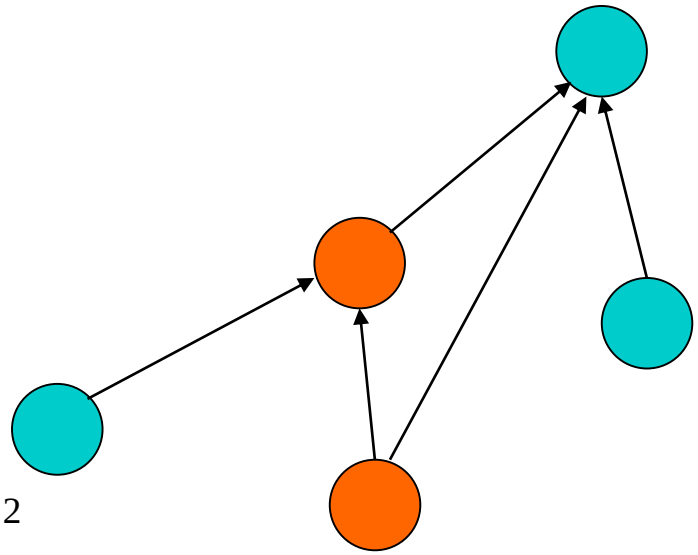
Artificial Neural Networks

Neural networks

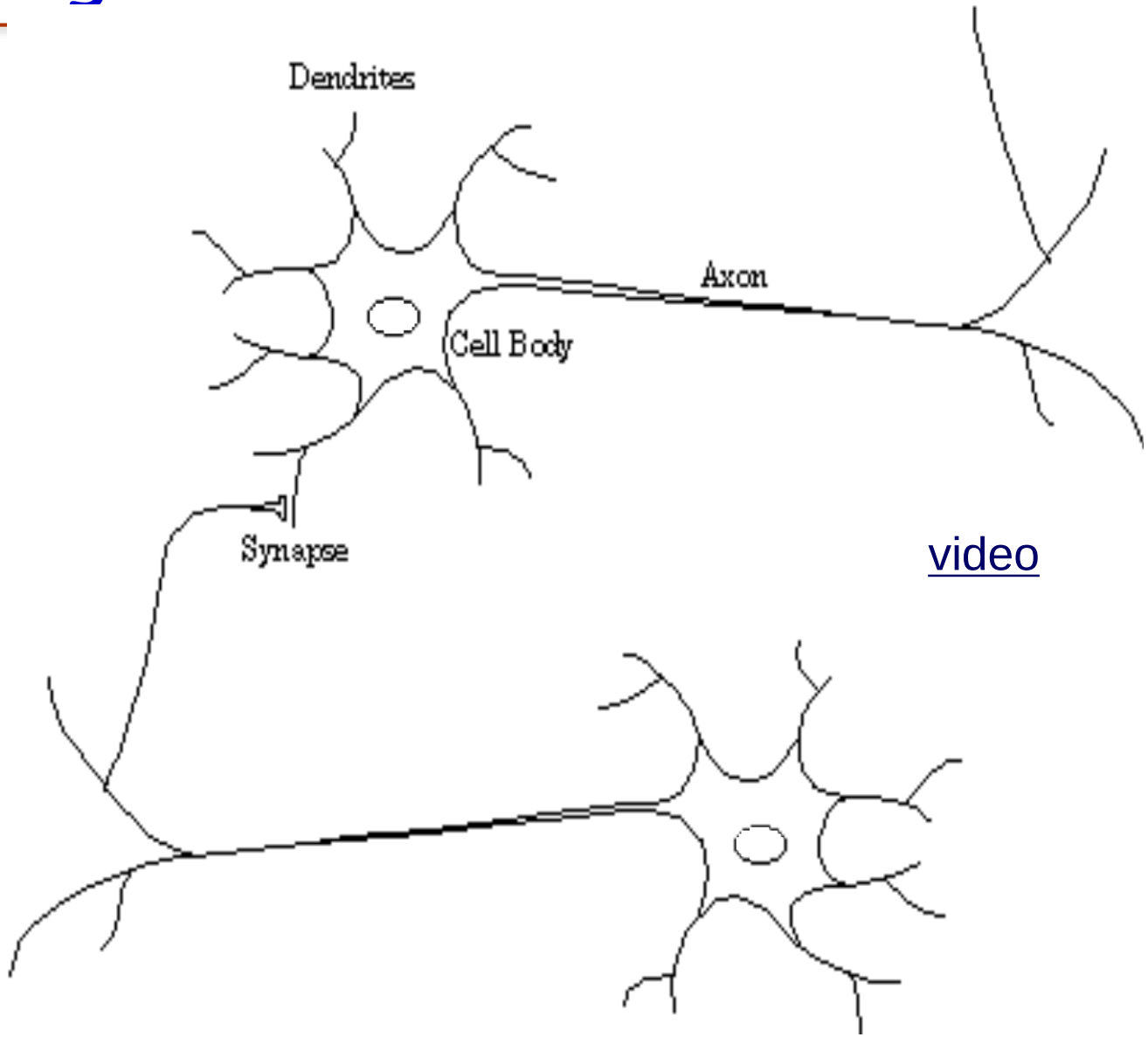
- Networks of processing units (neurons) with connections (synapses) between them
- Large number of neurons: 10^{10}
- Large connectitivity: 10^5
- Parallel processing
- Distributed computation/memory
- Robust to noise, failures



