Neural Networks

Part 1

Chapter 18

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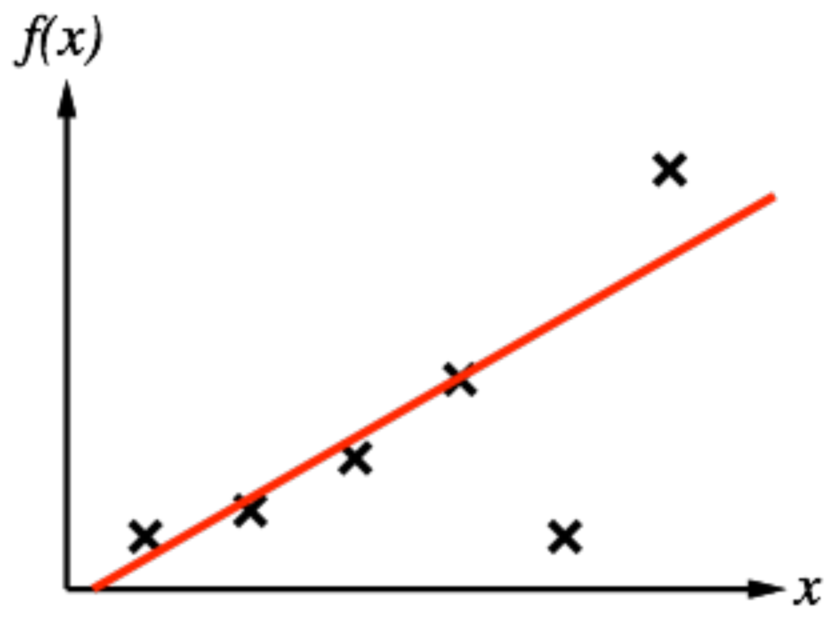
More Supervised Learning Methods

- Neural Networks
- Support Vector Machines (SVMs)
- k-Nearest Neighbors (KNN)
- Ensemble methods

Linear Regression

Linear Regression

Find the best linear fit to our data



Linear Regression

Find the best linear fit to our data

Hypothesis h parameterized by weights w

$$y = h(x; w) = w_1 x + w_0$$

Loss function $L(D;w)$ defines goodness of fit

$$L(D; w) = \sum_{j=1}^{N} (y_j - h(x_j; w))^2 = \sum_{j=1}^{N} (y_j - (w_1 x_j + w_0))^2$$

Find weight vector that minimizes loss:

$$w^* = \arg\min_w L(D; w) \quad \Rightarrow \quad \text{Solve } \frac{\partial L}{\partial w_i} = 0$$

Gradient Descent

$w \leftarrow$ Any point in parameter (weight) space

Loop until convergence **do**

For each i **do**

$$w_i \leftarrow \quad w_i - \alpha \frac{\partial L}{\partial w_i}$$

A variant of this method for discrete classification is called the *perceptron learning rule*

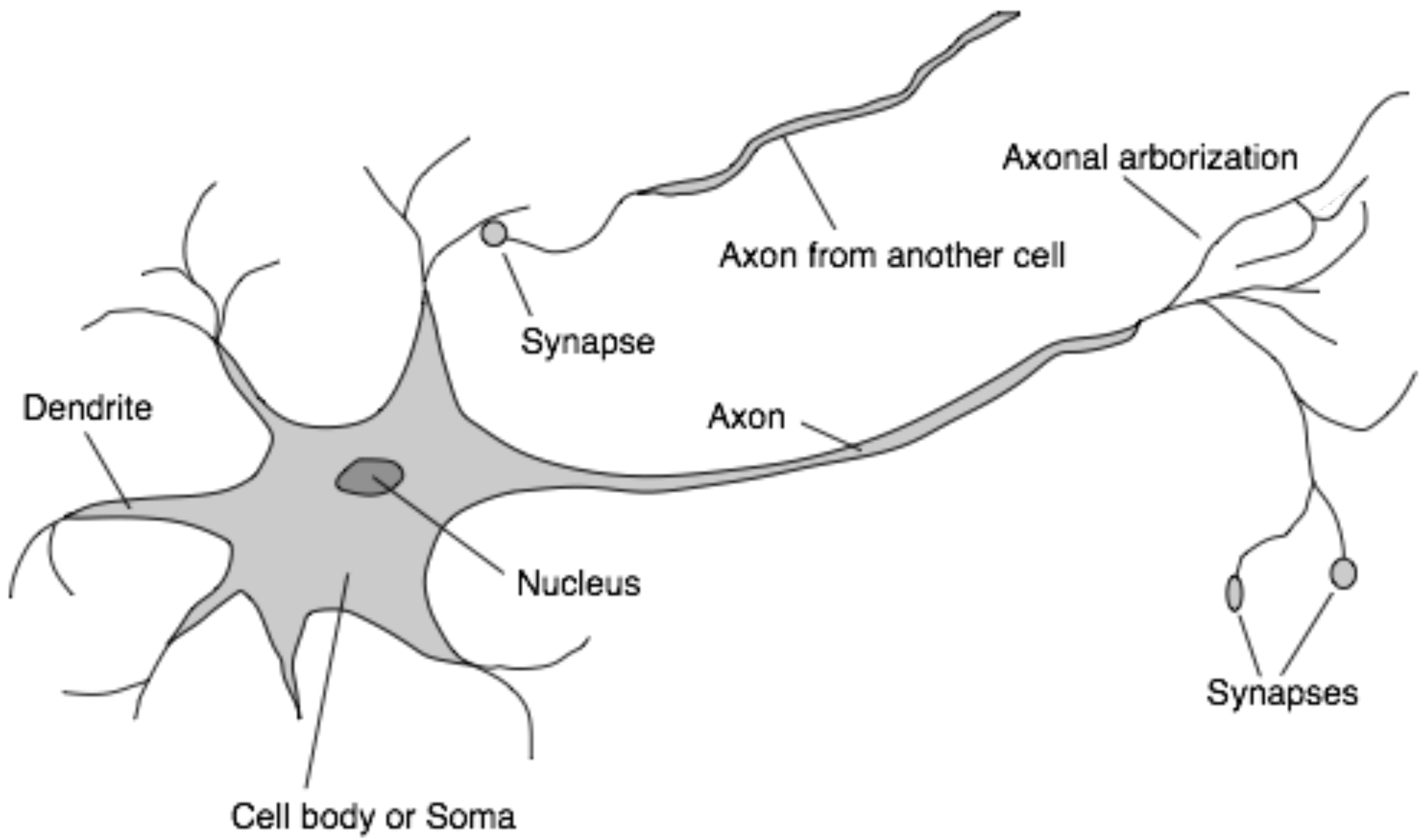
Neural Nets

Outline

- Brains
- Neural Networks
- Perceptrons
- Multilayer Perceptrons
- Applications of NNets

