Data Mining

3.7 Neural Networks

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Outline (I)

- How the Brain Works
- Artificial Neural Networks
- Simple Computing Elements
- Network Structures
- Perceptrons
- Perceptron Learning Method
- Backpropagation
- Defining a Network Topology
- Backpropagation Algorithm

Outline (II)

- Backpropagation and Interpretability
- Discussion
- References

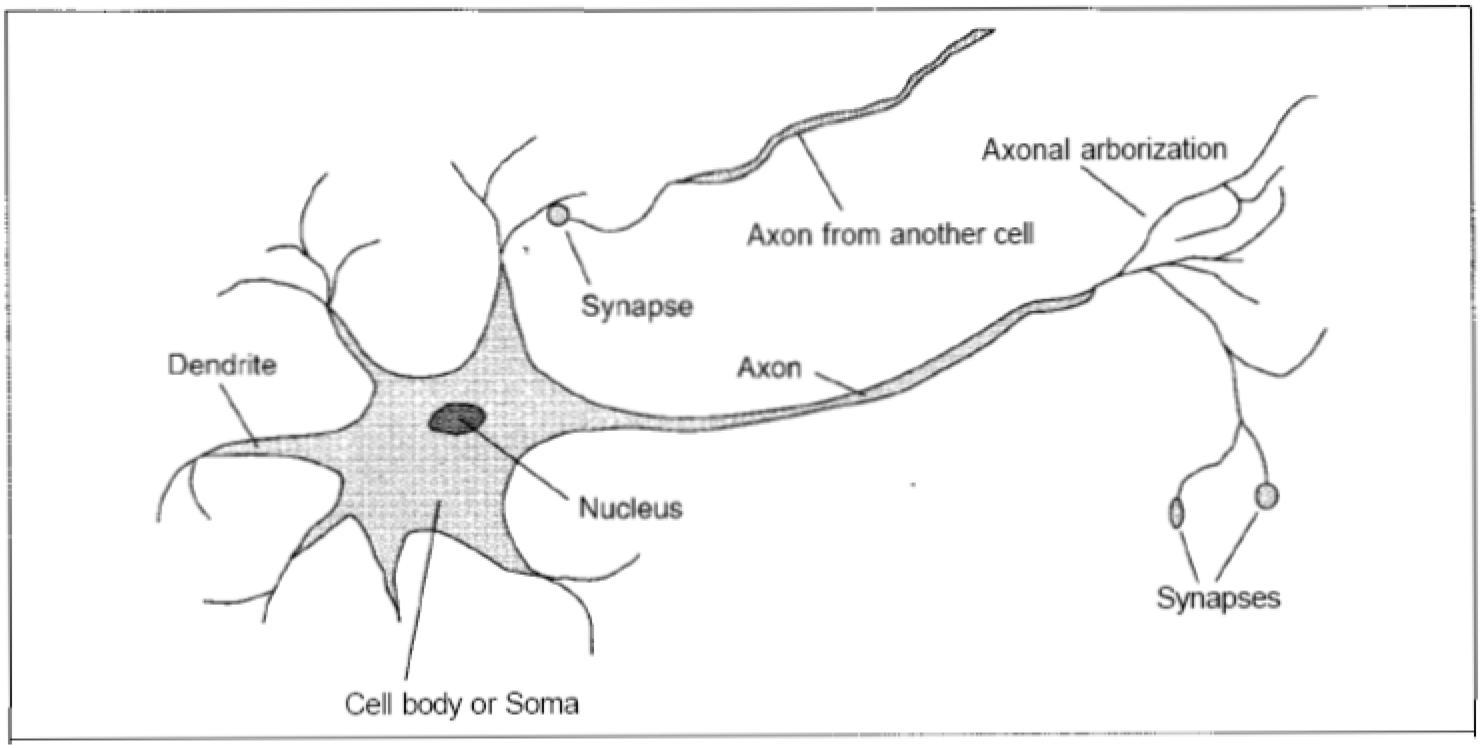
How the Brain Works

How the Brain Works

- **Neuron**, or nerve cell, is the fundamental functional unit of all nervous system tissue, including the brain.
- There 10^{11} neurons in the human brain
- Neuron components
  - **Soma** (cell body): provides the support functions and structure of the cell, that contains a cell **nucleus**.
  - **Dendrites**: consist of more branching fibers which receive signal from other nerve cells
  - **Axon**: a branching fiber which carries signals away from the neuron that connect to the dendrites and cell bodies of other neurons.
  - **Synapse**: The connecting junction between axon and dendrites.

How the Brain Works

- The parts of a nerve cell or neuron. In reality, the length of the axon should be about 100 times the diameter of the cell body.



Neuron Firing Process

1) Synapse receives incoming signals, change electrical potential of cell body
2) When a potential of cell body reaches some limit, neuron "fires", electrical signal (action potential) sent down axon
3) Axon propagates signal to other neurons, downstream

How the Brain Works

- Synapse
  - **Excitatory synapse**: increasing potential
  - **Synaptic connection**: plasticity
  - **Inhibitory synapse**: decreasing potential
- new connections or migration of neurons
  - Neurons also form new connections with other neurons
  - Sometimes entire collections of neurons can migrate from one place to another.
  - These mechanisms are thought to form the basis for learning in the brain.
- A collection of simple cells can lead to thoughts, action, and consciousness.

Comparing brains with digital computers

- Advantages of a human brain vs. a computer
  - **Parallelism**: all the neurons and synapses are active simultaneously, whereas most current computers have only one or at most a few CPUs.
  - **More fault-tolerant**: A hardware error that flips a single bit can doom an entire computation, but brain cells die all the time with no ill effect to the overall functioning of the brain.
  - **Inductive algorithm:** To be trained using an inductive learning algorithm

Artificial Neural Networks

Artificial Neural Networks

- Approximation of biological neural nets by ANN
- Started by psychologists and neurobiologists to develop and test computational analogues of neurons
- Other names: connectionist learning, parallel distributed processing, neural computation, adaptive networks, and collective computation

Artificial Neural Networks

- **Units**
  - A neural network is composed of a number of nodes, or units
  - Metaphor for nerve cell body
- **Links**
  - Units connected by links.
  - Links represent synaptic connections from one unit to another
- **Weight**
  - Each link has a numeric **weight**

Artificial Neural Networks

- Weights are the primary means of long-term storage in neural networks
- Learning usually takes place by adjusting the weights.
- Some of the units are connected to the external environment, and can be designated as input or output units.

Artificial Neural Networks

- Each unit has a set of input links from other units, a set of output links to other units, a current **activation level**, and a means of computing the activation level at the next step in time, given its inputs and weights.
- The idea is that each unit does a local computation based on inputs from its neighbors, but without the need for any global control over the set of units as a whole.

Artificial Neural Networks

- To build a neural network to perform some task first must decide
  - how many units are to be used
  - what kind of units are appropriate
  - how the units are to be connected to form a network.
- Then
  - initializes the weights of the network, and
  - trains the weights using a learning algorithm applied to a set of training examples for the task.
- The use of examples also implies that one must decide how to encode the examples in terms of inputs and outputs of the network.

Artificial Neural Networks

- Neural networks can be used for both
  - supervised learning, and
  - unsupervised learning
- For supervised learning neural networks can be used for both
  - classification (to predict the class label of a given tuple) and
  - prediction (to predict a continuous-valued output).
- In this chapter we want to discuss about application of neural networks for supervised learning

Simple Computing Elements

Simple computing elements

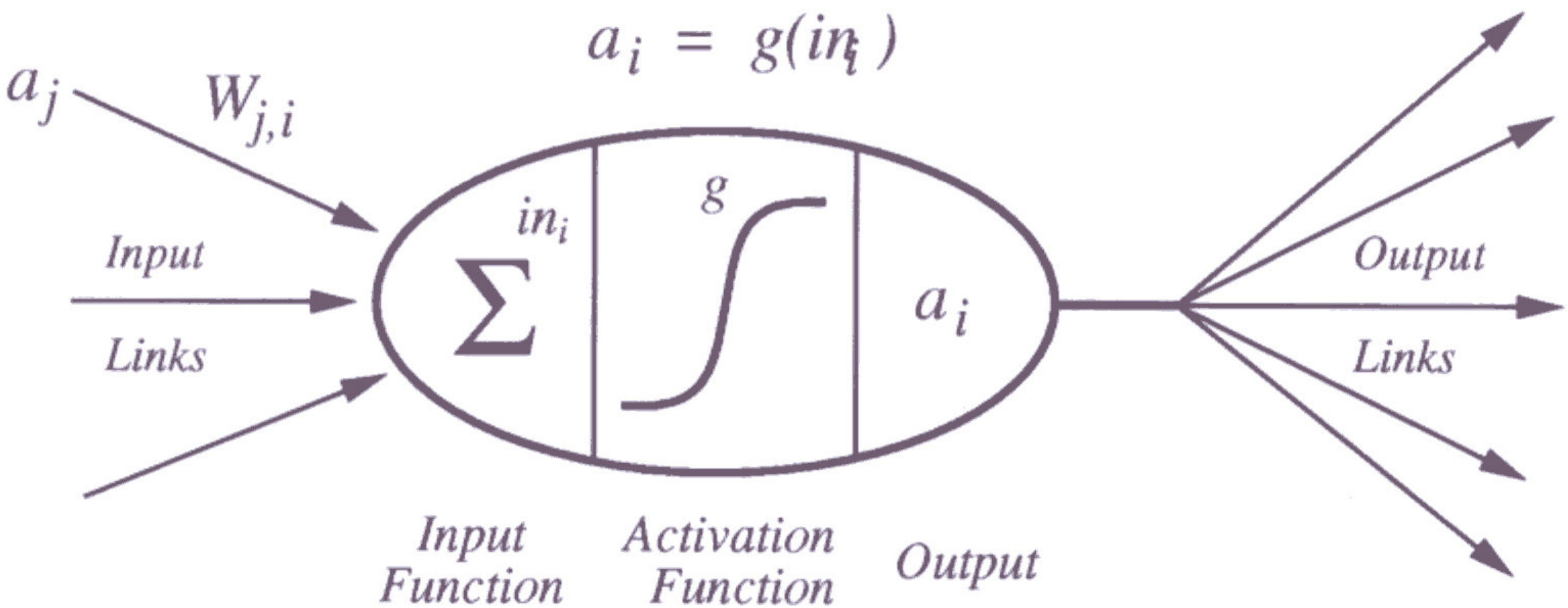
- Each unit performs a simple process:
  - Receives n-inputs
  - Multiplies each input by its weight
  - Applies activation function to the sum of results
  - Outputs result

Simple computing elements

- Two computational components
  - Linear component: **input function**, that in_i, that computes the weighted sum of the unit's input values.
  - Nonlinear component: **activation function**, g, that transforms the weighted sum into the final value that serves as the unit's activation value, a_i
    - Usually, all units in a network use the same activation function.