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



video

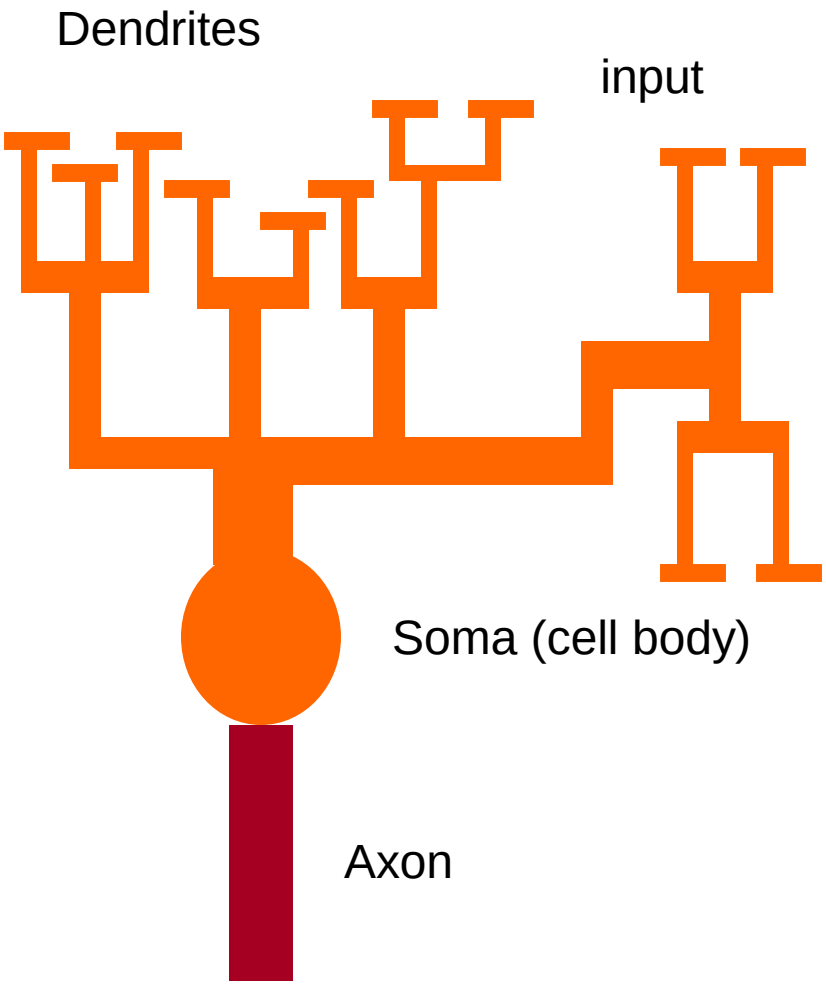
Biological neuron

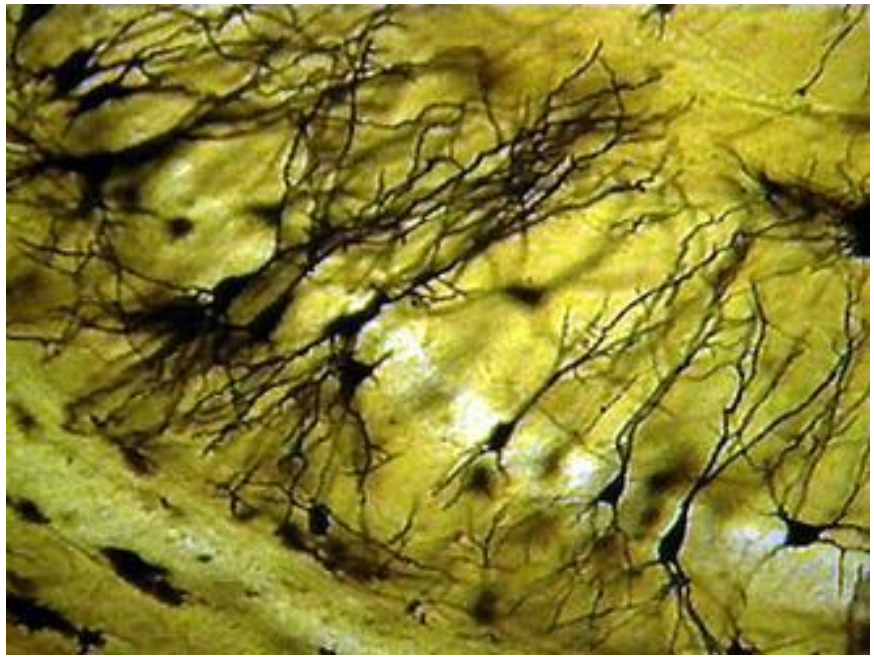
- dendrites: nerve fibres carrying electrical signals to the cell
- cell body: computes a non-linear function of its inputs
- axon: single long fiber that carries the electrical signal from the cell body to other neurons
- synapse: the point of contact between the axon of one cell and the dendrite of 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

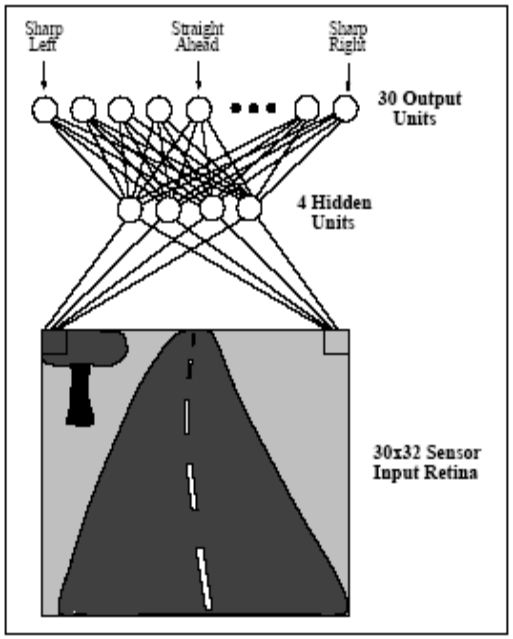
- Hodgkin and Huxley experimented on squids and discovered how the signal is produced within the neuron
- This model was published in *Jour. of Physiology* (1952)
- They were awarded the 1963 Nobel Prize

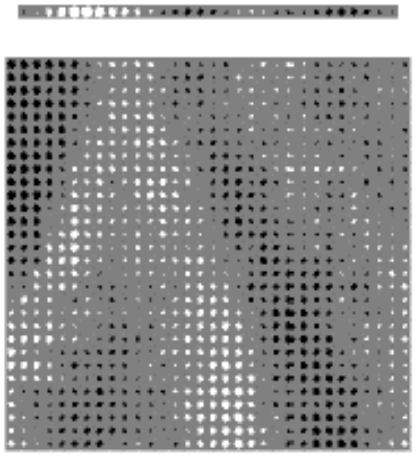
When to consider ANNs

- 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

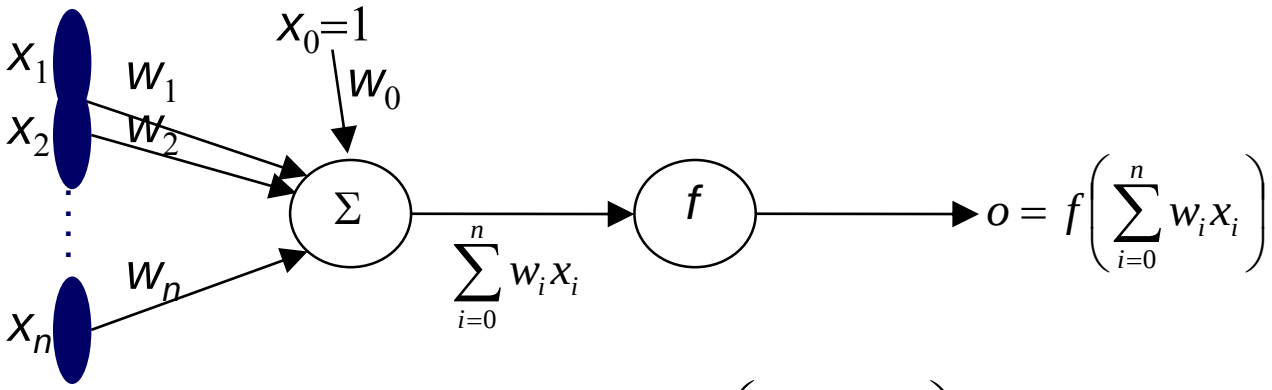
- ALVINN: a perception system which learns to control the NAVLAB vehicles by watching a person drive





How many weights need to be learned?