Brains

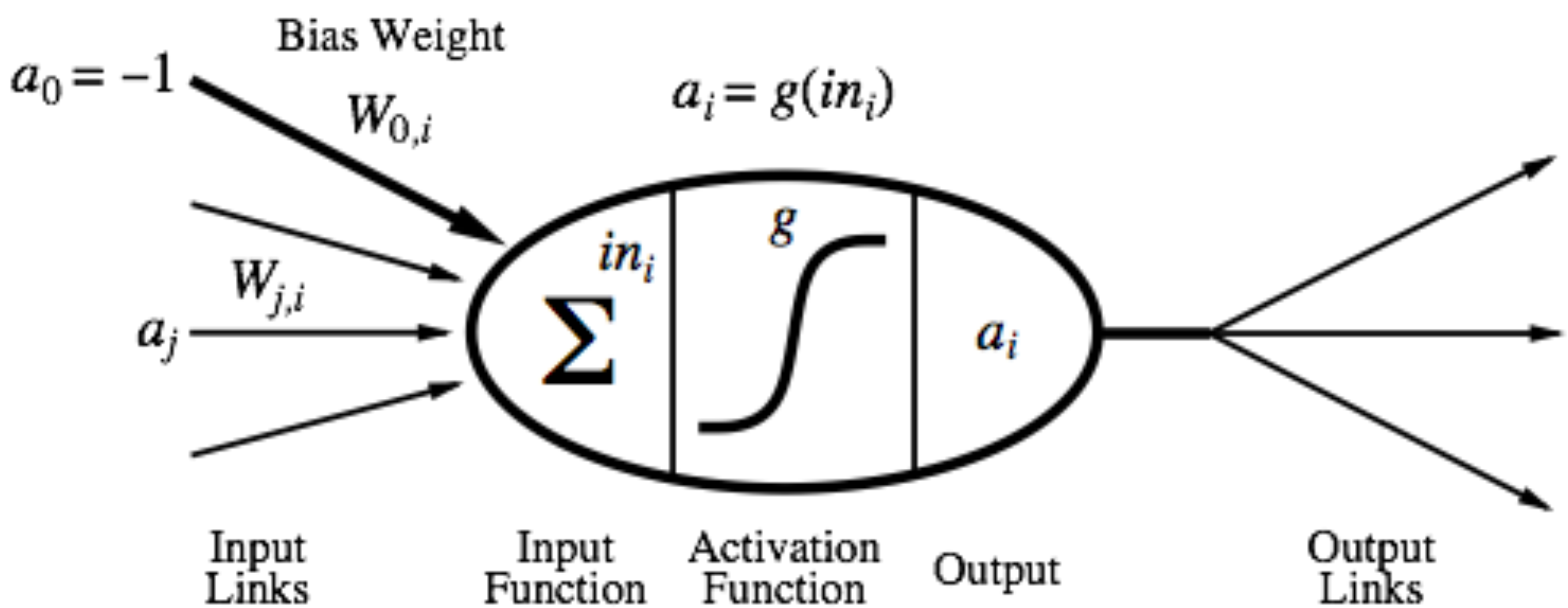
10^{11} neurons of > 20 types, 10^{14} synapses, 1ms–10ms cycle time
Signals are noisy "spike trains" of electrical potential



McCulloch-Pitts "unit"

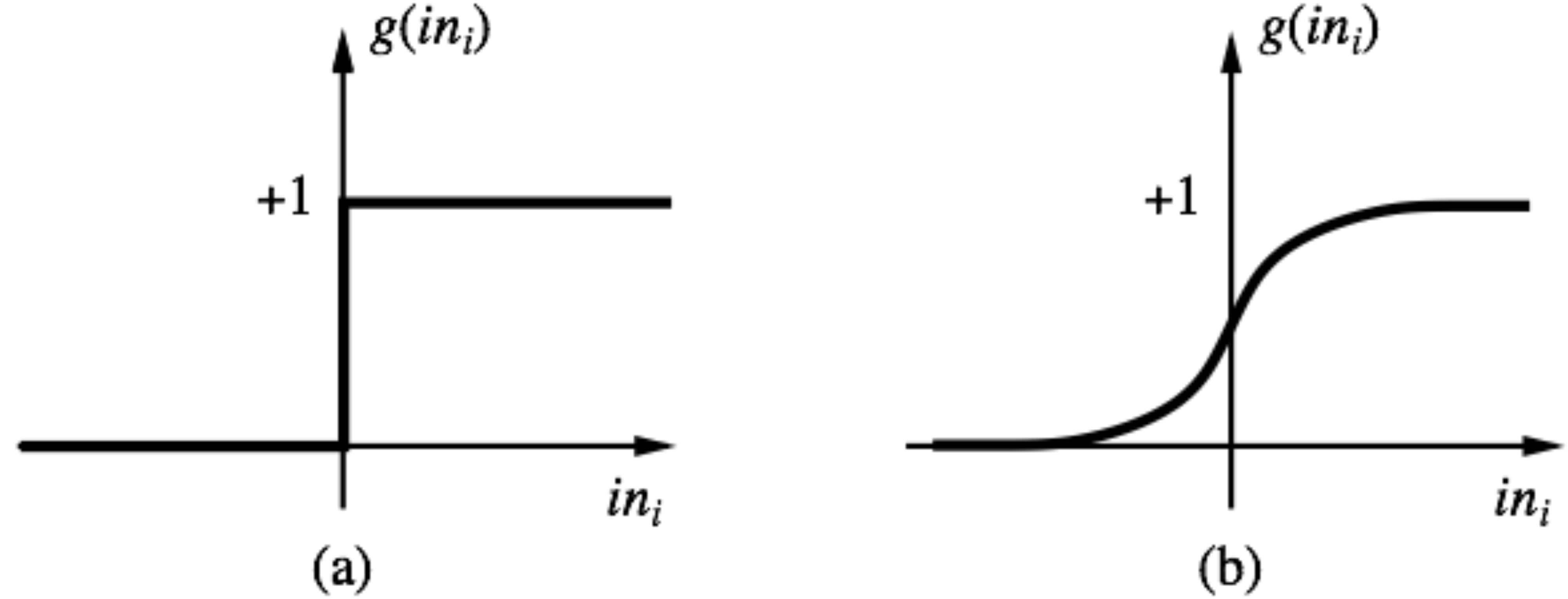
Output is a "squashed" linear function of the inputs:

$$a_i \leftarrow g(in_i) = g\left(\Sigma_j W_{j,i} a_j\right)$$



A gross oversimplification of real neurons, but its purpose is to develop understanding of what networks of simple units can do

Activation Functions

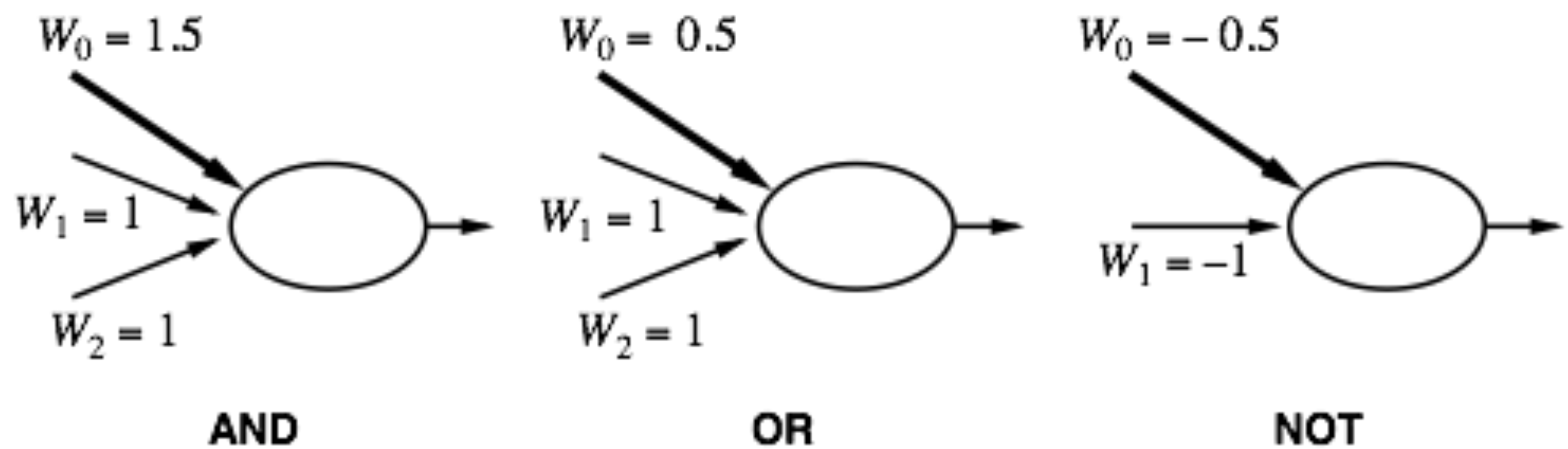


(a) is a step function or threshold function

(b) is a sigmoid function $1/(1 + e^{-x})$

Changing the bias weight $W_{0,i}$ moves the threshold location

Implementing Logic Functions



McCulloch and Pitts: every Boolean function can be implemented

Network Structures

Feed-forward networks:

