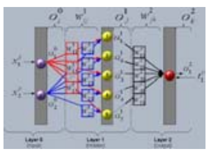
Machine Learning

10-701/15-781, Fall 2011

Neural Networks

Eric Xing

Lecture 5, September 26, 2011



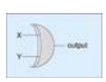
Reading: Chap. 5 CB

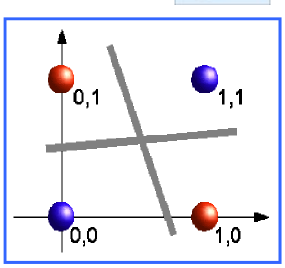
Learning highly non-linear functions

f: X → Y

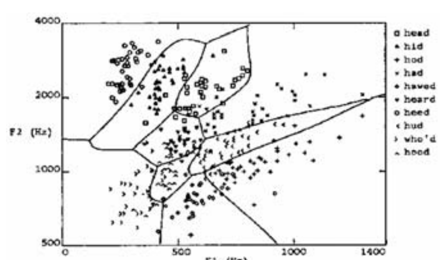
- f might be non-linear function
- X (vector of) continuous and/or discrete vars
- Y (vector of) continuous and/or discrete vars

The XOR gate



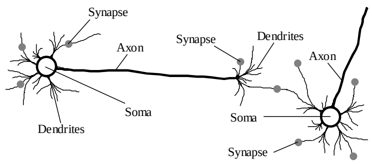


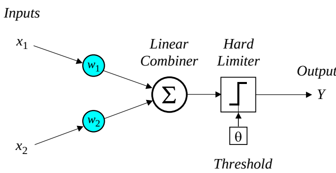
Speech recognition



Perceptron and Neural Nets

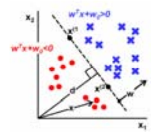
- From biological neuron to artificial neuron (perceptron)



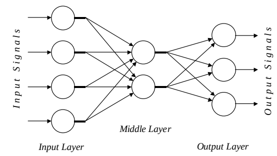


- Activation function

$$X = \sum_{i=1}^{n} x_i w_i \qquad Y = \begin{cases} +1, & \text{if } X \geq \omega_0 \\ -1, & \text{if } X < \omega_0 \end{cases}$$

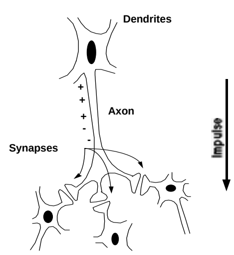


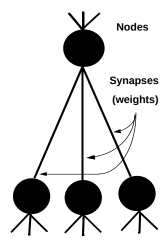
- Artificial neuron networks
  - supervised learning
  - gradient descent



Connectionist Models

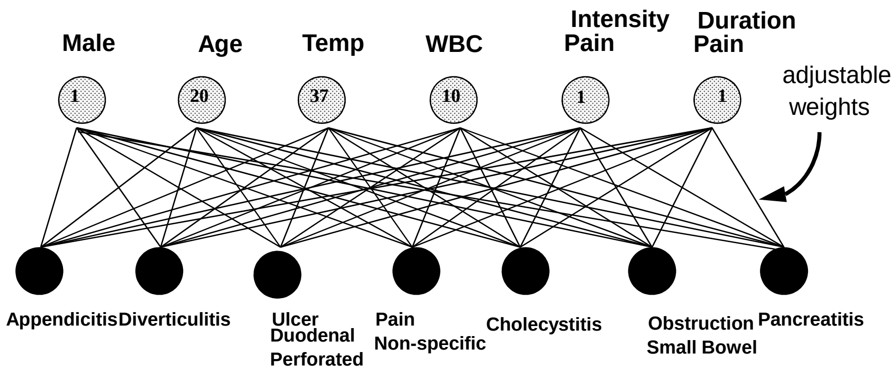
- Consider humans:
  - Neuron switching time
    ~ 0.001 second
  - Number of neurons
    ~ 10^{10}
  - Connections per neuron
    ~ 10^{4-5}
  - Scene recognition time
    ~ 0.1 second
  - 100 inference steps doesn't seem like enough
    → much parallel computation



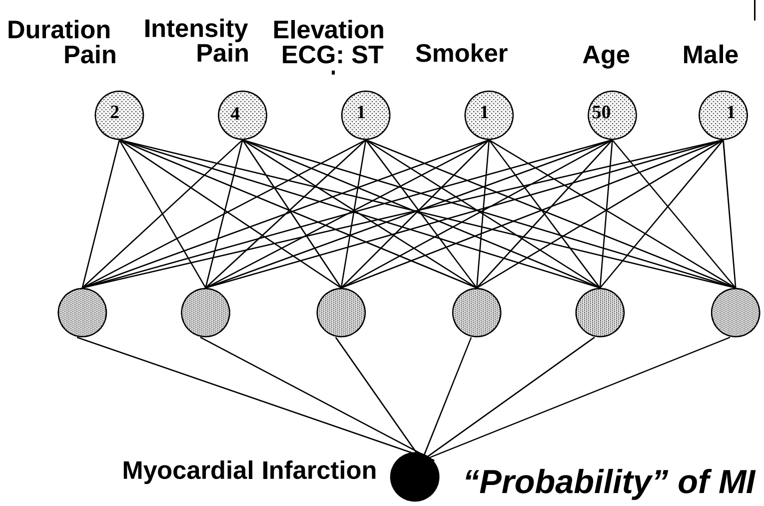


- Properties of artificial neural nets (ANN)
  - Many neuron-like threshold switching units
  - Many weighted interconnections among units
  - Highly parallel, distributed processes

Abdominal Pain Perceptron



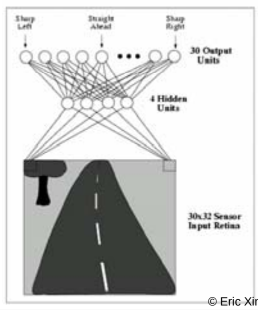
Myocardial Infarction Network

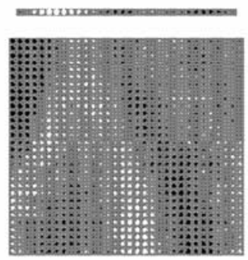


The "Driver" Network

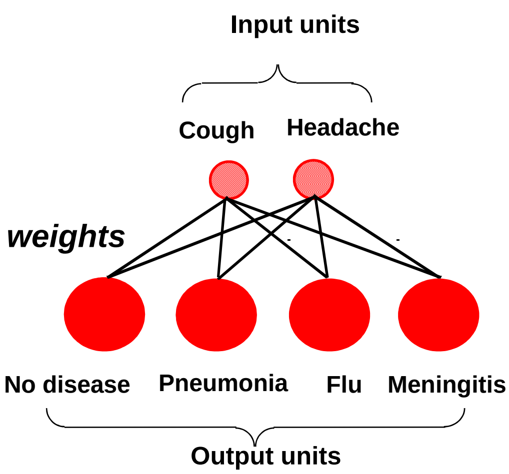
ALVINN

[Pomerleau 1993]





