Artificial Neural Networks

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

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Connectionist Models

Consider humans

- Neuron switching time ~.001 second
- Number of neurons ~1010
- Connections per neuron ~10⁴⁻⁵
- 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

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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

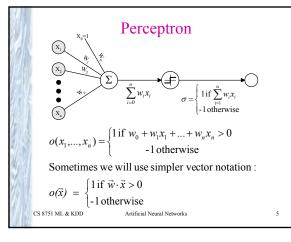
Examples:

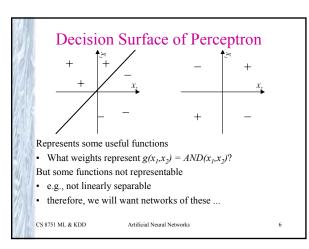
- · Speech phoneme recognition [Waibel]
- Image classification [Kanade, Baluja, Rowley]
- Financial prediction

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ALVINN drives 70 mph on highways Shurp Straight Shurp Right 4 Hidden Units 30x32 Sensor Input Retina CS 8751 MI. & KDD Artificial Neural Networks 4





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

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Gradient Descent

To understand, consider simple linear unit, where

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

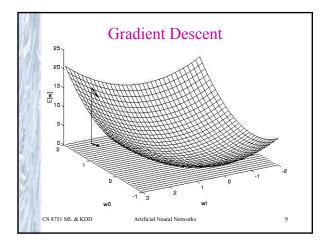
Idea: learn w_i 's that minimize the squared error

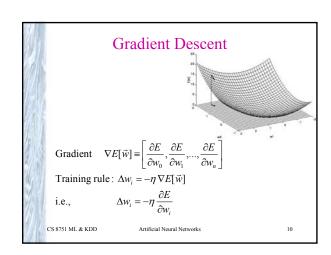
$$E[\vec{w}] = \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2$$

Where D is the set of training examples

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Gradient Descent

$$\begin{split} \frac{\partial E}{\partial w_i} &= \frac{\partial}{\partial w_i} \frac{1}{2} \sum_d (t_d - o_d)^2 \\ &= \frac{1}{2} \sum_d \frac{\partial}{\partial w_i} (t_d - o_d)^2 \\ &= \frac{1}{2} \sum_d 2 (t_d - o_d) \frac{\partial}{\partial w_i} (t_d - o_d) \\ &= \sum_d (t_d - o_d) \frac{\partial}{\partial w_i} (t_d - \vec{w} \cdot \vec{x}_d) \\ \frac{\partial E}{\partial w_i} &= \sum_d (t_d - o_d) (-x_{i,d}) \end{split}$$

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Gradient Descent

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).

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- 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

 $w_i \leftarrow w_i + \Delta w_i$

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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

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Incremental (Stochastic) Gradient Descent

Batch mode Gradient Descent:

Do until satisfied:

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

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

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

Incremental mode Gradient Descent:

Do until satisfied:

- For each training example d in D

1. Compute the gradient $\nabla E_a / \vec{w} /$

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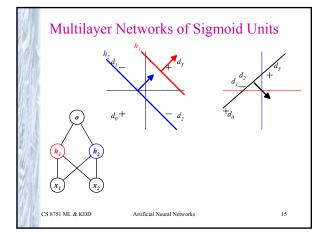
$$E_d[\vec{w}] = \frac{1}{2}(t_d - o_d)^2$$

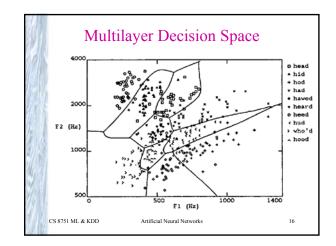
$$2.\vec{w} \leftarrow \vec{w} - \eta \nabla E_d[\vec{w}]$$

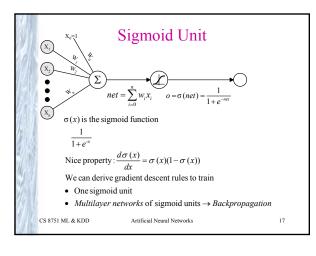
Incremental Gradient Descent can approximate Batch Gradient Descent arbitrarily closely if η made small enough

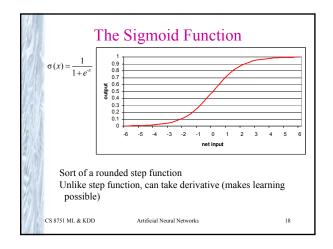
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Error Gradient for a Sigmoid Unit