Simple computing elements

- A typical unit



Simple computing elements

- Biological Neural Network vs. Artificial Neural Network

Biological Neural Network	**Artificial Neural Network**
Soma / Cell body	Neuron / Node / Unit
Dendrite	Input links
Axon	Output links
Synapse	Weight

Simple computing elements

- Total weighted input

$$in_i = \sum_j W_{j,i} a_j$$

  - the weights on links into node *i* from node *j are denoted by* $W_{j,i}$
  - *The input values is called* a_j

Example: Total weighted input

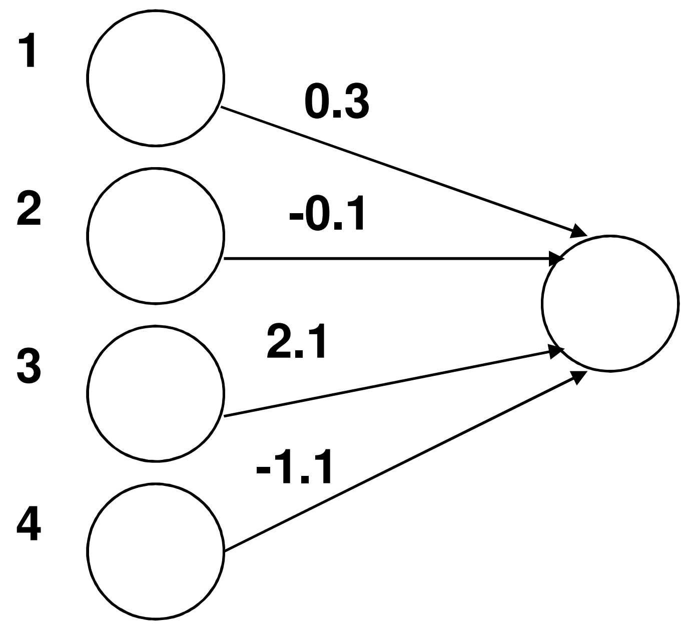
Input: (3, 1, 0, -2)

Processing:

3(0.3) + 1(-0.1) + 0(2.1) + -1.1(-2)

= 0.9 + (-0.1) + 2.2

Output: 3



Simple computing elements

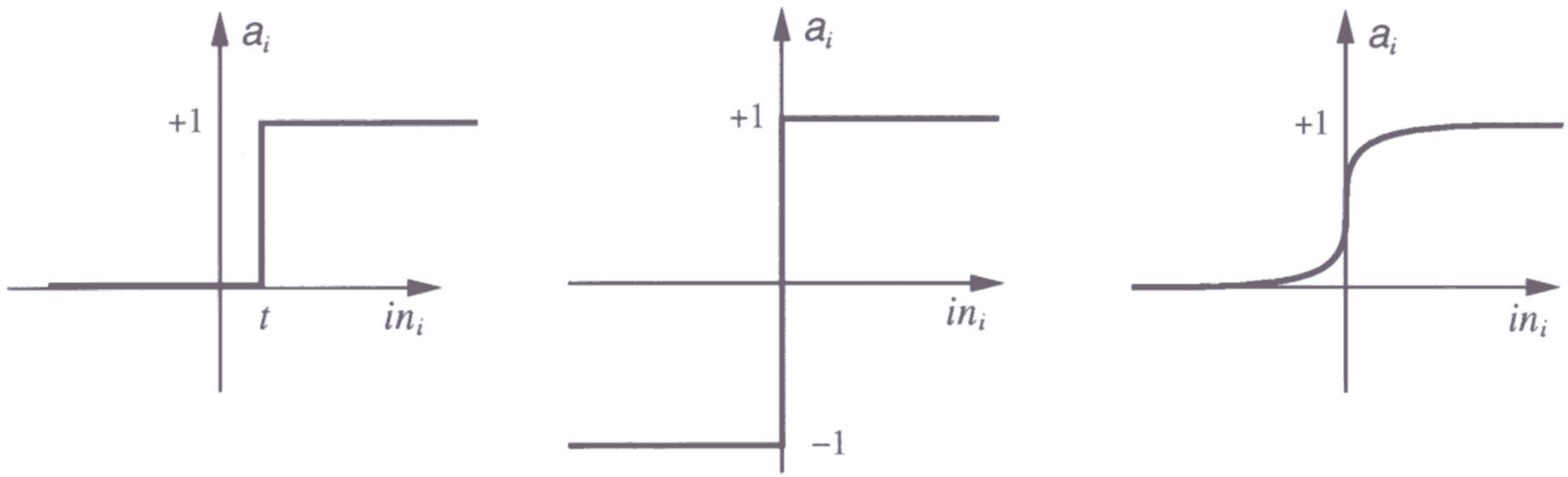
- The activation function g

$$a_i = g(in_i) = g(\sum_j W_{j,i} a_j)$$

- Three common mathematical functions for g are
  - **Step** function
  - **Sign** function
  - **Sigmoid** function

Simple computing elements

- Three common mathematical functions for *g*



(a) Step function (b) Sign function (c) Sigmoid function

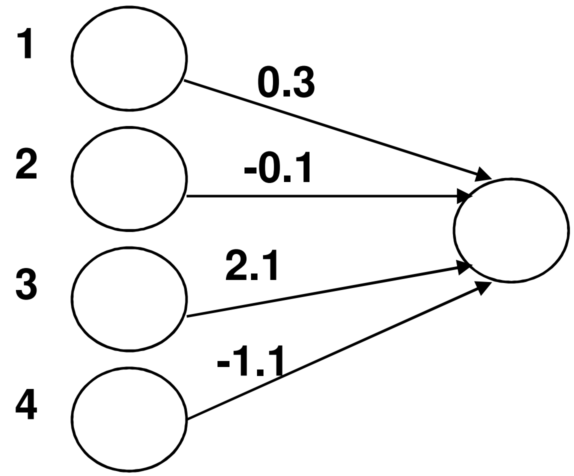
$$step_t(x) = \begin{cases} 1, & \text{if } x \geq t \\ 0, & \text{if } x < t \end{cases} \quad sign(x) = \begin{cases} +1, & \text{if } x \geq 0 \\ -1, & \text{if } x < 0 \end{cases} \quad sigmoid(x) = \frac{1}{1+e^{-x}}$$

Step Function

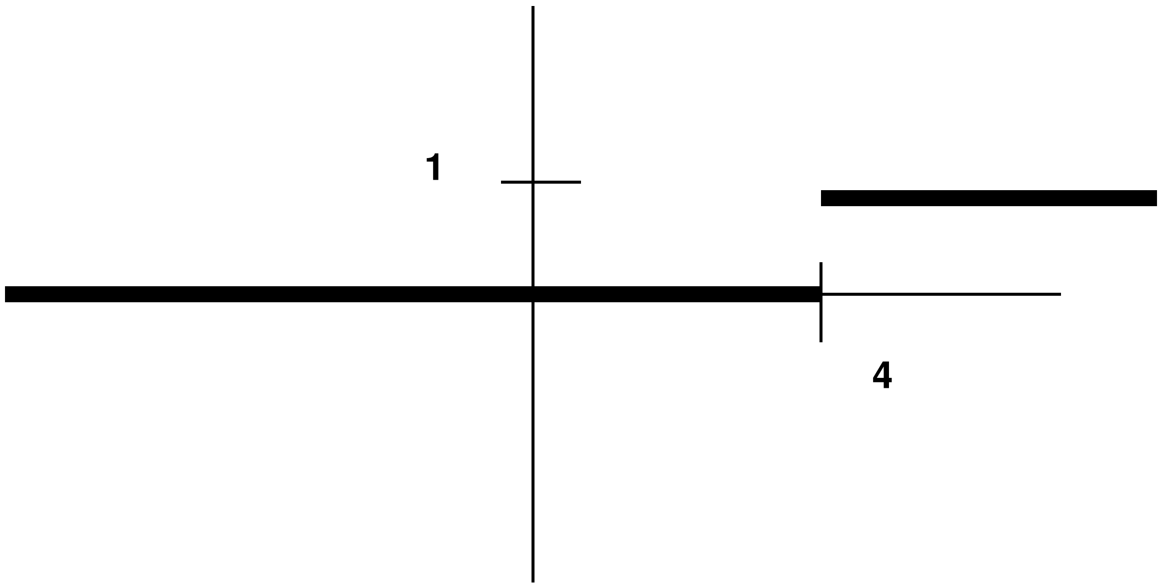
- The step function has a threshold t such that it outputs a 1 when the input is greater than its threshold, and outputs a 0 otherwise.
- The biological motivation is that a 1 represents the firing of a pulse down the axon, and a 0 represents no firing.
- The threshold represents the minimum total weighted input necessary to cause the neuron to fire.

Step Function Example

- Let t = 4



$$Step_4(3) = 0$$



Step Function

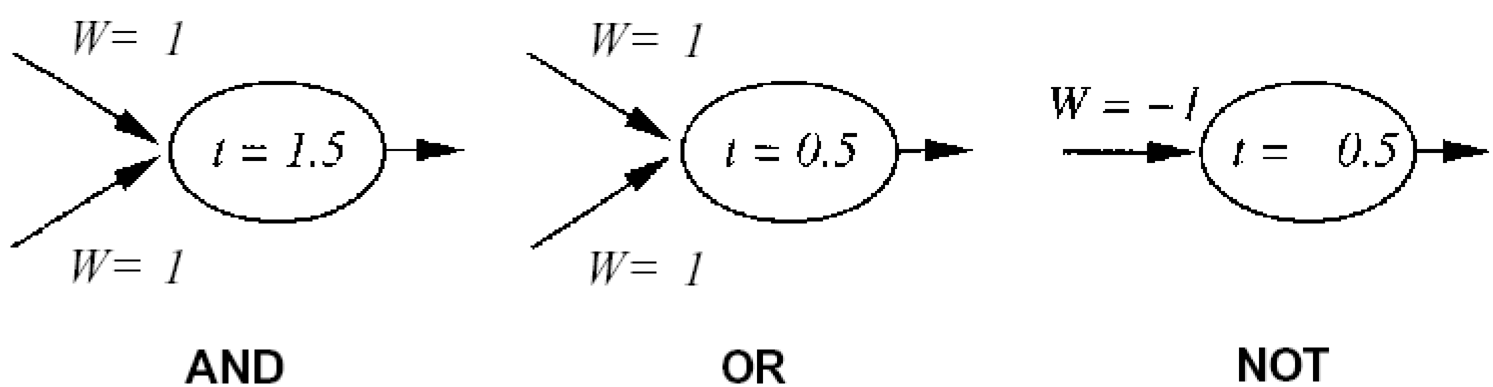
- it mathematically convenient to replace the threshold with an extra input weight.
- Because it need only worry about adjusting weights, rather than adjusting both weights and thresholds.
- Thus, instead of having a threshold *t* for each unit, we add an extra input whose activation a_0

$$a_i = step_t(\sum_{j=1}^{n} W_{j,i} a_j) = step_0(\sum_{j=0}^{n} W_{j,i} a_j)$$

Where $W_{0,i} = t$ and $a_0 = -1$ ← fixed

Step Function

- The Figure shows how the Boolean functions *AND, OR,* and *NOT* can be represented by units with a step function and suitable weights and thresholds.
- This is important because it means we can use these units to build a network to compute any Boolean function of the inputs.