Perceptrons



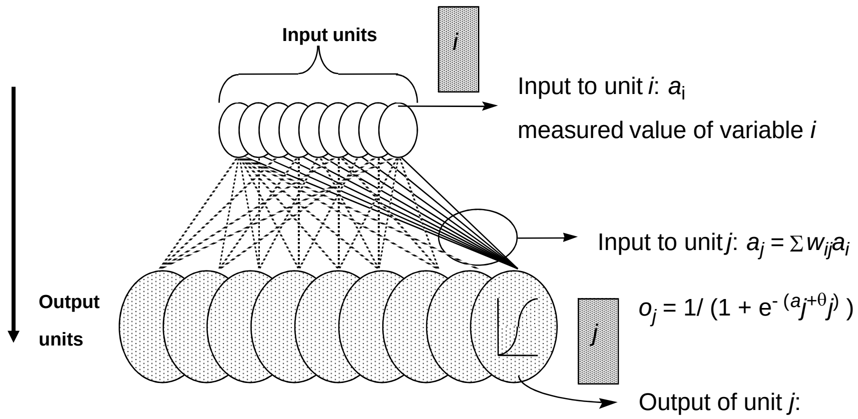
Δ **rule**

change weights to decrease the error

- what we got
  what we wanted

error

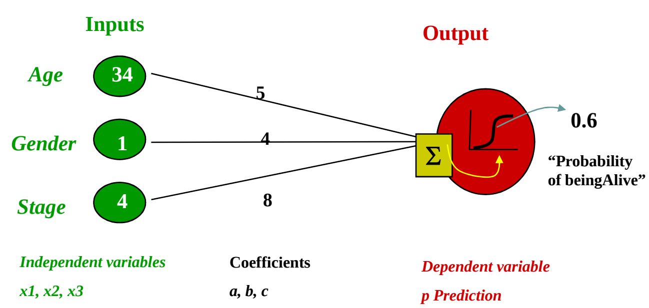
Perceptrons



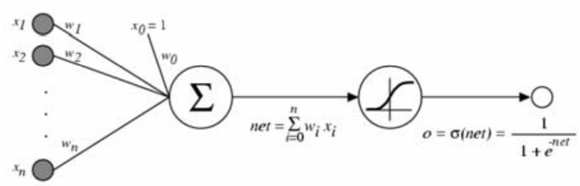
Jargon Pseudo-Correspondence

- Independent variable = input variable
- Dependent variable = output variable
- Coefficients = “weights”
- Estimates = “targets”

Logistic Regression Model (the sigmoid unit)



The perceptron learning algorithm



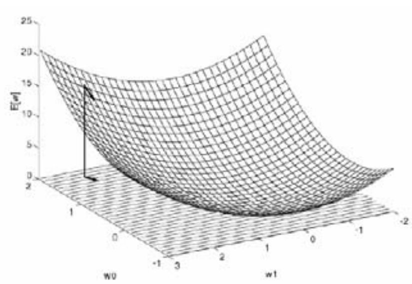
- Recall the nice property of sigmoid function $\frac{d\sigma}{dt} = \sigma(1-\sigma)$
- Consider regression problem f:X→Y , for scalar Y: $y = f(x) + \epsilon$
- Let's maximize the conditional data likelihood

$$\vec{w} = \arg\max_{\vec{w}} \ln \prod_i P(y_i | x_i; \vec{w})$$

$$\vec{w} = \arg\min_{\vec{w}} \sum_i \frac{1}{2}(y_i - \hat{f}(x_i; \vec{w}))^2$$

Gradient Descent

x_d = input
t_d = target output
o_d =observed unit output
w_i =weight i



$$\frac{\partial E[\vec{w}]}{\partial w_j} = \frac{\partial}{\partial w_i}\frac{1}{2}\sum (t_d - o_d)^2$$
$$=$$

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.,

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

The perceptron learning rules

x_d = input
t_d = target output
o_d =observed unit output
w_i =weight i

$$
\begin{aligned}
\frac{\partial E_D[\vec{w}])}{\partial w_j} &= \frac{\partial}{\partial w_i}\frac{1}{2}\sum_d (t_d - o_d)^2 \\
&= \frac{1}{2}\sum_d 2(t_d - o_d)\frac{\partial}{\partial w_i}(t_d - o_d) \\
&= \sum_d (t_d - o_d)(-\frac{\partial o_d}{\partial w_i}) \\
&= -\sum_d (t_d - o_d)\frac{\partial o_d}{\partial net_i}\frac{\partial net_d}{\partial w_i} \\
&= -\sum_d (t_d - o_d) o_d (1 - o_d) x_d^i
\end{aligned}
$$

Batch mode:

Do until converge:

1. compute gradient $\nabla E_D[w]$
2. $\vec{w} = \vec{w} - \eta \nabla E_D[\vec{w}]$

Incremental mode:

Do until converge:

- **For each training example *d* in *D***
  1. compute gradient $\nabla E_d[w]$
  2. $\vec{w} = \vec{w} - \eta \nabla E_d[\vec{w}]$

  where

  $\nabla E_d[\vec{w}] = -(t_d - o_d) o_d (1 - o_d) \vec{x}_d$

MLE vs MAP

- Maximum conditional likelihood estimate

$$\vec{w} = \arg\max_{\vec{w}} \ln \prod_i P(y_i | x_i; \vec{w})$$

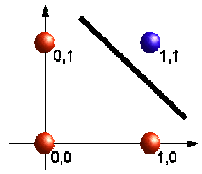
$$\boxed{\vec{w} \leftarrow \vec{w} + \eta \sum_d (t_d - o_d) o_d (1 - o_d) \vec{x}_d}$$

- Maximum a posteriori estimate

$$\vec{w} = \arg\max_{\vec{w}} \ln p(\vec{w}) \prod_i P(y_i | x_i; \vec{w})$$

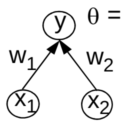
$$\boxed{\vec{w} \leftarrow \vec{w} + \eta (\sum_d (t_d - o_d) o_d (1 - o_d) \vec{x}_d - \lambda \vec{w})}$$

What decision surface does a perceptron define?



NAND

x	y	Z (color)
0	0	1
0	1	1
1	0	1
1	1	0



$\theta = 0.5$

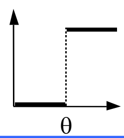
$f(x_1w_1 + x_2w_2) = y$

$f(0w_1 + 0w_2) = 1$

$f(0w_1 + 1w_2) = 1$

$f(1w_1 + 0w_2) = 1$

$f(1w_1 + 1w_2) = 0$

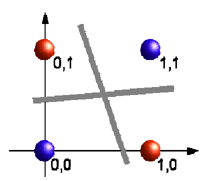


$$f(a) = \begin{cases} 1, \text{ for } a > \theta \\ 0, \text{ for } a \le \theta \end{cases}$$

some possible values for w_1 and w_2

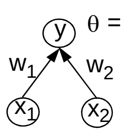
w_1	w_2
0.20	0.35
0.20	0.40
0.25	0.30
0.40	0.20

What decision surface does a perceptron define?



