Machine Learning 10-701

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March 24, 2011

Today:
- Non-linear regression
- Artificial neural networks
- Backpropagation
- Cognitive modeling
- Deep belief networks

Reading:
- Mitchell: Chapter 4
- Bishop: Chapter 5

Artificial Neural Networks to learn f: X → Y

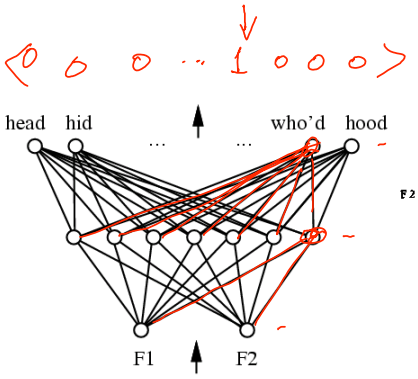
- f might be non-linear function
- X (vector of) continuous and/or discrete vars
- Y (vector of) continuous and/or discrete vars

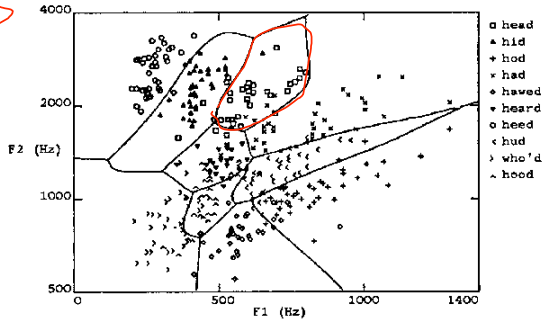
- Represent f by ***network*** of logistic units
- Each unit is a logistic function

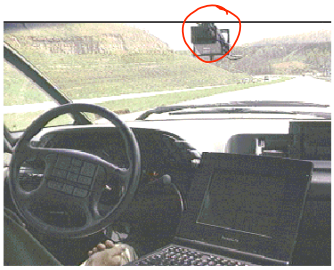
$$unit\ output = \frac{1}{1 + exp(w_0 + \sum_i w_i x_i)}$$

- MLE: train weights of all units to minimize sum of squared errors of predicted network outputs
- MAP: train to minimize sum of squared errors plus weight magnitudes

Multilayer Networks of Sigmoid Units

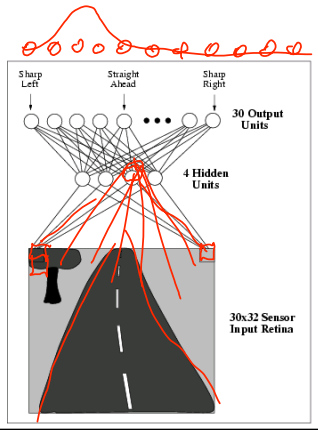


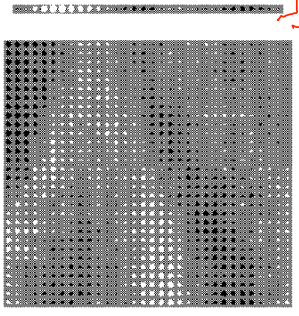




ALVINN

[Pomerleau 1993]





Connectionist Models

Consider humans:

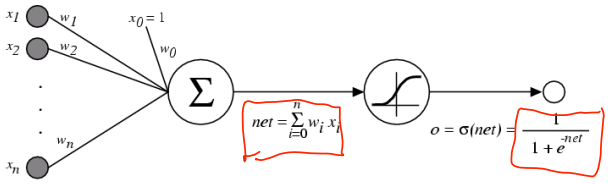
- Neuron switching time ~ .001 second
- Number of neurons ~ 10^{10}
- Connections per neuron ~ 10^{4-5}
- Scene recognition time ~ .1 second
- 100 inference steps doesn't seem like enough

