Machine learning: Part 3

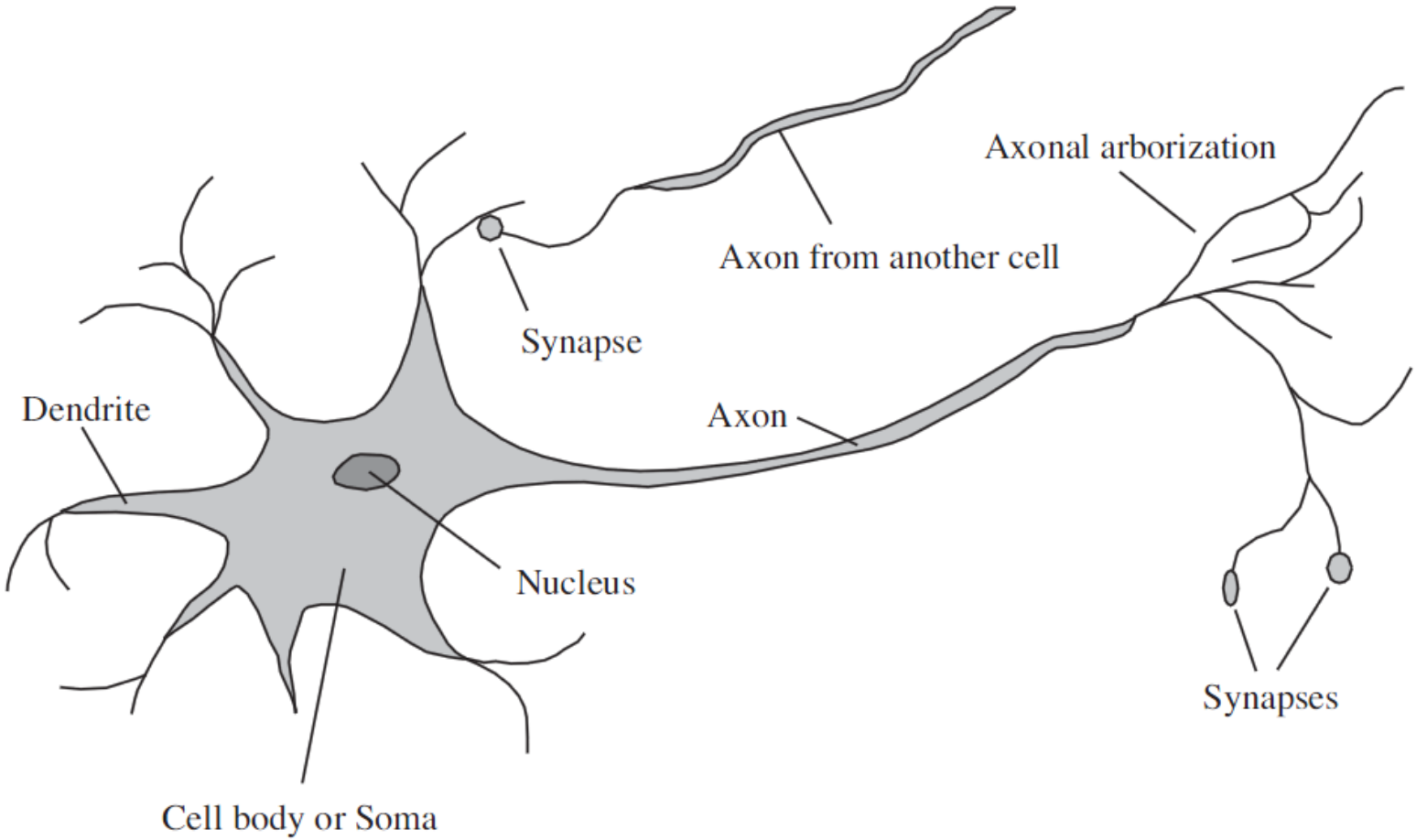
- Linear and logistic regression
- Backpropagation for neural nets

Slides based on those of Pascal Poupart

Brain

- Seat of human intelligence
- Where memory/knowledge resides
- Responsible for thoughts and decisions
- Can learn
- Consists of nerve cells called neurons

Neuron

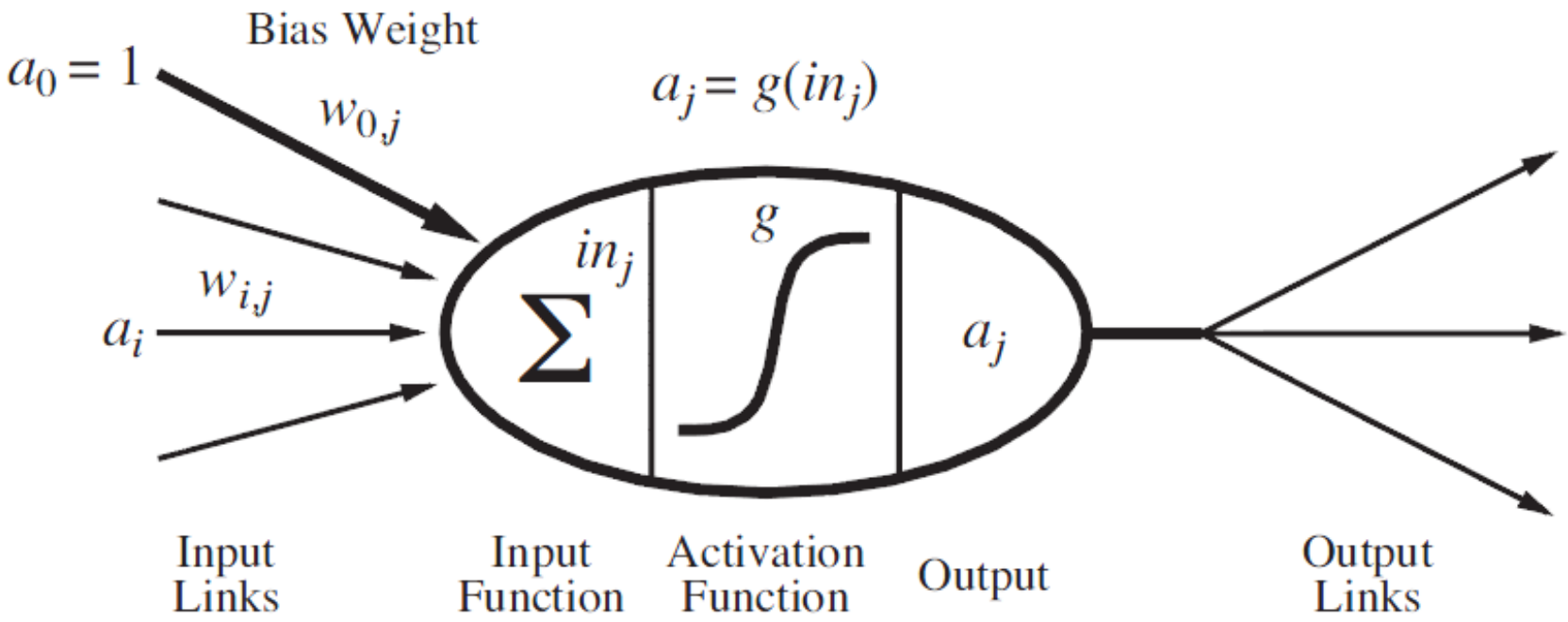


A neuron makes connections with 10 to 100,000 other neurons at junctions called synapse (突触)