Sigmoid Function

- A sigmoid function often used to approximate the step function

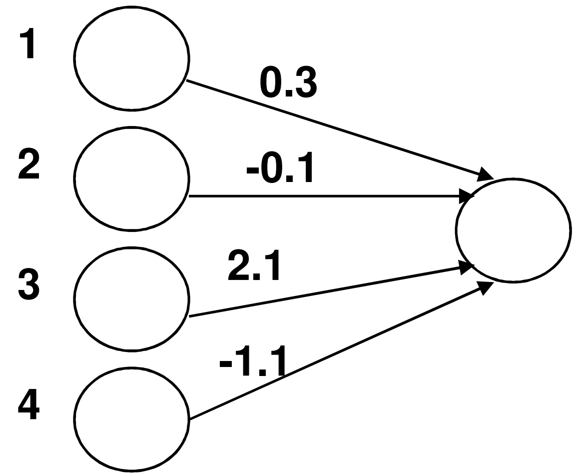
$$f(x) = \frac{1}{1 + e^{-\sigma x}}$$

σ : the steepness parameter

Sigmoid Function

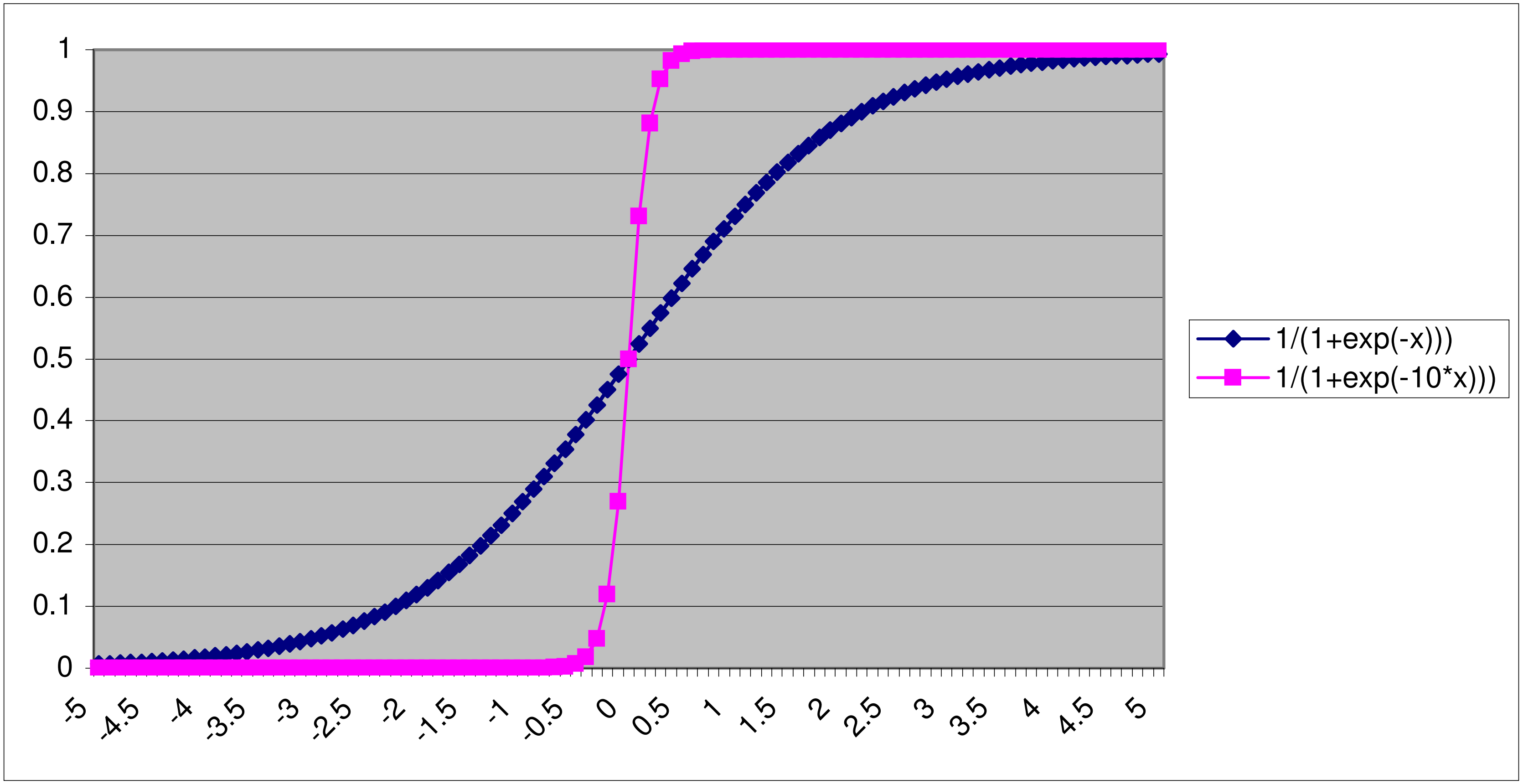
- *Input*: (3, 1, 0, -2), $\sigma = 1$

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



$$f(3) = \frac{1}{1 + e^{-x}} \approx .95$$

Sigmoid Function

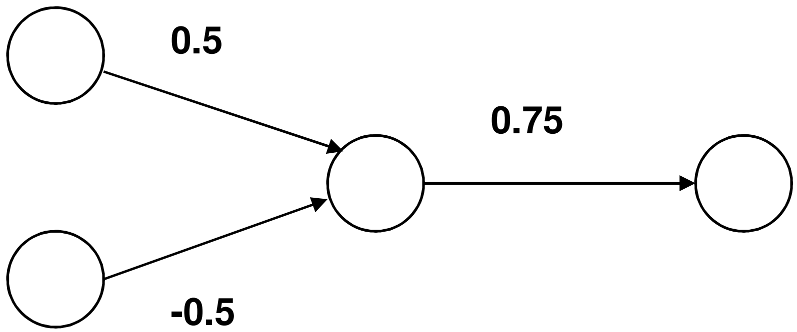


sigmoidal(0) = 0.5

Another Example

- A two weight layer, feedforward network
- Two inputs, one output, one ‘hidden’ unit
- *Input*: (3, 1)

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



- What is the output?

Computing in Multilayer Networks

- Start at leftmost layer
  - Compute activations based on inputs
- Then work from left to right, using computed activations as inputs to next layer
- Example solution
  - Activation of hidden unit
    - f(0.5(3) + -0.5(1)) =
      - f(1.5 – 0.5) =
      - f(1) = 0.731
  - Output activation
    - f(0.731(0.75)) =
      - f(0.548) = .634

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

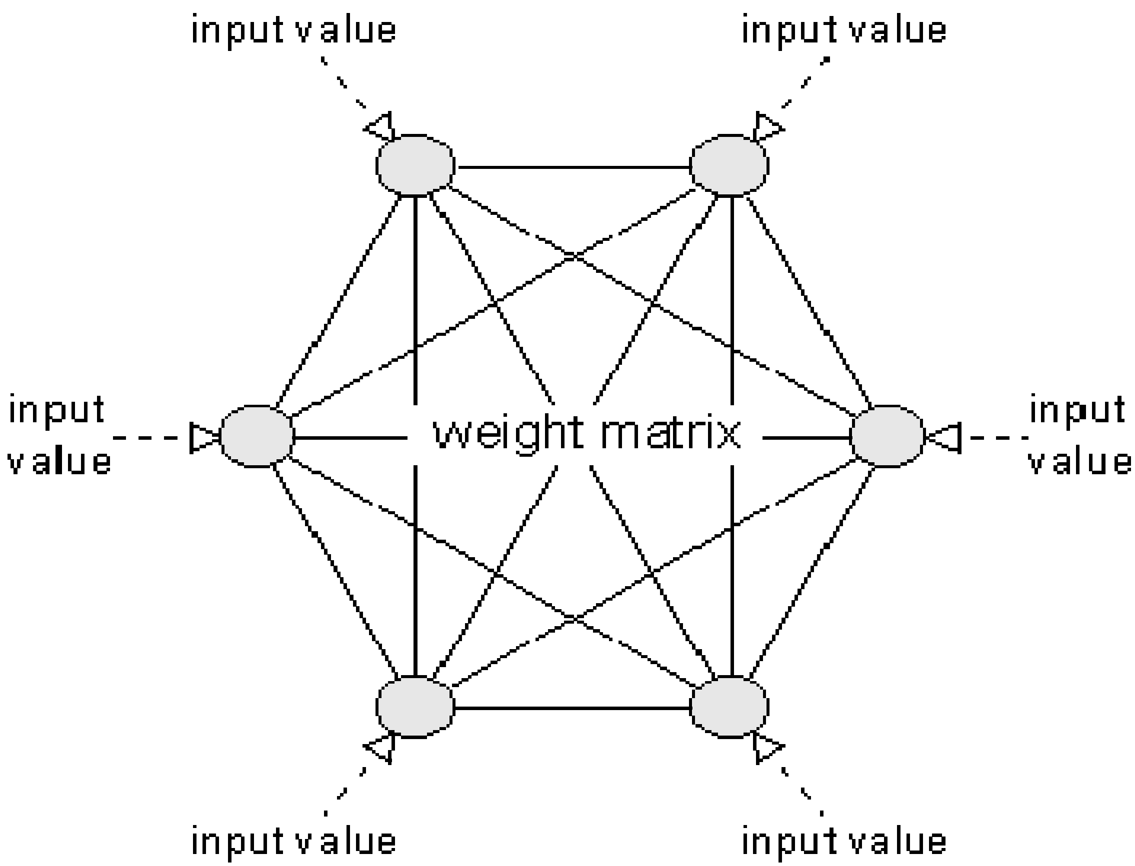
Network Structures

Network Structures

- Two main kinds of network structure are
  - **Recurrent networks**
    - The links can form arbitrary topologies
    - Long computation time
    - Need advanced mathematical method
    - The Brain similar to Recurrent Network has backward link
  - **Feed-forward networks**
    - Unidirectional links, no cycles
    - Directed acyclic graph (DAG)
    - No links between units in the same layer, no links backward to a previous layer, no links that skip a layer.
    - Uniformly processing from input units to output units

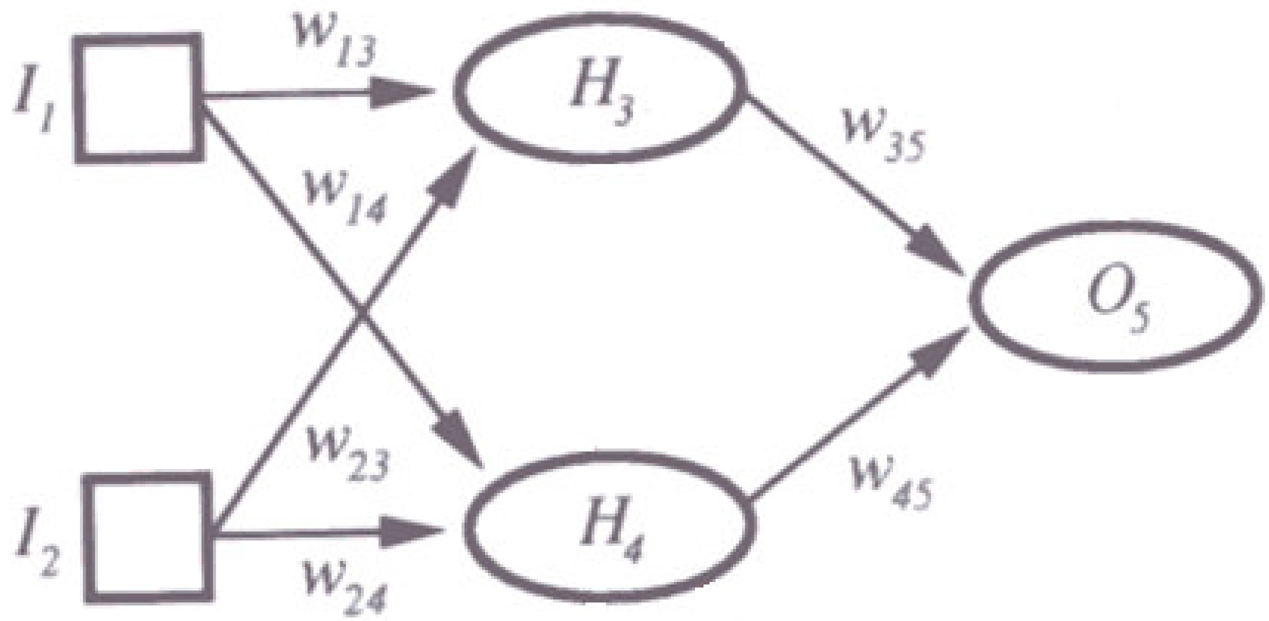
Network Structures

- An example of recurrent network (Hopfield Net)



Network Structures

- An example: A very simple, two-layer, feed-forward network with two inputs, two hidden nodes, and one output node.