→ 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

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 → Backpropagation

M(C)LE Training for Neural Networks

- Consider regression problem f:X→Y , for scalar Y

  $y = f(x) + \varepsilon$ ← assume noise N(0,σ_ε), iid

  deterministic

- Let's maximize the conditional data likelihood

$$W \leftarrow \arg\max_W \ln \prod_l P(Y^l | X^l, W)$$

$$W \leftarrow \arg\min_W \sum_l (y^l - \hat{f}(x^l))^2$$

Learned neural network

MAP Training for Neural Networks

- Consider regression problem f:X→Y , for scalar Y

  $y = f(x) + \varepsilon$ ← noise N(0,σ_ε)

  deterministic

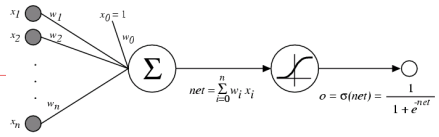
Gaussian P(W) = N(0,σI)

$$W \leftarrow \arg\max_W \ln P(W) \prod_l P(Y^l | X^l, W)$$

$$W \leftarrow \arg\min_W \left[c \sum_i w_i^2 \right] + \left[\sum_l (y^l - \hat{f}(x^l))^2 \right]$$

ln P(W) ↔ c $\sum_i w_i^2$

Error Gradient for a Sigmoid Unit



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

x_d = input

t_d = target output

o_d = observed unit output

w_i = weight i

But we know:

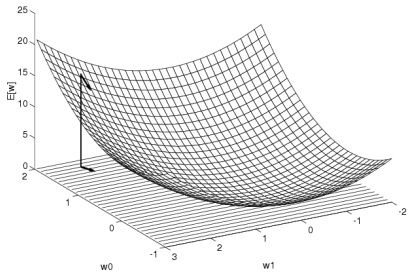
$$\frac{\partial o_d}{\partial net_d} = \frac{\partial \sigma(net_d)}{\partial net_d} = o_d(1 - o_d)$$

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

So:

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

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.,

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

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

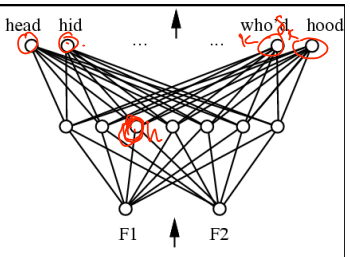
- For each training example d in D
  1. Compute the gradient $\nabla E_d[\vec{w}]$
  2. $\vec{w} \leftarrow \vec{w} - \eta \nabla E_d[\vec{w}]$

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

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

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

Backpropagation Algorithm (MLE)



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

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

x_d = input

t_d = target output

o_d = observed unit output

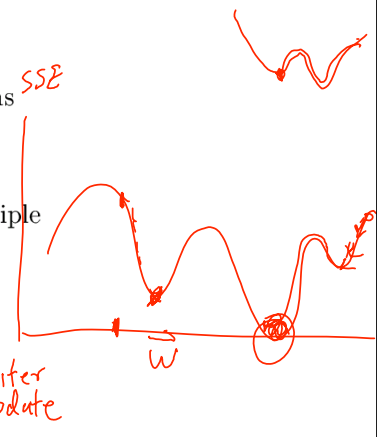
w_{ij} = wt from i to j

More on Backpropagation

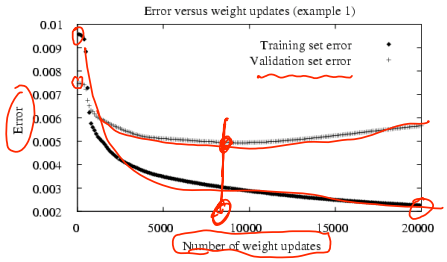
- Gradient descent over entire *network* weight vector
- Easily generalized to arbitrary directed graphs
- Will find a local, not necessarily global error minimum
  - In practice, often works well (can run multiple times)
- Often include weight *momentum* α

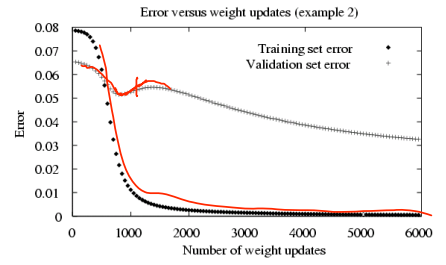
$$\Delta w_{i,j}(n) = \eta \delta_j x_{i,j} + \alpha \Delta w_{i,j}(n-1)$$

