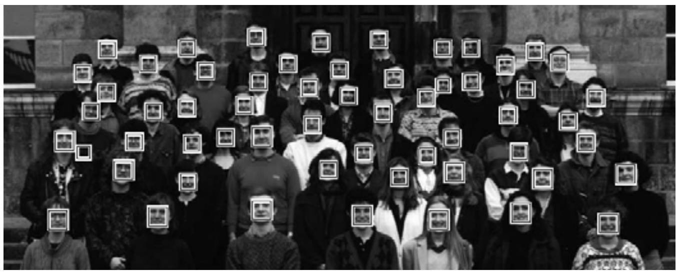
CSEP 573

Machine Learning I: Supervised Learning



(Rowley, Baluja & Kanade, 1998)

What's on our menu today?

Supervised Learning

- Classification
  - Decision trees
  - Cross validation
  - K-nearest neighbor
  - Neural networks
    - + Perceptrons
  - Support Vector Machines (SVMs)
- Regression
  - Backpropagation networks

Why Learning?

Learning is essential for unknown environments
- e.g., when designer lacks omniscience

Learning is necessary in dynamic environments
- Agent can adapt to changes in environment not foreseen at design time

Learning is useful as a system construction method
- Expose the agent to reality rather than trying to approximate it through equations etc.

Learning modifies the agent's decision mechanisms to improve performance

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Types of Learning

Supervised learning: correct answers for each input is provided
- E.g., decision trees, backpropagation neural networks

Unsupervised learning: correct answers not given, must discover patterns in input data
- E.g., clustering, principal component analysis

Reinforcement learning: occasional rewards (or punishments) given to guide behavior

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Inductive learning

We will focus on one form of supervised learning called Inductive Learning:

Learn a function from examples

f is the target function. Examples are pairs (x, $f(x)$)

Problem: learn a function ("hypothesis") *h*

such that $h \approx f$ (*h* approximates *f* as best as possible)

given a training set of examples

(This is a highly simplified model of real learning:

- Ignores prior knowledge
- Assumes examples are given)

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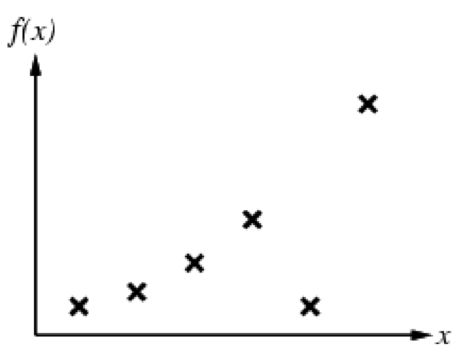
Inductive learning example

Construct *h* to agree with *f* on training set

- *h* is consistent if it agrees with *f* on all training examples

E.g., curve fitting (regression):



× = Input data point (training example)

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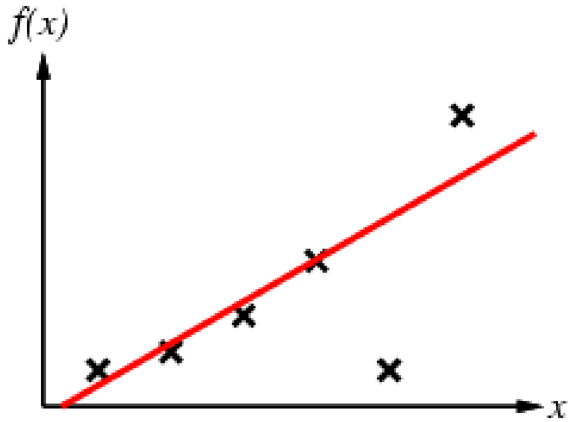
Inductive learning example

h = Straight line?



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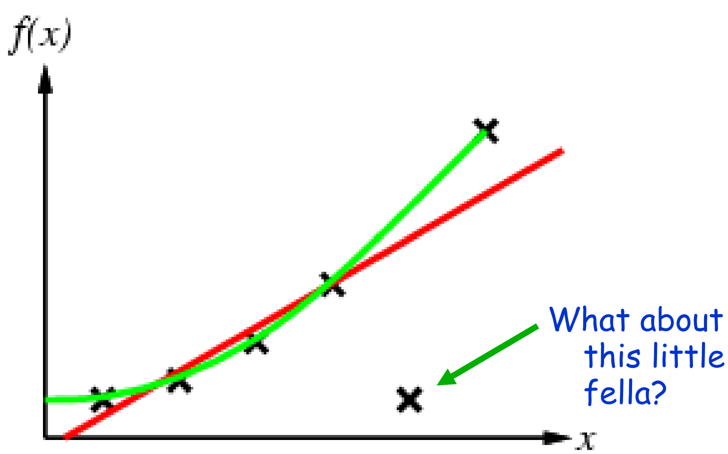
Inductive learning example

What about a quadratic function?



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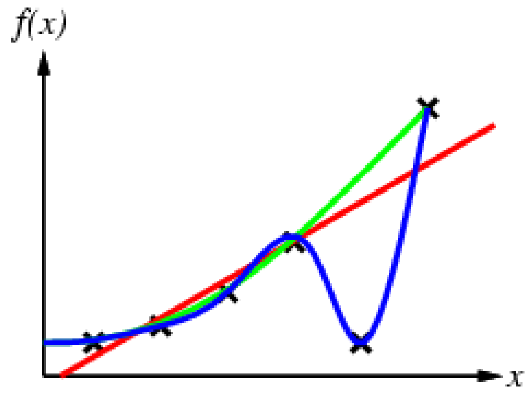
Inductive learning example

Finally, a function that satisfies all!



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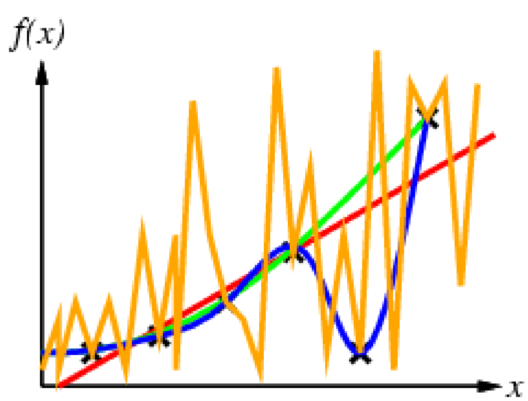
Inductive learning example

But so does this one…



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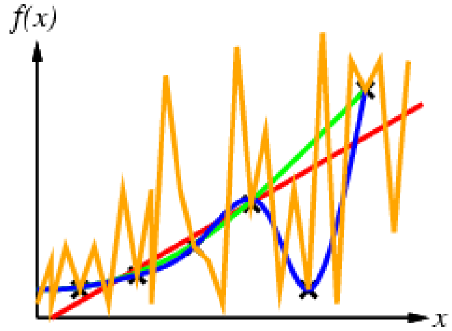
Ockham's Razor Principle



Ockham's razor: prefer the simplest hypothesis consistent with data

- Related to KISS principle ("keep it simple stupid")
- Smooth blue function preferable over wiggly yellow one
- If noise known to exist in this data, even linear might be better (the lowest x might be due to noise)

Supervised Learning Technique I: Decision Trees

http://www.sfgate.com/blogs/images/sfgate/sgreen/2007/09/05/2240773250x321.jpg

Example data for learning the concept "Good day for tennis"

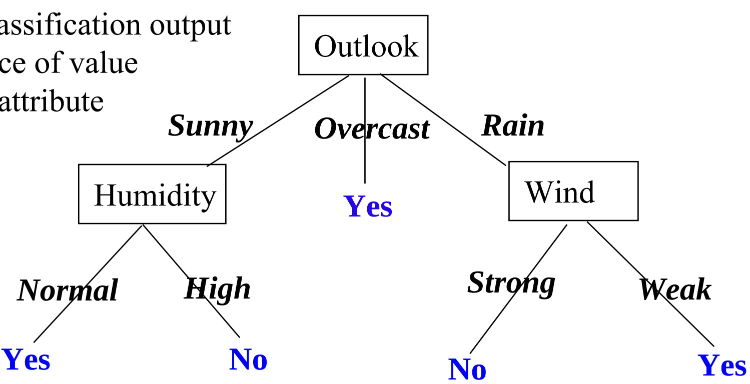
Day	Outlook	Humid	Wind	PlayTennis?
d1	s	h	w	n
d2	s	h	s	n
d3	o	h	w	y
d4	r	h	w	y
d5	r	n	w	y
d6	r	n	s	y
d7	o	n	s	y
d8	s	h	w	n
d9	s	n	w	y
d10	r	n	w	y
d11	s	n	s	y
d12	o	h	s	y
d13	o	n	w	y
d14	r	h	s	n

- Outlook = sunny, overcast, rain
- Humidity = high, normal
- Wind = weak, strong

A Decision Tree for the Same Data

Decision Tree for "PlayTennis?"