- single-layer perceptrons
- multi-layer perceptrons

Feed-forward networks implement functions, have no internal state

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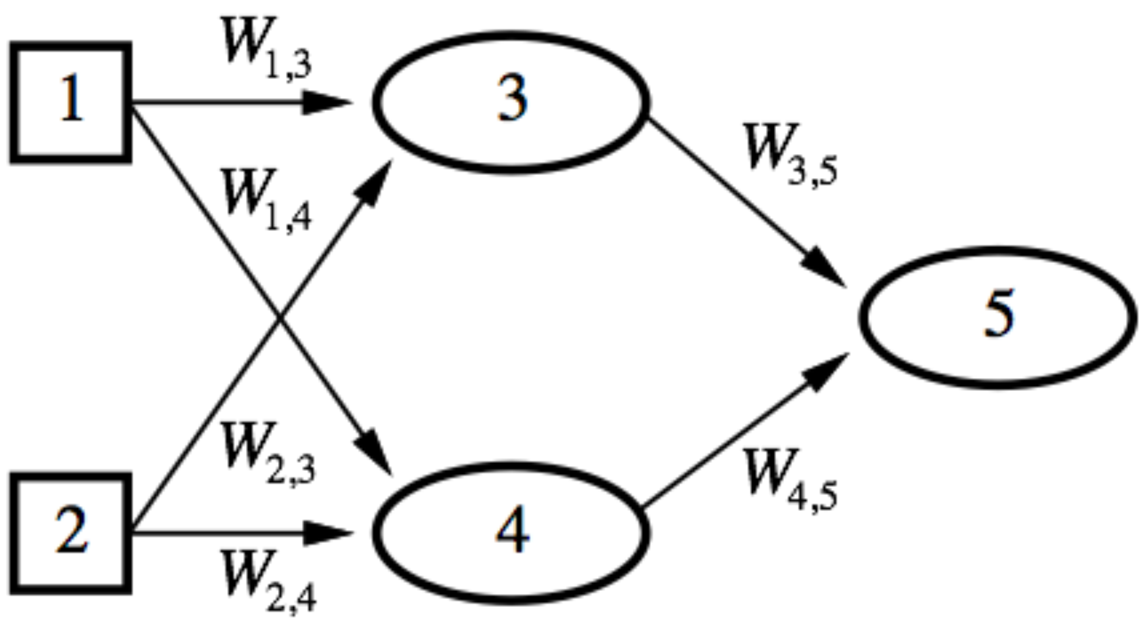
Recurrent networks:
- Hopfield networks have symmetric weights ($W_{i,j} = W_{j,i}$)
  $g(x) = \text{sign}(x)$, $a_i = \pm 1$; **holographic associative memory**
- Boltzmann machines use stochastic activation functions,
  $\approx$ MCMC in Bayes nets
- recurrent neural nets have directed cycles with delays
  $\Rightarrow$ have internal state (like flip-flops), can oscillate etc.

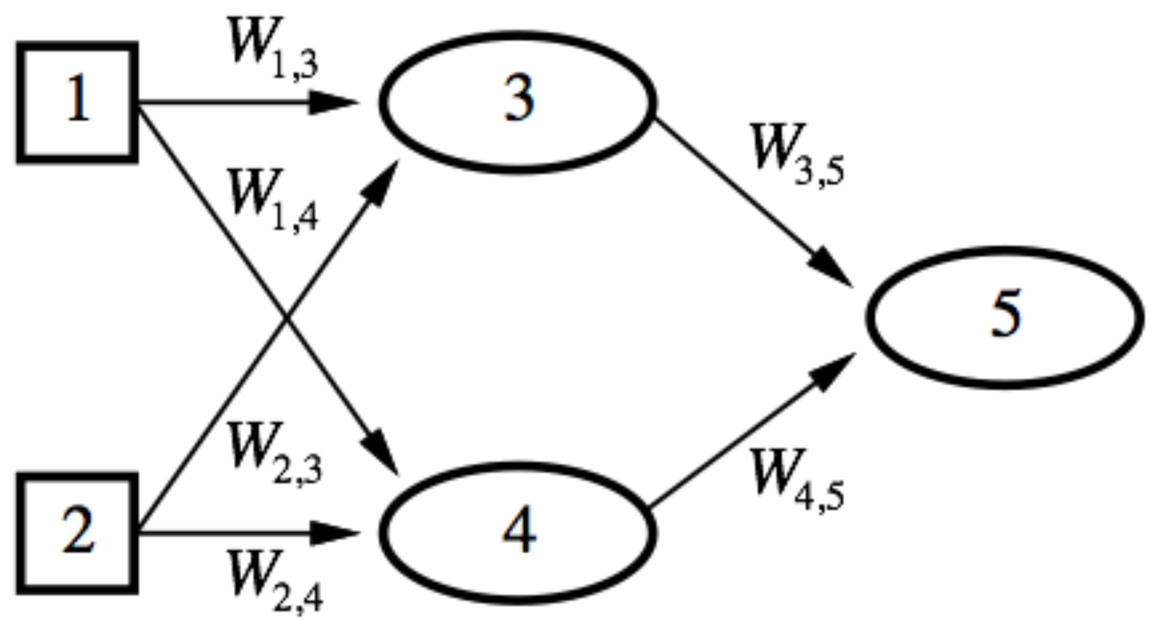
Feed-forward Example



Feed-forward network = a parameterized family of nonlinear functions:

$$a_5 = g(W_{3,5} \cdot a_3 + W_{4,5} \cdot a_4)$$

Feed-forward Example

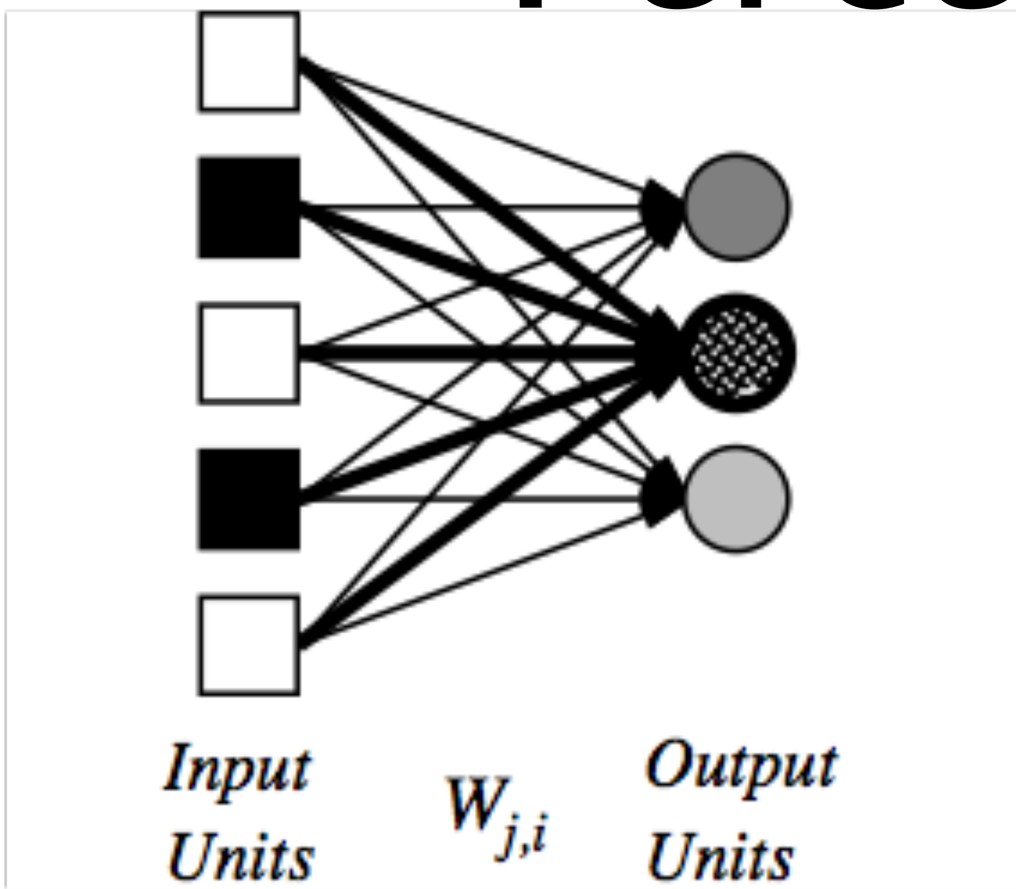


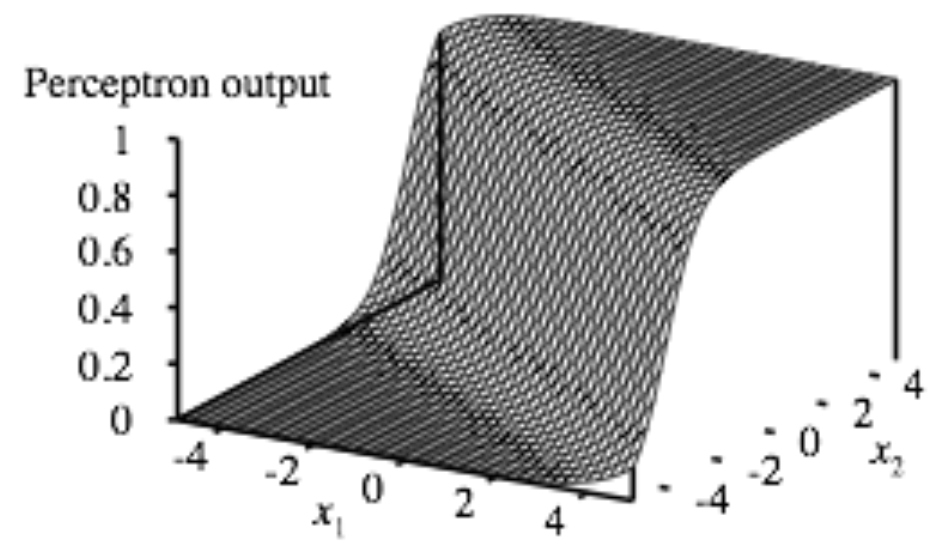
Feed-forward network = a parameterized family of nonlinear functions:

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

Adjusting weights changes the function: do learning this way!

Single-layer Perceptrons





Output units all operate separately—no shared weights

Adjusting weights moves the location, orientation, and steepness of cliff

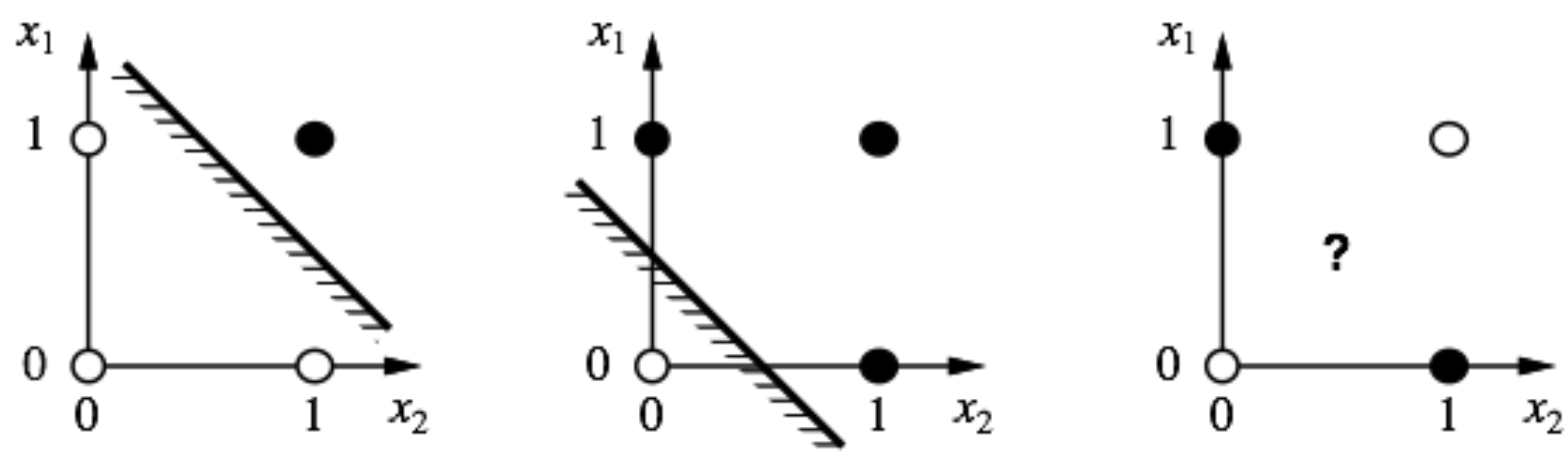
Single-layer Perceptrons

Consider a perceptron with g = step function (Rosenblatt, 1957, 1960)

Can represent AND, OR, NOT, majority, etc., but not XOR

Represents a linear separator in input space:

$$\Sigma_j W_j x_j > 0 \quad \text{or} \quad \mathbf{W} \cdot \mathbf{x} > 0$$



(a) x_1 **and** x_2 (b) x_1 **or** x_2 (c) x_1 **xor** x_2

Minsky & Papert (1969) pricked the neural network balloon

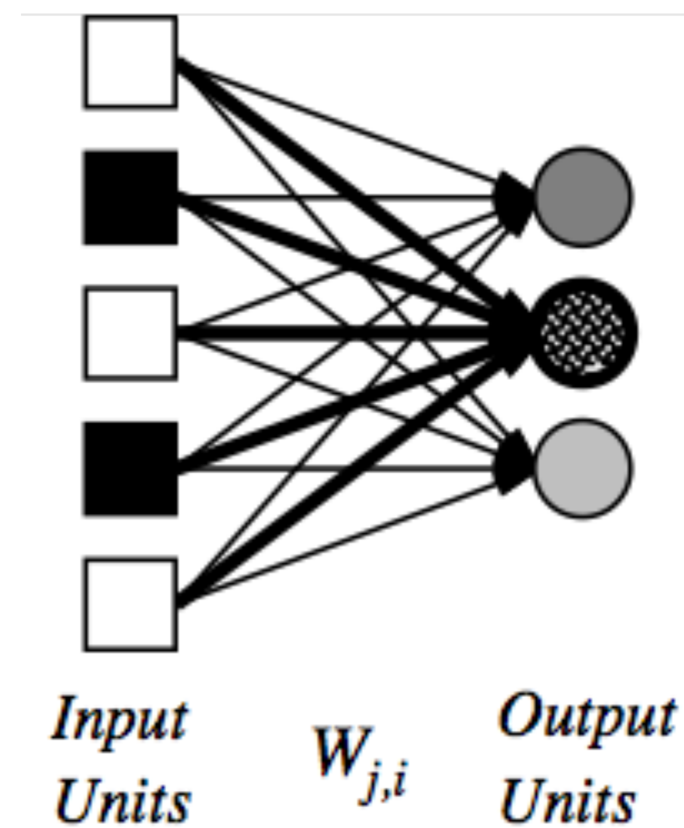
Perceptron Learning

Learn by adjusting weights to reduce error on training set

The squared error for an example with input $\mathbf{x}$ and true output y is

$$E = \frac{1}{2}Err^2 \equiv \frac{1}{2}(y - h_{\mathbf{W}}(\mathbf{x}))^2 \ ,$$

Why is it squared?



Perceptron Learning

Learn by adjusting weights to reduce error on training set

The squared error for an example with input $\mathbf{x}$ and true output y is

$$E = \frac{1}{2}Err^2 \equiv \frac{1}{2}(y - h_{\mathbf{W}}(\mathbf{x}))^2 \ ,$$

Perform optimization search by gradient descent:

$$\begin{aligned}\frac{\partial E}{\partial W_j} &= Err \times \frac{\partial Err}{\partial W_j} = Err \times \frac{\partial}{\partial W_j}\left(y - g(\Sigma_{j=0}^{n} W_j x_j)\right) \\ &= -Err \times g'(in) \times x_j\end{aligned}$$

Simple weight update rule:

$$W_j \leftarrow W_j + \alpha \times Err \times g'(in) \times x_j$$

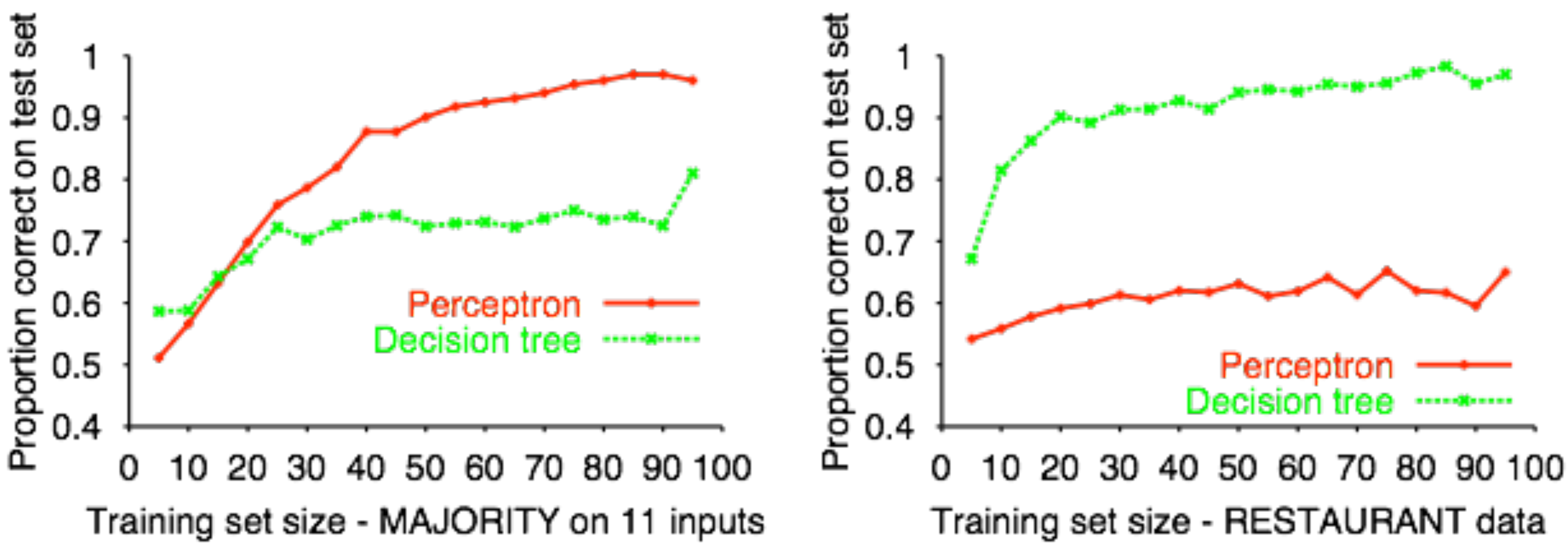
E.g., +ve error $\Rightarrow$ increase network output
$\Rightarrow$ increase weights on +ve inputs, decrease on -ve inputs

Perceptron Learning

- Algorithm:
  - Initialize network weights to random values
  - Consider each training example 1 at a time
  - Adjust weights after each example
  - One pass through the examples is an epoch,
  - Repeat for multiple epochs until a stopping condition is met: e.g, when changes to weights become small then a local minima in the search has been reached.

Perceptron Learning

Perceptron learning rule converges to a consistent function
for any linearly separable data set



Perceptron learns majority function easily, DTL is hopeless

DTL learns restaurant function easily, perceptron cannot represent it

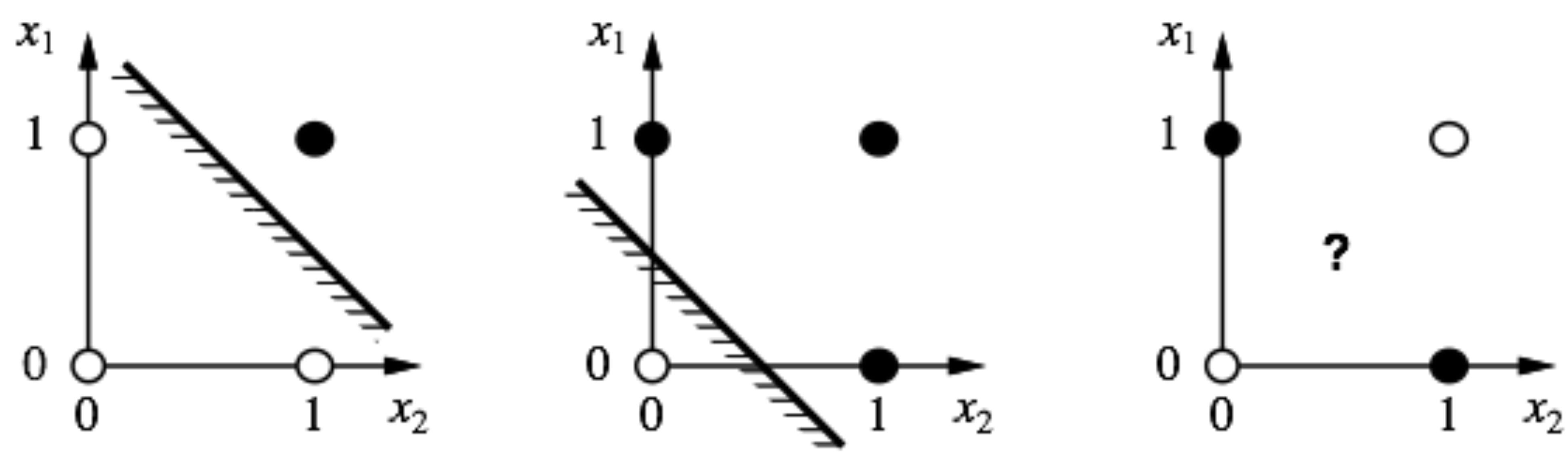
Single-layer Perceptrons

Consider a perceptron with $g =$ step function (Rosenblatt, 1957, 1960)

