Outline

- Why Machine Learning?
- What is a well-defined learning problem?
- An example: learning to play checkers
- What questions should we ask about Machine Learning?

Why Machine Learning

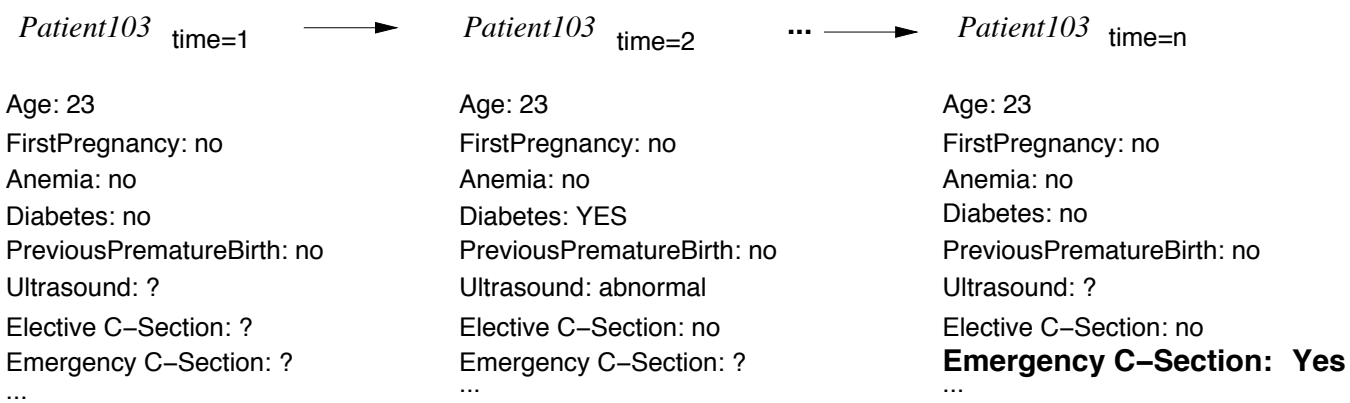
- Recent progress in algorithms and theory
- Growing flood of online data
- Computational power is available
- Budding industry

Three niches for machine learning:

- Data mining : using historical data to improve decisions
  - medical records → medical knowledge
- Software applications we can't program by hand
  - autonomous driving
  - speech recognition
- Self customizing programs
  - Newsreader that learns user interests

Typical Datamining Task

Data:



Given:

- 9714 patient records, each describing a pregnancy and birth
- Each patient record contains 215 features

Learn to predict:

- Classes of future patients at high risk for Emergency Cesarean Section

Datamining Result

Data:

Patient103 time=1	*Patient103* time=2	*Patient103* time=n
Age: 23	Age: 23	Age: 23
FirstPregnancy: no	FirstPregnancy: no	FirstPregnancy: no
Anemia: no	Anemia: no	Anemia: no
Diabetes: no	Diabetes: YES	Diabetes: no
PreviousPrematureBirth: no	PreviousPrematureBirth: no	PreviousPrematureBirth: no
Ultrasound: ?	Ultrasound: abnormal	Ultrasound: ?
Elective C–Section: ?	Elective C–Section: no	Elective C–Section: no
Emergency C–Section: ?	Emergency C–Section: ?	**Emergency C–Section: Yes**
...	...	...

One of 18 learned rules:

```
If   No previous vaginal delivery, and
     Abnormal 2nd Trimester Ultrasound, and
     Malpresentation at admission
Then Probability of Emergency C-Section is 0.6

 Over training data: 26/41 = .63,
 Over test data: 12/20 = .60
```

Credit Risk Analysis

Data:

Customer103: (time=t0)	*Customer103:* (time=t1)	...	*Customer103:* (time=tn)
Years of credit: 9	Years of credit: 9		Years of credit: 9
Loan balance: $2,400	Loan balance: $3,250		Loan balance: $4,500
Income: $52k	Income: ?		Income: ?
Own House: Yes	Own House: Yes		Own House: Yes
Other delinquent accts: 2	Other delinquent accts: 2		Other delinquent accts: 3
Max billing cycles late: 3	Max billing cycles late: 4		Max billing cycles late: 6
Profitable customer?: ?	Profitable customer?: ?		**Profitable customer?: No**
...	...		...

Rules learned from synthesized data:

```
If   Other-Delinquent-Accounts > 2, and
     Number-Delinquent-Billing-Cycles > 1
Then Profitable-Customer? = No
     [Deny Credit Card application]

If   Other-Delinquent-Accounts = 0, and
     (Income > $30k)  OR  (Years-of-Credit > 3)
Then Profitable-Customer? = Yes
     [Accept Credit Card application]
```

Other Prediction Problems

Customer purchase behavior:

Customer103: (time=t0)	*Customer103:* (time=t1)	...	*Customer103:* (time=tn)
Sex: M	Sex: M		Sex: M
Age: 53	Age: 53		Age: 53
Income: $50k	Income: $50k		Income: $50k
Own House: Yes	Own House: Yes		Own House: Yes
MS Products: Word	MS Products: Word		MS Products: Word
Computer: 386 PC	Computer: Pentium		Computer: Pentium
Purchase Excel?: ?	Purchase Excel?: ?		**Purchase Excel?: Yes**
...	...		...

Customer retention:

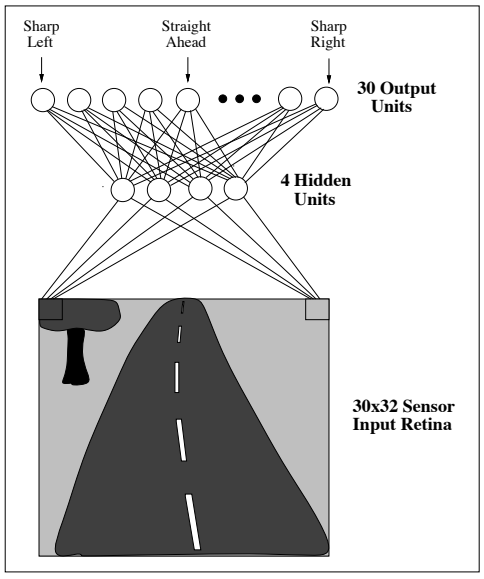
Customer103: (time=t0)	*Customer103:* (time=t1)	...	*Customer103:* (time=tn)
Sex: M	Sex: M		Sex: M
Age: 53	Age: 53		Age: 53
Income: $50k	Income: $50k		Income: $50k
Own House: Yes	Own House: Yes		Own House: Yes
Checking: $5k	Checking: $20k		Checking: $0
Savings: $15k	Savings: $0		Savings: $0
Current–customer?: yes	Current–customer?: yes		**Current–customer?: No**

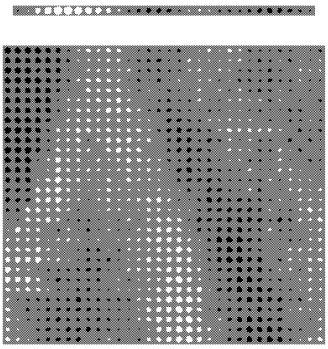
Process optimization:

Product72: (time=t0)	*Product72:* (time=t1)	...	*Product72:* (time=tn)
Stage: mix	Stage: cook		Stage: cool
Mixing–speed: 60rpm	Temperature: 325		Fan–speed: medium
Viscosity: 1.3	Viscosity: 3.2		Viscosity: 1.3
Fat content: 15%	Fat content: 12%		Fat content: 12%
Density: 2.8	Density: 1.1		Density: 1.2
Spectral peak: 2800	Spectral peak: 3200		Spectral peak: 3100
Product underweight?: ??	Product underweight?: ??		**Product underweight?: Yes**
...	...		...

Problems Too Difficult to Program by Hand

ALVINN [Pomerleau] drives 70 mph on highways





Software that Customizes to User

http://www.wisewire.com

Where Is this Headed?

Today: tip of the iceberg

- First-generation algorithms: neural nets, decision trees, regression ...
- Applied to well-formated database
- Budding industry

Opportunity for tomorrow: enormous impact

- Learn across full mixed-media data
- Learn across multiple internal databases, plus the web and newsfeeds
- Learn by active experimentation
- Learn decisions rather than predictions
- Cumulative, lifelong learning
- Programming languages with learning embedded?

Relevant Disciplines

- Artificial intelligence
- Bayesian methods
- Computational complexity theory
- Control theory
- Information theory
- Philosophy
- Psychology and neurobiology
- Statistics
- ...

What is the Learning Problem?

Learning = Improving with experience at some task

- Improve over task T,
- with respect to performance measure P,
- based on experience E.

E.g., Learn to play checkers

- T: Play checkers
- P: % of games won in world tournament
- E: opportunity to play against self

Learning to Play Checkers

- T: Play checkers
- P: Percent of games won in world tournament
- What experience?
- What exactly should be learned?
- How shall it be represented?
- What specific algorithm to learn it?

Type of Training Experience

- Direct or indirect?
- Teacher or not?

A problem: is training experience representative of performance goal?

Choose the Target Function

- $ChooseMove : Board \rightarrow Move$??
- $V : Board \rightarrow \Re$??
- ...

Possible Definition for Target Function V

- if b is a final board state that is won, then $V(b) = 100$
- if b is a final board state that is lost, then $V(b) = -100$
- if b is a final board state that is drawn, then $V(b) = 0$
- if b is a not a final state in the game, then $V(b) = V(b')$, where b' is the best final board state that can be achieved starting from b and playing optimally until the end of the game.

This gives correct values, but is not operational

Choose Representation for Target Function

- collection of rules?
- neural network ?
- polynomial function of board features?
- ...

A Representation for Learned Function

$w_0 + w_1 \cdot bp(b) + w_2 \cdot rp(b) + w_3 \cdot bk(b) + w_4 \cdot rk(b) + w_5 \cdot bt(b) + w_6 \cdot rt(b$

- $bp(b)$: number of black pieces on board b
- $rp(b)$: number of red pieces on b
- $bk(b)$: number of black kings on b
- $rk(b)$: number of red kings on b
- $bt(b)$: number of red pieces threatened by black (i.e., which can be taken on black's next turn)
- $rt(b)$: number of black pieces threatened by red

Obtaining Training Examples

- $V(b)$: the true target function
- $\hat{V}(b)$: the learned function
- $V_{train}(b)$: the training value

One rule for estimating training values:

- $V_{train}(b) \leftarrow \hat{V}(Successor(b))$

Choose Weight Tuning Rule

LMS Weight update rule:

Do repeatedly:

- Select a training example b at random

  1. Compute $error(b)$:

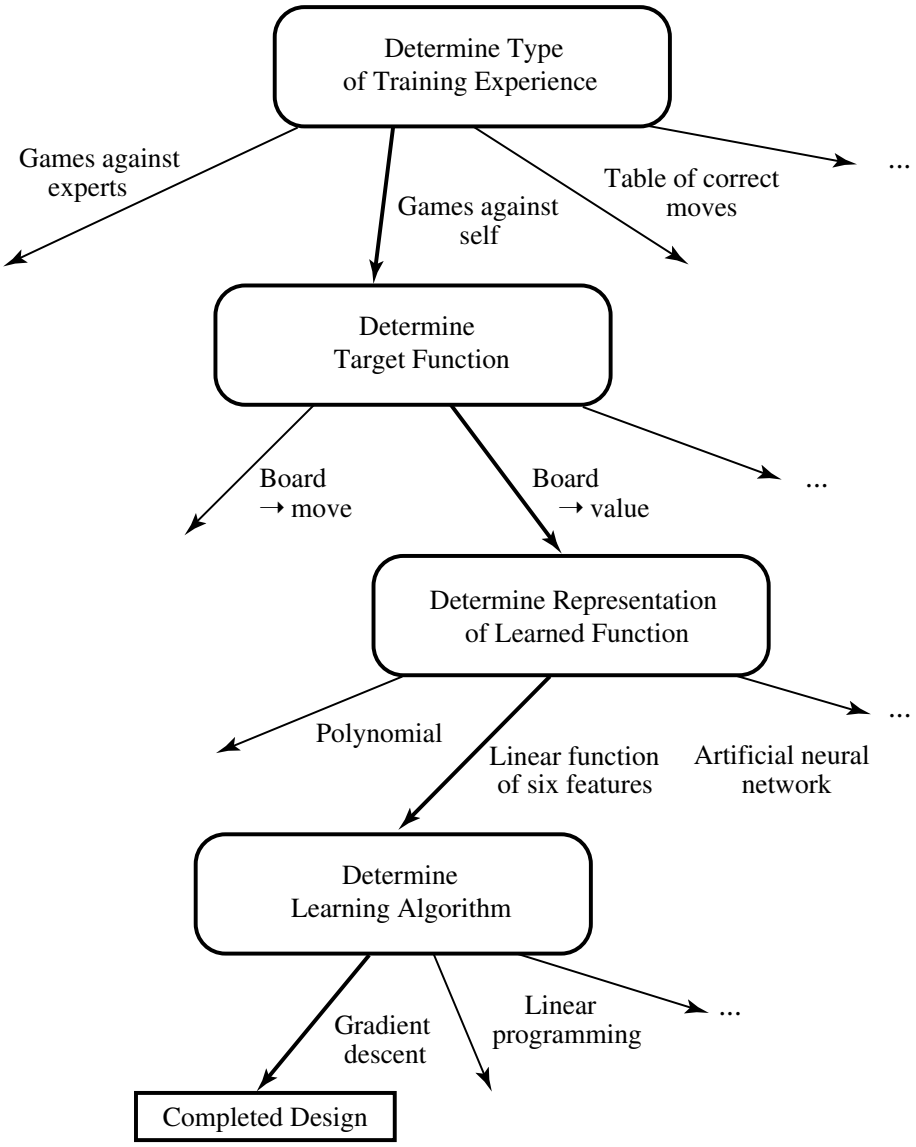
$$error(b) = V_{train}(b) - \hat{V}(b)$$

  2. For each board feature f_i, update weight w_i:

$$w_i \leftarrow w_i + c \cdot f_i \cdot error(b)$$

c is some small constant, say 0.1, to moderate the rate of learning

Design Choices



Some Issues in Machine Learning

- What algorithms can approximate functions well (and when)?
- How does number of training examples influence accuracy?
- How does complexity of hypothesis representation impact it?
- How does noisy data influence accuracy?
- What are the theoretical limits of learnability?
- How can prior knowledge of learner help?
- What clues can we get from biological learning systems?
- How can systems alter their own representations?

Outline

[read Chapter 2]
[suggested exercises 2.2, 2.3, 2.4, 2.6]

- Learning from examples
- General-to-specific ordering over hypotheses
- Version spaces and candidate elimination algorithm
- Picking new examples
- The need for inductive bias

Note: simple approach assuming no noise, illustrates key concepts

Training Examples for EnjoySport

Sky	Temp	Humid	Wind	Water	Forecst	EnjoySpt
Sunny	Warm	Normal	Strong	Warm	Same	Yes
Sunny	Warm	High	Strong	Warm	Same	Yes
Rainy	Cold	High	Strong	Warm	Change	No
Sunny	Warm	High	Strong	Cool	Change	Yes

What is the general concept?

Representing Hypotheses

Many possible representations

Here, h is conjunction of constraints on attributes

Each constraint can be

- a specfic value (e.g., $Water = Warm$)
- don't care (e.g., "$Water =?$")
- no value allowed (e.g.,"Water=$\emptyset$")

For example,

Sky	AirTemp	Humid	Wind	Water	Forecst
$\langle Sunny$	?	?	$Strong$	?	$Same\rangle$

Prototypical Concept Learning Task

- **Given:**
  - Instances X: Possible days, each described by the attributes *Sky, AirTemp, Humidity, Wind, Water, Forecast*
  - Target function c: $EnjoySport : X \rightarrow \{0, 1\}$
  - Hypotheses H: Conjunctions of literals. E.g.

$$\langle ?, Cold, High, ?, ?, ? \rangle.$$

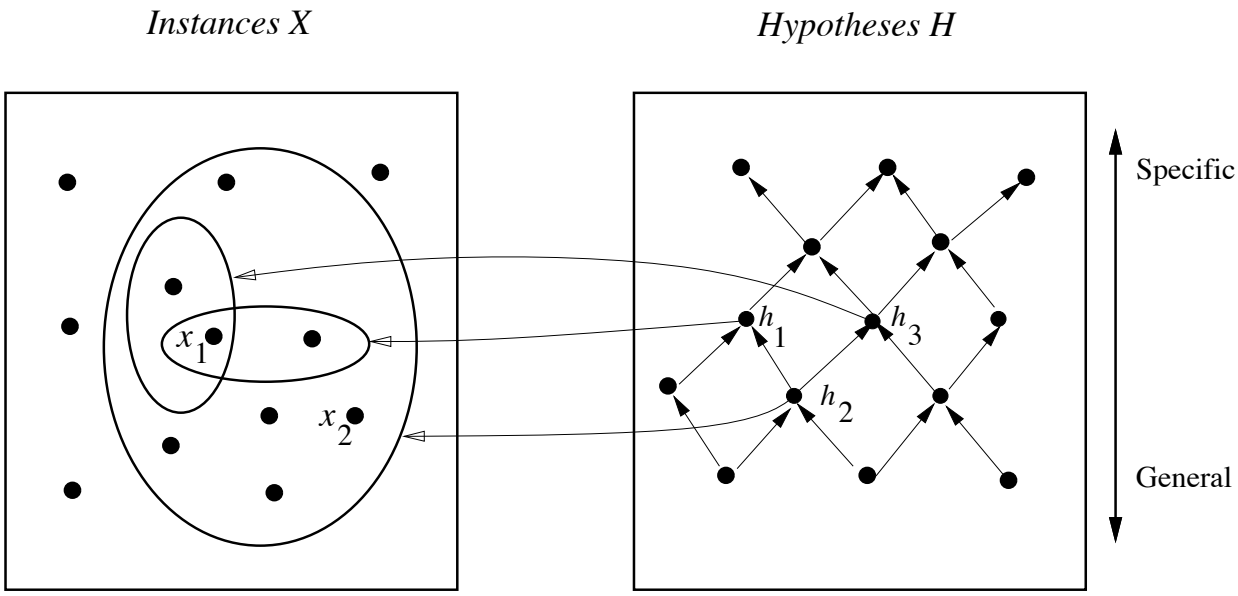
  - Training examples D: Positive and negative examples of the target function

$$\langle x_1, c(x_1) \rangle, \ldots \langle x_m, c(x_m) \rangle$$

- **Determine:** A hypothesis h in H such that $h(x) = c(x)$ for all x in D.

The inductive learning hypothesis: Any hypothesis found to approximate the target function well over a sufficiently large set of training examples will also approximate the target function well over other unobserved examples.

Instance, Hypotheses, and More-General-Than



x_1= <Sunny, Warm, High, Strong, Cool, Same>

x_2= <Sunny, Warm, High, Light, Warm, Same>

h_1= <Sunny, ?, ?, Strong, ?, ?>

h_2= <Sunny, ?, ?, ?, ?, ?>

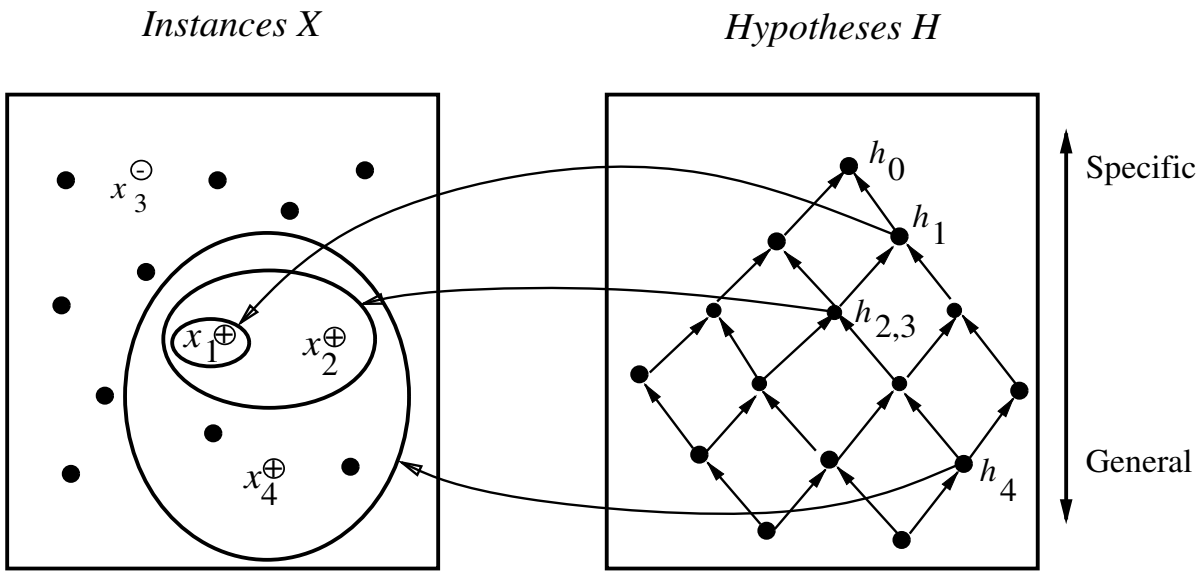
h_3= <Sunny, ?, ?, ?, Cool, ?>

Find-S **Algorithm**

1. Initialize h to the most specific hypothesis in H
2. For each positive training instance x
   - For each attribute constraint a_i in h

     If the constraint a_i in h is satisfied by x
     Then do nothing
     Else replace a_i in h by the next more general constraint that is satisfied by x
3. Output hypothesis h

Hypothesis Space Search by Find-S



x_1 = <*Sunny Warm Normal Strong Warm Same*>, +

x_2 = <*Sunny Warm High Strong Warm Same*>, +

x_3 = <*Rainy Cold High Strong Warm Change*>, -

x_4 = <*Sunny Warm High Strong Cool Change*>, +

h_0 = <∅, ∅, ∅, ∅, ∅, ∅, ∅>

h_1 = <*Sunny Warm Normal Strong Warm Sam*

h_2 = <*Sunny Warm ? Strong Warm Same*>

h_3 = <*Sunny Warm ? Strong Warm Same*>

h_4 = <*Sunny Warm ? Strong ? ?* >

Complaints about Find-S

- Can't tell whether it has learned concept
- Can't tell when training data inconsistent
- Picks a maximally specific h (why?)
- Depending on H, there might be several!

Version Spaces

A hypothesis h is **consistent** with a set of training examples D of target concept c if and only if $h(x) = c(x)$ for each training example $\langle x, c(x)\rangle$ in D.

$$Consistent(h, D) \equiv (\forall \langle x, c(x)\rangle \in D)\ h(x) = c(x)$$

The **version space**, $VS_{H,D}$, with respect to hypothesis space H and training examples D, is the subset of hypotheses from H consistent with all training examples in D.