Leaves = classification output
Arcs = choice of value
for parent attribute



Decision tree is equivalent to logic in disjunctive normal form
PlayTennis $\Leftrightarrow$ (Sunny $\wedge$ Normal) $\vee$ Overcast $\vee$ (Rain $\wedge$ Weak)

Decision Trees

Input: Description of an object or a situation through a set of **attributes**

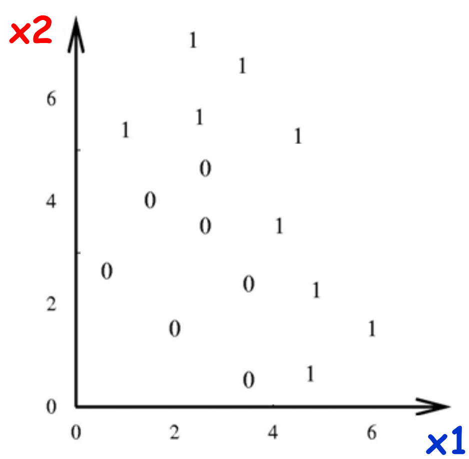
Output: a **decision** that is the predicted output value for the input

Both **input and output can be discrete or continuous**

Discrete-valued functions lead to **classification problems**

Example: Decision Tree for Continuous Valued Features and Discrete Output

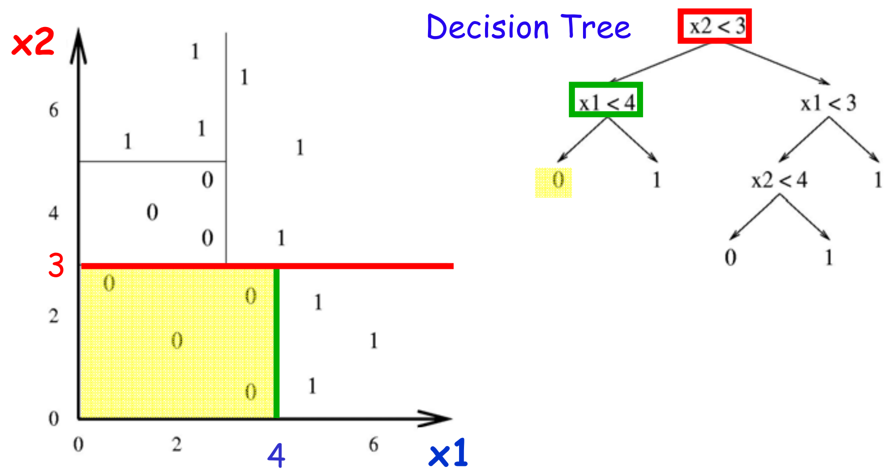
Input real number attributes (x1,x2), Classification output: 0 or 1



How do we branch using attribute values x1 and x2 to partition the space correctly?

Example: Classification of Continuous Valued Inputs

Decision trees divide the feature space into axis-parallel rectangles, and label each rectangle with one of the K classes.



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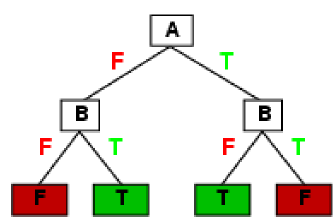
Expressiveness of Decision Trees

Decision trees can express any function of the input attributes.

E.g., for Boolean functions, truth table row = path to leaf:

A	B	A xor B
F	F	F
F	T	T
T	F	T
T	T	F



Trivially, there is a consistent decision tree for any training set with one path to leaf for each example

- But most likely won't generalize to new examples

Prefer to find more compact decision trees

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Learning Decision Trees

Example: When should I wait for a table at a restaurant?

Attributes (features) relevant to *Wait?* decision:

1. Alternate: is there an alternative restaurant nearby?
2. Bar: is there a comfortable bar area to wait in?
3. Fri/Sat: is today Friday or Saturday?
4. Hungry: are we hungry?
5. Patrons: number of people in the restaurant (None, Some, Full)
6. Price: price range ($, $$, $$$)
7. Raining: is it raining outside?
8. Reservation: have we made a reservation?
9. Type: kind of restaurant (French, Italian, Thai, Burger)
10. WaitEstimate: estimated waiting time (0-10, 10-30, 30-60, >60)

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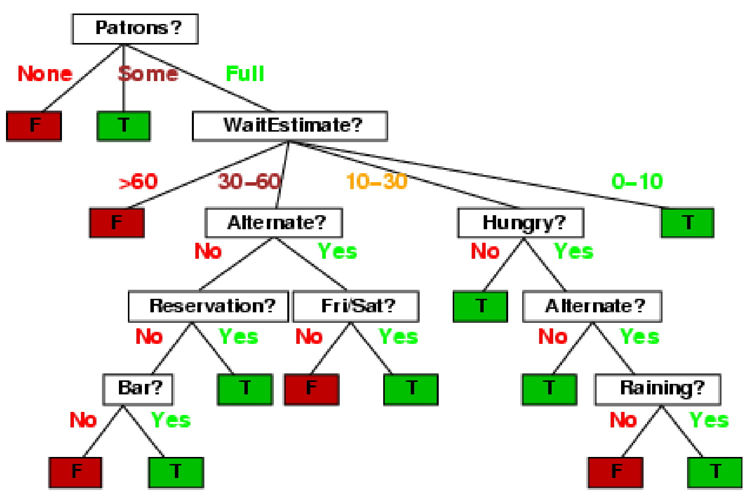
Example Decision tree

A decision tree for *Wait?* based on personal "rules of thumb":



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Input Data for Learning

Past examples when I did/did not wait for a table:

Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*Wait*
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

Classification of examples is positive (T) or negative (F)

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Decision Tree Learning

Aim: find a small tree consistent with training examples

Idea: (recursively) choose "most significant" attribute as root of (sub)tree

function DTL(*examples*, *attributes*, *default*) **returns** a decision tree
  if *examples* is empty **then return** *default*
  else if all *examples* have the same classification **then return** the classification
  else if *attributes* is empty **then return** MODE(*examples*)
  else
    $\boxed{best \leftarrow \text{CHOOSE-ATTRIBUTE}(attributes, examples)}$
    tree ← a new decision tree with root test *best*
    for each value v_i of *best* **do**
      $examples_i \leftarrow$ {elements of *examples* with $best = v_i$}
      $\boxed{subtree \leftarrow \text{DTL}(examples_i, attributes - best, \text{MODE}(examples))}$
      add a branch to *tree* with label v_i and subtree *subtree*
    return *tree*

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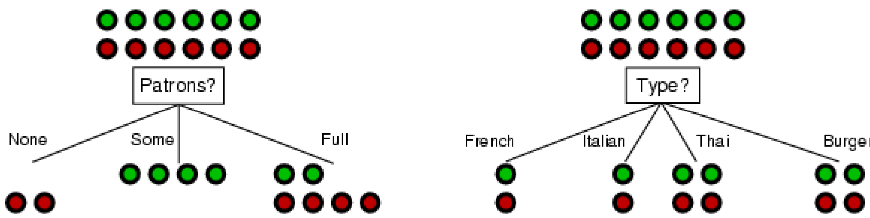
Choosing an attribute to split on

Idea: a good attribute should reduce uncertainty

- E.g., splits the examples into subsets that are (ideally) "all positive" or "all negative"



Patrons? is a better choice

For *Type?*, to wait or not to wait is still at 50%

How do we quantify uncertainty?

http://a.espncdn.com/media/ten/2006/0306/photo/g_mcenroe_195.jpg

Using information theory to quantify uncertainty

Entropy measures the amount of uncertainty in a probability distribution

Entropy (or Information Content) of an answer to a question with possible answers $v_1, \ldots, v_n$:

$$I(P(v_1), \ldots, P(v_n)) = \Sigma_{i=1} -P(v_i) \log_2 P(v_i)$$

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Using information theory

Imagine we have p examples with Wait = True (positive) and n examples with Wait = false (negative).

Our best estimate of the probabilities of Wait = true or false is given by:

$$P(true) \approx p / p + n$$
$$p(false) \approx n / p + n$$

Hence the entropy of Wait is given by:

$$I(\frac{p}{p+n}, \frac{n}{p+n}) = -\frac{p}{p+n} \log_2 \frac{p}{p+n} - \frac{n}{p+n} \log_2 \frac{n}{p+n}$$

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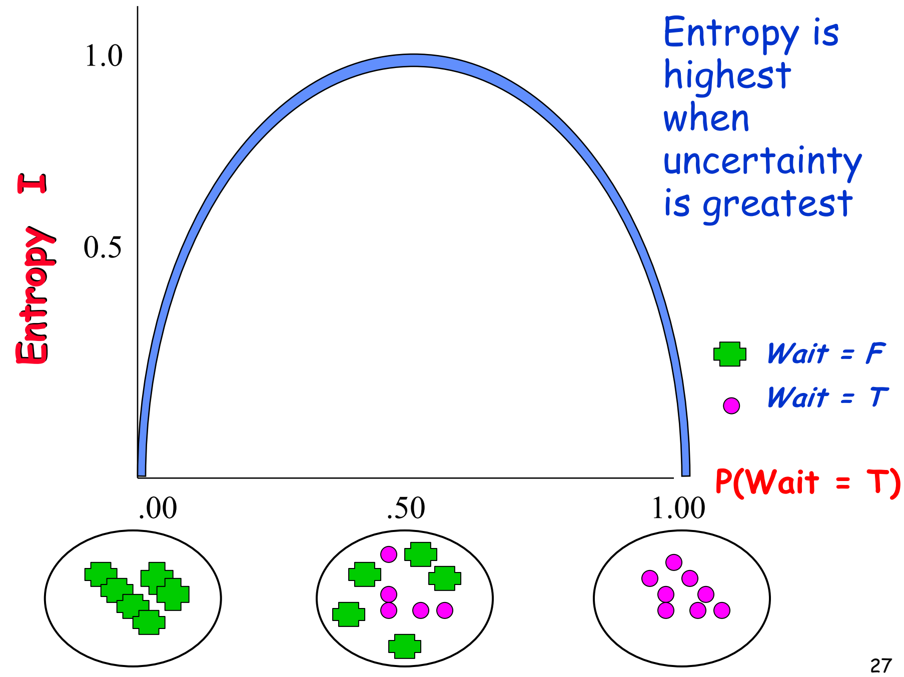

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Choosing an attribute to split on

Idea: a good attribute should reduce uncertainty and result in "gain in information"

How much information do we gain if we disclose the value of some attribute?

