Artificial Neural Networks

[Read Ch. 4]
[Recommended exercises 4.1, 4.2, 4.5, 4.9, 4.11]

- 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 steps doesn't seem like enough

$\rightarrow$ much parallel computation

Properties of artificial neural nets (ANN's):

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

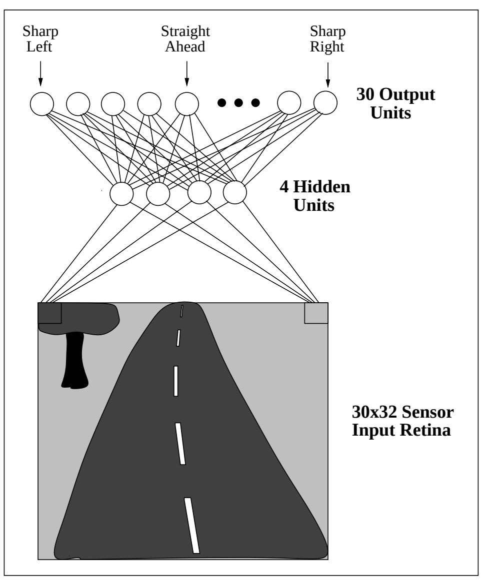
When to Consider Neural Networks

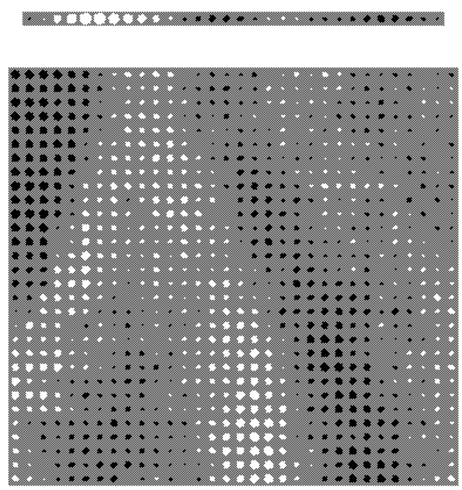
- Input is high-dimensional discrete or real-valued (e.g. raw sensor input)
- Output is discrete or real valued
- Output is a vector of values
- Possibly noisy data
- Form of target function is unknown
- Human readability of result is unimportant

Examples:

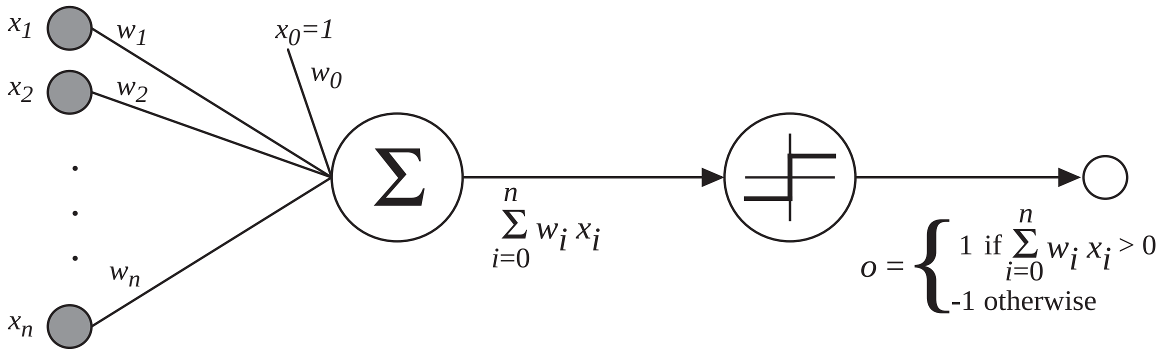
- Speech phoneme recognition [Waibel]
- Image classification [Kanade, Baluja, Rowley]
- Financial prediction

