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 ~10^{10}
- Connections per neuron ~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

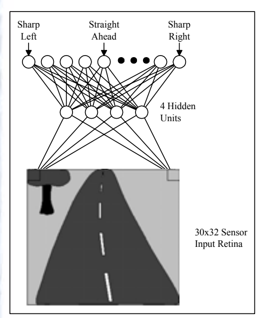
When to Consider Neural Networks

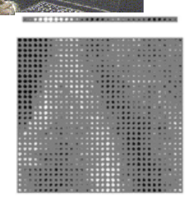
- Input is high-dimensional discrete or real-valued (e.g., raw sensor input)
- Output is discrete or real valued
- Output is a vector of values
- Possibly noisy data
- Form of target function is unknown
- Human readability of result is *unimportant*

Examples:

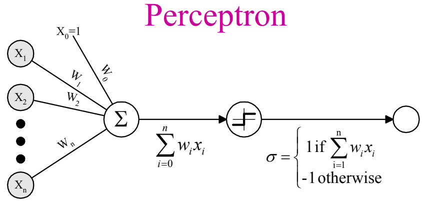
- Speech phoneme recognition [Waibel]
- Image classification [Kanade, Baluja, Rowley]
- Financial prediction

ALVINN drives 70 mph on highways





Perceptron

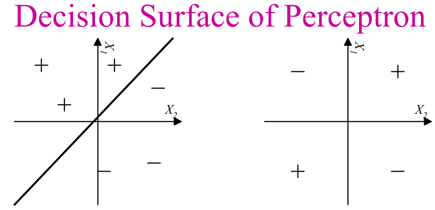


$$o(x_1,\ldots,x_n) = \begin{cases} 1 \text{ if } w_0 + w_1 x_1 + \ldots + w_n x_n > 0 \\ -1 \text{ otherwise} \end{cases}$$

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

Gradient Descent

To understand, consider simple *linear unit*, where

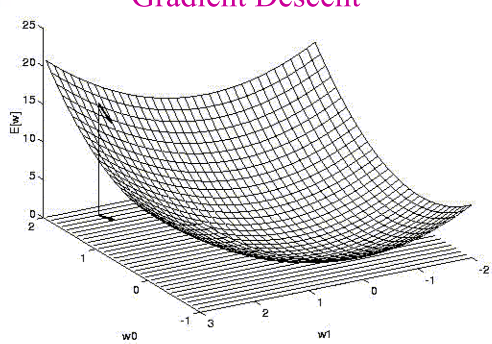
$$o = w_0 + w_1 x_1 + \ldots + w_n x_n$$

Idea : learn w_i's that minimize the squared error

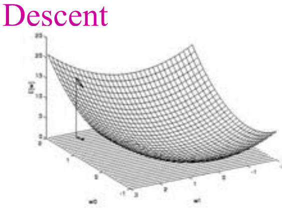
$$E[\vec{w}] \equiv \tfrac{1}{2}\sum_{d\in D}(t_d - o_d)^2$$

Where D is the set of training examples

Gradient Descent



Gradient Descent



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

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

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

Gradient Descent

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

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

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

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

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

Gradient Descent

GRADIENT – DESCENT(*training _ examples*, η)

Each training examples is a pair of the form $<\vec{x}, t>$ *, 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 $<\vec{x}, t>$ 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. $\vec{w} \leftarrow \vec{w} - \eta \nabla E_D[\vec{w}]$

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

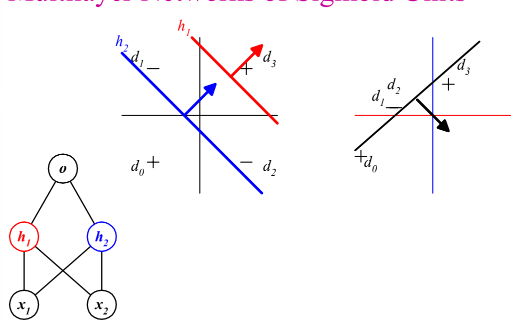
Incremental mode Gradient Descent:
Do until satisfied:

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

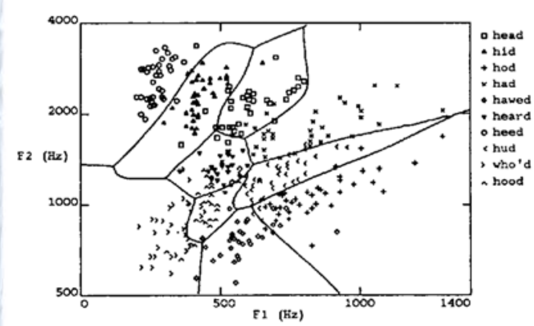
$$E_d[\vec{w}] \equiv \frac{1}{2}(t_d - o_d)^2$$

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

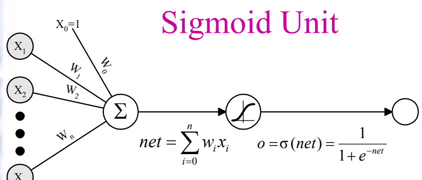
Multilayer Networks of Sigmoid Units



Multilayer Decision Space



Sigmoid Unit



$$net = \sum_{i=0}^{n} w_i x_i \qquad o = \sigma(net) = \frac{1}{1+e^{-net}}$$

$\sigma(x)$ is the sigmoid function

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

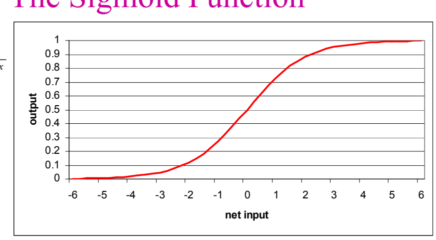
Nice property: $\frac{d\sigma(x)}{dx} = \sigma(x)(1-\sigma(x))$