Answer:

uncertainty before – uncertainty after

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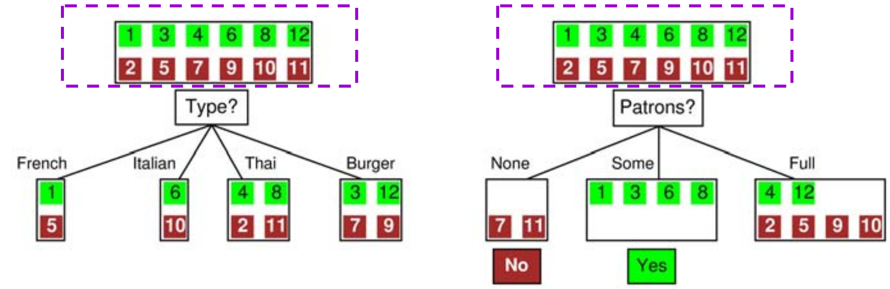
Back at the Restaurant



Before choosing an attribute:

Entropy = - 6/12 log(6/12) – 6/12 log(6/12)

= - log(1/2) = log(2) = 1 bit

There is “1 bit of information to be discovered”

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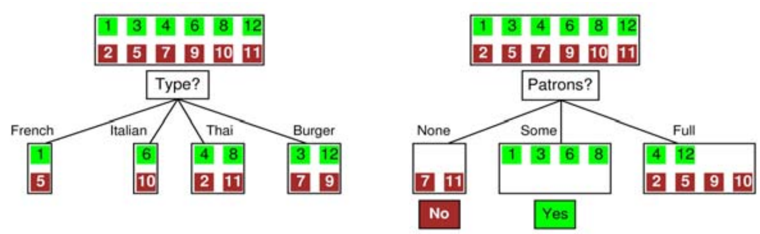
Back at the Restaurant



If we choose Type: Go along branch “French”: we have entropy = 1 bit; similarly for the others.

Information gain = 1-1 = 0 along any branch

If we choose Patrons:

In branch “None” and “Some”, entropy = 0

For “Full”, entropy = -2/6 log(2/6)-4/6 log(4/6) = 0.92

Info gain = (1-0) or (1-0.92) bits > 0 in both cases

So choosing Patrons gains more information!

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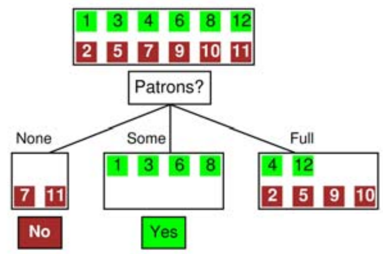
Entropy across branches

- How do we combine entropy of different branches?
- Answer: Compute average entropy
- Weight entropies according to probabilities of branches

  2/12 times we enter "None", so weight for "None" = 1/6

  "Some" has weight: 4/12 = 1/3

  "Full" has weight 6/12 = ½



$$AvgEntropy = \sum_{i=1}^{n} \frac{p_i + n_i}{p+n} Entropy\left(\frac{p_i}{p_i + n_i}, \frac{n_i}{p_i + n_i}\right)$$

weight for each branch

entropy for each branch

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Information gain

Information Gain (IG) or reduction in entropy from using attribute A:

IG(A) = Entropy before – AvgEntropy after choosing A

Choose the attribute with the largest IG

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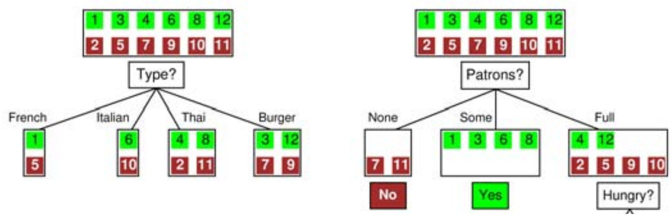
Information gain in our example



$$IG(Patrons) = 1 - [\frac{2}{12} I(0,1) + \frac{4}{12} I(1,0) + \frac{6}{12} I(\frac{2}{6}, \frac{4}{6})] = .541 \text{ bits}$$

$$IG(Type) = 1 - [\frac{2}{12} I(\frac{1}{2}, \frac{1}{2}) + \frac{2}{12} I(\frac{1}{2}, \frac{1}{2}) + \frac{4}{12} I(\frac{2}{4}, \frac{2}{4}) + \frac{4}{12} I(\frac{2}{4}, \frac{2}{4})] = 0 \text{ bits}$$

Patrons has the highest IG of all attributes

$\Rightarrow$ DTL algorithm chooses *Patrons* as the root

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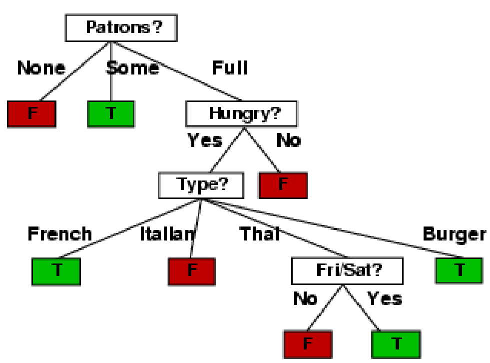
Should I stay or should I go? Learned Decision Tree

Decision tree learned from the 12 examples:



Substantially simpler than "rules-of-thumb" tree

- more complex hypothesis not justified by small amount of data

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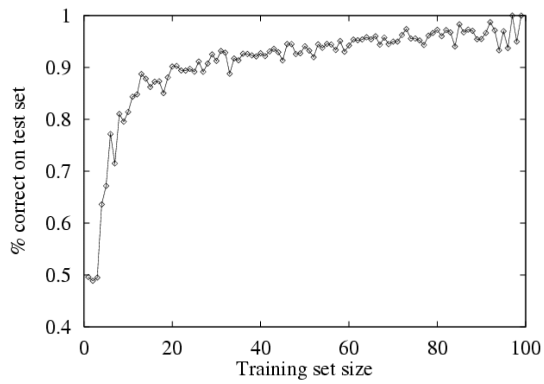
Performance Evaluation

How do we know that the learned tree $h \approx f$?

Answer: Try h on a new test set of examples

Learning curve = % correct on test set as a function of training set size



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Generalization

How do we know the classifier function we have learned is good?

- Look at generalization error on test data
  - Method 1: Split data in training vs test set (the "hold out" method)
  - Method 2: Cross-Validation

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Cross-validation

K-fold cross-validation:

- Divide data into k subsets of equal size
- Train learning algorithm K times, leaving out one of the subsets. Compute error on left-out subset
- Report average error over all subsets

Leave-1-out cross-validation:

- Train on all but 1 data point, test on that data point; repeat for each point
- Report average error over all points

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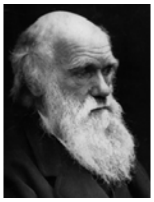
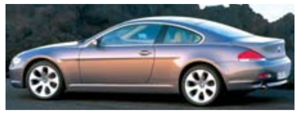
Decision trees are for girlie men – let's move on to more powerful learning algorithms

http://www.ipjnet.com/schwarzenegger2/pages/arnold_01.htm

Example Problem: Face Detection

How do we build a classifier to distinguish between faces and other objects?









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Images as Vectors

Binary handwritten characters

```
00000000010000000000
00000000110000000000
00000000101000000000
00000001000010000000
00000010000010000000
00000100000001000000
00001000000000100000
00001100111111110000
00001111111000001000
00011000000000011000
00010000000000001100
00110000000000000100
00110000000000000110
00100000000000000010
00100000000000000010
01100000000000000010
01000000000000000000
00000000000000000000
```