Network Structures

- Because the input units (square nodes) simply serve to pass activation to the next layer, they are not counted
- Input, output, and hidden units
  - **input units**: the activation value of each of these units is determined by the environment.
  - **output units**: at the right-hand end of the network units
  - **hidden units**: they have no direct connection to the outside world.

Network Structures

- Types of feed-forward networks:
  - **Perceptrons**: no hidden units, This makes the learning problem much simpler, but it means that perceptrons are very limited in what they can represent.
  - **Multilayer networks**: one or more hidden units

Network Structures

- Feed-forward networks have a fixed structure and fixed activation functions g
- Therefore, the functions have a specific parameterized structure
- The weights chosen for the network determine which of these functions is actually represented.
- For example, the network calculates the following function:

$$\begin{aligned} a_5 &= g(W_{3,5}a_3 + W_{4,5}a_4) \\ &= g(W_{3,5}g(W_{1,3}a_1 + W_{2,3}a_2) + W_{4,5}g(W_{1,4}a_1 + W_{2,4}a_2)) \end{aligned}$$

  – where g is the activation function, a_i and , is the output of node i.

What neural networks do

- Because the activation functions g are nonlinear, the whole network represents a complex nonlinear function.
- If you think of the weights as parameters or coefficients of this function, then learning just becomes:
  - a process of tuning the parameters to fit the data in the training set—a process that statisticians call **nonlinear regression**.

Optimal Network Structure

- Too small network: in capable of representation
- Too big network: not generalized well
  - Overfitting when there are too many parameters.
- Feed forward NN with one hidden layer
  - can approximate any continuous function
- Feed forward NN with 2 hidden layer
  - can approximate any function

Optimal Network Structure

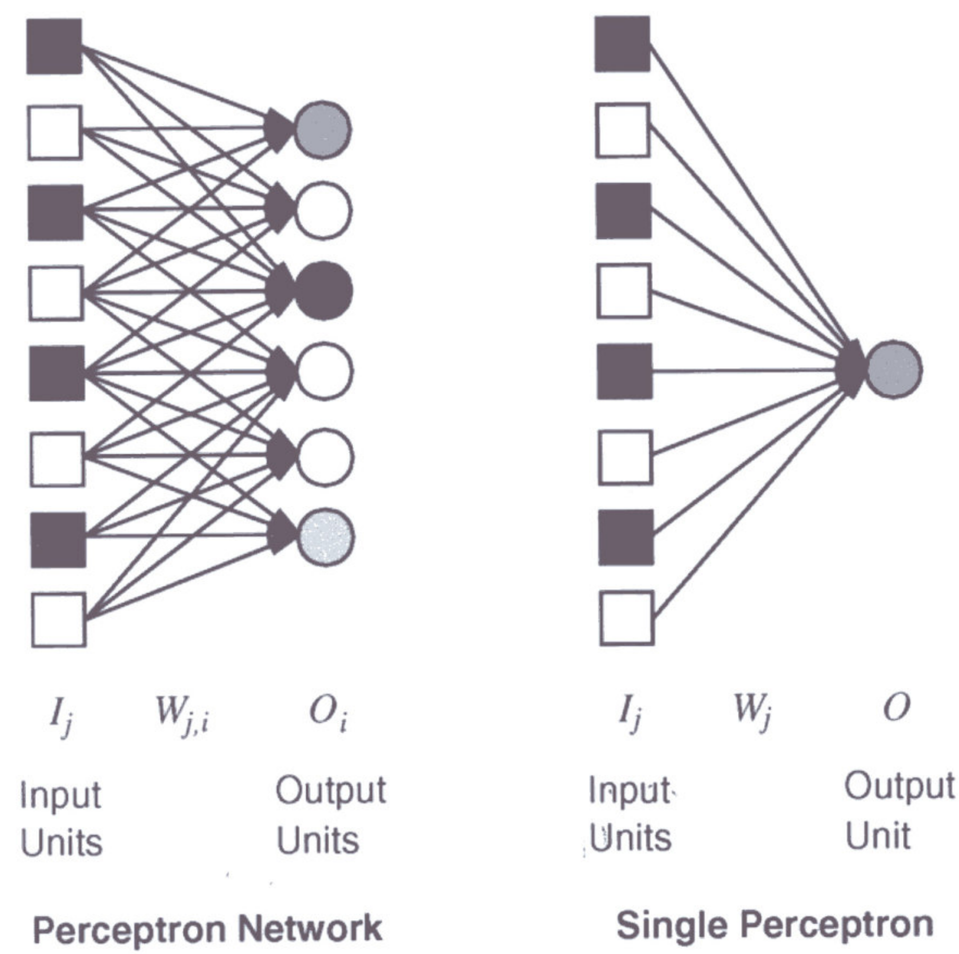
- Using **genetic algorithm**: for finding a good network structure
- Hill-climbing search (modifying an existing network structure)
  - Start with a big network: **optimal brain damage algorithm**
- Removing weights from fully connected model
  - Start with a small network: **tiling algorithm**
- Start with single unit and add subsequent units
- **Cross-validation techniques**: are useful for deciding when we have found a network of the right size.

Perceptrons

Perceptrons

- **Perceptrons**
  - Layered feed-forward networks
  - were first studied in the late 1950s
  - the name **perceptron** is usually used as a synonym for a single-layer, feed-forward network.

Perceptrons



Perceptrons

- Notice that each output unit is independent of the others — each weight only affects one of the outputs.
- That means that we can limit our study to perceptrons with a single output unit, as in the right-hand side of the Figure
- and we can use several of them to build up a **multi-output perceptron**.

Perceptrons

- Activation of output unit:

$$O = Step_0\left(\sum_j W_j I_j\right) = Step_0(\mathbf{W} \cdot \mathbf{I})$$

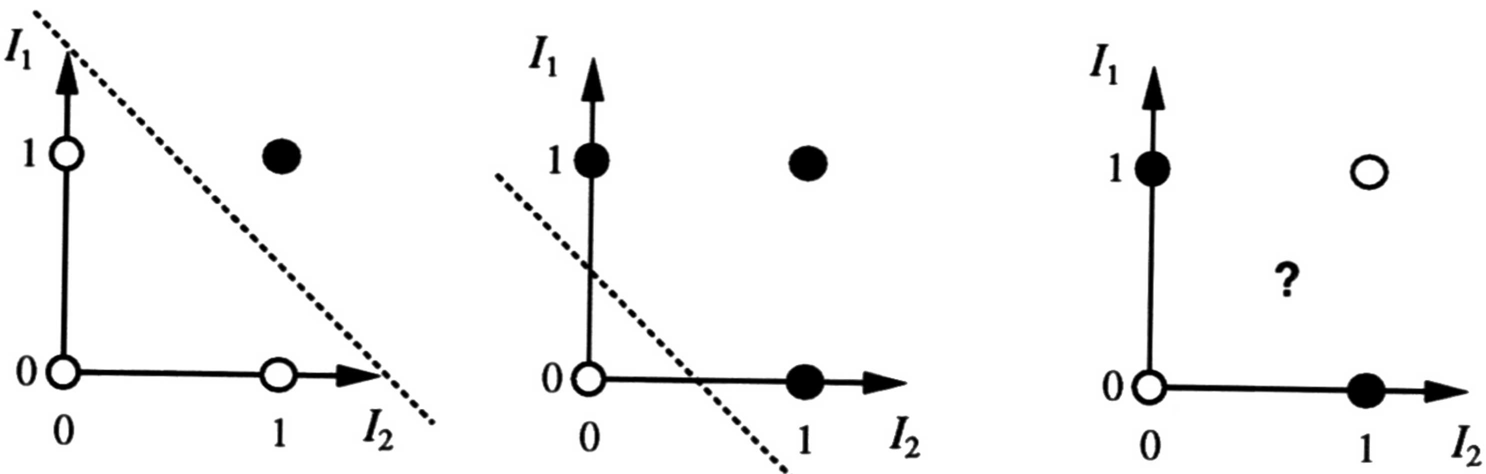
  - *the weight from input unit j Wj*
  - The activation of input unit j is given by I_j.
  - we have assumed an additional weight W_0 to provide a threshold for the step function, with $I_0 = -1$.

Perceptrons

- Perceptrons are severely limited in the Boolean functions they can represent.
- The problem is that any input I_j can only influence the final output in one direction, no matter what the other input values are.
- Consider some input vector a.
  - Suppose that this vector has $a_j = 0$ and that the vector produces a 0 as output. Furthermore, suppose that when a_j is replaced with *1*, the output changes to *1.* This implies that W_j must be positive.
  - It also implies that there can be no input vector b for which the output is 1 when $b_j = 0$, *but the output is* 0 when b_j *is replaced with 1.*

Perceptrons

- The Figure shows three different Boolean functions of two inputs, the AND, OR, and XOR functions.



(a) I_1 and I_2 (b) I_1 or I_2 (c) I_1 xor I_2

- Black dots indicate a point in the input space where the value of the function is 1, and white dots indicate a point where the value is 0.

Perceptrons

- As we will explain, a perceptron can represent a function only if there is some line that separates all the white dots from the black dots.
- Such functions are called **linearly separable.**
- Thus, a perceptron can represent AND and OR, but not XOR (if $I_1 \# I_2$)**.**

Perceptrons

- The fact that a perceptron can only represent linearly separable functions follows directly from Equation:

$$O = Step_0\left(\sum_j W_j I_j\right) = Step_0(\mathbf{W} \cdot \mathbf{I})$$

- A perceptron outputs a 1 only if W • I > 0.
  - This means that the entire input space is divided in two along a boundary defined by W • I = 0,
  - that is, a plane in the input space with coefficients given by the weights.