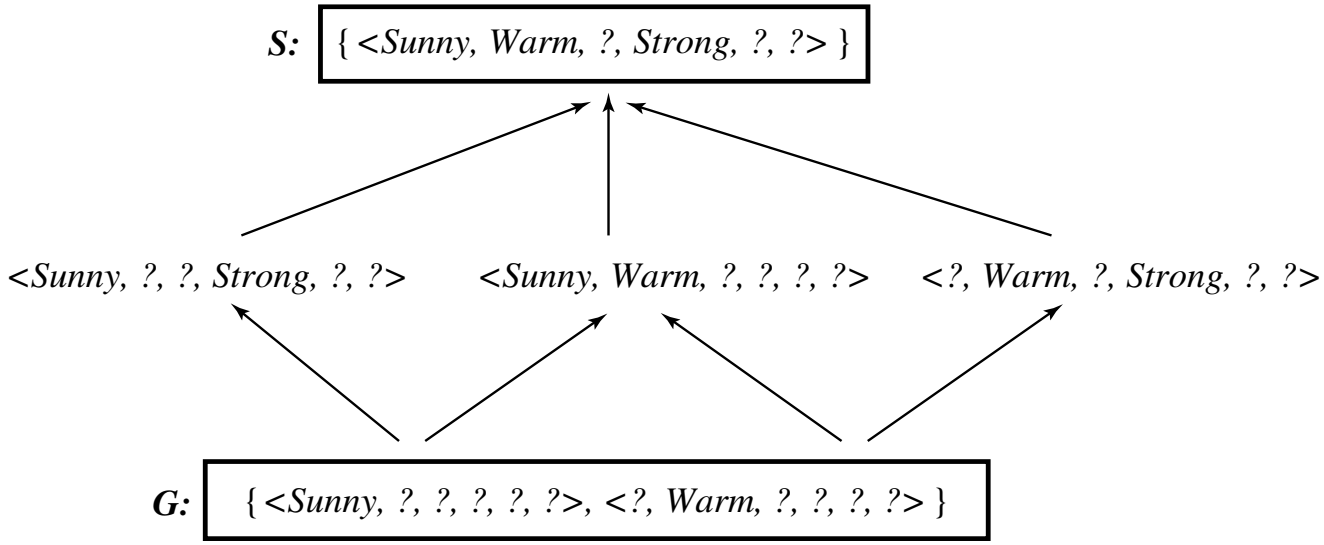
$$VS_{H,D} \equiv \{h \in H | Consistent(h, D)\}$$

The List-Then-Eliminate **Algorithm:**

1. $VersionSpace \leftarrow$ a list containing every hypothesis in H
2. For each training example, $\langle x, c(x) \rangle$

   remove from $VersionSpace$ any hypothesis h for which $h(x) \neq c(x)$
3. Output the list of hypotheses in $VersionSpace$

Example Version Space



Representing Version Spaces

The **General boundary**, G, of version space $VS_{H,D}$ is the set of its maximally general members

The **Specific boundary**, S, of version space $VS_{H,D}$ is the set of its maximally specific members

Every member of the version space lies between these boundaries

$$VS_{H,D} = \{h \in H | (\exists s \in S)(\exists g \in G)(g \geq h \geq s)\}$$

where $x \geq y$ means x is more general or equal to y

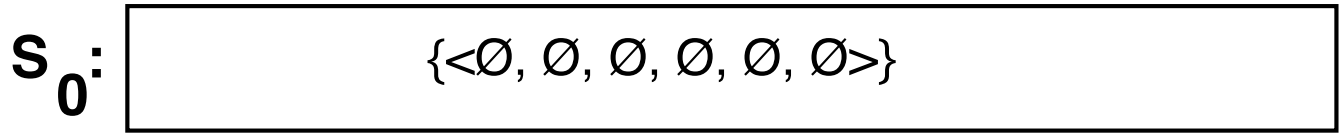
Candidate Elimination Algorithm

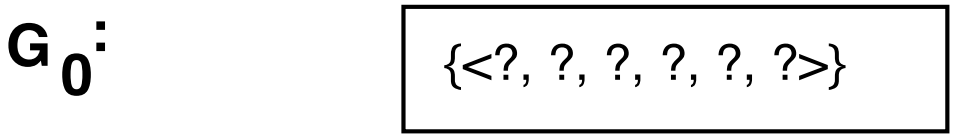
$G \leftarrow$ maximally general hypotheses in H
$S \leftarrow$ maximally specific hypotheses in H
For each training example d, do

- If d is a positive example
  - Remove from G any hypothesis inconsistent with d
  - For each hypothesis s in S that is not consistent with d
    - Remove s from S
    - Add to S all minimal generalizations h of s such that
      1. h is consistent with d, and
      2. some member of G is more general than h
    - Remove from S any hypothesis that is more general than another hypothesis in S
- If d is a negative example

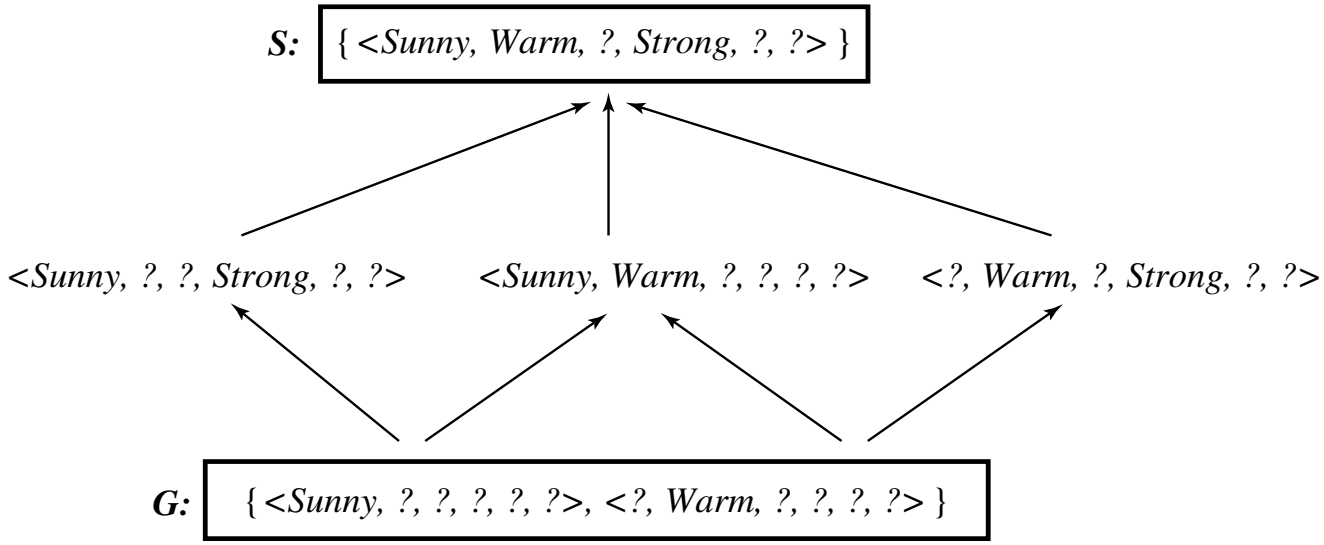
- Remove from S any hypothesis inconsistent with d
- For each hypothesis g in G that is not consistent with d
  - Remove g from G
  - Add to G all minimal specializations h of g such that
    1. h is consistent with d, and
    2. some member of S is more specific than h
  - Remove from G any hypothesis that is less general than another hypothesis in G

Example Trace

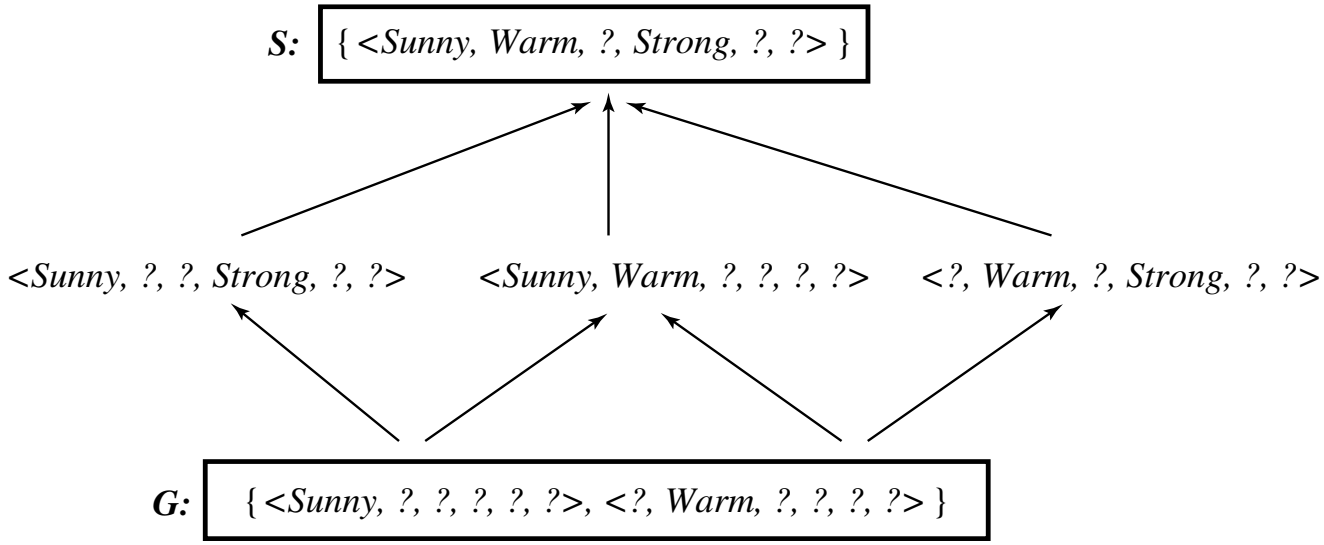




What Next Training Example?



How Should These Be Classified?



$\langle Sunny\ Warm\ Normal\ Strong\ Cool\ Change \rangle$

$\langle Rainy\ Cool\ Normal\ Light\ Warm\ Same \rangle$

$\langle Sunny\ Warm\ Normal\ Light\ Warm\ Same \rangle$

What Justifies this Inductive Leap?

$+ \ \langle Sunny\ Warm\ Normal\ Strong\ Cool\ Change \rangle$

$+ \ \langle Sunny\ Warm\ Normal\ Light\ Warm\ Same \rangle$

$S: \ \langle Sunny\ Warm\ Normal\ ?\ ?\ ? \rangle$

Why believe we can classify the unseen

$\langle Sunny\ Warm\ Normal\ Strong\ Warm\ Same \rangle$

An UNBiased Learner

Idea: Choose H that expresses every teachable concept (i.e., H is the power set of X)

Consider $H' =$ disjunctions, conjunctions, negations over previous H. E.g.,

$\langle Sunny\, Warm\, Normal\, ?\, ?\, ?\rangle \vee \neg\langle ?\, ?\, ?\, ?\, ?\, Change\rangle$

What are S, G in this case?

S $\leftarrow$

G $\leftarrow$

Inductive Bias

Consider

- concept learning algorithm L
- instances X, target concept c
- training examples $D_c = \{\langle x, c(x)\rangle\}$
- let $L(x_i, D_c)$ denote the classification assigned to the instance x_i by L after training on data D_c.

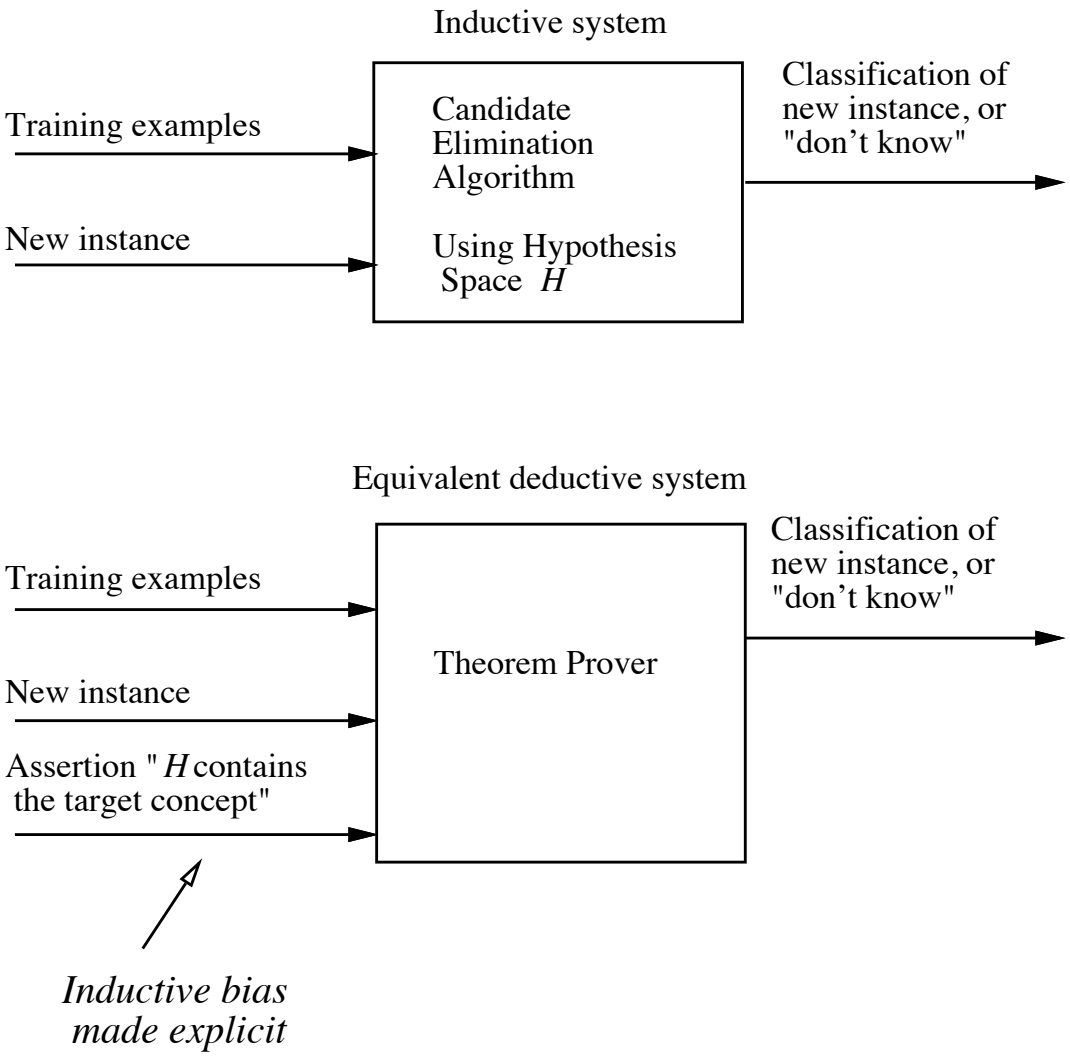
Definition:

The **inductive bias** of L is any minimal set of assertions B such that for any target concept c and corresponding training examples D_c

$$(\forall x_i \in X)[(B \wedge D_c \wedge x_i) \vdash L(x_i, D_c)]$$

where $A \vdash B$ means A logically entails B

Inductive Systems and Equivalent Deductive Systems



Three Learners with Different Biases

1. *Rote learner:* Store examples, Classify x iff it matches previously observed example.
2. *Version space candidate elimination algorithm*
3. *Find-S*

Summary Points

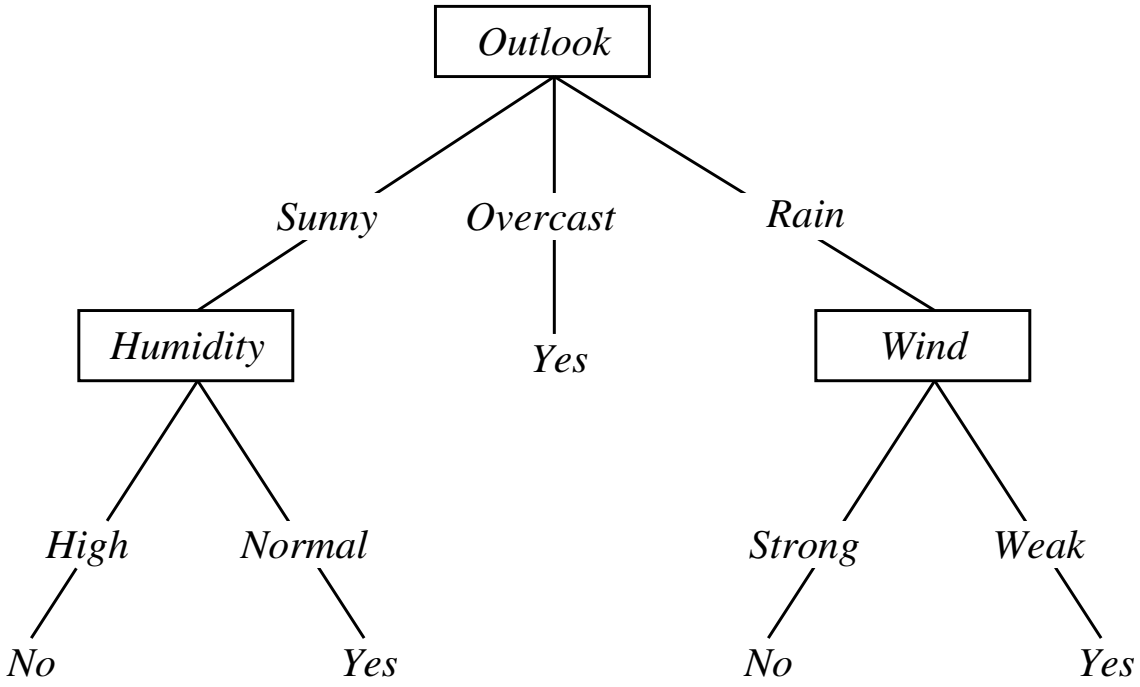
1. Concept learning as search through H
2. General-to-specific ordering over H
3. Version space candidate elimination algorithm
4. S and G boundaries characterize learner's uncertainty
5. Learner can generate useful queries
6. Inductive leaps possible only if learner is biased
7. Inductive learners can be modelled by equivalent deductive systems

Decision Tree Learning

[read Chapter 3]
[recommended exercises 3.1, 3.4]

- Decision tree representation
- ID3 learning algorithm
- Entropy, Information gain
- Overfitting

Decision Tree for *PlayTennis*



A Tree to Predict C-Section Risk

Learned from medical records of 1000 women

Negative examples are C-sections

```
[833+,167-] .83+ .17-
Fetal_Presentation = 1: [822+,116-] .88+ .12-
| Previous_Csection = 0: [767+,81-] .90+ .10-
| | Primiparous = 0: [399+,13-] .97+ .03-
| | Primiparous = 1: [368+,68-] .84+ .16-
| | | Fetal_Distress = 0: [334+,47-] .88+ .12-
| | | | Birth_Weight < 3349: [201+,10.6-] .95+ .05
| | | | Birth_Weight >= 3349: [133+,36.4-] .78+ .2
| | | Fetal_Distress = 1: [34+,21-] .62+ .38-
| Previous_Csection = 1: [55+,35-] .61+ .39-
Fetal_Presentation = 2: [3+,29-] .11+ .89-
Fetal_Presentation = 3: [8+,22-] .27+ .73-
```

Decision Trees

Decision tree representation:

- Each internal node tests an attribute
- Each branch corresponds to attribute value
- Each leaf node assigns a classification

How would we represent:

- $\wedge, \vee$, XOR
- $(A \wedge B) \vee (C \wedge \neg D \wedge E)$
- M of N

When to Consider Decision Trees

- Instances describable by attribute–value pairs
- Target function is discrete valued
- Disjunctive hypothesis may be required
- Possibly noisy training data

Examples:

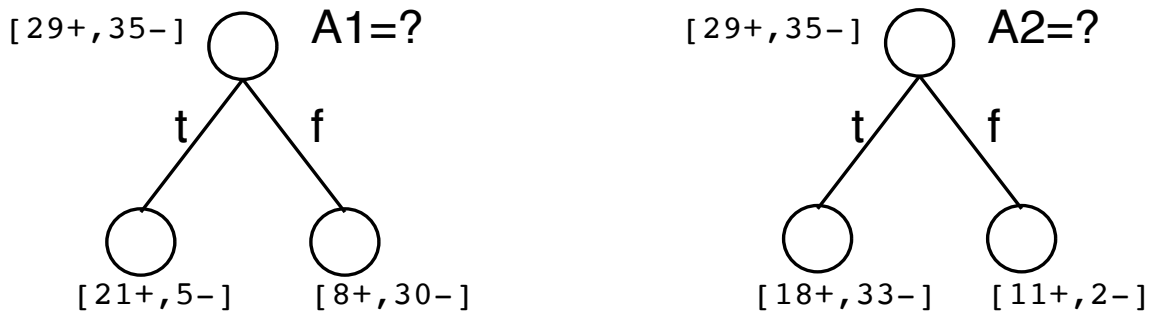
- Equipment or medical diagnosis
- Credit risk analysis
- Modeling calendar scheduling preferences

Top-Down Induction of Decision Trees

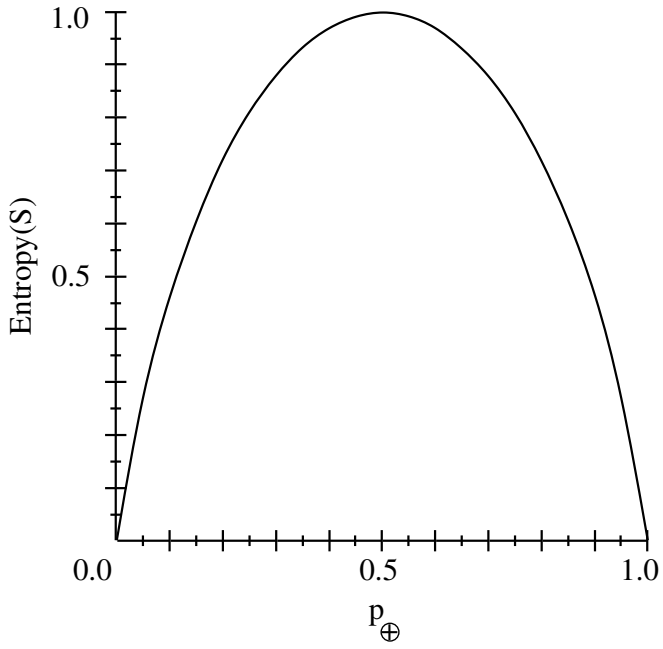
Main loop:

1. $A \leftarrow$ the "best" decision attribute for next *node*
2. Assign A as decision attribute for *node*
3. For each value of A, create new descendant of *node*
4. Sort training examples to leaf nodes
5. If training examples perfectly classified, Then STOP, Else iterate over new leaf nodes

Which attribute is best?



