Neural Networks

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Slides Courtesy: Tom Mitchell

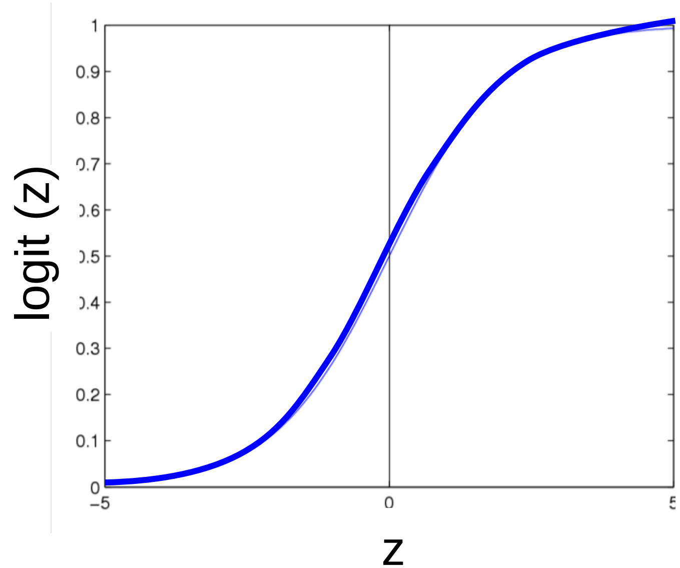
Logistic Regression

Assumes the following functional form for P(Y|X):

$$P(Y=1|X) = \frac{1}{1+\exp(-(w_0 + \sum_i w_i X_i))}$$

Logistic function applied to a linear function of the data

Logistic function (or Sigmoid): $\frac{1}{1+exp(-z)}$



Features can be discrete or continuous!

Logistic Regression is a Linear Classifier!

Assumes the following functional form for P(Y|X):

$$P(Y=1|X) = \frac{1}{1+\exp(-(w_0 + \sum_i w_i X_i))}$$

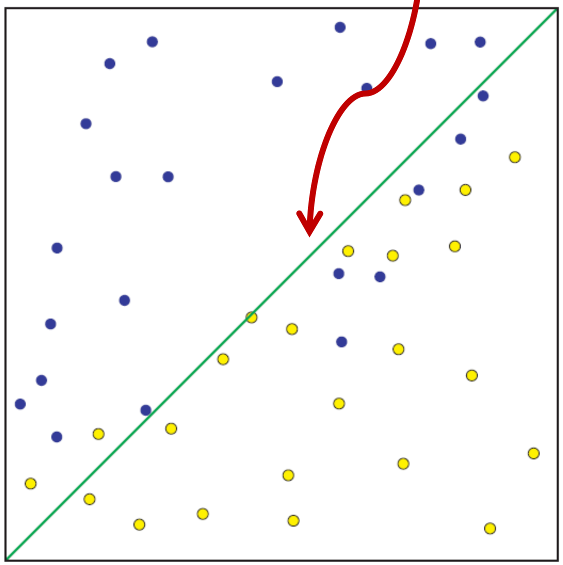
Decision boundary:

$$P(Y=0|X) \underset{1}{\overset{0}{\gtrless}} P(Y=1|X)$$

$$0 \underset{1}{\overset{0}{\gtrless}} w_0 + \sum_i w_i X_i$$

(Linear Decision Boundary)

$$w_0 + \sum_i w_i X_i = 0$$



Training Logistic Regression

How to learn the parameters w_0, w_1, … w_d?

Training Data $\{(X^{(j)}, Y^{(j)})\}_{j=1}^{n}$ $X^{(j)} = (X_1^{(j)}, \ldots, X_d^{(j)})$

Maximum (Conditional) Likelihood Estimates

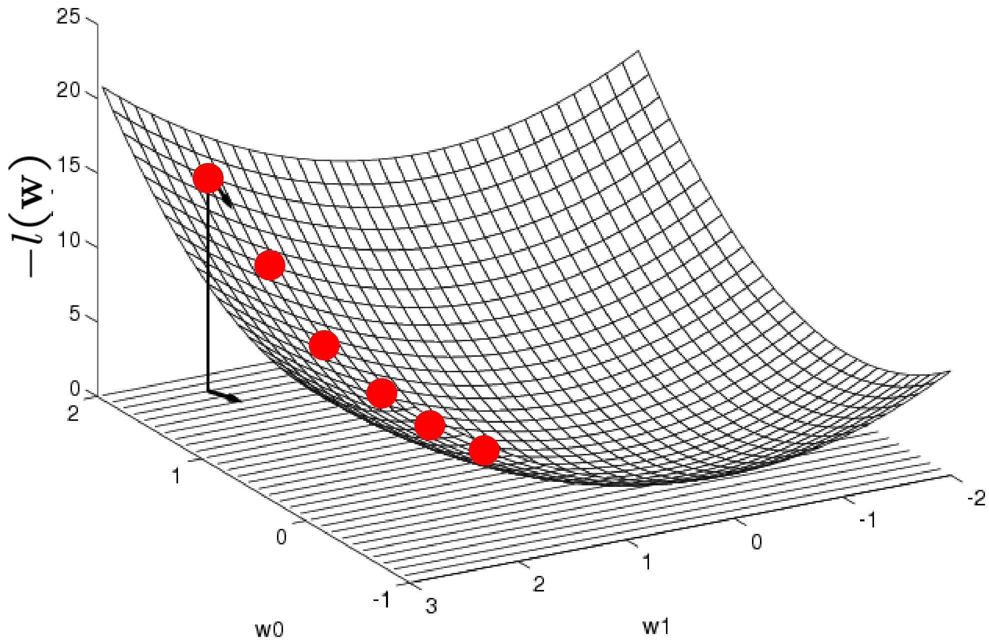
$$\hat{\mathbf{w}}_{MCLE} = \arg\max_{\mathbf{w}} \prod_{j=1}^{n} P(Y^{(j)} \mid X^{(j)}, \mathbf{w})$$