ALVINN drives 70 mph on highways





Perceptron

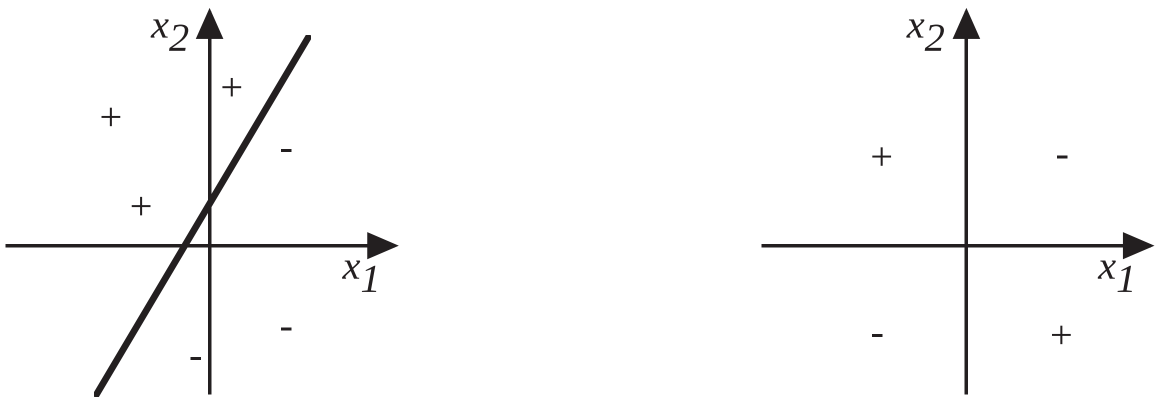


$$o(x_1, \ldots, x_n) = \begin{cases} 1 & \text{if } w_0 + w_1 x_1 + \cdots + w_n x_n > 0 \\ -1 & \text{otherwise.} \end{cases}$$

Sometimes we'll 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 a Perceptron



(a) (b)

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'll want networks of these...

Perceptron training rule

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

where

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

Where:

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

Perceptron training rule

Can prove it will converge

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

Gradient Descent

To understand, consider simpler *linear unit*, where

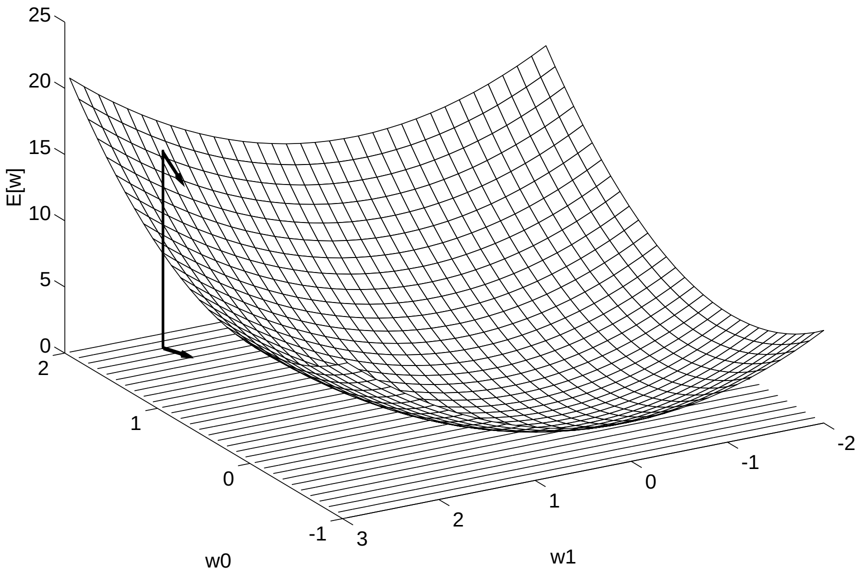
$$o = w_0 + w_1 x_1 + \cdots + w_n x_n$$

Let's 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 set of training examples

Gradient Descent



Gradient

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

Training rule:

$$\Delta \vec{w} = -\eta \nabla E[\vec{w}]$$

i.e.,

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

Gradient Descent

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

训练线性单元的梯度下降算法

GRADIENT-DESCENT(*training_examples, η*)

training_examples 中每一训练样例形式为序偶<**x,t**>，其中 **x** 式输入向量，**t** 是目标输出值，*η*是学习速率**(**例如 **0.05)**

- 初始化每个 **wi** 为某个小的随机值
- 遇到终止条件之前，做以下操作：
  - 初始化每个Δ**wi** 为 **0**
  - 对于训练样例 ***training_examples*** 中的每个<**x,t**>，做：
    - 把实例 **x** 输入到此单元，计算输出 **o**
    - 对于线性单元的每个权 **wi**，做

$$\Delta wi \leftarrow \Delta wi + \eta(t-o)xi \tag{4.8}$$

  - 对于线性单元的每个权 **wi**，做

$$wi \leftarrow wi + \Delta wi \tag{4.9}$$

Gradient Descent

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

Each training example 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 $\vec{x}$ to the unit and compute the 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_i, 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. $\vec{w} \leftarrow \vec{w} - \eta \nabla E_D[\vec{w}]$