Perceptrons

- It is easiest to understand for the case where *n = 2. In Figure (a),* one possible separating "plane" is the dotted line defined by the equation

$$I_1 = -I_2 + 1.5 \qquad \text{or} \qquad I_1 + I_2 = 1.5$$

- The region above the line, where the output is 1 , is therefore given by

$$-1.5 + I_1 + I_2 > 0$$

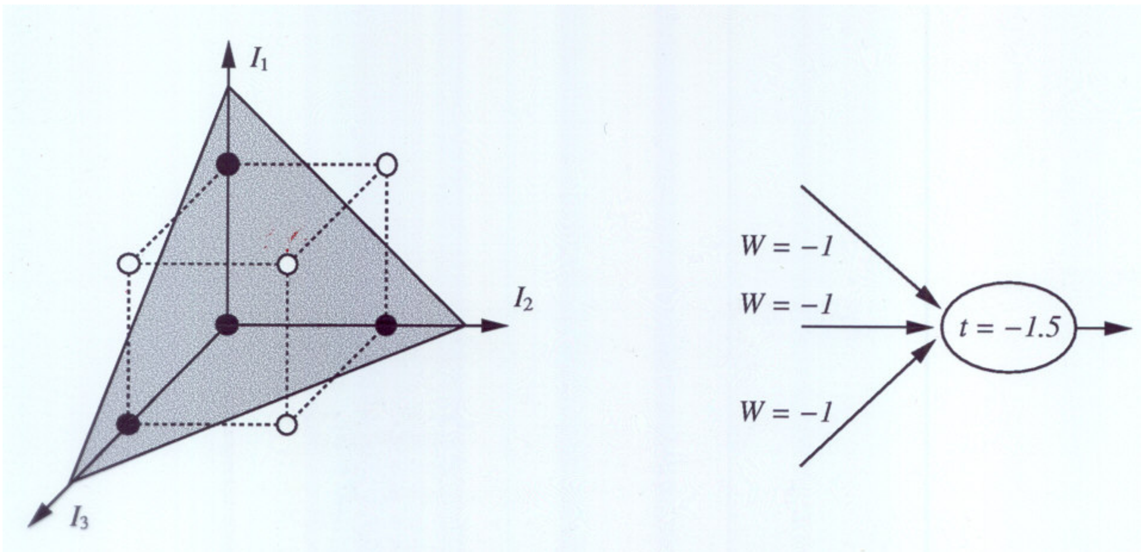
Perceptrons

- With three inputs, the separating plane can still be visualized.
- The shaded separating plane is defined by the equation

  $I1 + I2 + I3 = 1.5$

- This time the positive outputs lie below the plane, in the region

  $(-I1) + (-I2) + (-I3) = -1.5$



(a) Separating plane (b) Weights and threshold

Perceptron Learning Method

Perceptron Learning Method

- The initial network has randomly assigned weights, usually from the range [-0.5,0.5].
- The network is then updated to try to make it consistent with the examples.
- This is done by making small adjustments in the weights to reduce the difference between the observed and predicted values.
- The algorithm is the need to repeat the update phase several times for each example in order to achieve convergence.
- Typically, the updating process is divided into **epochs.**
- **Each** epoch involves updating all the weights for all the examples.

Perceptron Learning Method

- The generic neural network learning method

```
function NEURAL-NETWORK-LEARNING(examples) returns network

  network ← a network with randomly assigned weights
  repeat
     for each e in examples do
        O ← NEURAL-NETWORK-OUTPUT(network, e)
        T ← the observed output values from e
        update the weights in network based on e, O, and T
     end
  until all examples correctly predicted or stopping criterion is reached
  return network
```

epoch

Err = T-O

Figure 19.11 The generic neural network learning method: adjust the weights until predicted output values **O** and true values **T** agree.

Perceptron Learning Method

- The weight update rule
  - If the predicted output for the single output unit is *O*, and the correct output should be T, then the error is given by

$$Err = T - O$$

  - If the error is positive, then we need to increase *O; if it is negative, we need to decrease 0.*
  - Now each input unit contributes $W_j I_j$ to the total input, so if I_j is positive, an increase in *Wj* will tend to increase *O, and if* I_j *is negative, an increase in Wj* will tend to decrease *O.*

Perceptron Learning Method

- *Thus, we can achieve* the effect we want with the following rule:

$$W_j \leftarrow W_j + \alpha * I_j * Err$$

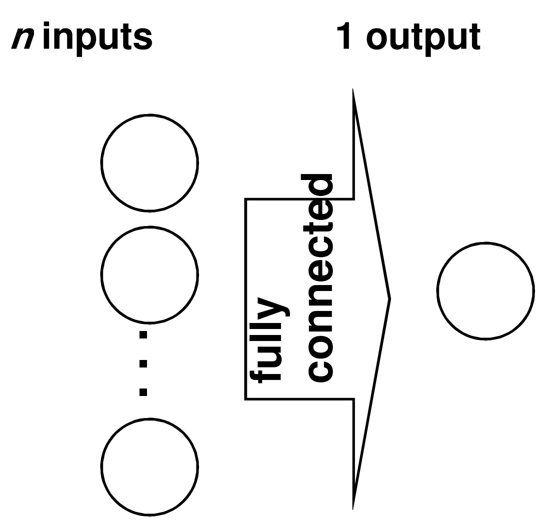
  – **α** : is the **learning rate**

- This rule is a slight variant of the **perceptron learning rule** proposed by Frank Rosenblatt.
- Rosenblatt proved that a learning system using the perceptron learning rule will converge to a set of weights that correctly represents the examples, as long as the examples represent a linearly separable function.

Delta Rule for a Single Output Unit

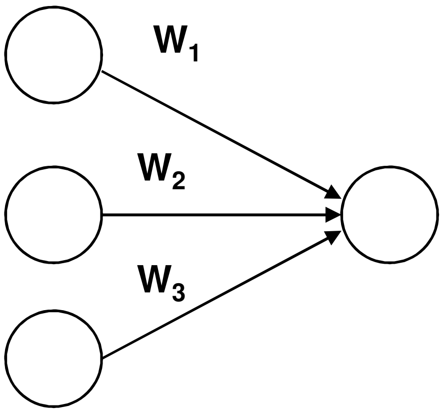
$$\Delta W_j = \alpha(T - O)I_j$$

ΔW_j	Change in *j* th weight of weight vector
α	Learning rate
T	Target or correct output
O	Net (summed, weighted) input to output unit
I_j	j th input value



Example

- W = (W1, W2, W3)
  - Initially: W= (.5 .2 .4)
- Let α = 0.5
- Apply delta rule



Sample	Input	Output
1	0 0 0	0
2	1 1 1	1
3	1 0 0	1
4	0 0 1	1

One Epoch of Training

Step	Input	Desired output (T)	Actual output (O)	Starting Weights	Weight updates
1	(0 0 0)	0	0	(.5 .2 .4)	
2	(1 1 1)	1			
3	(1 0 0)	1			
4	(0 0 1)	1			

Delta rule: $\Delta W_j = \alpha(T - O)I_j$

One Epoch of Training

Step	Input	Desired output (T)	Actual output (O)	Starting Weights	Weight updates
1	(0 0 0)	0	0	(.5 .2 .4)	W1: 0.1(0 – 0)0 W2: 0.1(0 – 0)0 W3: 0.1(0 – 0)0

Delta rule: $\Delta W_j = \alpha(T - O)l_j$

delta-rule1.xls

One Epoch of Training

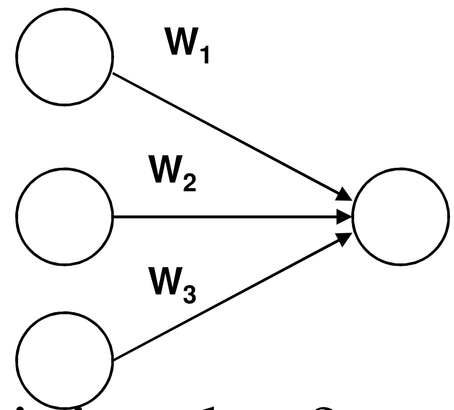
Step	Input	Desired output (T)	Actual output (O)	Starting Weights	Weight updates
1	(0 0 0)	0	0	(.5 .2 .4)	(0 0 0)
2	(1 1 1)	1		(.5 .2 .4)	
3	(1 0 0)	1			
4	(0 0 1)	1			

Remaining Steps in First Epoch of Training

Step	Input	Desired output (T)	Actual output (O)	Starting Weights	Weight updates
1	(0 0 0)	0	0	(.5 .2 .4)	(0 0 0)
2	(1 1 1)	1	1.1	(.5 .2 .4)	(-.05 -.05 -.05)
3	(1 0 0)	1	.45	(.45 .15 .35)	(.275 0 0)
4	(0 0 1)	1	.35	(.725 .15 .35)	(0 0 .325)

Completing the Example

- After 18 epochs
  - Weights
    - W1= 0.990735
    - W2= -0.970018005
    - W3= 0.98147



- Does this adequately approximate the training data?

Sample	Input	Output
1	0 0 0	0
2	1 1 1	1
3	1 0 0	1
4	0 0 1	1

Example

- Actual Outputs

Sample	Input	Desired Output	Actual Output
1	0 0 0	0	0
2	1 1 1	1	1.002187
3	1 0 0	1	0.990735
4	0 0 1	1	0.98147

Perceptron Learning Method

- There is a slight difference between the example descriptions used for neural networks and those used for other attribute-based methods such as decision trees.
- In a neural network, all inputs are real numbers in some fixed range, whereas decision trees allow for multivalued attributes with a discrete set of values.
- For example, an attribute may has values *None, Some, and Full.*

Perceptron Learning Method

- *There are* two ways to handle this.
  - **Local encoding**
    - we use a single input unit and pick an appropriate number of distinct values to correspond to the discrete attribute values.
    - For example, we can use *None = 0.0, Some = 0.5, and Full = 1.0.*
  - **Distributed encoding**
    - *we use one input unit for* each value of the attribute, turning on the unit that corresponds to the correct value.