Perceptron



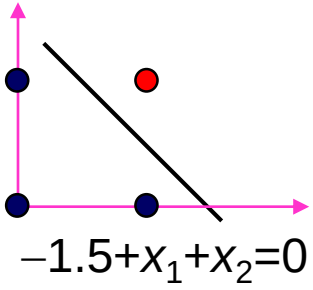
- $-w_0$: threshold value or bias $\left(\sum_{i=1}^{n} w_i x_i\right) - (-w_0)$

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

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

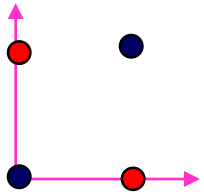
Decision surface of a perceptron

- 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, $x_1 \wedge x_2$?



- $x_1 \vee x_2$?
- x_1 XOR x_2 ?

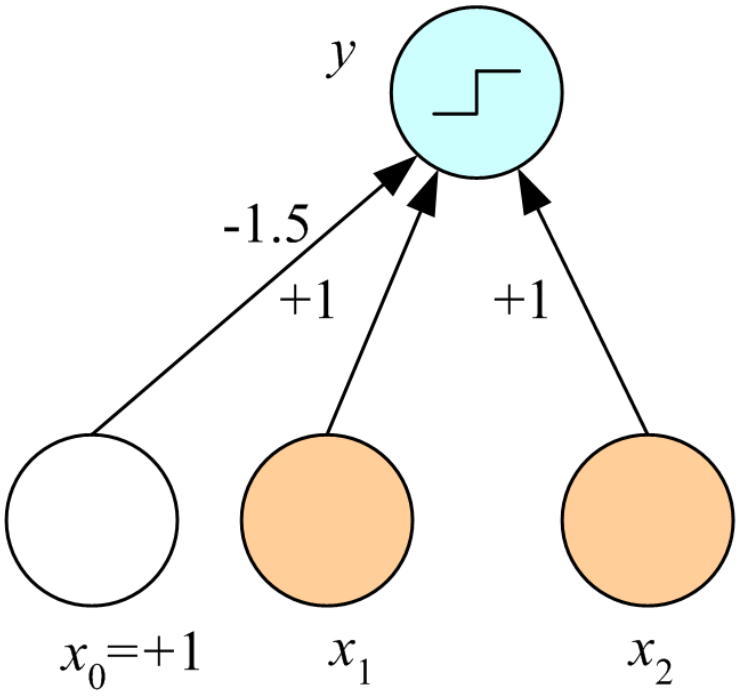
Not linearly separable!

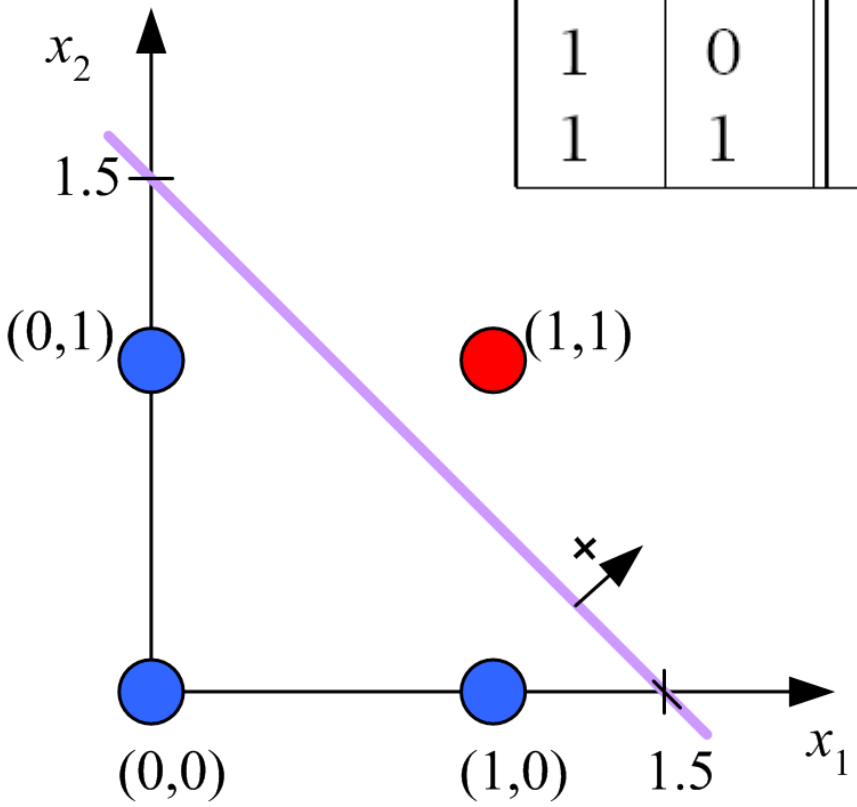


- Generalization to higher dimensions
  - Hyperplanes as decision surfaces

Learning Boolean AND

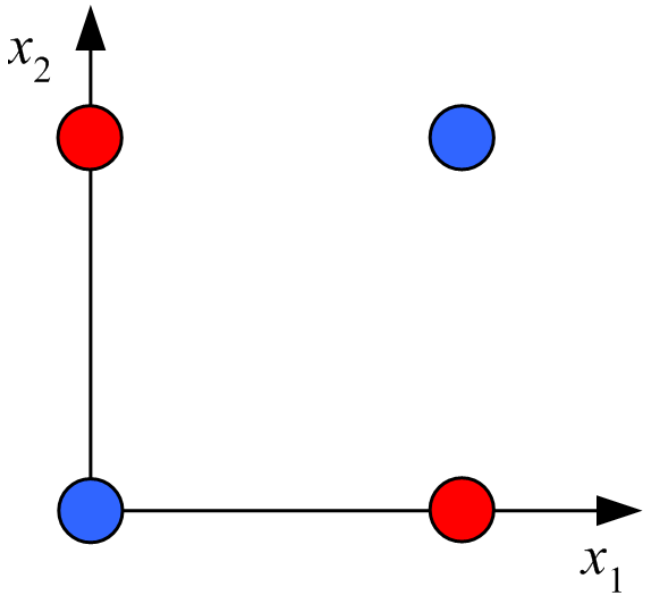
x_1	x_2	r
0	0	0
0	1	0
1	0	0
1	1	1





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, η = 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 $o(x) = w_0 + w_1 x_1 + \ldots + w_n x_n$
  - 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