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

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

But we know :

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

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

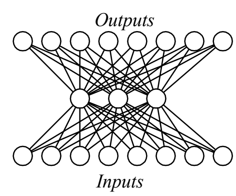
Initialize all weights to small random numbers. Until satisfied, do

- 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

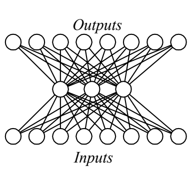
- Gradient descent over entire *network* weight vector
- Easily generalized to arbitrary directed graphs
- Will find a local, not necessarily global error minimum
  - In practice, often works well (can run multiple times)
- Often include weight *momentum* α
  $$\Delta w_{i,j}(n) = \eta\,\delta_j x_{i,j} + \alpha\,\Delta w_{i,j}(n-1)$$
- 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



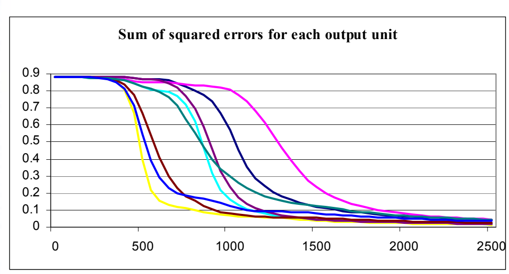
Input	Output
10000000 →	10000000
01000000 →	01000000
00100000 →	00100000
00010000 →	00010000
00001000 →	00001000
00000100 →	00000100
00000010 →	00000010
00000001 →	00000001

Learning Hidden Layer Representations

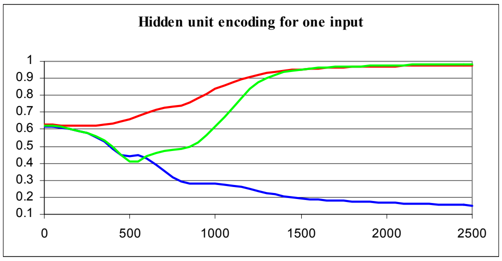


Input		Output
10000000 →	.89 .04 .08 →	10000000
01000000 →	.01 .11 .88 →	01000000
00100000 →	.01 .97 .27 →	00100000
00010000 →	.99 .97 .71 →	00010000
00001000 →	.03 .05 .02 →	00001000
00000100 →	.22 .99 .99 →	00000100
00000010 →	.80 .01 .98 →	00000010
00000001 →	.60 .94 .01 →	00000001

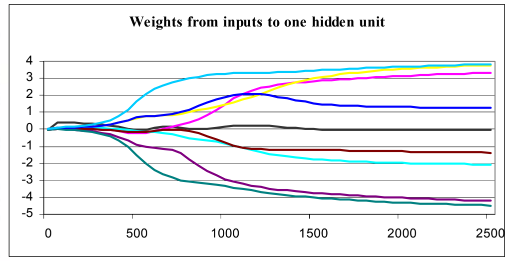
Output Unit Error during Training



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

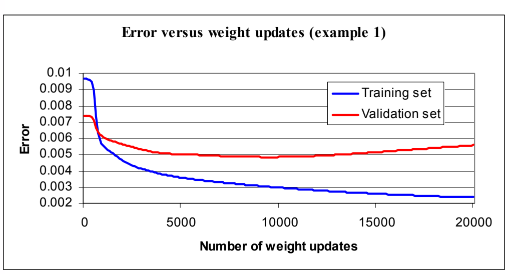
Boolean functions:

- 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

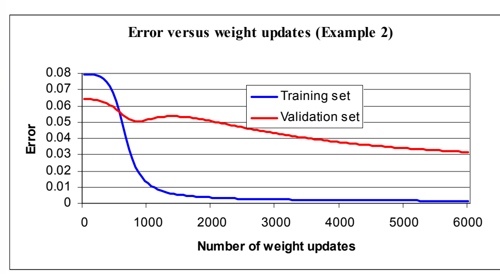
Continuous functions:

- 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]

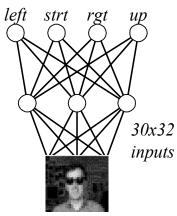
Overfitting in ANNs



Overfitting in ANNs



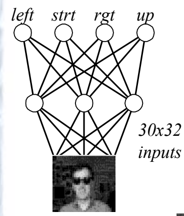
Neural Nets for Face Recognition



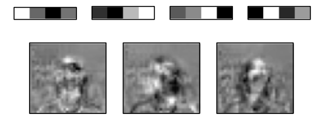
90% accurate learning head pose, and recognizing 1-of-20 faces

Typical Input Images

Learned Network Weights



Learned Weights



Typical Input Images

Alternative Error Functions

Penalize large weights:

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

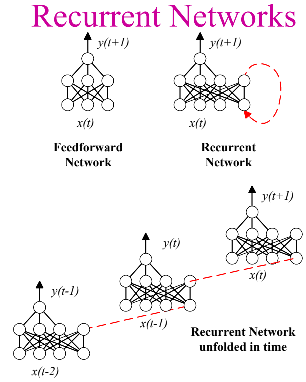
Train on target slopes as well as values:

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

Tie together weights:

- e.g., in phoneme recognition

Recurrent Networks



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