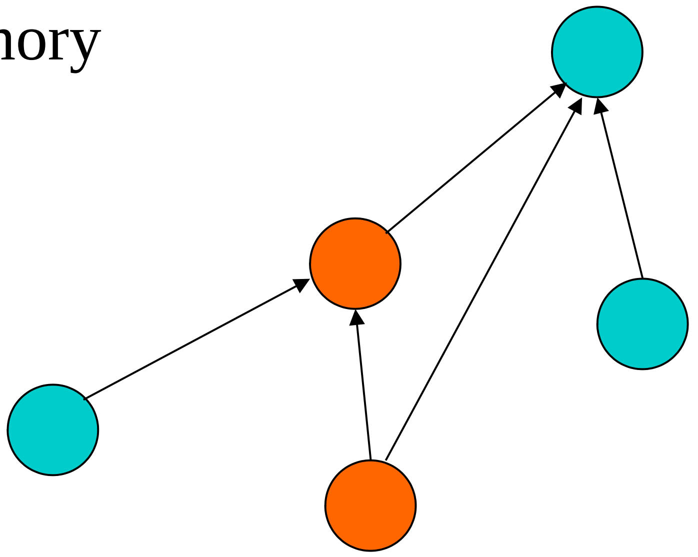
Machine Learning

CS60050

Artificial Neural Networks

Neural networks

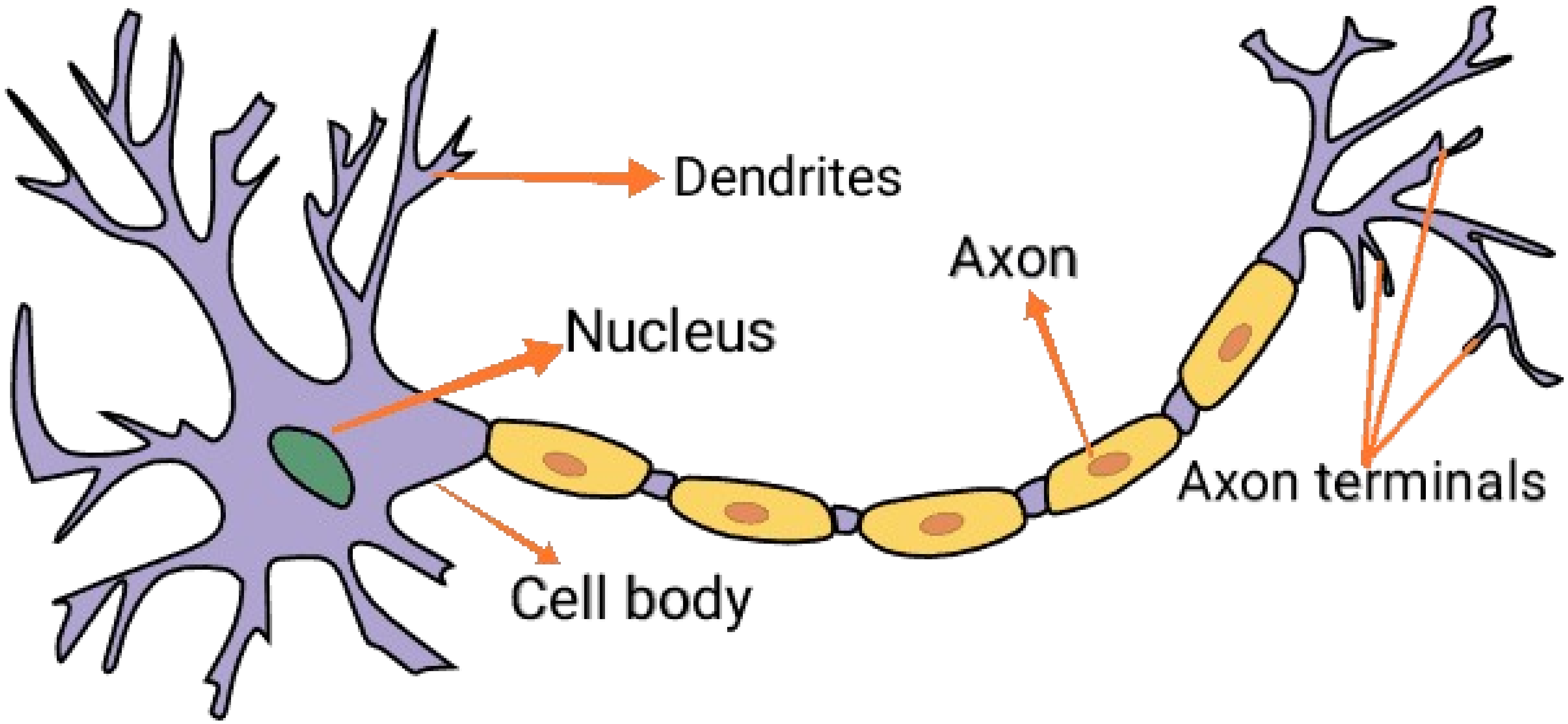
- Networks of processing units (neurons) with connections (synapses) between them
- Large number of neurons: 10^{10}
- Large connectitivity: 10^{5}
- Parallel processing
- Distributed computation/memory
- Robust to noise, failures



Connectionism

- Alternative to *symbolism*
- Humans and evidence of connectionism/parallelism:
  - Physical structure of brain:
  - Neuron switching time: 10^{-3} second
- Complex, short-time computations:
  - Scene recognition time: 10^{-1} second
  - 100 inference steps doesn’t seem like enough
  - much parallel computation
- Artificial Neural Networks (ANNs)
  - Many neuron-like threshold switching units
  - Many weighted interconnections among units
  - Highly parallel, distributed process
  - Emphasis on tuning weights automatically (search in weight space)

Biological neuron



Biological neuron

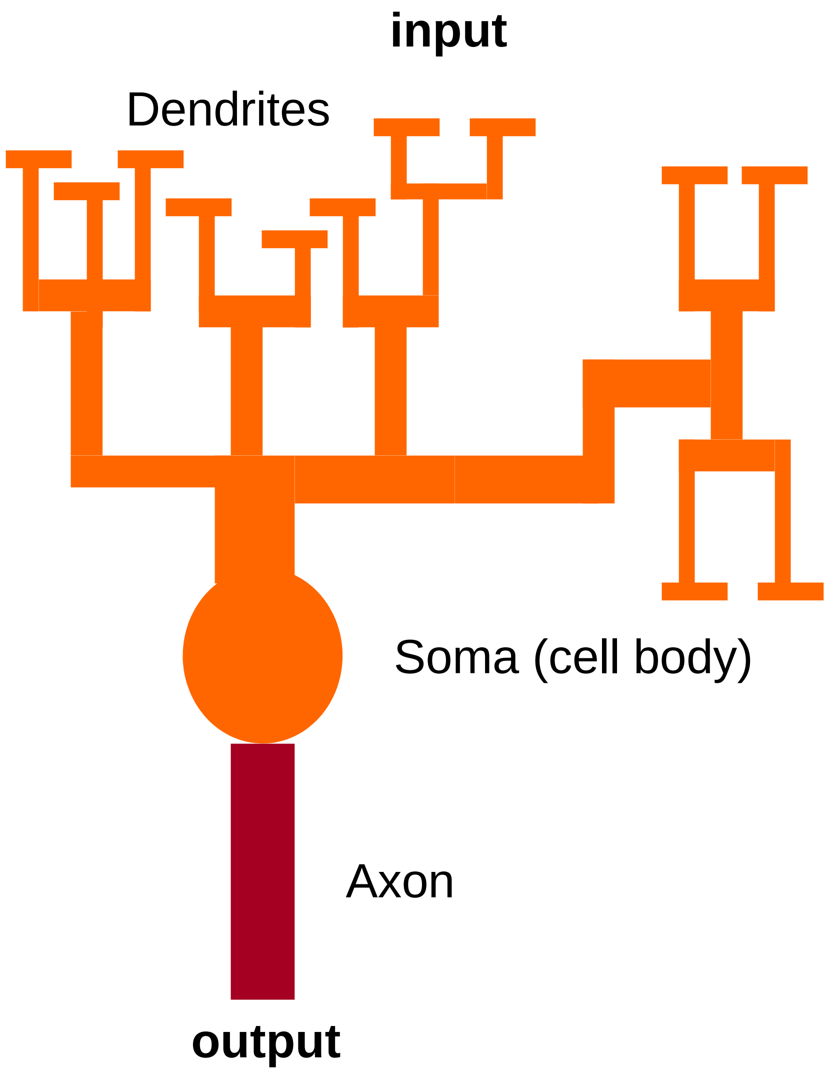
- dendrites: nerve fibres carrying electrical signals to the cell
- cell body: computes a non-linear function of its inputs
- axon: single long fiber that carries the electrical signal from the cell body to other neurons
- synapse: the point of contact between the axon of one cell and the dendrite of another, regulating a chemical connection whose strength affects the input to the cell.