Artificial Neural Networks

- Idea: mimic the brain to do computation
- Artificial neural network:
  - Nodes (a.k.a. units) correspond to neurons
  - Links correspond to synapses
- Computation:
  - Numerical signal transmitted between nodes corresponds to chemical signals between neurons
  - Nodes modifying numerical signal correspond to neurons firing rate

A simple mathematical model of neuron



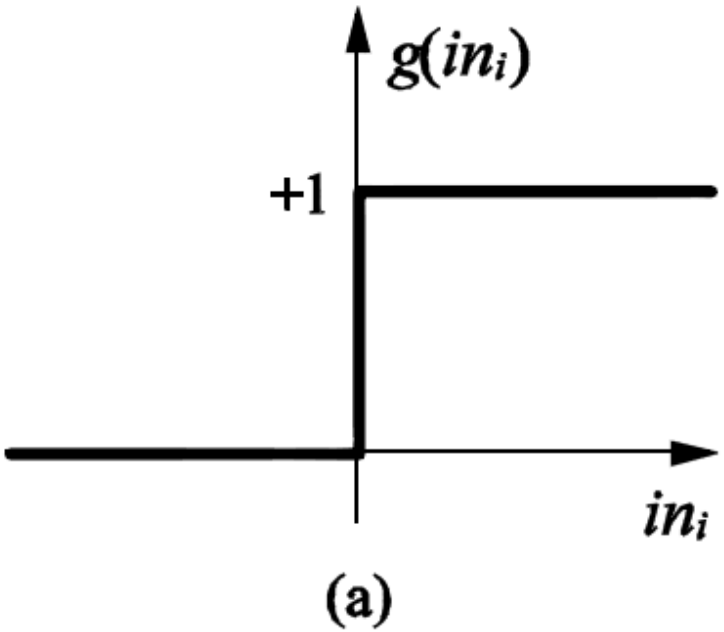
it "fires" when a linear combination of its inputs exceeds some (hard or soft) threshold

Activation Function

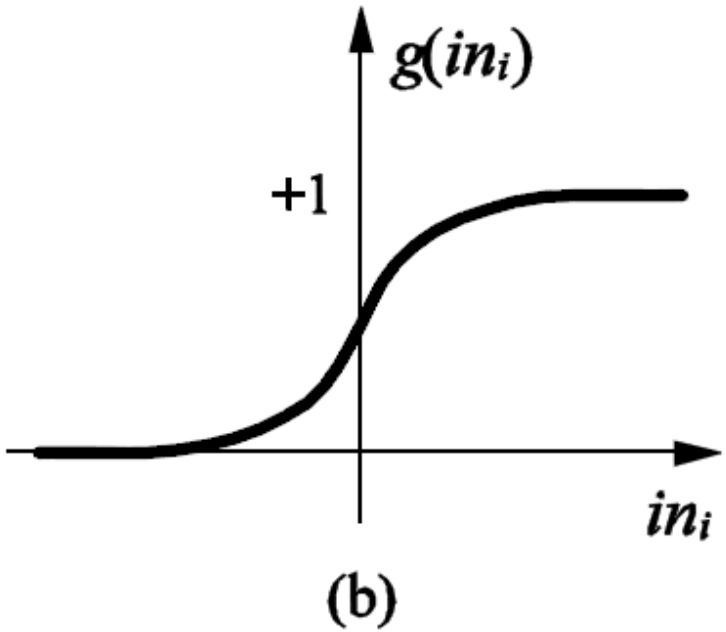
- Should be nonlinear
  - Otherwise network is just a linear function
- Often chosen to mimic firing in neurons
  - Unit should be "active" (output near 1) when fed with the "right" inputs
  - Unit should be "inactive" (output near 0) when fed with the "wrong" inputs

Common activation functions

Threshold



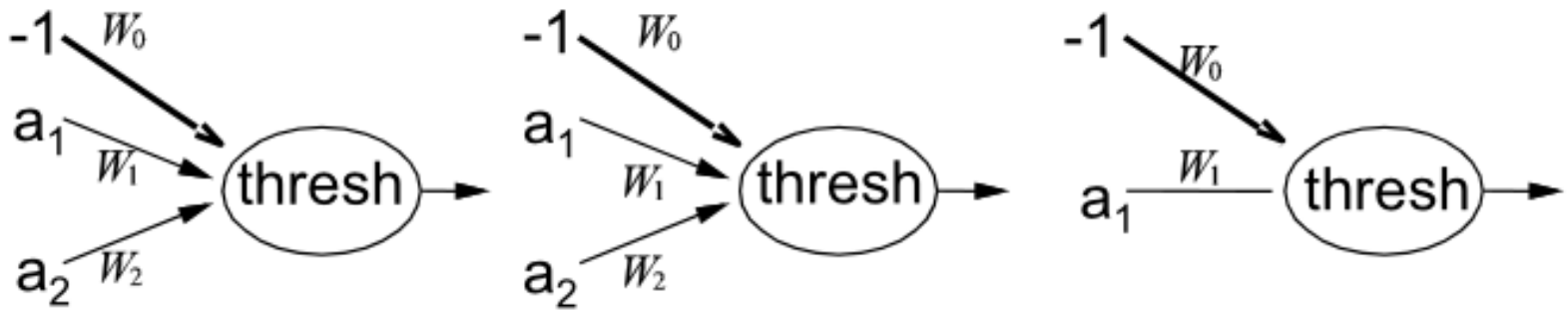
Sigmoid



$$g(x) = 1/(1+e^{-x})$$

Logic gates

- McCulloch and Pitts (1943)
  - Design ANNs to represent Boolean fns
- What should be the weights of the following units to code AND, OR, NOT ?