Discriminative philosophy – Don't waste effort learning P(X), focus on P(Y|X) – that's all that matters for classification!

Optimizing concave/convex function

- Conditional likelihood for Logistic Regression is concave
- Maximum of a concave function = minimum of a convex function

Gradient Ascent (concave)/ Gradient Descent (convex)



Gradient:

$$\nabla_{\mathbf{w}} l(\mathbf{w}) = [\frac{\partial l(\mathbf{w})}{\partial w_0}, \ldots, \frac{\partial l(\mathbf{w})}{\partial w_d}]'$$

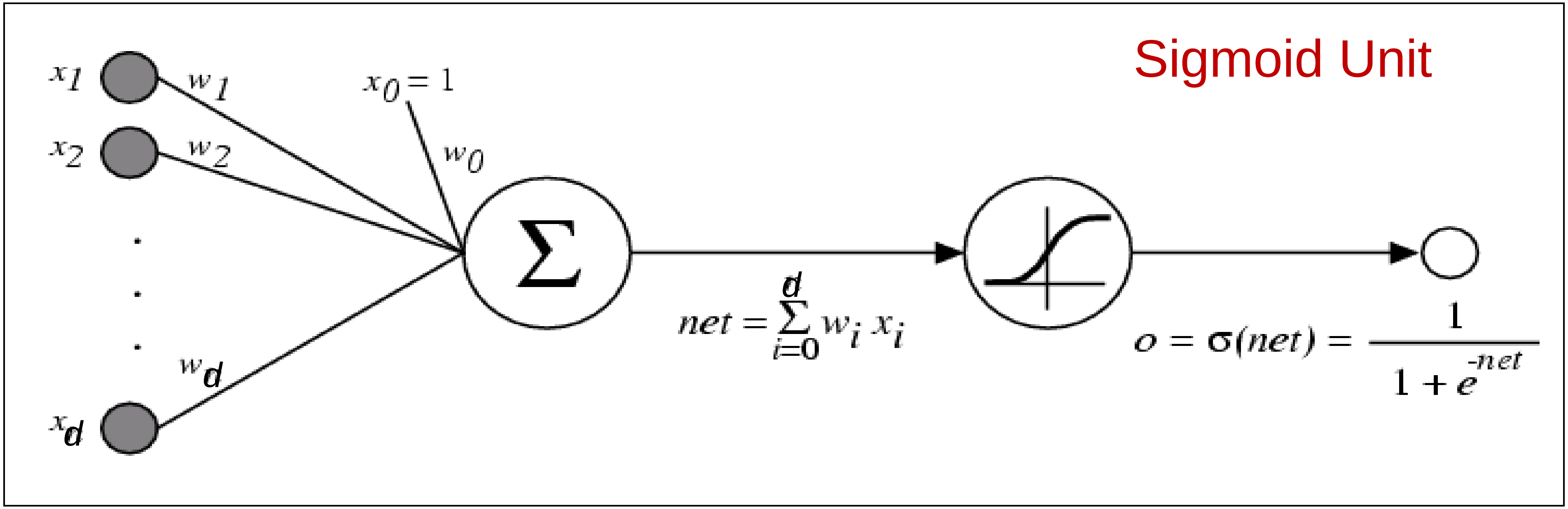
Update rule: Learning rate, η>0

$$\Delta \mathbf{w} = \eta \nabla_{\mathbf{w}} l(\mathbf{w})$$

$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \left. \frac{\partial l(\mathbf{w})}{\partial w_i} \right|_t$$