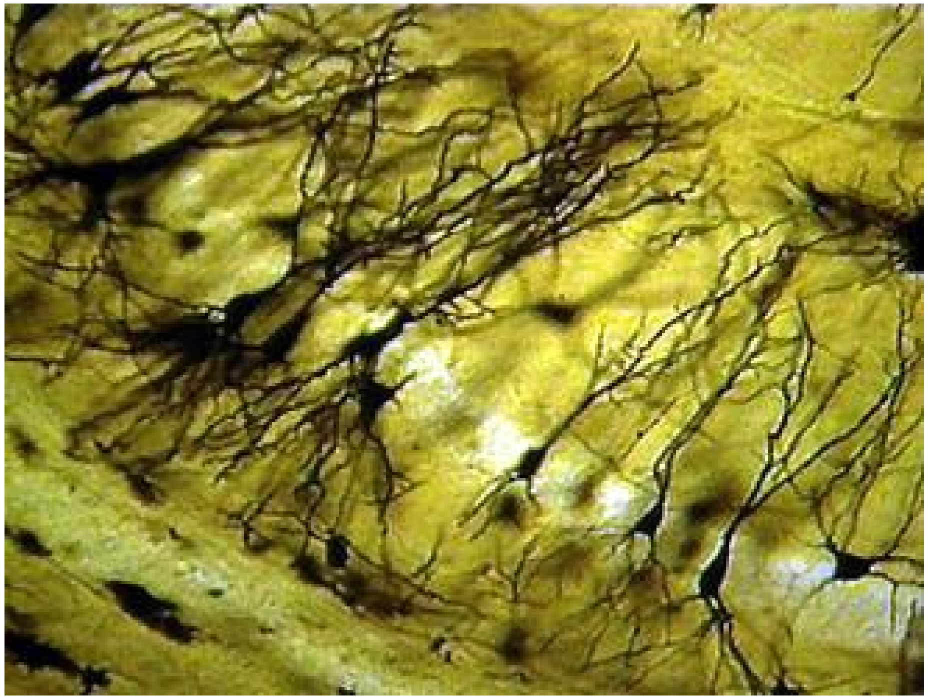
Biological neuron

- A variety of different neurons exist (motor neuron, on-center off-surround visual cells…), with different branching structures

- The connections of the network and the strengths of the individual synapses establish the function of the network.

Biological inspiration





Biological inspiration

- The spikes travelling along the axon of the pre-synaptic neuron trigger the release of neurotransmitter substances at the synapse.

- The neurotransmitters cause excitation or inhibition in the dendrite of the post-synaptic neuron.

- The integration of the excitatory and inhibitory signals may produce spikes in the post-synaptic neuron.

- The contribution of the signals depends on the strength of the synaptic connection.

Hodgkin and Huxley model

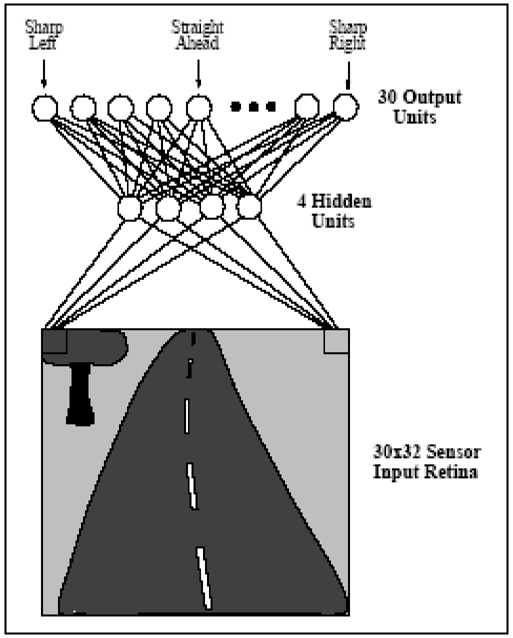
- Hodgkin and Huxley experimented on squids and discovered how the signal is produced within the neuron
- This model was published in *Jour. of Physiology* (1952)
- They were awarded the 1963 Nobel Prize

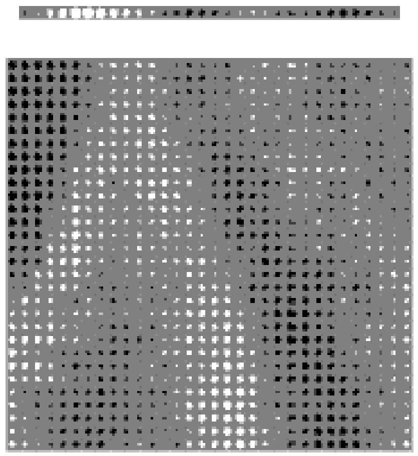
When to consider ANNs

- Input is
  - high-dimensional
  - discrete or real-valued
    - e.g., raw sensor inputs
  - noisy
- *Long training times*
- Form of target function is unknown
- *Human readability is unimportant*
- Especially good for complex recognition problems
  - Speech recognition
  - Image classification
  - Financial prediction

Problems too hard to program

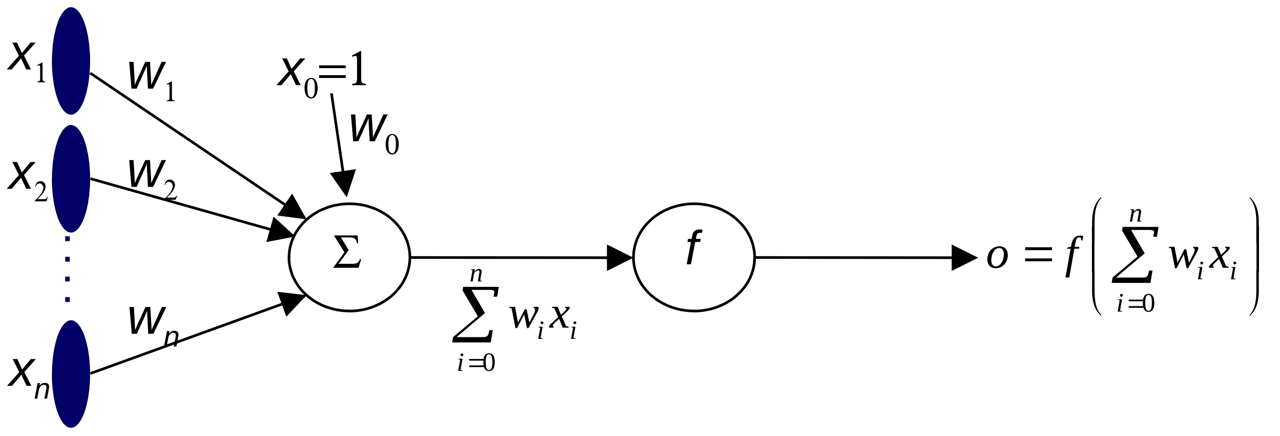
ALVINN: a perception system which learns to control the NAVLAB vehicles by watching a person drive





How many weights need to be learned?

Perceptron



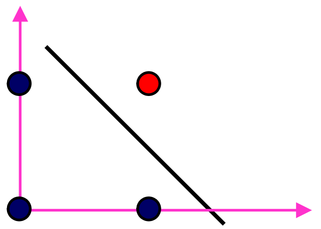
- $-w_0$: threshold value or bias $\left(\sum_{i=1}^{n} w_i x_i\right) - (-w_0)$

- *f (or o())* : activation function (thresholding unit), typically:

$$f(x) = \begin{cases} 1 & x > 0 \\ -1 & \text{otherwise} \end{cases}$$

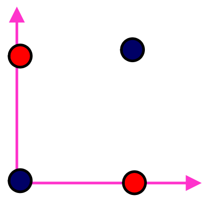
Decision surface of a perceptron

- Decision surface is a hyperplane given by $\sum_{i=0}^{n} w_i x_i = 0$
- 2D case: the decision surface is a line
- Represents many useful functions: for example, $x_1 \wedge x_2$?
  - $x_1 \wedge x_2$?



$-1.5+x_1+x_2=0$

x_1 XOR x_2?

