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.

$$\begin{array}{rr} P(cancer) = & P(\neg cancer) = \\ P(+|cancer) = & P(-|cancer) = \\ P(+|\neg cancer) = & P(-|\neg cancer) = \end{array}$$

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

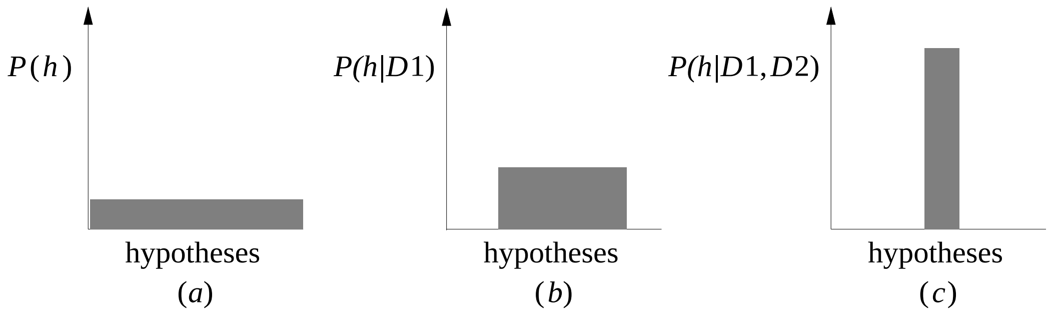
Choose $P(h)$ to be *uniform* distribution

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

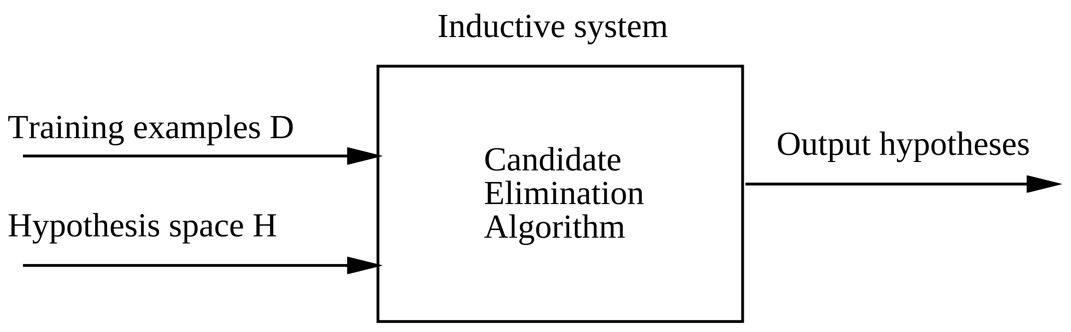
Then,

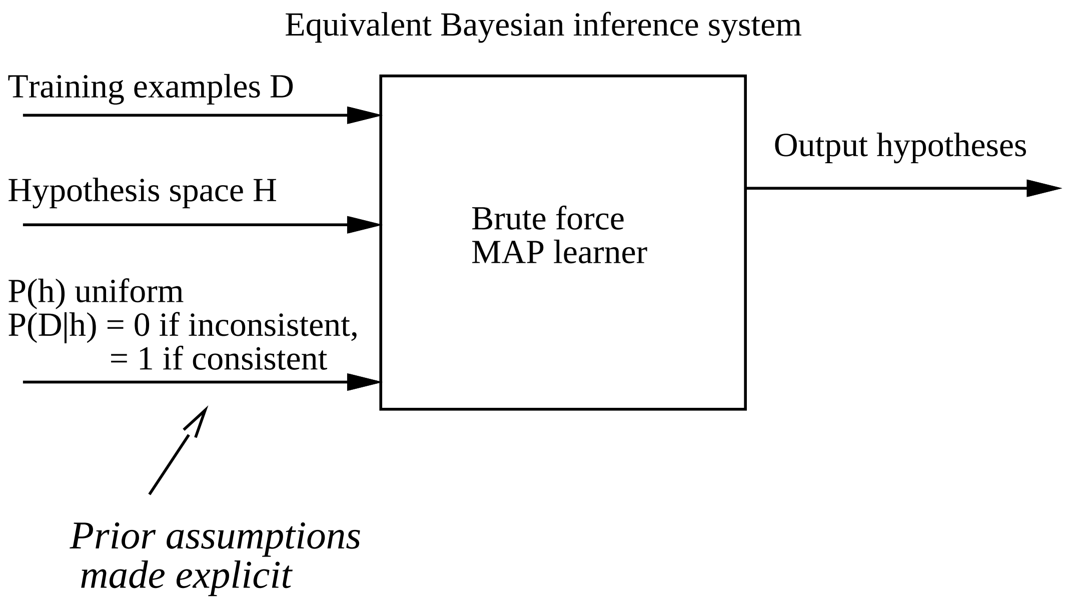
$$P(h|D) = \begin{cases} \frac{1}{|VS_{H,D}|} & \text{if } h \text{ is consistent with } D \\ \\ 0 & \text{otherwise} \end{cases}$$