Logistic Regression as a Graph

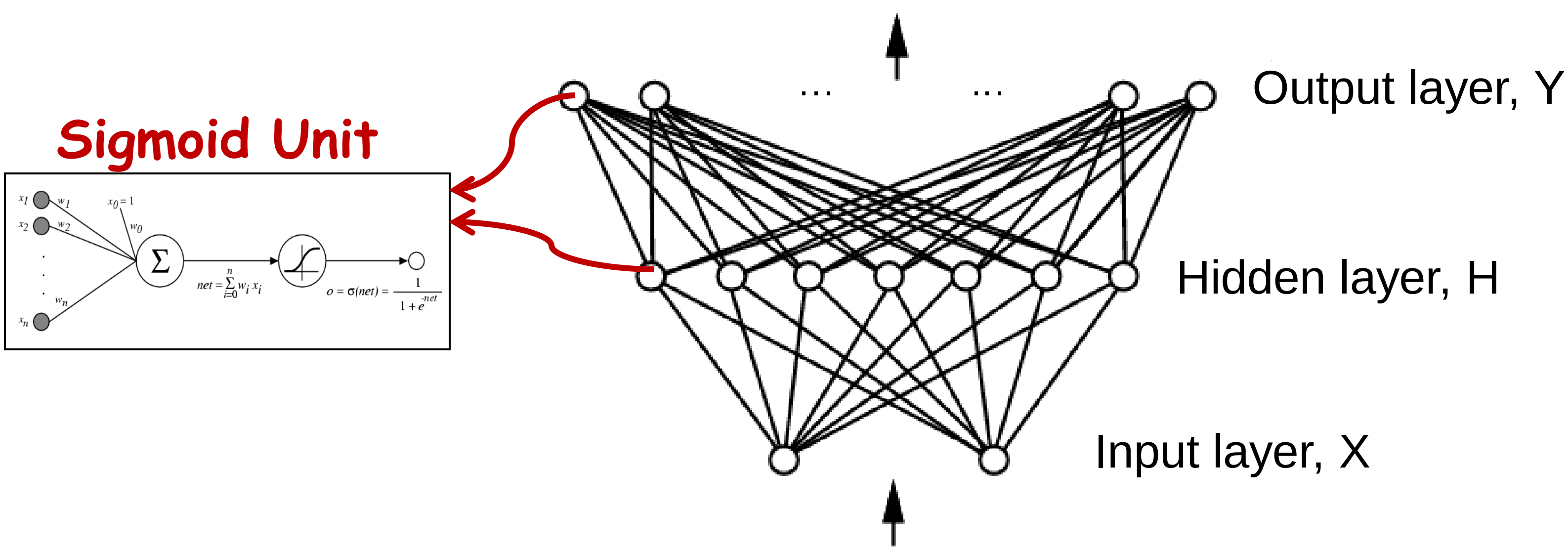
$$\text{Output, } o(\mathbf{x}) = \sigma(w_0 + \sum_i w_i X_i) = \frac{1}{1 + \exp(-(w_0 + \sum_i w_i X_i))}$$