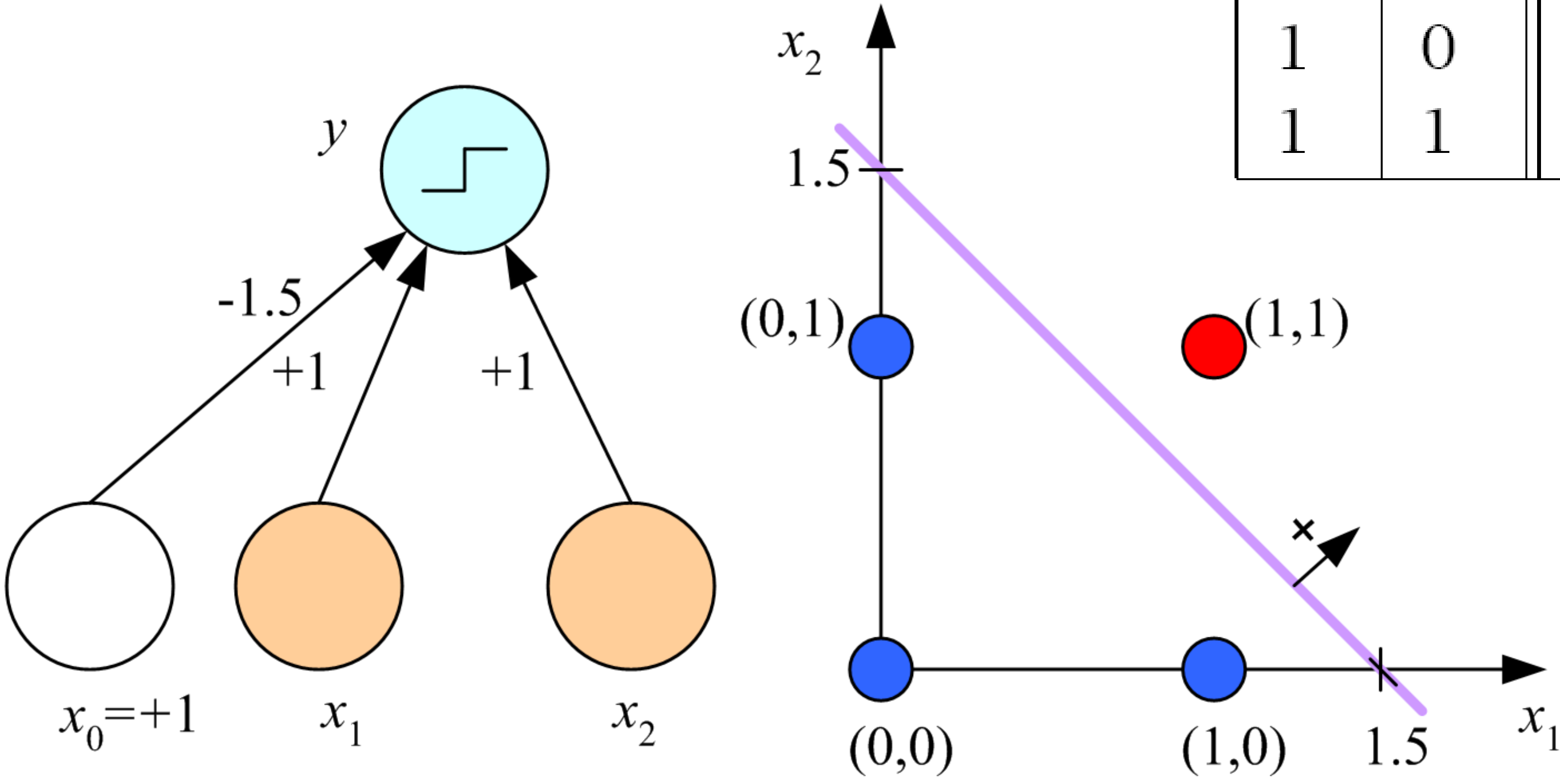


Not linearly separable!

- Generalization to higher dimensions
  - Hyperplanes as decision surfaces

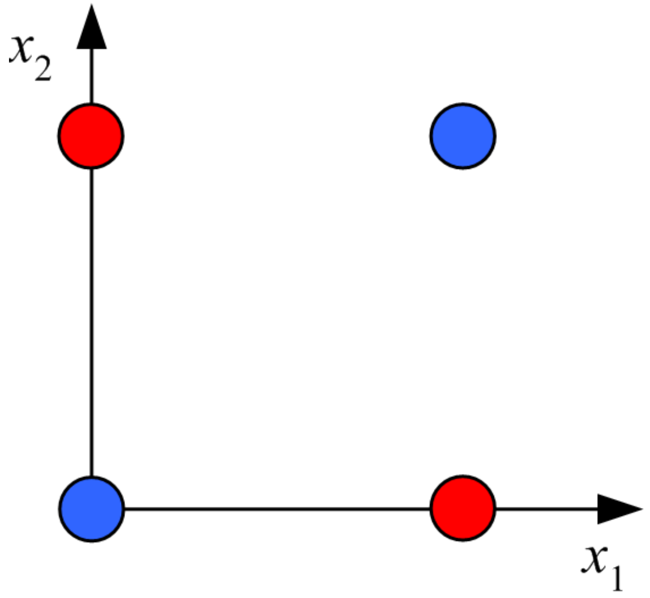
Learning Boolean AND

x_1	x_2	r
0	0	0
0	1	0
1	0	0
1	1	1



XOR

x_1	x_2	r
0	0	0
0	1	1
1	0	1
1	1	0



- No w_0, w_1, w_2 satisfy:

$$\begin{aligned} & & w_0 &\le 0 \\ & w_2 + & w_0 &> 0 \\ w_1 + & & w_0 &> 0 \\ w_1 + & w_2 + & w_0 &\le 0 \end{aligned}$$

(Minsky and Papert, 1969)

Boolean functions

- Solution:
  - network of perceptrons
  - Any boolean function representable as DNF
    - 2 layers
    - Disjunction (layer 1) of conjunctions (layer 2)
- Example of XOR
  - (X1=1 AND X2=0) OR (X1=0 AND X2=1)
- Practical problem of representing high-dimensional functions

Training rules

- Finding learning rules to build networks from TEs

- Will examine two major techniques
  - Perceptron training rule
  - Delta (gradient search) training rule (for more perceptrons as well as general ANNs)

- Both focused on learning weights
  - Hypothesis space can be viewed as set of weights

Perceptron training rule

- ITERATIVE RULE: $w_i := w_i + \Delta w_i$
  - where $\Delta w_i = \eta\ (t - o)\ x_i$
  - t is the target value
  - o is the perceptron output for x
  - η is small positive constant, called the learning rate

- Why rule works:
  - E.g., t = 1, o = -1, $x_i = 0.8$, $\eta = 0.1$
  - then $\Delta w_i = 0.16$ and $w_i x_i$ gets larger
  - o converges to t

Perceptron training rule

- The process will converge if
  - training data is linearly separable, and
  - η is sufficiently small

- But if the training data is not linearly separable, it may not converge (Minsky & Pappert)
  - Basis for Minsky/Pappert attack on NN approach

- Question: how to overcome problem:
  - different model of neuron?
  - different training rule?
  - both?

Gradient descent

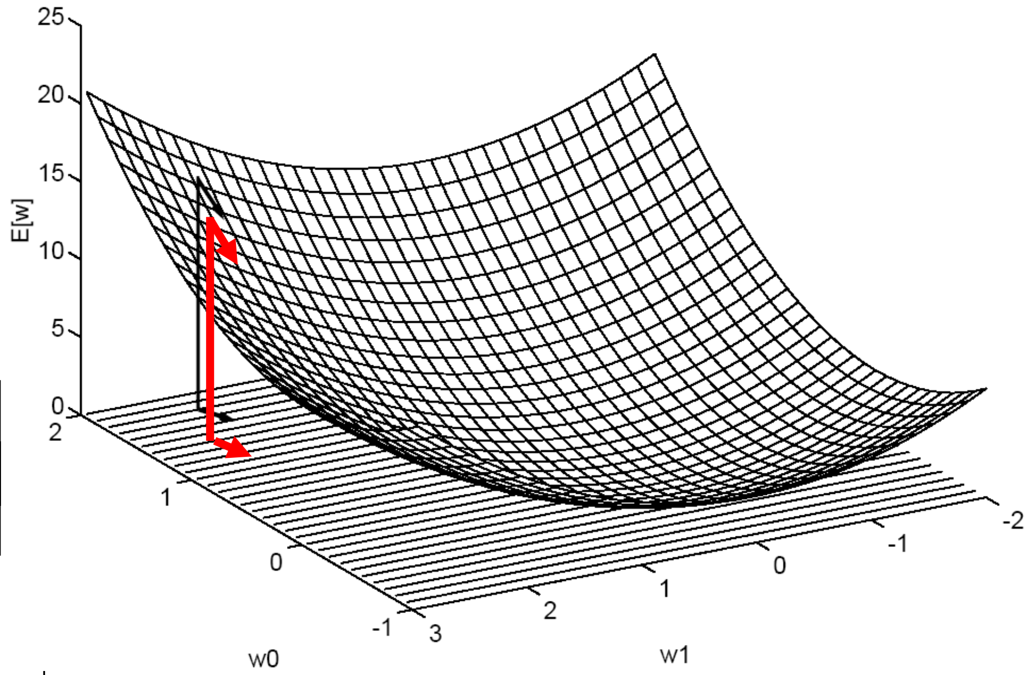
- Solution: use alternate rule
  - More general
  - Basis for networks of units
  - Works in non-linearly separable cases
- Let $o(x) = w_0 + w_1x_1 + \ldots + w_nx_n$
  - Simple example of linear unit (will generalize)
  - Omit the thresholding initially
- D is the set of training examples $\{d = \langle x, t_d \rangle\}$
- We will learn w_i's that minimize the squared error

$$E[\vec{w}] \equiv \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2$$

Error minimization

- Look at error E as a function of weights $\{w_i\}$
- Slide down gradient of E in weight space
- Reach values of $\{w_i\}$ that correspond to minimum error
  - Look for global minimum
- Example of 2-dimensional case:
  - $E = w_1 * w_1 + w_2 * w_2$
  - Minimum at $w_1 = w_2 = 0$
- Look at general case of n-dimensional space of weights

Gradient descent



Parabola with a single minima

- Gradient "points" to the steepest increase:

$$\nabla E[\vec{w}] \equiv \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \cdots, \frac{\partial E}{\partial w_n} \right]$$

- Training rule: $\Delta w = -\eta \nabla E[w]$
  where η is a positive constant (learning rate)

$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

- How might one interpret this update rule?