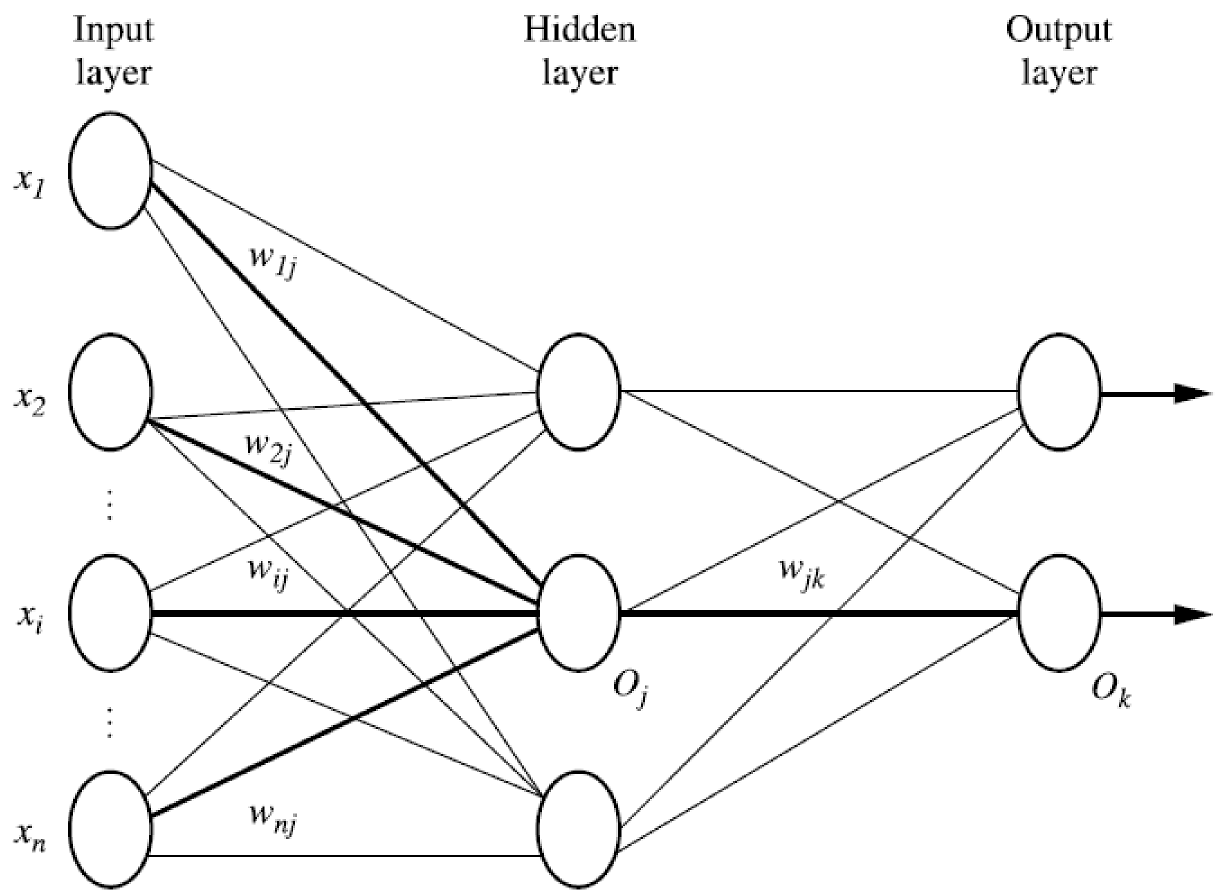
Backpropagation

Backpropagation

- The backpropagation algorithm performs learning on a **multilayer feed-forward** neural network.
- It is the most popular method for learning in multilayer networks
- Invented in 1969 by **Bryson** and **Ho**
- It iteratively learns a set of weights for prediction of the class label of tuples.
- A multilayer feed-forward neural network consists of an **input layer**, one or more **hidden layers**, and an **output layer**.

Backpropagation

- A multilayer feed-forward neural network

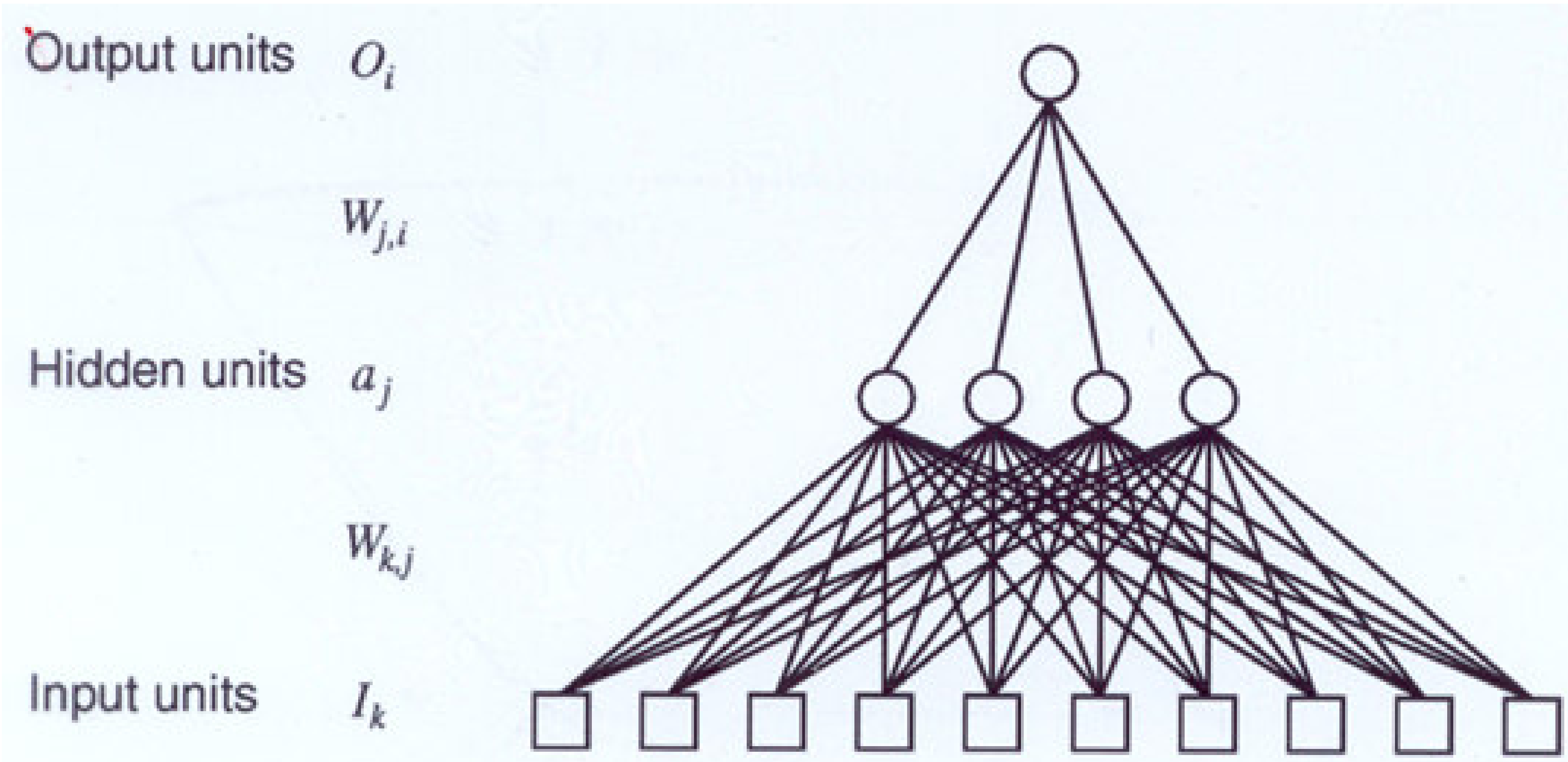


Backpropagation

- Suppose we want to construct a network for a problem.
- We have ten attributes describing each example, so we will need ten input units.
- How many hidden units are needed?
  - The problem of choosing the right number of hidden units in advance is still not well-understood.
- we use a network with four hidden units.

Backpropagation

- A two-layer feed-forward network



Backpropagation

- Each layer is made up of units.
- The **inputs** to the network correspond to the attributes measured for each training tuple.
- Inputs are fed simultaneously into the units making up the **input layer**
- They are then weighted and fed simultaneously to a **hidden layer**
- The number of hidden layers is arbitrary, although in practice, usually only one is used.
- The weighted outputs of the last hidden layer are input to units making up the **output layer**, which sends out the network's prediction.

Backpropagation

- A two-layer neural network has a hiden layer and an output layer.
- The input layer is not counted because it serves only to pass the input values to the next layer.
- A network containing two hidden layers is called a *three-layer neural network, and so on.*

Backpropagation

- The network is **feed-forward** in that none of the weights cycles back to an input unit or to an output unit of a previous layer
- From a statistical point of view, networks perform **nonlinear regression**
- Given enough hidden units and enough training samples, they can closely approximate any function

Backpropagation

- **Learning method** is the same way as for perceptrons
  - example inputs are presented to the network, and if the network computes an output vector that matches the target, nothing is done.
  - If there is an error (a difference between the output and target), then the weights are adjusted to reduce this error.
  - The trick is to assess the blame for an error and divide it among the contributing weights.
  - In perceptrons, this is easy, because there is only one weight between each input and the output.
  - But in multilayer networks, there are many weights connecting each input to an output, and each of these weights contributes to more than one output.

Backpropagation

- The weight update rule is very similar to the rule for the perceptron.
- There are two differences:
  - the activation of the hidden unit a_j is used instead of the input value; and
  - the rule contains a term for the gradient of the activation function.

Defining a Network Topology

Defining a Network Topology

- First decide the **network topology:**
  - the number of units in the *input layer*,
  - the number of *hidden layers* (if > 1),
  - the number of units in *each hidden layer*, and
  - the number of units in the *output layer*

- Normalizing the input values for each attribute measured in the training tuples to [0.0—1.0] will help speed up the learning phase.

Defining a Network Topology

- **Input units**
  - One input unit per domain value, each initialized to 0
  - Discrete-valued attributes may be encoded such that there is one input unit per domain value.
  - For example, if an attribute *A* has three possible or known values, namely $\{a_0, a_1, a_2\}$, then we may assign three input units to represent *A*.
  - That is, we may have, say, I_0, I_1, I_2 as input units.
  - Each unit is initialized to *0. If* $A=a_0$, *then* I_0 *is set* to 1, If $A = a_1$, I_1 *is set to 1, and so on.*

Defining a Network Topology

- **Output unit**
  - For classification, one output unit may be used to represent two classes (where the value 1 represents one class, and the value 0 represents the other).
  - If there are more than two classes, then one output unit per class is used.

Defining a Network Topology

- **Hidden layer units**
  - There are no clear rules as to the "best" number of hidden layer units
  - Network design is a trial-and-error process and may affect the accuracy of the resulting trained network.

- Once a network has been trained and its accuracy is **unacceptable**, repeat the training process with a *different network topology* or a *different set of initial weights*

Defining a Network Topology

- Cross-validation techniques for accuracy estimation (described later) can be used to help decide when an acceptable network has been found.
- A number of automated techniques have been proposed that search for a “good” network structure.
- These typically use a hill-climbing approach that starts with an initial structure that is selectively modified.

Backpropagation Algorithm

Backpropagation

- **Backpropagation** iteratively process a set of training tuples & compare the network's prediction with the actual known target value
- The target value may be the known class label of the training tuple (for classification problems) or a continuous value (for prediction problems).
- For each training tuple, the weights are modified to **minimize the mean squared error** between the network's prediction and the actual target value

Backpropagation

- Modifications are made in the "**backwards**" direction
  - from the output layer, through each hidden layer down to the first hidden layer, hence "**backpropagation**"
  - Although it is not guaranteed, in general the weights will eventually converge, and the learning process stops.

Backpropagation

- Steps
  - Initialize the weights
    - Initialize weights to small random and biases in the network
  - Propagate the inputs forward
    - by applying activation function
  - Backpropagate the error
    - by updating weights and biases
  - Terminating condition
    - when error is very small, etc.

Backpropagation Algorithm

- Algorithm:
  – Backpropagation. Neural network learning for classification or prediction, using the backpropagation algorithm.
- Input:
  – ***D**,* a data set consisting of the training tuples and their associated target values
  – ***l**,* the learning rate
  – ***network***, a multilayer feed-forward network
- Output:
  – A trained neural network.

Backpropagation Algorithm

Initialize all weights and biases in *network*;
while terminating condition is not satisfied {
    for each training tuple X in D {
        // Propagate the inputs forward:
        for each input layer unit j {
            $O_j = I_j$; // output of an input unit is its actual input value
        for each hidden or output layer unit j {
            $I_j = \sum_i w_{ij} O_i + \theta_j$; //compute the net input of unit j with respect to the previous layer, i
            $O_j = \frac{1}{1+e^{-I_j}}$; } // compute the output of each unit j
        // Backpropagate the errors:
        for each unit j in the output layer
            $Err_j = O_j(1 - O_j)(T_j - O_j)$; // compute the error
        for each unit j in the hidden layers, from the last to the first hidden layer
            $Err_j = O_j(1 - O_j) \sum_k Err_k w_{jk}$; // compute the error with respect to the next higher layer, k
        for each weight w_{ij} in *network* {
            $\Delta w_{ij} = (l) Err_j O_i$; // weight increment
            $w_{ij} = w_{ij} + \Delta w_{ij}$; } // weight update
        for each bias θ_j in *network* {
            $\Delta \theta_j = (l) Err_j$; // bias increment
            $\theta_j = \theta_j + \Delta \theta_j$; } // bias update
        } }

Initialize the weights

- The weights in the network are initialized to small random numbers
  - e.g., ranging from -1.0 to 1.0 or -0.5 to 0.5
- Each unit has a bias associated with it
  - The biases are similarly initialized to small random numbers.

