Artificial Neural Networks

- Threshold units
- Gradient descent
- Multilayer networks
- Backpropagation
- Hidden layer representations
- Example: Face recognition
- Advanced topics

Connectionist Models

Consider humans

- Neuron switching time ~.001 second
- Number of neurons $\sim 10^{10}$
- Connections per neuron $\sim 10^{4-5}$
- Scene recognition time ~.1 second
- 100 inference step does not seem like enough

must use lots of parallel computation!

Properties of artificial neural nets (ANNs):

- Many neuron-like threshold switching units
- Many weighted interconnections among units
- Highly parallel, distributed process
- Emphasis on tuning weights automatically

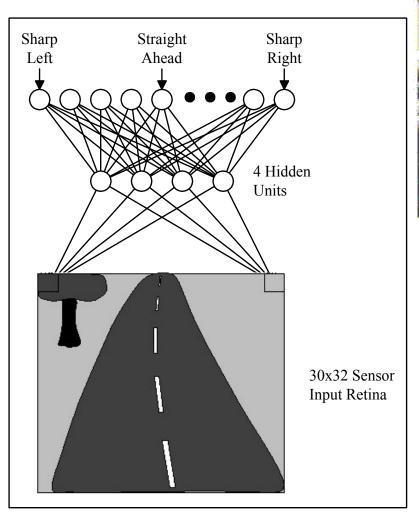
When to Consider Neural Networks

- Input is high-dimensional discrete or real-valued (e.g., raw sensor input)
- Output is discrete or real valued
- Output is a vector of values
- Possibly noisy data
- Form of target function is unknown
- Human readability of result is *unimportant*

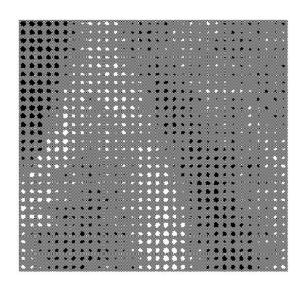
Examples:

- Speech phoneme recognition [Waibel]
- Image classification [Kanade, Baluja, Rowley]
- Financial prediction

ALVINN drives 70 mph on highways



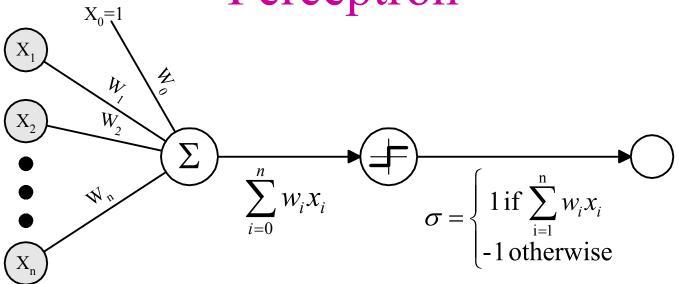




CS 5751 Machine Learning

Chapter 4 Artificial Neural Networks

Perceptron

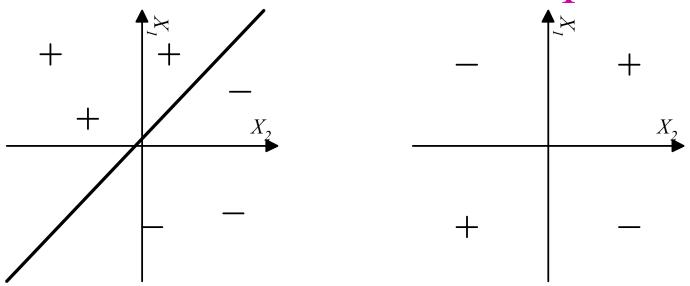


$$o(x_1,...,x_n) = \begin{cases} 1 \text{ if } w_0 + w_1 x_1 + ... + w_n x_n > 0 \\ -1 \text{ otherwise} \end{cases}$$

Sometimes we will use simpler vector notation:

$$o(\vec{x}) = \begin{cases} 1 & \text{if } \vec{w} \cdot \vec{x} > 0 \\ -1 & \text{otherwise} \end{cases}$$

Decision Surface of Perceptron



Represents some useful functions

• What weights represent $g(x_1, x_2) = AND(x_1, x_2)$?