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

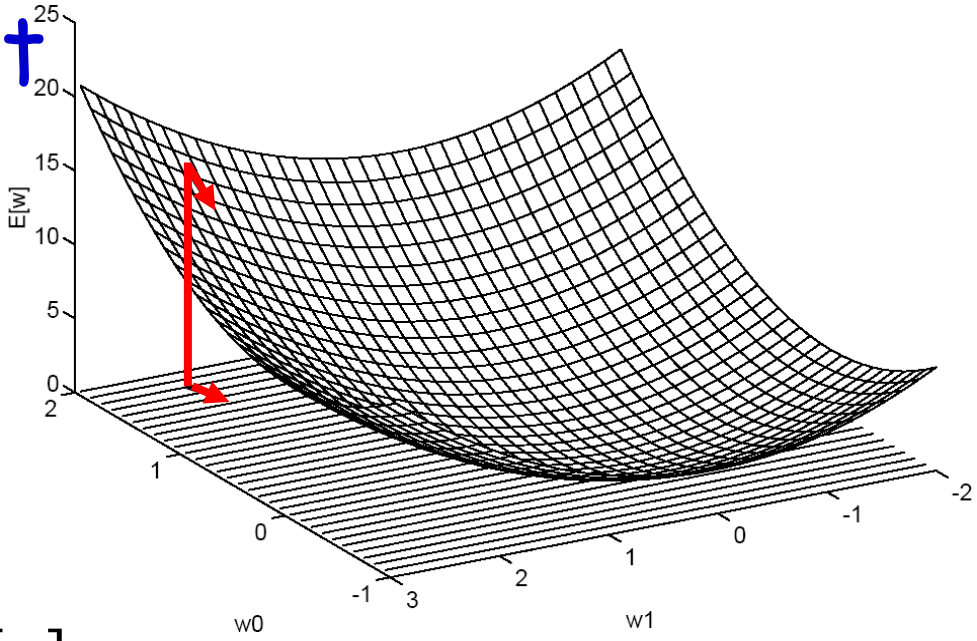
Error minimization

- Look at error E as a function of weights {wi}
- Slide down gradient of E in weight space
- Reach values of {wi} that correspond to minimum error
  - Look for global minimum
- Example of 2-dimensional case:
  - E = w1*w1 + w2*w2
  - Minimum at w1=w2=0
- Look at general case of n-dimensional space of weights

Gradient descent

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

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

Parabola with a single minima

- How might one interpret this update rule?

Gradient descent

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

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

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

$$= \sum_{d\in D}\left(t_d - o_d\right)\frac{\partial}{\partial w_i}\left(t_d - \vec{w}_d \cdot \vec{x}_d\right)$$

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

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

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

Gradient descent algorithm

Gradient-Descent (*training examples*, η)

Each training example is a pair $\langle x, t \rangle$*:* 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 training example $\langle x, t \rangle$
     - 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 $\nabla E_D[\vec{w}]$
  2. $\vec{w} \leftarrow \vec{w} - \eta \nabla E_D[\vec{w}]$

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 $\nabla E_d[\vec{w}]$
    2. $\vec{w} \leftarrow \vec{w} - \eta \nabla E_d[\vec{w}]$
- 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 $\langle x, t \rangle$*:* 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 $\langle x, t \rangle$
     - 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