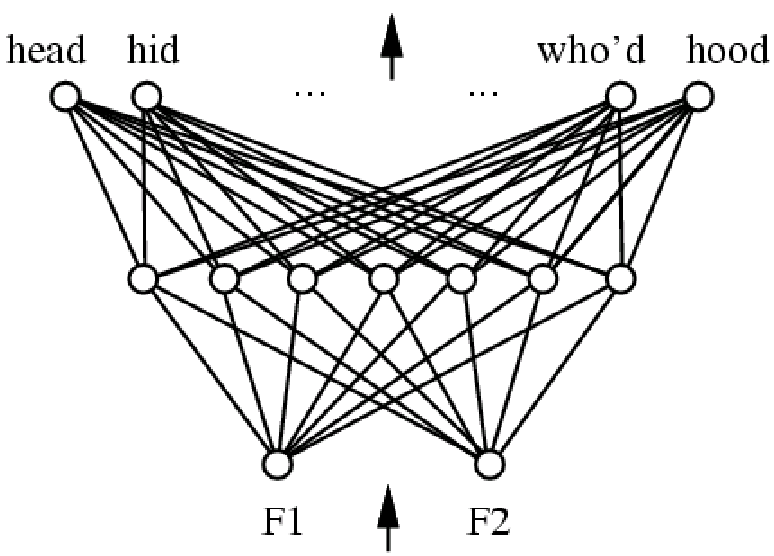
Neural Networks to learn f: X → Y

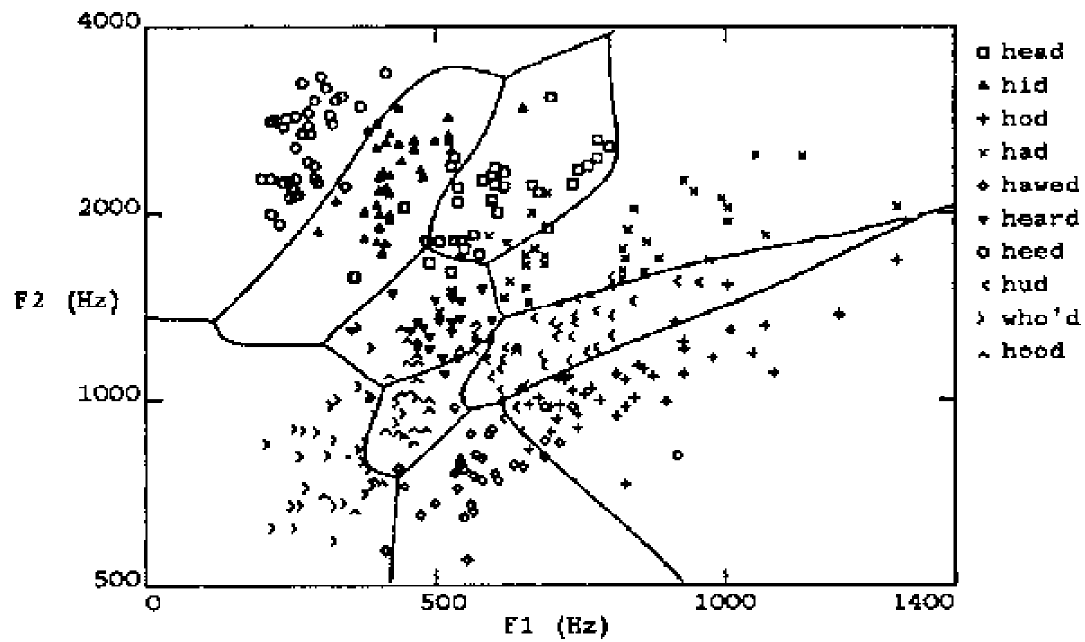
- f can be a non-linear function
- X (vector of) continuous and/or discrete variables
- Y (vector of) continuous and/or discrete variables

- Neural networks - Represent f by *network* of logistic/sigmoid units, we will focus on feedforward networks:



Multilayer Networks of Sigmoid Units





Connectionist Models

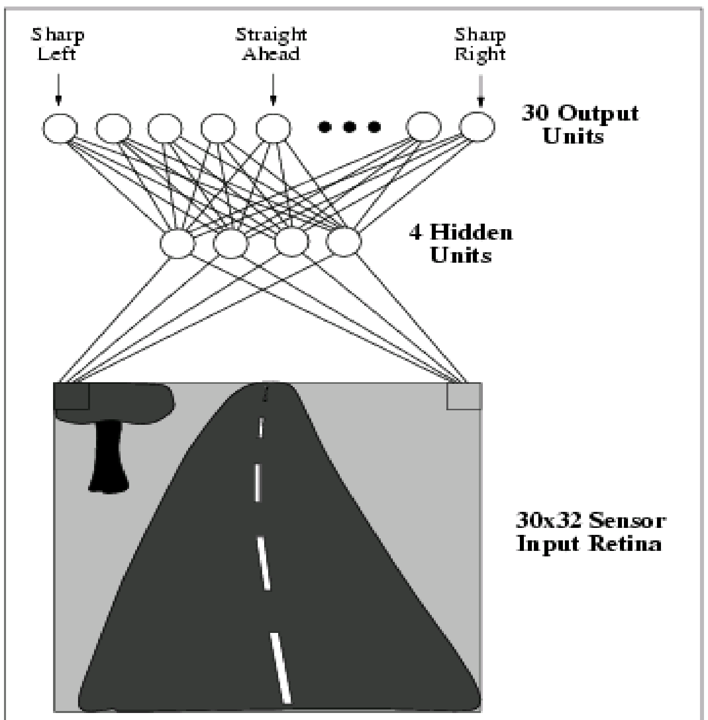
Consider humans:

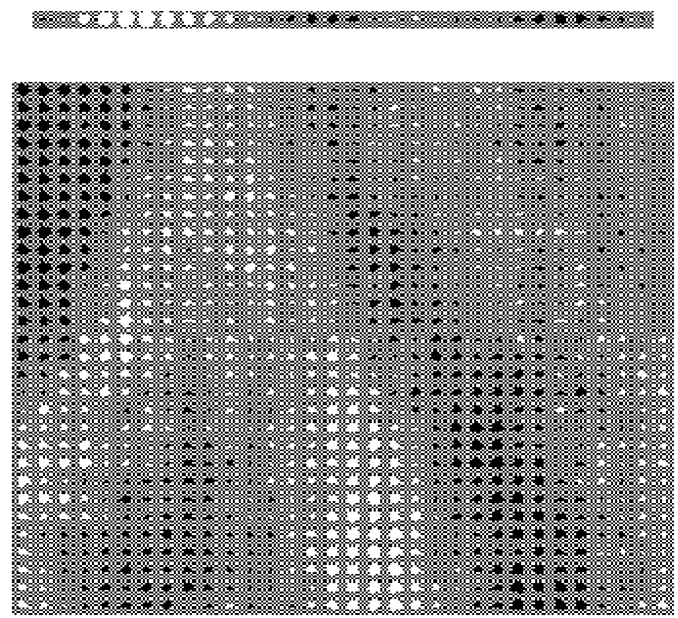
- Neuron switching time ~ .001 second
- Number of neurons ~ 10^{10}
- Connections per neuron ~ 10^{4-5}
- Scene recognition time ~ .1 second
- 100 inference steps doesn't seem like enough