But some functions not representable

- e.g., not linearly separable
- therefore, we will want networks of these ...

Perceptron Training Rule

$$w_i \leftarrow w_i + \Delta w_i$$

where

$$\Delta w_i = \eta (t - o) x_i$$

- $t = c(\vec{x})$ is target value
- o is perceptron output
- η is small constant (e.g., .1) called learning rate

Can prove it will converge

- If training data is linearly separable
- and η is sufficiently small

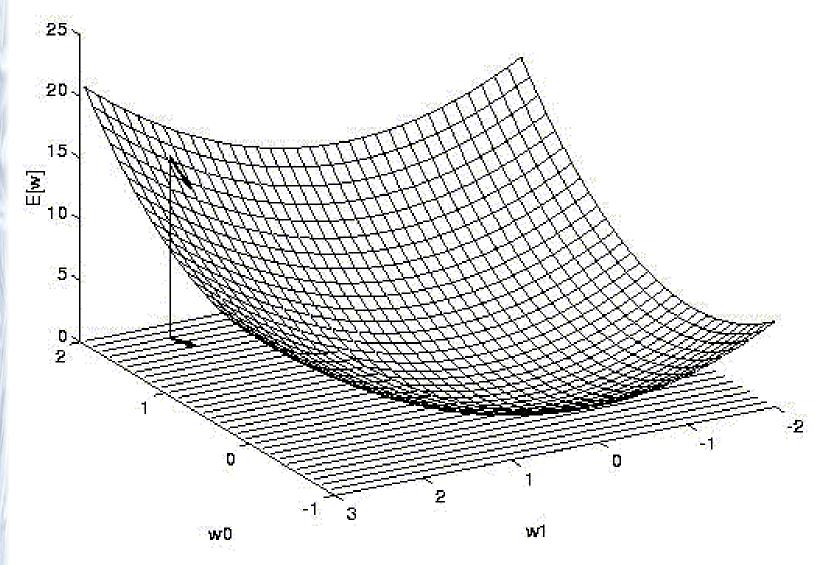
To understand, consider simple linear unit, where

$$o = w_0 + w_1 x_1 + \dots + w_n x_n$$

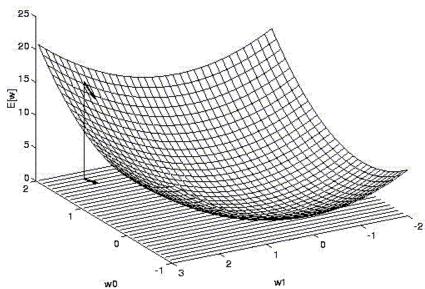
Idea: learn w_i 's that minimize the squared error

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

Where D is the set of training examples



Chapter 4 Artificial Neural Networks



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

Training rule: $\Delta w_i = -\eta \nabla E[\vec{w}]$

i.e.,
$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

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

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

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

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

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

GRADIENT – DESCENT(training $_examples, \eta$)

Each training examples is a pair of the form $\langle \vec{x}, t \rangle$, where \vec{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
- Until the termination condition is met, do
 - Initialize each Δw_i to zero.
 - For each $\langle \vec{x}, t \rangle$ in *training _examples*, do
 - * Input the instance \vec{x} and compute output o
 - * For each linear unit weight w_i , do

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

- For each linear unit weight w, do

$$w_i \leftarrow w_i + \Delta w_i$$

Summary

Perceptron training rule guaranteed to succeed if

- Training examples are linearly separable
- Sufficiently small learning rate η

Linear unit training rule uses gradient descent

- Guaranteed to converge to hypothesis with minimum squared error
- Given sufficiently small learning rate η
- Even when training data contains noise
- Even when training data not separable by *H*

Incremental (Stochastic) Gradient Descent

Batch mode Gradient Descent:

Do until satisfied:

1. Compute the gradient $\nabla E_D[\vec{w}]$

$$2.\vec{w} \leftarrow \vec{w} - \eta \nabla E_D[\vec{w}]$$

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

Incremental mode Gradient Descent:

Do until satisfied:

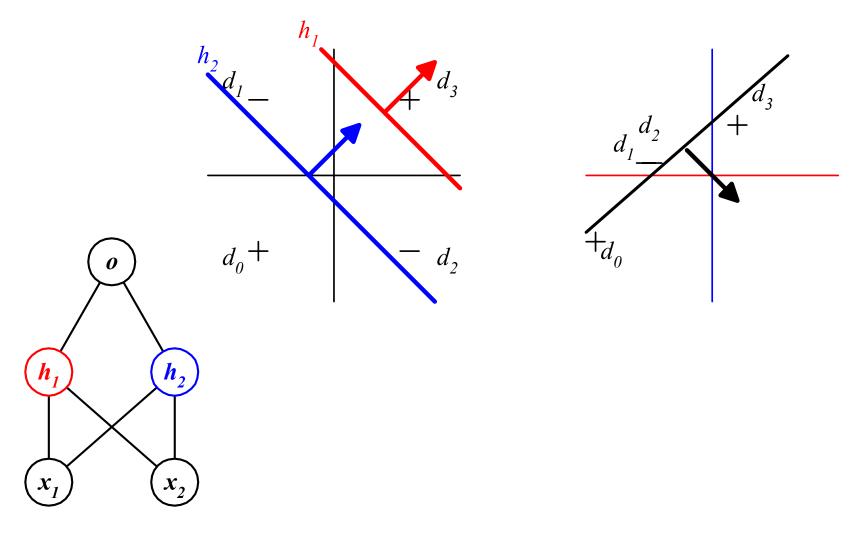
- For each training example *d* in *D*
 - 1. Compute the gradient $\nabla E_d[\vec{w}]$

$$2.\vec{w} \leftarrow \vec{w} - \eta \nabla E_d[\vec{w}]$$

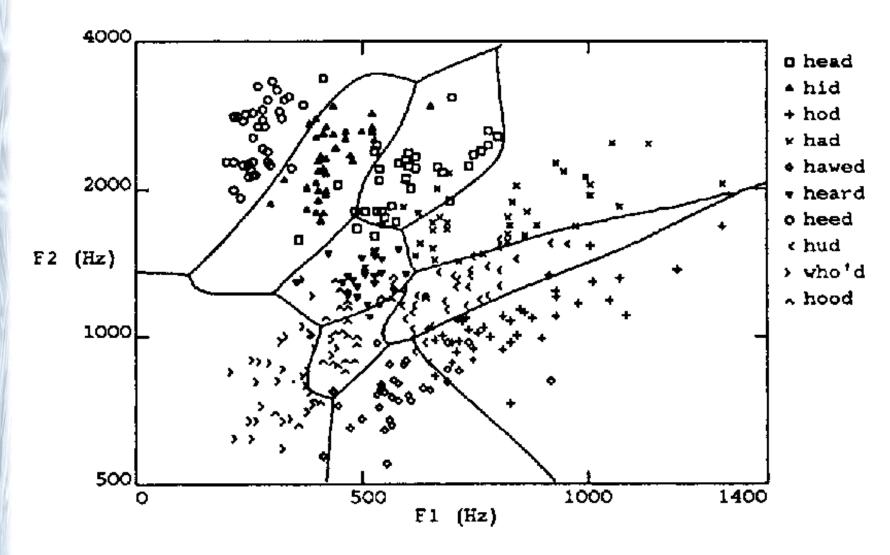
$$E_d[\vec{w}] \equiv \frac{1}{2} (t_d - o_d)^2$$

Incremental Gradient Descent can approximate Batch Gradient Descent arbitrarily closely if η made small enough