NAND

x	y	Z (color)
0	0	0
0	1	1
1	0	1
1	1	0



$\theta = 0.5$

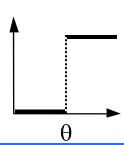
$f(x_1w_1 + x_2w_2) = y$

$f(0w_1 + 0w_2) = 0$

$f(0w_1 + 1w_2) = 1$

$f(1w_1 + 0w_2) = 1$

$f(1w_1 + 1w_2) = 0$

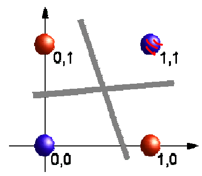


$$f(a) = \begin{cases} 1, \text{ for } a > \theta \\ 0, \text{ for } a \le \theta \end{cases}$$

some possible values for w_1 and w_2

w_1	w_2

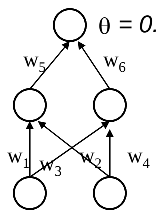
What decision surface does a perceptron define?

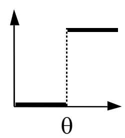


NAND

x	y	Z (color)
0	0	**0**
0	1	**1**
1	0	**1**
1	1	**0**

θ = 0.5 for all units





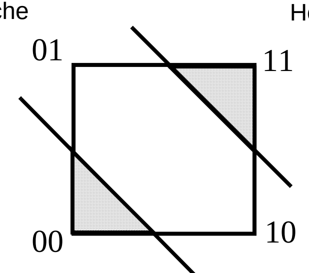
$$f(a) = \begin{cases} 1, \text{ for } a > \theta \\ 0, \text{ for } a \le \theta \end{cases}$$

a possible set of values for $(w_1, w_2, w_3, w_4, w_5, w_6)$:
$(0.6,-0.6,-0.7,0.8,1,1)$