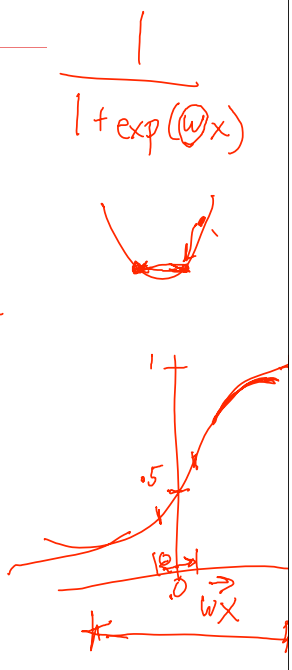
- Minimizes error over *training* examples
  - Will it generalize well to subsequent examples?
- Training can take thousands of iterations → slow!
- Using network after training is very fast



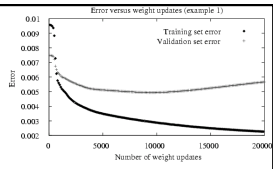
Overfitting in ANNs







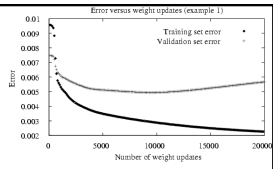
Dealing with Overfitting



Our learning algorithm involves a parameter
n=number of gradient descent iterations
How do we choose n to optimize future error?
(note: similar issue for logistic regression, decision trees, …)

e.g. the n that minimizes error rate of neural net over future data

Dealing with Overfitting



Our learning algorithm involves a parameter
n=number of gradient descent iterations
How do we choose n to optimize future error?

- Separate available data into training and validation set
- Use training to perform gradient descent
- n ← number of iterations that optimizes validation set error

→ *gives unbiased estimate of optimal n*
(but a biased estimate of true error)

K-Fold Cross Validation

Idea: train multiple times, leaving out a disjoint subset of data each time for test. Average the test set accuracies.

Partition data into K disjoint subsets
For k=1 to K
    testData = kth subset
    h ← classifier trained* on all data except for testData
    accuracy(k) = accuracy of h on testData
end
FinalAccuracy = mean of the K recorded testset accuracies

* might withhold some of this to choose number of gradient decent steps

Leave-One-Out Cross Validation

This is just k-fold cross validation leaving out one example each iteration

---

Partition data into K disjoint subsets, *each containing one example*
For k=1 to K
    testData = kth subset
    h ← classifier trained* on all data except for testData
    accuracy(k) = accuracy of h on testData
end
FinalAccuracy = mean of the K recorded testset accuracies

* might withhold some of this to choose number of gradient decent steps

Expressive Capabilities of ANNs

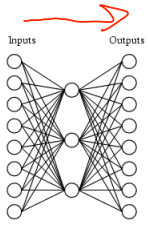
Boolean functions:

- 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].

Learning Hidden Layer Representations



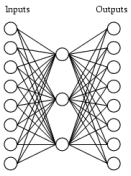
A target function:

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

Can this be learned??

Learning Hidden Layer Representations

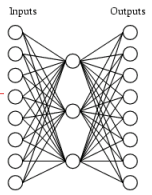
A network:

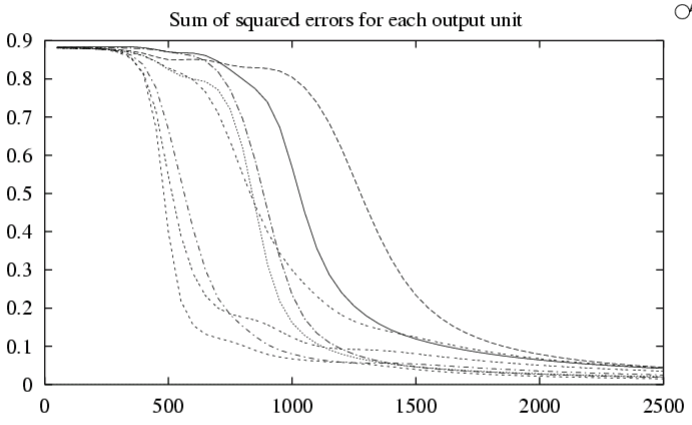


Learned hidden layer representation:

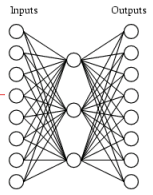
Input		Hidden Values				Output
10000000	→	.89	.04	.08	→	10000000
01000000	→	.01	.11	.88	→	01000000
00100000	→	.01	.97	.27	→	00100000
00010000	→	.99	.97	.71	→	00010000
00001000	→	.03	.05	.02	→	00001000
00000100	→	.22	.99	.99	→	00000100
00000010	→	.80	.01	.98	→	00000010
00000001	→	.60	.94	.01	→	00000001

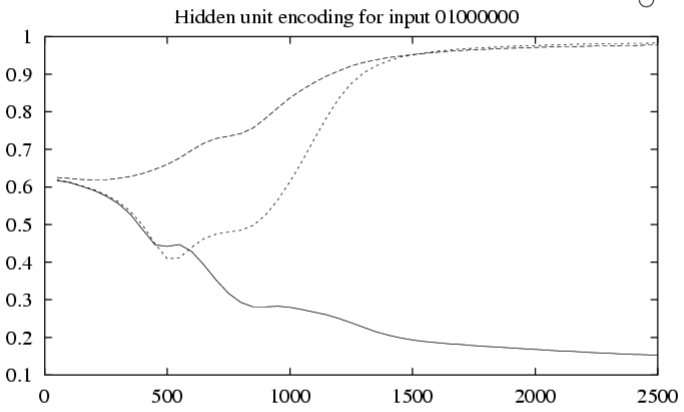
Training



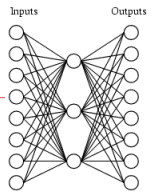


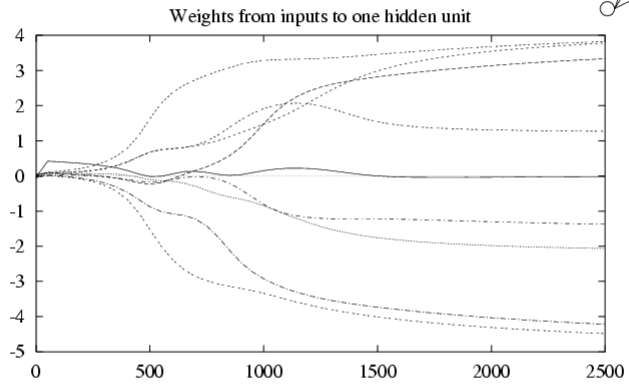
Training



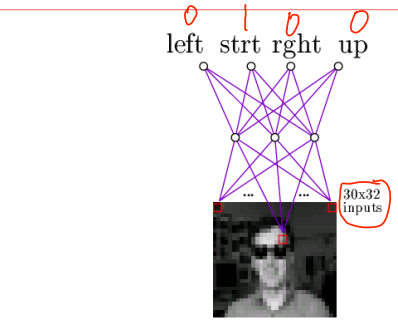


Training





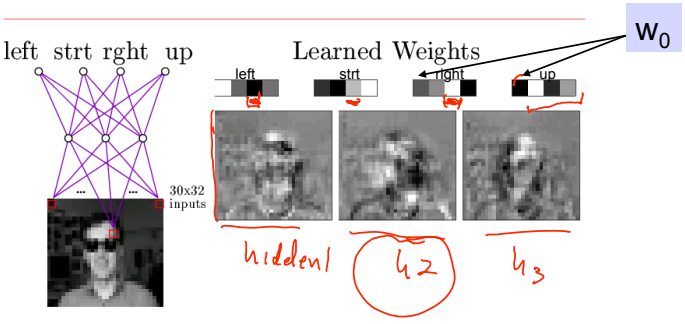
Neural Nets for Face Recognition



Typical input images

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

Learned Hidden Unit Weights



Typical input images

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