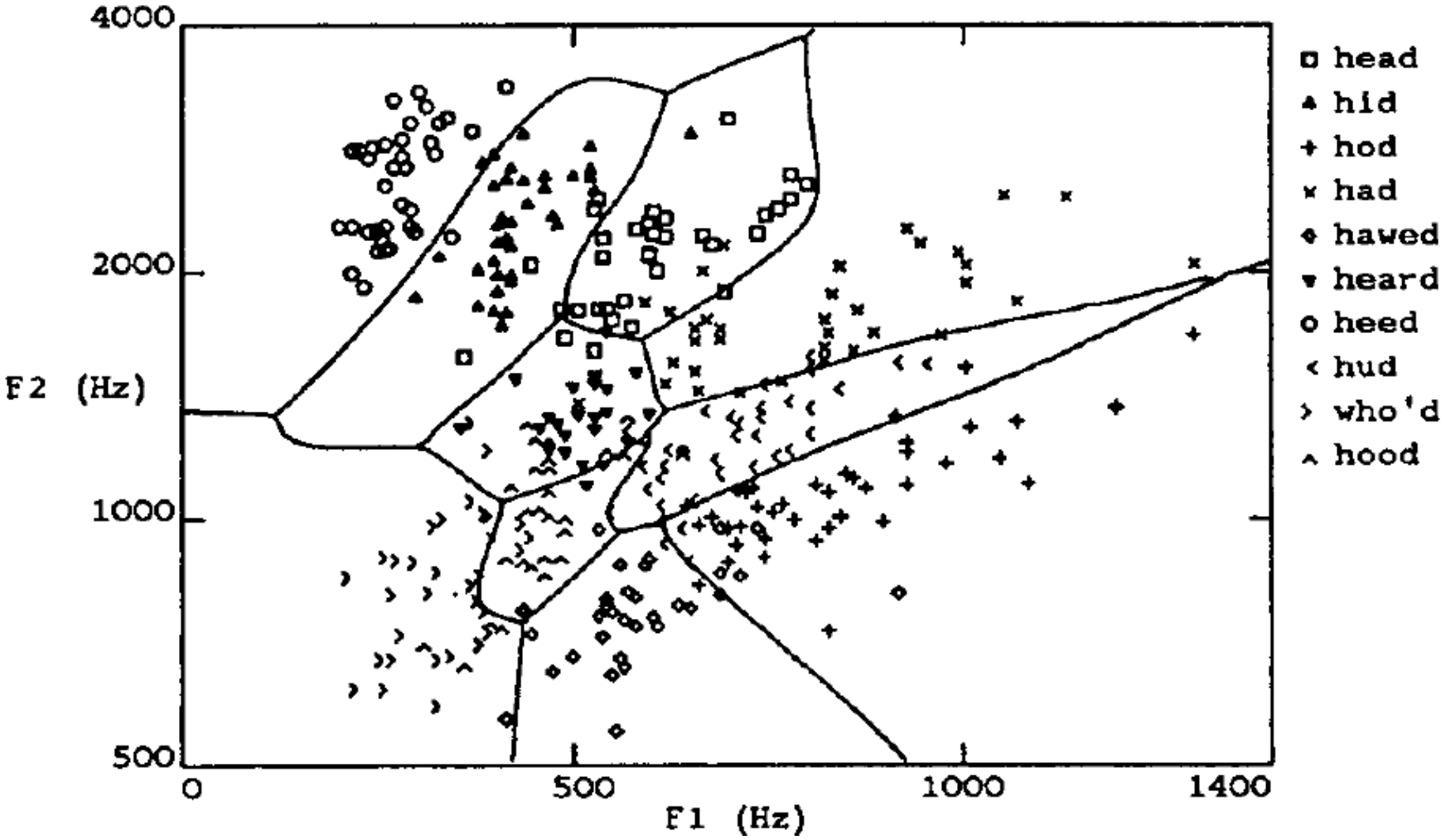
Perceptron vs. Delta rule training

- 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

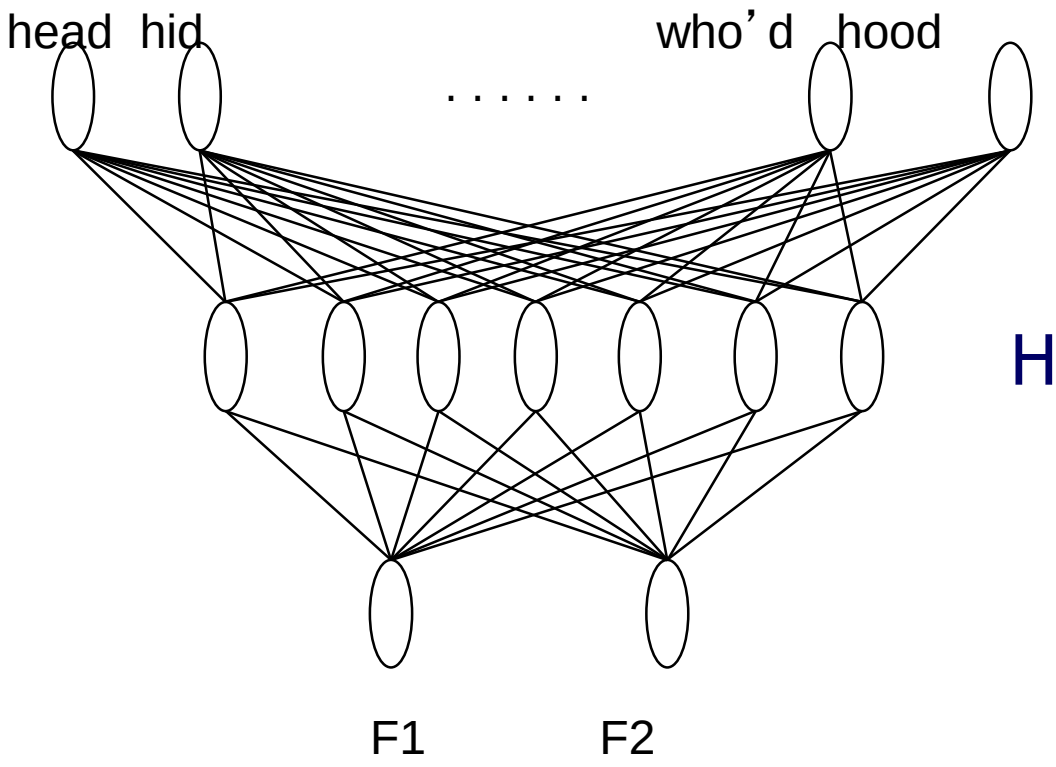
Multilayer networks of *sigmoid* units

- 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



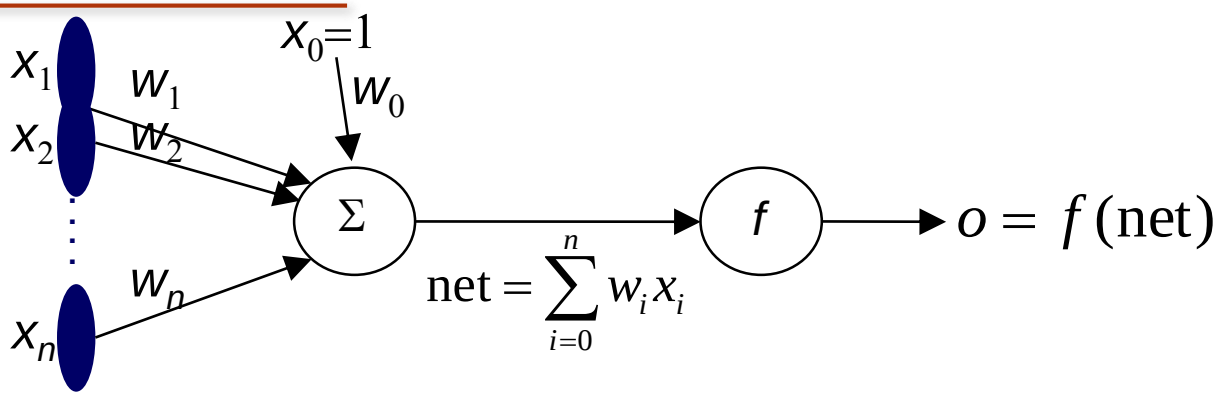
Multilayer networks



Hidden layer

- Can have more than one hidden layer

Sigmoid unit



- f is the sigmoid function

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

- Derivative can be easily computed:

$$\frac{df(x)}{dx} = f(x)\big(1 - f(x)\big)$$

- 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

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

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

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

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

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

net: linear combination
o (output): logistic function

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

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

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

… Incremental Version

- Batch gradient descent for a single Sigmoid unit

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

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

- Stochastic approximation

$$E_d = \frac{1}{2}(t_d - o_d)^2$$

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

Backpropagation procedure

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

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

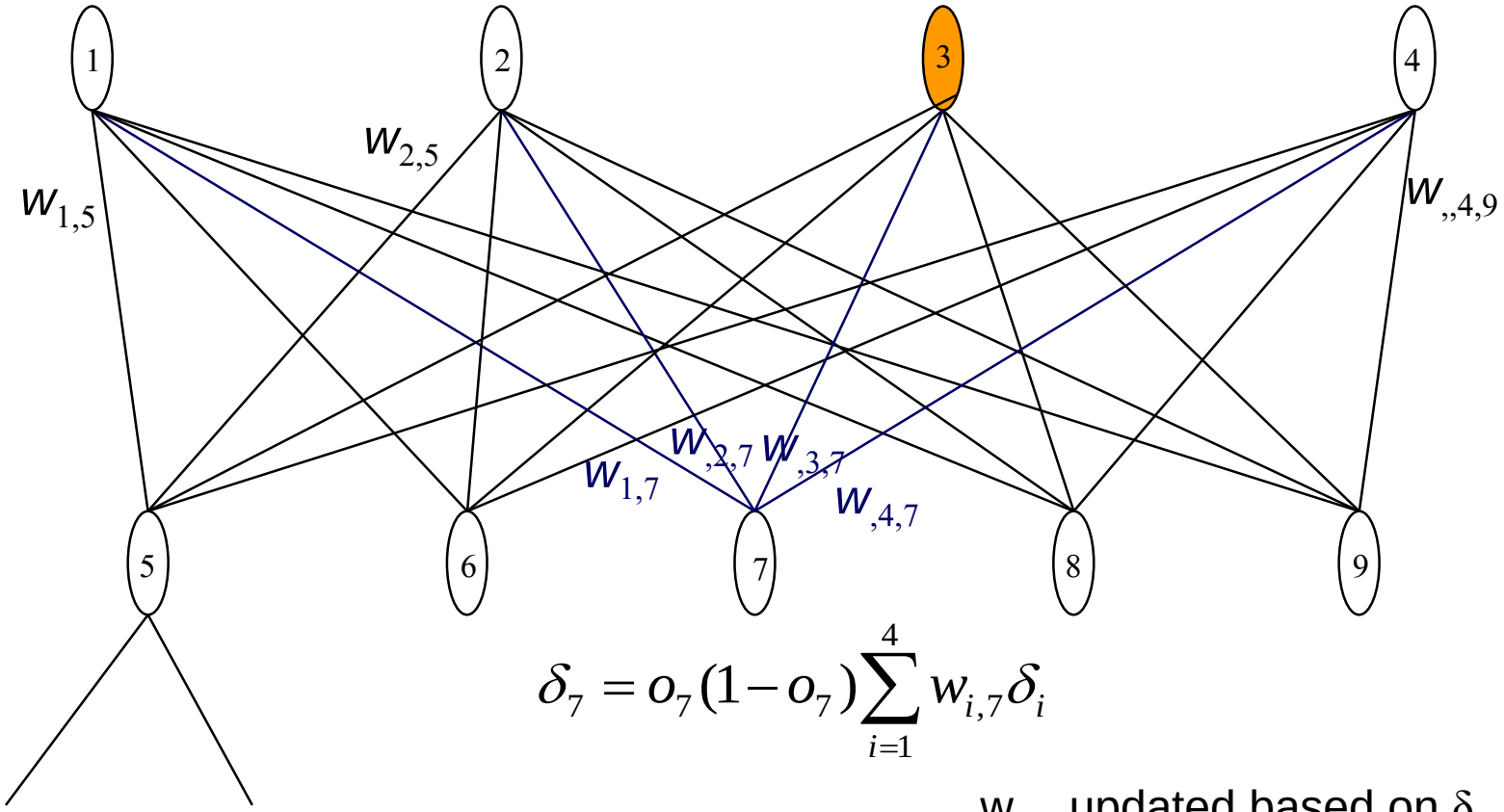
  4. Update each network weight $w_{j,i}$