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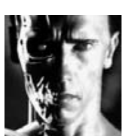
00000000011110000000
00000001100001100000
00000011000000110000
00001100000000011000
00001000000000001000
00001100000000010000
00000111000000100000
00000011100111100000
00000000111100000000
00000011000111000000
00001100000000110000
00011000000000011000
00110000000000001000
00100000000000001100
00010000000000011000
00011000000000010000
00001000000000110000
00000011111110000000
```

Greyscale images



62	79	23	119	120	105	4	0
10	10	9	62	12	78	34	0
10	58	197	46	46	0	0	48
176	135	5	188	191	68	0	49
2	1	1	29	26	37	0	77
0	89	144	147	187	102	62	208
255	252	0	166	123	62	0	31
166	63	127	17	1	0	99	30

.....

⋮

Treat an image as a high-dimensional vector
(e.g., by reading pixel values left to right, top to bottom row)

$$\mathbf{I} = \begin{bmatrix} p_1 \\ p_2 \\ \vdots \\ p_{N-2} \\ p_N \end{bmatrix}$$

Pixel value p_i can be 0 or 1 (binary image) or 0 to 255 (greyscale)

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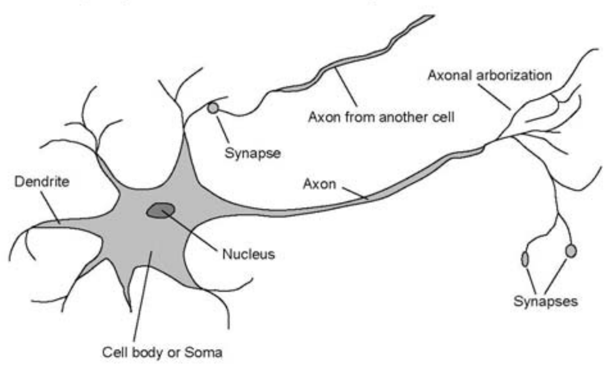
The human brain is extremely good at classifying images

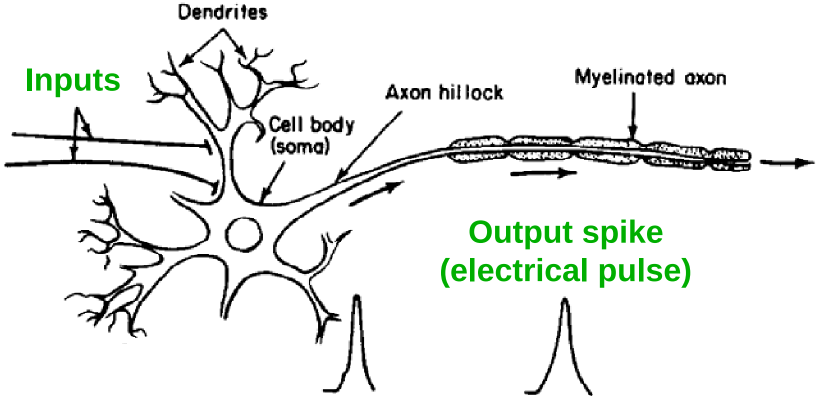
Can we develop classification methods by emulating the brain?

Brains

10^{11} neurons of > 20 types, 10^{14} synapses, 1ms–10ms cycle time
Signals are noisy "spike trains" of electrical potential



Neurons communicate via spikes



Output spike roughly dependent on whether sum of all inputs reaches a threshold

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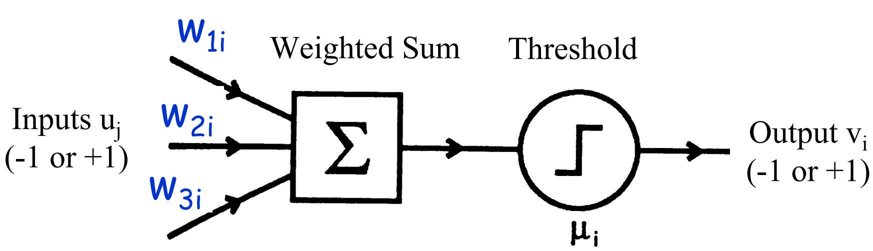
Neurons as "Threshold Units"

Artificial neuron:

- **m binary inputs (-1 or 1), 1 output (-1 or 1)**
- **Synaptic weights w_{ji}**
- **Threshold μ_i**



$$v_i = \Theta(\sum_j w_{ji} u_j - \mu_i)$$

$\Theta(x) = 1$ if $x > 0$ and -1 if $x \leq 0$

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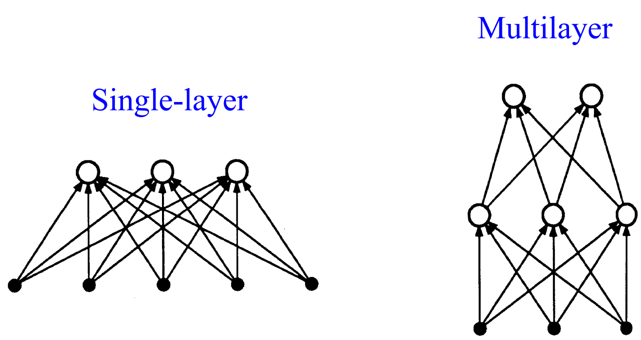
"Perceptrons" for Classification

Fancy name for a type of layered "feed-forward" networks (no loops)

Uses artificial neurons ("units") with binary inputs and outputs



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Perceptrons and Classification

Consider a single-layer perceptron

- Weighted sum forms a *linear hyperplane*

$$\sum_j w_{ji} u_j - \mu_i = 0$$

- Everything *on one side* of this hyperplane is in class 1 (output = +1) and everything *on other side* is class 2 (output = -1)

Any function that is linearly separable can be computed by a perceptron

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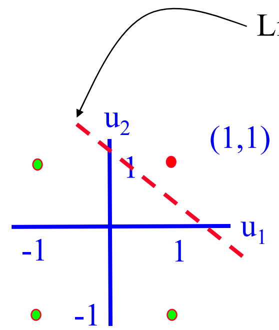
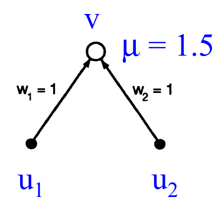
Linear Separability

Example: AND is linearly separable

u_1	u_2	AND
-1	-1	-1
1	-1	-1
-1	1	-1
1	1	1





$v = 1$ iff $u_1 + u_2 - 1.5 > 0$

Similarly for OR and NOT

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How do we *learn* the appropriate weights given only examples of (input,output)?

Idea: Change the weights to decrease the error in ouput

Perceptron Learning Rule

Given input pair (u, v^d) where $v^d \in \{+1,-1\}$ is the desired output, adjust w and μ as follows:

1. Calculate current output v of neuron

$$v = \Theta(\sum_j w_j u_j - \mu) = \Theta(\mathbf{w}^T \mathbf{u} - \mu)$$

2. Compute error signal $e = (v^d - v)$

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Perceptron Learning Rule

3. Change w and μ according to error $(v^d - v)$:

If input is positive and error is positive, then w not large enough $\Rightarrow$ increase w

If input is positive and error is negative, then w too large $\Rightarrow$ decrease w

Similar reasoning for other cases yields:

$$\mathbf{w} \to \mathbf{w} + \alpha(v^d - v)\mathbf{u}$$

$$\mu \to \mu - \alpha(v^d - v)$$

$A \to B$ means replace A with B

α is the "learning rate" (a small positive number, e.g., 0.05)

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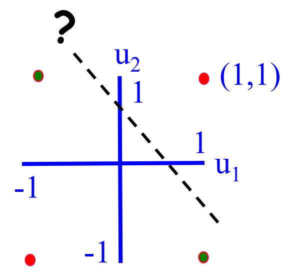
What about the XOR function?

u_1	u_2	XOR
-1	-1	1
1	-1	-1
-1	1	-1
1	1	1



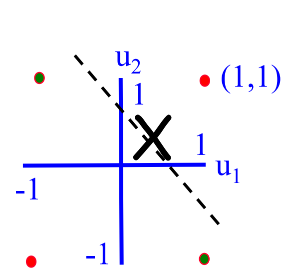
Can a perceptron separate the +1 outputs from the -1 outputs?

