# The Naïve Bayes Algorithm 

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## Probabilistic Approach to Learning

## Instead of learning $\mathrm{F}: \mathrm{X} \rightarrow \mathrm{Y}$, learn $\mathrm{P}(\mathrm{Y} \mid \mathrm{X})$.

Can design algorithms that learn functions with uncertain outcomes (e.g., predicting tomorrow's stock price) and that incorporate prior knowledge to guide learning (e.g., a bias that tomorrow's stock price is likely to be similar to today's price).

## Bayes Rule

Bayes Rule: $\quad \mathbf{P}(\mathbf{A} \mid \mathbf{B})=\frac{\mathbf{P}(\mathbf{B} \mid \mathbf{A}) \mathbf{P}(\mathbf{A})}{\mathbf{P}(\mathbf{B})}$

## $\mathrm{P}(\mathrm{A}) \quad$ prior

## $\mathrm{P}(\mathrm{A} \mid \mathrm{B})$ posterior

...by no means merely a curious speculation in the doctrine of chances, but necessary to be solved in order to a sure foundation for all our reasonings concerning past facts, and what is likely to be hereafter. necessary to be considered by any that would give a clear account of the strength of analogical or inductive reasoning...


Bayes, Thomas (1763) An essay towards solving a problem in the doctrine of chances. Philosophical Transactions of the Royal Society of London, 53:370-418

## Naïve Bayes in a Nutshell, Y, $X_{i}$ Discrete

Pick the most probably $Y$ for $X^{\text {new }}=\left(X_{1}^{\text {new }}, X_{2}^{\text {new }}, \ldots, X_{n}^{\text {new }}\right)$

$$
Y^{\text {new }}=\operatorname{argmax}_{y_{k}} P\left(Y=y_{k} \mid X_{1}^{\text {new }}, \ldots, X_{n}^{\text {new }}\right)
$$

Bayes Rule: $\mathrm{P}\left(\mathrm{Y}=\mathrm{y}_{\mathrm{k}} \mid \mathrm{X}_{1}, \ldots, \mathrm{X}_{\mathrm{n}}\right)=\frac{\mathrm{P}\left(\mathrm{Y}=\mathrm{y}_{\mathrm{k}}\right) \mathrm{P}\left(\mathrm{X}_{1}, \ldots, \mathrm{X}_{\mathrm{n}} \mid \mathrm{Y}=\mathrm{y}_{\mathrm{k}}\right)}{\mathrm{P}\left(\mathrm{X}_{1}, \ldots, \mathrm{X}_{\mathrm{n}}\right)}$

## Main problem: learning $P(X \mid Y)$ might require more data than we have...

## Example:

$\mathrm{n}=100$ attributes
Number of rows in this table? $\quad 2^{100} \sim 100^{10} \sim 10^{30}$
Number of people on Earth? $10^{9}$
Fraction of rows with 0 training examples: 0.9999

## Naïve Bayes algorithms assume Conditional Independence

$\mathrm{X}_{\mathrm{i}}$ and $\mathrm{X}_{\mathrm{j}}$ are conditionally independent given Y, for all $\mathrm{i} \neq \mathrm{j}$

$$
\mathrm{P}\left(\mathrm{X}_{1}, \mathrm{X}_{2}, \ldots, \mathrm{X}_{\mathrm{n}} \mid \mathrm{Y}\right)=\prod_{\mathrm{i}} \mathrm{P}\left(\mathrm{X}_{\mathrm{i}} \mid \mathrm{Y}\right)
$$

If $\mathrm{X}_{1}, \ldots, \mathrm{X}_{\mathrm{n}}, \mathrm{Y}$ are all Boolean, how many parameters do we need to describe $P\left(X_{1}, X_{2}, \ldots, X_{n} \mid Y\right)$ ?

- Without the conditional independence assumption: $2\left(2^{n}-1\right)$
- With conditional independence assumption: $2 n$


## Naïve Bayes in a Nutshell

Bayes Rule: $\mathrm{P}\left(\mathrm{Y}=\mathrm{y}_{\mathrm{k}} \mid \mathrm{X}_{1}, \ldots, \mathrm{X}_{\mathrm{n}}\right)=\frac{\mathrm{P}\left(\mathrm{Y}=\mathrm{y}_{\mathrm{k}}\right) \mathrm{P}\left(\mathrm{X}_{1}, \ldots, \mathrm{X}_{\mathrm{n}} \mid \mathrm{Y}=\mathrm{y}_{\mathrm{k}}\right)}{\mathrm{P}\left(\mathrm{X}_{1}, \ldots, \mathrm{X}_{\mathrm{n}}\right)}$