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

  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 network after training is fast

Convergence of Backpropagation

- Convergence
  - Training can take thousands of iterations → 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

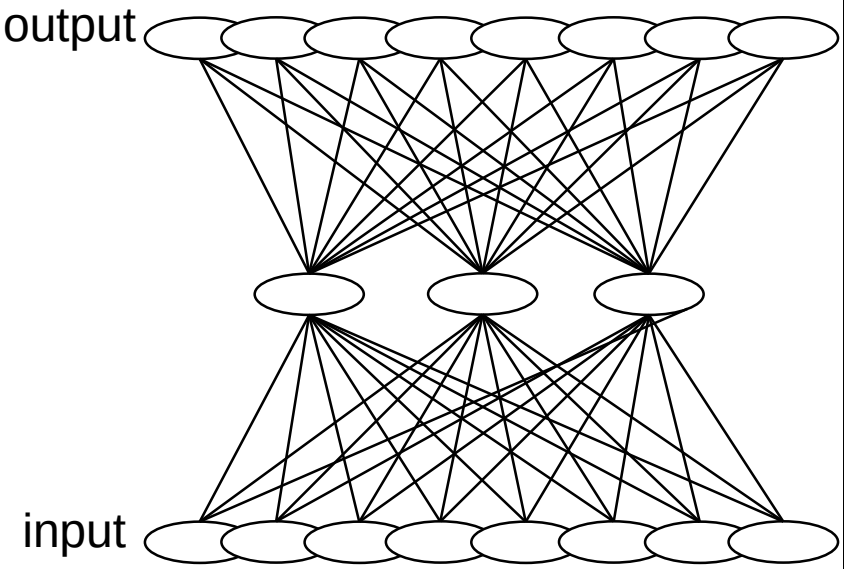
$$\Delta w_{i,j}(t_n) = \eta\, \delta_j\, x_{i,j} + \alpha\, \Delta w_{i,j}(t_{n-1})$$

➢ Momentum avoids local max/min and plateaus

Example of learning a simple function

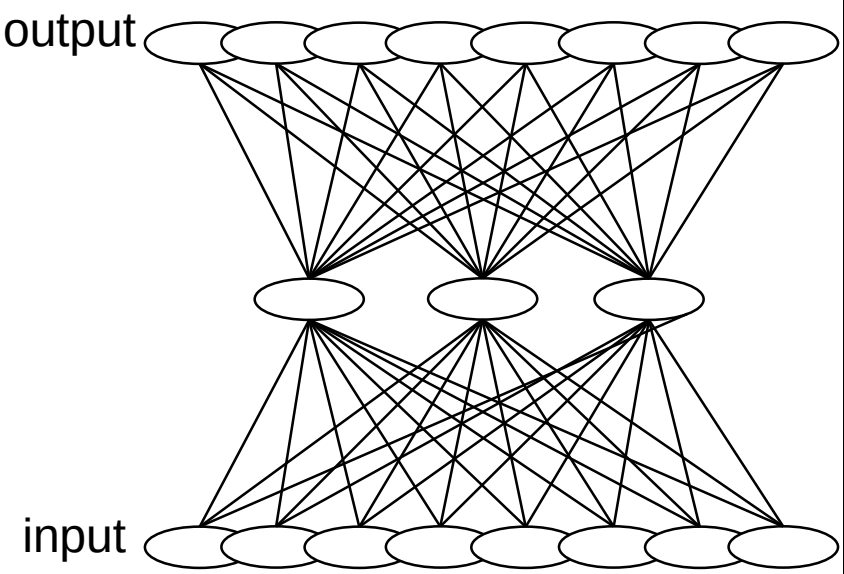
- Learn to recognize 8 simple inputs
  - Interest in how to interpret hidden units
  - System learns binary representation!
- Trained with
  - initial w_i between –0.1, +0.1,
  - eta=0.3
- 5000 iterations (most change in first 50%)
- Target output values:
  - .1 for 0
  - .9 for 1