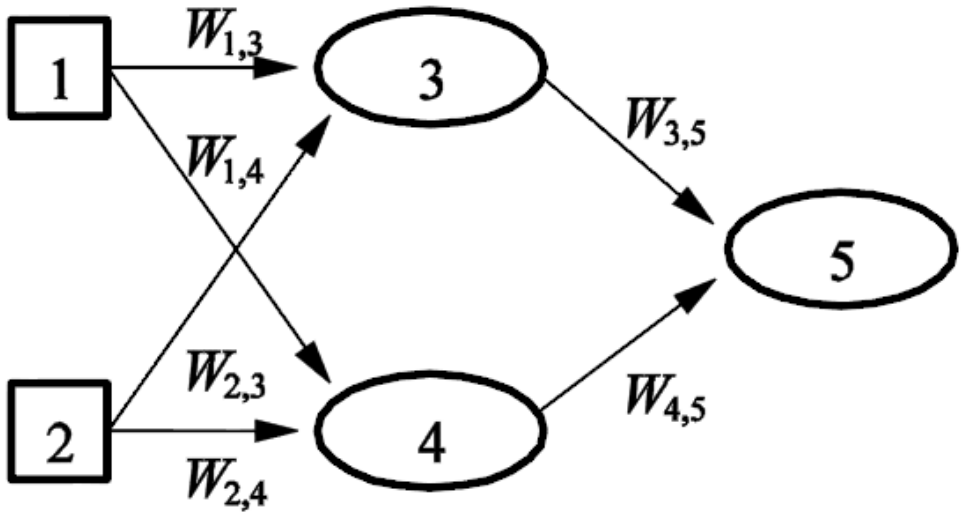


Network structures

- Feed-forward network (前馈网络)
  - Directed acyclic graph
  - No internal state
  - Simply computes outputs from inputs
- Recurrent network (循环网络)
  - Directed cyclic graph
  - Dynamical system with internal states
  - Can memorize information

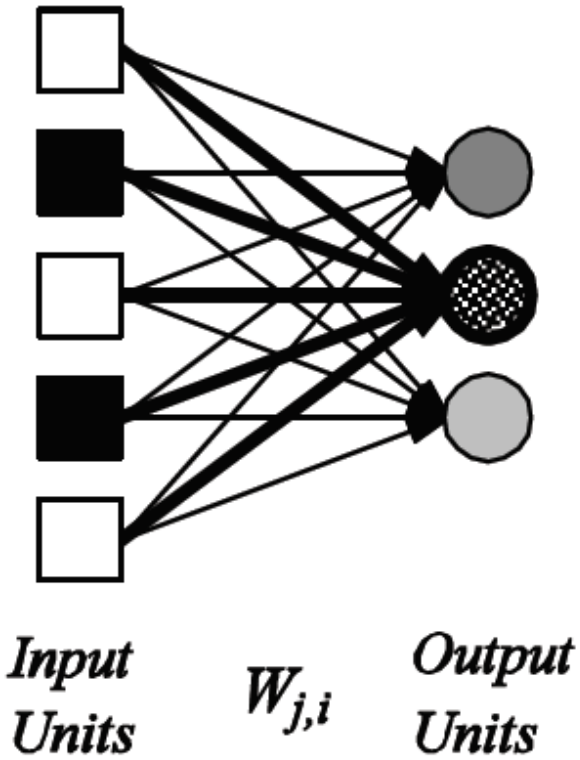
An example

Simple network with two inputs, one hidden layer of two units, one output unit



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

Single layer feed-forward network



Threshold Perceptron Hypothesis Space

- Hypothesis space h_w: All binary classifications with parameters w s.t. $w \cdot x \geq 0 \rightarrow 1$, $w \cdot x < 0 \rightarrow 0$
- Since $w \cdot x$ is linear in x, perceptron is called a linear separator (线性分离器)

Are all Boolean gates linearly separable?

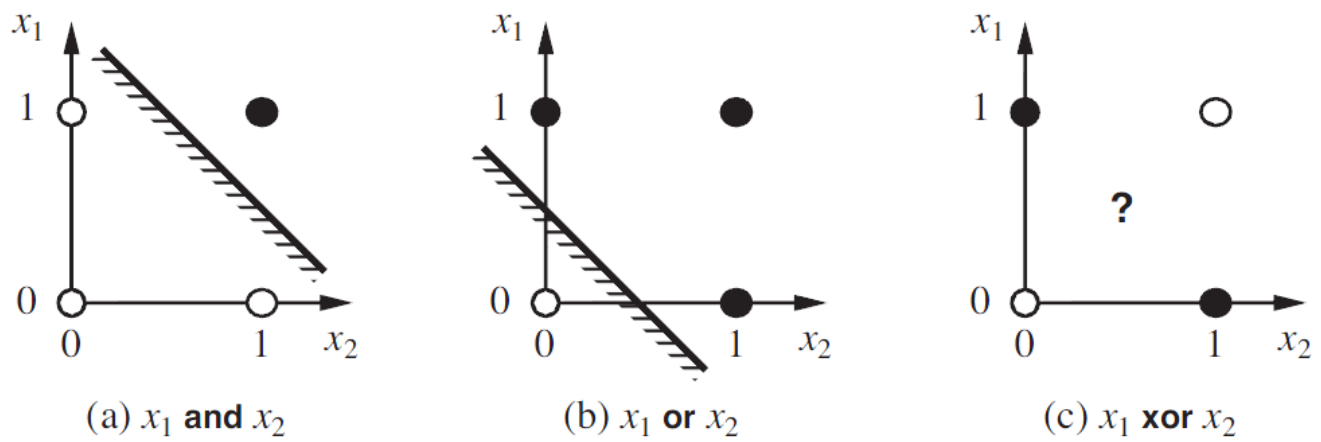
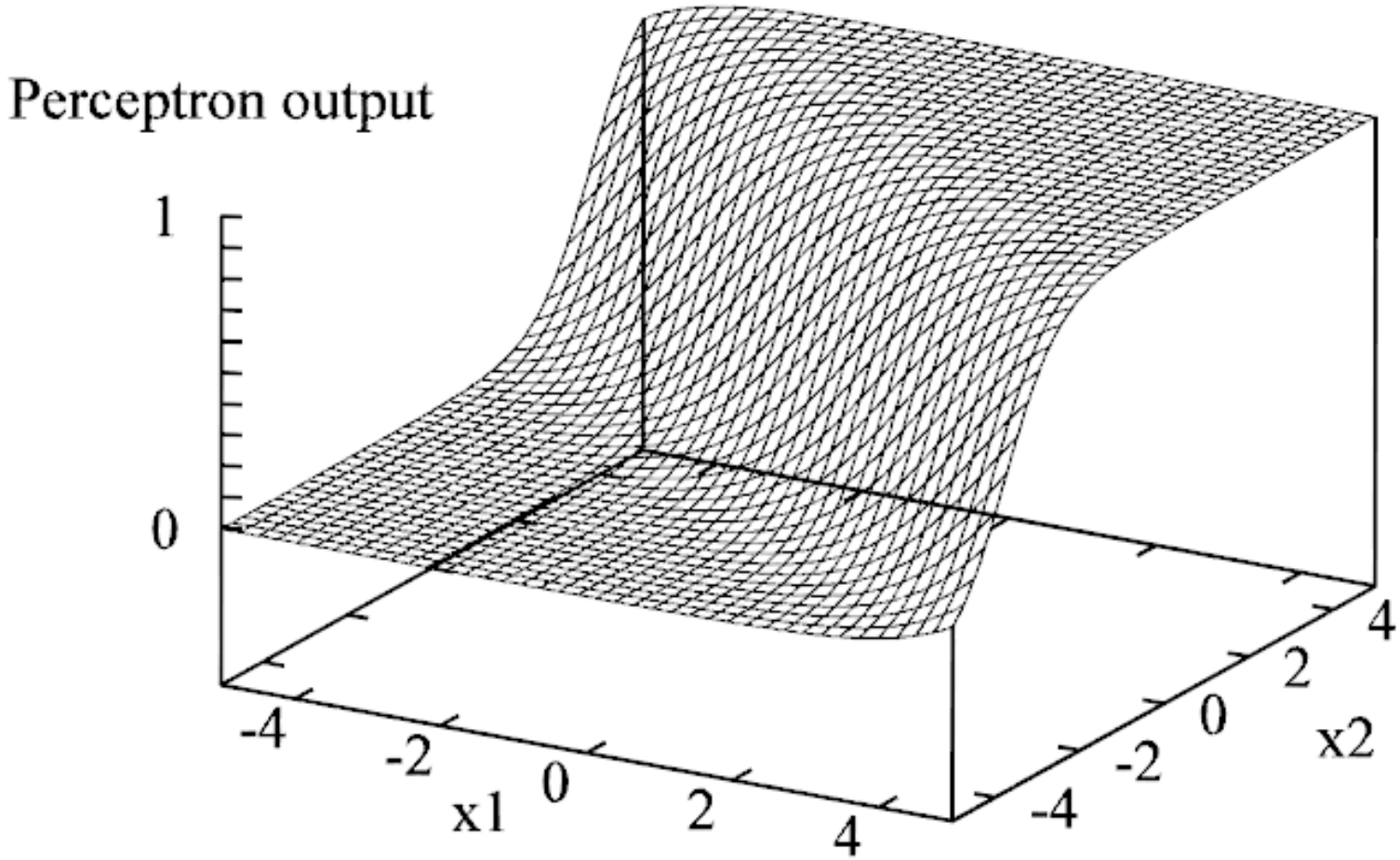


