Machine Learning

Bayesian Learning

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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

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

Remark on Conditional Probabilities and Priors

- $P((d_1, \ldots, d_m)|h)$: probability that a hypothesis h generated a certain classification for a fixed input data set $(\mathbf{x}_1, \ldots, \mathbf{x}_m)$
- $P((\mathbf{x}_1, \ldots, \mathbf{x}_m)|\mu, \sigma^2)$ probability that input data set was generated by a Gaussian distribution with specific parameter values μ, σ
- $=$ Likelihood of these values
- For a hypothesis h (e.g., a decision tree) $P(h)$ should be seen as prior knowledge about hypothesis:
- For instance: smaller trees are more probable than more complex trees
- Or: uniform distribution, if no prior knowledge
- $\rightarrow$ subjective probability$\approx$ probability as belief

Bayes Theorem

- In the following: fixed training set $\mathbf{x}_1, \ldots, \mathbf{x}_m$
- Classifications $D = (d_1, \ldots, d_m)$
- This allows to determine the most probable hypothesis given the data using 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 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

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

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

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

Relation to Concept Learning

Consider our usual concept learning task

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

What would Bayes rule produce as the 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
$D = \langle c(x_1), \ldots, c(x_m) \rangle = \langle d_1, \ldots, d_m \rangle$

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

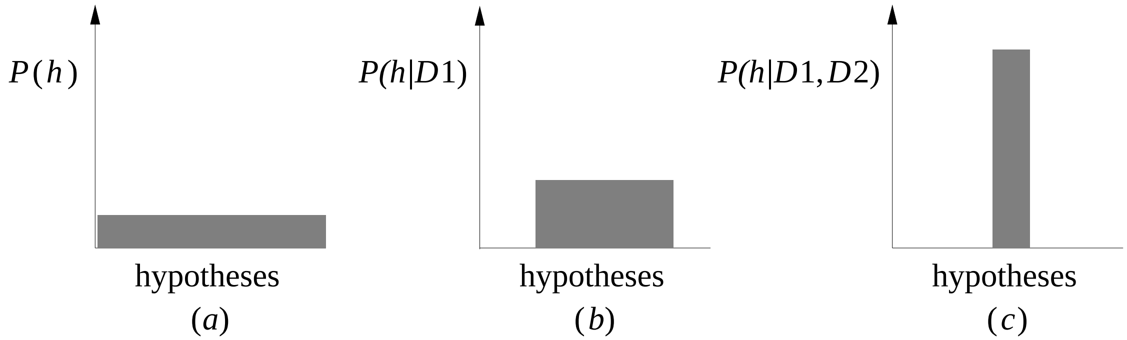
Choose $P(h)$ to be *uniform* distribution

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

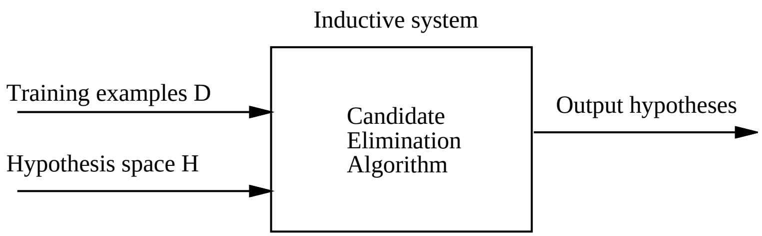
Then,

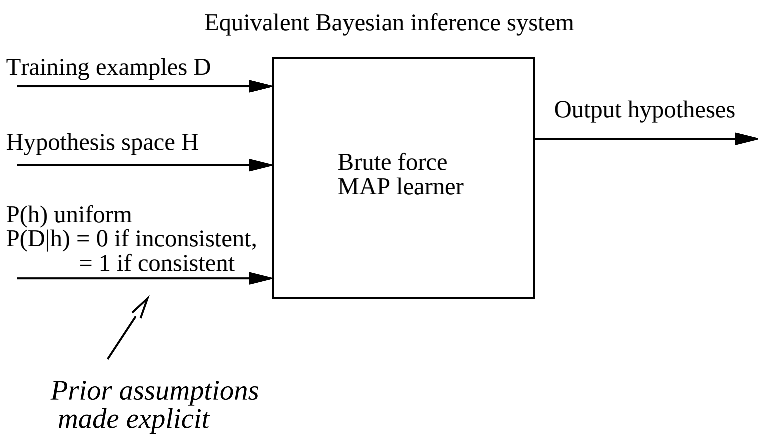
$$P(h|D) = \begin{cases} \frac{1}{|VS_{H,D}|} & \text{if } h \text{ is consistent with } D \\ 0 & \text{otherwise} \end{cases}$$