Can represent AND, OR, NOT, majority, etc., but not XOR

Represents a linear separator in input space:

$\Sigma_j W_j x_j > 0$ or $\mathbf{W} \cdot \mathbf{x} > 0$

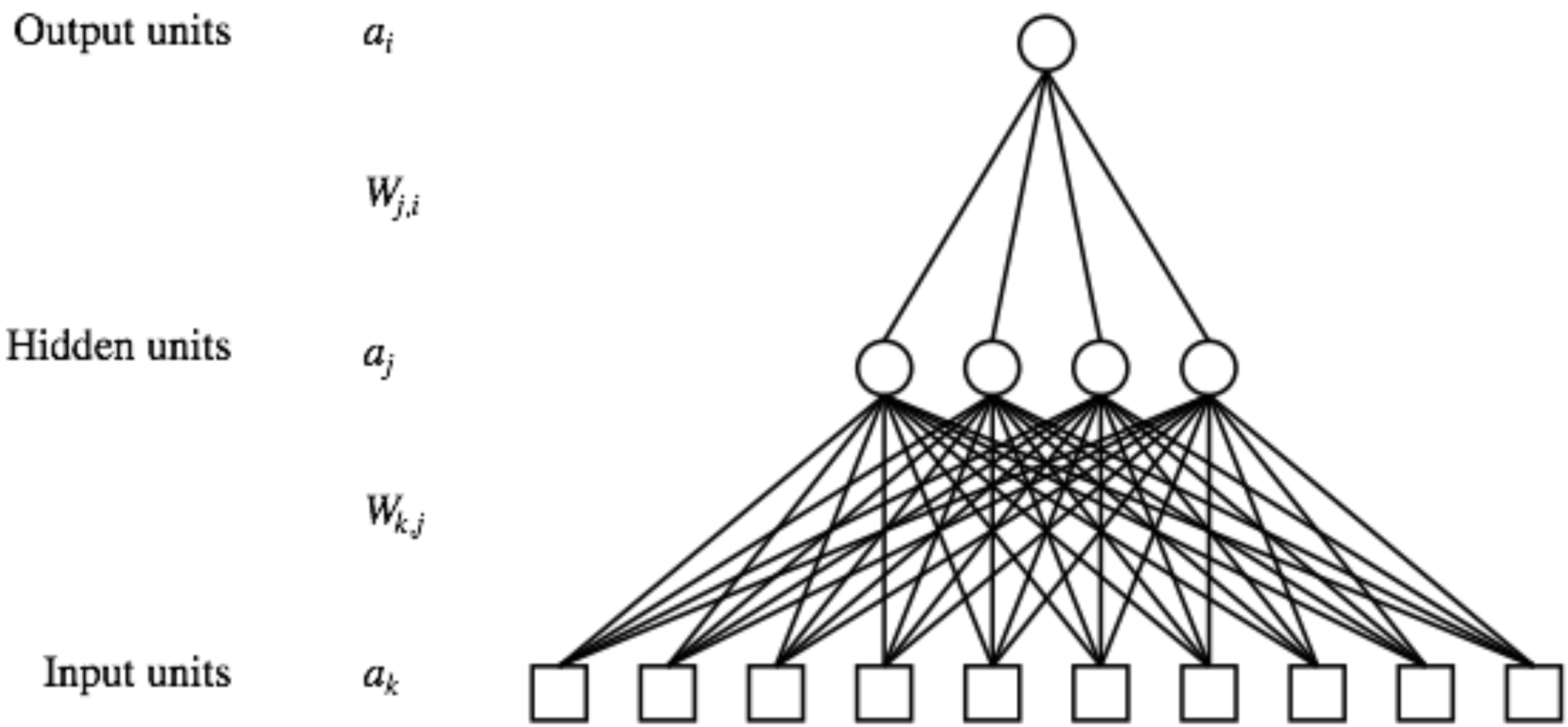


(a) x_1 **and** x_2 (b) x_1 **or** x_2 (c) x_1 **xor** x_2

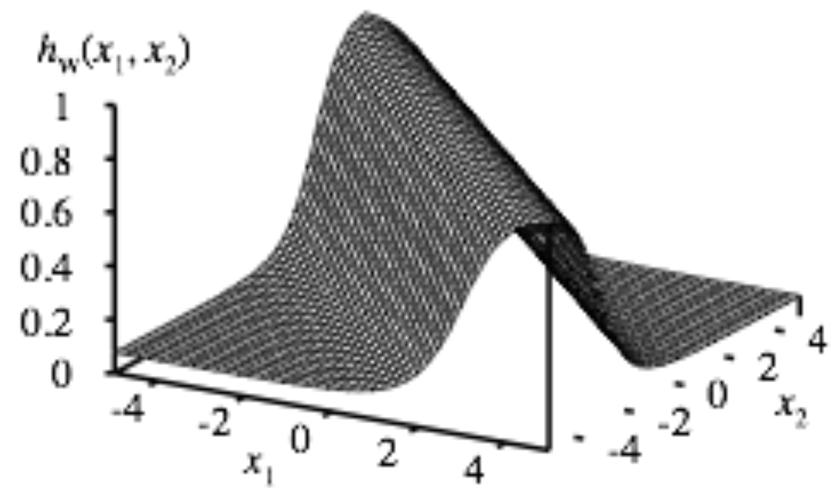
Minsky & Papert (1969) pricked the neural network balloon

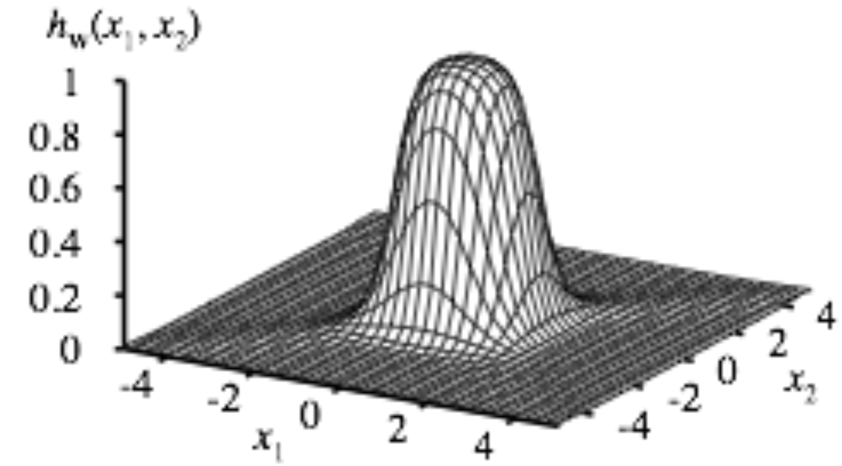
Multi-layer Perceptrons

Layers are usually fully connected;
numbers of hidden units typically chosen by hand



Multi-layer Perceptrons





Combine two opposite-facing threshold functions to make a ridge

Combine two perpendicular ridges to make a bump

Add bumps of various sizes and locations to fit any surface

Proof requires exponentially many hidden units (cf DTL proof)