Incremental mode Gradient Descent:
Do until satisfied

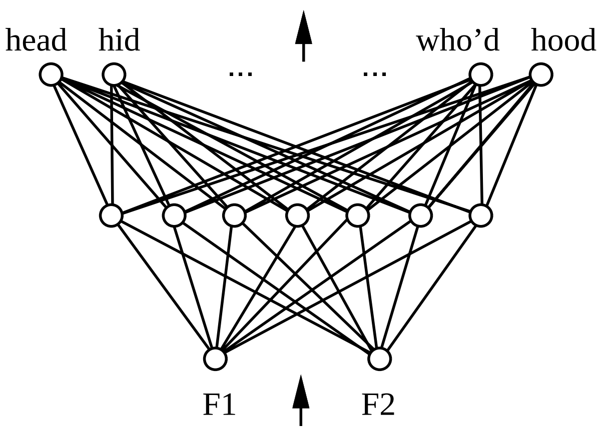
- For each training example d in D
  1. Compute the gradient $\nabla E_d[\vec{w}]$
  2. $\vec{w} \leftarrow \vec{w} - \eta \nabla E_d[\vec{w}]$

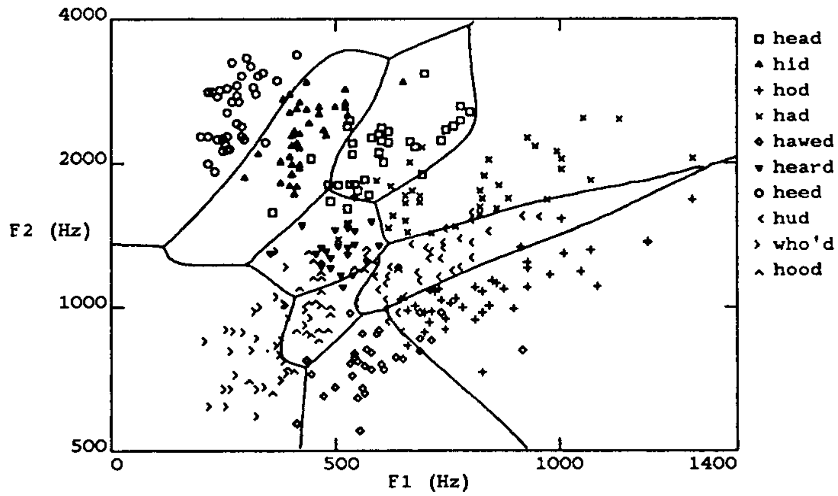
$$E_D[\vec{w}] \equiv \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2$$

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

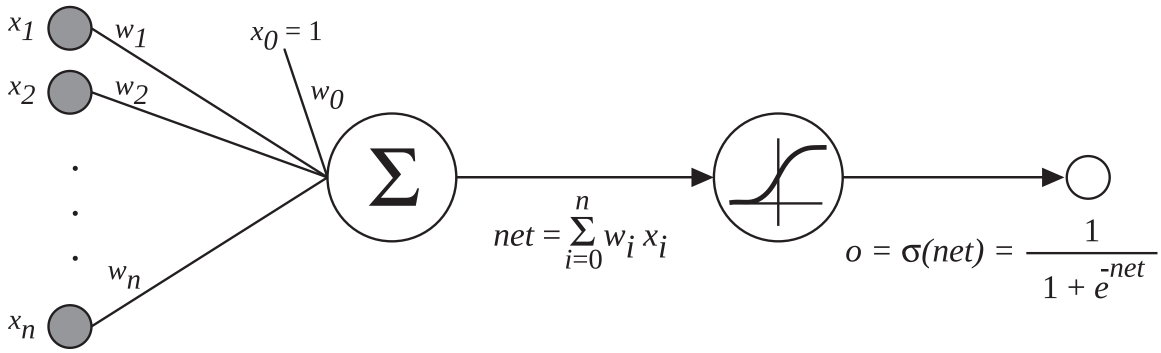
Incremental Gradient Descent can approximate *Batch Gradient Descent* arbitrarily closely if η made small enough