Non Linear Separation

Meningitis
No cough
Headache

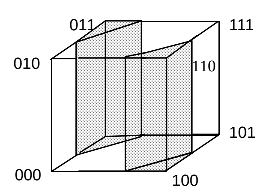
Flu
Cough
Headache



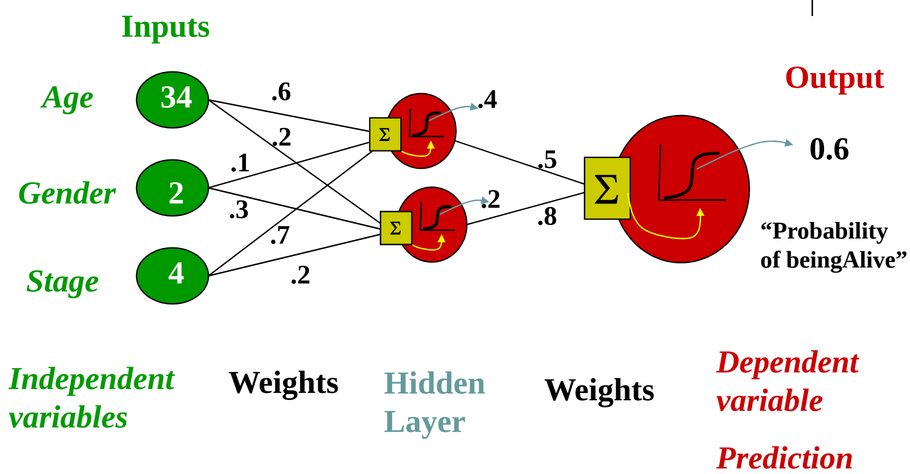
No treatment
Treatment

No disease
No cough
No headache

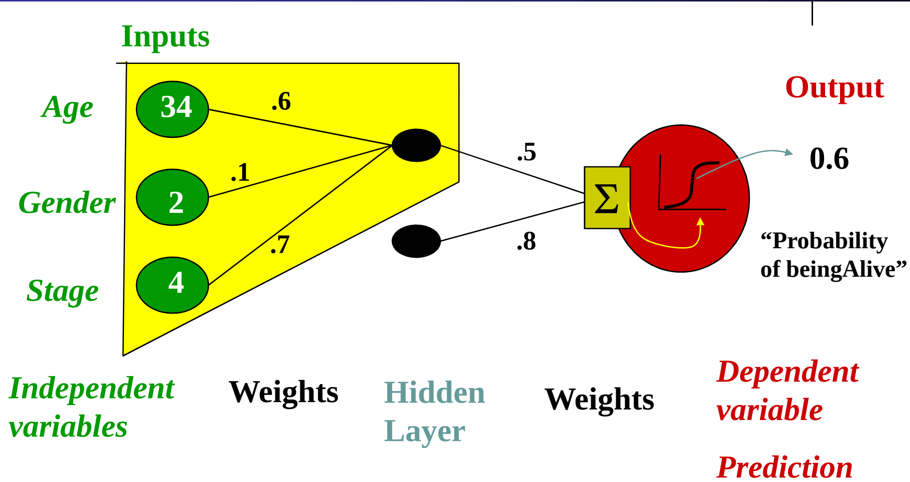
Pneumonia
Cough
No headache

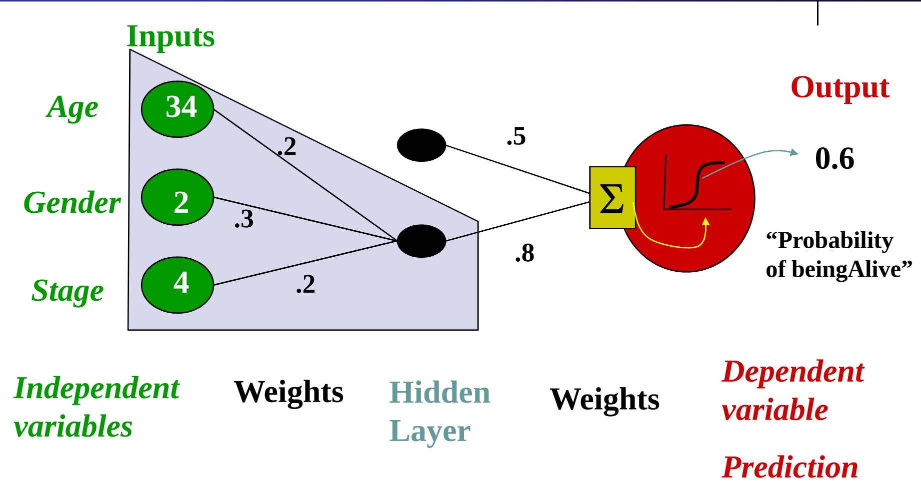


Neural Network Model

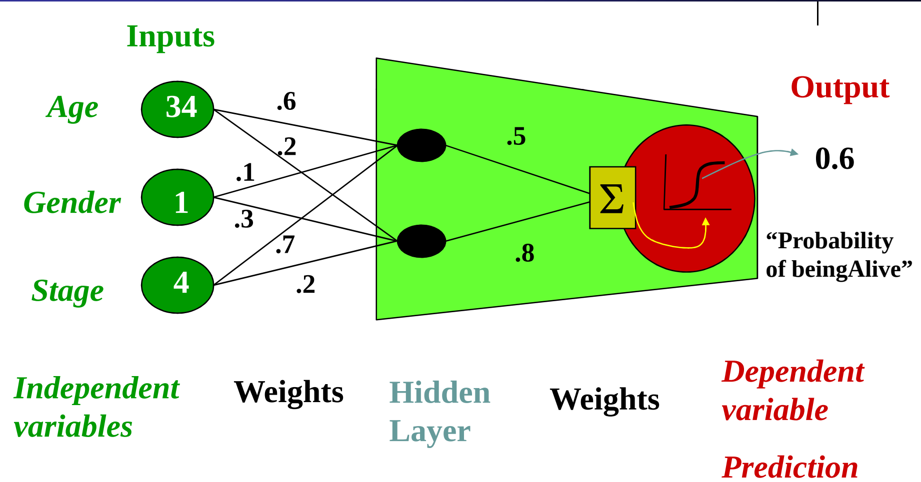


"Combined logistic models"



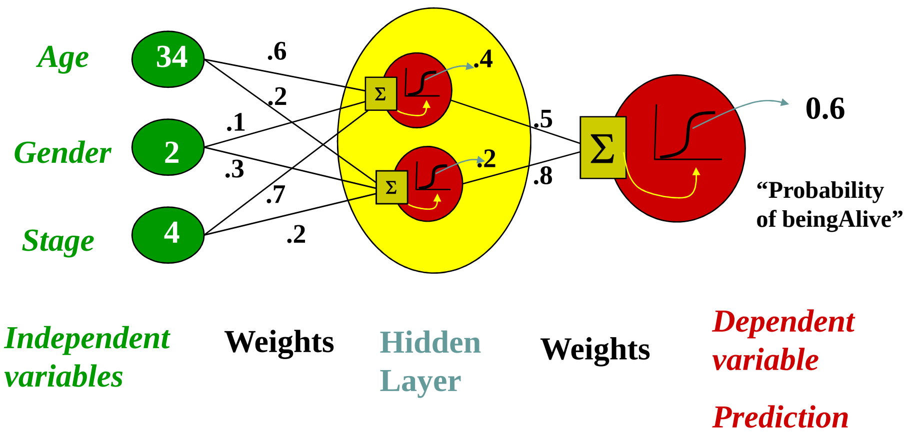


Inputs
Age
34
Gender
2
Stage
4
.2
.3
.2
.5
.8
Σ
Output
0.6
"Probability of beingAlive"
Independent variables
Weights
Hidden Layer
Weights
Dependent variable
Prediction



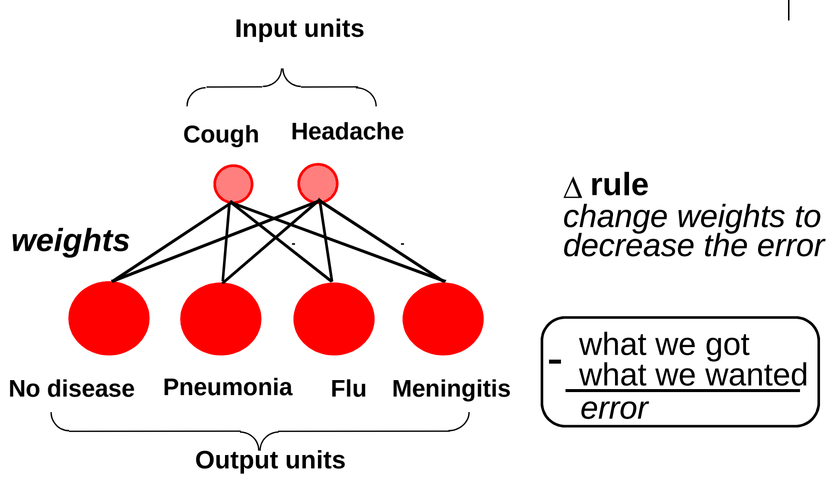
Inputs
Age
34
Gender
1
Stage
4
.6
.2
.1
.3
.7
.2
.5
.8
Σ
Output
0.6
"Probability of beingAlive"
Independent variables
Weights
Hidden Layer
Weights
Dependent variable
Prediction

Not really, no target for hidden units...

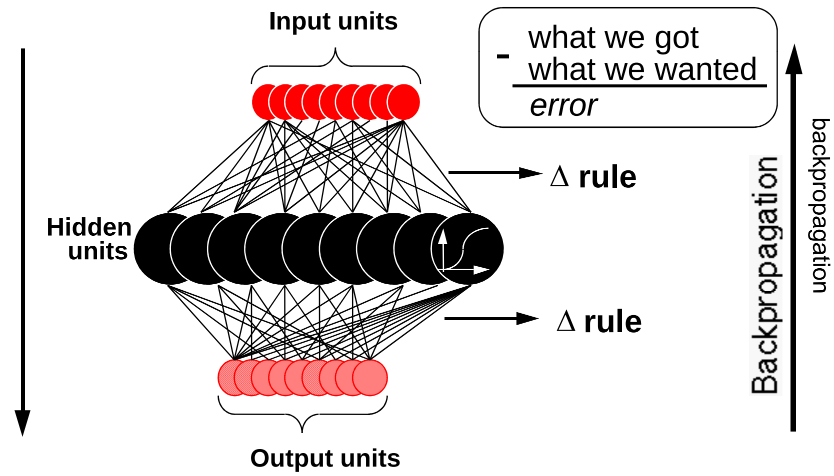


Recall perceptrons

$$\vec{w} \leftarrow \vec{w} + \eta \sum_d (t_d - o_d) o_d (1 - o_d) \vec{x}_d$$



Hidden Units and Backpropagation



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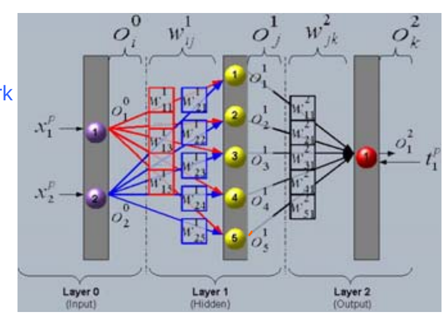
Backpropagation Algorithm

x_d = input
t_d = target output
o_d =observed unit output
w_i =weight i

- Initialize all weights to small random numbers
  Until convergence, Do



1. Input the training example to the network and compute the network outputs
1. For each output unit k

$$\delta_k \leftarrow o_k^2(1-o_k^2)(t-o_k^2)$$

2. For each hidden unit h

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

3. Undate each network weight $w_{i,j}$

$$w_{i,j} \leftarrow w_{i,j} + \Delta w_{i,j} \text{ where } \Delta w_{i,j} = \eta \delta_j x^j$$

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More on Backpropatation

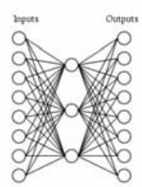
- It is doing gradient descent over entire network weight vector
- Easily generalized to arbitrary directed graphs
- Will find a local, not necessarily global error minimum
  - In practice, often works well (can run multiple times)
- Often include weight *momentum* α