Learning Multi-layer NNets

- Before we just updated a single layer of weights based on the error
- Now we need to propagate the error from the 2nd layer back to the 1st layer
- Algorithm: Back-propagation

Back-propagation Learning

Output layer: same as for single-layer perceptron,

$$W_{j,i} \leftarrow W_{j,i} + \alpha \times a_j \times \Delta_i$$

where $\Delta_i = Err_i \times g'(in_i)$

Hidden layer: **back-propagate** the error from the output layer:

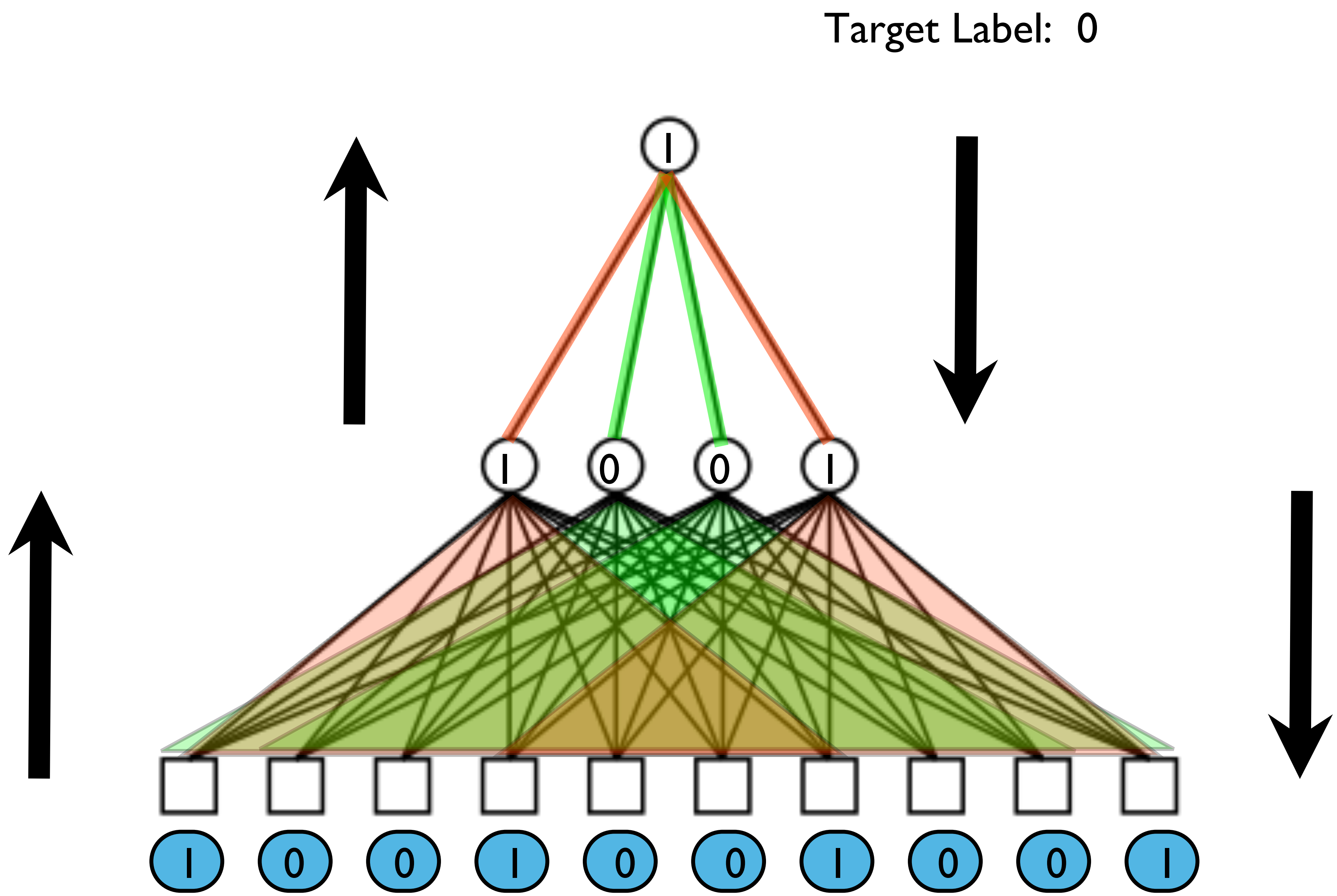
$$\Delta_j = g'(in_j) \sum_i W_{j,i} \Delta_i \ .$$

Update rule for weights in hidden layer:

$$W_{k,j} \leftarrow W_{k,j} + \alpha \times a_k \times \Delta_j \ .$$

(Most neuroscientists deny that back-propagation occurs in the brain)

Ex: Back Propagation



BackProp Learning

- Algorithm -- similar to Perceptron
  - Initialize network weights to random values
  - Consider each training example 1 at a time
  - Compute error at each output node, update weights
  - Propagate error back to previous layer, update weights
  - One pass through the examples is an epoch, repeat for multiple epochs until a stopping condition

Back-propagation Derivation

The squared error on a single example is defined as

$$E = \frac{1}{2}\sum_i (y_i - a_i)^2 \ ,$$

where the sum is over the nodes in the output layer.

$$\begin{aligned}
\frac{\partial E}{\partial W_{j,i}} &= -(y_i - a_i)\frac{\partial a_i}{\partial W_{j,i}} = -(y_i - a_i)\frac{\partial g(in_i)}{\partial W_{j,i}} \\
&= -(y_i - a_i)g'(in_i)\frac{\partial in_i}{\partial W_{j,i}} = -(y_i - a_i)g'(in_i)\frac{\partial}{\partial W_{j,i}}\left(\sum_j W_{j,i}a_j\right) \\
&= -(y_i - a_i)g'(in_i)a_j = -a_j\Delta_i
\end{aligned}$$