Multilayer Networks of Sigmoid Units





Sigmoid Unit



$\sigma(x)$ 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 decent rules to train

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

$$E(\vec{w}) = \frac{1}{2}\sum_{d \in D}\sum_{k \in output}(t_{kd} - o_{kd})^2$$

$$E_d(\vec{w}) = \frac{1}{2}\sum_{k \in output}(t_k - o_k)^2$$

$$\frac{\partial E_d}{\partial w_{ji}} = \frac{\partial E_d}{\partial net_j}\frac{\partial net_j}{\partial w_{ji}} = \frac{\partial E_d}{\partial net_j} x_{ji}$$

情况 **1**：输出单元的权值训练法则

$$\frac{\partial E_d}{\partial net_j} = \frac{\partial E_d}{\partial o_j}\frac{\partial o_j}{\partial net_j}$$

情况 **2**：隐藏单元的权值训练法则

$$\frac{\partial E_d}{\partial net_j} = \sum_{k \in Downstream(j)} \frac{\partial E_d}{\partial net_k}\frac{\partial net_k}{\partial net_j}$$

Error Gradient for a Sigmoid Unit

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

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:

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

包含两层 **sigmoid** 单元的前馈网络的反向传播算法**(**随机梯度下降版本**)**

BACPROPAGATION(*training_examples,* η ***,***n_{in}***,*** n_{out}***,***n_{hidden}**)**

training_examples中每一训练样例形式为序偶**<x,t>**，其中**x**式输入向量，**t**是目标输出值，η是学习速率**(**例如 **0.05)**。n_{in}是网络输入的数量，n_{hidden}是隐藏层单元数，n_{out}是输出单元数。

从单元 **i** 到单元 **j** 的输入表示为 **xji,** 单元 **i** 到单元 **j** 的权值表示为 **wji**。

•创建具有n_{in}个输入，n_{hidden}个隐藏单元，n_{out}个输出单元的网络

•初始化所有的网络权值为小的随机值**(**例如**-0.05** 和 **0.05** 之间的数**)**

•在遇到终止条件前：

•对于训练样例 ***training_examples*** 中的每个$<\vec{x},\vec{t}>$：

把输入沿网络前向传播

1. 把实例**x**输入网络，并计算网络中每个单元**u**的输出o_u

使误差沿网络反向传播

2. 对于网络的每个输出单元**k**，计算它的误差项δ_k

$$\delta_k \leftarrow o_k(1-o_k)(t_k-o_k)$$

3. 对于网络的每个隐藏单元**h**，计算它的误差项δ_h

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

4. 更新每个网络权值 **wji**

$$wji \leftarrow wji + \Delta wji$$

其中

$$\Delta wji = \eta \delta j x_{ji}$$

Backpropagation Algorithm

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

- For each training example, Do
  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
  $$\delta_h \leftarrow o_h(1 - o_h) \sum_{k \in outputs} w_{h,k} \delta_k$$
  4. Update each network weight $w_{i,j}$
  $$w_{i,j} \leftarrow w_{i,j} + \Delta w_{i,j}$$
  where
  $$\Delta w_{i,j} = \eta \delta_j x_{i,j}$$

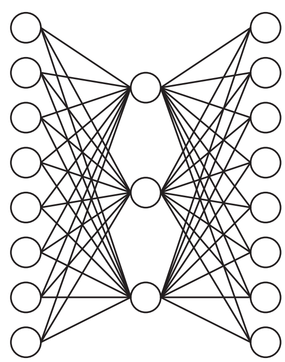
More on Backpropagation

- 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 $\rightarrow$ slow!
- Using network after training is very fast

Learning Hidden Layer Representations



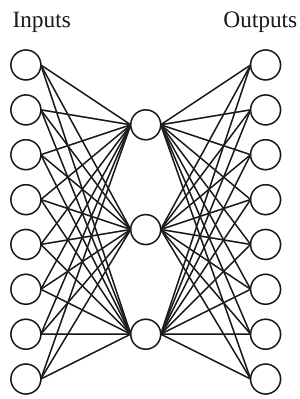
A target function:

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

Can this be learned??