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

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

Learning Hidden Layer Representation

- A network:



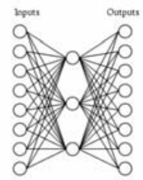
- A target function:

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 Representation

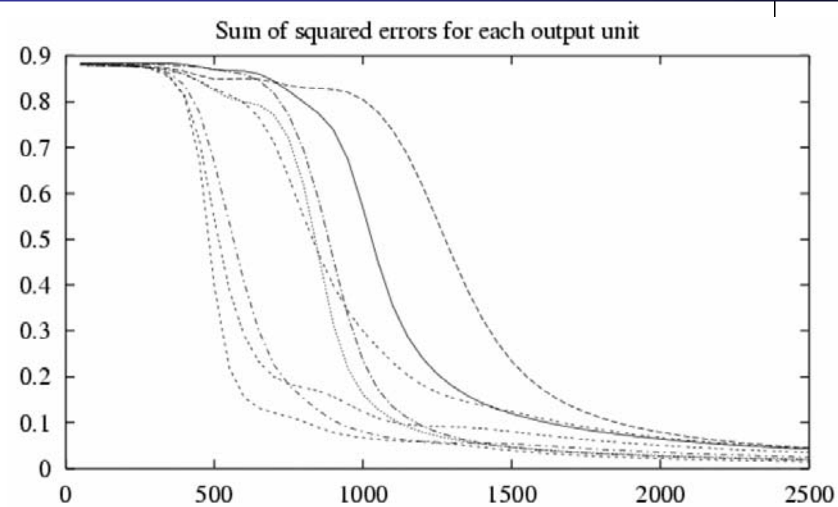
- A network:



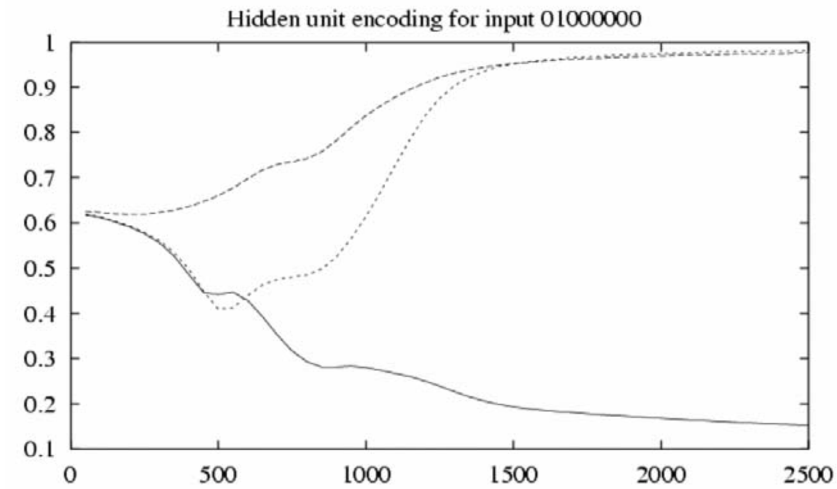
- Learned hidden layer representation:

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



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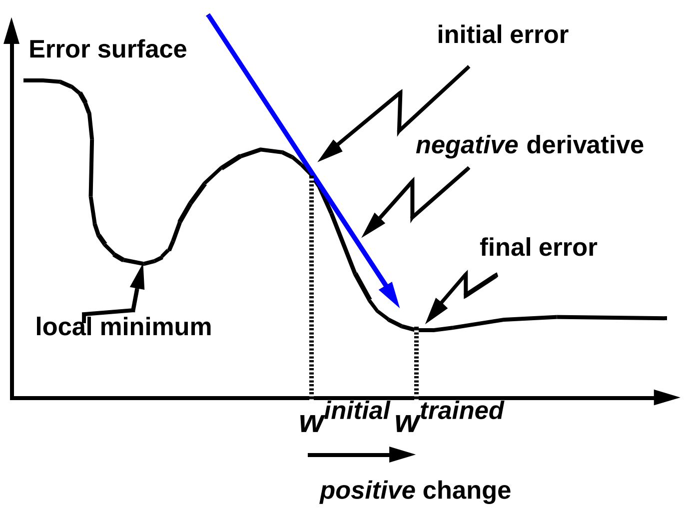
Minimizing the Error



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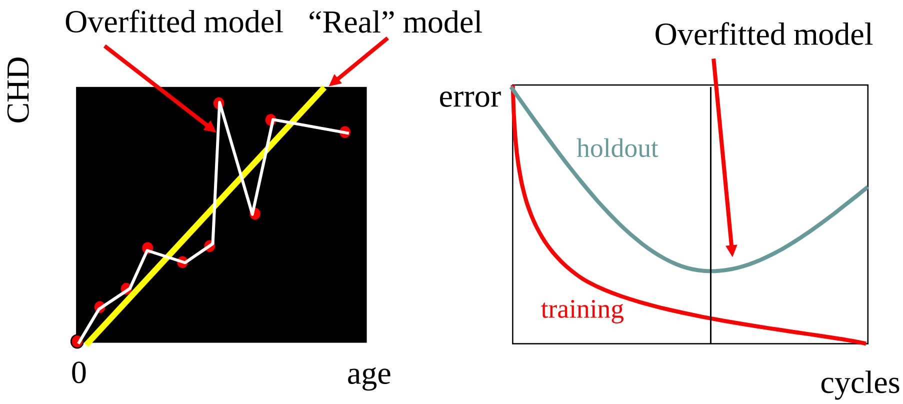
Overfitting in Neural Nets



Alternative Error Functions

- Penalize large weights:

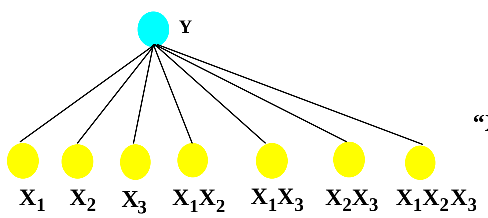
$$E[\vec{w}] \equiv \frac{1}{2} \sum_{d \in D} \sum_{k \in outputs} (t_{k,d} - o_{k,d})^2 + \gamma \sum_{i,j} w_{j,i}^2$$

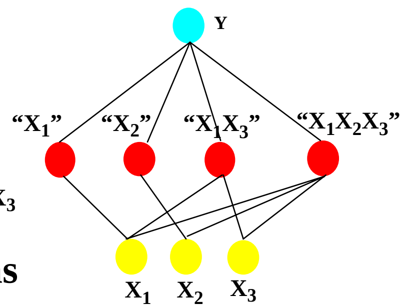
- Training on target slopes as well as values