$\rightarrow$ much parallel computation

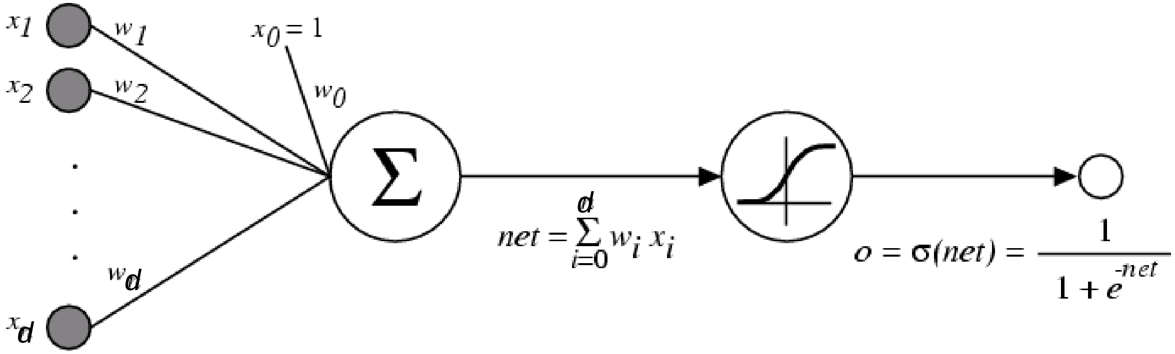
Properties of artificial neural nets (ANN's):

- Many neuron-like threshold switching units
- Many weighted interconnections among units
- Highly parallel, distributed process


Sharp Left
Straight Ahead
Sharp Right
30 Output Units
4 Hidden Units
30x32 Sensor Input Retina



Sigmoid Unit



$\sigma(x)$ is the sigmoid function/activation function (also linear, threshold)

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

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

We can derive gradient decent rules to train

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

Forward Propagation for prediction

Sigmoid unit:

$$o(\mathbf{x}) = \sigma(w_0 + \sum_i w_i x_i)$$

1-Hidden layer,
1 output NN:

$$o(\mathbf{x}) = \sigma \underbrace{\left(w_0 + \sum_h w_h \underbrace{\sigma(w_0^h + \sum_i w_i^h x_i)}_{o_h} \right)}$$

Prediction – Given neural network (hidden units and weights), use it to predict the label of a test point

Forward Propagation –

Start from input layer
For each subsequent layer, compute output of sigmoid unit

M(C)LE Training for Neural Networks

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

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

deterministic

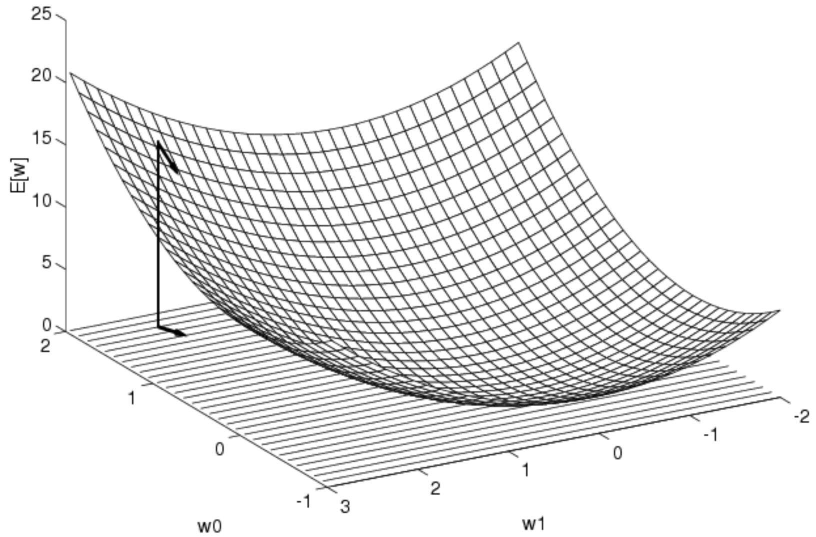
Gaussian $P(W) = N(0,\sigma I)$

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

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

$\ln P(W) \leftrightarrow c \sum_i w_i^2$

Gradient Descent



E – Mean Square Error

Gradient

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

Training rule:

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

i.e.,

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

For Neural Networks,
E[*w*] no longer convex in w

Incremental (Stochastic) Gradient Descent

Batch mode Gradient Descent:
Do until satisfied

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

Using all training data *D*

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

$$E_D[\vec{w}] \equiv \frac{1}{2} \sum_{l \in D} (y^l - o^l)^2$$

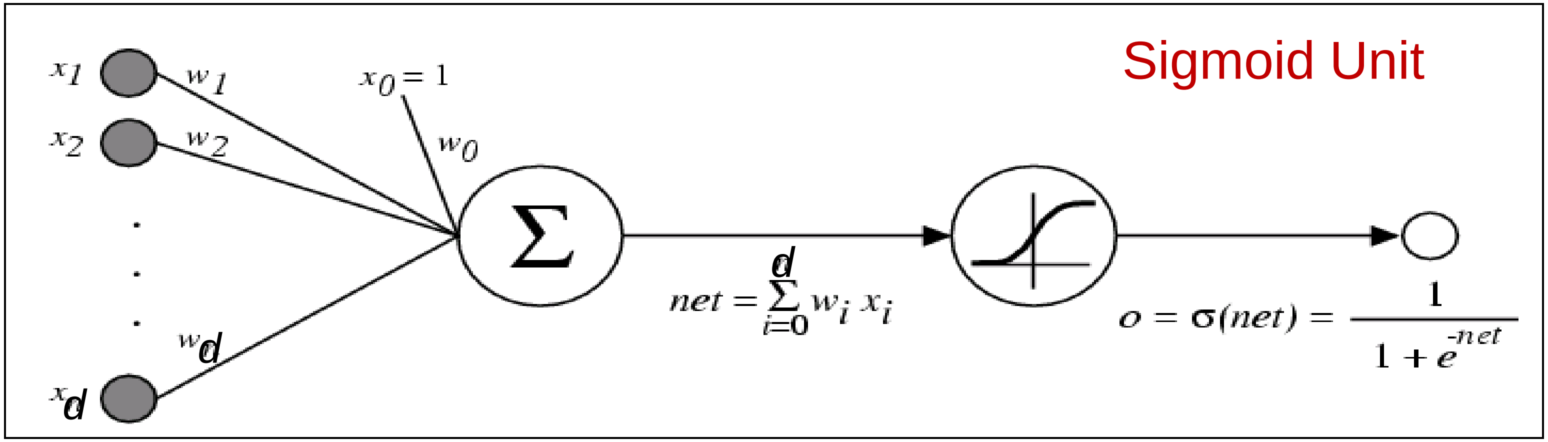
Incremental mode Gradient Descent:
Do until satisfied

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

$$E_l[\vec{w}] \equiv \frac{1}{2} (y^l - o^l)^2$$

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

Error Gradient for a Sigmoid Unit



$$\frac{\partial E}{\partial w_i} = \frac{\partial}{\partial w_i} \frac{1}{2} \sum_{l \in D} (y^l - o^l)^2$$

$$= \frac{1}{2} \sum_l \frac{\partial}{\partial w_i} (y^l - o^l)^2$$

$$= \frac{1}{2} \sum_l 2(y^l - o^l) \frac{\partial}{\partial w_i} (y^l - o^l)$$

$$= \sum_l (y^l - o^l) \left(- \frac{\partial o^l}{\partial w_i} \right)$$

$$= - \sum_l (y^l - o^l) \frac{\partial o^l}{\partial net^l} \frac{\partial net^l}{\partial w_i}$$

But we know:

$$\frac{\partial o^l}{\partial net^l} = \frac{\partial \sigma(net^l)}{\partial net^l} = o^l (1 - o^l)$$

$$\frac{\partial net^l}{\partial w_i} = \frac{\partial (\vec{w} \cdot \vec{x}^l)}{\partial w_i} = x_i^l$$

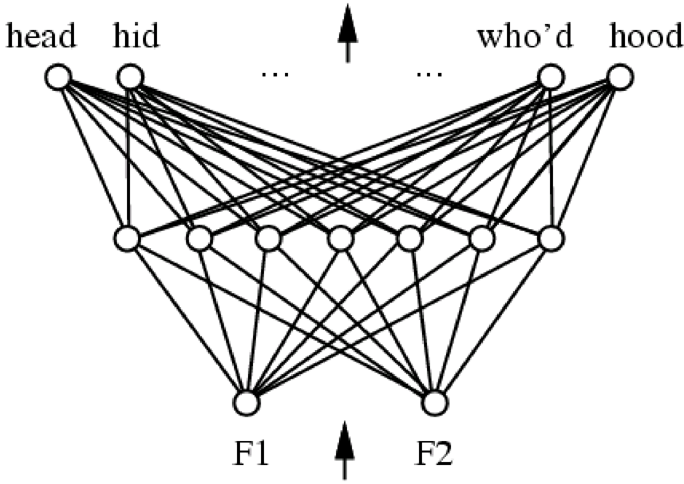
So:

$$\frac{\partial E}{\partial w_i} = - \sum_{l \in D} (y^l - o^l) o^l (1 - o^l) x_i^l$$