Learning Hidden Layer Representations

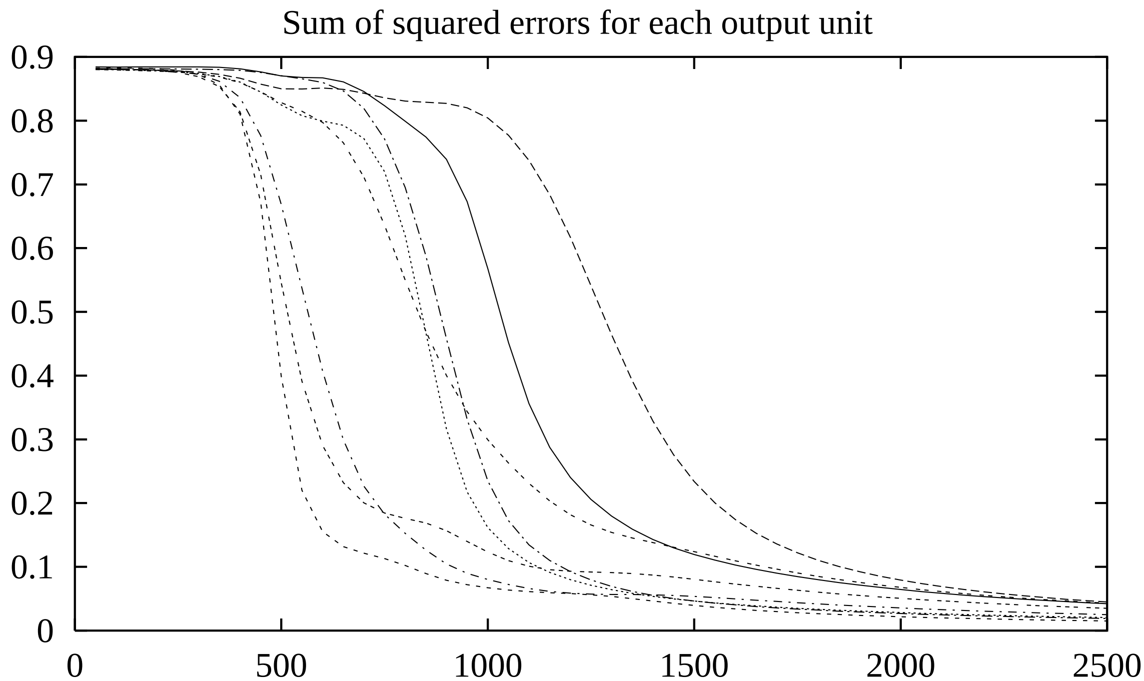
A network:



Learned hidden layer representation:

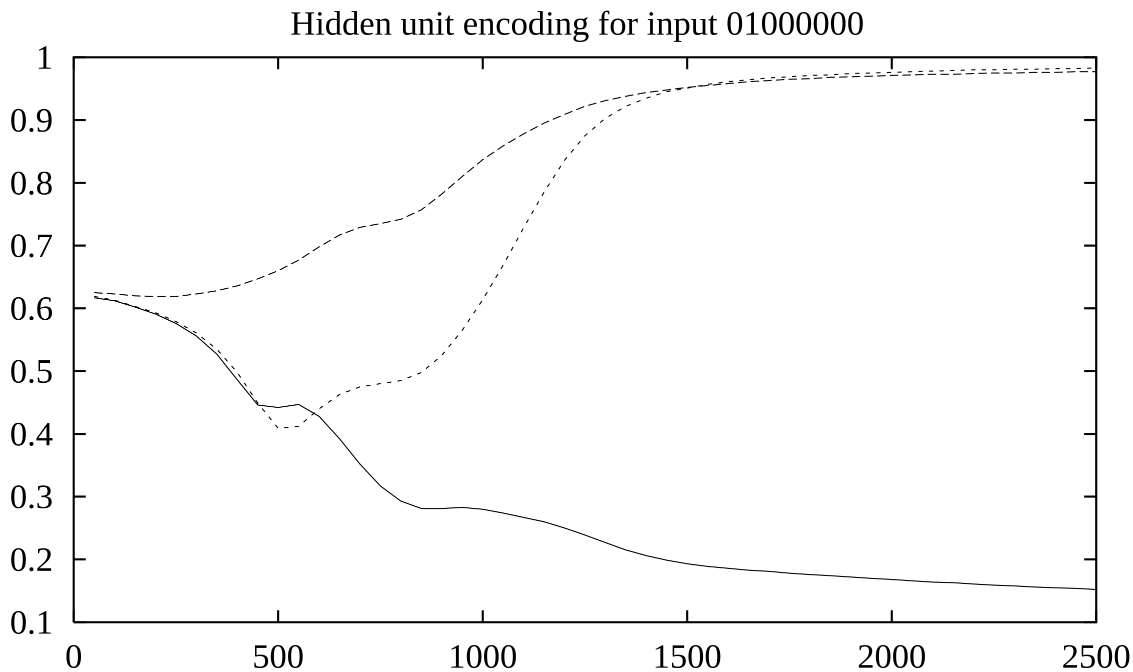
Input		Hidden Values				Output
10000000	$\rightarrow$	.89	.04	.08	$\rightarrow$	10000000
01000000	$\rightarrow$	.01	.11	.88	$\rightarrow$	01000000
00100000	$\rightarrow$	.01	.97	.27	$\rightarrow$	00100000
00010000	$\rightarrow$	.99	.97	.71	$\rightarrow$	00010000
00001000	$\rightarrow$	.03	.05	.02	$\rightarrow$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