Evolution of Posterior Probabilities



Characterizing Learning Algorithms by Equivalent MAP Learners

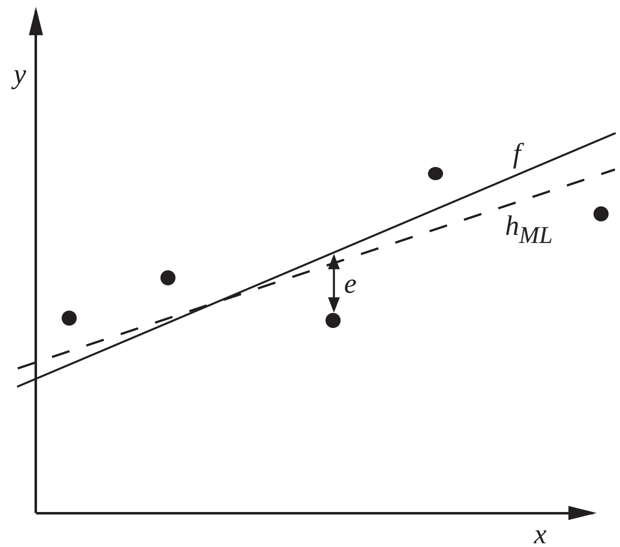




Does $FindS$ output a MAP hypothesis?

Yes, if $P(h)$ is chosen such it prefers more specific over more general hypothesis.

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:

$d_i = f(x_i) + e_i$ and

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 (cont'd)

Proof:

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

Maximize logarithm of this instead...

$h_{ML} = \mathrm{argmax}_{h \in H} \ln(\prod_{i=1}^{m} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(\frac{d_i - h(x_i)}{\sigma})^2})$

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

Learning to Predict Probabilities

- 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 only a 0 or 1)
- example: predicting probability that (insert your favourite soccer team here) wins.
- how to do this?

1. building relative frequencies from training examples, train regression model
2. use different errorfunction (shown here)

In this case we can show that

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

Situation: given p training examples $\{(x_i, d_i)\}_{i=1}^p$. d_i are class labels, i.e. $d_i \in \{0, 1\}$.

Idea: $h(x) \stackrel{!}{=} P(c(x) = 1)$ (output value should equal to class probability of correct class $c(x)$ given x).

ML-approach: maximize $P(D|h)$.
$P(D|h) = P(x_1, d_1|h) \ \ldots \ P(x_p, d_p|h)$
x_i is independent from h. Therefore (with product rule):
$P(x_i, d_i|h) = P(d_i|x_i, h)\, P(x_i|h) = P(d_i|x_i, h)\, P(x_i)$

What is $P(d_i|x_i, h)$? Recall: $h(i)$ should compute probabilty for d_i being 1. Therefore

$$P(d_i|x_i, h) = \begin{cases} h(x_i) & , \quad \text{if } d_i = 1 \\ 1 - h(x_i) & , \quad \text{if } d_i = 0 \end{cases} \tag{1}$$

in short notation:
$P(d_i|x_i, h) = h(x_i)^{d_i}\, (1 - h(x_i))^{(1-d_i)}$
Therefore: $P(D|h) = \Pi_{i=1}^p P(x_i, d_i|h) = \Pi_{i=1}^p P(d_i|x_i, h)\, P(x_i) =$
$\Pi_{i=1}^p h(x_i)^{d_i}\, (1 - h(x_i))^{(1-d_i)}\, P(x_i)$

Maximum-likelihood:

$h_{ML} = \text{argmax}_h \, P(D|h) =$
$\text{argmax}_h \, \Pi_{i=1}^{p} h(x_i)^{d_i} \, (1 - h(x_i))^{(1-d_i)} \, P(x_i)$

taking logarithm finally yields:

$h_{ML} = \text{argmax}_h \sum_i^n d_i \ln(h(x_i)) + (1 - d_i) \ln(1 - h(x_i)) =$
$\text{argmin}_h - \sum_i^n d_i \ln(h(x_i)) + (1 - d_i) \ln(1 - h(x_i))$

This expression is often termed the 'cross-entropy'-error function

$$h_{ML} = \underset{h}{\operatorname{argmin}} - \sum_{i}^{n} d_i \ln(h(x_i)) + (1 - d_i)\ \ln(1 - h(x_i))$$

What does this mean for a machine learning setup? E.g. multilayer-perceptrons?

Use the 'cross-entropy' errorfunction (instead of the usual mean-square errorfunction) to learn probabilities of classification.

Remark: fits particularly well to sigmoid activation function, since some terms cancel out then.

Minimum Description Length Principle

Occam's razor: prefer the shortest hypothesis

MDL: prefer the hypothesis h that minimizes

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

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

$$
\begin{aligned}
h_{MAP} &= \arg\max_{h \in H} P(D|h)P(h) \\
&= \arg\max_{h \in H} \log_2 P(D|h) + \log_2 P(h) \\
&= \arg\min_{h \in H} - \log_2 P(D|h) - \log_2 P(h) \qquad (2)
\end{aligned}
$$

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! Why?

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:

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

'Optimal': No other classification method using the same hypothesis space and the same prior knowledge can outperform this method in average.

Bayes Optimal Classifier

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

Example:

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

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

Thus,

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

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 (Haussler et al, 1994):

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

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:

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

Naive Bayes assumption:

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

cond. independence assumption: individual features are independent given the class

('correct computation' example: $P(a_1, a_2, a_3|v_j) =$
$P(a_1, a_2|a_3, v_j)\, P(a_3|v_j) = P(a_1|a_2, a_3, v_j)\, P(a_2|a_3, v_j)\, P(a_3|v_j)$
using conditional independence assumption:
$= P(a_1|v_j)\, P(a_2|v_j)\, P(a_3|v_j)$)

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

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)

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

Naive Bayes: Example

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

How to derive $\hat{P}(v_j)$, $\hat{P}(a_i|v_j)$?

simply by counting, e.g.

$\hat{P}('yes') = \frac{9}{14}$

$\hat{P}(strong|'yes') = \frac{3}{9}$

Why is this easier than computing

$\hat{P}(strong, rain, mild, normal, sunny|'yes')$?

Much less training examples of exactly that combination in the latter case.

Naive Bayes: Example

Consider *PlayTennis* again, and new instance

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

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

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

is often violated (e.g: $P(word_t =' machine' | word_{t+1} =' learning', Author =' TomMitchell') \neq P(word_t =' machine' | Author =' TomMitchell')$

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

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

- 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

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

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

$\textsc{Learn\_naive\_Bayes\_text}(Examples, V)$

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

Random guessing: 5%

Article from rec.sport.hockey

```
Path: cantaloupe.srv.cs.cmu.edu!das-news.harvard.edu!ogicse!uwm
From: xxx@yyy.zzz.edu (John Doe)
Subject: Re: This year's biggest and worst (opinion)...
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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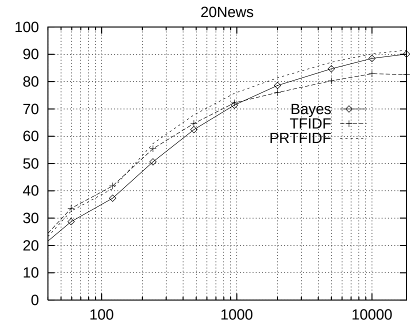
Learning Curve for 20 Newsgroups



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

Summary

- Probability theory offers a powerful framework to design and analyse learning methods
- probabilistic analysis offers insight in learning algorithms
- even if not directly manipulating probabilities, algorithms might be seen fruitfully in a probabilistic perspective