Gradient descent

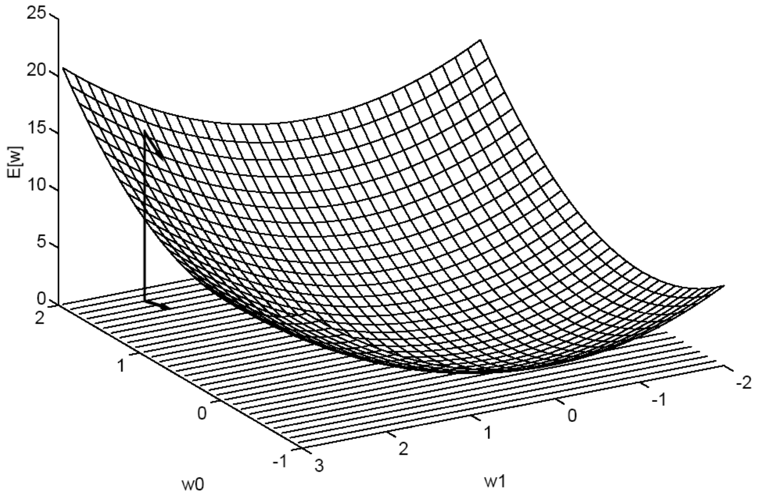
$$\frac{\partial E}{\partial w_i} = \frac{\partial}{\partial w_i}\frac{1}{2}\sum_{d\in D}(t_d - o_d)^2$$

$$= \frac{1}{2}\sum_{d\in D}\frac{\partial}{\partial w_i}(t_d - o_d)^2$$

$$= \frac{1}{2}\sum_{d\in D}2(t_d - o_d)\frac{\partial}{\partial w_i}(t_d - o_d)$$

$$= \sum_{d\in D}(t_d - o_d)\frac{\partial}{\partial w_i}(t_d - \vec{w_d}\cdot\vec{x_d})$$

$$= \sum_{d\in D}(t_d - o_d)(-x_{i,d})$$



$$\Delta w_i = -\eta\frac{\partial E}{\partial w_i} = -\eta\sum_{d\in D}(t_d - o_d)(-x_{i,d}) = \eta\sum_{d\in D}(t_d - o_d)x_{i,d}$$

$$\Delta w_i = \sum_{d\in D}\left(\eta(t_d - o_d)x_{i,d}\right)$$

Gradient descent algorithm

Gradient-Descent (*training examples, η*)

Each training example is a pair <x, t>: x is the vector of input values, and t is the target output value. η is the learning rate (e.g., .05).

- Initialize each w_i to some small random value
- Repeat until the termination condition is met

```
1. Initialize each $\Delta w_i$ to zero
2. For each training example <x, t>
     ♦ Input x to the unit and compute the output o
     ♦ For each linear unit weight $w_i$
           $\Delta w_i \leftarrow \Delta w_i + \eta (t - o) x_i$
3. For each linear unit weight $w_i$
           $w_i \leftarrow w_i + \Delta w_i$
```

- At each iteration, consider reducing η

Also called
- LMS (Least Mean Square) rule
- Delta rule

Incremental (Stochastic) Gradient Descent

Batch mode Gradient Descent: $E_D[\vec{w}] \equiv \frac{1}{2}\sum_{d \in D}(t_d - o_d)^2$

- Repeat
  1. Compute the gradient $\nabla E_D[w]$
  2. $w \leftarrow w - \eta \nabla E_D[w]$

Incremental mode Gradient Descent: $E_d[\vec{w}] \equiv \frac{1}{2}(t_d - o_d)^2$

- Repeat
  - For each training example *d* in *D*
    1. Compute the gradient $\nabla E_d[w]$
    2. $w \leftarrow w - \eta \nabla E_d[w]$
- Incremental can approximate batch if η is small enough

Incremental Gradient Descent Algorithm

Incremental-Gradient-Descent (*training examples*, η)

Each training example is a pair <x, t>: x is the vector of input values, and t is the target output value. η is the learning rate (e.g., .05).

- Initialize each w_i to some small random value
- Repeat until the termination condition is met
  1. *Initialize each Δw_i to zero*
  2. *For each <x, t>*
     - ♦ *Input x to the unit and compute output o*
     - ♦ *For each linear unit weight w_i*

$$w_i \leftarrow w_i + \eta (t - o) x_i$$

Perceptron vs. Delta rule training

- Perceptron training rule guaranteed to succeed if
  - Training examples are linearly separable
  - Sufficiently small learning rate
- Delta training rule uses gradient descent
  - Guaranteed to converge to hypothesis with minimum squared error
    - Given sufficiently small learning rate
    - Even when training data contains noise
    - Even when training data not linearly separable
- Can generalize linear units to units with threshold
  - Just threshold the results

Perceptron vs. Delta rule training

- Delta/perceptron training rules appear same *but*
  - Perceptron rule trains discontinuous units
    - Guaranteed to converge under limited conditions
    - May not converge in general
  - Gradient rules trains over continuous response (unthresholded outputs)
    - Gradient rule always converges
      - Even with noisy training data
      - Even with non-separable training data
  - Gradient descent generalizes to other continuous responses
  - Can train perceptron with LMS rule
    - get prediction by thresholding outputs