- Each training tuple, ***X,*** is processed by the following steps.

Propagate the inputs forward

- a) determining the output of input layer units
  - the training tuple is fed to the input layer of the network.
  - The inputs pass through the input units, unchanged.
  - For an input unit, *j*,
    - its input value, I_j
    - its output, O_j, is equal to its input value, I_j.

Propagate the inputs forward

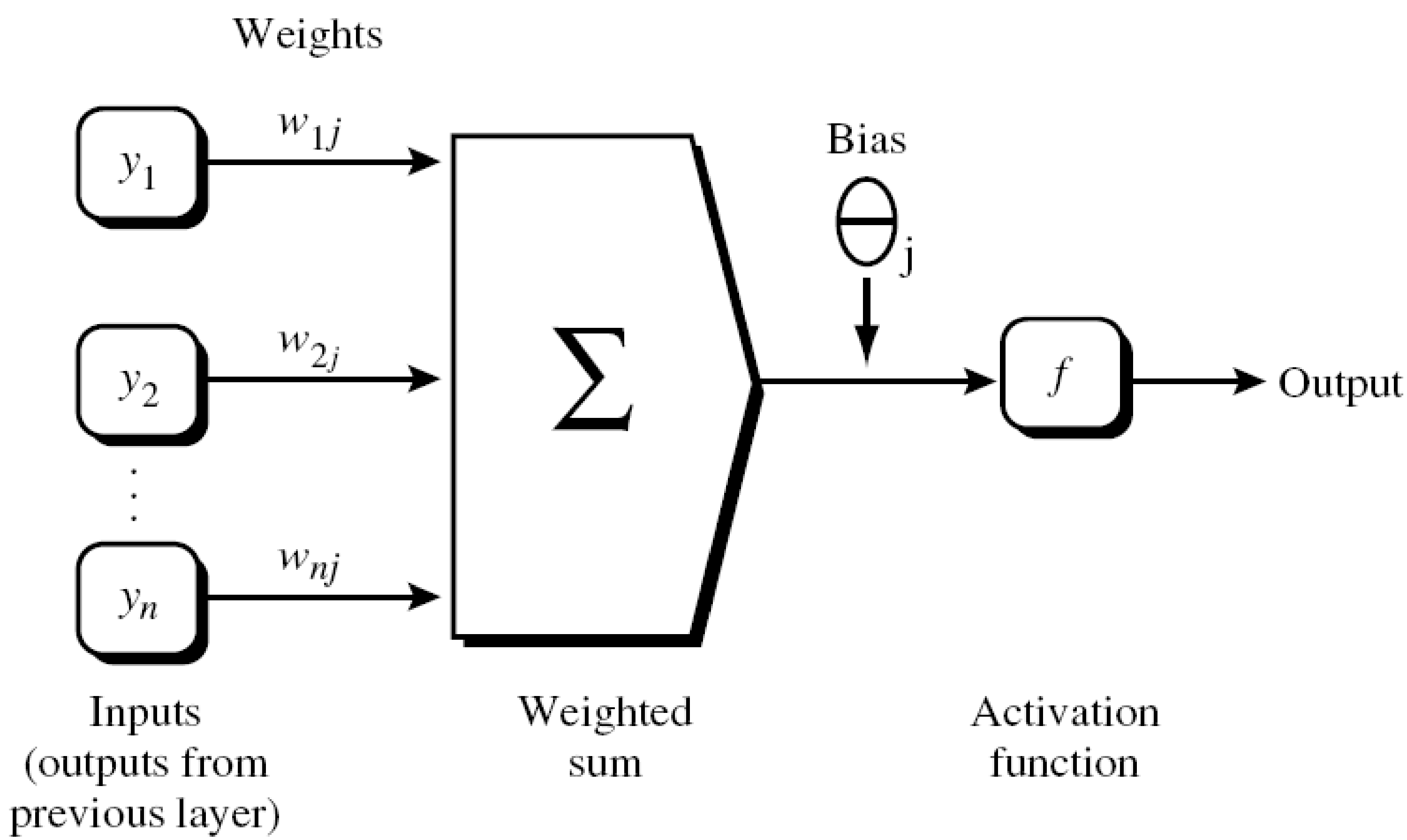
- b) compute the net input of each unit in the hidden and output layers
  - The net input to a unit in the hidden or output layers is computed as a linear combination of its inputs.
  - Given a unit *j* in a hidden or output layer, the net input, I_j, to unit *j* is

$$I_j = \sum_i w_{ij} O_i + \theta_j$$

    - where w_{ij} is the weight of the connection from unit i in the previous layer to unit j
    - O_i is the output of unit i from the previous layer
    - Θ_j is the bias of the unit

Propagate the inputs forward

- A hidden or output layer unit *j*



Propagate the inputs forward

- c) compute the output of each unit j in the hidden and output layers
  - The output of each unit is calculating by applying an activation function to its net input
  - The function symbolizes the activation of the neuron represented by the unit.
  - The **logistic**, or **sigmoid**, function is used.
  - Given the net input I_j to unit j, then O_j, the output of unit j, is computed as:

$$O_j = \frac{1}{1+e^{-I_j}}$$

Backpropagate the Error

- The error is propagated backward by updating the weights and biases to reflect the error of the network's prediction.
- a) compute the error for each unit j in the output layer
  - For a unit j in the output layer, the error Err_j is computed by

$$Err_j = O_j(1 - O_j)(T_j - O_j)$$

    - O_j is the actual output of unit j,
    - T_j is the known target value of the given training tuple
    - Note that O_j (1 - O_j) is the derivative of the logistic function.

Backpropagate the Error

- b) compute the error for each unit j in the hidden layers, from the last to the first hidden layer
  - The error of a hidden layer unit j is

$$Err_j = O_j(1 - O_j)\sum_k Err_k w_{jk}$$

    - w_{jk} is the weight of the connection from unit j to a unit k in the next higher layer, and
    - Err_k is the error of unit k.

Backpropagate the Error

- c) update the weights for each weight w_{ij} in network
  - Weights are updated by the following equations

$$w_{ij} = w_{ij} + \Delta w_{ij}$$

$$\Delta w_{ij} = (l) Err_j O_i$$

- Δw_{ij} is the change in weight w_{ij}
- The variable l is the **learning rate**, a constant typically having a value between 0.0 and 1.0

Backpropagate the Error

- Learning rate
  - Backpropagation learns using a method of gradient descent to search for a set of weights that fits the training data so as to minimize the mean squared distance between the network's class prediction and the known target value of the tuples.
  - The learning rate helps avoid getting stuck at a local minimum in decision space (i.e., where the weights appear to converge, but are not the optimum solution) and encourages finding the global minimum.
  - If the learning rate is too small, then learning will occur at a very slow pace.
  - If the learning rate is too large, then oscillation between inadequate solutions may occur.
  - A rule of thumb is to set the learning rate to 1/t, where t is the number of iterations through the training set so far.

Backpropagate the Error

- d) update the for each bias Θ_j in network
  - Biases are updated by the following equations below:

$$\theta_j = \theta_j + \Delta\theta_j$$

$$\Delta\theta_j = (l)Err_j$$

    - $\Delta\Theta_j$ is the change in bias Θ_j
  - Note that here we are updating the weights and biases after the presentation of each tuple.

Backpropagate the Error

- Updating strategies:
  - **Case updating**
    - updating the weights and biases after the presentation of each tuple.
    - case updating is more common because it tends to yield more accurate result
  - **Epoch updating**
    - the weight and bias increments could be accumulated in variables, so that the weights and biases are updated after all of the tuples in the training set have been presented.
    - one iteration through the training set is an epoch.

Terminating Condition

- Training stops when
  - All Δw_{ij} in the previous epoch were so small as to be below some specified threshold, or
  - The percentage of tuples misclassified in the previous epoch is below some threshold, or
  - A prespecified number of epochs has expired.

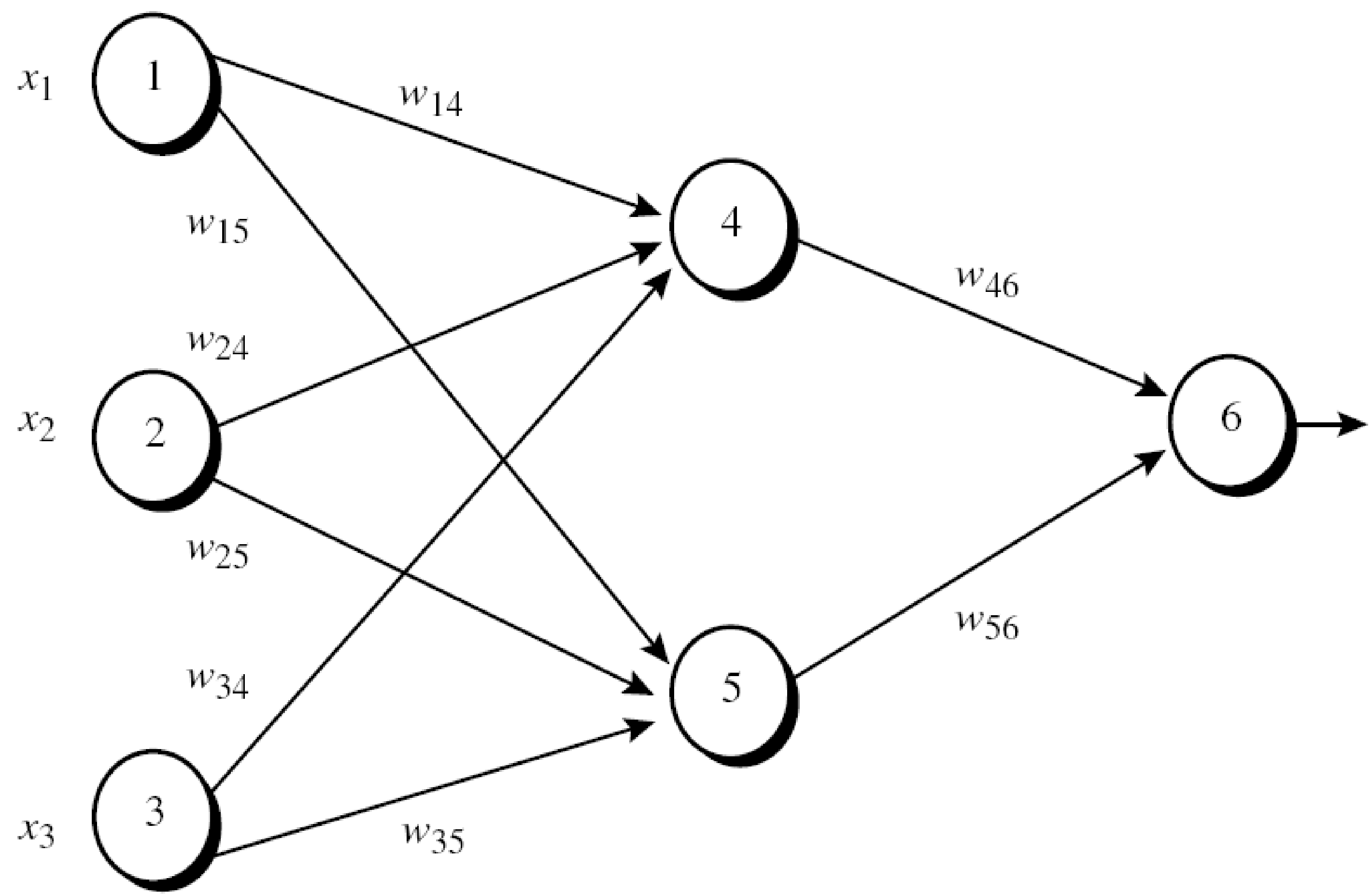
- In practice, several hundreds of thousands of epochs may be required before the weights will converge.