Linear Inseparability

Perceptron with threshold units fails if classification task is not linearly separable

- **Example: XOR**
- **No single line can separate the "yes" (+1) outputs from the "no" (-1) outputs!**

Minsky and Papert's book showing such negative results put a damper on neural networks research for over a decade!



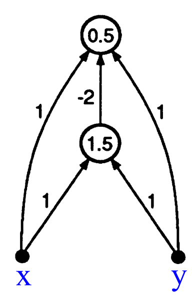
How do we deal with linear inseparability?

Idea 1: Multilayer Perceptrons

Removes limitations of single-layer networks

- Can solve XOR

Example: Two-layer perceptron that computes XOR



Output is +1 if and only if $x + y - 2\Theta(x + y - 1.5) - 0.5 > 0$

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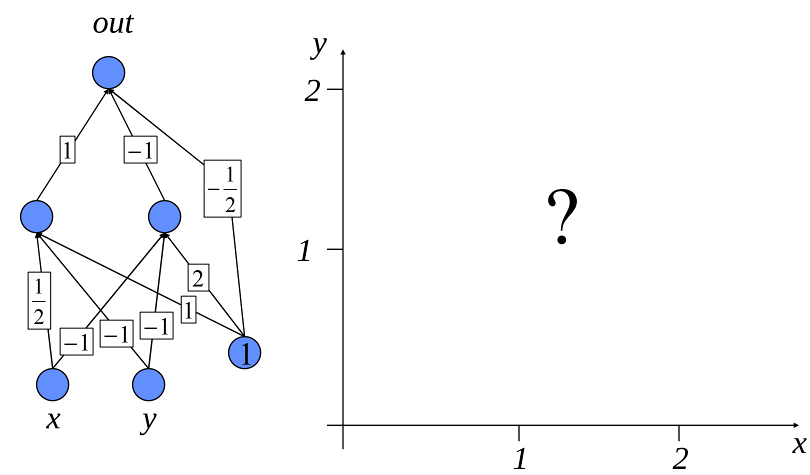
Multilayer Perceptron: What does it do?



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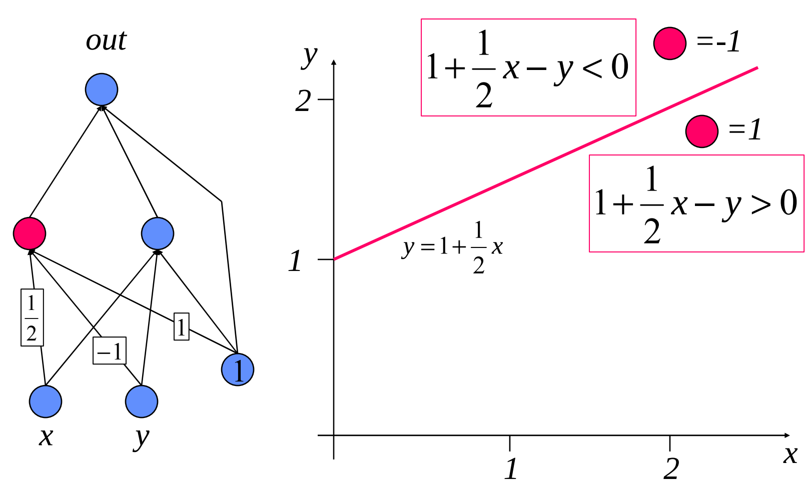
Multilayer Perceptron: What does it do?



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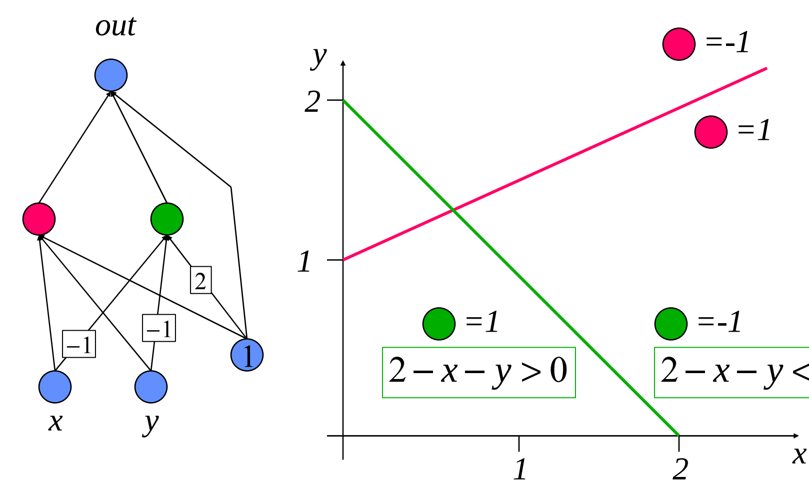
Multilayer Perceptron: What does it do?



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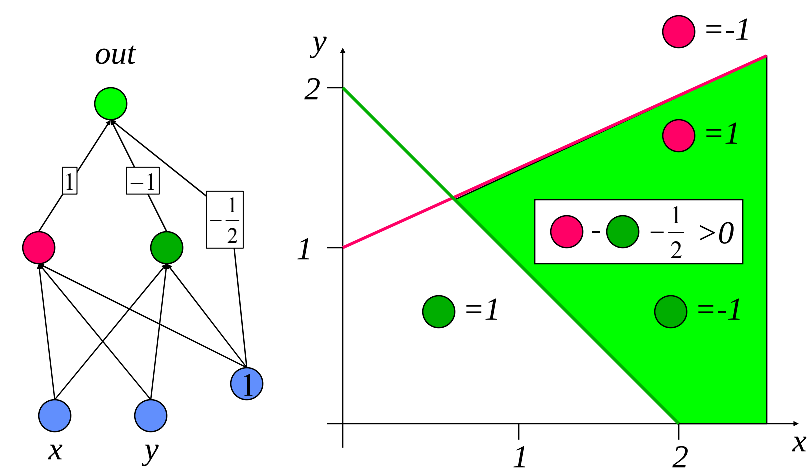
Multilayer Perceptron: What does it do?



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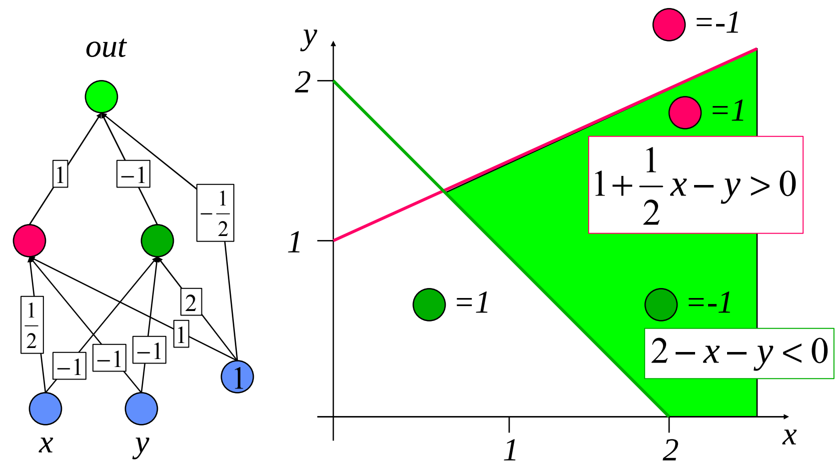
Perceptrons as Constraint Satisfaction Networks



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Back to Linear Separability

- **Recall: Weighted sum in perceptron forms a *linear hyperplane***

$$\sum_i w_i x_i + b = 0$$

- Due to threshold function, everything *on one side* of this hyperplane is labeled as class 1 (output = +1) and everything *on other side* is labeled as class 2 (output = -1)

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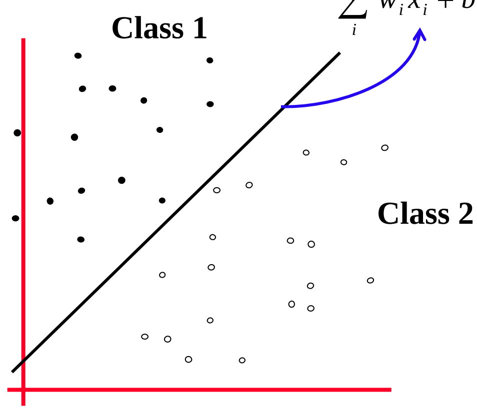
Separating Hyperplane

$$\sum_i w_i x_i + b = 0$$



- denotes +1 output
- ◦ denotes -1 output

Need to choose **w** and *b* based on training data

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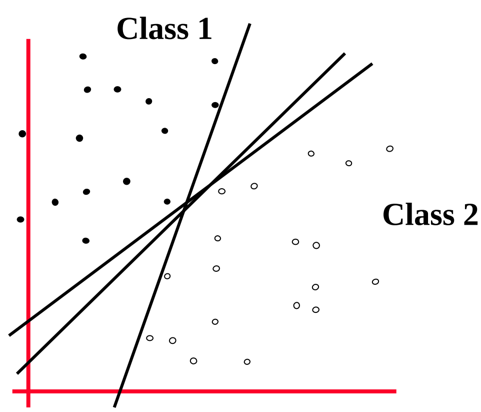
Separating Hyperplanes

Different choices of **w** and *b* give different hyperplanes



- denotes +1 output
- ◦ denotes -1 output

(This and next few slides adapted from Andrew Moore's)

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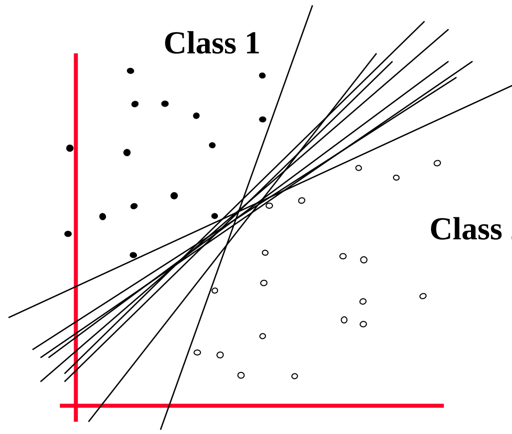
Which hyperplane is best?



- denotes +1 output
- ◦ denotes -1 output

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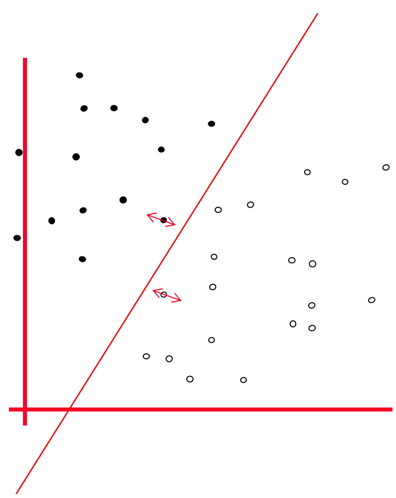
How about the one right in the middle?



Intuitively, this boundary seems good

Avoids misclassification of new test points if they are generated from the same distribution as training points

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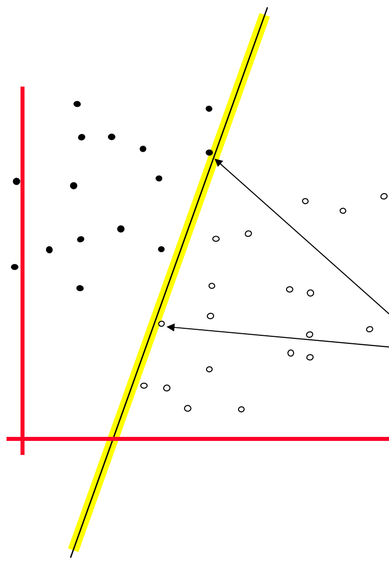
Margin



Define the margin of a linear classifier as the width that the boundary could be increased by before hitting a datapoint.

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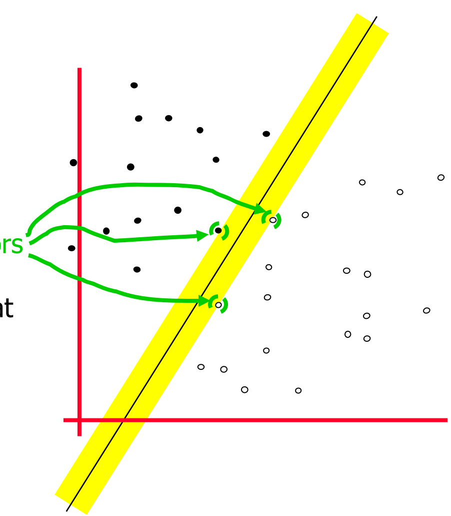
Maximum Margin and Support Vector Machine

Support Vectors are those datapoints that the margin pushes up against



The maximum margin classifier is called a Support Vector Machine (in this case, a Linear SVM or LSVM)

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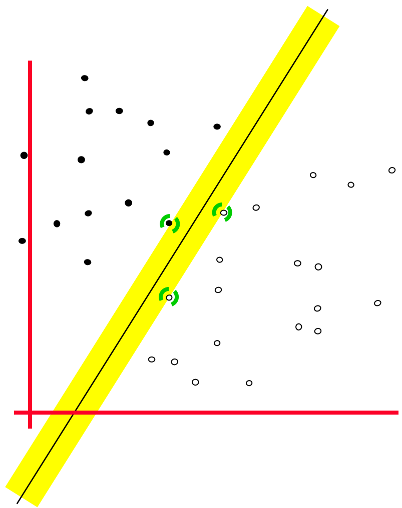
Why Maximum Margin?



- Robust to small perturbations of data points near boundary
- There exists theory showing this is best for generalization to new points
- Empirically works great

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Support Vector Machines: The Math

Suppose the training data points $(\mathbf{x}_i, y_i)$ satisfy :

$\mathbf{w} \cdot \mathbf{x}_i + b \geq +1$ for $y_i = +1$

$\mathbf{w} \cdot \mathbf{x}_i + b \leq -1$ for $y_i = -1$

This can be rewritten as

$y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq +1$

We can always do this by rescaling **w** and *b*, without affecting the separating hyperplane:

$$\mathbf{w} \cdot \mathbf{x} + b = 0$$

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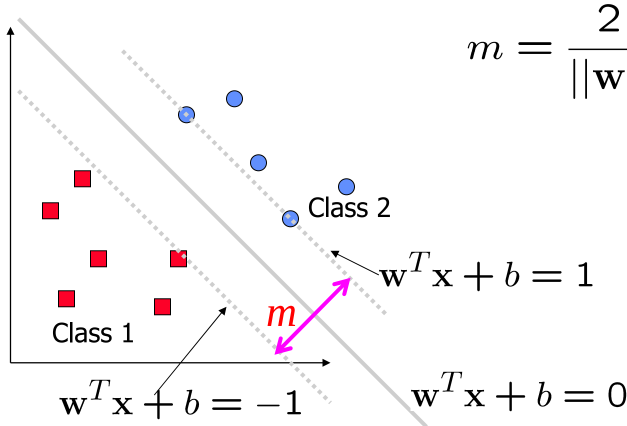