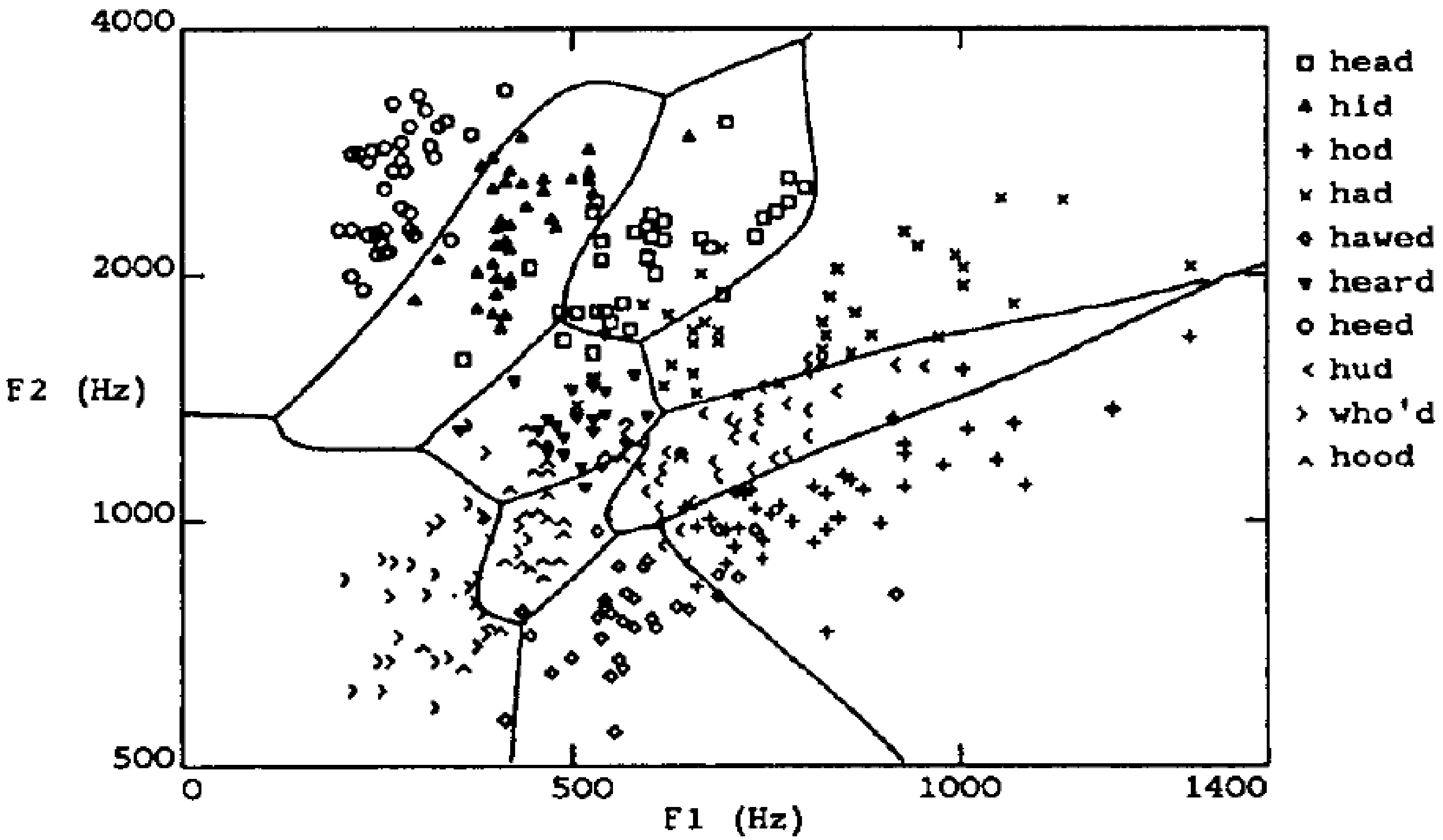
Multilayer networks of sigmoid units

- Needed for relatively complex (i.e., typical) functions

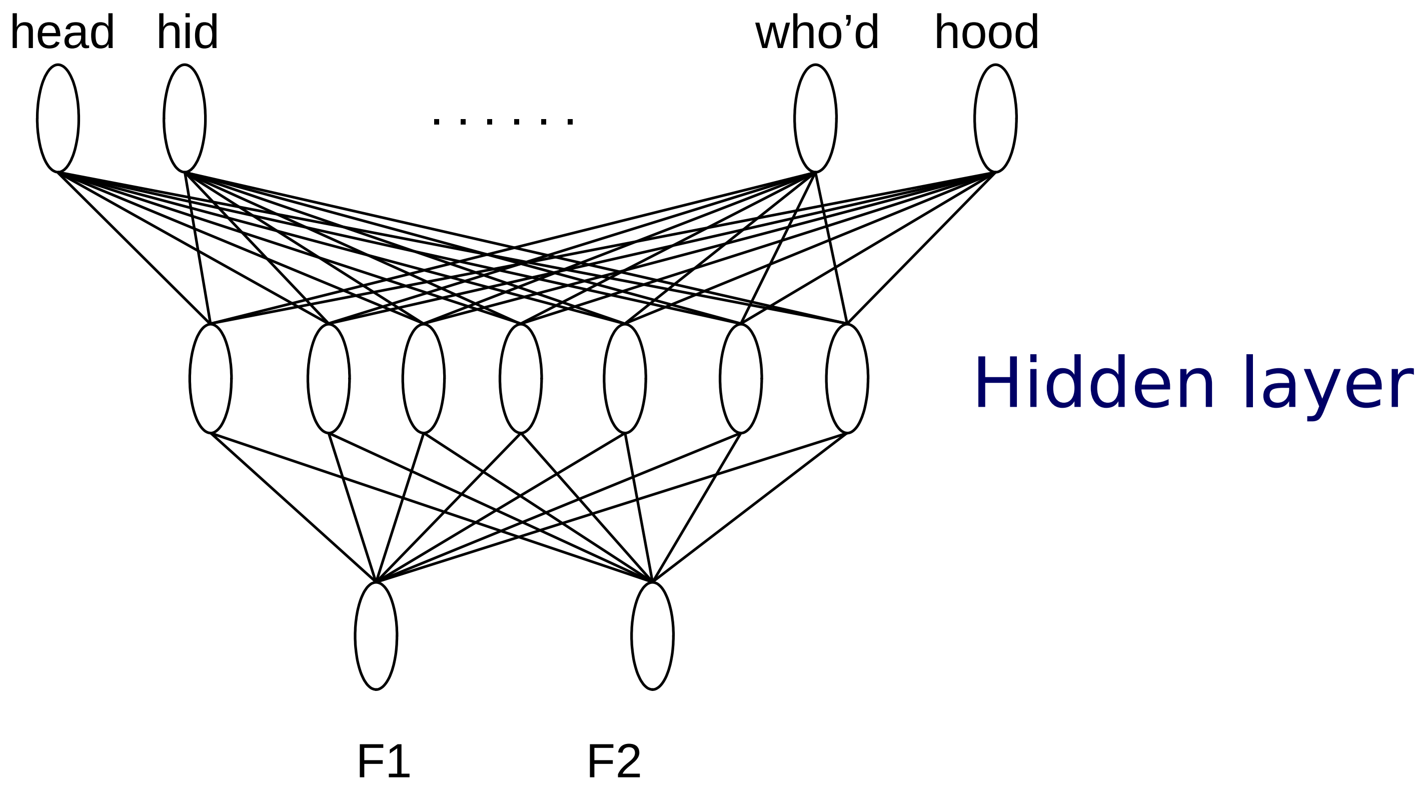
- Want non-linear response units in many systems
  - Example (next slide) of phoneme recognition
  - Cascaded nets of linear units only give linear response
  - Sigmoid unit as example of many possibilities

- Want differentiable functions of weights
  - So can apply gradient descent
    - Minimization of error function
  - Step function perceptrons non-differentiable

Speech recognition example

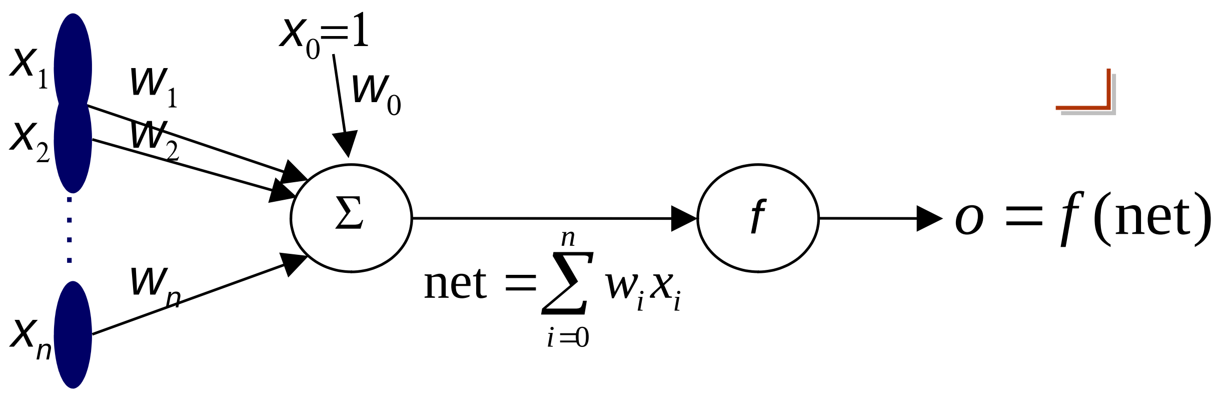


Multilayer networks



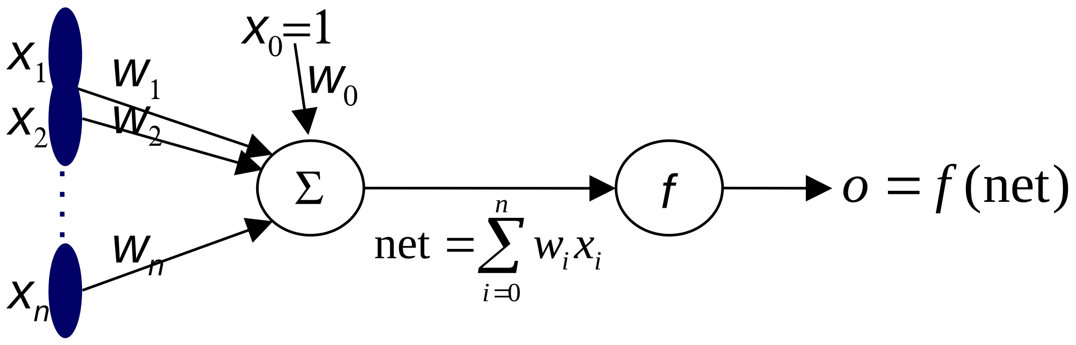
- Can have more than one hidden layer

Sigmoid unit



- f is the sigmoid function $f(x) = \dfrac{1}{1+e^{-x}}$
- Derivative can be easily computed: $\dfrac{df(x)}{dx} = f(x)\left(1 - f(x)\right)$
- Logistic equation
    - used in many applications
    - other functions possible (tanh)
- Single unit:
    - apply gradient descent rule
- Multilayer networks: **backpropagation**

Error Gradient for a Sigmoid Unit



$$\frac{\partial E}{\partial w_i} = \frac{\partial}{\partial w_i} \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2$$

$$= \frac{1}{2} \sum_{d \in D} \frac{\partial}{\partial w_i} (t_d - o_d)^2$$

$$= \frac{1}{2} \sum_{d \in D} 2(t_d - o_d) \frac{\partial}{\partial w_i} (t_d - o_d)$$

$$= \sum_{d \in D} (t_d - o_d) \left(- \frac{\partial o_d}{\partial w_i} \right)$$

$$= - \sum_{d \in D} (t_d - o_d) \frac{\partial o_d}{\partial \text{net}_d} \frac{\partial \text{net}_d}{\partial w_i}$$

net: linear combination
o (output): logistic function

$$\frac{\partial o_d}{\partial \text{net}_d} = \frac{\partial f(\text{net}_d)}{\partial \text{net}_d} = f(\text{net}_d)(1 - f(\text{net}_d)) = o_d (1 - o_d)$$

$$\frac{\partial \text{net}_d}{\partial w_i} = \frac{\partial (\vec{w} \cdot \vec{x}_d)}{\partial w_i} = x_{i,d}$$

$$\frac{\partial E}{\partial w_i} = - \sum_{d \in D} (t_d - o_d) o_d (1 - o_d) x_{i,d}$$

… Incremental Version

- Batch gradient descent for a single Sigmoid unit

$$E_D = \frac{1}{2}\sum_{d\in D}(t_d - o_d)^2 \qquad \frac{\partial E_D}{\partial w_i} = -\sum_{d\in D}(t_d - o_d)o_d(1 - o_d)x_{i,d}$$

- Stochastic approximation

$$E_d = \frac{1}{2}(t_d - o_d)^2 \qquad \frac{\partial E_d}{\partial w_i} = -(t_d - o_d)o_d(1 - o_d)x_{i,d}$$

Backpropagation procedure

- Create FFnet
  - n_i inputs, n_o output units, n hidden layers
  - Define error by considering *all* output units
- Train the net by propagating errors backwards from output units
  - First output units
  - Then hidden units
- Notation: $x_{j,i}$ is input from unit i to unit j

  $w_{j,i}$ is the corresponding weight
- Note: various termination conditions
  - error
  - # iterations,…
- Issues of under/over fitting, etc.