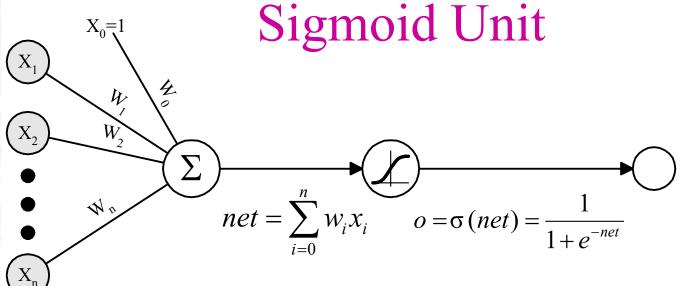
Multilayer Networks of Sigmoid Units



Multilayer Decision Space



Chapter 4 Artificial Neural Networks



 $\sigma(x)$ is the sigmoid function

$$\frac{1}{1+e^{-x}}$$

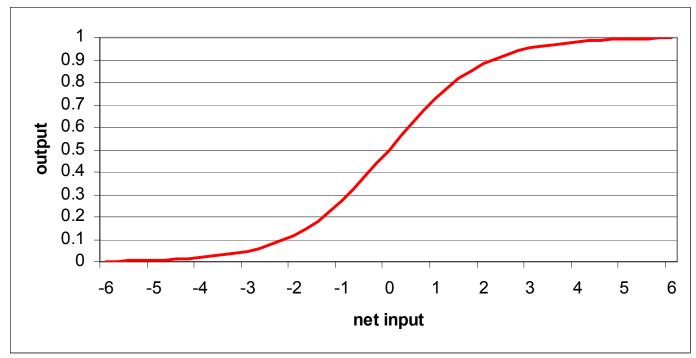
Nice property:
$$\frac{d\sigma(x)}{dx} = \sigma(x)(1 - \sigma(x))$$

We can derive gradient descent rules to train

- One sigmoid unit
- Multilayer networks of sigmoid units \rightarrow Backpropagation

The Sigmoid Function

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



Sort of a rounded step function Unlike step function, can take derivative (makes learning possible)

Error Gradient for a Sigmoid Unit

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

But we know:

$$\begin{split} \frac{\partial o_d}{\partial net_d} &= \frac{\partial \sigma \left(net_d \right)}{\partial net_d} = o_d (1 - o_d) \\ \frac{\partial net_d}{\partial w_i} &= \frac{\partial (\vec{w} \cdot \vec{x}_d)}{\partial w_i} = x_{i,d} \end{split}$$

So:

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

Backpropagation Algorithm

Initialize all weights to small random numbers. Until satisfied, do

- For each training example, do
 - 1. Input the training example and compute the 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

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

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

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

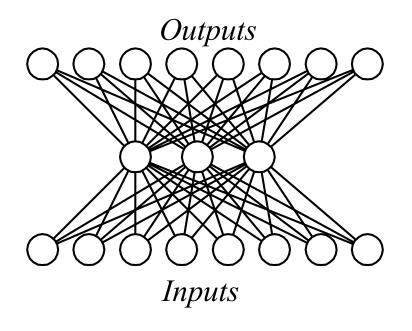
where

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

More on Backpropagation

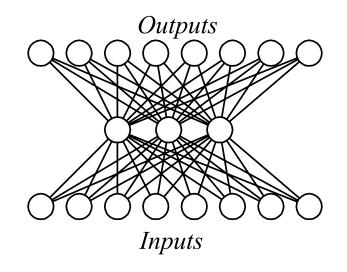
- Gradient descent over entire *network* weight vector
- Easily generalized to arbitrary directed graphs
- Will find a local, not necessarily global error minimum
 - In practice, often works well (can run multiple times)
- Often include weight momentum α $\Delta w_{i,j}(n) = \eta \, \delta_i x_{i,j} + \alpha \, \Delta w_{i,j}(n-1)$
- Minimizes error over training examples
- Will it generalize well to subsequent examples?
- Training can take thousands of iterations -- slow!
 - Using network after training is fast

