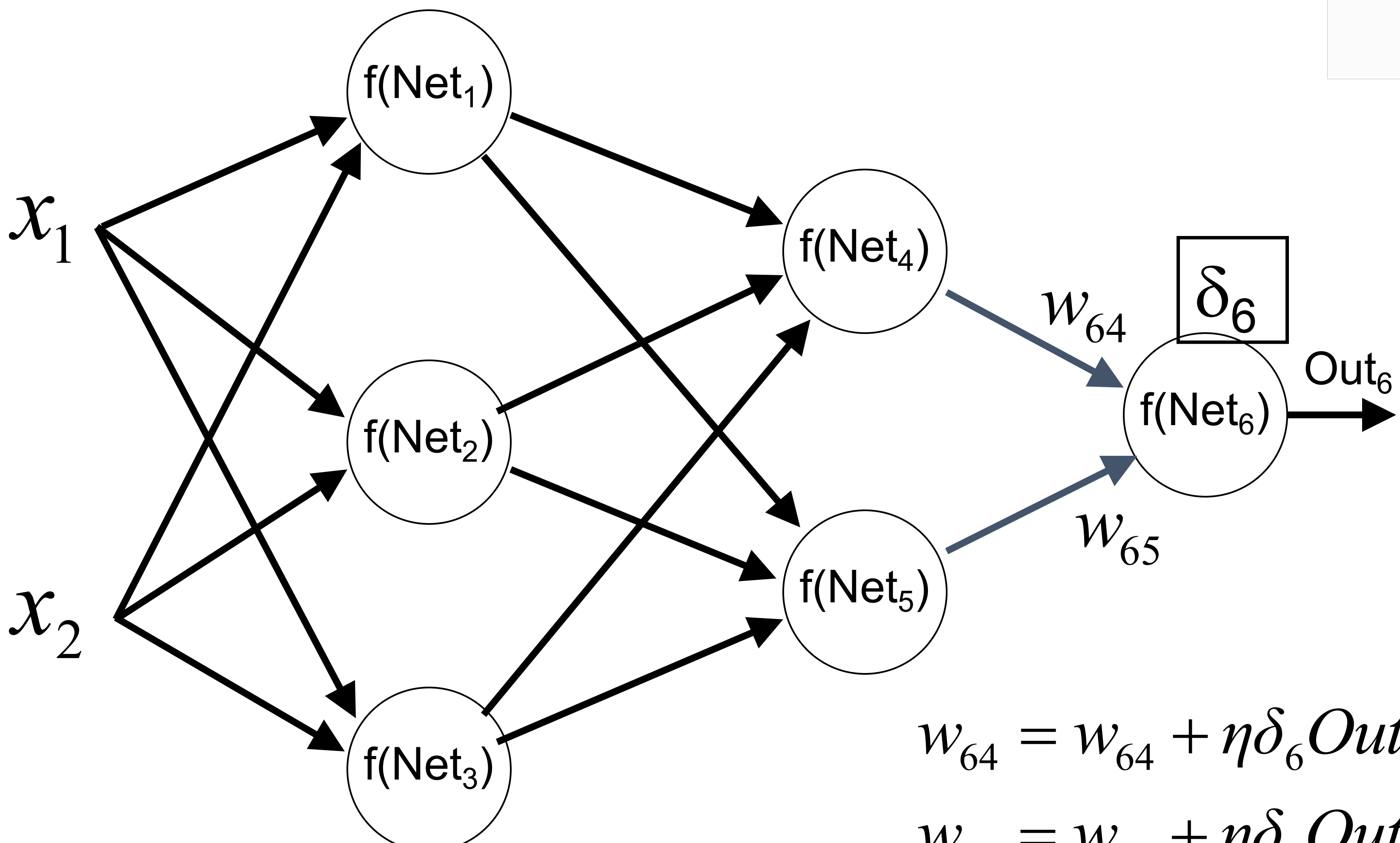


$$w_{51} = w_{51} + \eta\delta_5 Out_1$$

$$w_{52} = w_{52} + \eta\delta_5 Out_2$$

$$w_{53} = w_{53} + \eta\delta_5 Out_3$$

BP algorithm: Update weight(6)



$$w_{64} = w_{64} + \eta \delta_6 Out_4$$

$$w_{65} = w_{65} + \eta \delta_6 Out_5$$

BP algorithm: Initialize weights

- Normally, weights are initialized with random small values
- If the weights have large initial values
  - Sigmoid functions will reach saturation soon
  - The system will deadlock at a saddle / stationary points