$$\begin{split} \frac{\partial E}{\partial w_i} &= \frac{\partial}{\partial w_i} \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2 \\ &= \frac{1}{2} \sum_{d} \frac{\partial}{\partial w_i} (t_d - o_d)^2 \\ &= \frac{1}{2} \sum_{d} \frac{\partial}{\partial w_i} (t_d - o_d)^2 \\ &= \frac{1}{2} \sum_{d} 2 (t_d - o_d) \frac{\partial}{\partial w_i} (t_d - o_d) \\ &= \sum_{d} (t_d - o_d) \left(-\frac{\partial o_d}{\partial w_i} \right) \\ &= -\sum_{d} (t_d - o_d) \frac{\partial o_d}{\partial net_d} \frac{\partial net_d}{\partial w_i} \end{split}$$
But we know:
$$\frac{\partial o_d}{\partial net_d} = \frac{\partial \sigma \left(net_d \right)}{\partial net_d} \\ &= \frac{\partial \sigma \left(net_d \right)}{\partial w_i} = a_{i,d} \\ &\text{So:} \\ &= \sum_{d} (t_d - o_d) o_d (1 - o_d) x_{i,d} \\ &= -\sum_{d} (t_d - o_d) \frac{\partial o_d}{\partial net_d} \frac{\partial net_d}{\partial w_i} \end{split}$$

$$\begin{split} \frac{\partial o_d}{\partial net_d} &= \frac{\partial \sigma \left(net_d\right)}{\partial net_d} = o_d (1 - o_d) \\ \frac{\partial net_d}{\partial w_i} &= \frac{\partial (\vec{w} \cdot \vec{x}_d)}{\partial w_i} = x_{i,d} \\ 0 &= 0 \end{split}$$

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

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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

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

4. Update each network weight w_i

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

where

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

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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

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

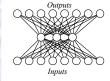
- · Minimizes error over training examples
- · Will it generalize well to subsequent examples?
- Training can take thousands of iterations -- slow!
 - Using network after training is fast

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Learning Hidden Layer Representations Input Output $10000000 \rightarrow 10000000$ $01000000 \rightarrow 01000000$ $00100000 \rightarrow 00100000$ $00010000 \rightarrow 00010000$ $00001000 \rightarrow 00001000$ $00000100 \rightarrow 00000100$ $00000010 \rightarrow 00000010$ $00000001 \rightarrow 00000001$ CS 8751 ML & KDD Artificial Neural Networks

Learning Hidden Layer Representations



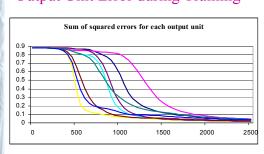
Input Output $10000000 \rightarrow .89.04.08 \rightarrow 10000000$ $01000000 \rightarrow .01.11.88 \rightarrow 01000000$ $00100000 \rightarrow .01.97.27 \rightarrow 00100000$ $00010000 \rightarrow .99.97.71 \rightarrow 00010000$ $00001000 \rightarrow .03.05.02 \rightarrow 00001000$ $00000100 \rightarrow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

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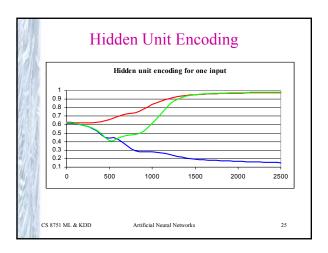
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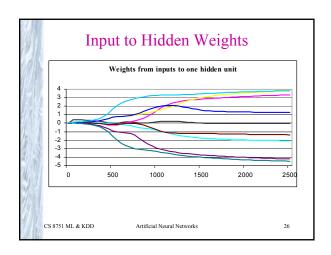
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Output Unit Error during Training



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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

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Expressive Capabilities of ANNs

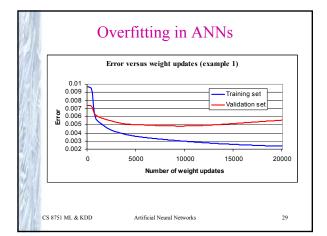
Boolean functions:

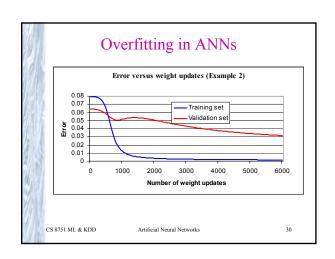
- Every Boolean function can be represented by network with a single hidden layer
- But that might require an exponential (in the number of inputs) hidden units

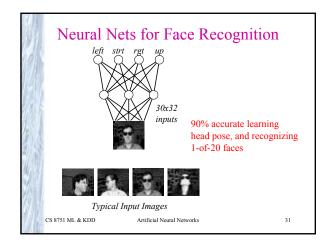
Continuous functions:

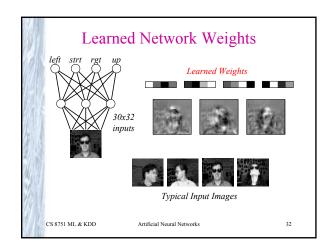
- Every bounded continuous function can be approximated with arbitrarily small error by a network with one hidden layer [Cybenko 1989; Hornik et al. 1989]
- Any function can be approximated to arbitrary accuracy by a network with two hidden layers [Cybenko 1988]

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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:

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

Tie together weights:

• e.g., in phoneme recognition

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