Figure 18.21 Linear separability in threshold perceptrons. Black dots indicate a point in the input space where the value of the function is 1, and white dots indicate a point where the value is 0. The perceptron returns 1 on the region on the non-shaded side of the line. In (c), no such line exists that correctly classifies the inputs.

Sigmoid Perceptron

Represent "soft" linear separators



Loss function

- The loss function $L(x, y, y')$ is defined as the amount of utility lost by predicting $h(x) = y'$ when the correct answer is $f(x) = y$
- Often a simplified version is used, $L(y, y')$, that is independent of x
- Three commonly used loss functions:
  - Absolute value loss: $L_1(y, y') = |y - y'|$
  - Squared error loss: $L_2(y, y') = (y - y')^2$
  - 0/1 loss: $L_{0/1}(y, y') = 0$ if $y = y'$, else 1
- Let E be the set of examples. Total loss $L(E) = \sum_{e \in E} L(e)$

Linear regression

- Regression with linear functions
- As an optimization search in weight space
- Use gradient descent (梯度下降)
- An iterative method to find the minimum of a function
- Start with any initial set of weights
- In each step, decrease each weight in proportion to its partial derivative:

$$w_i \leftarrow w_i - \alpha \partial Loss(w)/\partial w_i$$

- α is called the learning rate

Linear regression

- $h_w(x) = w \cdot x = \sum_i w_i x_i$
- Squared error loss: $Loss(w) = (y - h_w(x))^2$
- Chain rule: $\partial g(f(x))/\partial x = g'(f(x))\partial f(x)/\partial x$
- $\partial Loss(w)/\partial w_i = -2(y - h_w(x))x_i$
- $w_i \leftarrow w_i + \alpha(y - h_w(x))x_i$

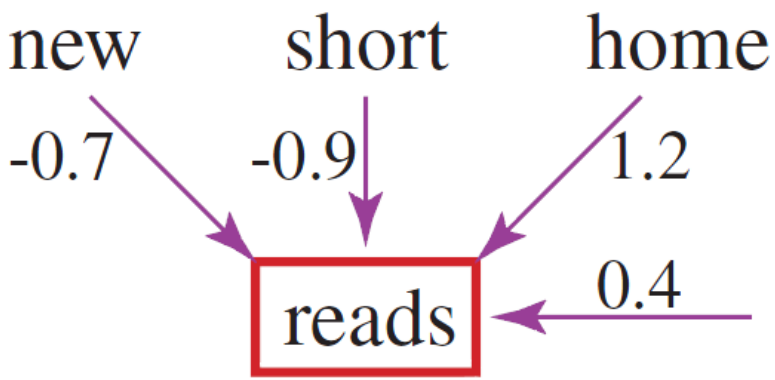
Logistic regression

- A logistic function is the sigmoid of a linear function
- Logistic regression: regression with logistic functions
- $g(x) = 1/(1 + e^{-x})$
- $h_w(x) = g(w \cdot x)$
- $g' = g(1 - g)$
- $Loss(w) = (y - h_w(x))^2$
- $\partial Loss(w)/\partial w_i = -2(y - h_w(x))g'(w \cdot x)x_i$
  $= -2(y - h_w(x))h_w(x)(1 - h_w(x))x_i$
- $w_i \leftarrow w_i + \alpha(y - h_w(x))h_w(x)(1 - h_w(x))x_i$

The algorithm

initialize w arbitrarily
repeat
    for each e in examples do
        $p \leftarrow g(w \cdot x(e))$
        $\delta \leftarrow y(e) - p$
        for each i do
            $w_i \leftarrow w_i + \alpha\delta p(1-p)x_i$
until some stopping criterion is satisfied
return w