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

- Tie together weights
  - E.g., in phoneme recognition

Regression vs. Neural Networks





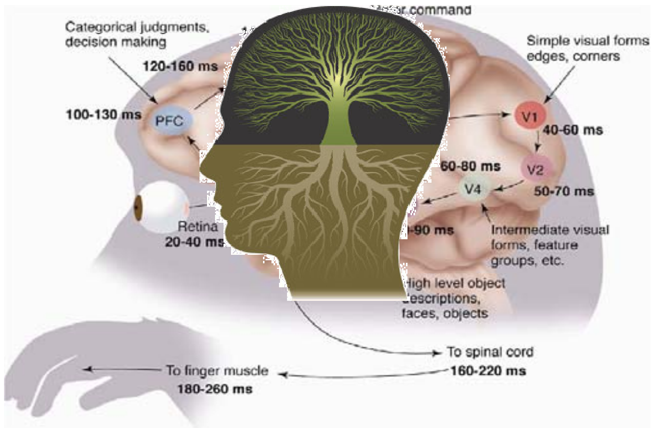
(2^3-1) possible combinations

$$Y = a(X_1) + b(X_2) + c(X_3) + d(X_1X_2) + ...$$

Artificial neural networks – what you should know

- Highly expressive non-linear functions
- Highly parallel network of logistic function units
- Minimizing sum of squared training errors
  - Gives MLE estimates of network weights if we assume zero mean Gaussian noise on output values
- Minimizing sum of sq errors plus weight squared (regularization)
  - MAP estimates assuming weight priors are zero mean Gaussian
- Gradient descent as training procedure
  - How to derive your own gradient descent procedure
- Discover useful representations at hidden units
- Local minima is greatest problem
- Overfitting, regularization, early stopping

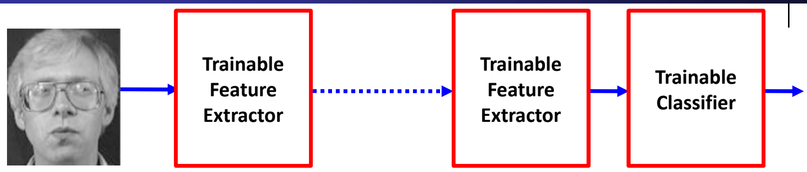
Modern ANN topics: "Deep" Learning



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 arbitrary 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].

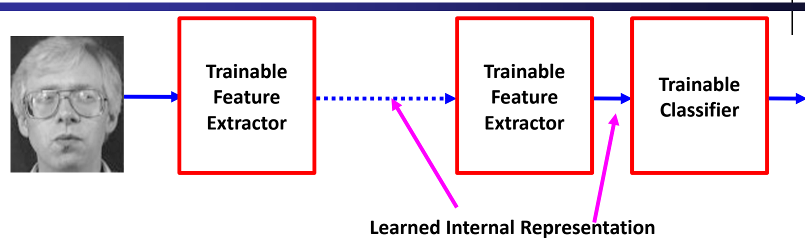
Using ANN to hierarchical representation



Good Representations are hierarchical

- In Language: hierarchy in syntax and semantics
  - Words->Parts of Speech->Sentences->Text
  - Objects,Actions,Attributes...-> Phrases -> Statements -> Stories
- In Vision: part-whole hierarchy
  - Pixels->Edges->Textons->Parts->Objects->Scenes

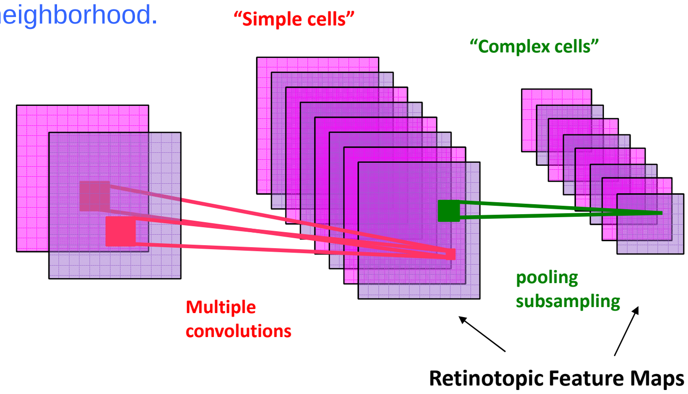
"Deep" learning: learning hierarchical representations



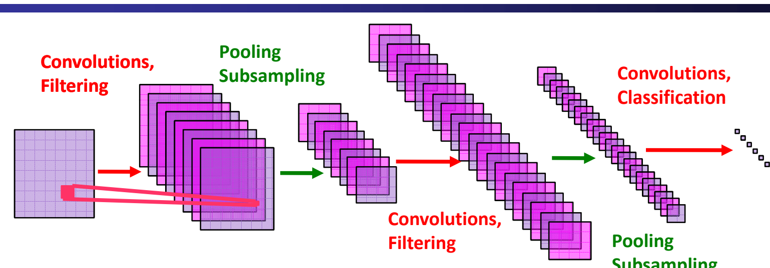
- Deep Learning: learning a hierarchy of internal representations
- From low-level features to mid-level invariant representations, to object identities
- Representations are increasingly invariant as we go up the layers
- using multiple stages gets around the specificity/invariance dilemma

Filtering+NonLinearity+Pooling = 1 stage of a Convolutional Net

- [Hubel & Wiesel 1962]:
  - simple cells detect local features
  - complex cells “pool” the outputs of simple cells within a retinotopic neighborhood.

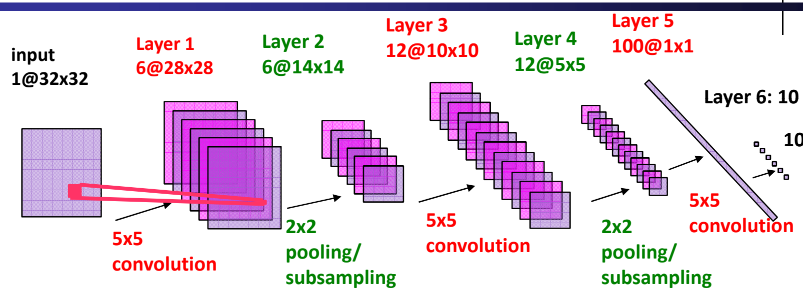


Convolutional Network: Multi-Stage Trainable Architecture



- **Hierarchical Architecture**
  - Representations are more global, more invariant, and more abstract as we go up the layers
- **Alternated Layers of Filtering and Spatial Pooling**
  - Filtering detects conjunctions of features
  - Pooling computes local disjunctions of features
- **Fully Trainable**
  - All the layers are trainable

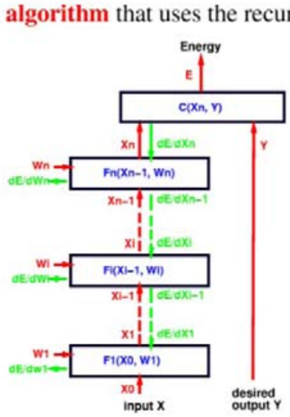
Convolutional Net Architecture for Hand-writing recognition