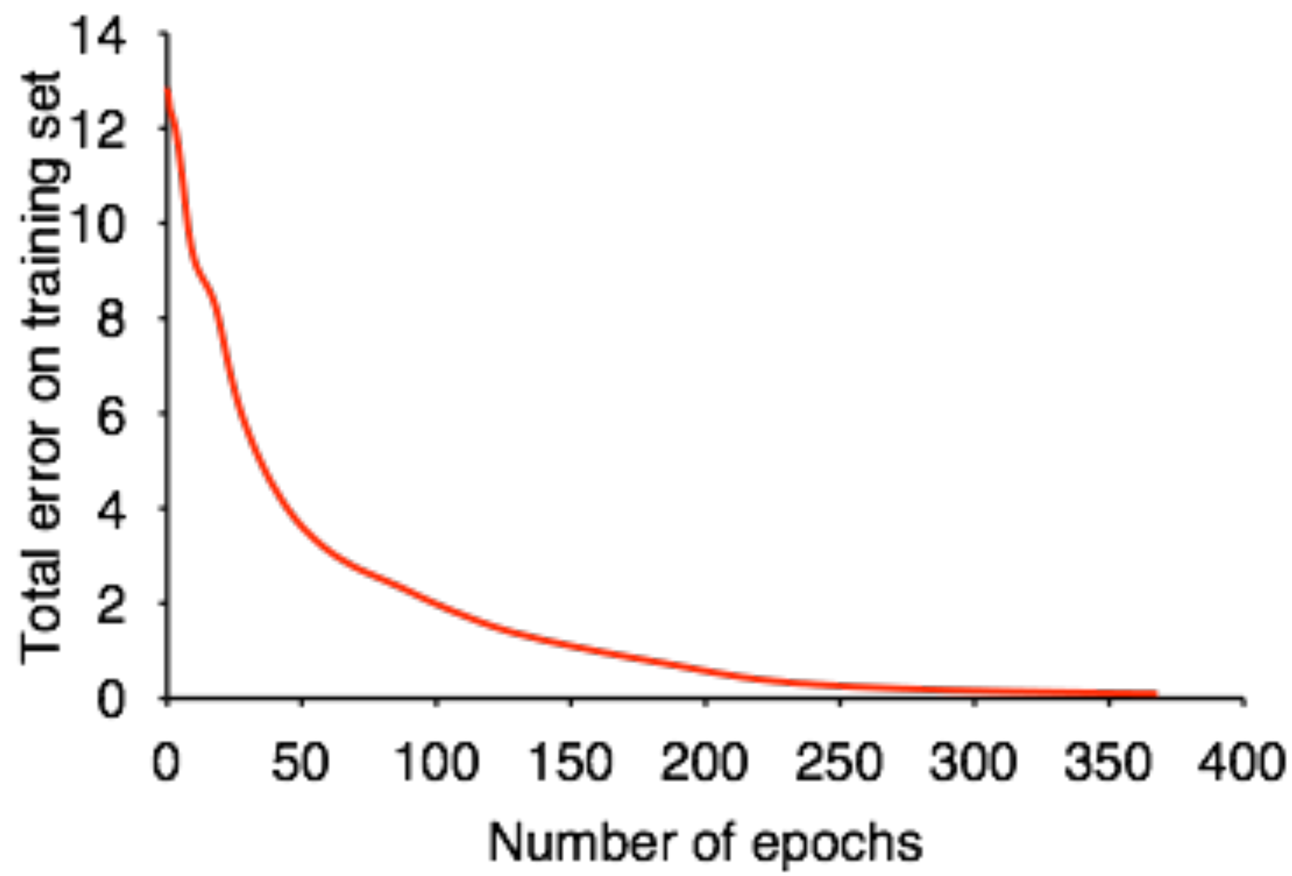
Back-propagation Derivation

$$
\begin{aligned}
\frac{\partial E}{\partial W_{k,j}} &= -\sum_i (y_i - a_i)\frac{\partial a_i}{\partial W_{k,j}} = -\sum_i (y_i - a_i)\frac{\partial g(in_i)}{\partial W_{k,j}} \\
&= -\sum_i (y_i - a_i) g'(in_i)\frac{\partial in_i}{\partial W_{k,j}} = -\sum_i \Delta_i \frac{\partial}{\partial W_{k,j}}\left(\sum_j W_{j,i} a_j\right) \\
&= -\sum_i \Delta_i W_{j,i}\frac{\partial a_j}{\partial W_{k,j}} = -\sum_i \Delta_i W_{j,i}\frac{\partial g(in_j)}{\partial W_{k,j}} \\
&= -\sum_i \Delta_i W_{j,i} g'(in_j)\frac{\partial in_j}{\partial W_{k,j}} \\
&= -\sum_i \Delta_i W_{j,i} g'(in_j)\frac{\partial}{\partial W_{k,j}}\left(\sum_k W_{k,j} a_k\right) \\
&= -\sum_i \Delta_i W_{j,i} g'(in_j) a_k = -a_k \Delta_j
\end{aligned}
$$

Back-propagation Learning

At each epoch, sum gradient updates for all examples and apply

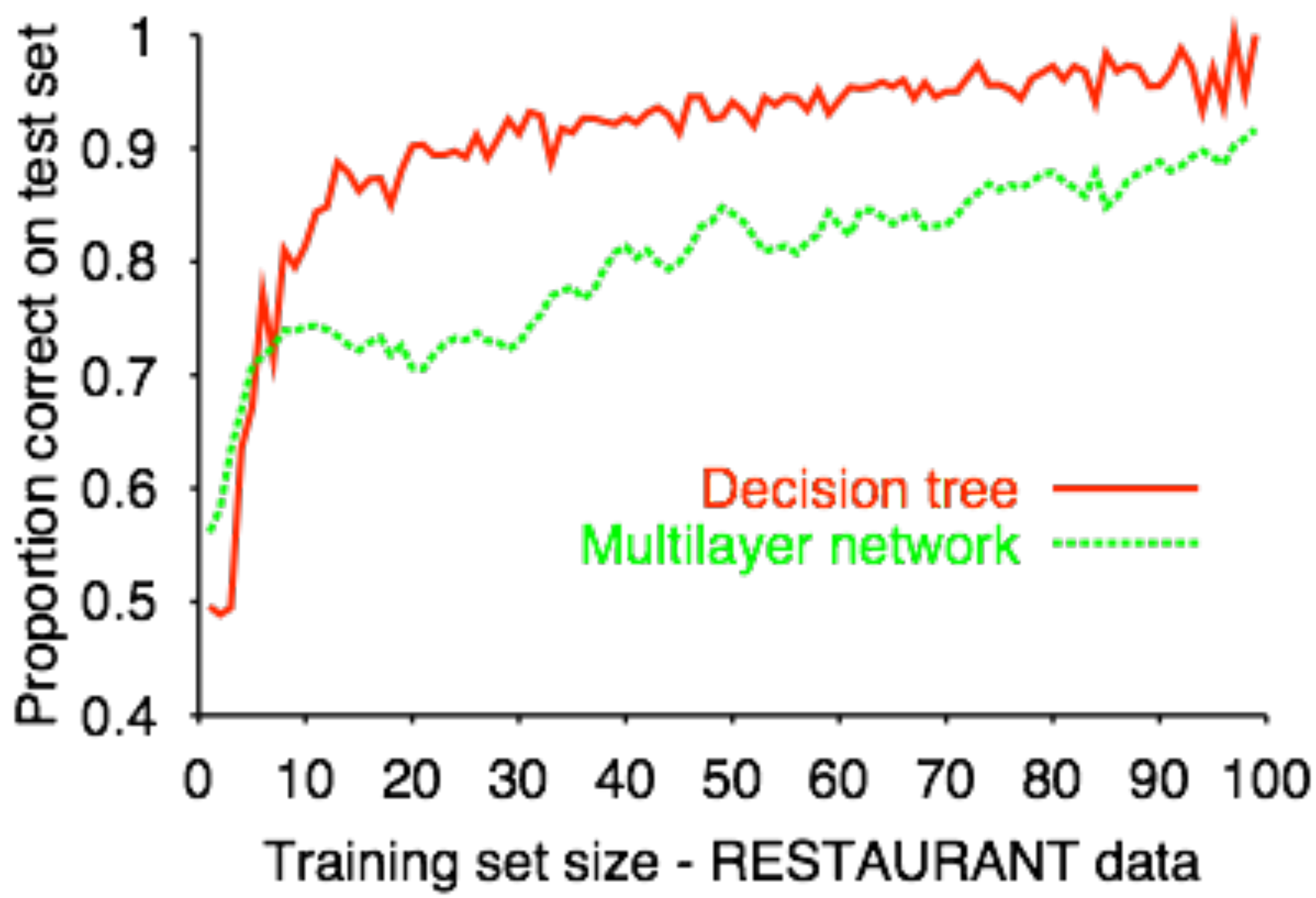
Training curve for 100 restaurant examples: finds exact fit



Typical problems: slow convergence, local minima

Back-propagation Learning

Learning curve for MLP with 4 hidden units:



MLPs are quite good for complex pattern recognition tasks, but resulting hypotheses cannot be understood easily