Estimating the Margin

The margin is given by (see Burges tutorial online):

$$m = \frac{2}{||\mathbf{w}||}$$



Margin can be calculated based on expression for distance from a point to a line, see, e.g., http://mathworld.wolfram.com/Point-LineDistance2-Dimensional.html

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Learning the Maximum Margin Classifier

Want to maximize margin:

$$2/\|\mathbf{w}\| \text{ subject to } \quad y_i(\mathbf{w}\cdot\mathbf{x}_i + b) \geq +1, \forall i$$

Equivalent to finding w and b that minimize:

$$\frac{1}{2}\|\mathbf{w}\|^2 \text{ subject to } \quad y_i(\mathbf{w}\cdot\mathbf{x}_i + b) \geq +1, \forall i$$

Constrained optimization problem that can be solved using Lagrange multiplier method

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Learning the Maximum Margin Classifier

Using Lagrange formulation and Lagrangian multipliers α_i, we get (see Burges tutorial online):

$$\mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i$$

where the α_i are obtained by maximizing:

$$\sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j)$$

subject to $\alpha_i \geq 0$ and $\sum_i \alpha_i y_i = 0$

This is a quadratic programming (QP) problem
- A global maximum can always be found

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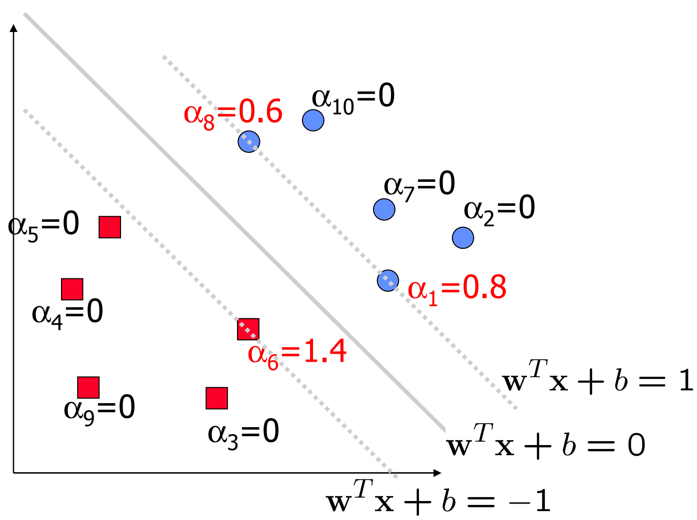
Geometrical Interpretation

$\mathbf{x}_i$ with non-zero α_i are called support vectors



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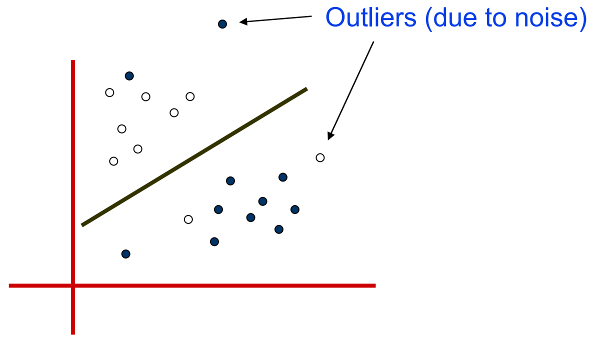
What if data is not linearly separable?



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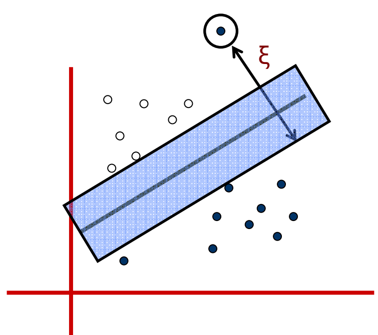
Approach 1: Soft Margin SVMs



Allow *errors* ξ_i (deviations from margin)

Trade off margin with errors.

Minimize: $\frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i \xi_i$ subject to :

$y_i(\mathbf{w}\cdot\mathbf{x}_i + b) \geq 1 - \xi_i \quad \text{and} \quad \xi_i \geq 0, \forall i$

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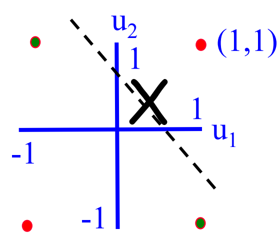
What if data is not linearly separable: Other ideas?

u_1	u_2	XOR
-1	-1	1
1	-1	-1
-1	1	-1
1	1	1



Can we do something to the inputs?

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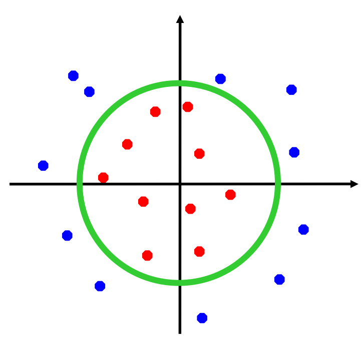
Another Example



Not linearly separable

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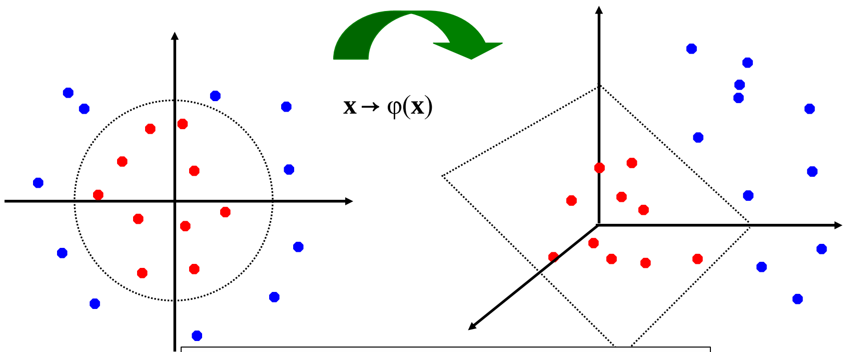
What if data is not linearly separable?

Approach 2: Map original input space to higher-dimensional feature space; use linear classifier in higher-dim. space



$$\Phi : \mathbb{R}^2 \rightarrow \mathbb{R}^3$$
$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{2}\, x_1 x_2, x_2^2)$$

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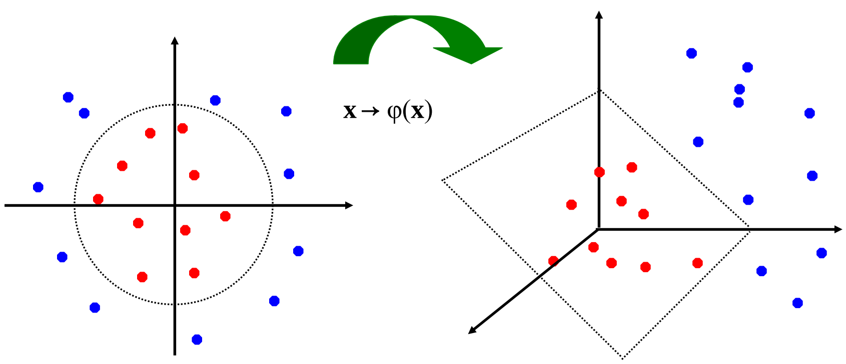
Problem with high dimensional spaces



Computation in high-dimensional feature space can be costly

The high dimensional projection function $\varphi(x)$ may be too complicated to compute

Kernel trick to the rescue!

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The Kernel Trick

Recall: SVM maximizes the quadratic function:

$$\sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j)$$

subject to $\alpha_i \geq 0$ and $\sum_i \alpha_i y_i = 0$

Insight:

The data points only appear as inner product

- No need to compute high-dimensional $\varphi(x)$ explicitly! Just replace inner product $x_i \cdot x_j$ with a kernel function $K(x_i,x_j) = \varphi(x_i) \cdot \varphi(x_j)$
- E.g., Gaussian kernel

  $K(x_i,x_j) = \exp(-||x_i-x_j||^2/2\sigma^2)$
- E.g., Polynomial kernel

  $K(x_i,x_j) = (x_i \cdot x_j+1)^d$

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An Example for $\phi(.)$ and $K(.,.)$

Suppose $\phi(.)$ is given as follows

$$\phi(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}) = (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

An inner product in the feature space is

$$\langle \phi(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}), \phi(\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}) \rangle = (1 + x_1y_1 + x_2y_2)^2$$