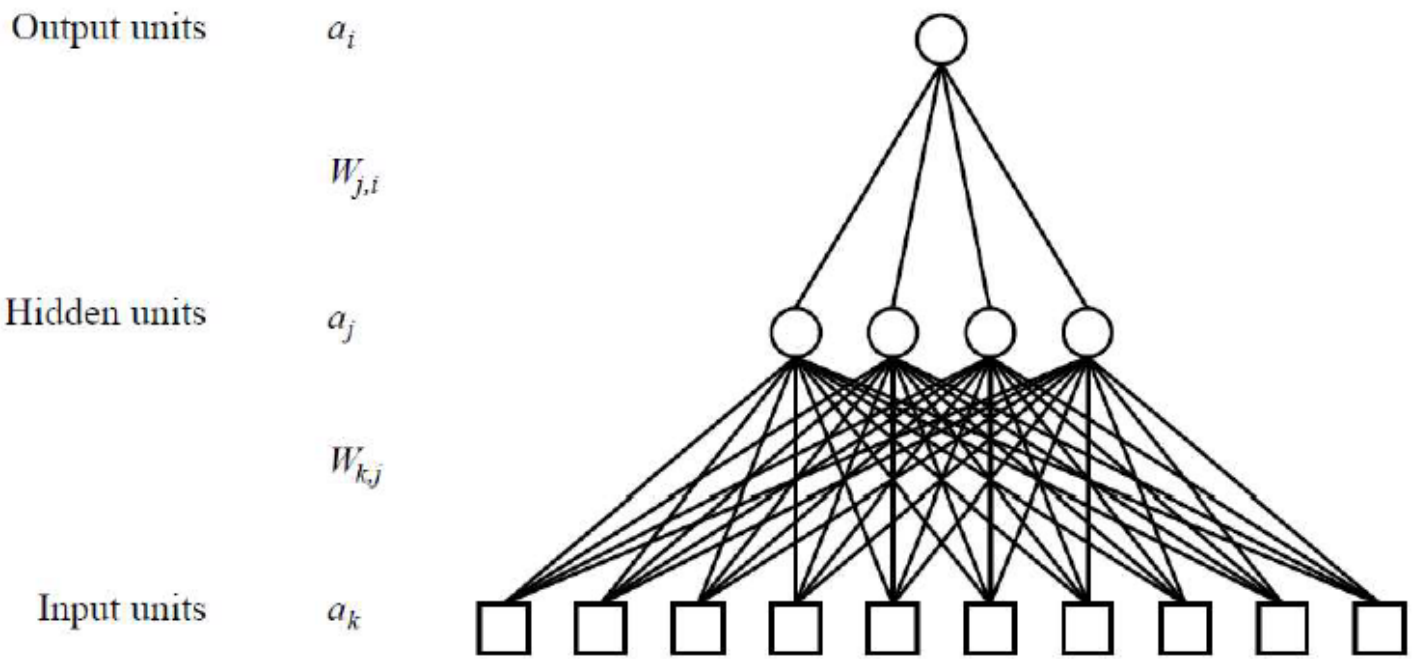
A simple example



Ex	new	short	home	reads		δ	error
				Predicted	Obs		
e1	0	0	0	$f(0.4) = 0.6$	0	-0.6	0.36
e2	1	1	0	$f(-1.2) = 0.23$	0	-0.23	0.053
e3	1	0	1	$f(0.9) = 0.71$	1	0.29	0.084

Multilayer Feed-forward Neural Networks

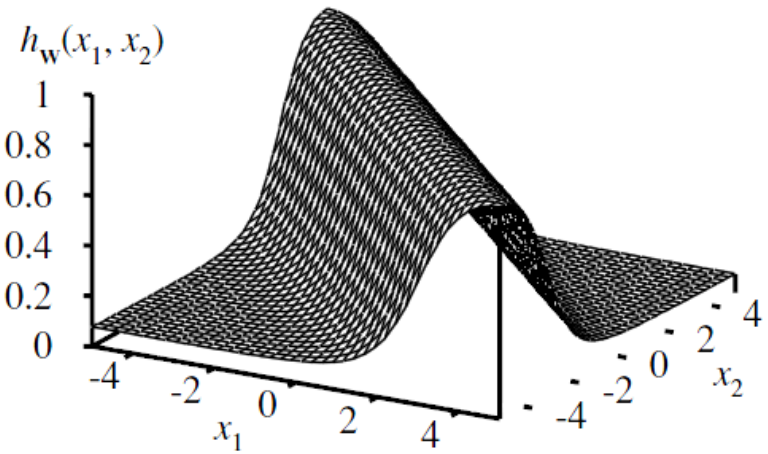
- Perceptron can only represent (soft) linear separators
- With multiple layers, what functions can be represented? Virtually any function!

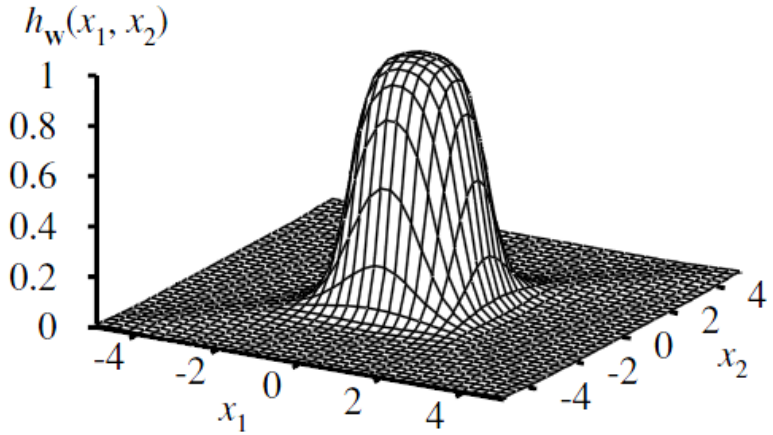


$$a_i = g\left(\sum_j W_{ji} g\left(\sum_k W_{kj} a_k\right)\right)$$

Multilayer networks

- Adding two sigmoid units with parallel but opposite "cliffs" produces a ridge
- Adding two intersecting ridges (and thresholding) produces a bump