Efficiency of Backpropagation

- The computational efficiency depends on the time spent training the network.
- However, in the worst-case scenario, the number of epochs can be exponential in n, the number of inputs.
- In practice, the time required for the networks to converge is highly variable.
- A number of techniques exist that help speed up the training time.
  - For example, a technique known as **simulated annealing** can be used, which also ensures convergence to a global optimum.

Sample Calculations

- The Figure shows a multilayer feed-forward neural network



Sample Calculations

- Let the learning rate be 0.9.
- The initial weight and bias values of the network are given in the Table, along with the first training tuple, X = (1, 0, 1), whose class label is 1.

x_1	x_2	x_3	w_{14}	w_{15}	w_{24}	w_{25}	w_{34}	w_{35}	w_{46}	w_{56}	θ_4	θ_5	θ_6
1	0	1	0.2	−0.3	0.4	0.1	−0.5	0.2	−0.3	−0.2	−0.4	0.2	0.1

- This example shows the calculations for backpropagation, given the first training tuple, ***X.***

Sample Calculations

- The net input and output calculations:

Unit j	Net input, I_j	Output, O_j
4	$0.2+0-0.5-0.4=-0.7$	$1/(1+e^{0.7})=0.332$
5	$-0.3+0+0.2+0.2=0.1$	$1/(1+e^{-0.1})=0.525$
6	$(-0.3)(0.332)-(0.2)(0.525)+0.1=-0.105$	$1/(1+e^{0.105})=0.474$

- Calculation of the error at each node:

Unit j	Err_j
6	$(0.474)(1-0.474)(1-0.474)=0.1311$
5	$(0.525)(1-0.525)(0.1311)(-0.2)=-0.0065$
4	$(0.332)(1-0.332)(0.1311)(-0.3)=-0.0087$

Sample Calculations

- Calculations for weight and bias updating:

Weight or bias	*New value*
w_{46}	$-0.3+(0.9)(0.1311)(0.332)=-0.261$
w_{56}	$-0.2+(0.9)(0.1311)(0.525)=-0.138$
w_{14}	$0.2+(0.9)(-0.0087)(1)=0.192$
w_{15}	$-0.3+(0.9)(-0.0065)(1)=-0.306$
w_{24}	$0.4+(0.9)(-0.0087)(0)=0.4$
w_{25}	$0.1+(0.9)(-0.0065)(0)=0.1$
w_{34}	$-0.5+(0.9)(-0.0087)(1)=-0.508$
w_{35}	$0.2+(0.9)(-0.0065)(1)=0.194$
θ_6	$0.1+(0.9)(0.1311)=0.218$
θ_5	$0.2+(0.9)(-0.0065)=0.194$
θ_4	$-0.4+(0.9)(-0.0087)=-0.408$

Sample Calculations

- Several variations and alternatives to the backpropagation algorithm have been proposed for classification in neural networks.
- These may involve:
  - the dynamic adjustment of the network topology and of the learning rate or
  - other parameters, or
  - the use of different error functions.

Backpropagation and Interpretability

Backpropagation and Interpretability

- Neural networks are like a black box.
- A major disadvantage of neural networks lies in their knowledge representation.
- Acquired knowledge in the form of a network of units connected by weighted links is difficult for humans to interpret.
- This factor has motivated research in extracting the knowledge embedded in trained neural networks and in representing that knowledge symbolically.
- Methods include:
  - **extracting rules from networks**
  - **sensitivity analysis**

Backpropagation and Interpretability

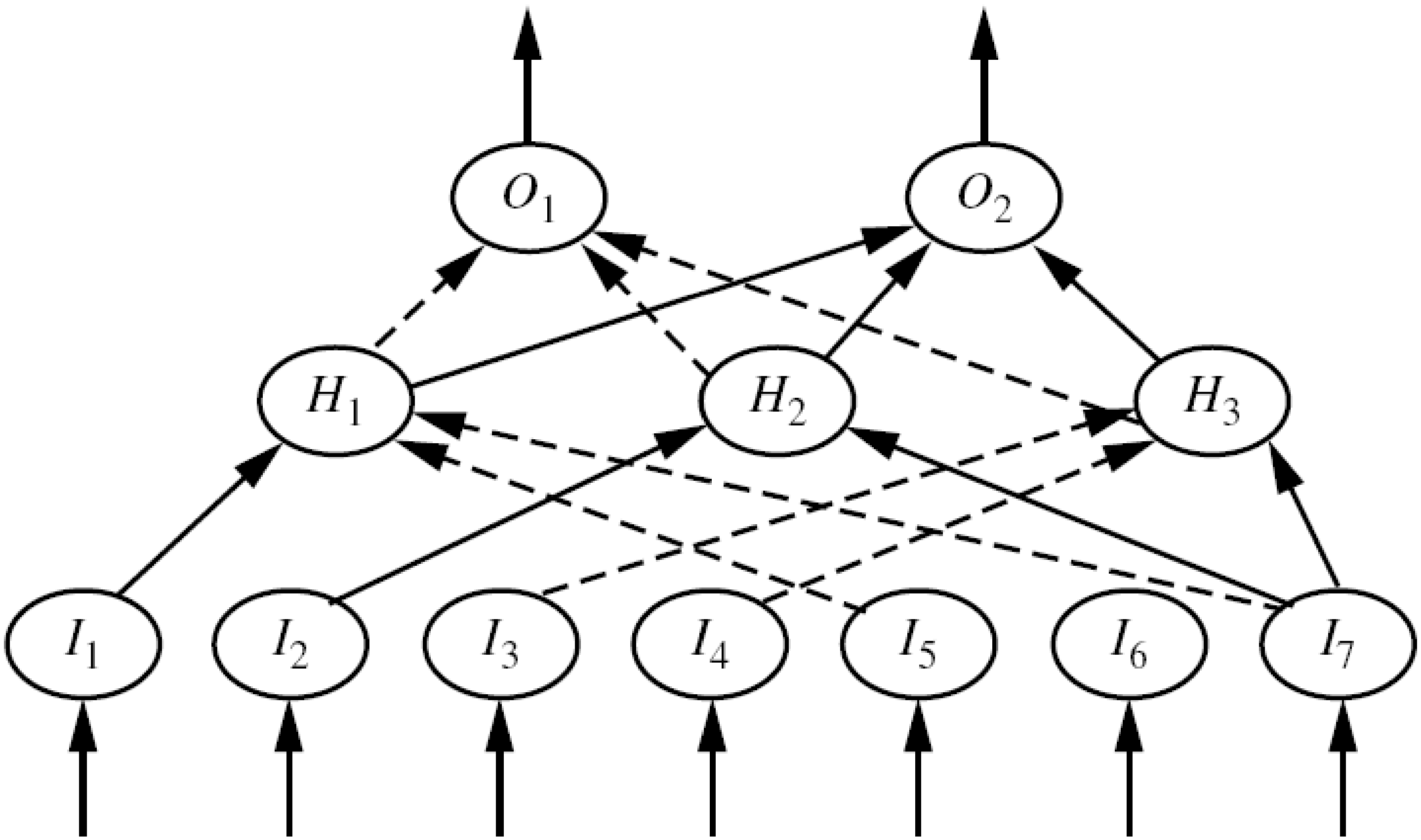
- Often the first step toward extracting rules from neural networks is **network pruning**
  - This consists of simplifying the network structure by removing weighted links that have the least effect on the trained network.

Backpropagation and Interpretability

- Rule extraction from networks
  - Often, the first step toward extracting rules from neural networks is **network pruning**.
    - This consists of simplifying the network structure by removing weighted links that have the least effect on the trained network
  - Then perform link, unit, or activation value clustering
    - In one method, for example, clustering is used to find the set of common activation values for each hidden unit in a given trained two-layer neural network.
  - The set of input and activation values are studied to derive rules describing the relationship between the input and hidden unit layers

Backpropagation and Interpretability

- Rules can be extracted from training neural networks



Backpropagation and Interpretability

Identify sets of common activation values for each hidden node, H_i:

for H_1: (–1,0,1)

for H_2: (0.1)

for H_3: (–1,0.24,1)

Derive rules relating common activation values with output nodes, O_j:

IF ($H_2 = 0$ AND $H_3 = -1$) OR

($H_1 = -1$ AND $H_2 = 1$ AND $H_3 = -1$) OR

($H_1 = -1$ AND $H_2 = 0$ AND $H_3 = 0.24$)

THEN $O_1 = 1$, $O_2 = 0$

ELSE $O_1 = 0$, $O_2 = 1$

Derive rules relating input nodes, I_j, to output nodes, O_j:

IF ($I_2 = 0$ AND $I_7 = 0$) THEN $H_2 = 0$

IF ($I_4 = 1$ AND $I_6 = 1$) THEN $H_3 = -1$

IF ($I_5 = 0$) THEN $H_3 = -1$

Obtain rules relating inputs and output classes:

IF ($I_2 = 0$ AND $I_7 = 0$ AND $I_4 = 1$ AND $I_6 = 1$) THEN class = 1

IF ($I_2 = 0$ AND $I_7 = 0$ AND $I_5 = 0$) THEN class = 1

Backpropagation and Interpretability

- **Sensitivity analysis**
  - assess the impact that a given input variable has on a network output.
  - The knowledge gained from this analysis can be represented in rules
  - Such as “IF X decreases 5% THEN Y increases 8%.”

Discussion

Discussion

- Weakness of neural networks
  - Long training time
  - Require a number of parameters typically best determined empirically, e.g., the network topology or ``structure."
  - Poor interpretability: Difficult to interpret the symbolic meaning behind the learned weights and of “hidden units” in the network

Discussion

- Strength of neural networks
  - High tolerance to noisy data
  - It can be used when you may have little knowledge of the relationships between attributes and classes
  - Well-suited for continuous-valued inputs and outputs
  - Successful on a wide array of real-world data
  - Algorithms are inherently parallel
  - Techniques have recently been developed for the extraction of rules from trained neural networks

Research Areas

- Finding optimal network structure
  - e.g. by genetic algorithms
- Increasing learning speed (efficiency)
  - e.g. by simulated annealing
- Increasing accuracy (effectiveness)
- Extracting rules from networks
- Stack generalization

References

References

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- S. J. Russell and P. Norvig, **Artificial Intelligence, A Modern Approach**, Prentice Hall,1995. (Chapter 19)

The end