- Convolutional net for handwriting recognition (400,000 synapses)
  - Convolutional layers (simple cells): all units in a feature plane share the same weights
  - Pooling/subsampling layers (complex cells): for invariance to small distortions.
  - Supervised gradient-descent learning using back-propagation
  - The entire network is trained end-to-end. All the layers are trained simultaneously.
  - [LeCun et al. Proc IEEE, 1998]

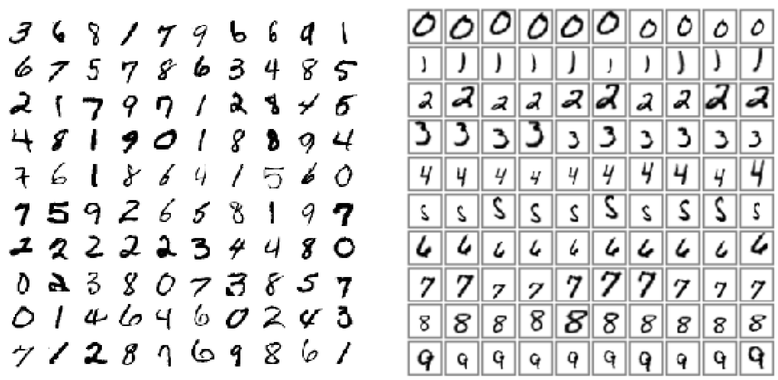
How to train?

To compute all the derivatives, we use a backward sweep called the **back-propagation algorithm** that uses the recurrence equation for $\frac{\partial E}{\partial X_i}$



- $\frac{\partial E}{\partial X_n} = \frac{\partial C(X_n, Y)}{\partial X_n}$
- $\frac{\partial E}{\partial X_{n-1}} = \frac{\partial E}{\partial X_n} \frac{\partial F_n(X_{n-1}, W_n)}{\partial X_{n-1}}$
- $\frac{\partial E}{\partial W_n} = \frac{\partial E}{\partial X_n} \frac{\partial F_n(X_{n-1}, W_n)}{\partial W_n}$
- $\frac{\partial E}{\partial X_{n-2}} = \frac{\partial E}{\partial X_{n-1}} \frac{\partial F_{n-1}(X_{n-2}, W_{n-1})}{\partial X_{n-2}}$
- $\frac{\partial E}{\partial W_{n-1}} = \frac{\partial E}{\partial X_{n-1}} \frac{\partial F_{n-1}(X_{n-2}, W_{n-1})}{\partial W_{n-1}}$
- ....etc, until we reach the first module.
- we now have all the $\frac{\partial E}{\partial W_i}$ for $i \in [1, n]$.

Application: MNIST Handwritten Digit Dataset



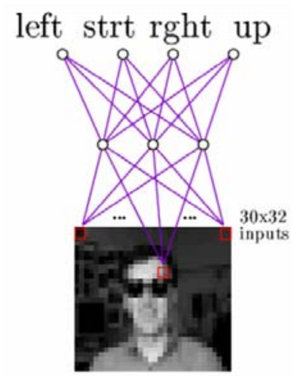
Handwritten Digit Dataset MNIST: 60,000 training samples, 10,000 test samples

Results on MNIST Handwritten Digits

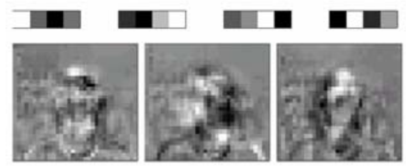
CLASSIFIER	DEFORMATION	PREPROCESSING	ERROR (%)	Reference
linear classifier (1-layer NN)		none	12.00	LeCun et al. 1998
linear classifier (1-layer NN)		deskewing	8.40	LeCun et al. 1998
pairwise linear classifier		deskewing	7.60	LeCun et al. 1998
K-nearest-neighbors, (L2)		none	3.09	Kenneth Wilder, U. Chicago
K-nearest-neighbors, (L2)		deskewing	2.40	LeCun et al. 1998
K-nearest-neighbors, (L2)		deskew, clean, blur	1.80	Kenneth Wilder, U. Chicago
K-NN L3, 2 pixel jitter		deskew, clean, blur	1.22	Kenneth Wilder, U. Chicago
K-NN, shape context matching		shape context feature	0.63	Belongie et al. IEEE PAMI 2002
40 PCA + quadratic classifier		none	3.30	LeCun et al. 1998
1000 RBF + linear classifier		none	3.60	LeCun et al. 1998
K-NN, Tangent Distance		subsamp 16x16 pixels	1.10	LeCun et al. 1998
SVM, Gaussian Kernel		none	1.40	
SVM deg 4 polynomial		deskewing	1.10	LeCun et al. 1998
Reduced Set SVM deg 5 poly		deskewing	1.00	LeCun et al. 1998
Virtual SVM deg-9 poly	Affine	none	0.80	LeCun et al. 1998
V-SVM, 2-pixel jittered		none	0.68	DeCoste and Scholkopf, MLJ2002
V-SVM, 2-pixel jittered		deskewing	0.56	DeCoste and Scholkopf, MLJ2002
2-layer NN, 300 HU, MSE		none	4.70	LeCun et al. 1998
2-layer NN, 300 HU, MSE,	Affine	none	3.60	LeCun et al. 1998
2-layer NN, 300 HU		deskewing	1.60	LeCun et al. 1998
3-layer NN, 500+ 150 HU		none	2.95	LeCun et al. 1998
3-layer NN, 500+ 150 HU	Affine	none	2.45	LeCun et al. 1998
3-layer NN, 500+ 300 HU, CE, reg		none	1.53	Hinton, unpublished, 2005
2-layer NN, 800 HU, CE		none	1.60	Simard et al., ICDAR 2003
2-layer NN, 800 HU, CE	Affine	none	1.10	Simard et al., ICDAR 2003
2-layer NN, 800 HU, MSE	Elastic	none	0.90	Simard et al., ICDAR 2003
2-layer NN, 800 HU, CE	Elastic	none	0.70	Simard et al., ICDAR 2003
Convolutional net LeNet-1		subsamp 16x16 pixels	1.70	LeCun et al. 1998
Convolutional net LeNet-4		none	1.10	LeCun et al. 1998
Convolutional net LeNet-5,		none	0.95	LeCun et al. 1998
Conv. net LeNet-5,	Affine	none	0.80	LeCun et al. 1998
Boosted LeNet-4	Affine	none	0.70	LeCun et al. 1998
Conv. net, CE	Affine	none	0.60	Simard et al., ICDAR 2003
Comv net, CE	Elastic	none	0.40	Simard et al., ICDAR 2003

Application: ANN for Face Reco.