Learning Hidden Layer Representations



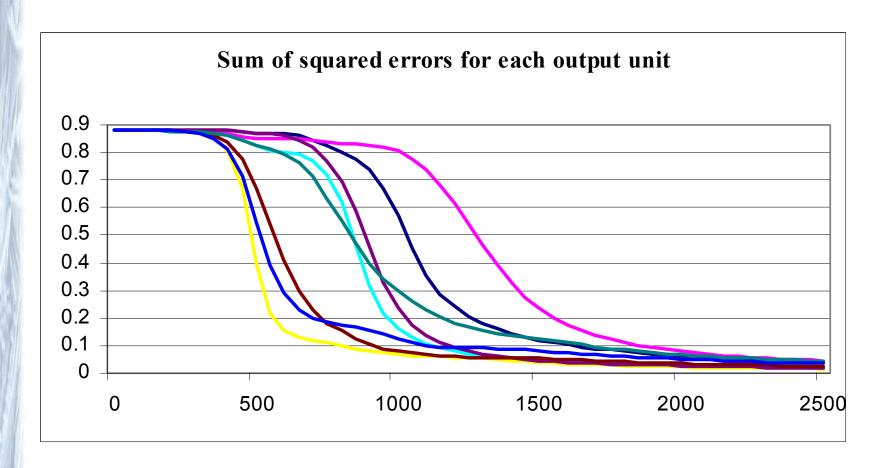
Input Output
$10000000 \rightarrow 10000000$
$01000000 \rightarrow 01000000$
$00100000 \rightarrow 00100000$
$00010000 \rightarrow 00010000$
$00001000 \rightarrow 00001000$
$00000100 \rightarrow 00000100$
$00000010 \rightarrow 00000010$
$00000001 \rightarrow 00000001$

Learning Hidden Layer Representations

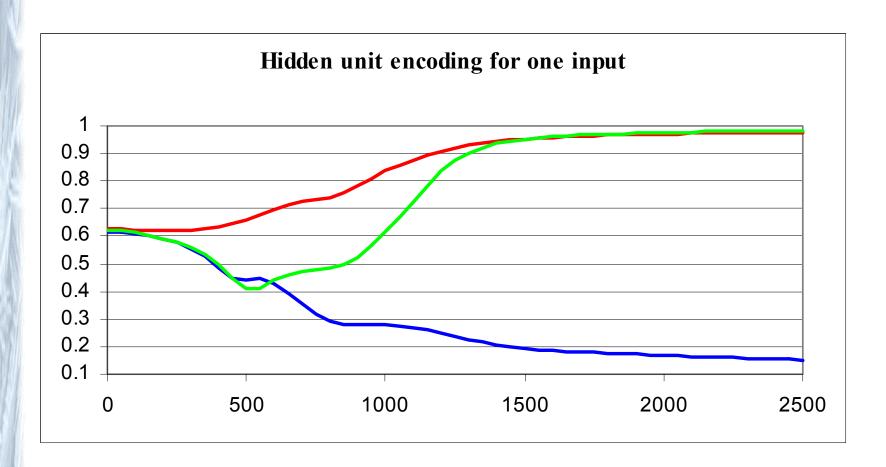


Input Output
$10000000 \rightarrow .89.04.08 \rightarrow 10000000$
$01000000 \rightarrow .01.11.88 \rightarrow 01000000$
$00100000 \rightarrow .01.97.27 \rightarrow 00100000$
$00010000 \rightarrow .99.97.71 \rightarrow 00010000$
$00001000 \rightarrow .03.05.02 \rightarrow 00001000$
$00000100 \rightarrow .22.99.99 \rightarrow 00000100$
$00000010 \rightarrow .80.01.98 \rightarrow 00000010$
$00000001 \rightarrow .60.94.01 \rightarrow 00000001$

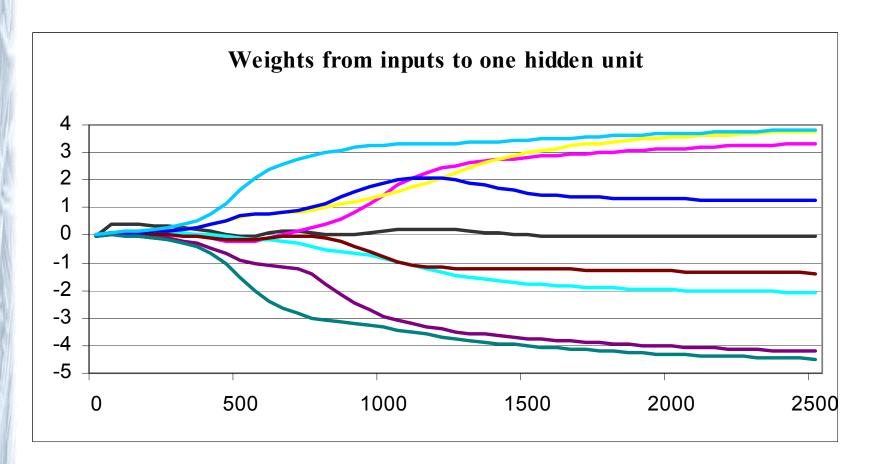
Output Unit Error during Training



Hidden Unit Encoding



Input to Hidden Weights



Convergence of Backpropagation

Gradient descent to some local minimum

- Perhaps not global minimum
- Momentum can cause quicker convergence
- Stochastic gradient descent also results in faster convergence
- Can train multiple networks and get different results (using different initial weights)