Backpropagation (stochastic case)

- Initialize all weights to small random numbers
- Repeat

For each training example

1. Input the training example to the network and compute the network outputs
2. For each output unit k

$$\delta_k \leftarrow o_k (1 - o_k)\,(t_{k\,-}\, o_k)$$

3. For each hidden unit h

$$\delta_h \leftarrow o_h (1 - o_h)\,\Sigma_{k \in \text{outputs}}\, w_{k,h} \delta_k$$

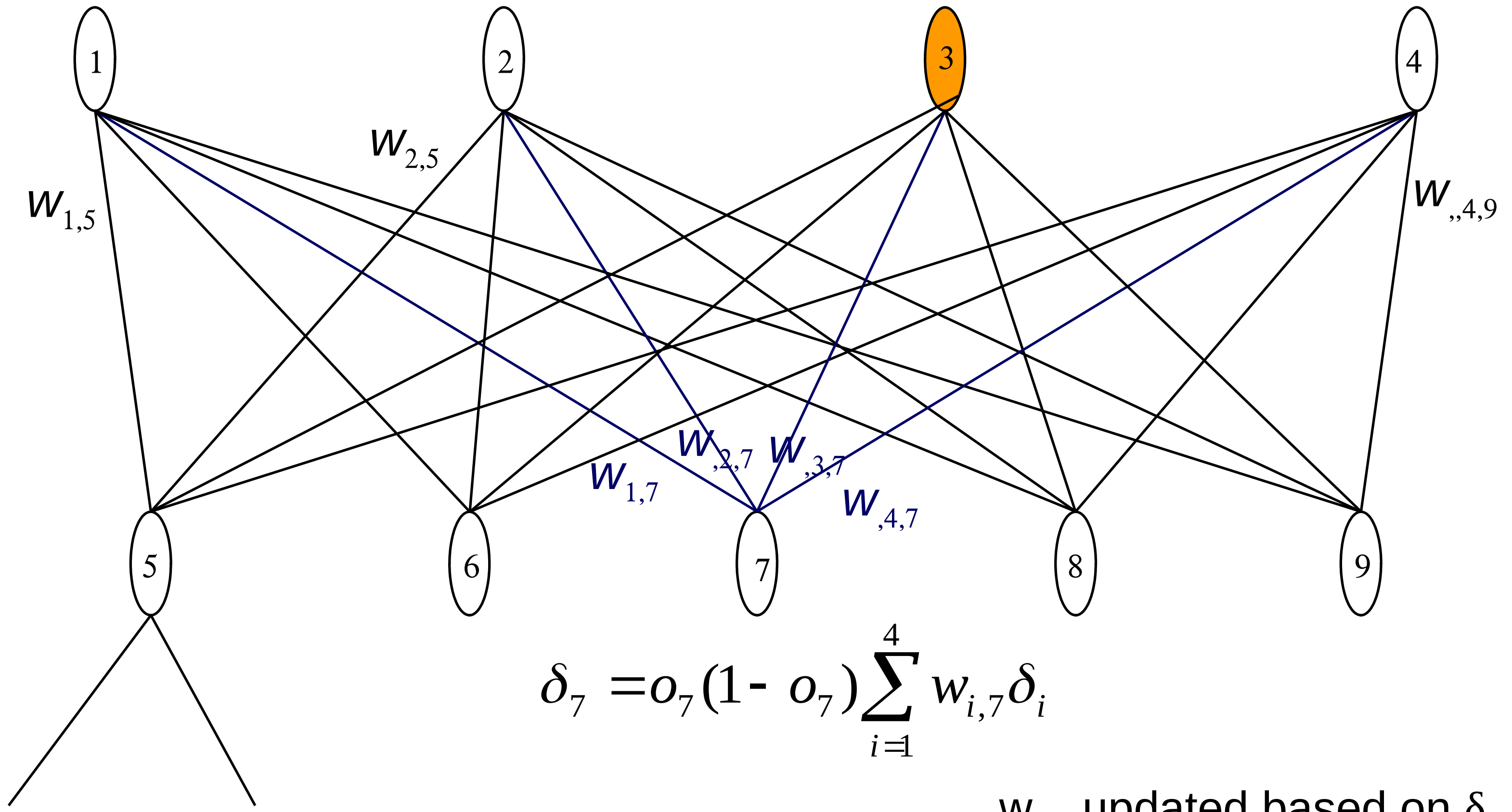
4. Update each network weight $w_{j,i}$

$$w_{j,i} \leftarrow w_{j,i} + \Delta w_{j,i}$$

where $\Delta w_{j,i} = \eta\, \delta_j x_{j,i}$

Errors propagate backwards

$$\delta_3 = o_3(1 - o_3)(t_3 - o_3)$$



$$\delta_7 = o_7(1 - o_7)\sum_{i=1}^{4} w_{i,7}\delta_i$$

$w_{1,7}$ updated based on δ_1 and $x_{1,7}$

- Same process repeats if we have more layers

Properties of Backpropagation

- Easily generalized to arbitrary directed acyclic graphs
  - Backpropagate errors through the different layers

- Training is slow but applying it to networks after training is fast

Convergence of Backpropagation

- Convergence
  - Training can take thousands of iterations $\rightarrow$ slow!
    - Gradient descent over entire network weight vector
    - Speed up using small initial values of weights:
      - – Linear response initially
  - Generally will find local minimum
    - Typically can find good approximation to global minimum
  - Solutions to local minimum trap problem
    - Stochastic gradient descent
    - Can run multiple times – Over different initial weights
    - Committee of networks
    - Can modify to find better approximation to global minimum
      - – include weight momentum α

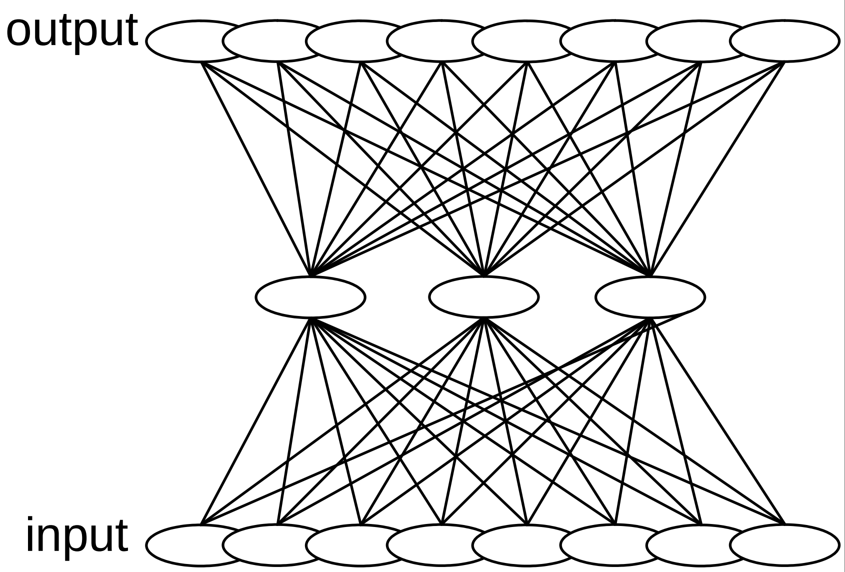
$$\Delta w_{i,j}(t_n) = \eta\, \delta_j x_{i,j} + \alpha\, \Delta w_{i,j}(t_{n-1})$$

➢ Momentum avoids local max/min and plateaus

Example of learning a simple function

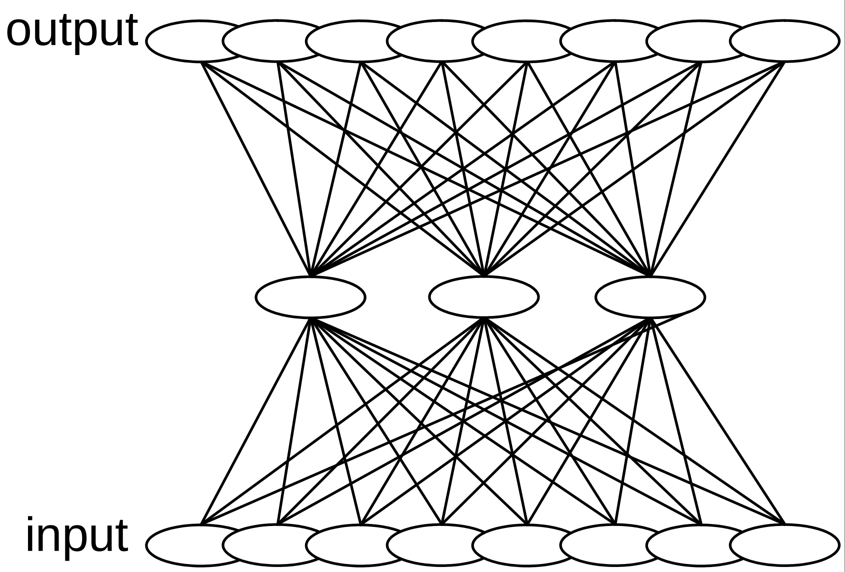
- Learn to recognize 8 simple inputs
  - Interest in how to interpret hidden units
  - System learns binary representation!
- Trained with
  - initial w_i between –0.1, +0.1,
  - eta=0.3
- 5000 iterations (most change in first 50%)
- Target output values:
  - 0.1 for 0
  - 0.9 for 1

Hidden layer representations



Input		Hidden values				Output
10000000	→				→	10000000
01000000	→				→	01000000
00100000	→				→	00100000
00010000	→	?	?	?	→	00010000
00001000	→				→	00001000
00000100	→				→	00000100
00000010	→				→	00000010
00000001	→				→	00000001

Hidden layer representations



Input		Hidden values				Output
10000000	→	.89	.04	.08	→	10000000
01000000	→	.01	.11	.88	→	01000000
00100000	→	.01	.97	.27	→	00100000
00010000	→	.99	.97	.71	→	00010000
00001000	→	.03	.05	.02	→	00001000
00000100	→	.22	.99	.99	→	00000100
00000010	→	.80	.01	.98	→	00000010
00000001	→	.60	.94	.01	→	00000001