Error Gradient for 1-Hidden layer, 1-output neural network

see Notes.pdf

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 → Using Forward propagation
  2. For each output unit k

$$\delta_k^l \leftarrow o_k^l(1 - o_k^l)(y_k^l - o_k^l)$$

  3. For each hidden unit h

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

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

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

where

$$\Delta w_{i,j}^l = \eta \delta_j^l o_i^l$$

y_k = target output (label) of output unit k

$o_{k(h)}$ = unit output (obtained by forward propagation)

w_{ij} = wt from i to j

Note: if i is input variable, $o_i = x_i$

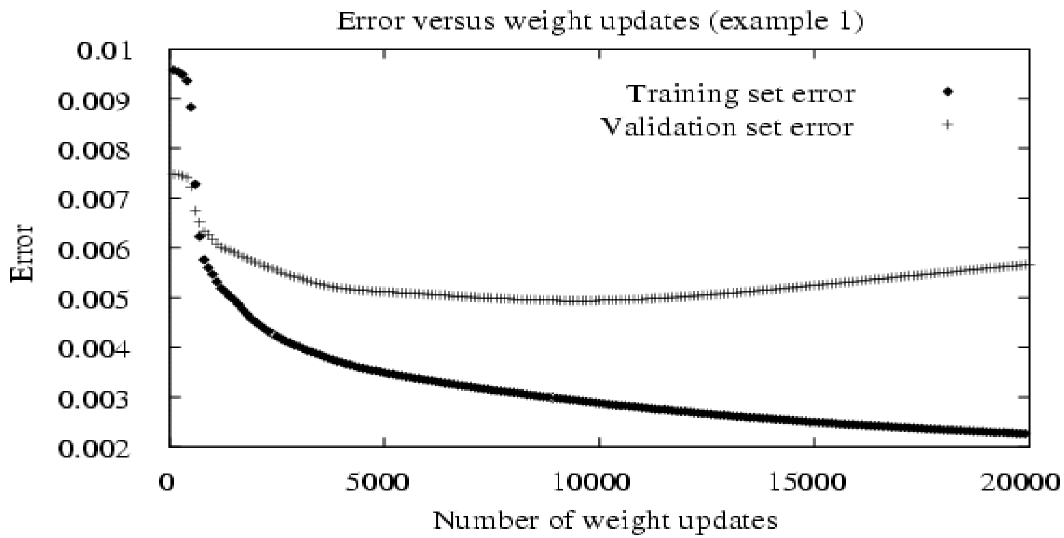
More on Backpropagation

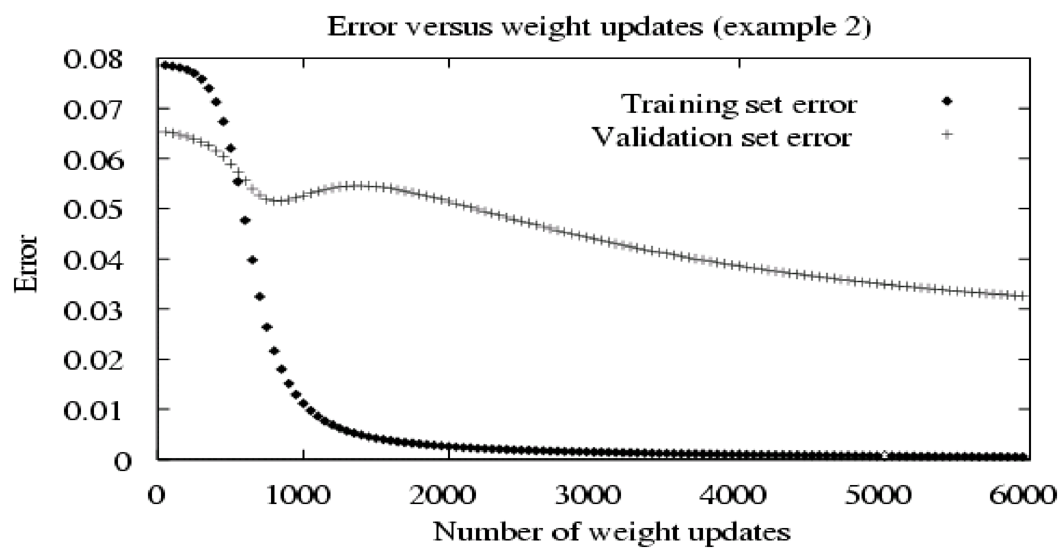
- Gradient descent over entire *network* weight vector
- Easily generalized to arbitrary directed graphs
- Will find a local, not necessarily global error minimum
  - In practice, often works well (can run multiple times)

Objective/Error no longer convex in weights

- 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

Overfitting in ANNs





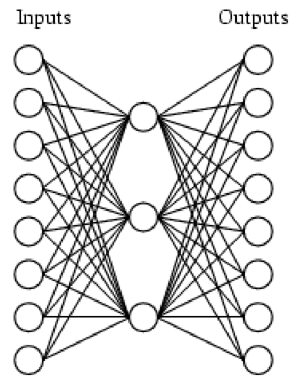
How to avoid overfitting?