Entropy



- S is a sample of training examples
- $p_{\oplus}$ is the proportion of positive examples in S
- $p_{\ominus}$ is the proportion of negative examples in S
- Entropy measures the impurity of S

$$Entropy(S) \equiv -p_{\oplus} \log_2 p_{\oplus} - p_{\ominus} \log_2 p_{\ominus}$$

Entropy

$Entropy(S)$ = expected number of bits needed to encode class ($\oplus$ or $\ominus$) of randomly drawn member of S (under the optimal, shortest-length code)

Why?

Information theory: optimal length code assigns $-\log_2 p$ bits to message having probability p.

So, expected number of bits to encode $\oplus$ or $\ominus$ of random member of S:

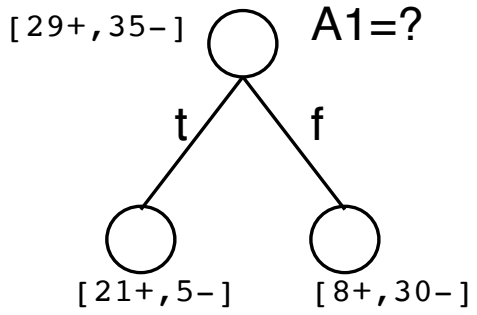
$$p_{\oplus}(-\log_2 p_{\oplus}) + p_{\ominus}(-\log_2 p_{\ominus})$$

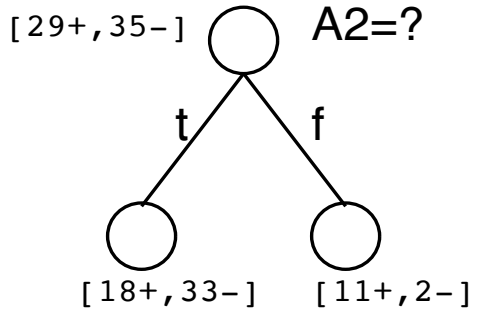
$$Entropy(S) \equiv -p_{\oplus}\log_2 p_{\oplus} - p_{\ominus}\log_2 p_{\ominus}$$

Information Gain

$Gain(S, A)$ = expected reduction in entropy due to sorting on A

$$Gain(S, A) \equiv Entropy(S) - \sum_{v \in Values(A)} \frac{|S_v|}{|S|} Entropy(S_v)$$



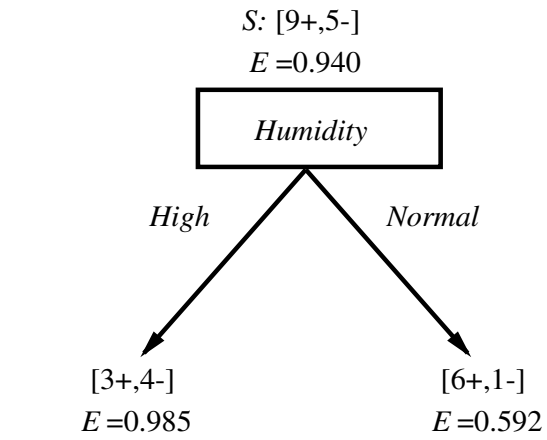


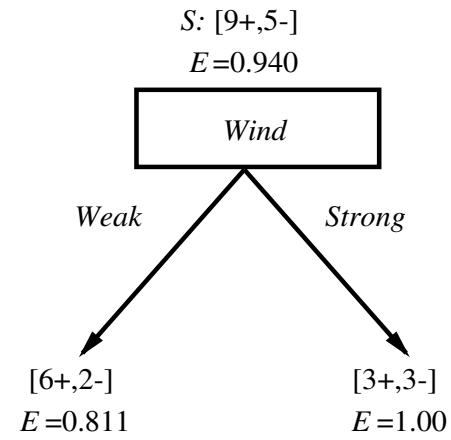
Training Examples

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Selecting the Next Attribute

Which attribute is the best classifier?



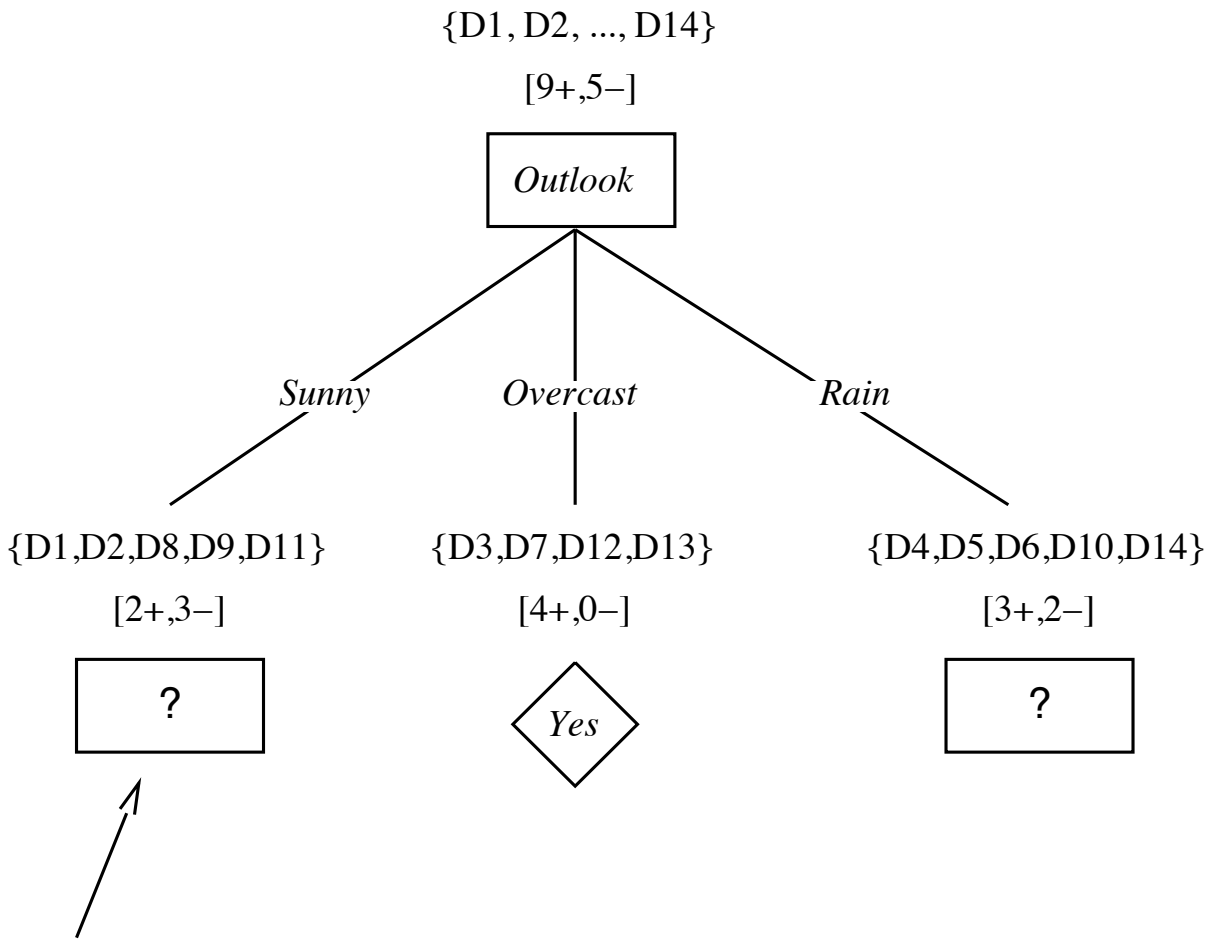


Gain (S, Humidity)

= .940 - (7/14).985 - (7/14).592
= .151

Gain (S, Wind)

= .940 - (8/14).811 - (6/14)1.0
= .048



Which attribute should be tested here?

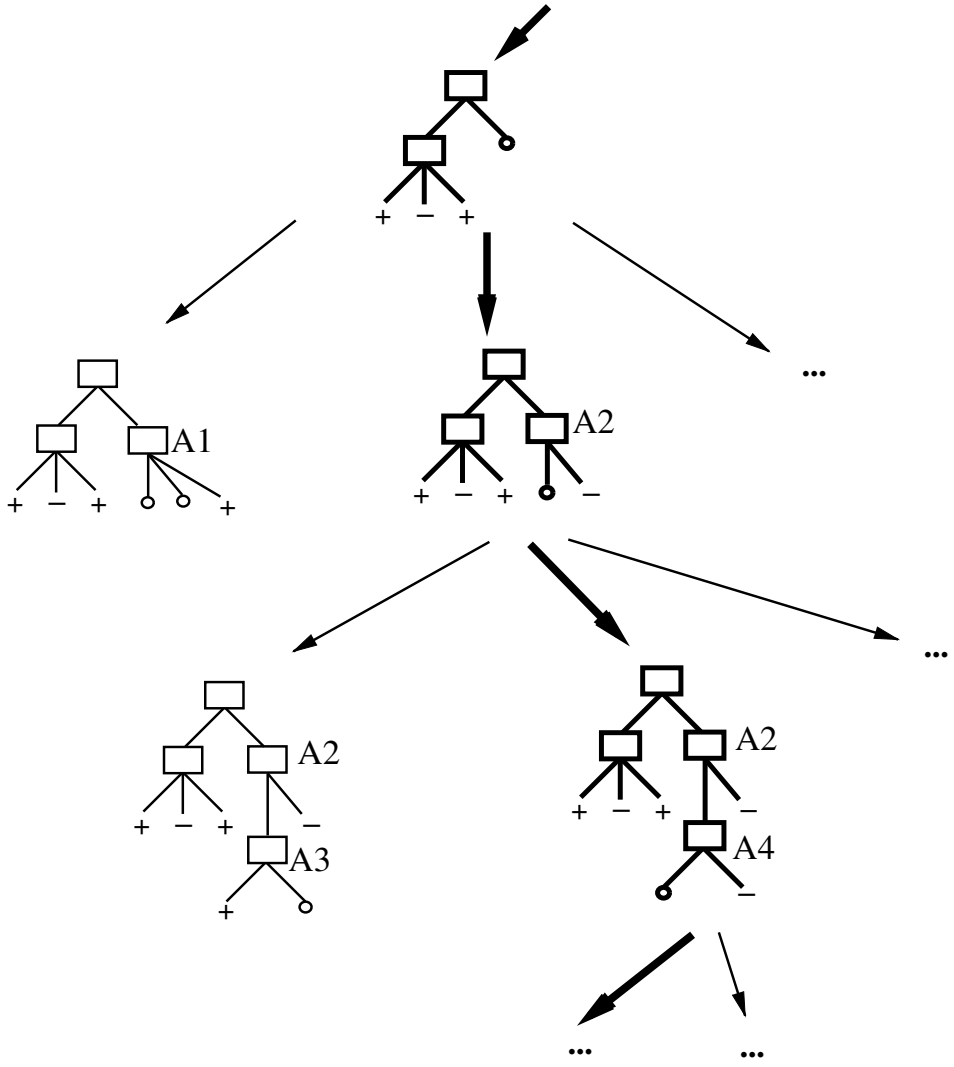
S_{sunny} = {D1,D2,D8,D9,D11}

Gain (S_{sunny} , *Humidity*) = .970 – (3/5) 0.0 – (2/5) 0.0 = .970

Gain (S_{sunny} , *Temperature*) = .970 – (2/5) 0.0 – (2/5) 1.0 – (1/5) 0.0 = .570

Gain (S_{sunny} , *Wind*) = .970 – (2/5) 1.0 – (3/5) .918 = .019

Hypothesis Space Search by ID3



Hypothesis Space Search by ID3

- Hypothesis space is complete!
  - Target function surely in there...
- Outputs a single hypothesis (which one?)
  - Can't play 20 questions...
- No back tracking
  - Local minima...
- Statisically-based search choices
  - Robust to noisy data...
- Inductive bias: approx "prefer shortest tree"

Inductive Bias in ID3

Note H is the power set of instances X

$\rightarrow$Unbiased?

Not really...

- Preference for short trees, and for those with high information gain attributes near the root
- Bias is a *preference* for some hypotheses, rather than a *restriction* of hypothesis space H
- Occam's razor: prefer the shortest hypothesis that fits the data

Occam's Razor

Why prefer short hypotheses?

Argument in favor:

- Fewer short hyps. than long hyps.

→ a short hyp that fits data unlikely to be coincidence

→ a long hyp that fits data might be coincidence

Argument opposed:

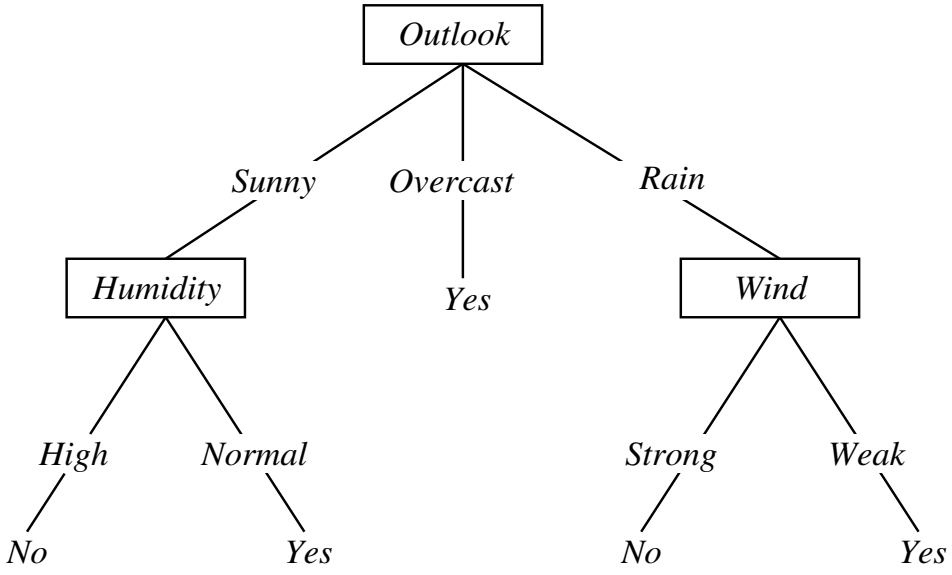
- There are many ways to define small sets of hyps
- e.g., all trees with a prime number of nodes that use attributes beginning with "Z"
- What's so special about small sets based on *size* of hypothesis??

Overfitting in Decision Trees

Consider adding noisy training example #15:

$Sunny,\ Hot,\ Normal,\ Strong,\ PlayTennis = No$

What effect on earlier tree?



Overfitting

Consider error of hypothesis h over

- training data: $error_{train}(h)$
- entire distribution $\mathcal{D}$ of data: $error_{\mathcal{D}}(h)$

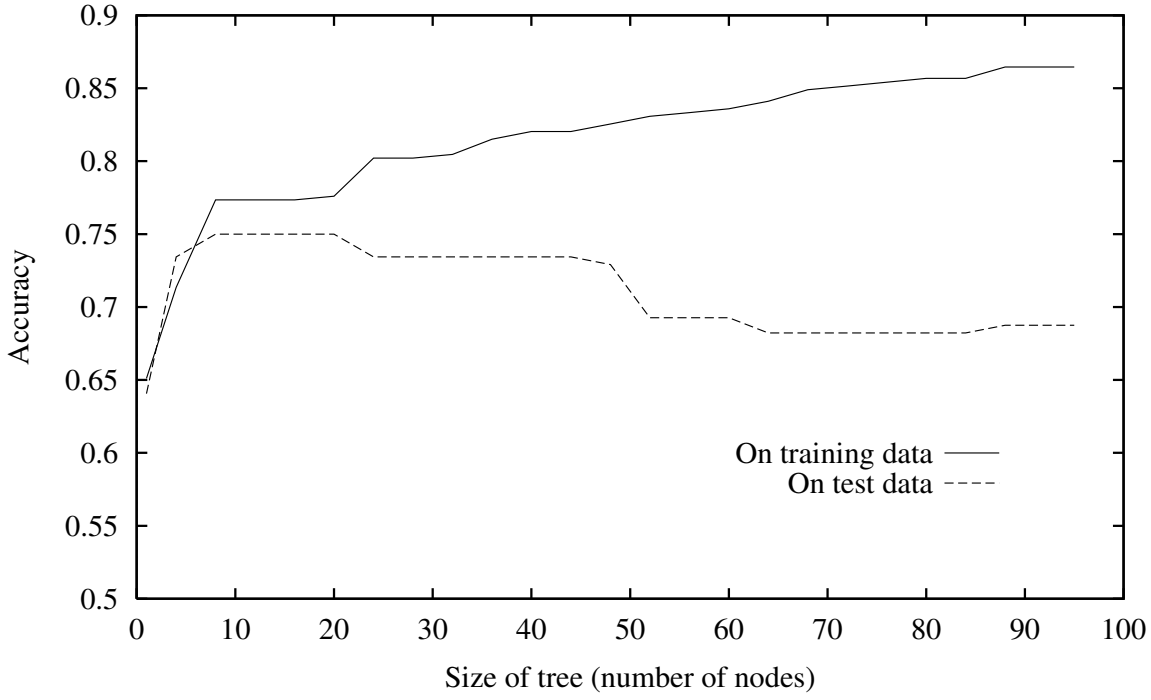
Hypothesis $h \in H$ **overfits** training data if there is an alternative hypothesis $h' \in H$ such that

$$error_{train}(h) < error_{train}(h')$$

and

$$error_{\mathcal{D}}(h) > error_{\mathcal{D}}(h')$$

Overfitting in Decision Tree Learning



Avoiding Overfitting

How can we avoid overfitting?

- stop growing when data split not statistically significant
- grow full tree, then post-prune

How to select "best" tree:

- Measure performance over training data
- Measure performance over separate validation data set
- MDL: minimize
  $size(tree) + size(misclassifications(tree))$

Reduced-Error Pruning

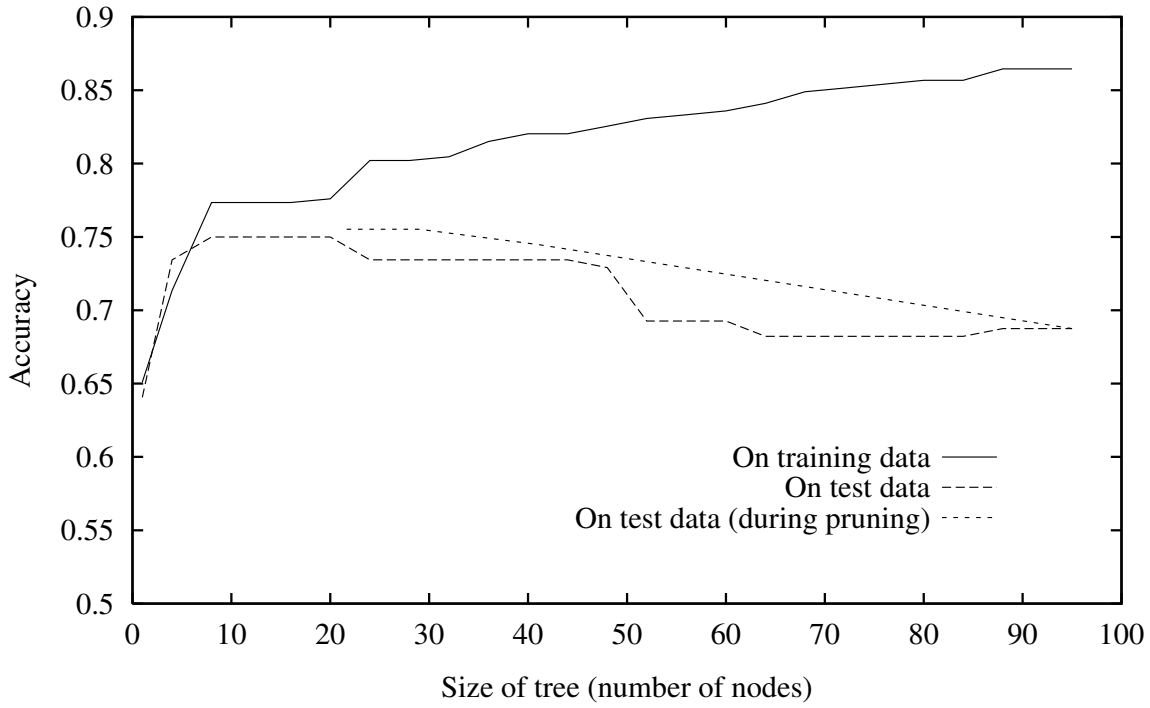
Split data into *training* and *validation* set

Do until further pruning is harmful:

1. Evaluate impact on *validation* set of pruning each possible node (plus those below it)
2. Greedily remove the one that most improves *validation* set accuracy

- produces smallest version of most accurate subtree
- What if data is limited?

Effect of Reduced-Error Pruning

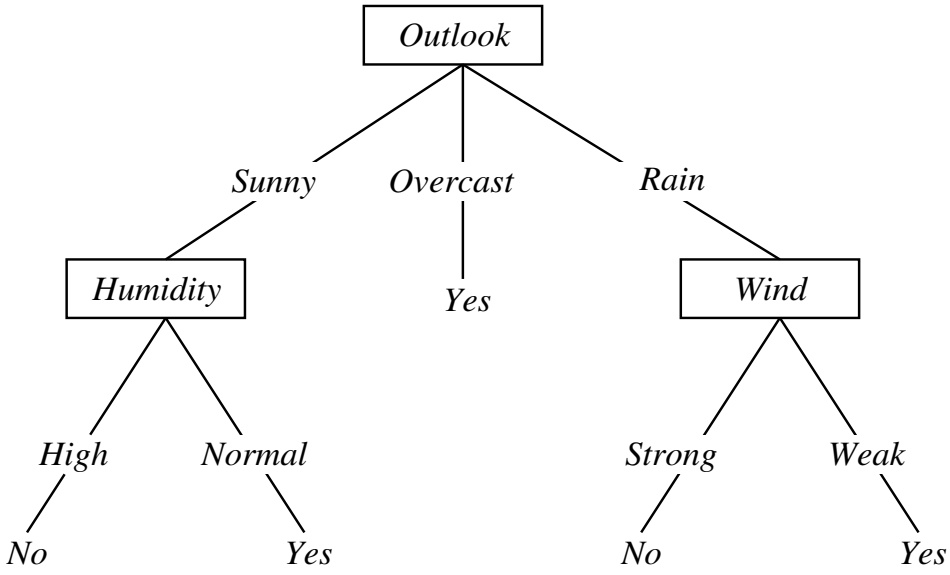


Rule Post-Pruning

1. Convert tree to equivalent set of rules
2. Prune each rule independently of others
3. Sort final rules into desired sequence for use

Perhaps most frequently used method (e.g., C4.5)

Converting A Tree to Rules



IF $(Outlook = Sunny) \wedge (Humidity = High)$
THEN $PlayTennis = No$

IF $(Outlook = Sunny) \wedge (Humidity = Normal)$
THEN $PlayTennis = Yes$

...