Example of head/face recognition

- Task: recognize faces from sample of
  - 20 people in 32 poses
  - Choose output of 4 values for direction of gaze
  - 120x128 images (256 gray levels)
- Can compute many functions
  - Identity/direction of face (used in book)/…
- Design issues
  - Input encoding (pixels/features/?)
    - Reduced image encoding (30x32)
  - Output encoding (1 or 4 values?)
    - Convergence to 0.1/0.9 and not 0/1
  - Network structure (1 layer of 3 hidden units)
  - Algorithm parameters
    - η =0.3; α =0.3; stochastic descent method
- Training/validation sets
- Results: 90% accurate for head pose

Some issues with ANNs

- Interpretation of hidden units
  - Hidden units "discover" new patterns/regularities
  - Often difficult to interpret

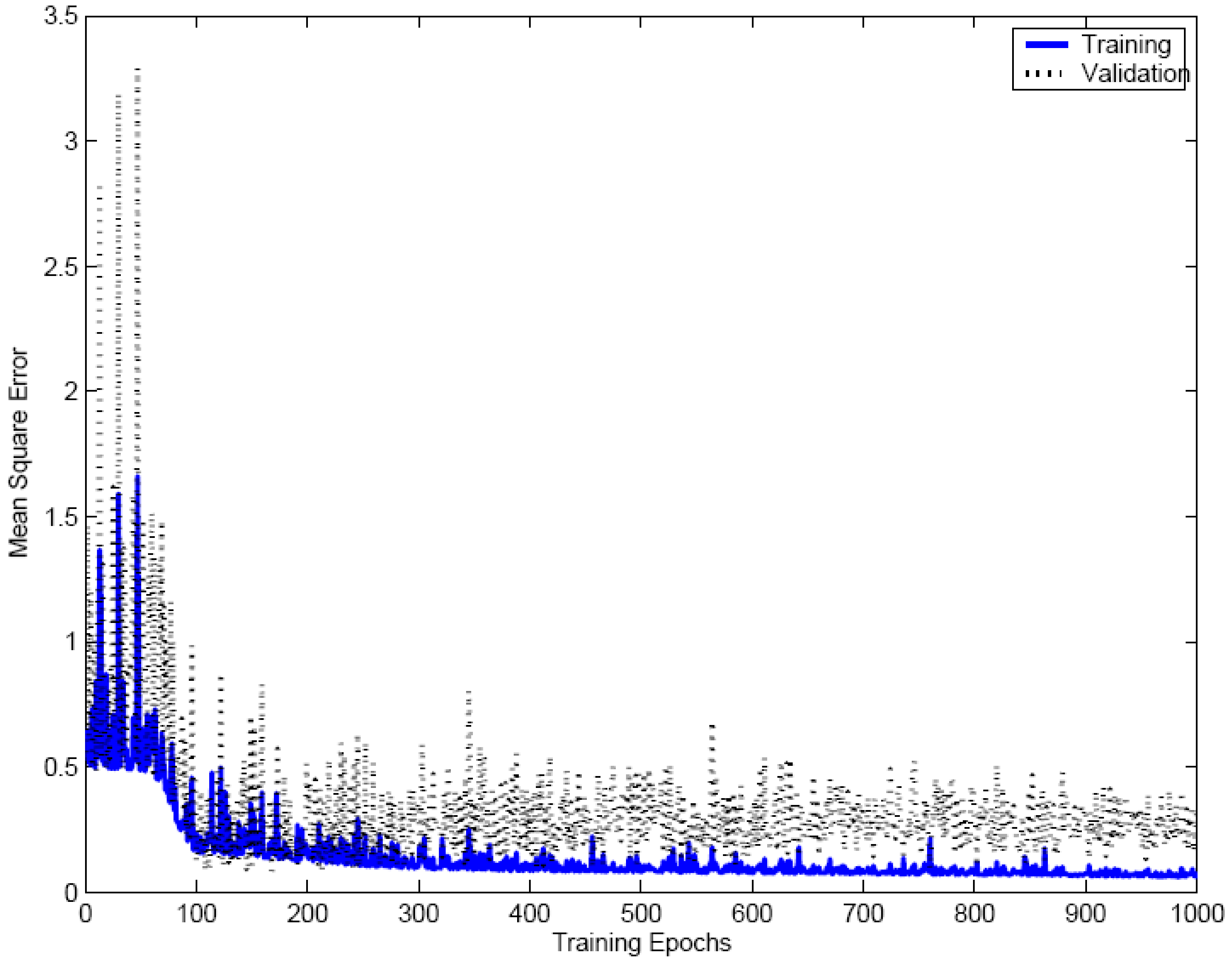
- Overfitting

- Expressiveness
  - Generalization to different classes of functions

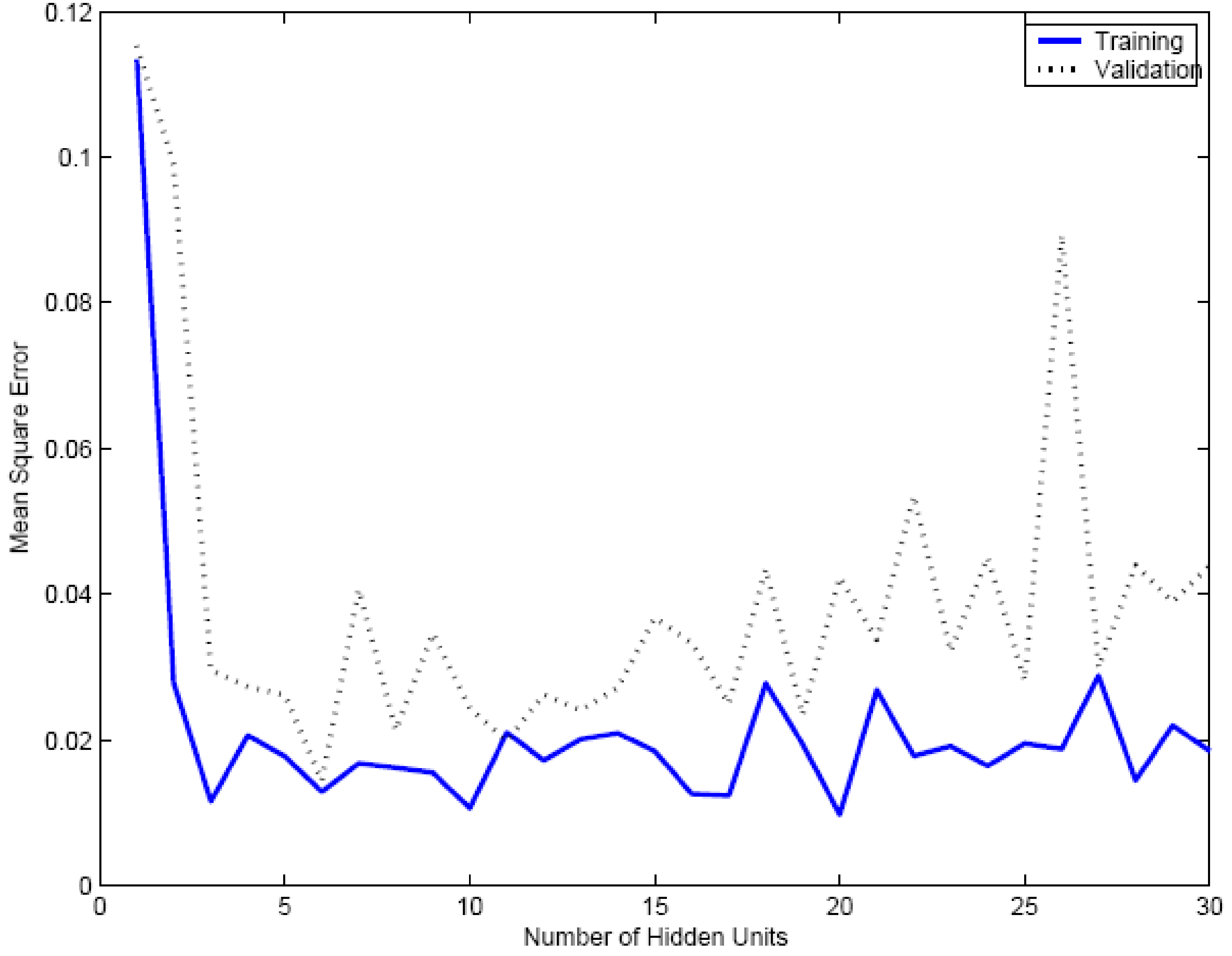
Dealing with overfitting

- Complex decision surface
- Divide sample into
  - Training set
  - Validation set
- Solutions
  - Return to weight set occurring near minimum over validation set
  - Prevent weights from becoming too large
    - Reduce weights by (small) proportionate amount at each iteration

Training vs. Validation



Effect of hidden units



Expressiveness

- Every Boolean function can be represented by network with a single hidden layer
  - Create 1 hidden unit for each possible input
  - Create OR-gate at output unit
  - *but* might require exponential (in number of inputs) hidden units
- Every bounded continuous function can be approximated with arbitrarily small error, by network with one hidden layer (Cybenko et al ‘89)
  - Hidden layer of sigmoid functions
  - Output layer of linear functions
- Any function can be approximated to arbitrary accuracy by a network with two hidden layers (Cybenko ‘88)
  - Sigmoid units in both hidden layers
  - Output layer of linear functions