Nature of convergence

- Initialize weights near zero
- Therefore, initial networks near-linear
- Increasingly non-linear functions as training progresses

Expressive Capabilities of ANNs

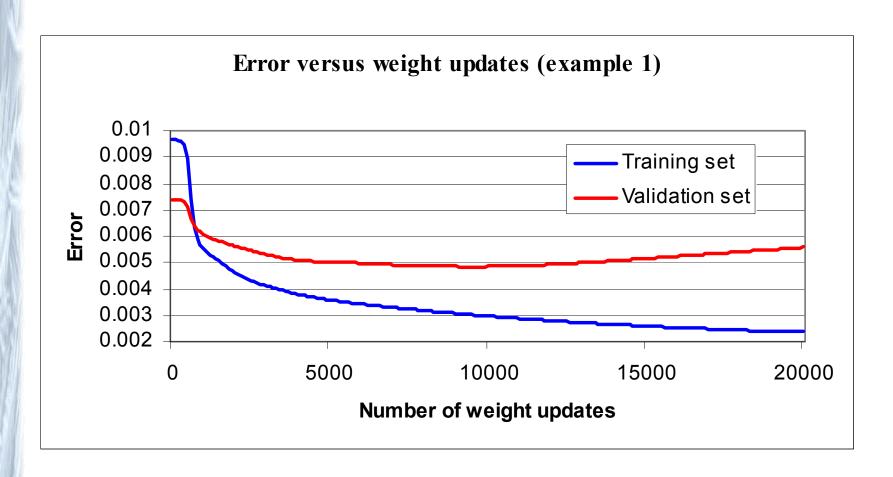
Boolean functions:

- Every Boolean function can be represented by network with a single hidden layer
- But that might require an exponential (in the number of inputs) hidden units

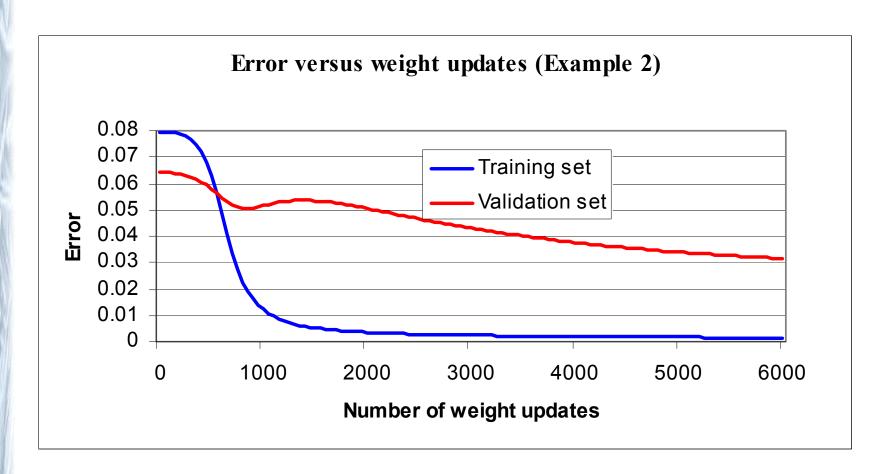
Continuous functions:

- Every bounded continuous function can be approximated with arbitrarily small error by a network with one hidden layer [Cybenko 1989; Hornik et al. 1989]
- Any function can be approximated to arbitrary accuracy by a network with two hidden layers [Cybenko 1988]