Continuous Valued Attributes

Create a discrete attribute to test continuous

- $Temperature = 82.5$
- $(Temperature > 72.3) = t, f$

Temperature:	40	48	60	72	80	90
PlayTennis:	No	No	Yes	Yes	Yes	No

Attributes with Many Values

Problem:

- If attribute has many values, $Gain$ will select it
- Imagine using $Date = Jun\_3\_1996$ as attribute

One approach: use $GainRatio$ instead

$$GainRatio(S, A) \equiv \frac{Gain(S, A)}{SplitInformation(S, A)}$$

$$SplitInformation(S, A) \equiv -\sum_{i=1}^{c} \frac{|S_i|}{|S|} \log_2 \frac{|S_i|}{|S|}$$

where S_i is subset of S for which A has value v_i

Attributes with Costs

Consider

- medical diagnosis, $BloodTest$ has cost \$150
- robotics, $Width\_from\_1ft$ has cost 23 sec.

How to learn a consistent tree with low expected cost?
One approach: replace gain by

- Tan and Schlimmer (1990)

$$\frac{Gain^2(S, A)}{Cost(A)}.$$

- Nunez (1988)

$$\frac{2^{Gain(S,A)} - 1}{(Cost(A) + 1)^w}$$

where $w \in [0, 1]$ determines importance of cost

Unknown Attribute Values

What if some examples missing values of A?
Use training example anyway, sort through tree

- If node n tests A, assign most common value of A among other examples sorted to node n
- assign most common value of A among other examples with same target value
- assign probability p_i to each possible value v_i of A
  - assign fraction p_i of example to each descendant in tree

Classify new examples in same fashion

Artificial Neural Networks

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

- Threshold units
- Gradient descent
- Multilayer networks
- Backpropagation
- Hidden layer representations
- Example: Face Recognition
- Advanced topics

Connectionist Models

Consider humans:

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

$\rightarrow$ much parallel computation

Properties of artificial neural nets (ANN's):

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

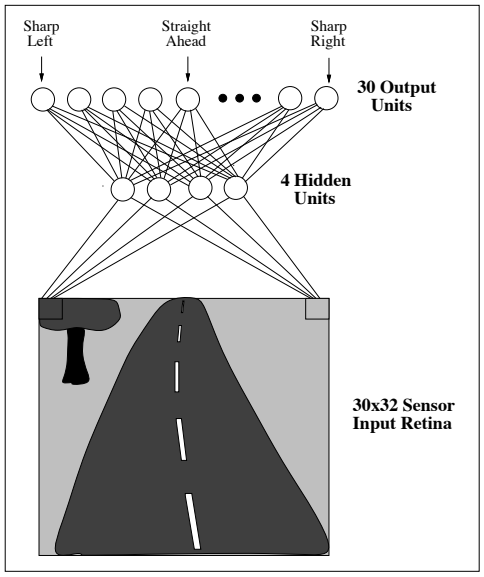
When to Consider Neural Networks

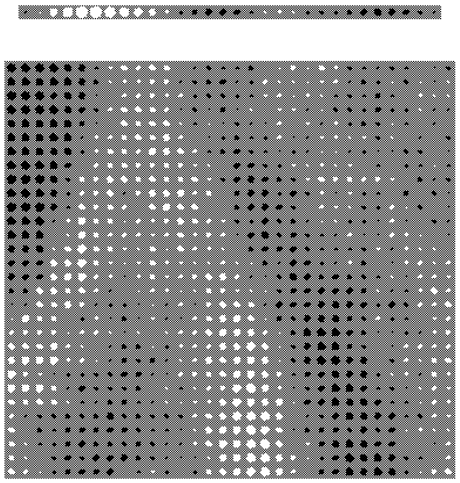
- Input is high-dimensional discrete or real-valued (e.g. raw sensor input)
- Output is discrete or real valued
- Output is a vector of values
- Possibly noisy data
- Form of target function is unknown
- Human readability of result is unimportant

Examples:

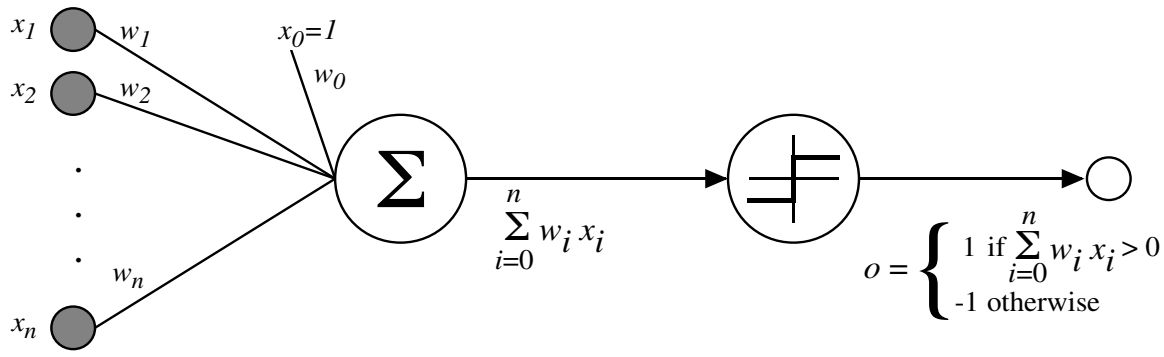
- Speech phoneme recognition [Waibel]
- Image classification [Kanade, Baluja, Rowley]
- Financial prediction

ALVINN drives 70 mph on highways





Perceptron

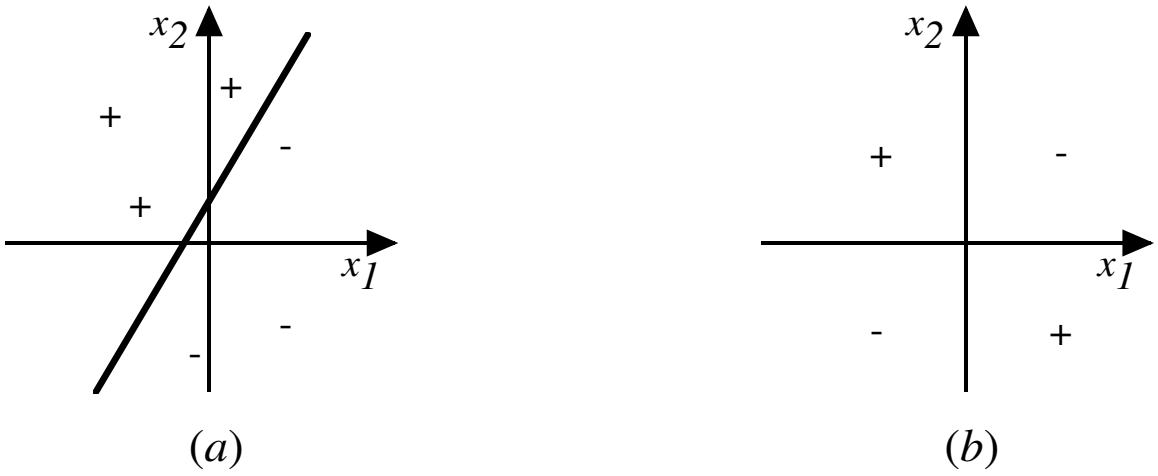


$$o(x_1, \ldots, x_n) = \begin{cases} 1 & \text{if } w_0 + w_1 x_1 + \cdots + w_n x_n > 0 \\ -1 & \text{otherwise.} \end{cases}$$

Sometimes we'll use simpler vector notation:

$$o(\vec{x}) = \begin{cases} 1 & \text{if } \vec{w} \cdot \vec{x} > 0 \\ -1 & \text{otherwise.} \end{cases}$$

Decision Surface of a Perceptron



Represents some useful functions

- What weights represent $g(x_1, x_2) = AND(x_1, x_2)$?

But some functions not representable

- e.g., not linearly separable
- Therefore, we'll want networks of these...

Perceptron training rule

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

where

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

Where:

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

Perceptron training rule

Can prove it will converge

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

Gradient Descent

To understand, consider simpler *linear unit*, where

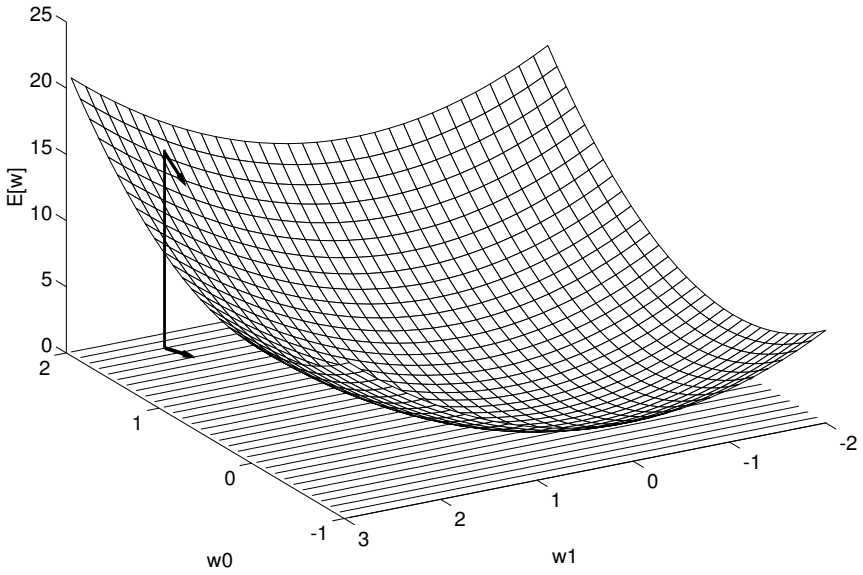
$$o = w_0 + w_1 x_1 + \cdots + w_n x_n$$

Let's learn w_i's that minimize the squared error

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

Where D is set of training examples

Gradient Descent



Gradient

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

Training rule:

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

i.e.,

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

Gradient Descent

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

Gradient Descent

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

Each training example is a pair of the form $\langle \vec{x}, t \rangle$*, where* $\vec{x}$ *is the vector of input values, and* t *is the target output value.* η *is the learning rate (e.g., .05).*

- Initialize each w_i to some small random value
- Until the termination condition is met, Do
  - Initialize each Δw_i to zero.
  - For each $\langle \vec{x}, t \rangle$ in *training_examples*, Do
    - Input the instance $\vec{x}$ to the unit and compute the output o
    - For each linear unit weight w_i, Do

$$\Delta w_i \leftarrow \Delta w_i + \eta(t - o)x_i$$

  - For each linear unit weight w_i, Do

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

Summary

Perceptron training rule guaranteed to succeed if

- Training examples are linearly separable
- Sufficiently small learning rate η

Linear unit training rule uses gradient descent

- Guaranteed to converge to hypothesis with minimum squared error
- Given sufficiently small learning rate η
- Even when training data contains noise
- Even when training data not separable by H

Incremental (Stochastic) Gradient Descent

Batch mode Gradient Descent:
Do until satisfied

1. Compute the gradient $\nabla E_D[\vec{w}]$
2. $\vec{w} \leftarrow \vec{w} - \eta \nabla E_D[\vec{w}]$

Incremental mode Gradient Descent:
Do until satisfied

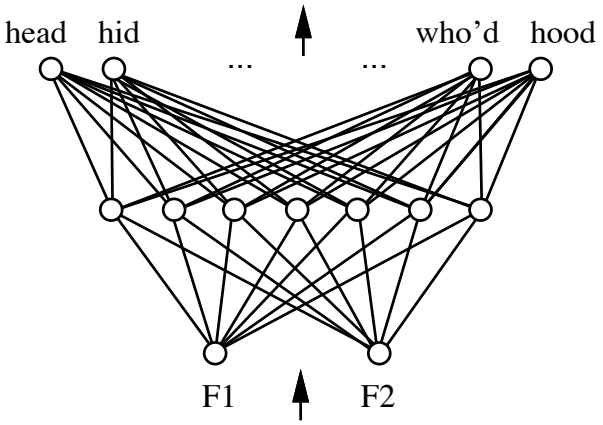
- For each training example d in D
  1. Compute the gradient $\nabla E_d[\vec{w}]$
  2. $\vec{w} \leftarrow \vec{w} - \eta \nabla E_d[\vec{w}]$

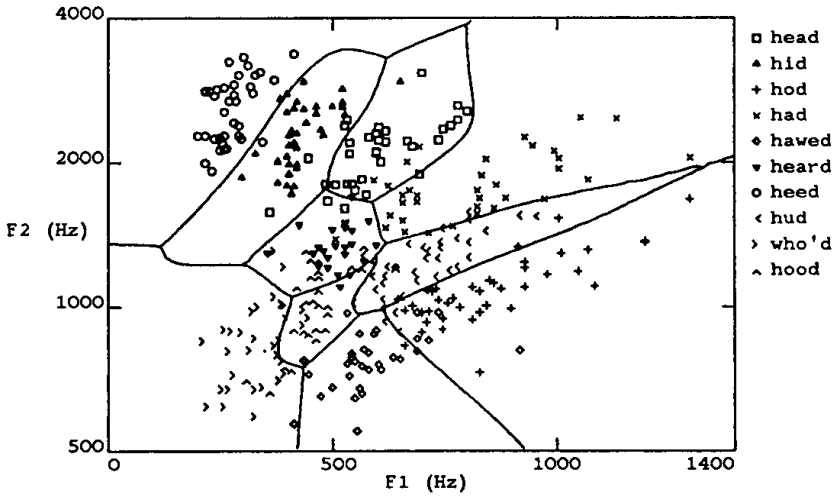
$$E_D[\vec{w}] \equiv \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2$$

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

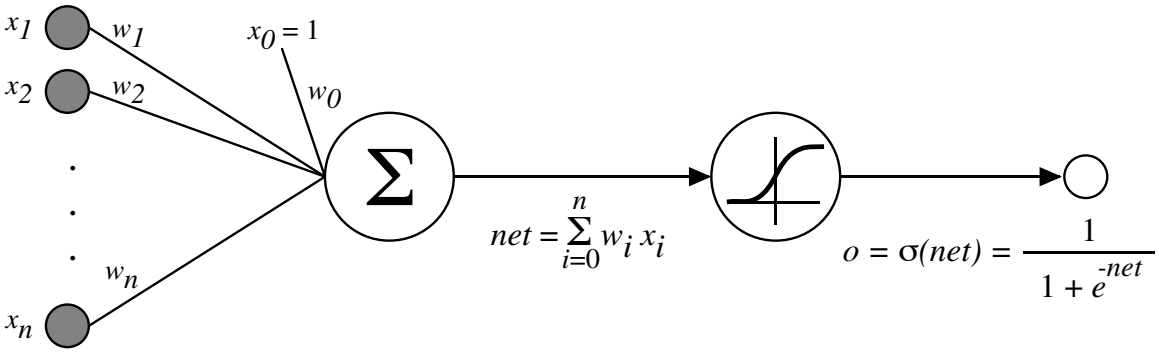
Incremental Gradient Descent can approximate *Batch Gradient Descent* arbitrarily closely if η made small enough

Multilayer Networks of Sigmoid Units





Sigmoid Unit



$\sigma(x)$ is the sigmoid function

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

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

We can derive gradient decent rules to train

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

Error Gradient for a Sigmoid Unit

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

But we know:

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

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

So:

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

Backpropagation Algorithm

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

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

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

  3. For each hidden unit h

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

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

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

  where

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

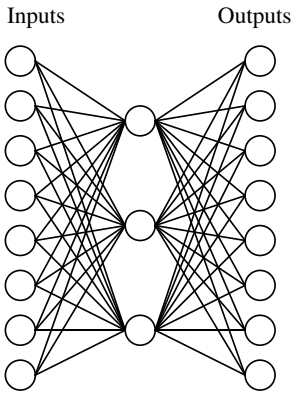
More on Backpropagation

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

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

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

Learning Hidden Layer Representations



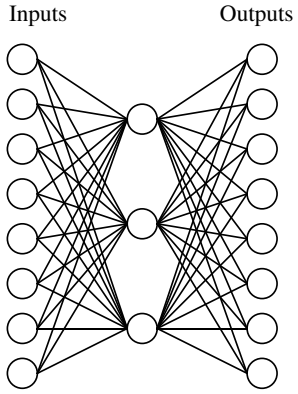
A target function:

Input		Output
10000000	$\rightarrow$	10000000
01000000	$\rightarrow$	01000000
00100000	$\rightarrow$	00100000
00010000	$\rightarrow$	00010000
00001000	$\rightarrow$	00001000
00000100	$\rightarrow$	00000100
00000010	$\rightarrow$	00000010
00000001	$\rightarrow$	00000001

Can this be learned??

Learning Hidden Layer Representations

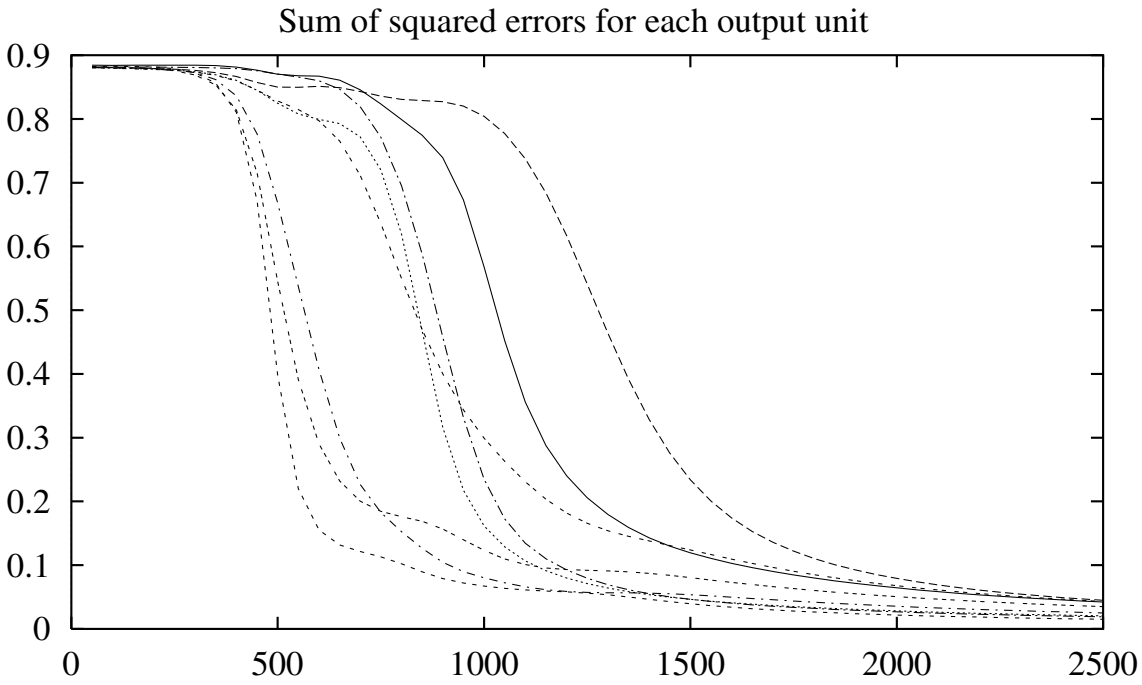
A network:



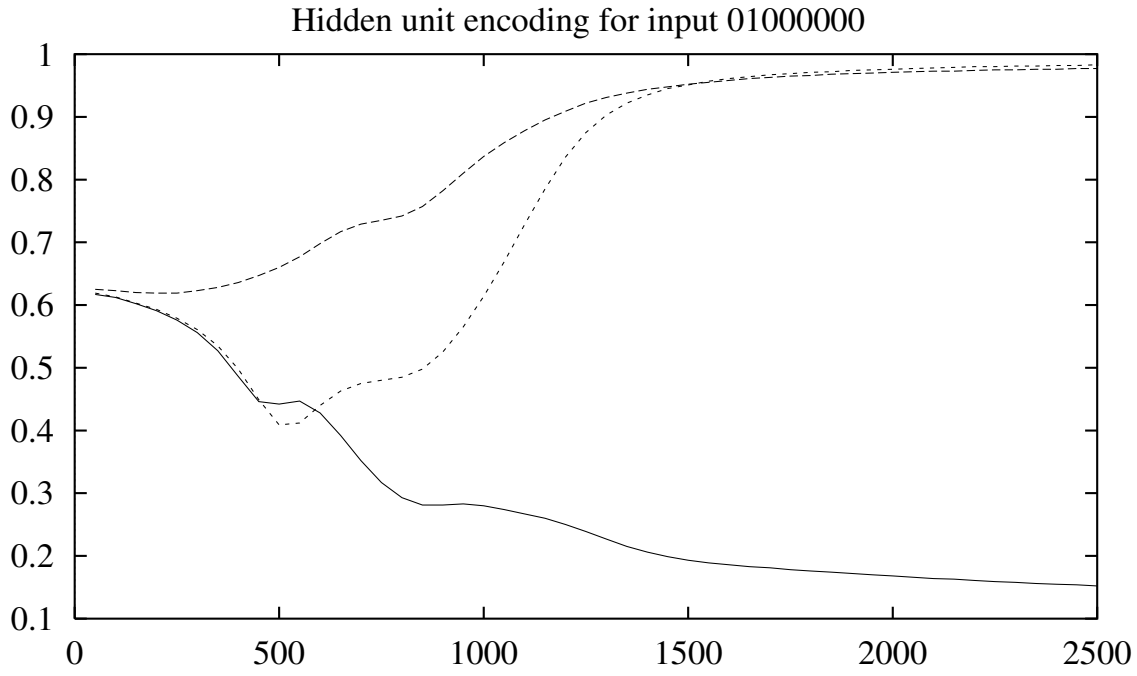
Learned hidden layer representation:

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

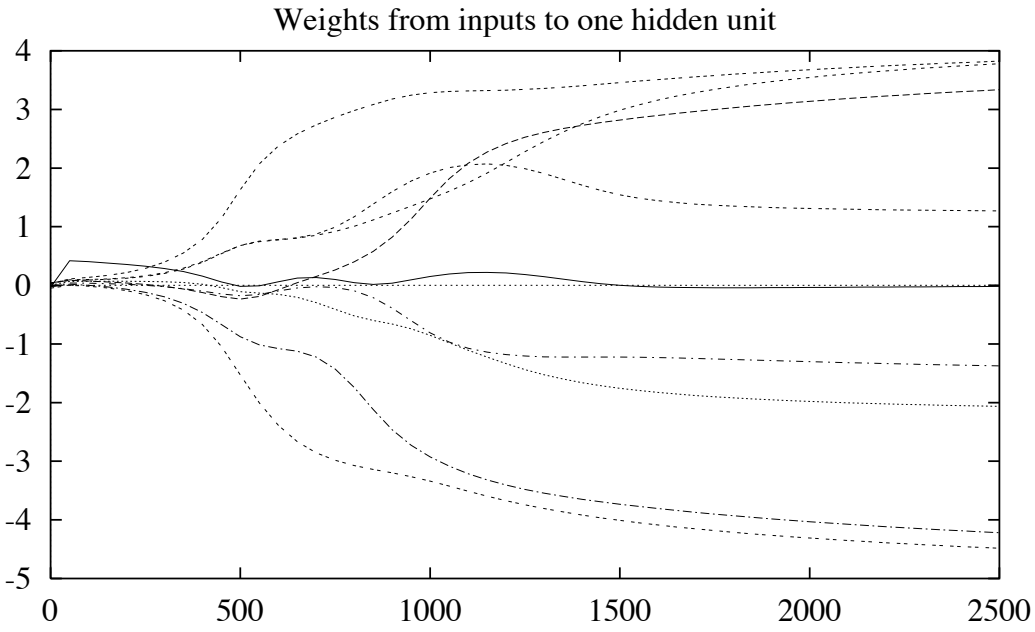
Training


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

Training


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

Training


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

Convergence of Backpropagation

Gradient descent to some local minimum

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

Nature of convergence

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

Expressive Capabilities of ANNs

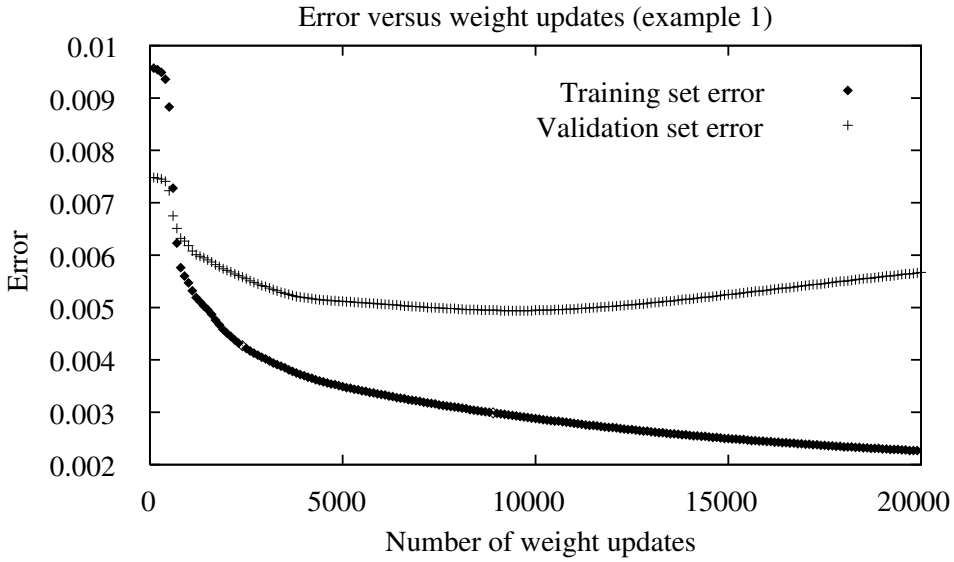
Boolean functions:

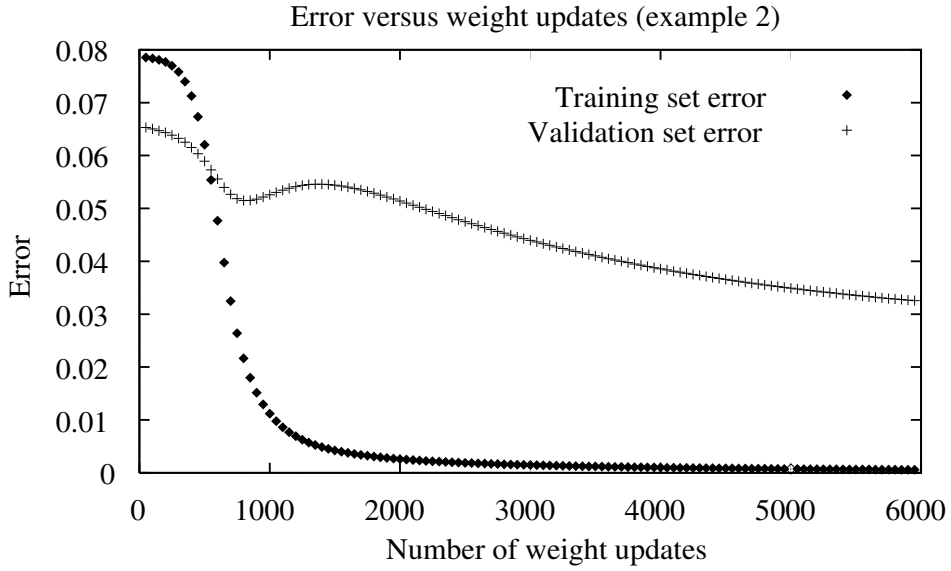
- Every boolean function can be represented by network with single hidden layer
- but might require exponential (in number of inputs) hidden units

Continuous functions:

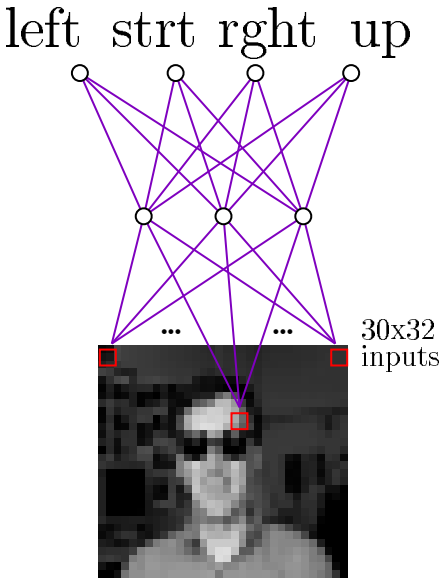
- Every bounded continuous function can be approximated with arbitrarily small error, by network with one hidden layer [Cybenko 1989; Hornik et al. 1989]
- Any function can be approximated to arbitrary accuracy by a network with two hidden layers [Cybenko 1988].

Overfitting in ANNs





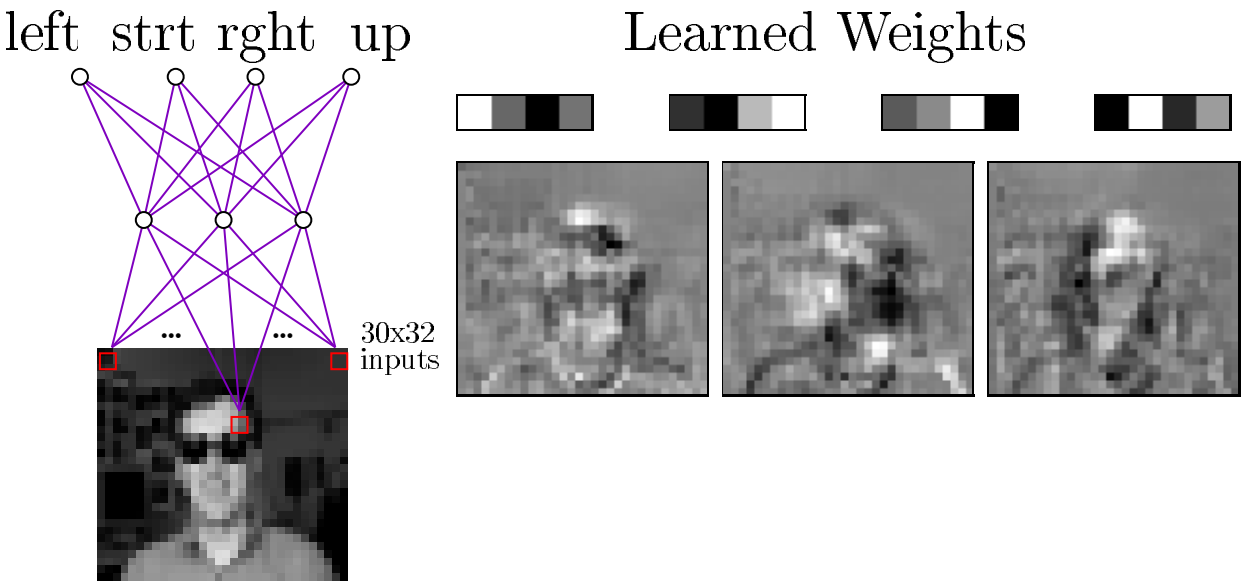
Neural Nets for Face Recognition



Typical input images

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

Learned Hidden Unit Weights



Typical input images

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

Alternative Error Functions

Penalize large weights:

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

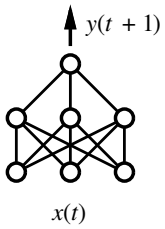
Train on target slopes as well as values:

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

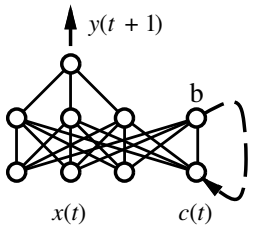
Tie together weights:

- e.g., in phoneme recognition network

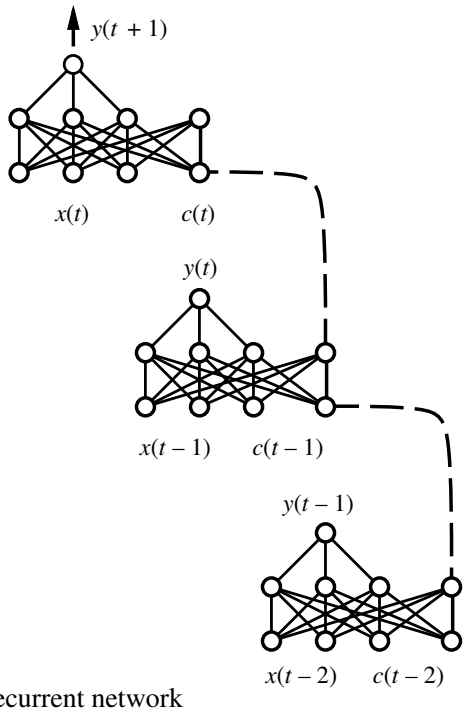
Recurrent Networks



(*a*) Feedforward network



(*b*) Recurrent network



(*c*) Recurrent network unfolded in time

Evaluating Hypotheses

[Read Ch. 5]
[Recommended exercises: 5.2, 5.3, 5.4]

- Sample error, true error
- Confidence intervals for observed hypothesis error
- Estimators
- Binomial distribution, Normal distribution, Central Limit Theorem
- Paired t tests
- Comparing learning methods

Two Definitions of Error

The **true error** of hypothesis h with respect to target function f and distribution $\mathcal{D}$ is the probability that h will misclassify an instance drawn at random according to $\mathcal{D}$.

$$error_{\mathcal{D}}(h) \equiv \Pr_{x \in \mathcal{D}}[f(x) \neq h(x)]$$

The **sample error** of h with respect to target function f and data sample S is the proportion of examples h misclassifies

$$error_S(h) \equiv \frac{1}{n} \sum_{x \in S} \delta(f(x) \neq h(x))$$

Where $\delta(f(x) \neq h(x))$ is 1 if $f(x) \neq h(x)$, and 0 otherwise.

How well does $error_S(h)$ estimate $error_{\mathcal{D}}(h)$?

Problems Estimating Error

1. *Bias:* If S is training set, $error_S(h)$ is optimistically biased

$$bias \equiv E[error_S(h)] - error_{\mathcal{D}}(h)$$

   For unbiased estimate, h and S must be chosen independently

2. *Variance:* Even with unbiased S, $error_S(h)$ may still *vary* from $error_{\mathcal{D}}(h)$

Example

Hypothesis h misclassifies 12 of the 40 examples in S

$$error_S(h) = \frac{12}{40} = .30$$

What is $error_{\mathcal{D}}(h)$?

Estimators

Experiment:

1. choose sample S of size n according to distribution $\mathcal{D}$
2. measure $error_S(h)$

$error_S(h)$ is a random variable (i.e., result of an experiment)

$error_S(h)$ is an unbiased *estimator* for $error_{\mathcal{D}}(h)$

Given observed $error_S(h)$ what can we conclude about $error_{\mathcal{D}}(h)$?

Confidence Intervals

If

- S contains n examples, drawn independently of h and each other
- $n \geq 30$

Then

- With approximately 95% probability, $error_{\mathcal{D}}(h)$ lies in interval

$$error_S(h) \pm 1.96\sqrt{\frac{error_S(h)(1 - error_S(h))}{n}}$$

Confidence Intervals

If

- S contains n examples, drawn independently of h and each other
- $n \geq 30$

Then

- With approximately N% probability, $error_{\mathcal{D}}(h)$ lies in interval

$$error_S(h) \pm z_N \sqrt{\frac{error_S(h)(1 - error_S(h))}{n}}$$

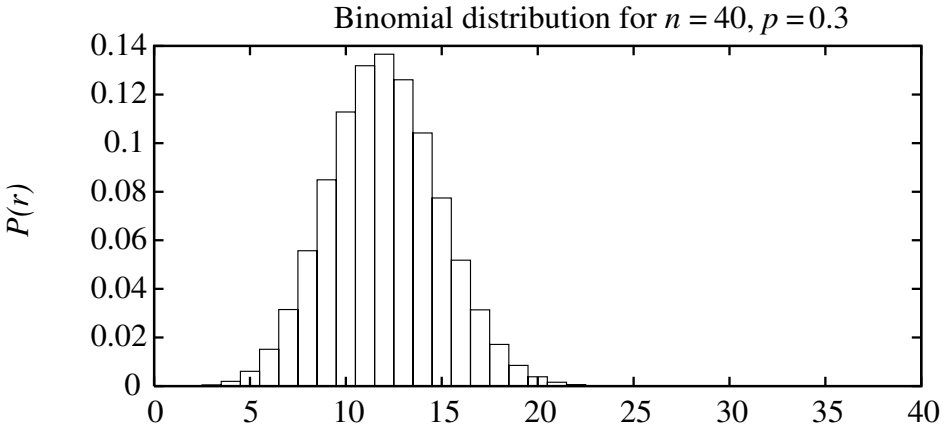
where

$N\%$:	50%	68%	80%	90%	95%	98%	99%
z_N:	0.67	1.00	1.28	1.64	1.96	2.33	2.58

$error_S(h)$ is a Random Variable

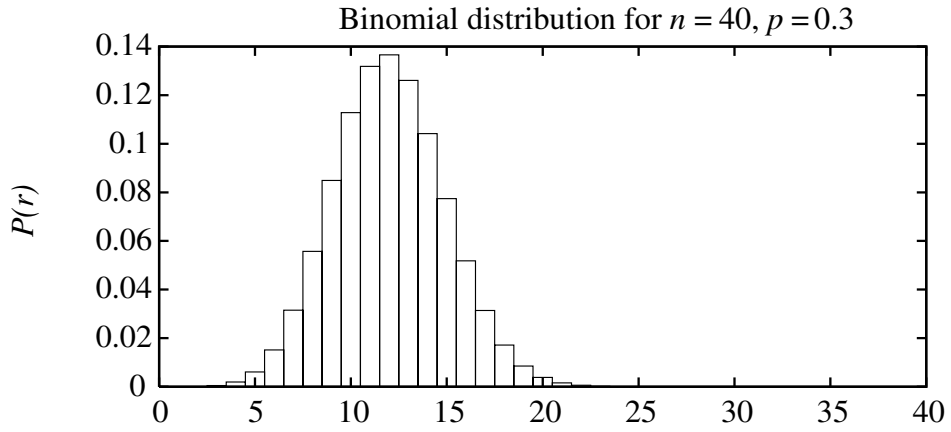
Rerun the experiment with different randomly drawn S (of size n)

Probability of observing r misclassified examples:



$$P(r) = \frac{n!}{r!(n-r)!} error_{\mathcal{D}}(h)^r (1 - error_{\mathcal{D}}(h))^{n-r}$$

Binomial Probability Distribution



$$P(r) = \frac{n!}{r!(n-r)!} p^r (1-p)^{n-r}$$

Probability $P(r)$ of r heads in n coin flips, if $p = \Pr(heads)$

- Expected, or mean value of X, $E[X]$, is

$$E[X] \equiv \sum_{i=0}^{n} iP(i) = np$$

- Variance of X is

$$Var(X) \equiv E[(X - E[X])^2] = np(1-p)$$

- Standard deviation of X, σ_X, is

$$\sigma_X \equiv \sqrt{E[(X - E[X])^2]} = \sqrt{np(1-p)}$$

Normal Distribution Approximates Binomial

$error_S(h)$ follows a *Binomial* distribution, with

- mean $\mu_{error_S(h)} = error_{\mathcal{D}}(h)$
- standard deviation $\sigma_{error_S(h)}$

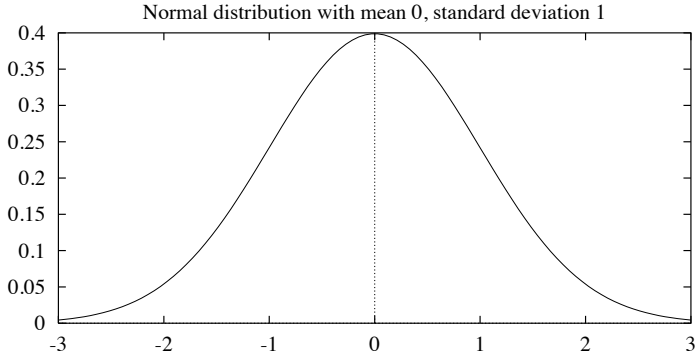
$$\sigma_{error_S(h)} = \sqrt{\frac{error_{\mathcal{D}}(h)(1 - error_{\mathcal{D}}(h))}{n}}$$

Approximate this by a *Normal* distribution with

- mean $\mu_{error_S(h)} = error_{\mathcal{D}}(h)$
- standard deviation $\sigma_{error_S(h)}$

$$\sigma_{error_S(h)} \approx \sqrt{\frac{error_S(h)(1 - error_S(h))}{n}}$$

Normal Probability Distribution



$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^2}$$

The probability that X will fall into the interval (a, b) is given by

$$\int_a^b p(x)dx$$

- Expected, or mean value of X, $E[X]$, is

$$E[X] = \mu$$

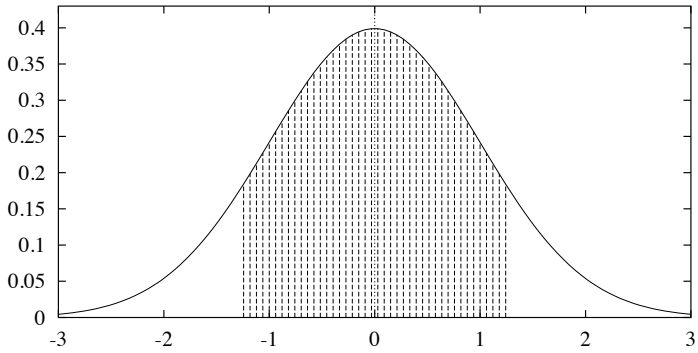
- Variance of X is

$$Var(X) = \sigma^2$$

- Standard deviation of X, σ_X, is

$$\sigma_X = \sigma$$

Normal Probability Distribution



80% of area (probability) lies in $\mu \pm 1.28\sigma$

N% of area (probability) lies in $\mu \pm z_N \sigma$

$N\%$:	50%	68%	80%	90%	95%	98%	99%
z_N:	0.67	1.00	1.28	1.64	1.96	2.33	2.58

Confidence Intervals, More Correctly

If

- S contains n examples, drawn independently of h and each other
- $n \geq 30$

Then

- With approximately 95% probability, $error_S(h)$ lies in interval

$$error_{\mathcal{D}}(h) \pm 1.96\sqrt{\frac{error_{\mathcal{D}}(h)(1-error_{\mathcal{D}}(h))}{n}}$$

equivalently, $error_{\mathcal{D}}(h)$ lies in interval

$$error_S(h) \pm 1.96\sqrt{\frac{error_{\mathcal{D}}(h)(1-error_{\mathcal{D}}(h))}{n}}$$

which is approximately

$$error_S(h) \pm 1.96\sqrt{\frac{error_S(h)(1-error_S(h))}{n}}$$

Central Limit Theorem

Consider a set of independent, identically distributed random variables $Y_1 \ldots Y_n$, all governed by an arbitrary probability distribution with mean μ and finite variance σ^2. Define the sample mean,

$$\bar{Y} \equiv \frac{1}{n} \sum_{i=1}^{n} Y_i$$

Central Limit Theorem. As $n \to \infty$, the distribution governing $\bar{Y}$ approaches a Normal distribution, with mean μ and variance $\frac{\sigma^2}{n}$.

Calculating Confidence Intervals

1. Pick parameter p to estimate
   - $error_{\mathcal{D}}(h)$
2. Choose an estimator
   - $error_S(h)$
3. Determine probability distribution that governs estimator
   - $error_S(h)$ governed by Binomial distribution, approximated by Normal when $n \geq 30$
4. Find interval (L, U) such that N% of probability mass falls in the interval
   - Use table of z_N values

Difference Between Hypotheses

Test h_1 on sample S_1, test h_2 on S_2

1. Pick parameter to estimate

$$d \equiv error_{\mathcal{D}}(h_1) - error_{\mathcal{D}}(h_2)$$

2. Choose an estimator

$$\hat{d} \equiv error_{S_1}(h_1) - error_{S_2}(h_2)$$

3. Determine probability distribution that governs estimator

$$\sigma_{\hat{d}} \approx \sqrt{\frac{\text{error}_{S_1}(h_1)(1-\text{error}_{S_1}(h_1))}{n_1} + \frac{\text{error}_{S_2}(h_2)(1-\text{error}_{S_2}(h_2))}{n_2}}$$

4. Find interval (L, U) such that N% of probability mass falls in the interval

$$\hat{d} \pm z_N \sqrt{\frac{error_{S_1}(h_1)(1-error_{S_1}(h_1))}{n_1} + \frac{error_{S_2}(h_2)(1-error_{S}}{n_2}}$$

Paired t test to compare h_A,h_B

1. Partition data into k disjoint test sets $T_1, T_2, \ldots, T_k$ of equal size, where this size is at least 30.
2. For i from 1 to k, do

$$\delta_i \leftarrow error_{T_i}(h_A) - error_{T_i}(h_B)$$

3. Return the value $\bar{\delta}$, where

$$\bar{\delta} \equiv \frac{1}{k} \sum_{i=1}^{k} \delta_i$$

$N\%$ confidence interval estimate for d:

$$\bar{\delta} \pm t_{N,k-1}\ s_{\bar{\delta}}$$

$$s_{\bar{\delta}} \equiv \sqrt{\frac{1}{k(k-1)} \sum_{i=1}^{k} (\delta_i - \bar{\delta})^2}$$

Note δ_i approximately Normally distributed

Comparing learning algorithms L_A and L_B

What we'd like to estimate:

$$E_{S \subset \mathcal{D}}[error_{\mathcal{D}}(L_A(S)) - error_{\mathcal{D}}(L_B(S))]$$

where $L(S)$ is the hypothesis output by learner L using training set S

i.e., the expected difference in true error between hypotheses output by learners L_A and L_B, when trained using randomly selected training sets S drawn according to distribution $\mathcal{D}$.