Training



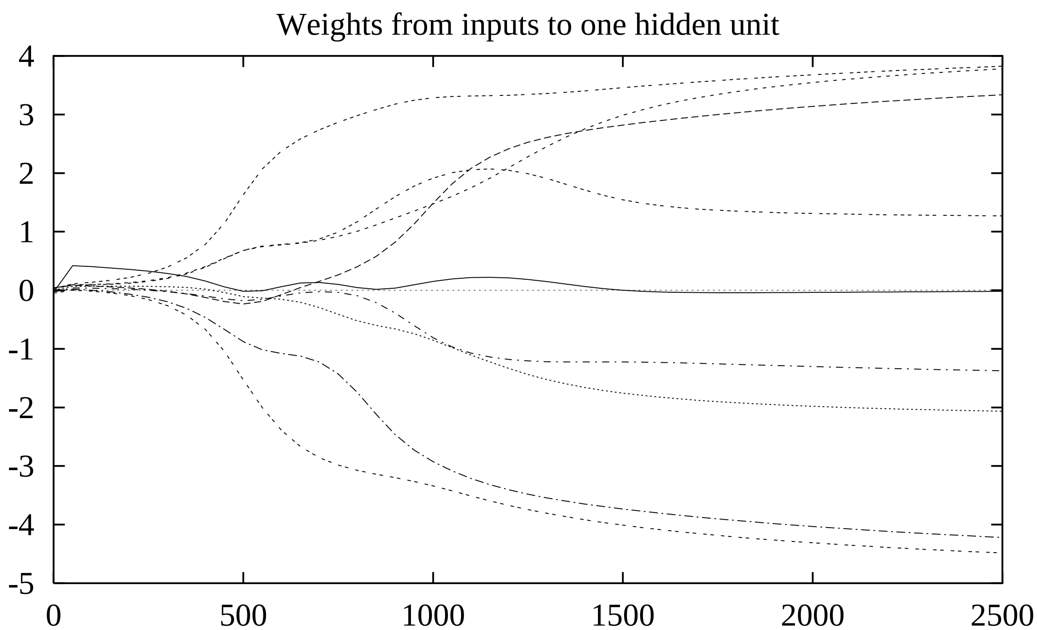
Sum of squared errors for each output unit
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
500
1000
1500
2000
2500

Training



Hidden unit encoding for input 01000000
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
500
1000
1500
2000
2500

Training


Weights from inputs to one hidden unit
4
3
2
1
0
-1
-2
-3
-4
-5
0
500
1000
1500
2000
2500

Convergence of Backpropagation

Gradient descent to some local minimum

- Perhaps not global minimum...
- Add momentum
- Stochastic gradient descent
- Train multiple nets with different inital weights