- The model



- The learned hidden unit weights

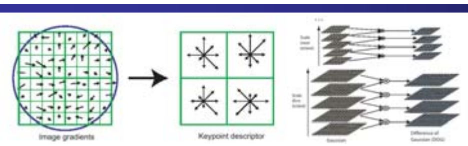


Typical input images

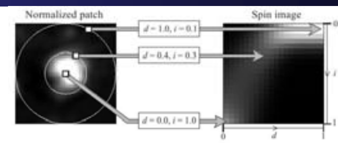
http://www.cs.cmu.edu/~tom/faces.html

Face Detection with a Convolutional Net

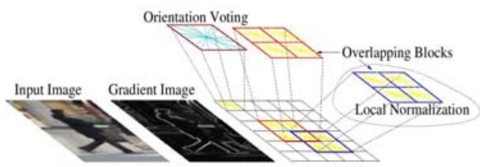
Computer vision features

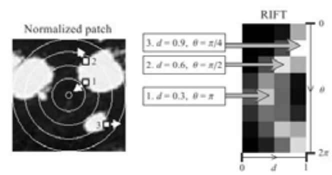


SIFT



Spin image





Drawbacks of feature engineering

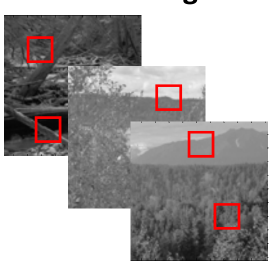
1. Needs expert knowledge
2. Time consuming hand-tuning

Textons GLOH

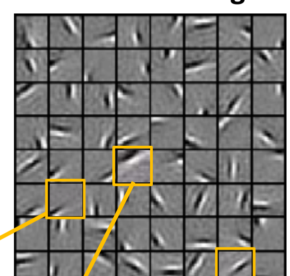
Courtesy: Lee and Ng

Sparse coding on images

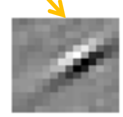
Natural Images



Learned bases: "Edges"



New example

 $= 0.8 *$  $+ 0.3 *$  $+ 0.5 *$ 

$$x = 0.8 * b_{36} + 0.3 * b_{42} + 0.5 * b_{65}$$

[0, 0, … 0.8, …, 0.3, …, 0.5, …] = coefficients (feature representation)

Courtesy: Lee and Ng

Basis (or features) can be learned by Optimization

Given input data $\{x^{(1)}, \ldots, x^{(m)}\}$, we want to find good bases $\{b_1, \ldots, b_n\}$:

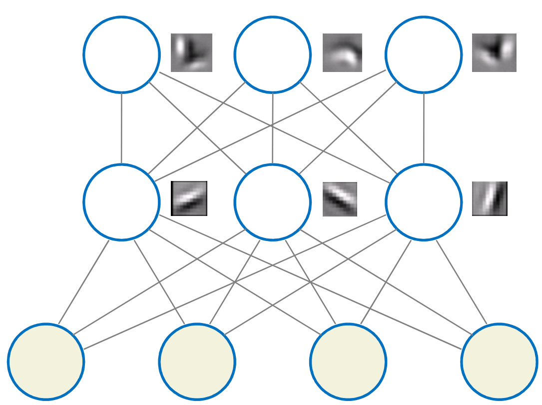
$$\min_{b,a} \sum_i \underbrace{\| x^{(i)} - \sum_j a_j^{(i)} b_j \|_2^2}_{\text{Reconstruction error}} + \beta \underbrace{\sum_i \| a^{(i)} \|_1}_{\text{Sparsity penalty}}$$

$$\forall j: \; \| b_j \| \le 1$$ Normalization constraint

Solve by alternating minimization:
-- Keep *b* fixed, find optimal *a*.
-- Keep *a* fixed, find optimal *b*.

Courtesy: Lee and Ng

Learning Feature Hierarchy



Higher layer (Combinations of edges)

"Sparse coding" (edges)

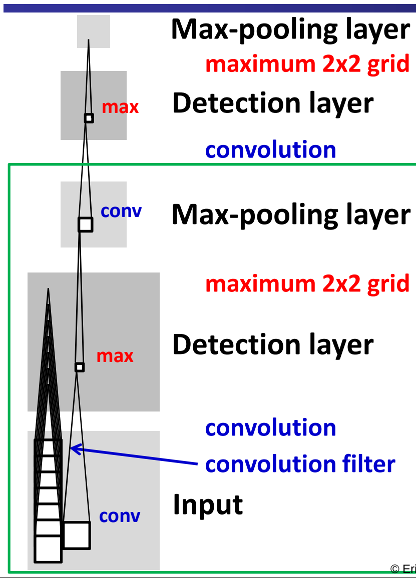
Input image (pixels)

DBN (Hinton et al., 2006) with additional sparseness constraint.

[Related work: Hinton, Bengio, LeCun, and others.]

Courtesy: Lee and Ng

Convolutional architectures



- **Weight sharing by convolution (e.g., [Lecun et al., 1989])**
- **"Max-pooling"**
  Invariance
  Computational efficiency
  Deterministic and feed-forward
- **One can develop convolutional Restricted Boltzmann machine (CRBM).**
- **One can define *probabilistic max-pooling* that *combine bottom-up and top-down information*.**

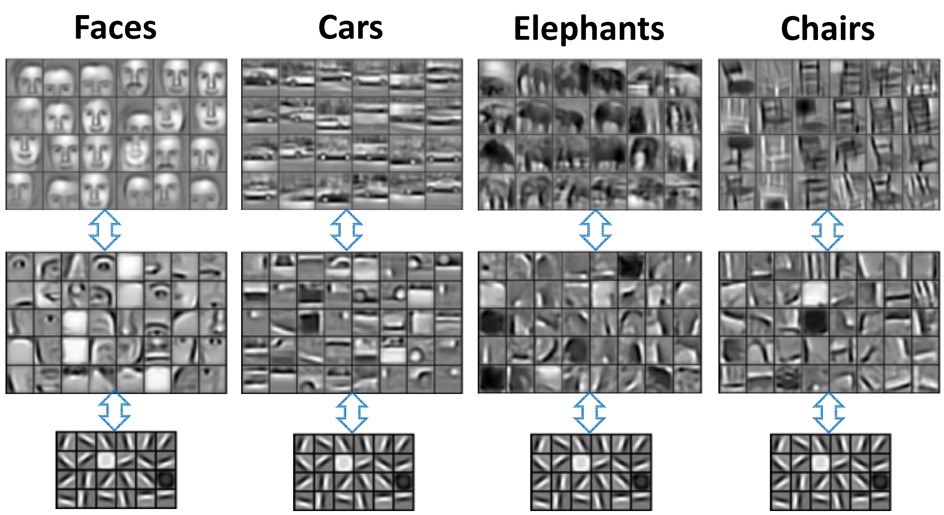
Courtesy: Lee and Ng

Convolutional Deep Belief Networks

- Bottom-up (greedy), layer-wise training
  - Train one layer (convolutional RBM) at a time.
- Inference (approximate)
  - Undirected connections for all layers (Markov net)
    [Related work: Salakhutdinov and Hinton, 2009]
  - Block Gibbs sampling or mean-field
  - Hierarchical probabilistic inference

Courtesy: Lee and Ng

Unsupervised learning of object-parts



Courtesy: Lee and Ng

Weaknesses & Criticisms

- Learning everything. Better to encode prior knowledge about structure of images.

  A: Compare with machine learning vs. linguists debate in NLP.

- Results not yet competitive with best engineered systems.

  A: Agreed. True for some domains.

Courtesy: Lee and Ng