But, given limited data D_0, what is a good estimator?

- could partition D_0 into training set S and training set T_0, and measure

$$error_{T_0}(L_A(S_0)) - error_{T_0}(L_B(S_0))$$

- even better, repeat this many times and average the results (next slide)

Comparing learning algorithms L_A and L_B

---

1. Partition data D_0 into k disjoint test sets $T_1, T_2, \ldots, T_k$ of equal size, where this size is at least 30.
2. For i from 1 to k, do

   use T_i for the test set, and the remaining data for training set S_i

   - $S_i \leftarrow \{D_0 - T_i\}$
   - $h_A \leftarrow L_A(S_i)$
   - $h_B \leftarrow L_B(S_i)$
   - $\delta_i \leftarrow error_{T_i}(h_A) - error_{T_i}(h_B)$
3. Return the value $\bar{\delta}$, where

$$\bar{\delta} \equiv \frac{1}{k} \sum_{i=1}^{k} \delta_i$$

Comparing learning algorithms L_A and L_B

Notice we'd like to use the paired t test on $\bar{\delta}$ to obtain a confidence interval

but not really correct, because the training sets in this algorithm are not independent (they overlap!)

more correct to view algorithm as producing an estimate of

$$E_{S \subset D_0}[error_{\mathcal{D}}(L_A(S)) - error_{\mathcal{D}}(L_B(S))]$$

instead of

$$E_{S \subset \mathcal{D}}[error_{\mathcal{D}}(L_A(S)) - error_{\mathcal{D}}(L_B(S))]$$

but even this approximation is better than no comparison

Bayesian Learning

[Read Ch. 6]
[Suggested exercises: 6.1, 6.2, 6.6]

- Bayes Theorem
- MAP, ML hypotheses
- MAP learners
- Minimum description length principle
- Bayes optimal classifier
- Naive Bayes learner
- Example: Learning over text data
- Bayesian belief networks
- Expectation Maximization algorithm

Two Roles for Bayesian Methods

Provides practical learning algorithms:

- Naive Bayes learning
- Bayesian belief network learning
- Combine prior knowledge (prior probabilities) with observed data
- Requires prior probabilities

Provides useful conceptual framework

- Provides "gold standard" for evaluating other learning algorithms
- Additional insight into Occam's razor

Bayes Theorem

$$P(h|D) = \frac{P(D|h)P(h)}{P(D)}$$

- $P(h)$ = prior probability of hypothesis h
- $P(D)$ = prior probability of training data D
- $P(h|D)$ = probability of h given D
- $P(D|h)$ = probability of D given h

Choosing Hypotheses

$$P(h|D) = \frac{P(D|h)P(h)}{P(D)}$$

Generally want the most probable hypothesis given the training data

Maximum a posteriori hypothesis h_{MAP}:

$$\begin{aligned} h_{MAP} &= \arg\max_{h \in H} P(h|D) \\ &= \arg\max_{h \in H} \frac{P(D|h)P(h)}{P(D)} \\ &= \arg\max_{h \in H} P(D|h)P(h) \end{aligned}$$

If assume $P(h_i) = P(h_j)$ then can further simplify, and choose the *Maximum likelihood* (ML) hypothesis

$$h_{ML} = \arg\max_{h_i \in H} P(D|h_i)$$

Bayes Theorem

Does patient have cancer or not?

A patient takes a lab test and the result comes back positive. The test returns a correct positive result in only 98% of the cases in which the disease is actually present, and a correct negative result in only 97% of the cases in which the disease is not present. Furthermore, .008 of the entire population have this cancer.

$$P(cancer) = \qquad P(\neg cancer) =$$
$$P(+|cancer) = \qquad P(-|cancer) =$$
$$P(+|\neg cancer) = \qquad P(-|\neg cancer) =$$

Basic Formulas for Probabilities

- *Product Rule*: probability $P(A \wedge B)$ of a conjunction of two events A and B:

$$P(A \wedge B) = P(A|B)P(B) = P(B|A)P(A)$$

- *Sum Rule*: probability of a disjunction of two events A and B:

$$P(A \vee B) = P(A) + P(B) - P(A \wedge B)$$

- *Theorem of total probability*: if events $A_1, \ldots, A_n$ are mutually exclusive with $\Sigma_{i=1}^{n} P(A_i) = 1$, then

$$P(B) = \sum_{i=1}^{n} P(B|A_i)P(A_i)$$

Brute Force MAP Hypothesis Learner

1. For each hypothesis h in H, calculate the posterior probability

$$P(h|D) = \frac{P(D|h)P(h)}{P(D)}$$

2. Output the hypothesis h_{MAP} with the highest posterior probability

$$h_{MAP} = \underset{h \in H}{\operatorname{argmax}} P(h|D)$$

Relation to Concept Learning

Consider our usual concept learning task

- instance space X, hypothesis space H, training examples D
- consider the FindS learning algorithm (outputs most specific hypothesis from the version space $VS_{H,D}$)

What would Bayes rule produce as the MAP hypothesis?

Does *FindS* output a MAP hypothesis??

Relation to Concept Learning

Assume fixed set of instances $\langle x_1, \ldots, x_m \rangle$
Assume D is the set of classifications
$D = \langle c(x_1), \ldots, c(x_m) \rangle$

Choose $P(D|h)$:

Relation to Concept Learning

Assume fixed set of instances $\langle x_1, \ldots, x_m \rangle$
Assume D is the set of classifications
$D = \langle c(x_1), \ldots, c(x_m) \rangle$
Choose $P(D|h)$

- $P(D|h) = 1$ if h consistent with D
- $P(D|h) = 0$ otherwise

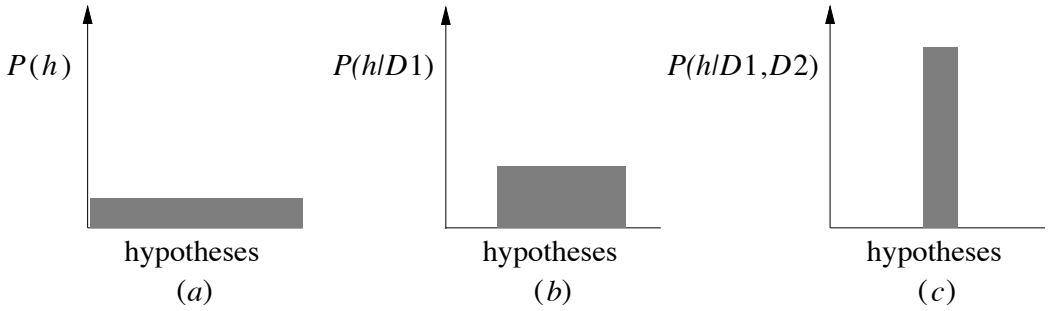
Choose $P(h)$ to be *uniform* distribution

- $P(h) = \frac{1}{|H|}$ for all h in H

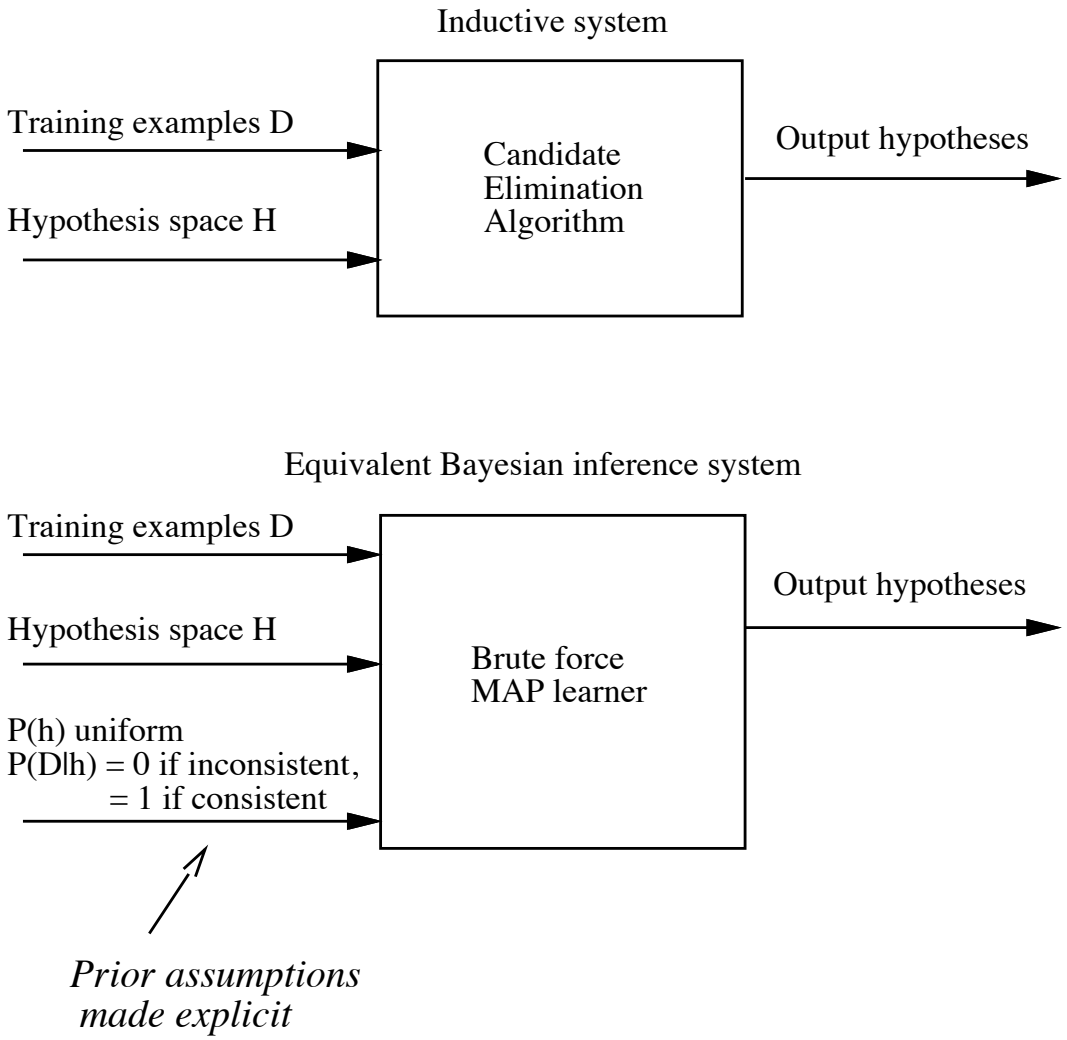
Then,

$$P(h|D) = \begin{cases} \frac{1}{|VS_{H,D}|} & \text{if } h \text{ is consistent with } D \\ 0 & \text{otherwise} \end{cases}$$

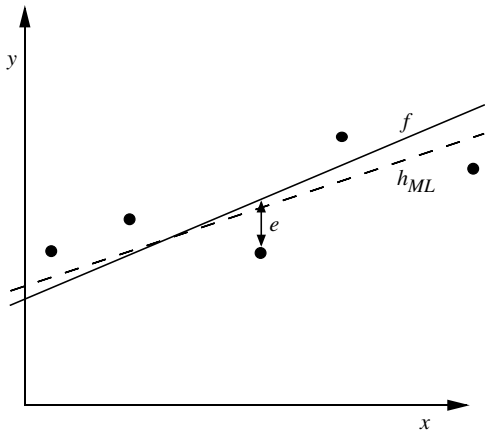
Evolution of Posterior Probabilities



Characterizing Learning Algorithms by Equivalent MAP Learners



Learning A Real Valued Function



Consider any real-valued target function f
Training examples $\langle x_i, d_i \rangle$, where d_i is noisy training value

- $d_i = f(x_i) + e_i$
- e_i is random variable (noise) drawn independently for each x_i according to some Gaussian distribution with mean=0

Then the maximum likelihood hypothesis h_{ML} is the one that minimizes the sum of squared errors:

$$h_{ML} = \arg\min_{h \in H} \sum_{i=1}^{m} (d_i - h(x_i))^2$$

Learning A Real Valued Function

$$
\begin{aligned}
h_{ML} &= \underset{h \in H}{\operatorname{argmax}} p(D|h) \\
&= \underset{h \in H}{\operatorname{argmax}} \prod_{i=1}^{m} p(d_i|h) \\
&= \underset{h \in H}{\operatorname{argmax}} \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{d_i - h(x_i)}{\sigma}\right)^2}
\end{aligned}
$$

Maximize natural log of this instead...

$$
\begin{aligned}
h_{ML} &= \underset{h \in H}{\operatorname{argmax}} \sum_{i=1}^{m} \ln \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2}\left(\frac{d_i - h(x_i)}{\sigma}\right)^2 \\
&= \underset{h \in H}{\operatorname{argmax}} \sum_{i=1}^{m} -\frac{1}{2}\left(\frac{d_i - h(x_i)}{\sigma}\right)^2 \\
&= \underset{h \in H}{\operatorname{argmax}} \sum_{i=1}^{m} -\left(d_i - h(x_i)\right)^2 \\
&= \underset{h \in H}{\operatorname{argmin}} \sum_{i=1}^{m} \left(d_i - h(x_i)\right)^2
\end{aligned}
$$

Learning to Predict Probabilities

Consider predicting survival probability from patient data

Training examples $\langle x_i, d_i \rangle$, where d_i is 1 or 0

Want to train neural network to output a *probability* given x_i (not a 0 or 1)

In this case can show

$$h_{ML} = \underset{h \in H}{\operatorname{argmax}} \sum_{i=1}^{m} d_i \ln h(x_i) + (1 - d_i) \ln(1 - h(x_i))$$

Weight update rule for a sigmoid unit:

$$w_{jk} \leftarrow w_{jk} + \Delta w_{jk}$$

where

$$\Delta w_{jk} = \eta \sum_{i=1}^{m} (d_i - h(x_i))\ x_{ijk}$$

Minimum Description Length Principle

Occam's razor: prefer the shortest hypothesis

MDL: prefer the hypothesis h that minimizes

$$h_{MDL} = \underset{h \in H}{\operatorname{argmin}} L_{C_1}(h) + L_{C_2}(D|h)$$

where $L_C(x)$ is the description length of x under encoding C

Example: H = decision trees, D = training data labels

- $L_{C_1}(h)$ is # bits to describe tree h
- $L_{C_2}(D|h)$ is # bits to describe D given h
  - Note $L_{C_2}(D|h) = 0$ if examples classified perfectly by h. Need only describe exceptions
- Hence h_{MDL} trades off tree size for training errors

Minimum Description Length Principle

$$\begin{aligned} h_{MAP} &= \arg\max_{h \in H} P(D|h)P(h) \\ &= \arg\max_{h \in H} \log_2 P(D|h) + \log_2 P(h) \\ &= \arg\min_{h \in H} -\log_2 P(D|h) - \log_2 P(h) \quad (1) \end{aligned}$$

Interesting fact from information theory:

> The optimal (shortest expected coding length) code for an event with probability p is $-\log_2 p$ bits.

So interpret (1):

- $-\log_2 P(h)$ is length of h under optimal code
- $-\log_2 P(D|h)$ is length of D given h under optimal code

$\rightarrow$ prefer the hypothesis that minimizes

$$length(h) + length(misclassifications)$$

Most Probable Classification of New Instances

So far we've sought the most probable *hypothesis* given the data D (i.e., h_{MAP})

Given new instance x, what is its most probable *classification*?

- $h_{MAP}(x)$ is not the most probable classification!

Consider:

- Three possible hypotheses:

  $$P(h_1|D) = .4,\ P(h_2|D) = .3,\ P(h_3|D) = .3$$

- Given new instance x,

  $$h_1(x) = +,\ h_2(x) = -,\ h_3(x) = -$$

- What's most probable classification of x?

Bayes Optimal Classifier

Bayes optimal classification:

$$\arg\max_{v_j \in V} \sum_{h_i \in H} P(v_j|h_i)P(h_i|D)$$

Example:

$$P(h_1|D) = .4,\ P(-|h_1) = 0,\ P(+|h_1) = 1$$
$$P(h_2|D) = .3,\ P(-|h_2) = 1,\ P(+|h_2) = 0$$
$$P(h_3|D) = .3,\ P(-|h_3) = 1,\ P(+|h_3) = 0$$

therefore

$$\sum_{h_i \in H} P(+|h_i)P(h_i|D) = .4$$
$$\sum_{h_i \in H} P(-|h_i)P(h_i|D) = .6$$

and

$$\arg\max_{v_j \in V} \sum_{h_i \in H} P(v_j|h_i)P(h_i|D) = -$$

Gibbs Classifier

Bayes optimal classifier provides best result, but can be expensive if many hypotheses.
Gibbs algorithm:

1. Choose one hypothesis at random, according to $P(h|D)$
2. Use this to classify new instance

Surprising fact: Assume target concepts are drawn at random from H according to priors on H. Then:

$$E[error_{Gibbs}] \leq 2E[error_{BayesOptimal}]$$

Suppose correct, uniform prior distribution over H, then

- Pick any hypothesis from VS, with uniform probability
- Its expected error no worse than twice Bayes optimal

Naive Bayes Classifier

Along with decision trees, neural networks, nearest nbr, one of the most practical learning methods.

When to use

- Moderate or large training set available
- Attributes that describe instances are conditionally independent given classification

Successful applications:

- Diagnosis
- Classifying text documents

Naive Bayes Classifier

Assume target function $f : X \rightarrow V$, where each instance x described by attributes $\langle a_1, a_2 \ldots a_n \rangle$. Most probable value of $f(x)$ is:

$$\begin{aligned} v_{MAP} &= \underset{v_j \in V}{\text{argmax}} P(v_j | a_1, a_2 \ldots a_n) \\ v_{MAP} &= \underset{v_j \in V}{\text{argmax}} \frac{P(a_1, a_2 \ldots a_n | v_j) P(v_j)}{P(a_1, a_2 \ldots a_n)} \\ &= \underset{v_j \in V}{\text{argmax}} P(a_1, a_2 \ldots a_n | v_j) P(v_j) \end{aligned}$$

Naive Bayes assumption:

$$P(a_1, a_2 \ldots a_n | v_j) = \prod_i P(a_i | v_j)$$

which gives

Naive Bayes classifier: $v_{NB} = \underset{v_j \in V}{\text{argmax}} P(v_j) \prod_i P(a_i | v_j)$

Naive Bayes Algorithm

Naive_Bayes_Learn($examples$)

For each target value v_j

$\hat{P}(v_j) \leftarrow$ estimate $P(v_j)$

For each attribute value a_i of each attribute a

$\hat{P}(a_i|v_j) \leftarrow$ estimate $P(a_i|v_j)$

Classify_New_Instance(x)

$$v_{NB} = \underset{v_j \in V}{\operatorname{argmax}} \hat{P}(v_j) \prod_{a_i \in x} \hat{P}(a_i|v_j)$$

Naive Bayes: Example

Consider *PlayTennis* again, and new instance

$\langle Outlk = sun, Temp = cool, Humid = high, Wind = strong$

Want to compute:

$$v_{NB} = \underset{v_j \in V}{\operatorname{argmax}} P(v_j) \prod_i P(a_i|v_j)$$

$P(y)\ P(sun|y)\ P(cool|y)\ P(high|y)\ P(strong|y) = .005$

$P(n)\ P(sun|n)\ P(cool|n)\ P(high|n)\ P(strong|n) = .021$

$$\rightarrow v_{NB} = n$$

Naive Bayes: Subtleties

1. Conditional independence assumption is often violated

$$P(a_1, a_2 \ldots a_n | v_j) = \prod_i P(a_i | v_j)$$

   - ...but it works surprisingly well anyway. Note don't need estimated posteriors $\hat{P}(v_j|x)$ to be correct; need only that

$$\underset{v_j \in V}{\text{argmax}}\, \hat{P}(v_j) \prod_i \hat{P}(a_i|v_j) = \underset{v_j \in V}{\text{argmax}}\, P(v_j) P(a_1 \ldots, a_n | v_j)$$

   - see [Domingos & Pazzani, 1996] for analysis
   - Naive Bayes posteriors often unrealistically close to 1 or 0

Naive Bayes: Subtleties

2. what if none of the training instances with target value v_j have attribute value a_i? Then

$$\hat{P}(a_i|v_j) = 0, \text{ and...}$$

$$\hat{P}(v_j) \prod_i \hat{P}(a_i|v_j) = 0$$

Typical solution is Bayesian estimate for $\hat{P}(a_i|v_j)$

$$\hat{P}(a_i|v_j) \leftarrow \frac{n_c + mp}{n + m}$$

where

- n is number of training examples for which $v = v_j$,
- n_c number of examples for which $v = v_j$ and $a = a_i$
- p is prior estimate for $\hat{P}(a_i|v_j)$
- m is weight given to prior (i.e. number of "virtual" examples)

Learning to Classify Text

Why?

- Learn which news articles are of interest
- Learn to classify web pages by topic

Naive Bayes is among most effective algorithms

What attributes shall we use to represent text documents??