Nature of convergence

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

Expressive Capabilities of ANNs

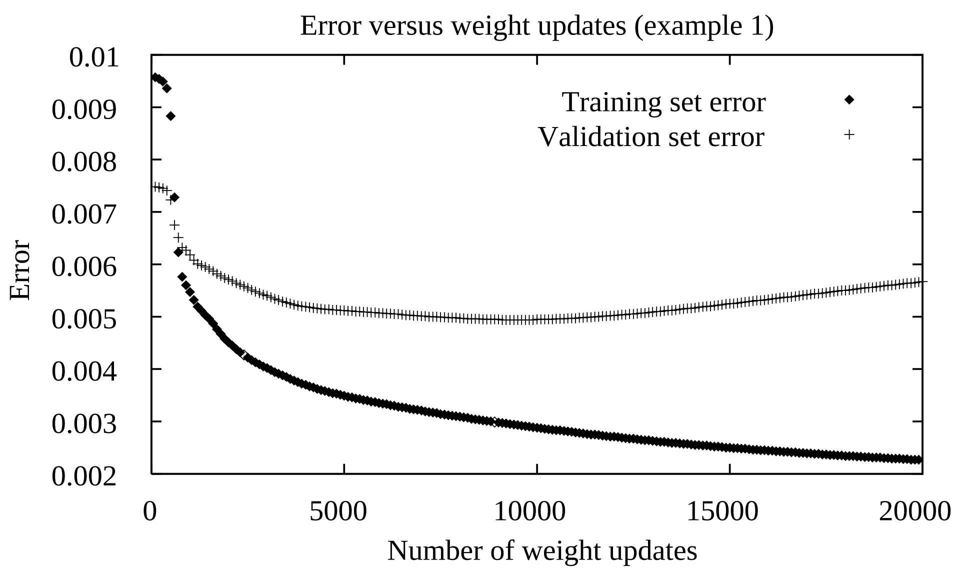
Boolean functions:

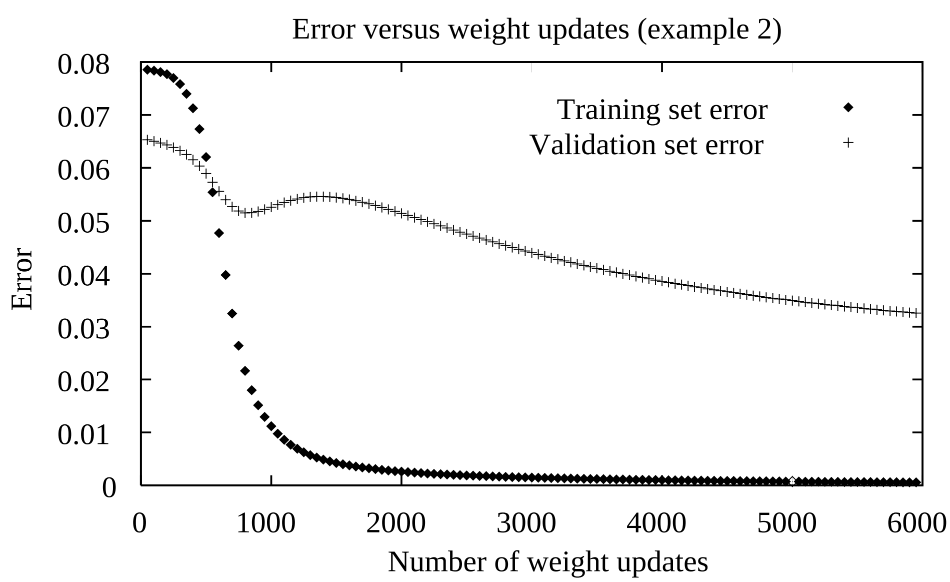
- Every boolean function can be represented by network with single hidden layer
- but might require exponential (in number of inputs) hidden units

Continuous functions:

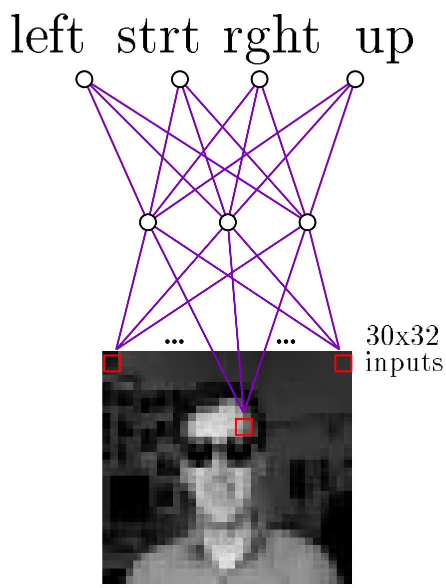
- Every bounded continuous function can be approximated with arbitrarily small error, by network with one hidden layer [Cybenko 1989; Hornik et al. 1989]
- Any function can be approximated to arbitrary accuracy by a network with two hidden layers [Cybenko 1988].