Evolution of Posterior Probabilities

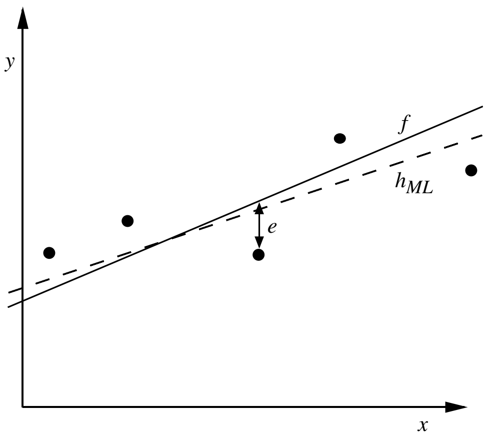


Characterizing Learning Algorithms by Equivalent MAP Learners





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

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

Maximize natural log of this instead...

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

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

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

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

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

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

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

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

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($x$)
```

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

Naive Bayes: Example

Consider *PlayTennis* again, and new instance

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

Want to compute:

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

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

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

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

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

$$v_{NB} = \operatorname*{argmax}_{v_j \in V} P(v_j) \prod_{i \in positions} P(a_i|v_j)$$

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
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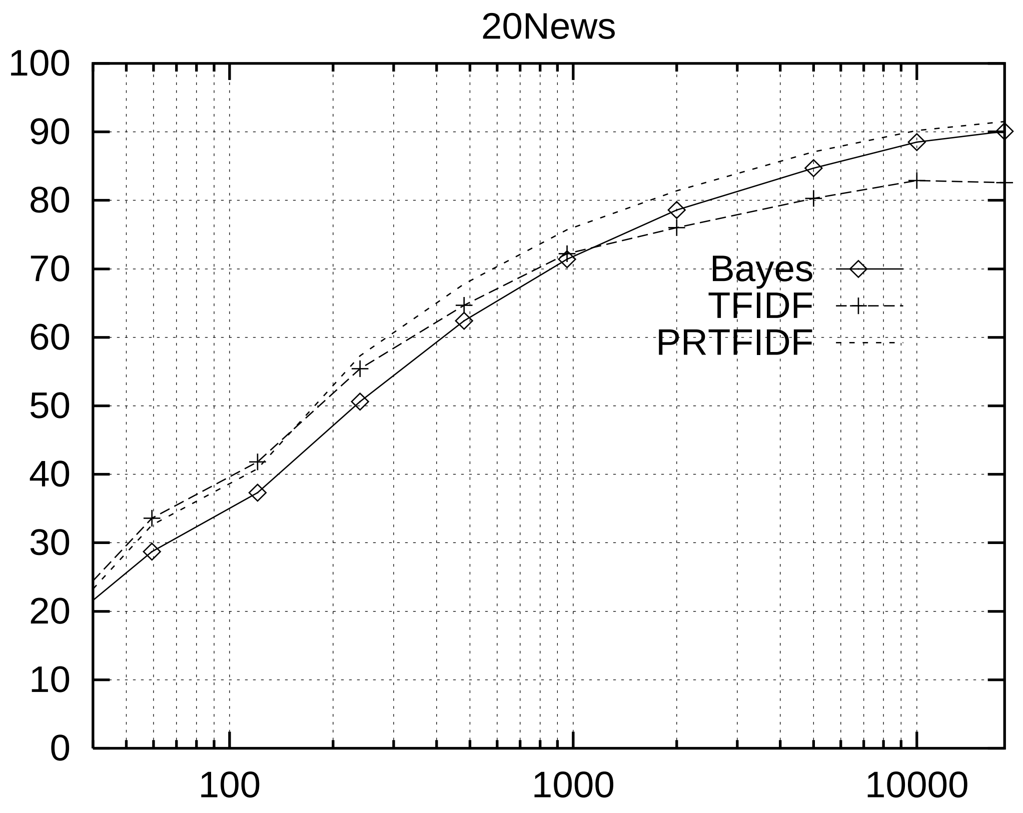
Learning Curve for 20 Newsgroups



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

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

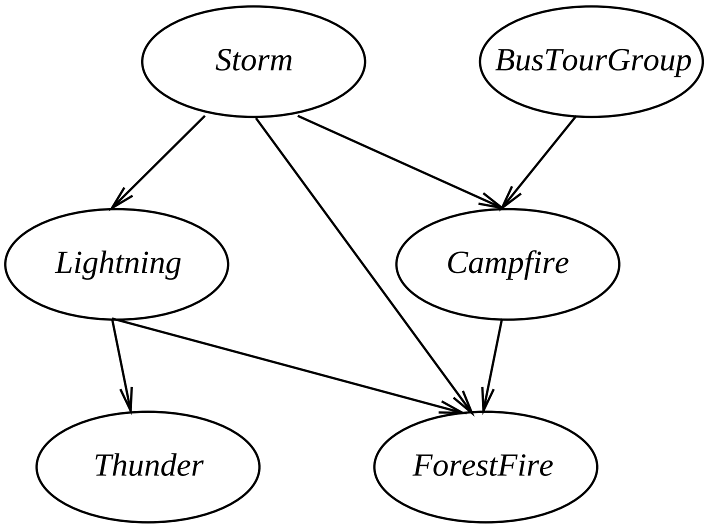