So, if we define the kernel function as follows, there is no need to compute $\phi(.)$ explicitly

$$K(\mathbf{x}, \mathbf{y}) = (1 + x_1y_1 + x_2y_2)^2$$

This use of kernel function to avoid computing $\phi(.)$ explicitly is known as the kernel trick

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Summary: Steps for Classification using SVMs

- Prepare the data matrix
- Select the kernel function to use
- Select parameters of the kernel function
  - You can use the values suggested by the SVM software, or use cross-validation
- Execute the training algorithm and obtain the parameters α_i
- Classify new data using the learned parameters

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Face Detection using SVMs

	Test Set A		Test Set B	
	Detect Rate	False Alarms	Detect Rate	False Alarms
SVM	97.1 %	4	74.2%	20
Sung *et al.*	94.6 %	2	74.2%	11

Kernel used: Polynomial of degree 2

(Osuna, Freund, Girosi, 1998)

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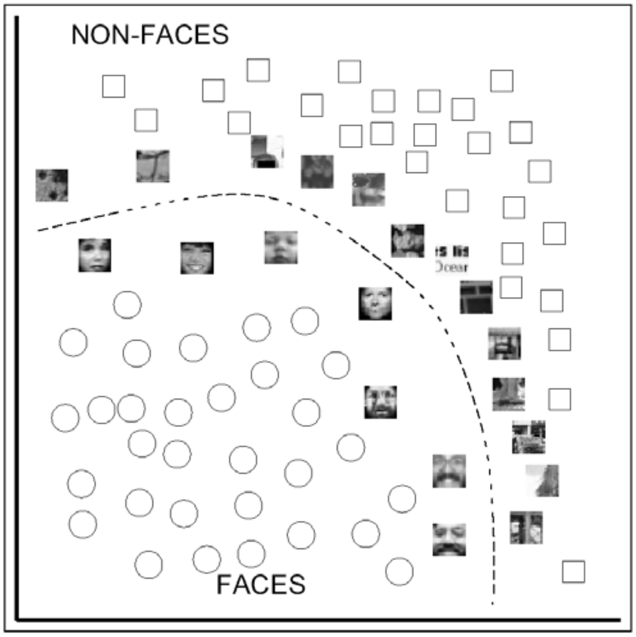
Support Vectors



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K-Nearest Neighbors

A simple non-parametric classification algorithm

Idea:

- Look around you to see how your neighbors classify data
- Classify a new data-point according to a *majority vote* of your k nearest neighbors

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Distance Metric

How do we measure what it means to be a neighbor (what is "close")?

Appropriate distance metric depends on the problem

Examples:

- x discrete (e.g., strings): Hamming distance
  $d(x_1,x_2)$ = # features on which x_1 and x_2 differ
- x continuous (e.g., vectors over reals): Euclidean distance
  $d(x_1,x_2) = || x_1-x_2 ||$ = square root of sum of squared differences between corresponding elements of data vectors

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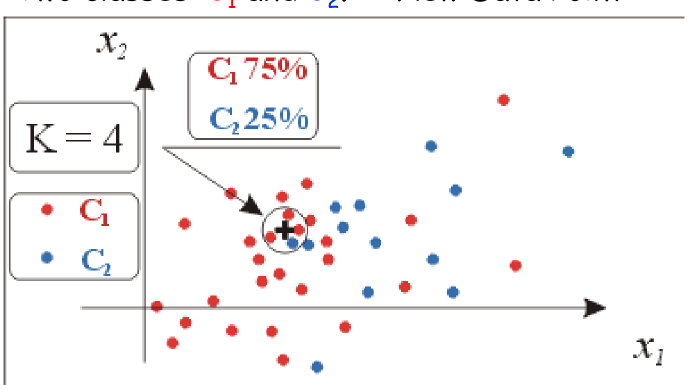
Example

Input Data: 2-D points (x_1,x_2)

Two classes: C_1 and C_2. New Data Point +



K = 4: Look at 4 nearest neighbors of +
3 are in C_1, so classify + as C_1

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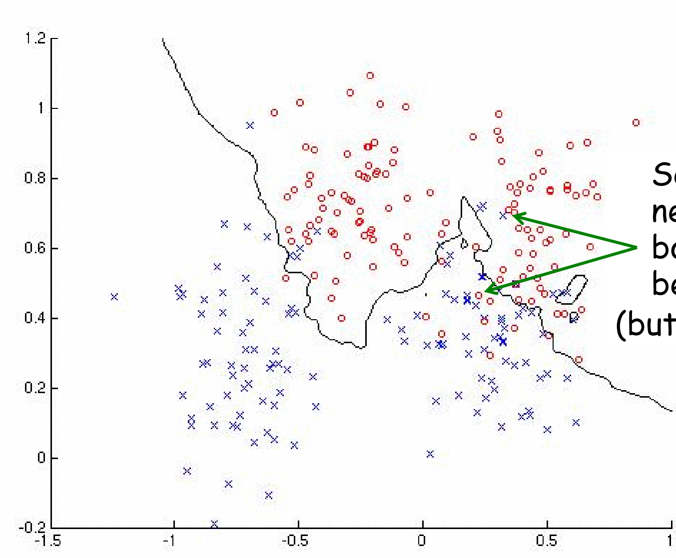
Decision Boundary using K-NN



Some points near the boundary may be misclassified (but maybe noise)

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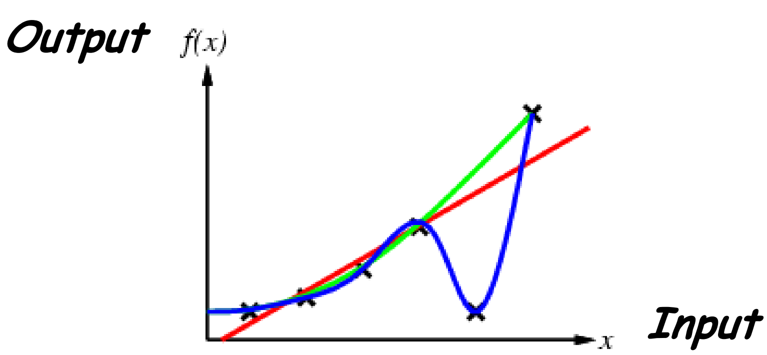
What if we want to learn continuous-valued functions?



Example: Learning to Drive

Can you use a neural network to drive?

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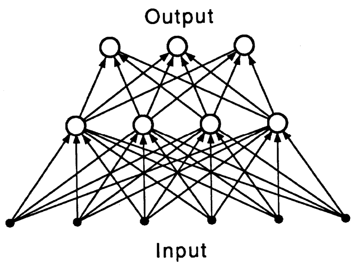
Regression using Networks

We want networks that can learn a function

- Network maps real-valued inputs to real-valued output
- Idea: Given data, *minimize errors* between network's output and desired output by changing weights



Continuous output values → Can't use binary threshold units anymore

To minimize errors, a *differentiable* output function is desirable

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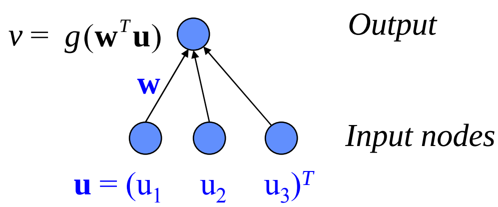
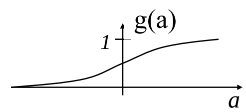
Sigmoidal Networks



The most common activation function:

Sigmoid function:

$$g(a) = \frac{1}{1 + e^{-\beta a}}$$



Non-linear "squashing" function: Squashes input to be between 0 and 1. The parameter β controls the slope.

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Gradient-Descent Learning ("Hill-Climbing")

Given training examples (u^m, d^m) $(m = 1, \ldots, N)$, define an <u>error function</u> (cost function or "energy" function)

$$E(\mathbf{w}) = \frac{1}{2}\sum_m (d^m - v^m)^2$$

where $v^m = g(\mathbf{w}^T \mathbf{u}^m)$

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Gradient-Descent Learning ("Hill-Climbing")

Would like to change w so that E(w) is minimized

- Gradient Descent: Change w in proportion to $-dE/d\mathbf{w}$ (why?)

$$\mathbf{w} \rightarrow \mathbf{w} - \varepsilon \frac{dE}{d\mathbf{w}}$$

$$\frac{dE}{d\mathbf{w}} = -\sum_m (d^m - v^m)\frac{dv^m}{d\mathbf{w}} = -\sum_m (d^m - v^m)g'(\mathbf{w}^T\mathbf{u}^m)\mathbf{u}^m$$