BP algorithm: Learning rate

- Important effect on the efficiency and convergence of BP algorithm
  - A large value of η can accelerate the convergence of the learning process, but can cause the system to ignore the global optimal point or focus on bad points (saddle points).
  - A small η value can make the learning process take a long time
- Often select it empirically
- Good values of learning rate at the beginning (learning process) may not be good at a later time
  - Using an adaptive (dynamic) learning rate?

BP algorithm: Momentum

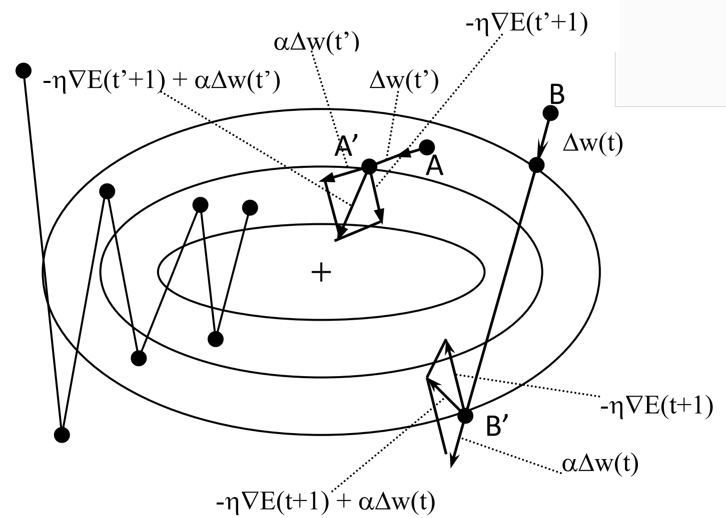
- The gradient descent method can be very slow if η is small and can fluctuate greatly if η is too large
- To reduce the level of fluctuations, it is necessary to add a momentum component

$$\Delta w^{(t)} = -\eta \nabla E^{(t)} + \alpha \Delta w^{(t-1)}$$

- where α ($\in$[0,1]) is a momentum parameter (usually assign = 0.9)
- We should choose reasonable values for learning rate and satisfying momentum

$$(\eta + \alpha) \gtrsim 1$$

where $\alpha > \eta$ to avoid fluctuations



Gradient descent for a simple square error function.

The left trajectory does not use momentum.

The right trajectory uses momentum.

BP algorithm: Number of neurons

- The size (number of neurons) of the hidden layer is an important question for the application of multi-layer neural network to solve practical problems
- In fact, it is difficult to identify the exact number of neurons needed to achieve the desired system accuracy
- The size of the hidden layer is usually determined through experiments (experiment/trial and test)

ANN: Learning limit

- Boolean functions
  - Any binary function can be learnt (approximately well) by an ANN using one hidden layer
- Continuous functions
  - Any bounded continuous function can be learnt (approximately) by an ANN using one hidden layer
    [Cybenko, 1989; Hornik et al., 1991]

ANN: advantages, disadvantages

- Advantages
  - Nature (structure) supports high-level parallel computation
  - Obtain high accuracy in many problems (photos, video, audio, text)
  - Very flexible in network architecture
- Disadvantages
  - There are no general rules for determining the network architecture and optimal parameters for a given problem
  - There is no general method for assessing ANN's inner workings (thus, the ANN system is viewed as a "black box").
  - It is difficult (impossible) to give explanations to the user
  - Fundamental theories are few, to help explain the real successes

ANN: When?

- The form of the function does not predetermined
- It is not necessary (or unimportant) to provide an explanation to the user about the results
- Accept long time for the training process
- Can collect a large number of labels for data
- Domains related to image, video, speech, text

Open library

Keras

Caffe2

TensorFlow

PYTORCH

References

- Cybenko, G. (1989) "Approximations by superpositions of sigmoidal functions", Mathematics of Control, Signals, and Systems, 2 (4), 303-314
- Kurt Hornik (1991) "Approximation Capabilities of Multilayer Feedforward Networks", Neural Networks, 4(2), 251–257