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

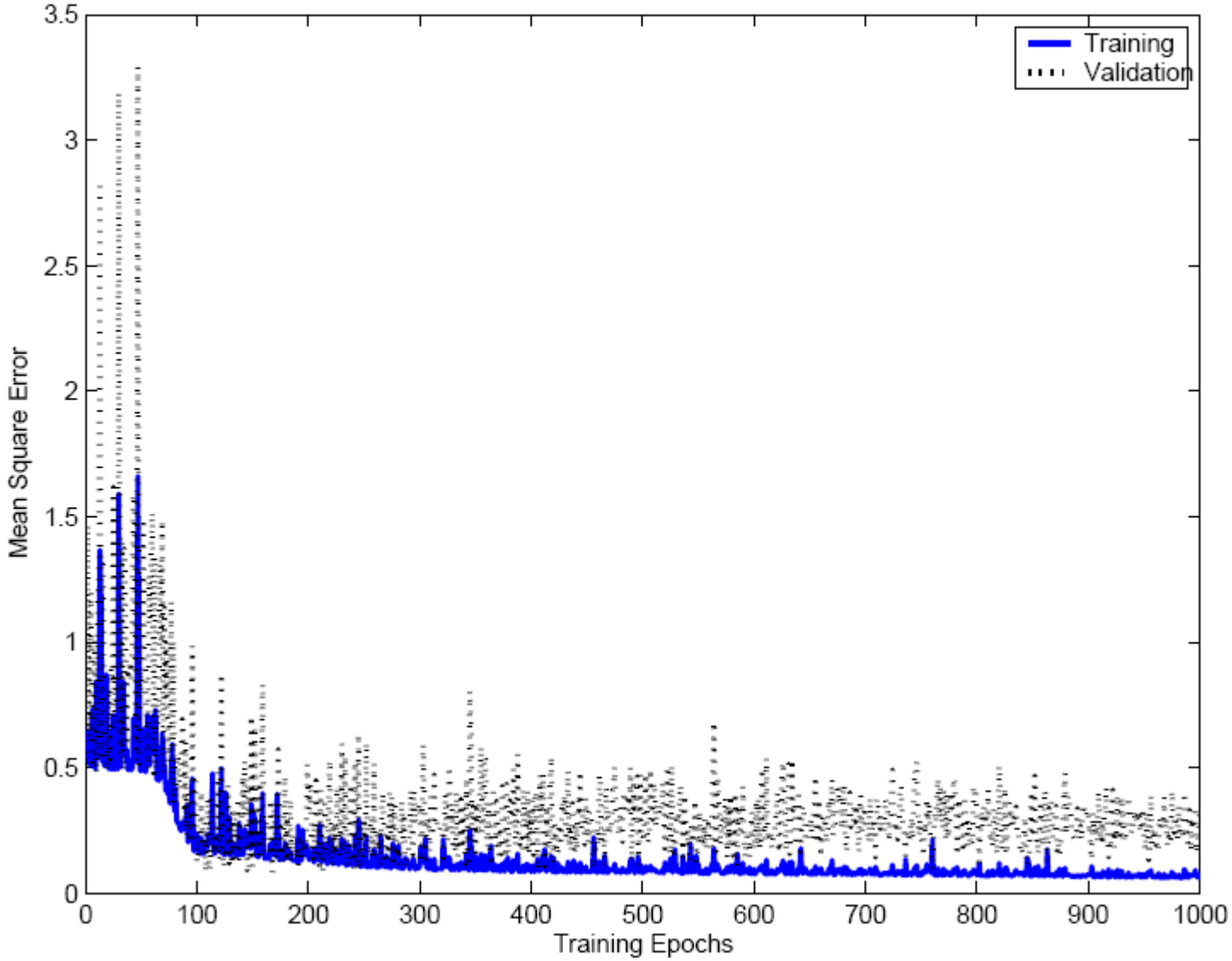
- Task: recognize faces from sample of
  - 20 people in 32 poses
  - Choose output of 4 values for direction of gaze
  - 120x128 images (256 gray levels)
- Can compute many functions
  - Identity/direction of face (used in book)/…
- Design issues
  - Input encoding (pixels/features/?)
    - Reduced image encoding (30x32)
  - Output encoding (1 or 4 values?)
    - Convergence to .1/.9 and not 0/1
  - Network structure (1 layer of 3 hidden units)
  - Algorithm parameters
    - Eta=.3; alpha=.3; stochastic descent method
- Training/validation sets
- Results: 90% accurate for head pose

Some issues with ANNs

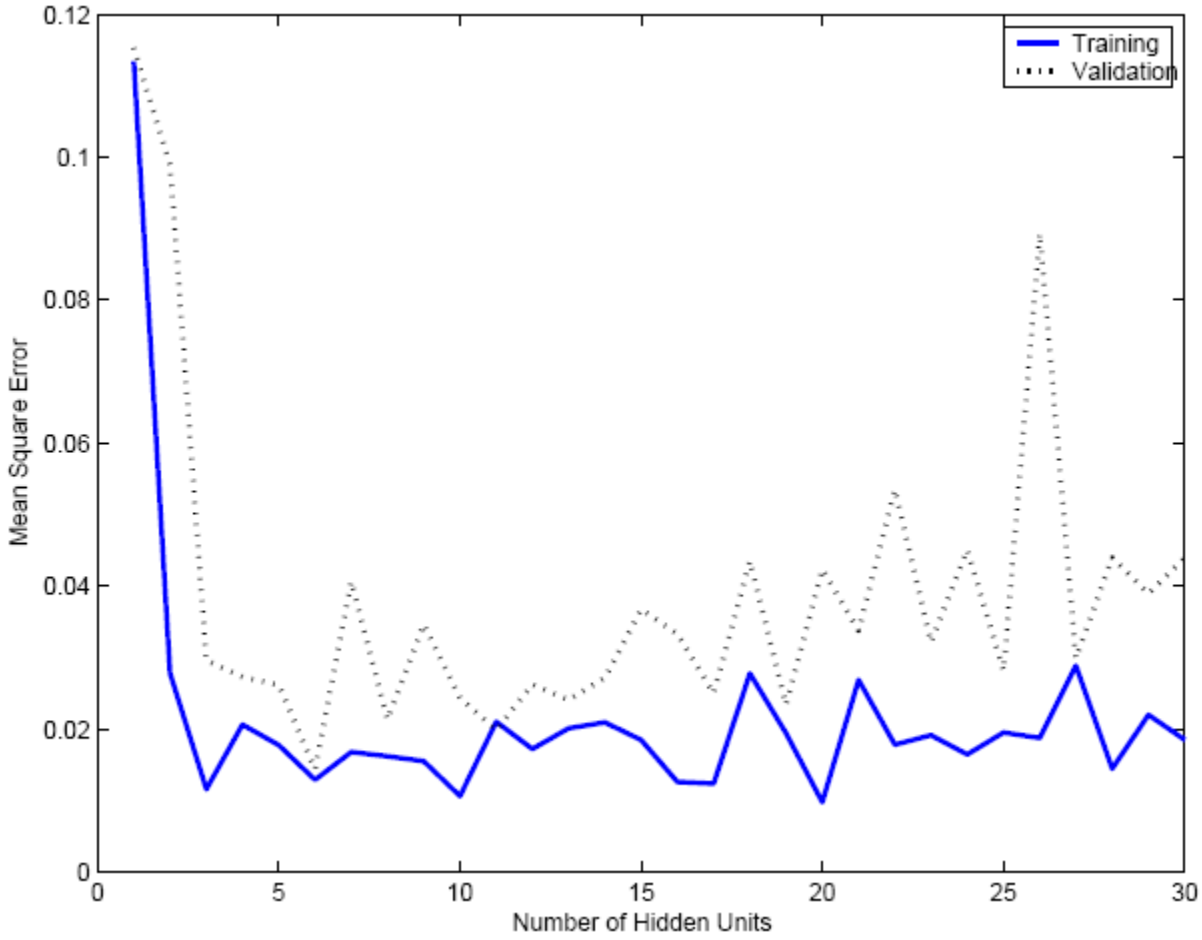
- Interpretation of hidden units
  - Hidden units "discover" new patterns/regularities
  - Often difficult to interpret
- Overfitting
- Expressiveness
  - Generalization to different classes of functions