Learning to Classify Text

Target concept $Interesting? : Document \rightarrow \{+, -\}$

1. Represent each document by vector of words
   - one attribute per word position in document
2. Learning: Use training examples to estimate
   - $P(+)$
   - $P(-)$
   - $P(doc|+)$
   - $P(doc|-)$

Naive Bayes conditional independence assumption

$$P(doc|v_j) = \prod_{i=1}^{length(doc)} P(a_i = w_k|v_j)$$

where $P(a_i = w_k|v_j)$ is probability that word in position i is w_k, given v_j

one more assumption:
$P(a_i = w_k|v_j) = P(a_m = w_k|v_j), \forall i, m$

LEARN_NAIVE_BAYES_TEXT($Examples, V$)

1. collect all words and other tokens that occur in Examples

- $Vocabulary \leftarrow$ all distinct words and other tokens in $Examples$

2. calculate the required $P(v_j)$ and $P(w_k|v_j)$ probability terms

- For each target value v_j in V do
  - $docs_j \leftarrow$ subset of $Examples$ for which the target value is v_j
  - $P(v_j) \leftarrow \frac{|docs_j|}{|Examples|}$
  - $Text_j \leftarrow$ a single document created by concatenating all members of $docs_j$
  - $n \leftarrow$ total number of words in $Text_j$ (counting duplicate words multiple times)
  - for each word w_k in $Vocabulary$
    - $n_k \leftarrow$ number of times word w_k occurs in $Text_j$
    - $P(w_k|v_j) \leftarrow \frac{n_k+1}{n+|Vocabulary|}$

CLASSIFY_NAIVE_BAYES_TEXT(Doc)

- $positions \leftarrow$ all word positions in Doc that contain tokens found in $Vocabulary$
- Return v_{NB}, where

$$v_{NB} = \underset{v_j \in V}{\text{argmax}} P(v_j) \prod_{i \in positions} P(a_i | v_j)$$

Twenty NewsGroups

Given 1000 training documents from each group
Learn to classify new documents according to
which newsgroup it came from

comp.graphics	misc.forsale
comp.os.ms-windows.misc	rec.autos
comp.sys.ibm.pc.hardware	rec.motorcycles
comp.sys.mac.hardware	rec.sport.baseball
comp.windows.x	rec.sport.hockey
alt.atheism	sci.space
soc.religion.christian	sci.crypt
talk.religion.misc	sci.electronics
talk.politics.mideast	sci.med
talk.politics.misc	
talk.politics.guns	

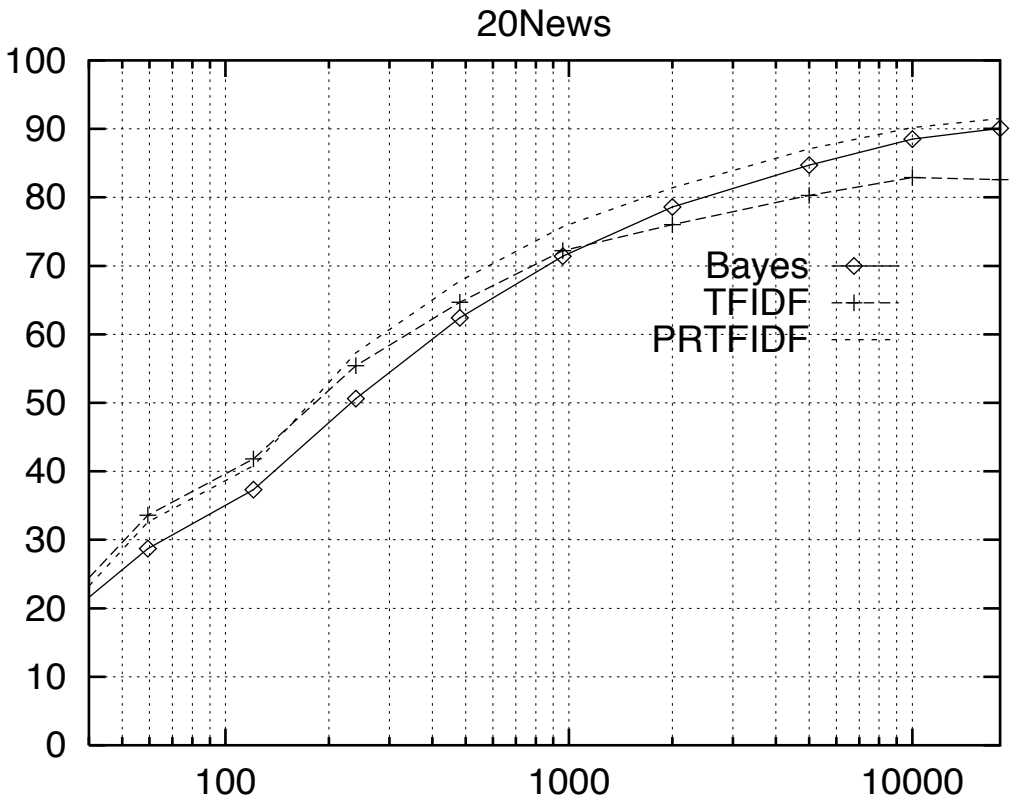
Naive Bayes: 89% classification accuracy

Article from rec.sport.hockey

Path: cantaloupe.srv.cs.cmu.edu!das-news.harvard.e
From: xxx@yyy.zzz.edu (John Doe)
Subject: Re: This year's biggest and worst (opinio
Date: 5 Apr 93 09:53:39 GMT

I can only comment on the Kings, but the most obvious candidate for pleasant surprise is Alex Zhitnik. He came highly touted as a defensive defenseman, but he's clearly much more than that. Great skater and hard shot (though wish he were more accurate). In fact, he pretty much allowed the Kings to trade away that huge defensive liability Paul Coffey. Kelly Hrudey is only the biggest disappointment if you thought he was any good to begin with. But, at best, he's only a mediocre goaltender. A better choice would be Tomas Sandstrom, though not through any fault of his own, but because some thugs in Toronto decided

Learning Curve for 20 Newsgroups



Accuracy vs. Training set size (1/3 withheld for test)

Bayesian Belief Networks

Interesting because:

- Naive Bayes assumption of conditional independence too restrictive
- But it's intractable without some such assumptions...
- Bayesian Belief networks describe conditional independence among *subsets* of variables

→ allows combining prior knowledge about (in)dependencies among variables with observed training data

(also called Bayes Nets)

Conditional Independence

Definition: X is *conditionally independent* of Y given Z if the probability distribution governing X is independent of the value of Y given the value of Z; that is, if

$$(\forall x_i, y_j, z_k)\ P(X = x_i | Y = y_j, Z = z_k) = P(X = x_i | Z = z_k$$

more compactly, we write

$$P(X|Y,Z) = P(X|Z)$$

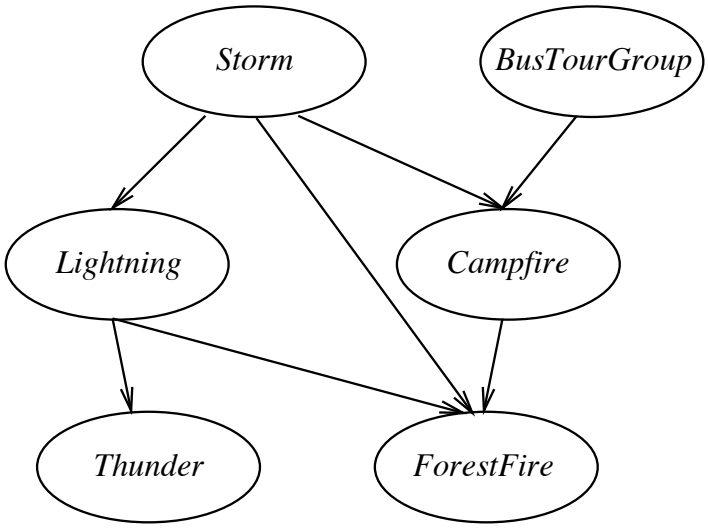
Example: $Thunder$ is conditionally independent of $Rain$, given $Lightning$

$$P(Thunder|Rain, Lightning) = P(Thunder|Lightning)$$

Naive Bayes uses cond. indep. to justify

$$\begin{aligned} P(X,Y|Z) &= P(X|Y,Z)P(Y|Z) \\ &= P(X|Z)P(Y|Z) \end{aligned}$$

Bayesian Belief Network



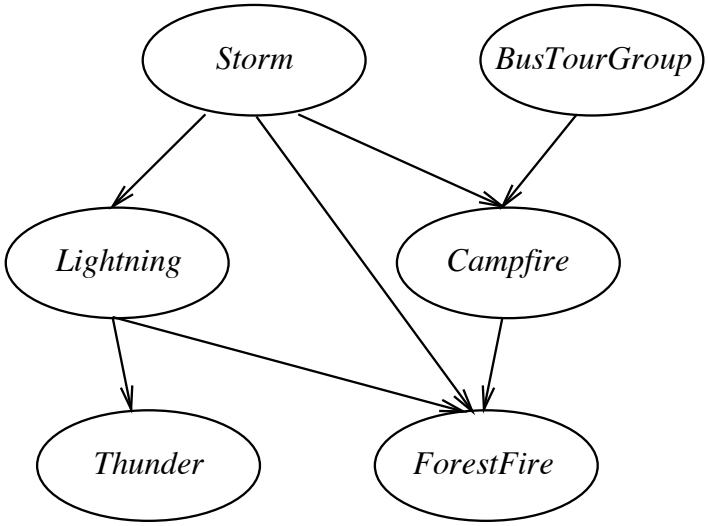
	S,B	$S,\neg B$	$\neg S,B$	$\neg S,\neg B$
C	0.4	0.1	0.8	0.2
$\neg C$	0.6	0.9	0.2	0.8

Campfire

Network represents a set of conditional independence assertions:

- Each node is asserted to be conditionally independent of its nondescendants, given its immediate predecessors.
- Directed acyclic graph

Bayesian Belief Network



	S,B	S,¬B	¬S,B	¬S,¬B
C	0.4	0.1	0.8	0.2
¬C	0.6	0.9	0.2	0.8

Campfire

Represents joint probability distribution over all variables

- e.g., $P(Storm, BusTourGroup, \ldots, ForestFire)$
- in general,

$$P(y_1, \ldots, y_n) = \prod_{i=1}^{n} P(y_i | Parents(Y_i))$$

  where $Parents(Y_i)$ denotes immediate predecessors of Y_i in graph

- so, joint distribution is fully defined by graph, plus the $P(y_i|Parents(Y_i))$

Inference in Bayesian Networks

How can one infer the (probabilities of) values of one or more network variables, given observed values of others?

- Bayes net contains all information needed for this inference
- If only one variable with unknown value, easy to infer it
- In general case, problem is NP hard

In practice, can succeed in many cases

- Exact inference methods work well for some network structures
- Monte Carlo methods "simulate" the network randomly to calculate approximate solutions

Learning of Bayesian Networks

Several variants of this learning task

- Network structure might be *known* or *unknown*
- Training examples might provide values of *all* network variables, or just *some*

If structure known and observe all variables

- Then it's easy as training a Naive Bayes classifier

Learning Bayes Nets

Suppose structure known, variables partially observable

e.g., observe *ForestFire, Storm, BusTourGroup, Thunder*, but not *Lightning, Campfire...*

- Similar to training neural network with hidden units
- In fact, can learn network conditional probability tables using gradient ascent!
- Converge to network h that (locally) maximizes $P(D|h)$

Gradient Ascent for Bayes Nets

Let w_{ijk} denote one entry in the conditional probability table for variable Y_i in the network

$w_{ijk} = P(Y_i = y_{ij} | Parents(Y_i) = \text{the list } u_{ik} \text{ of values})$

e.g., if $Y_i = Campfire$, then u_{ik} might be $\langle Storm = T, BusTourGroup = F \rangle$

Perform gradient ascent by repeatedly

1. update all w_{ijk} using training data D

$$w_{ijk} \leftarrow w_{ijk} + \eta \sum_{d \in D} \frac{P_h(y_{ij}, u_{ik} | d)}{w_{ijk}}$$

2. then, renormalize the w_{ijk} to assure
   - $\Sigma_j w_{ijk} = 1$
   - $0 \leq w_{ijk} \leq 1$

More on Learning Bayes Nets

EM algorithm can also be used. Repeatedly:

1. Calculate probabilities of unobserved variables, assuming h
2. Calculate new w_{ijk} to maximize $E[\ln P(D|h)]$ where D now includes both observed and (calculated probabilities of) unobserved variables

When structure unknown...

- Algorithms use greedy search to add/substract edges and nodes
- Active research topic

Summary: Bayesian Belief Networks

- Combine prior knowledge with observed data
- Impact of prior knowledge (when correct!) is to lower the sample complexity
- Active research area
  - Extend from boolean to real-valued variables
  - Parameterized distributions instead of tables
  - Extend to first-order instead of propositional systems
  - More effective inference methods
  - ...

Expectation Maximization (EM)

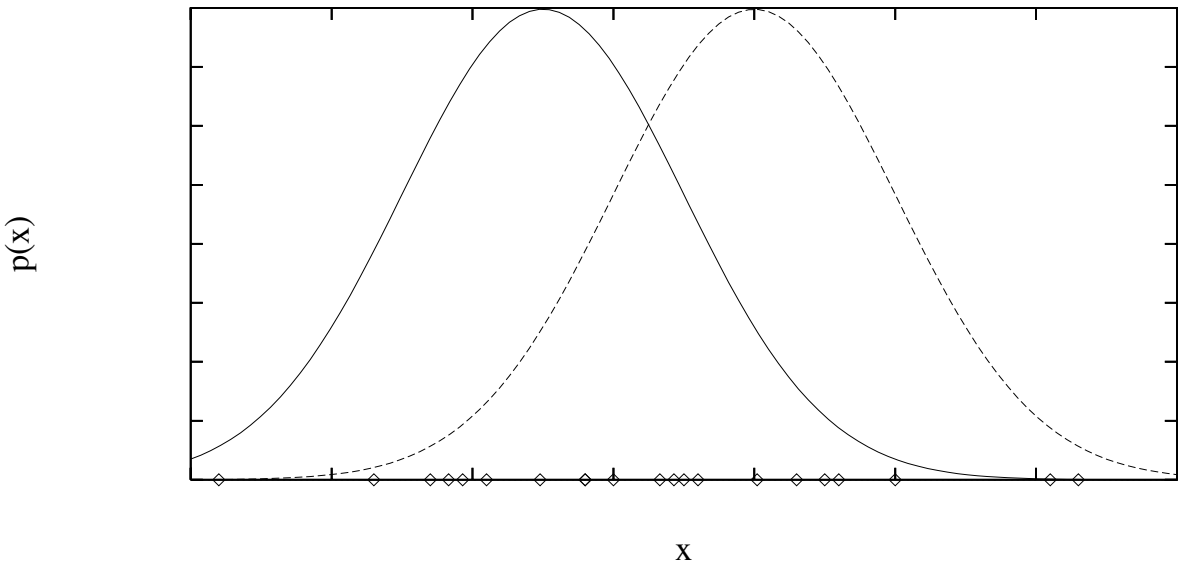
When to use:

- Data is only partially observable
- Unsupervised clustering (target value unobservable)
- Supervised learning (some instance attributes unobservable)

Some uses:

- Train Bayesian Belief Networks
- Unsupervised clustering (AUTOCLASS)
- Learning Hidden Markov Models

Generating Data from Mixture of k Gaussians



Each instance x generated by

1. Choosing one of the k Gaussians with uniform probability
2. Generating an instance at random according to that Gaussian

EM for Estimating k Means

Given:

- Instances from X generated by mixture of k Gaussian distributions
- Unknown means $\langle \mu_1, \ldots, \mu_k \rangle$ of the k Gaussians
- Don't know which instance x_i was generated by which Gaussian

Determine:

- Maximum likelihood estimates of $\langle \mu_1, \ldots, \mu_k \rangle$

Think of full description of each instance as $y_i = \langle x_i, z_{i1}, z_{i2} \rangle$, where

- z_{ij} is 1 if x_i generated by jth Gaussian
- x_i observable
- z_{ij} unobservable

EM for Estimating k Means

EM Algorithm: Pick random initial $h = \langle \mu_1, \mu_2 \rangle$, then iterate

E step: Calculate the expected value $E[z_{ij}]$ of each hidden variable z_{ij}, assuming the current hypothesis $h = \langle \mu_1, \mu_2 \rangle$ holds.

$$E[z_{ij}] = \frac{p(x = x_i | \mu = \mu_j)}{\sum_{n=1}^{2} p(x = x_i | \mu = \mu_n)}$$

$$= \frac{e^{-\frac{1}{2\sigma^2}(x_i - \mu_j)^2}}{\sum_{n=1}^{2} e^{-\frac{1}{2\sigma^2}(x_i - \mu_n)^2}}$$

M step: Calculate a new maximum likelihood hypothesis $h' = \langle \mu'_1, \mu'_2 \rangle$, assuming the value taken on by each hidden variable z_{ij} is its expected value $E[z_{ij}]$ calculated above. Replace $h = \langle \mu_1, \mu_2 \rangle$ by $h' = \langle \mu'_1, \mu'_2 \rangle$.

$$\mu_j \leftarrow \frac{\sum_{i=1}^{m} E[z_{ij}] \; x_i}{\sum_{i=1}^{m} E[z_{ij}]}$$

EM Algorithm

Converges to local maximum likelihood h
and provides estimates of hidden variables z_{ij}

In fact, local maximum in $E[\ln P(Y|h)]$

- Y is complete (observable plus unobservable variables) data
- Expected value is taken over possible values of unobserved variables in Y

General EM Problem

Given:

- Observed data $X = \{x_1, \ldots, x_m\}$
- Unobserved data $Z = \{z_1, \ldots, z_m\}$
- Parameterized probability distribution $P(Y|h)$, where
  - $Y = \{y_1, \ldots, y_m\}$ is the full data $y_i = x_i \cup z_i$
  - h are the parameters

Determine:

- h that (locally) maximizes $E[\ln P(Y|h)]$

Many uses:

- Train Bayesian belief networks
- Unsupervised clustering (e.g., k means)
- Hidden Markov Models

General EM Method

Define likelihood function $Q(h'|h)$ which calculates $Y = X \cup Z$ using observed X and current parameters h to estimate Z

$$Q(h'|h) \leftarrow E[\ln P(Y|h')|h, X]$$

EM Algorithm:

Estimation (E) step: Calculate $Q(h'|h)$ using the current hypothesis h and the observed data X to estimate the probability distribution over Y.

$$Q(h'|h) \leftarrow E[\ln P(Y|h')|h, X]$$

Maximization (M) step: Replace hypothesis h by the hypothesis h' that maximizes this Q function.

$$h \leftarrow \underset{h'}{\operatorname{argmax}} Q(h'|h)$$

Computational Learning Theory

[read Chapter 7]
[Suggested exercises: 7.1, 7.2, 7.5, 7.8]

- Computational learning theory
- Setting 1: learner poses queries to teacher
- Setting 2: teacher chooses examples
- Setting 3: randomly generated instances, labeled by teacher
- Probably approximately correct (PAC) learning
- Vapnik-Chervonenkis Dimension
- Mistake bounds

Computational Learning Theory

What general laws constrain inductive learning?

We seek theory to relate:

- Probability of successful learning
- Number of training examples
- Complexity of hypothesis space
- Accuracy to which target concept is approximated
- Manner in which training examples presented

Prototypical Concept Learning Task

- **Given:**
  - Instances X: Possible days, each described by the attributes *Sky*, *AirTemp*, *Humidity*, *Wind*, *Water*, *Forecast*
  - Target function c: $EnjoySport : X \rightarrow \{0, 1\}$
  - Hypotheses H: Conjunctions of literals. E.g.

$$\langle ?, Cold, High, ?, ?, ? \rangle.$$

  - Training examples D: Positive and negative examples of the target function

$$\langle x_1, c(x_1) \rangle, \ldots \langle x_m, c(x_m) \rangle$$

- **Determine:**
  - A hypothesis h in H such that $h(x) = c(x)$ for all x in D?
  - A hypothesis h in H such that $h(x) = c(x)$ for all x in X?

Sample Complexity

How many training examples are sufficient to learn the target concept?

1. If learner proposes instances, as queries to teacher
   - Learner proposes instance x, teacher provides $c(x)$
2. If teacher (who knows c) provides training examples
   - teacher provides sequence of examples of form $\langle x, c(x) \rangle$
3. If some random process (e.g., nature) proposes instances
   - instance x generated randomly, teacher provides $c(x)$

Sample Complexity: 1

Learner proposes instance x, teacher provides $c(x)$ (assume c is in learner's hypothesis space H)

Optimal query strategy: play 20 questions

- pick instance x such that half of hypotheses in VS classify x positive, half classify x negative
- When this is possible, need $\lceil \log_2 |H| \rceil$ queries to learn c
- when not possible, need even more

Sample Complexity: 2

Teacher (who knows c) provides training examples (assume c is in learner's hypothesis space H)

Optimal teaching strategy: depends on H used by learner

Consider the case H = conjunctions of up to n boolean literals and their negations

e.g., $(AirTemp = Warm) \wedge (Wind = Strong)$, where $AirTemp, Wind, \ldots$ each have 2 possible values.

- if n possible boolean attributes in H, $n + 1$ examples suffice
- why?