Extension of ANNs

- Many possible variations
  - Alternative error functions
    - Penalize large weights
      - Add weighted sum of squares of weights to error term
  - Structure of network
    - Start with small network, and grow
    - Start with large network and diminish

- Use other learning algorithms to learn weights

Extensions of ANNs

- Recurrent networks
  - Example of time series
    - Would like to have representation of behavior at t+1 from arbitrary past intervals (no set number)
    - Idea of simple recurrent network
      – hidden units that have feedback to inputs

- Dynamically growing and shrinking networks

Inductive bias of Backpropagation

- Smooth interpolation between data points

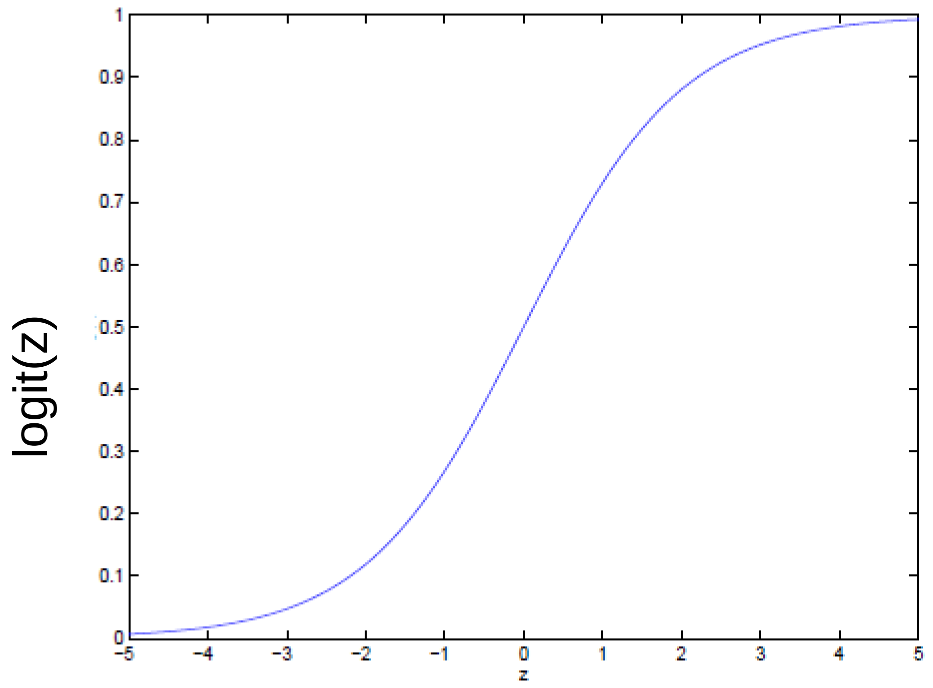
Summary

- Practical method for learning continuous functions over continuous and discrete attributes
- Robust to noise
- Slow to train but fast afterwards
- Gradient descent search over space of weights
- Overfitting can be a problem
- Hidden layers can invent new features

Logistic function (Logit function)

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

This term lies in [0, infinity]



- σ(z) is always bounded between [0,1] (a nice property),
- as z increase σ(z) approaches 1,
- as z decreases σ(z) approaches to 0.

Segway: Logistic regression

- Logistic regression is often used because the relationship between the dependent discrete variable and a predictor is non-linear

- Example: the probability of heart disease changes very little with a ten-point difference among people with low-blood pressure, but a ten point change can mean a drastic change in the probability of heart disease in people with high blood-pressure.

Logistic regression

Learn a function to map X values to Y given data

$$(X^1, Y^1), .., (X^N, Y^N)$$

Discrete

$$f : X \to Y$$

X can be continuous or discrete

The function we try to learn is P(Y|X)

Logistic regression (Classification)

Classification

$$1 < \frac{P(Y=0|X)}{P(Y=1|X)} \longrightarrow$$

If this holds Y=0 is more probable than Y=1 given X

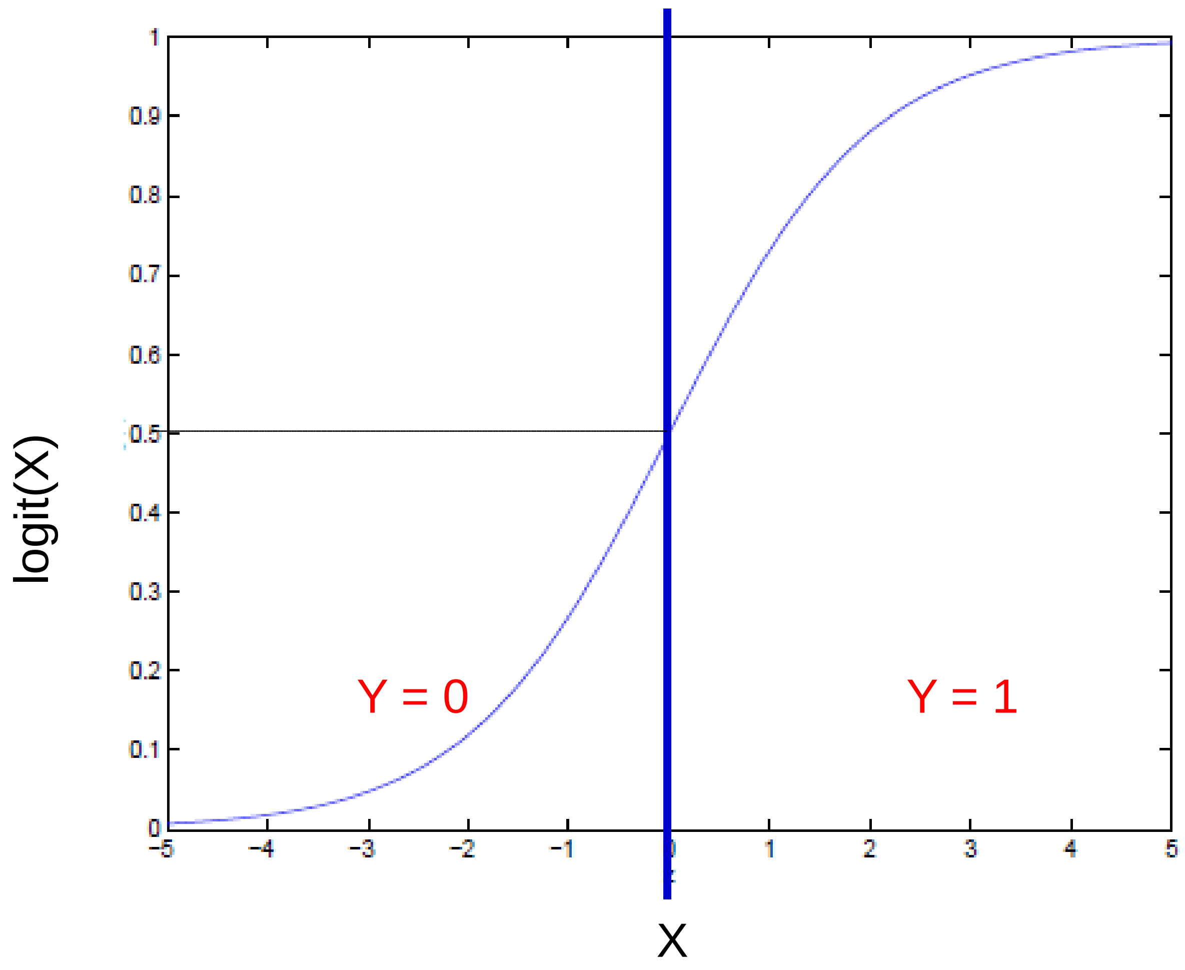
Classification

$$1 < \frac{P(Y=0|X)}{P(Y=1|X)}$$

Take log both sides

Classification rule: if this holds Y=0

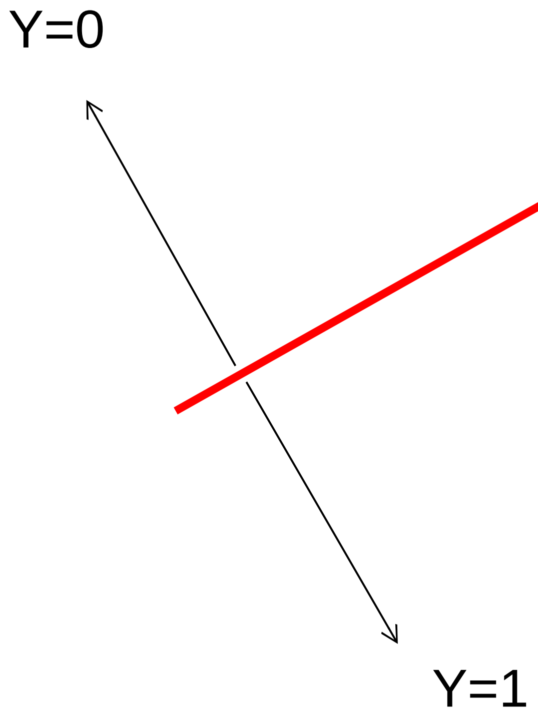
Logistic Function (Logit function)



Logistic regression is a linear classifier

Decision boundary

$$w_0 + \sum_1^N w_i X_i = 0$$



Learn parameters using sigmoid unit training (gradient descent)

Thank You!