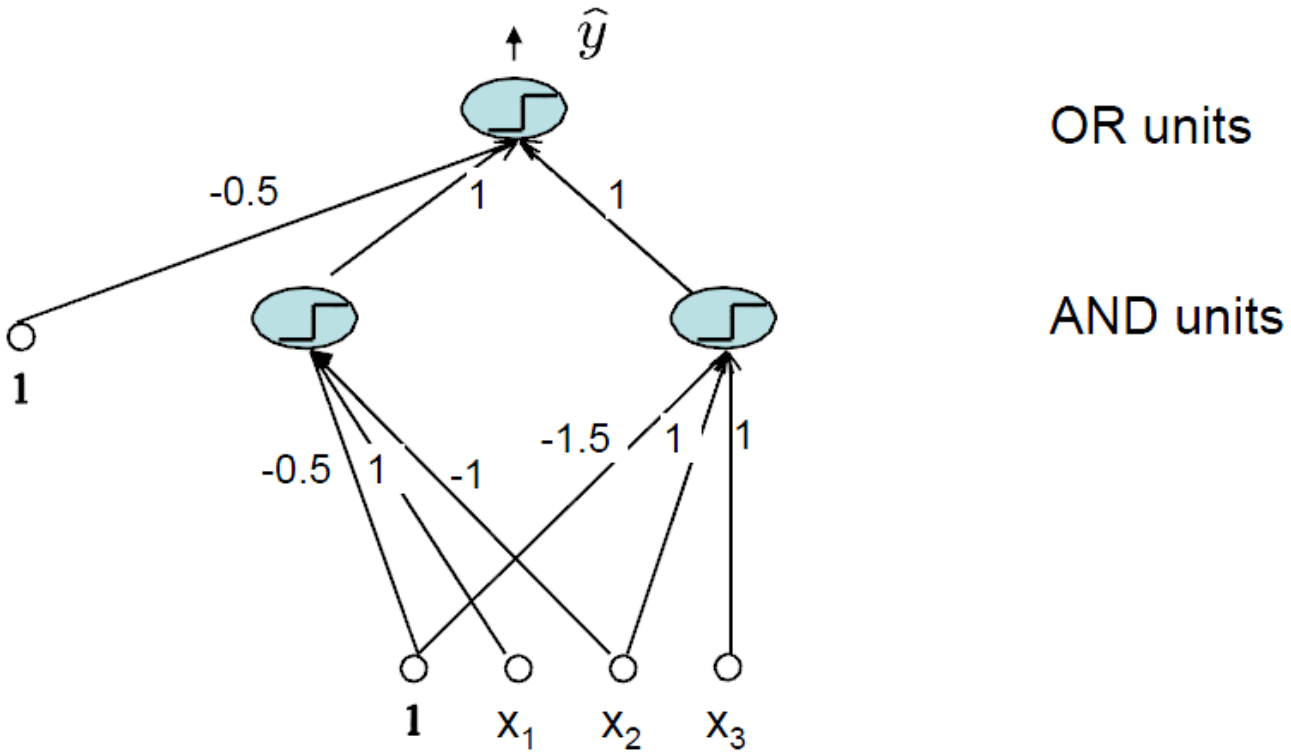
Multilayer networks

By tiling bumps of various heights together, we can approximate any function

Theorem: Neural networks with at least one hidden layer of sufficiently many sigmoid units can approximate any function arbitrarily closely.

Neural nets for Boolean functions: an example

Boolean function: $x_1 \wedge \neg x_2 \vee x_2 \wedge x_3$



Any Boolean function can be put into CNF or DNF, and hence can be represented with a neural network with one hidden layer

Weight training

- A set of examples, each with input vector x and output vector y
- Squared error loss: $Loss = \sum_k Loss_k$, $Loss_k = (y_k - a_k)^2$, where a_k is the k-th output of the neural net
- The weights are adjusted as follows: $w_{ij} \leftarrow w_{ij} - \alpha \partial Loss / \partial w_{ij}$
- How can we compute the gradient efficiently given an arbitrary network structure?
- Answer: backpropagation algorithm

Forward and backward phases

Forward phase:

- Propagate inputs forward to compute the output of each unit
- Output a_j at unit j: $a_j = g(in_j)$ where $in_j = \sum_i w_{ij} a_i$

Backward phase:

- Propagate errors backward
- For an output unit j: $\Delta_j = g'(in_j)(y_j - a_j)$
- For an hidden unit i: $\Delta_i = g'(in_i) \sum_j w_{ij} \Delta_j$

function BACK-PROP-LEARNING($examples$, $network$) **returns** a neural network

inputs: $examples$, a set of examples, each with input vector **x** and output vector **y**
$network$, a multilayer network with L layers, weights $w_{i,j}$, activation function g

local variables: Δ, a vector of errors, indexed by network node

repeat
  for each weight $w_{i,j}$ in $network$ **do**
    $w_{i,j} \leftarrow$ a small random number
  for each example (**x**, **y**) **in** $examples$ **do**
    /* *Propagate the inputs forward to compute the outputs* */
    for each node i in the input layer **do**
      $a_i \leftarrow x_i$
    for $\ell = 2$ **to** L **do**
      for each node j in layer ℓ **do**
        $in_j \leftarrow \sum_i w_{i,j} \, a_i$
        $a_j \leftarrow g(in_j)$
    /* *Propagate deltas backward from output layer to input layer* */
    for each node j in the output layer **do**
      $\Delta[j] \leftarrow g'(in_j) \times (y_j - a_j)$
    for $\ell = L - 1$ **to** 1 **do**
      for each node i in layer ℓ **do**
        $\Delta[i] \leftarrow g'(in_i) \sum_j w_{i,j} \, \Delta[j]$
    /* *Update every weight in network using deltas* */
    for each weight $w_{i,j}$ in $network$ **do**
      $w_{i,j} \leftarrow w_{i,j} + \alpha \times a_i \times \Delta[j]$
until some stopping criterion is satisfied
return $network$

Output layer

$$\begin{aligned}
\frac{\partial Loss_k}{\partial w_{j,k}} &= -2(y_k - a_k)\frac{\partial a_k}{\partial w_{j,k}} = -2(y_k - a_k)\frac{\partial g(in_k)}{\partial w_{j,k}} \\
&= -2(y_k - a_k)g'(in_k)\frac{\partial in_k}{\partial w_{j,k}} = -2(y_k - a_k)g'(in_k)\frac{\partial}{\partial w_{j,k}}\left(\sum_j w_{j,k}a_j\right) \\
&= -2(y_k - a_k)g'(in_k)a_j = -a_j\Delta_k \ ,
\end{aligned}$$

Hidden layers

$$
\begin{aligned}
\frac{\partial Loss_k}{\partial w_{i,j}} &= -2(y_k - a_k)\frac{\partial a_k}{\partial w_{i,j}} = -2(y_k - a_k)\frac{\partial g(in_k)}{\partial w_{i,j}} \\
&= -2(y_k - a_k)g'(in_k)\frac{\partial in_k}{\partial w_{i,j}} = -2\Delta_k \frac{\partial}{\partial w_{i,j}}\left(\sum_j w_{j,k}a_j\right) \\
&= -2\Delta_k w_{j,k}\frac{\partial a_j}{\partial w_{i,j}} = -2\Delta_k w_{j,k}\frac{\partial g(in_j)}{\partial w_{i,j}} \\
&= -2\Delta_k w_{j,k}g'(in_j)\frac{\partial in_j}{\partial w_{i,j}} \\
&= -2\Delta_k w_{j,k}g'(in_j)\frac{\partial}{\partial w_{i,j}}\left(\sum_i w_{i,j}a_i\right) \\
&= -2\Delta_k w_{j,k}g'(in_j)a_i = -a_i\Delta_j \ ,
\end{aligned}
$$

Forward and backward phases

Forward phase:

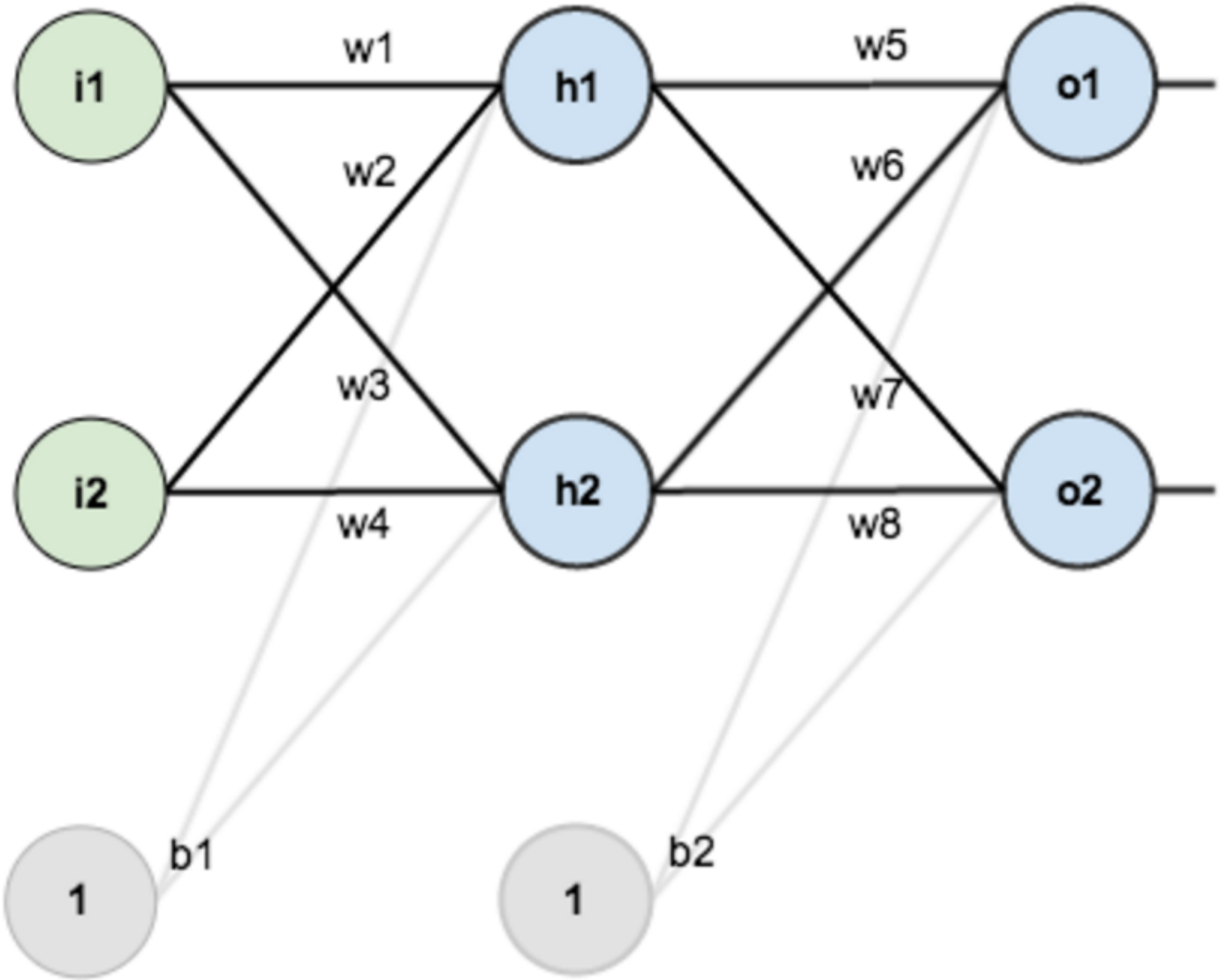
- Propagate inputs forward to compute the output of each unit
- Output a_j at unit j: $a_j = g(in_j)$ where $in_j = \sum_i w_{ij} a_i$

Backward phase:

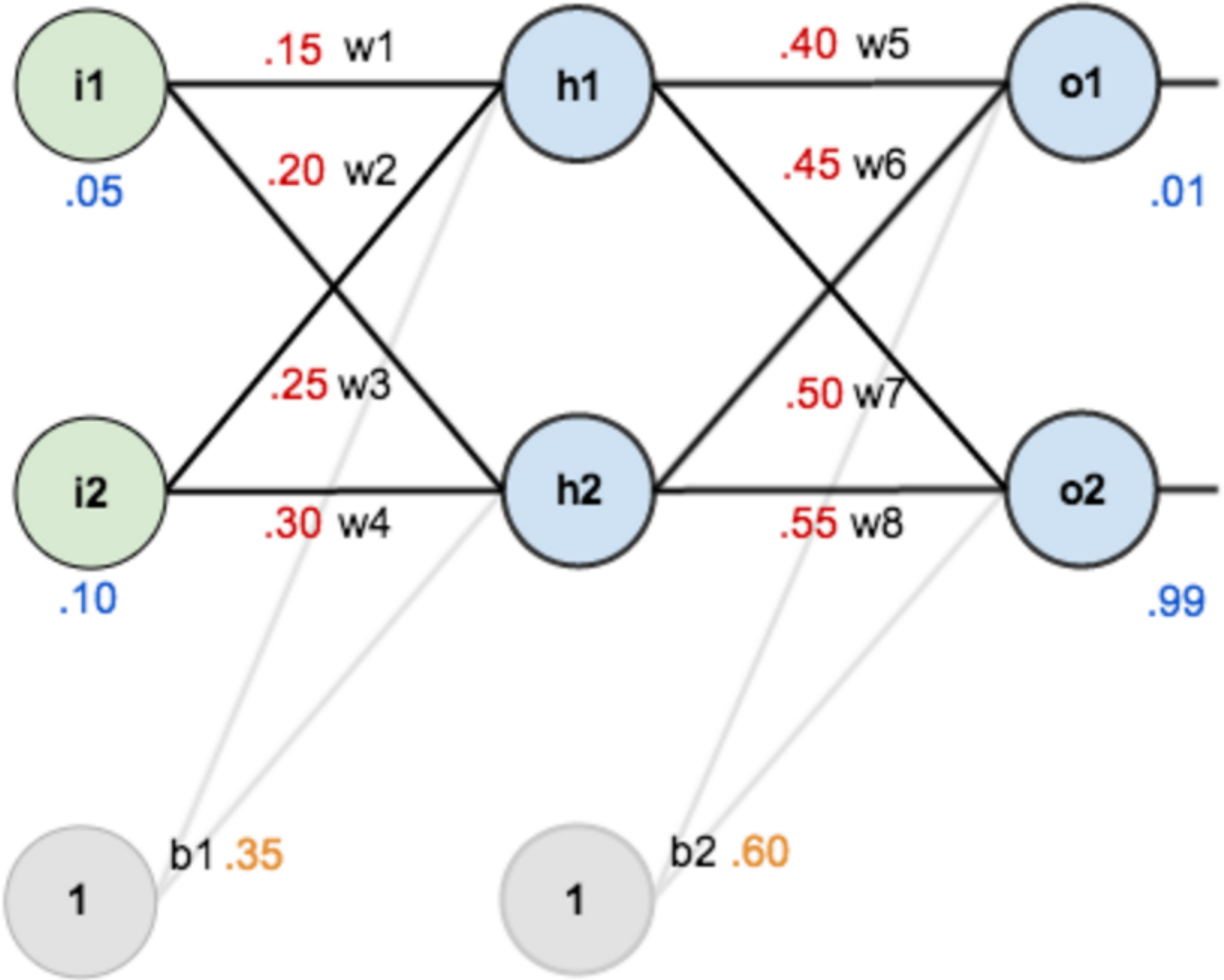
- Propagate errors backward
- For an output unit j:
  $\Delta_j = g'(in_j)(y_j - a_j) = a_j(1 - a_j)(y_j - a_j)$
- For an hidden unit i:
  $\Delta_i = g'(in_i) \sum_j w_{ij} \Delta_j = a_i(1 - a_i) \sum_j w_{ij} \Delta_j$