Sample Complexity: 3

Given:

- set of instances X
- set of hypotheses H
- set of possible target concepts C
- training instances generated by a fixed, unknown probability distribution $\mathcal{D}$ over X

Learner observes a sequence D of training examples of form $\langle x, c(x)\rangle$, for some target concept $c \in C$

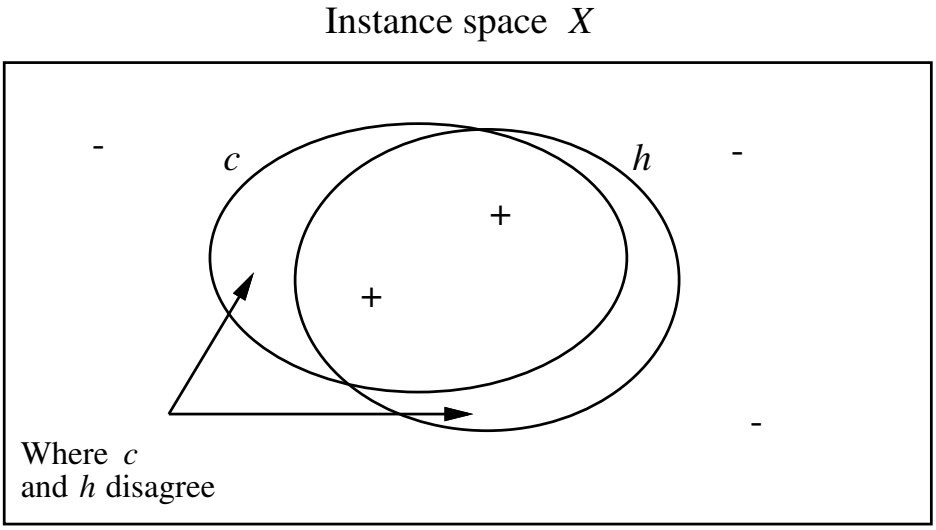
- instances x are drawn from distribution $\mathcal{D}$
- teacher provides target value $c(x)$ for each

Learner must output a hypothesis h estimating c

- h is evaluated by its performance on subsequent instances drawn according to $\mathcal{D}$

Note: randomly drawn instances, noise-free classifications

True Error of a Hypothesis



Definition: The **true error** (denoted $error_{\mathcal{D}}(h)$) of hypothesis h with respect to target concept c and distribution $\mathcal{D}$ is the probability that h will misclassify an instance drawn at random according to $\mathcal{D}$.

$$error_{\mathcal{D}}(h) \equiv \Pr_{x \in \mathcal{D}}[c(x) \neq h(x)]$$

Two Notions of Error

Training error of hypothesis h with respect to target concept c

- How often $h(x) \neq c(x)$ over training instances

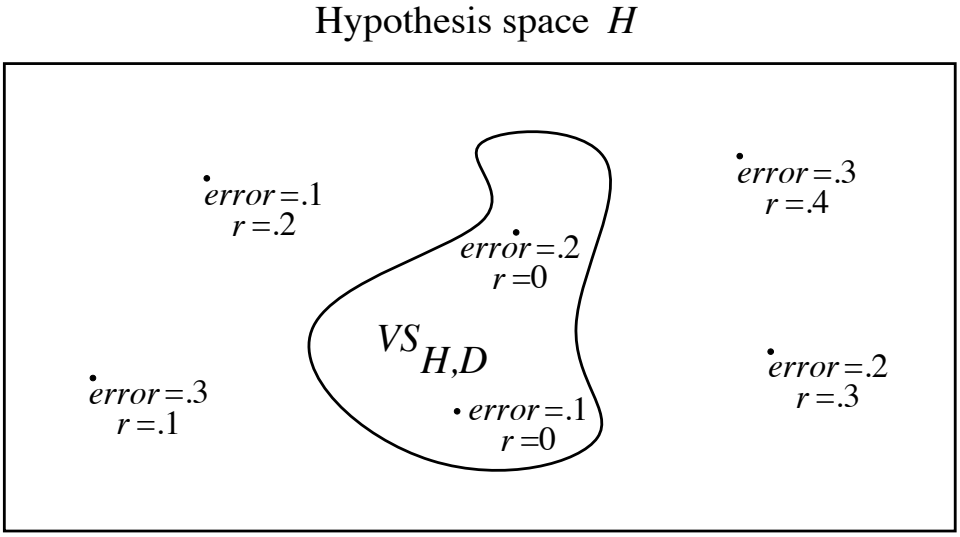
True error of hypothesis h with respect to c

- How often $h(x) \neq c(x)$ over future random instances

Our concern:

- Can we bound the true error of h given the training error of h?
- First consider when training error of h is zero (i.e., $h \in VS_{H,D}$)

Exhausting the Version Space



(r = training error, $error$ = true error)

Definition: The version space $VS_{H,D}$ is said to be ϵ-**exhausted** with respect to c and $\mathcal{D}$, if every hypothesis h in $VS_{H,D}$ has error less than ϵ with respect to c and $\mathcal{D}$.

$$(\forall h \in VS_{H,D})\ error_{\mathcal{D}}(h) < \epsilon$$

How many examples will ϵ-exhaust the VS?

Theorem: [Haussler, 1988].

If the hypothesis space H is finite, and D is a sequence of $m \geq 1$ independent random examples of some target concept c, then for any $0 \leq \epsilon \leq 1$, the probability that the version space with respect to H and D is not ϵ-exhausted (with respect to c) is less than

$$|H|e^{-\epsilon m}$$

Interesting! This bounds the probability that any consistent learner will output a hypothesis h with $error(h) \geq \epsilon$

If we want to this probability to be below δ

$$|H|e^{-\epsilon m} \leq \delta$$

then

$$m \geq \frac{1}{\epsilon}(\ln |H| + \ln(1/\delta))$$

Learning Conjunctions of Boolean Literals

How many examples are sufficient to assure with probability at least $(1 - \delta)$ that

every h in $VS_{H,D}$ satisfies $error_{\mathcal{D}}(h) \leq \epsilon$

Use our theorem:

$$m \geq \frac{1}{\epsilon}(\ln |H| + \ln(1/\delta))$$

Suppose H contains conjunctions of constraints on up to n boolean attributes (i.e., n boolean literals). Then $|H| = 3^n$, and

$$m \geq \frac{1}{\epsilon}(\ln 3^n + \ln(1/\delta))$$

or

$$m \geq \frac{1}{\epsilon}(n \ln 3 + \ln(1/\delta))$$

How About *EnjoySport*?

$$m \geq \frac{1}{\epsilon}(\ln |H| + \ln(1/\delta))$$

If H is as given in *EnjoySport* then $|H| = 973$, and

$$m \geq \frac{1}{\epsilon}(\ln 973 + \ln(1/\delta))$$

... if want to assure that with probability 95%, VS contains only hypotheses with $error_{\mathcal{D}}(h) \leq .1$, then it is sufficient to have m examples, where

$$m \geq \frac{1}{.1}(\ln 973 + \ln(1/.05))$$

$$m \geq 10(\ln 973 + \ln 20)$$

$$m \geq 10(6.88 + 3.00)$$

$$m \geq 98.8$$

PAC Learning

Consider a class C of possible target concepts defined over a set of instances X of length n, and a learner L using hypothesis space H.

> *Definition:* C is **PAC-learnable** by L using H if for all $c \in C$, distributions $\mathcal{D}$ over X, ϵ such that $0 < \epsilon < 1/2$, and δ such that $0 < \delta < 1/2$,
>
> learner L will with probability at least $(1 - \delta)$ output a hypothesis $h \in H$ such that $error_{\mathcal{D}}(h) \leq \epsilon$, in time that is polynomial in $1/\epsilon$, $1/\delta$, n and $size(c)$.

Agnostic Learning

So far, assumed $c \in H$

Agnostic learning setting: don't assume $c \in H$

- What do we want then?
  - The hypothesis h that makes fewest errors on training data
- What is sample complexity in this case?

$$m \geq \frac{1}{2\epsilon^2}(\ln |H| + \ln(1/\delta))$$

derived from Hoeffding bounds:

$$Pr[error_D(h) > error_D(h) + \epsilon] \leq e^{-2m\epsilon^2}$$

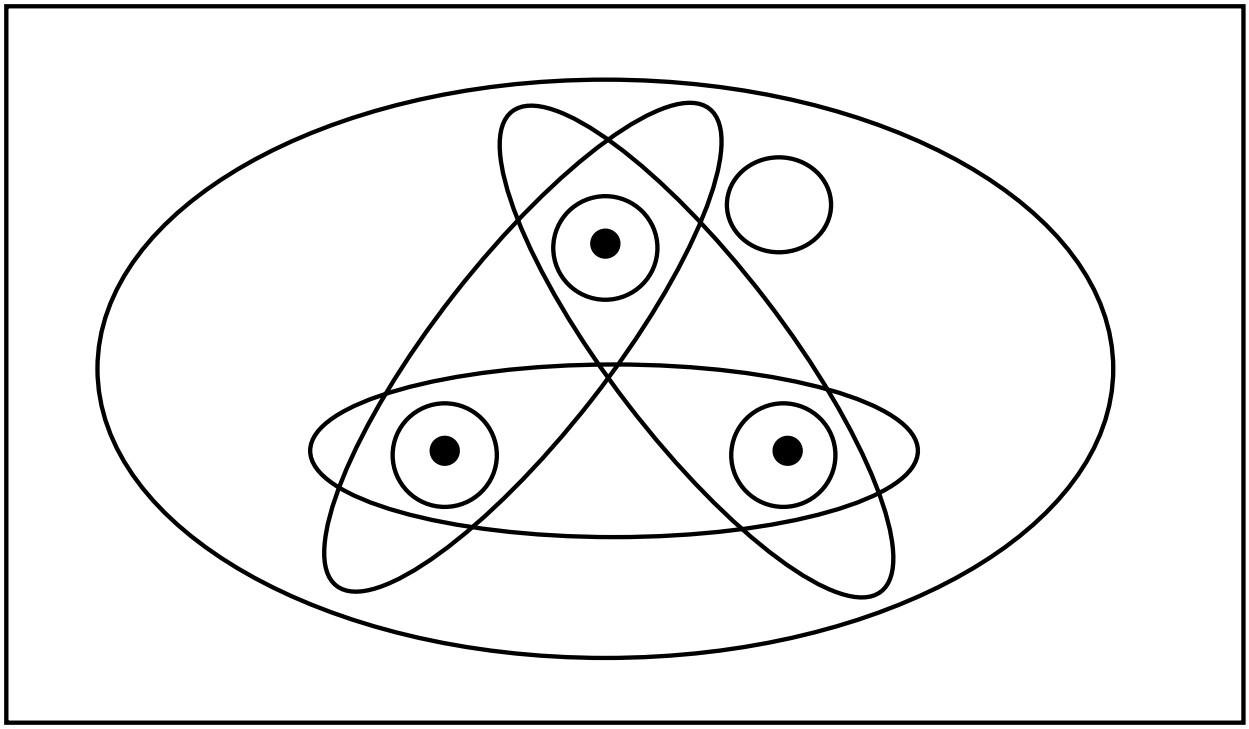
Shattering a Set of Instances

Definition: a **dichotomy** of a set S is a partition of S into two disjoint subsets.

Definition: a set of instances S is **shattered** by hypothesis space H if and only if for every dichotomy of S there exists some hypothesis in H consistent with this dichotomy.

Three Instances Shattered

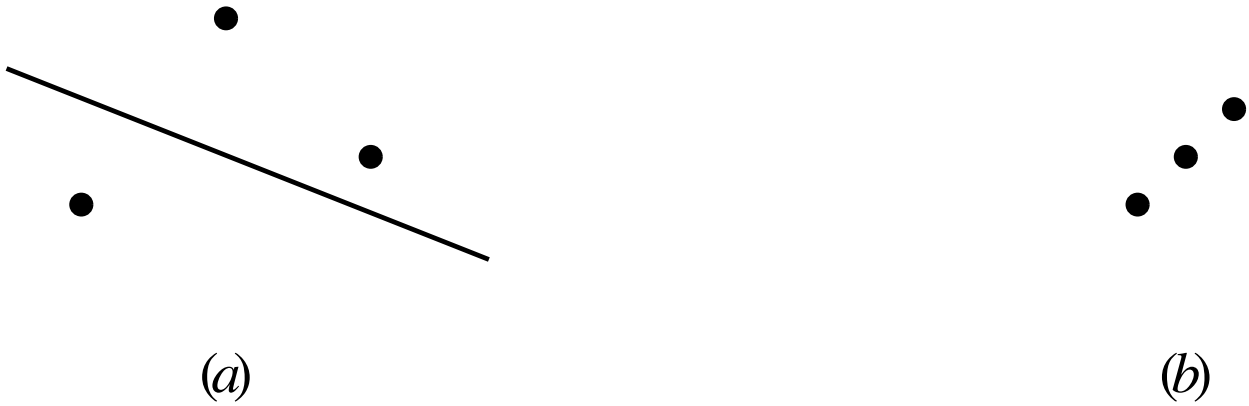
Instance space X



The Vapnik-Chervonenkis Dimension

Definition: The **Vapnik-Chervonenkis dimension**, $VC(H)$, of hypothesis space H defined over instance space X is the size of the largest finite subset of X shattered by H. If arbitrarily large finite sets of X can be shattered by H, then $VC(H) \equiv \infty$.

VC Dim. of Linear Decision Surfaces



Sample Complexity from VC Dimension

How many randomly drawn examples suffice to ϵ-exhaust $VS_{H,D}$ with probability at least $(1-\delta)$?

$$m \geq \frac{1}{\epsilon}(4\log_2(2/\delta) + 8VC(H)\log_2(13/\epsilon))$$

Mistake Bounds

So far: how many examples needed to learn?

What about: how many mistakes before convergence?

Let's consider similar setting to PAC learning:

- Instances drawn at random from X according to distribution $\mathcal{D}$
- Learner must classify each instance before receiving correct classification from teacher
- Can we bound the number of mistakes learner makes before converging?

Mistake Bounds: Find-S

Consider Find-S when H = conjunction of boolean literals

FIND-S:

- Initialize h to the most specific hypothesis $l_1 \wedge \neg l_1 \wedge l_2 \wedge \neg l_2 \ldots l_n \wedge \neg l_n$
- For each positive training instance x
  - Remove from h any literal that is not satisfied by x
- Output hypothesis h.

How many mistakes before converging to correct h?

Mistake Bounds: Halving Algorithm

Consider the Halving Algorithm:

- Learn concept using version space CANDIDATE-ELIMINATION algorithm
- Classify new instances by majority vote of version space members

How many mistakes before converging to correct h?

- ... in worst case?
- ... in best case?

Optimal Mistake Bounds

Let $M_A(C)$ be the max number of mistakes made by algorithm A to learn concepts in C. (maximum over all possible $c \in C$, and all possible training sequences)

$$M_A(C) \equiv \max_{c \in C} M_A(c)$$

Definition: Let C be an arbitrary non-empty concept class. The **optimal mistake bound** for C, denoted $Opt(C)$, is the minimum over all possible learning algorithms A of $M_A(C)$.

$$Opt(C) \equiv \min_{A \in learning\ algorithms} M_A(C)$$

$$VC(C) \leq Opt(C) \leq M_{Halving}(C) \leq log_2(|C|).$$

Instance Based Learning

[Read Ch. 8]

- k-Nearest Neighbor
- Locally weighted regression
- Radial basis functions
- Case-based reasoning
- Lazy and eager learning

Instance-Based Learning

Key idea: just store all training examples $\langle x_i, f(x_i) \rangle$

Nearest neighbor:

- Given query instance x_q, first locate nearest training example x_n, then estimate $\hat{f}(x_q) \leftarrow f(x_n)$

k-Nearest neighbor:

- Given x_q, take vote among its k nearest nbrs (if discrete-valued target function)
- take mean of f values of k nearest nbrs (if real-valued)

$$\hat{f}(x_q) \leftarrow \frac{\Sigma_{i=1}^{k} f(x_i)}{k}$$

When To Consider Nearest Neighbor

- Instances map to points in $\Re^n$
- Less than 20 attributes per instance
- Lots of training data

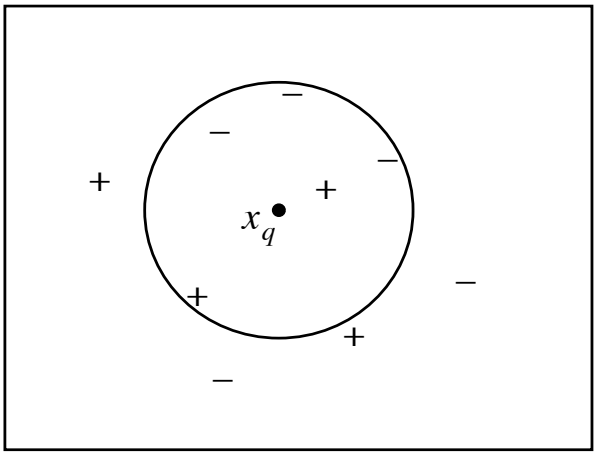
Advantages:

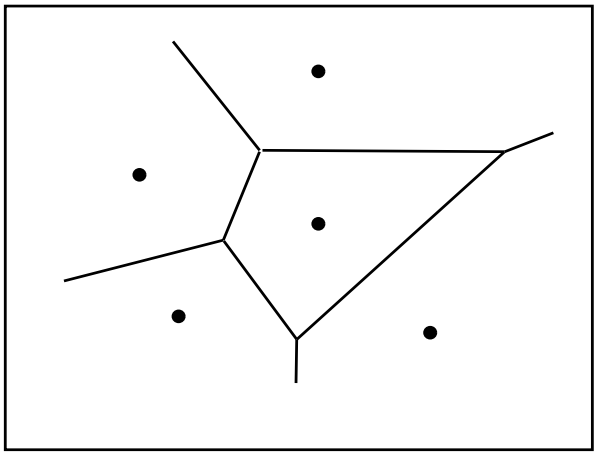
- Training is very fast
- Learn complex target functions
- Don't lose information

Disadvantages:

- Slow at query time
- Easily fooled by irrelevant attributes

Voronoi Diagram





Behavior in the Limit

Consider $p(x)$ defines probability that instance x will be labeled 1 (positive) versus 0 (negative).

Nearest neighbor:

- As number of training examples $\rightarrow \infty$, approaches Gibbs Algorithm

  Gibbs: with probability $p(x)$ predict 1, else 0

k-Nearest neighbor:

- As number of training examples $\rightarrow \infty$ and k gets large, approaches Bayes optimal

  Bayes optimal: if $p(x) > .5$ then predict 1, else 0

Note Gibbs has at most twice the expected error of Bayes optimal

Distance-Weighted kNN

Might want weight nearer neighbors more heavily...

$$\hat{f}(x_q) \leftarrow \frac{\Sigma_{i=1}^{k} w_i f(x_i)}{\Sigma_{i=1}^{k} w_i}$$

where

$$w_i \equiv \frac{1}{d(x_q, x_i)^2}$$

and $d(x_q, x_i)$ is distance between x_q and x_i

Note now it makes sense to use *all* training examples instead of just k

$\rightarrow$ Shepard's method

Curse of Dimensionality

Imagine instances described by 20 attributes, but only 2 are relevant to target function

Curse of dimensionality: nearest nbr is easily mislead when high-dimensional X

One approach:

- Stretch jth axis by weight z_j, where $z_1, \ldots, z_n$ chosen to minimize prediction error
- Use cross-validation to automatically choose weights $z_1, \ldots, z_n$
- Note setting z_j to zero eliminates this dimension altogether

see [Moore and Lee, 1994]

Locally Weighted Regression

Note kNN forms local approximation to f for each query point x_q

Why not form an explicit approximation $\hat{f}(x)$ for region surrounding x_q

- Fit linear function to k nearest neighbors
- Fit quadratic, ...
- Produces "piecewise approximation" to f

Several choices of error to minimize:

- Squared error over k nearest neighbors

$$E_1(x_q) \equiv \frac{1}{2} \sum_{x \in \ k \ nearest \ nbrs \ of \ x_q} (f(x) - \hat{f}(x))^2$$

- Distance-weighted squared error over all nbrs

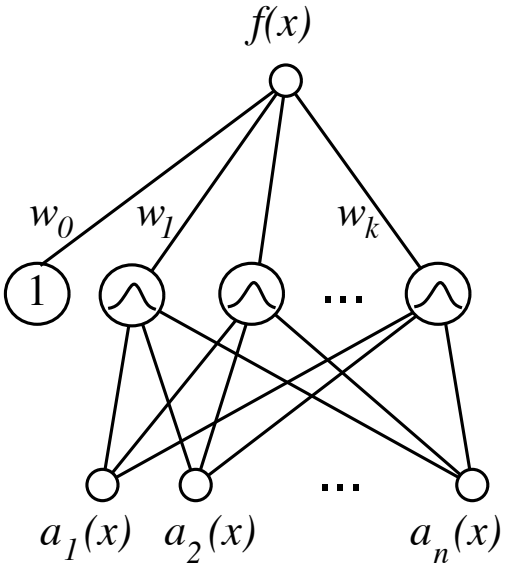
$$E_2(x_q) \equiv \frac{1}{2} \sum_{x \in D} (f(x) - \hat{f}(x))^2 \ K(d(x_q, x))$$

- ...

Radial Basis Function Networks

- Global approximation to target function, in terms of linear combination of local approximations
- Used, e.g., for image classification
- A different kind of neural network
- Closely related to distance-weighted regression, but "eager" instead of "lazy"

Radial Basis Function Networks



where $a_i(x)$ are the attributes describing instance x, and

$$f(x) = w_0 + \sum_{u=1}^{k} w_u K_u(d(x_u, x))$$

One common choice for $K_u(d(x_u, x))$ is

$$K_u(d(x_u, x)) = e^{-\frac{1}{2\sigma_u^2} d^2(x_u, x)}$$

Training Radial Basis Function Networks

Q1: What x_u to use for each kernel function $K_u(d(x_u, x))$

- Scatter uniformly throughout instance space
- Or use training instances (reflects instance distribution)

Q2: How to train weights (assume here Gaussian K_u)

- First choose variance (and perhaps mean) for each K_u
  - e.g., use EM
- Then hold K_u fixed, and train linear output layer
  - efficient methods to fit linear function

Case-Based Reasoning

Can apply instance-based learning even when $X \neq \Re^n$

$\rightarrow$ need different "distance" metric

Case-Based Reasoning is instance-based learning applied to instances with symbolic logic descriptions

```
((user-complaint error53-on-shutdown)
 (cpu-model PowerPC)
 (operating-system Windows)
 (network-connection PCIA)
 (memory 48meg)
 (installed-applications Excel Netscape VirusScan)
 (disk 1gig)
 (likely-cause ???))
```

Case-Based Reasoning in CADET

CADET: 75 stored examples of mechanical devices

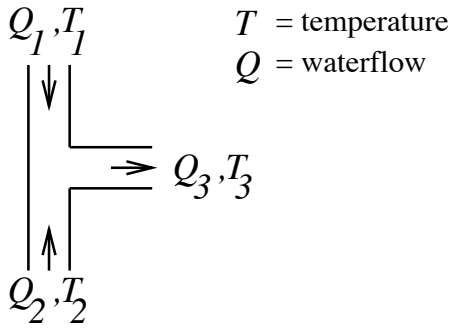
- each training example: $\langle$ qualitative function, mechanical structure$\rangle$
- new query: desired function,
- target value: mechanical structure for this function

Distance metric: match qualitative function descriptions

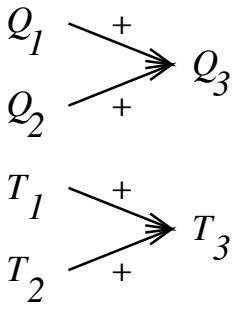
Case-Based Reasoning in CADET

A stored case: T–junction pipe

Structure:



Function:

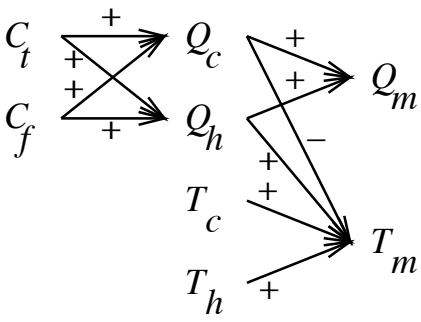


A problem specification: Water faucet

Structure:

?

Function:



Case-Based Reasoning in CADET

- Instances represented by rich structural descriptions
- Multiple cases retrieved (and combined) to form solution to new problem
- Tight coupling between case retrieval and problem solving

Bottom line:

- Simple matching of cases useful for tasks such as answering help-desk queries
- Area of ongoing research

Lazy and Eager Learning

Lazy: wait for query before generalizing

- k-NEAREST NEIGHBOR, Case based reasoning

Eager: generalize before seeing query

- Radial basis function networks, ID3, Backpropagation, NaiveBayes, ...

Does it matter?

- Eager learner must create global approximation
- Lazy learner can create many local approximations
- if they use same H, lazy can represent more complex fns (e.g., consider H = linear functions)