Example: *Thunder* is conditionally independent of *Rain*, given *Lightning*

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

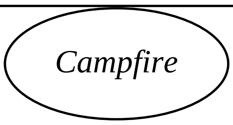
Naive Bayes uses cond. indep. to justify

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

Bayesian Belief Network



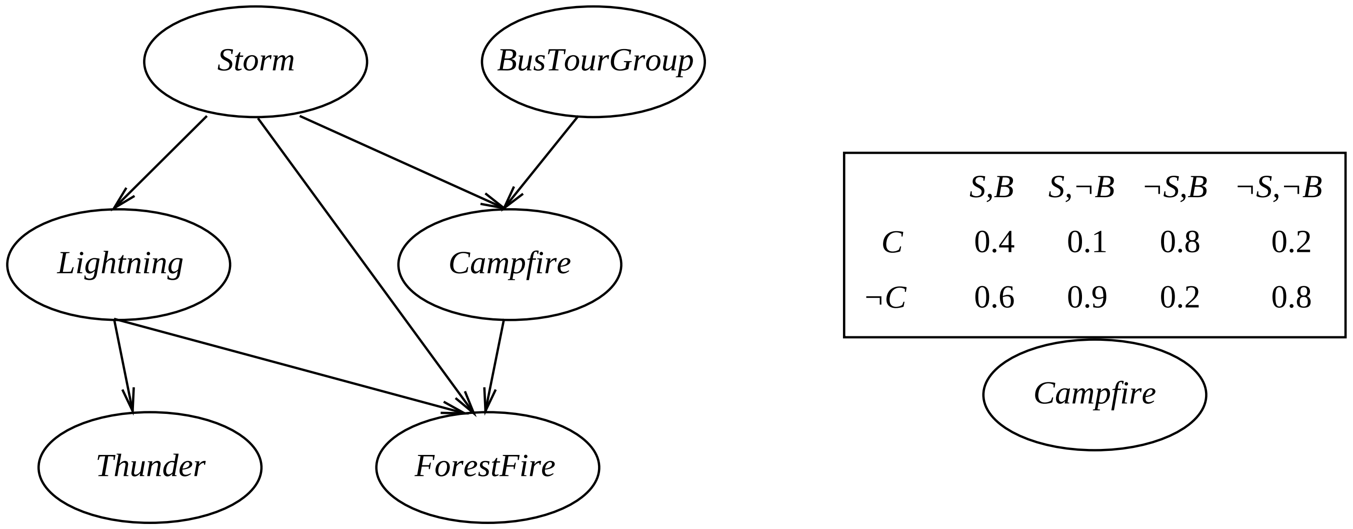
	S,B	S,¬B	¬S,B	¬S,¬B
C	0.4	0.1	0.8	0.2
¬C	0.6	0.9	0.2	0.8



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

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

$w_{ijk} = P(Y_i = y_{ij} | Parents(Y_i) =$ the list u_{ik} 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
   - $\sum_j w_{ijk} = 1$
   - $0 \leq w_{ijk} \leq 1$

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)

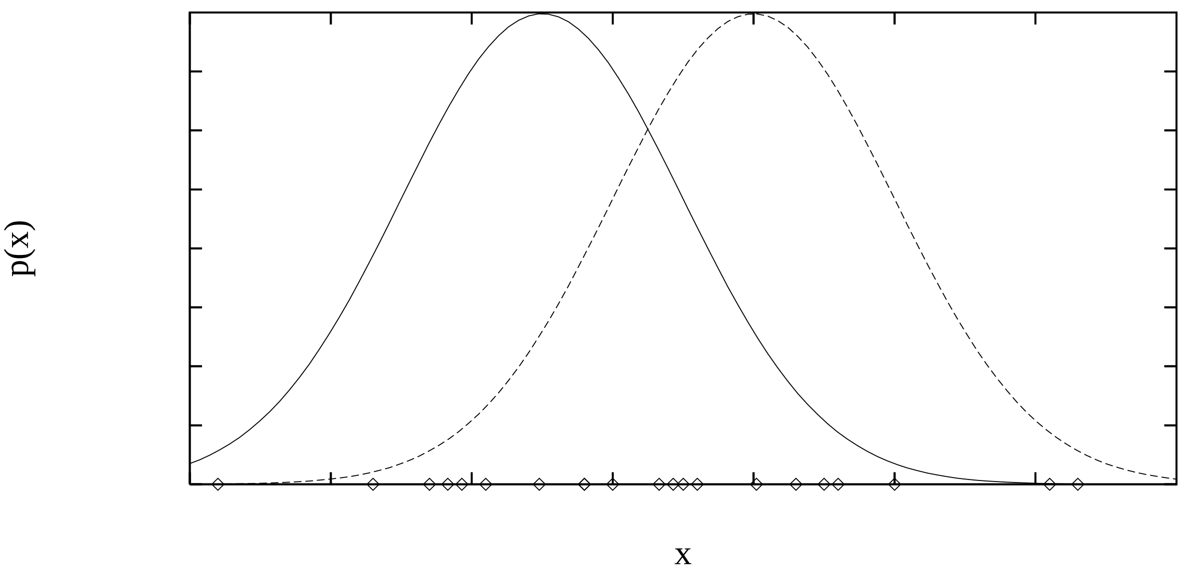
When to use:

- 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.