Weight updating: $w_{ij} \leftarrow w_{ij} + \alpha a_i \delta_j$

The network structure



The numbers


i1
i2
h1
h2
o1
o2
.15 w1
.20 w2
.25 w3
.30 w4
.40 w5
.45 w6
.50 w7
.55 w8
.05
.10
.01
.99
1
b1 .35
1
b2 .60

Forward pass

- $in_{h_1} = w_1 i_1 + w_2 i_2 + b_1 = 0.05 * 0.15 + 0.10 * 0.20 + 0.35 = 0.3775$
- $out_{h_1} = g(in_{h_1}) = \frac{1}{1+e^{-0.3775}} = 0.593269992$
- $out_{h_2} = 0.596884378$
- $in_{o_1} = w_5 out_{h_1} + w_6 out_{h_2} + b_2 = 0.40 * 0.593269992 + 0.45 * 0.596884378 + 0.60 = 1.105905967$
- $out_{o_1} = g(in_{o_1}) = \frac{1}{1+e^{-1.105905967}} = 0.75136507$
- $out_{o_2} = 0.772928465$

Backward pass

Let $\alpha = 0.5$

- $\Delta_{o_1} = 0.75136507(1 - 0.75136507)(0.01 - 0.75136507) = -0.138498562$
- $w_5^+ = w_5 + \alpha \cdot out_{h_1} \cdot \Delta_{o_1} =$
  $0.40 - 0.5 * 0.593269992 * 0.138498562 = 0.35891648$
- $w_6^+ = w_6 + \alpha \cdot out_{h_2} \cdot \Delta_{o_1} =$
  $0.45 - 0.5 * 0.596884378 * 0.138498562 = 0.408666186$

Backward pass

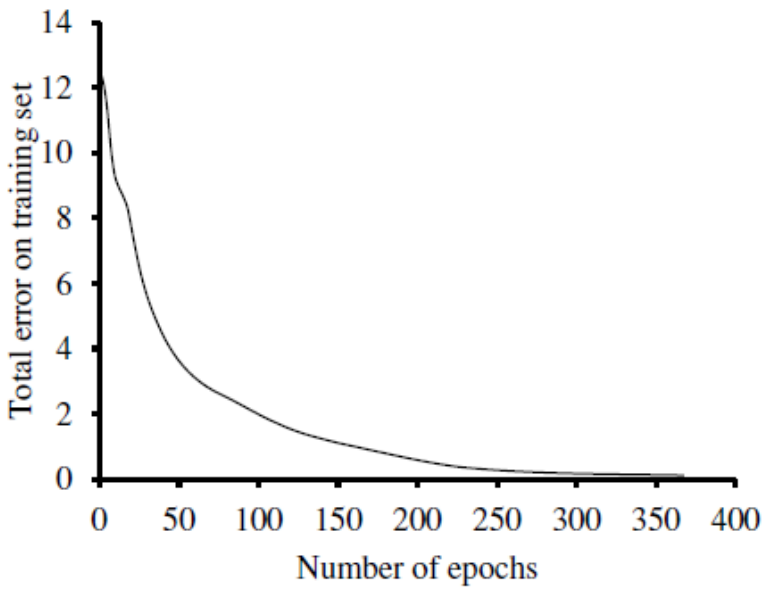
- $\Delta_{o_2} = 0.772928465(1 - 0.772928465)(0.99 - 0.772928465) = 0.0380982366$
- $w_7^+ = w_7 + \alpha \cdot out_{h_1} \cdot \Delta_{o_2} = 0.50 + 0.5 * 0.593269992 * 0.0380982366 = 0.511301270$
- $w_8^+ = w_8 + \alpha \cdot out_{h_2} \cdot \Delta_{o_2} = 0.55 + 0.5 * 0.596884378 * 0.0380982366 = 0.561370121$

Backward pass

- $\Delta_{h_1} = g'(in_{h_1})(w_5\Delta_{o_1} + w_7\Delta_{o_2}) =$
  $0.593269992(1 - 0.593269992)(0.40 * (-0.138498562) +$
  $0.50 * 0.0380982366) = -0.241300709 * 0.036350306$
- $w_1^+ = w_1 + \alpha \cdot i_1 \cdot \Delta_{h_1} =$
  $0.15 - 0.5 * 0.05 * 0.241300709 * 0.036350306 = 0.149780716$
- $w_2^+ = 0.19956143$
- $w_3^+ = 0.24975114$
- $w_4^+ = 0.29950229$

The restaurant example

- First, we need to determine the structure of the network.
- We have 10 attributes, so we will need 10 input units.
- Should we have one hidden layer or two? How many nodes in each layer? Should they be fully connected?
- There is no good theory that will tell us the answer.
- We can use cross-validation: try several different structures and see which one works best.
- It turns out that a network with one hidden layer containing four nodes is about right for this problem.



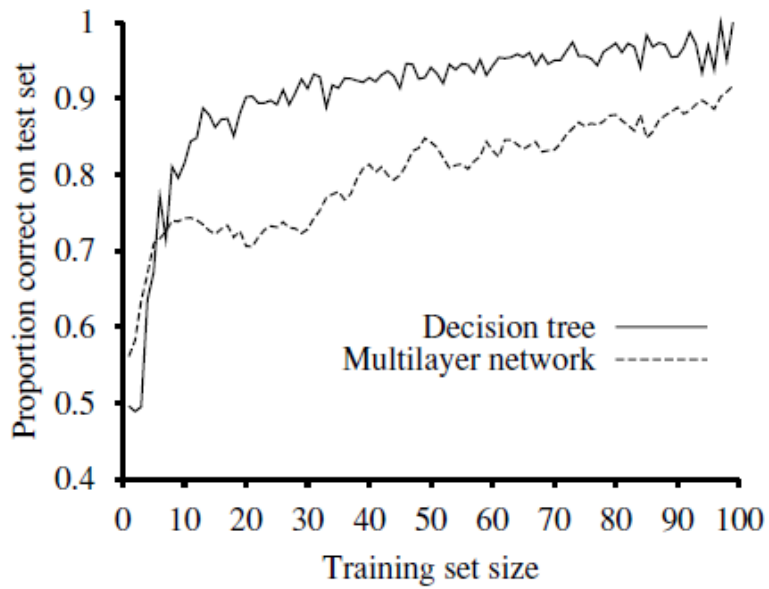


Figure 18.25 (a) Training curve showing the gradual reduction in error as weights are modified over several epochs, for a given set of examples in the restaurant domain. (b) Comparative learning curves showing that decision-tree learning does slightly better on the restaurant problem than back-propagation in a multilayer network.