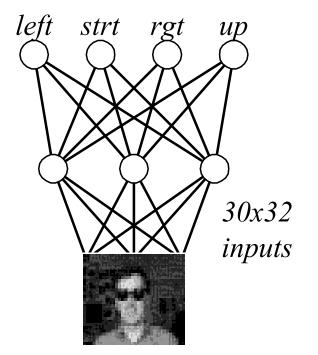
Overfitting in ANNs



Overfitting in ANNs



Neural Nets for Face Recognition



90% accurate learning head pose, and recognizing 1-of-20 faces



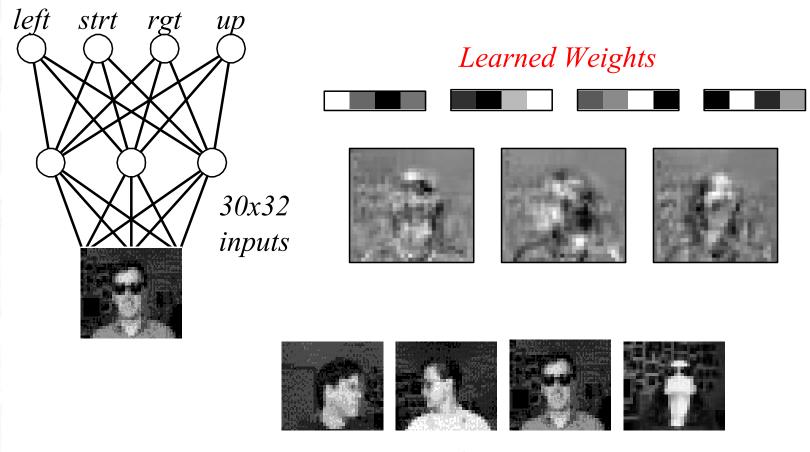






Typical Input Images

Learned Network Weights



Typical Input Images

Alternative Error Functions

Penalize large weights:

$$E(\vec{w}) \equiv \frac{1}{2} \sum_{d \in D} \sum_{k \in outputs} (t_{kd} - o_{kd})^2 + \gamma \sum_{i,j} w^2_{ji}$$

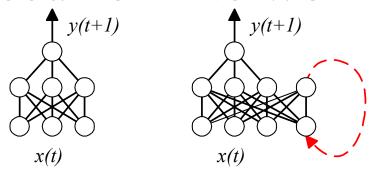
Train on target slopes as well as values:

$$E(\vec{w}) = \frac{1}{2} \sum_{d \in D} \sum_{k \in outputs} \left[(t_{kd} - o_{kd})^2 + \mu \left(\frac{\partial t_{kd}}{\partial x^j_d} - \frac{\partial o_{kd}}{\partial x^j_d} \right)^2 \right]$$

Tie together weights:

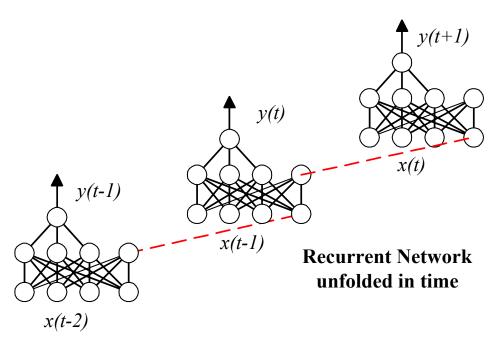
e.g., in phoneme recognition

Recurrent Networks



Feedforward Network

Recurrent Network



Chapter 4 Artificial Neural Networks

Neural Network Summary

- physiologically (neurons) inspired model
- powerful (accurate), slow, opaque (hard to understand resulting model)
- bias: preferential
 - based on gradient descent
 - finds local minimum
 - effect by initial conditions, parameters
- neural units
 - linear
 - linear threshold
 - sigmoid

Neural Network Summary (cont)

- gradient descent
 - convergence
- linear units
 - limitation: hyperplane decision surface
 - learning rule
- multilayer network
 - advantage: can have non-linear decision surface
 - backpropagation to learn
 - backprop learning rule
- learning issues
 - units used

Neural Network Summary (cont)

- learning issues (cont)
 - batch versus incremental (stochastic)
 - parameters
 - initial weights
 - learning rate
 - momentum
 - cost (error) function
 - sum of squared errors
 - can include penalty terms
- recurrent networks
 - simple
 - backpropagation through time