Derivative of sigmoid

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"Stochastic" Gradient Descent

What if the inputs only arrive one-by-one?

Stochastic gradient descent approximates sum over all inputs with an "on-line" running sum:

$$\mathbf{w} \rightarrow \mathbf{w} - \varepsilon \frac{dE_1}{d\mathbf{w}}$$

$$\frac{dE_1}{d\mathbf{w}} = -\underbrace{(d^m - v^m)}_{\text{delta = error}}g'(\mathbf{w}^T\mathbf{u}^m)\mathbf{u}^m$$

Also known as the "delta rule" or "LMS (least mean square) rule"

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But wait….

Delta rule tells us how to modify the connections from input to output (one layer network)

- One layer networks are not that interesting (remember XOR?)

What if we have multiple layers?

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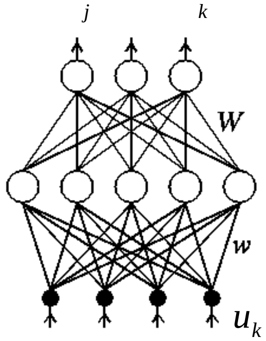
Learning Multilayer Networks

$$v_i = g(\sum_j W_{ji} g(\sum_k w_{kj} u_k))$$



Start with random weights **W**, **w**

Given input **u**, network produces output **v**

Find **W** and **w** that minimize total squared output error over all output units (labeled *i*):

$$E(\mathbf{W},\mathbf{w}) = \frac{1}{2}\sum_i (d_i - v_i)^2$$

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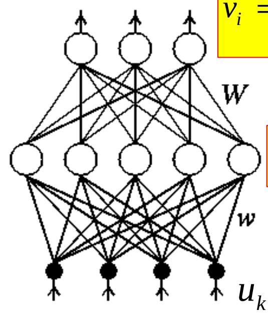
Backpropagation: Output Weights

$$E(\mathbf{W},\mathbf{w}) = \frac{1}{2}\sum_i (d_i - v_i)^2$$

$$\boxed{v_i = g(\sum_j W_{ji} x_j)}$$



$$\boxed{x_j}$$

Learning rule for <u>hidden-output weights **W**</u>:

$$W_{ji} \rightarrow W_{ji} - \varepsilon \frac{dE}{dW_{ji}} \qquad \{\textit{gradient descent}\}$$

$$\frac{dE}{dW_{ji}} = -(d_i - v_i) g'(\sum_j W_{ji} x_j) x_j \qquad \{\textit{delta rule}\}$$

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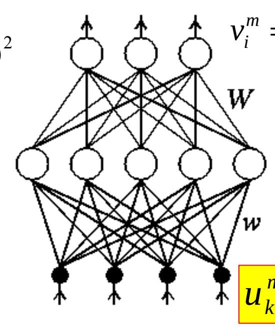
Backpropagation: Hidden Weights

$$E(\mathbf{W},\mathbf{w}) = \frac{1}{2}\sum_i (d_i - v_i)^2$$

$$v_i^m = g(\sum_j W_{ji} x_j)$$



$$\boxed{x_j^m = g(\sum_k w_{kj} u_k^m)}$$

$$\boxed{u_k^m}$$

Learning rule for <u>input-hidden weights **w**</u>:

$$w_{kj} \rightarrow w_{kj} - \varepsilon \frac{dE}{dw_{kj}} \qquad \text{But}: \frac{dE}{dw_{kj}} = \frac{dE}{dx_j} \cdot \frac{dx_j}{dw_{kj}} \qquad \{\textit{chain rule}\}$$

$$\frac{dE}{dw_{kj}} = \left[-\sum_{m,i} (d_i^m - v_i^m) g'(\sum_j W_{ji} x_j^m) W_{ji} \right] \cdot \left[g'(\sum_k w_{kj} u_k^m) u_k^m \right]$$

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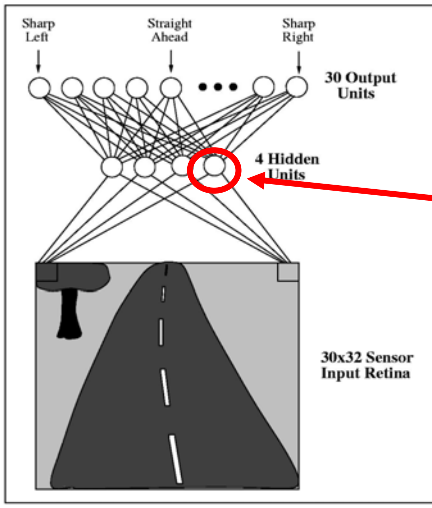
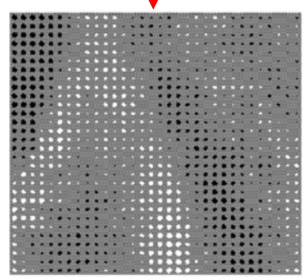
Learning to Drive using Backprop



One of the learned "road features" w_i



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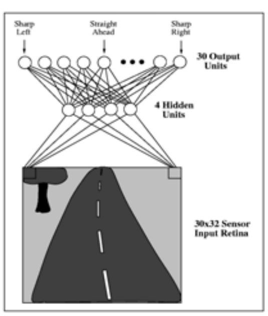
ALVINN (Autonomous Land Vehicle in a Neural Network)



CMU Navlab

Trained using human driver + camera images

After learning:

- Drove up to 70 mph on highway
- Up to 22 miles without intervention
- Drove cross-country largely autonomously

(Pomerleau, 1992)

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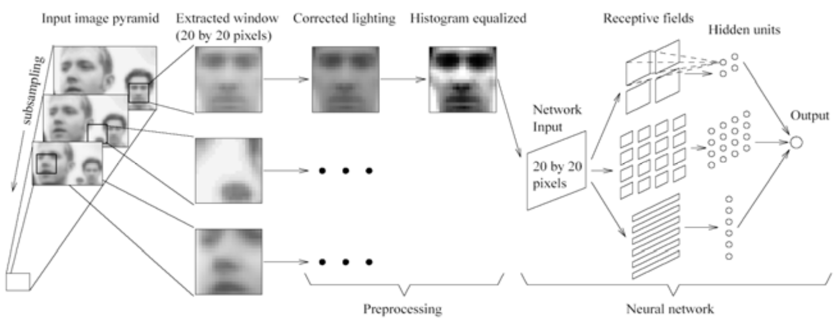
Another Example: Face Detection



Output between -1 (no face) and +1 (face present)

(Rowley, Baluja & Kanade, 1998)

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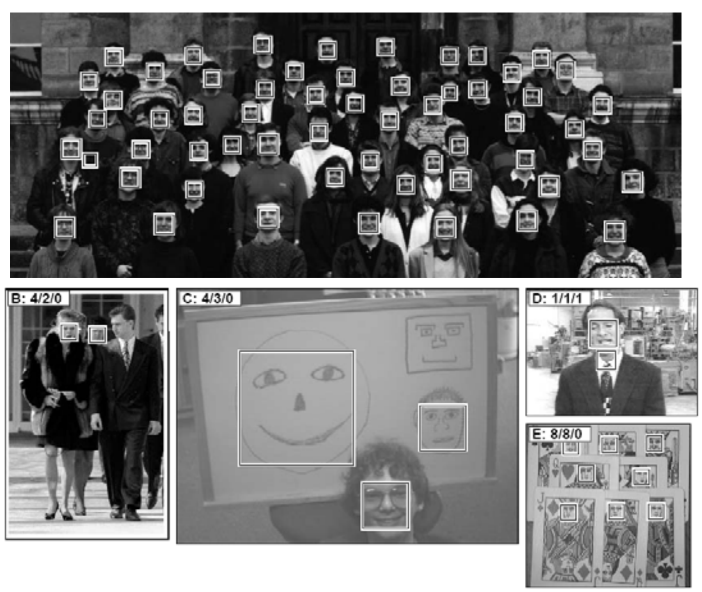
Face Detection Results



(Rowley, Baluja & Kanade, 1998)

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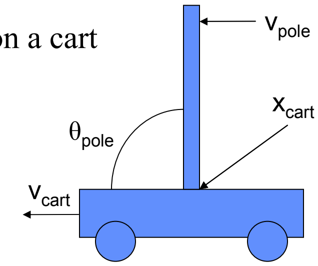
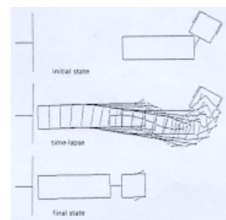
Demos: Pole Balancing and Backing up a Truck

(courtesy of Keith Grochow, CSE 599)

- Neural network learns to balance a pole on a cart
  - System:
    - 4 state variables: x_{cart}, v_{cart}, θ_{pole}, v_{pole}
    - 1 input: Force on cart
  - Backprop Network:
    - Input: State variables
    - Output: New force on cart



- NN learns to back a truck into a loading dock
  - System (Nyugen and Widrow, 1989):
    - State variables: x_{cab}, y_{cab}, θ_{cab}
    - 1 input: new $\theta_{steering}$
  - Backprop Network:
    - Input: State variables
    - Output: Steering angle $\theta_{steering}$



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