Regularization – train neural network by maximize M(C)AP

Early stopping

Regulate # hidden units – prevents overly complex models
≡ dimensionality reduction

Learning Hidden Layer Representations



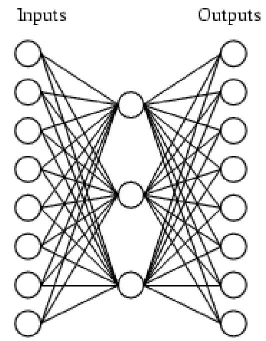
A target function:

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

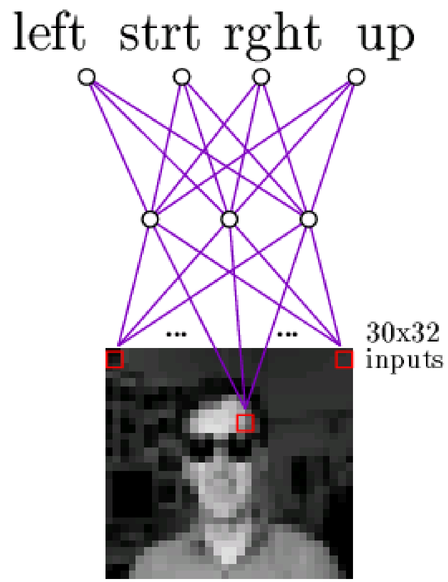
A network:



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

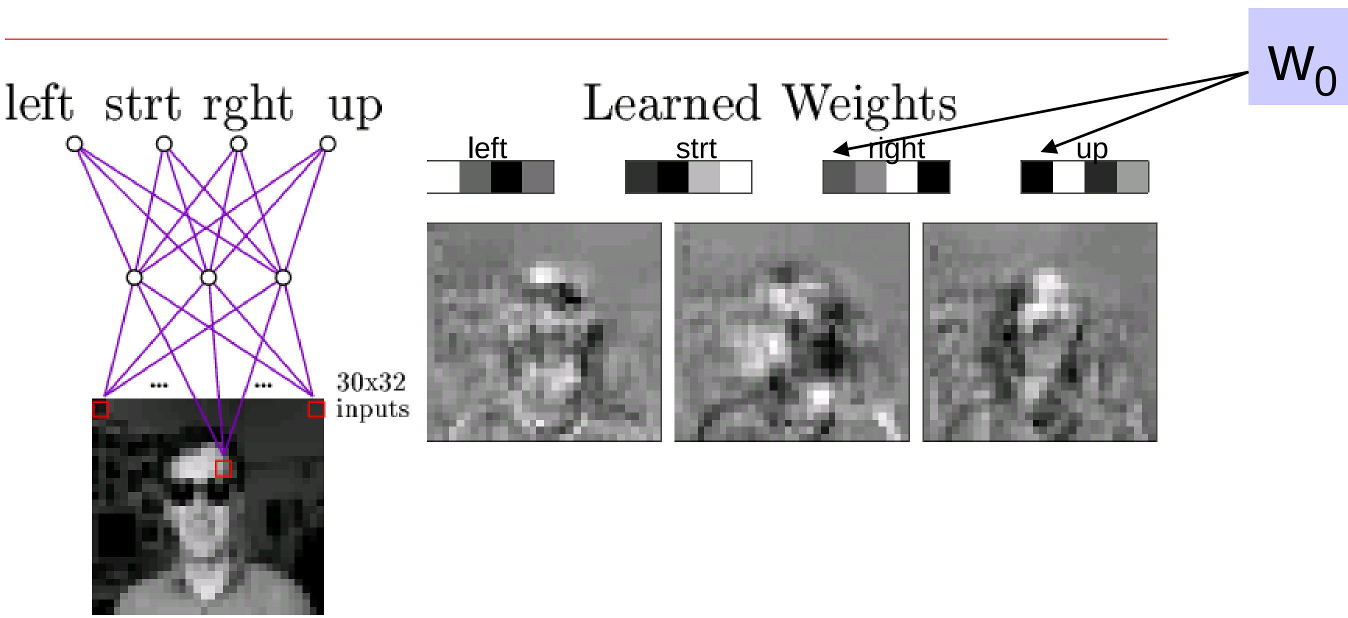
Neural Nets for Face Recognition

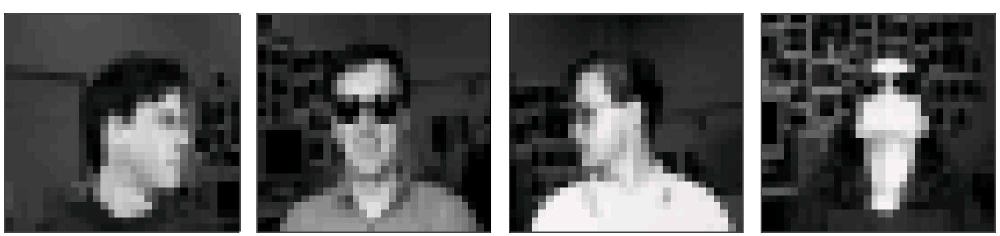


Typical input images

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

Artificial Neural Networks: Summary

- Actively used to model distributed computation in brain
- Highly non-linear regression/classification
- Vector-valued inputs and outputs
- Potentially millions of parameters to estimate - overfitting
- Hidden layers learn intermediate representations – how many to use?

- Prediction – Forward propagation
- Gradient descent (Back-propagation), local minima problems

- Mostly obsolete – kernel tricks are more popular, but coming back in new form as deep belief networks (probabilistic interpretation)