Overfitting in ANNs





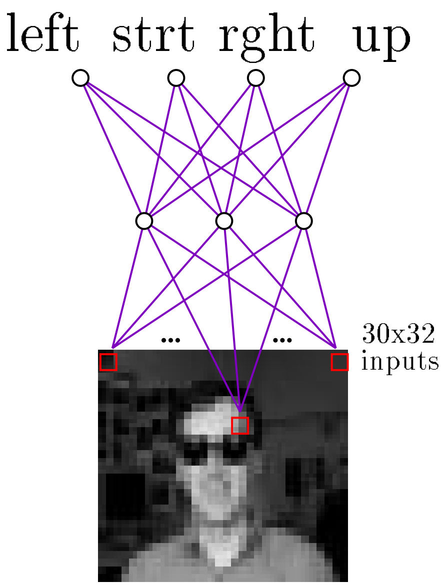
Neural Nets for Face Recognition



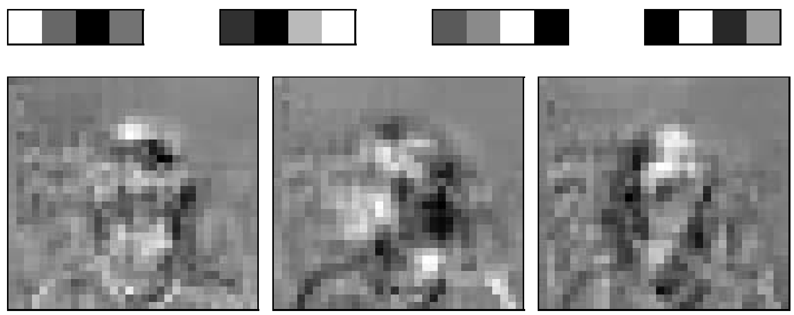
Typical input images

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

Learned Hidden Unit Weights



Learned Weights



Typical input images

http://www.cs.cmu.edu/~tom/faces.html

Alternative Error Functions

Penalize large weights:

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

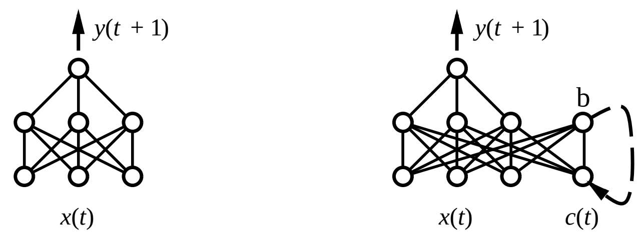
Train on target slopes as well as values:

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

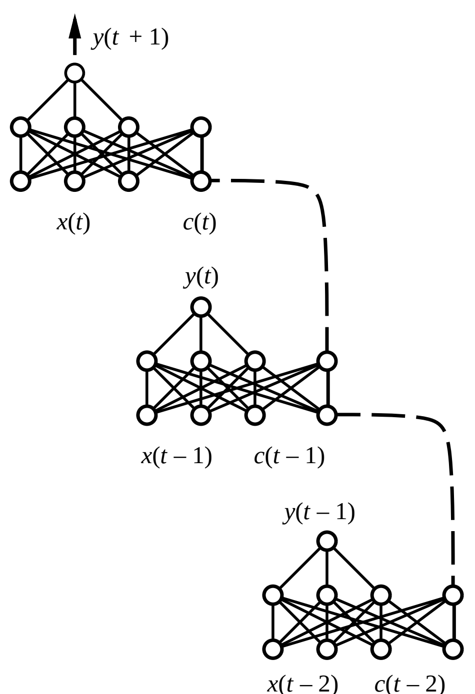
Tie together weights:

- e.g., in phoneme recognition network

Recurrent Networks



(*a*) Feedforward network (*b*) Recurrent network



(*c*) Recurrent network unfolded in time