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
Validation
Mean Square Error
Training Epochs
0
0.5
1
1.5
2
2.5
3
3.5
0
100
200
300
400
500
600
700
800
900
1000

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

Expressiveness

- 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

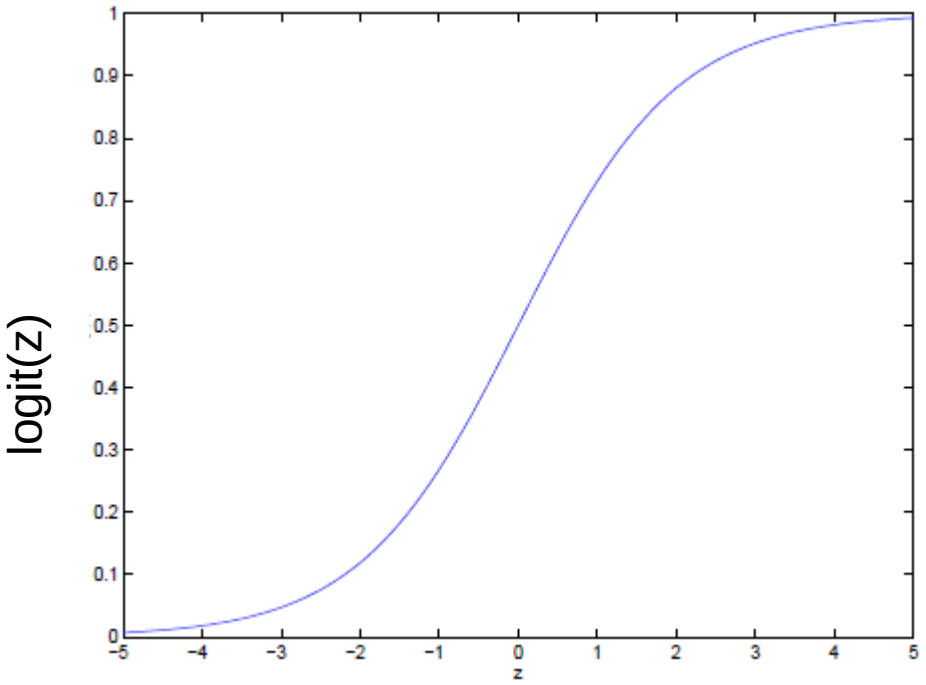
Summary

- 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

$$f : X \rightarrow Y$$

X can be continuous or discrete

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

Logistic regression (Classification)

$$P(Y=1|\mathbf{X}) = \frac{1}{1+e^{-w0-\sum_1^N w_i X_i}}$$

$$P(Y=0|\mathbf{X}) = 1- P(Y=1|\mathbf{X}) = \frac{e^{-w0-\sum_1^N w_i X_i}}{1+e^{-w0-\sum_1^N w_i X_i}}$$

$$P(Y=1|\mathbf{X}=0) = P(Y=0|\mathbf{X}=0) = \frac{1}{2}$$

Classification

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

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

Classification

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

$$P(Y=0|\mathbf{X}) = \frac{e^{-w_0 - \sum_1^N w_i X_i}}{1+e^{-w_0 - \sum_1^N w_i X_i}}$$

$$P(Y=1|\mathbf{X}) = \frac{1}{1+e^{-w_0 - \sum_1^N w_i X_i}}$$

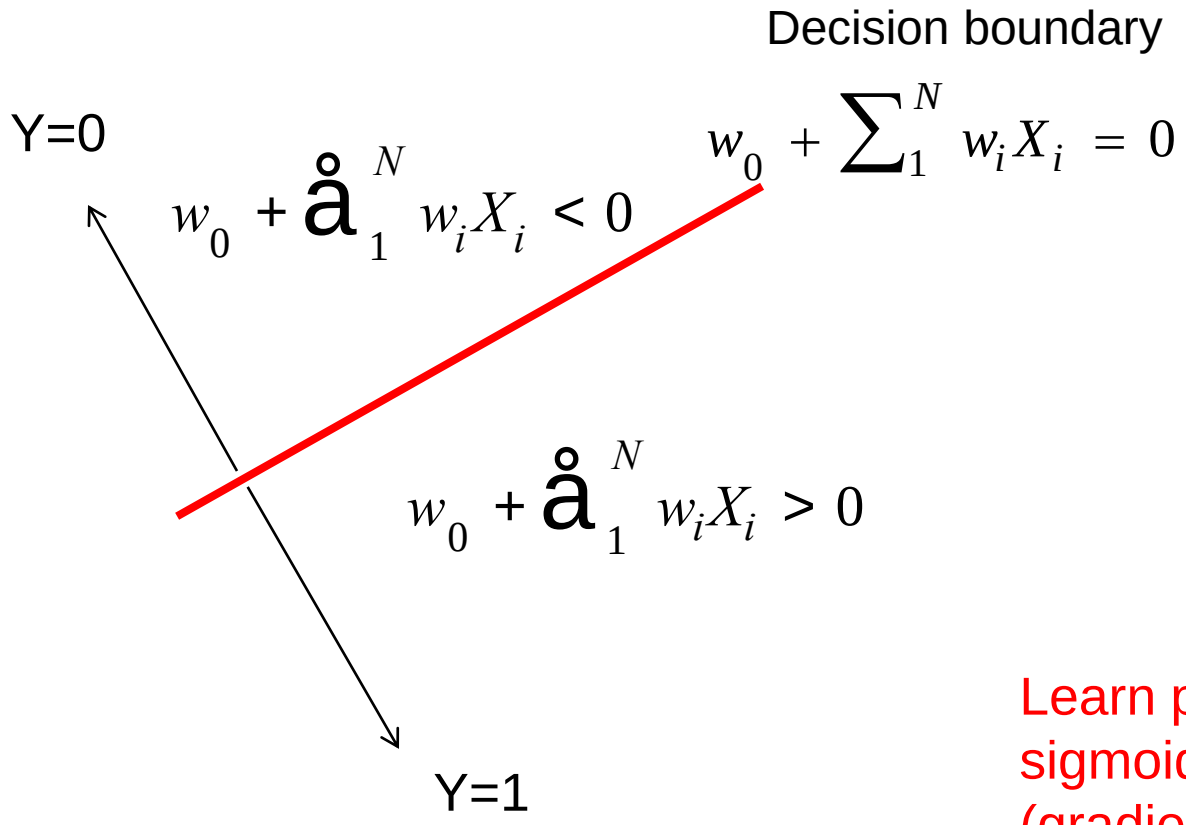
$$1 < e^{-w_0 - \sum_1^N w_i X_i}$$

Take log both sides

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

Classification rule: if this holds Y=0

Logistic regression is a linear classifier



Learn parameters using sigmoid unit training (gradient descent)

Logistic Function (Logit function)