$$\begin{aligned} E[z_{ij}] &= \frac{p(x = x_i | \mu = \mu_j)}{\Sigma_{n=1}^{2} p(x = x_i | \mu = \mu_n)} \\ &= \frac{e^{-\frac{1}{2\sigma^2}(x_i - \mu_j)^2}}{\Sigma_{n=1}^{2} e^{-\frac{1}{2\sigma^2}(x_i - \mu_n)^2}} \end{aligned}$$

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 $h' = \langle \mu'_1, \mu'_2 \rangle$.

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

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 $c \in C$

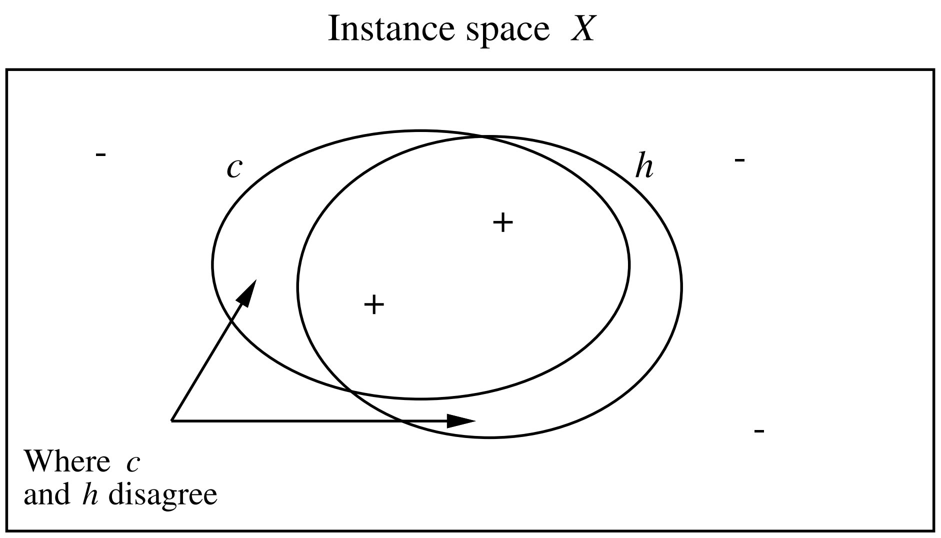
- instances x are drawn from distribution $\mathcal{D}$
- teacher provides target value $c(x)$ for each

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

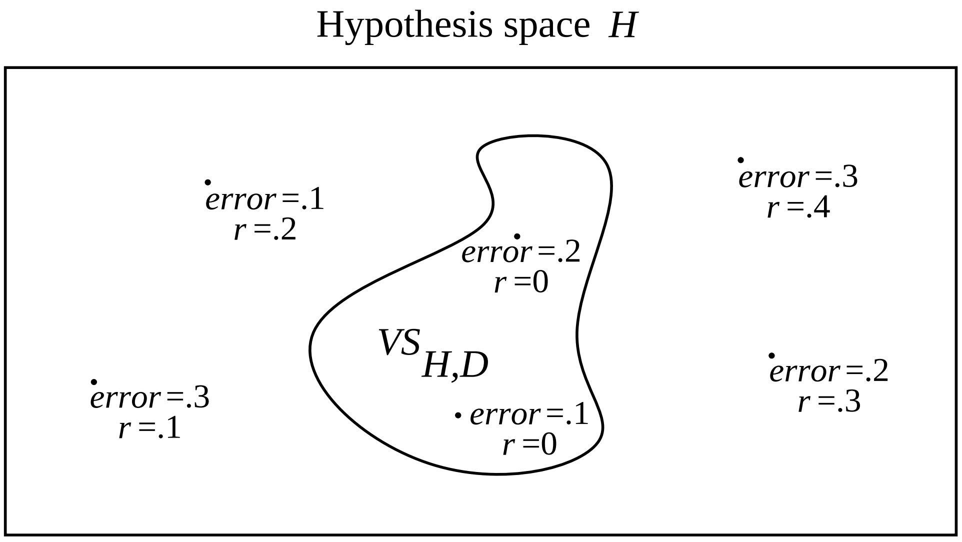
True error of hypothesis h with respect to c

- 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:

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

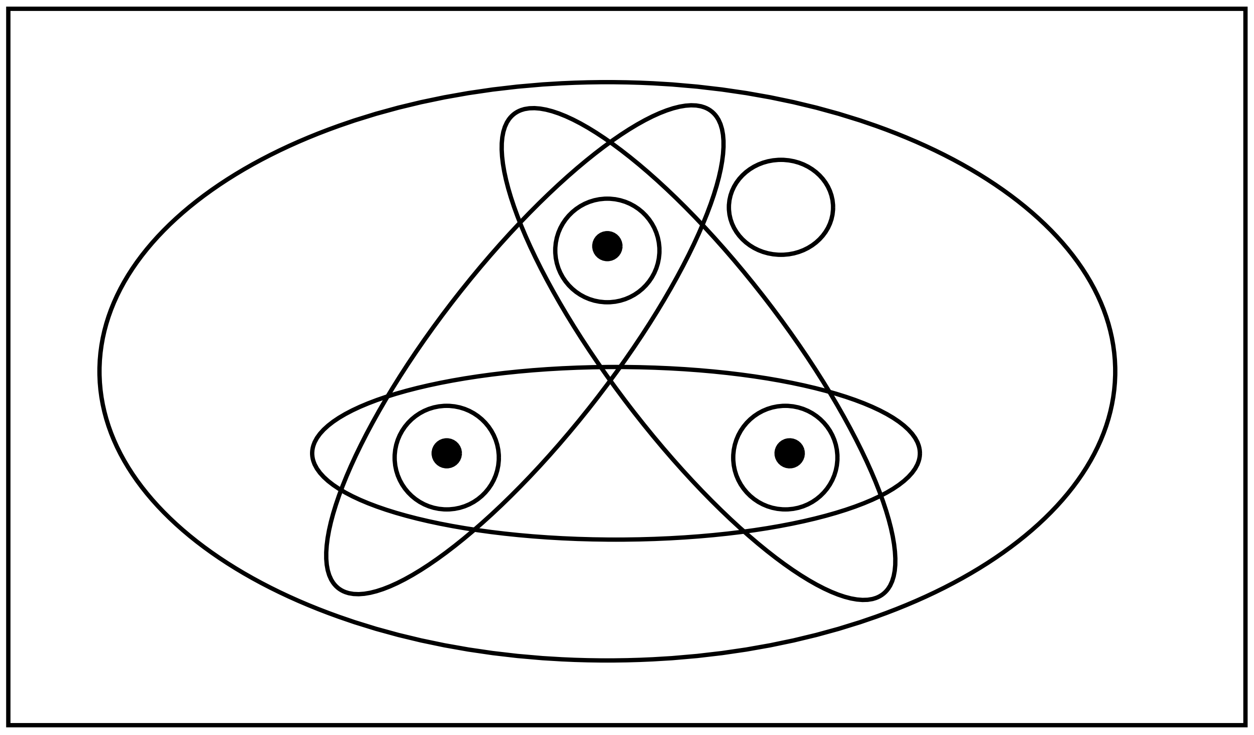
Shattering a Set of Instances

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

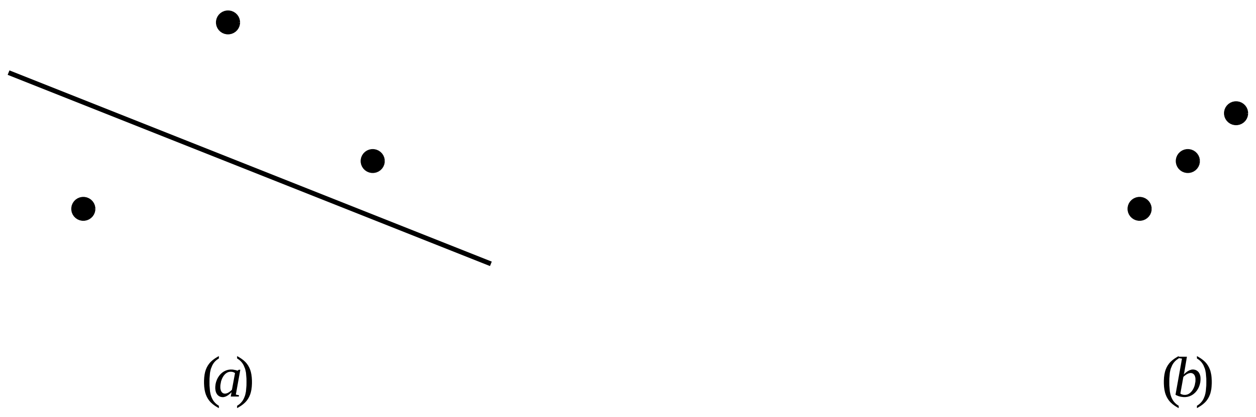
Instance space X



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)

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

When To Consider Nearest Neighbor

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

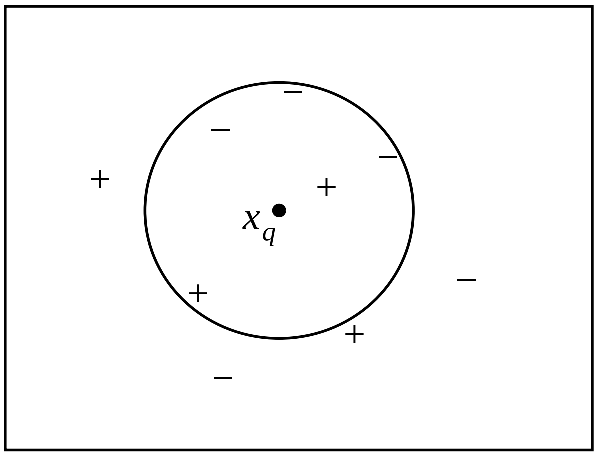
Advantages:

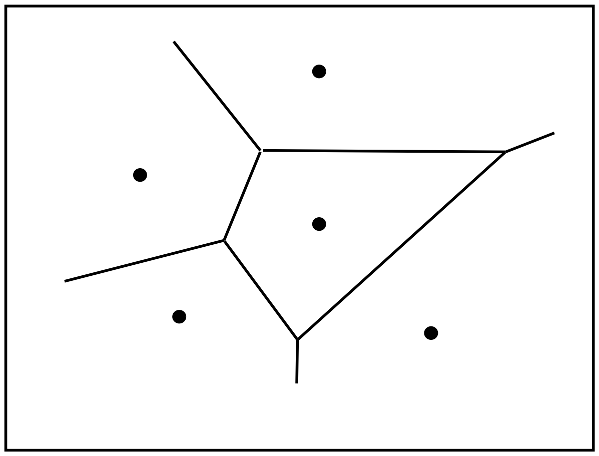
- Training is very fast
- Learn complex target functions
- Don't lose information

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

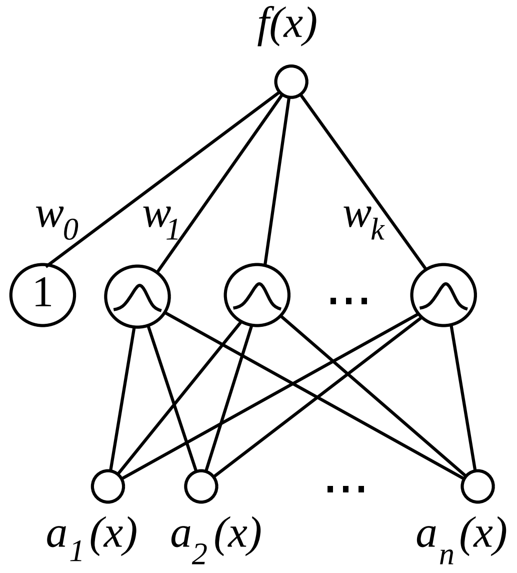
$$E_2(x_q) \equiv \frac{1}{2} \sum_{x \in D} (f(x) - \hat{f}(x))^2 \ K(d(x_q, x))$$

- ...

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

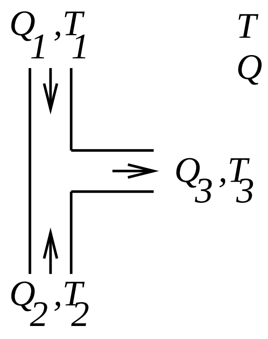
- each training example: $\langle$ qualitative function, mechanical structure$\rangle$
- new query: desired function,
- target value: mechanical structure for this function

Distance metric: match qualitative function descriptions

Case-Based Reasoning in CADET

A stored case: T−junction pipe

Structure:



T = temperature
Q = waterflow

Function:

$$\begin{tikzcd}
Q_1 \arrow[dr, "+"] & \\
& Q_3 \\
Q_2 \arrow[ur, "+"'] & \\
T_1 \arrow[dr, "+"] & \\
& T_3 \\
T_2 \arrow[ur, "+"'] &
\end{tikzcd}$$

A problem specification: Water faucet

Structure:

?

Function:

$$\begin{tikzcd}
C_t \arrow[r, "+"] \arrow[ddr, "+"'] & Q_c \arrow[dr, "+"] \arrow[ddddr, "-"] & \\
& & Q_m \\
C_f \arrow[r, "+"'] \arrow[uur, "+"] & Q_h \arrow[ur, "+"] \arrow[ddr, "+"] & \\
& T_c \arrow[dr, "+"] & \\
& & T_m \\
& T_h \arrow[ur, "+"'] &
\end{tikzcd}$$

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)