If $X_{i}$ and $X_{j}$ are conditionally independent given $Y$, for all $i \neq j$

$$
\mathrm{P}\left(\mathrm{Y}=\mathrm{y}_{\mathrm{k}} \mid \mathrm{X}_{1}, \ldots, \mathrm{X}_{\mathrm{n}}\right)=\frac{\mathrm{P}\left(\mathrm{Y}=\mathrm{y}_{\mathrm{k}}\right) \prod_{\mathrm{i}} \mathrm{P}\left(\mathrm{X}_{\mathrm{i}} \mid \mathrm{Y}=\mathrm{y}_{\mathrm{k}}\right)}{\mathrm{P}\left(\mathrm{X}_{1}, \ldots, \mathrm{X}_{\mathrm{n}}\right)}
$$

So, to pick the most probably Y for $\mathrm{X}^{\text {new }}=\left(\mathrm{X}_{1}^{\text {new }}, \mathrm{X}_{2}^{\text {new }}, \ldots, \mathrm{X}_{\mathrm{n}}^{\text {new }}\right)$

$$
Y^{\text {new }}=\operatorname{argmax}_{y_{k}} P\left(Y=y_{k}\right) \prod_{i} P\left(X_{i}^{\text {new }} \mid Y=y_{k}\right)
$$

## Naïve Bayes: discrete $X_{i}$

## Training phase (input: training examples)

- For each value $y_{k}$, estimate $\pi_{k}=P\left(Y=y_{k}\right)$; get $\widehat{\pi_{k}}$
- For each value $\mathrm{x}_{\mathrm{ij}}$ of attribute $\mathrm{X}_{\mathrm{i}}$ estimate $\theta_{\mathrm{i}, \mathrm{j}, \mathrm{k}}=\mathrm{P}\left(\mathrm{X}_{\mathrm{i}}=\mathrm{x}_{\mathrm{ij}} \mid \mathrm{Y}=\mathrm{y}_{\mathrm{k}}\right)$; get $\widehat{\theta_{\mathrm{i}, \mathrm{j}, \mathrm{k}}}$

Testing phase:

- Classify $X^{\text {new }}=\left(X_{1}^{\text {new }}, X_{2}^{\text {new }}, \ldots, X_{n}^{\text {new }}\right)$

$$
Y^{\text {new }}=\operatorname{argmax}_{y_{k}} \widehat{\pi_{k}} \prod_{\mathrm{i}} \widehat{\theta_{\mathrm{i}, \mathrm{new}, \mathrm{k}}}
$$

[Ideal rule: $\mathrm{Y}^{\text {new }}=\operatorname{argmax}_{\mathrm{y}_{\mathrm{k}}} \mathrm{P}\left(\mathrm{Y}=\mathrm{y}_{\mathrm{k}}\right) \prod_{\mathrm{i}} \mathrm{P}\left(\mathrm{X}_{\mathrm{i}}^{\text {new }} \mid \mathrm{Y}=\mathrm{y}_{\mathrm{k}}\right)$ ]

## Estimating parameters $\mathrm{Y}, \mathrm{X}_{\mathrm{i}}$ discrete

## Maximum Likelihood Estimation

- For each value $y_{k}$, get $\widehat{\pi_{k}}=\widehat{P}\left(Y=y_{k}\right)=\frac{\# D\left(Y=y_{k}\right)}{|D|}$
number of training data points with $Y=y_{k}$ divided by the total number of training data points
- For each value $\mathrm{x}_{\mathrm{ij}}$ of attribute $\mathrm{X}_{\mathrm{i}}$ estimate $\theta_{\mathrm{i}, \mathrm{j}, \mathrm{k}}=\mathrm{P}\left(\mathrm{X}_{\mathrm{i}}=\mathrm{x}_{\mathrm{ij}} \mid Y=\mathrm{y}_{\mathrm{k}}\right)$;

$$
\text { get } \widehat{\theta_{\mathrm{i}, \mathrm{j}, \mathrm{k}}}=\widehat{\mathrm{P}}\left(\mathrm{X}_{\mathrm{i}}=\mathrm{x}_{\mathrm{ij}} \mid Y=\mathrm{y}_{\mathrm{k}}\right)=\frac{\# \mathrm{D}\left(\mathrm{X}_{\mathrm{i}}=\mathrm{x}_{\mathrm{ij}} \wedge \mathrm{Y}=\mathrm{y}_{\mathrm{k}}\right)}{\# \mathrm{D}\left(\mathrm{Y}=\mathrm{y}_{\mathrm{k}}\right)}
$$

The fraction of datapoints with $\mathrm{Y}=\mathrm{y}_{\mathrm{k}}$ that also have $\mathrm{X}=\mathrm{x}_{\mathrm{i}, \mathrm{j}}$.

## Sublety 1: Violation of the Naïve Bayes Assumption

- Usually features are not conditionally independent given the label

$$
P\left(X_{1}, X_{2}, \ldots, X_{n} \mid Y\right) \neq \prod_{i} P\left(X_{i} \mid Y\right)
$$

- Nonetheless, NB is widely used:
- NB often performs well, even when assumption is violated
- [Domingos \& Pazzani '96] discuss some conditions for good performance


## Subtlety 2: Need to use MAP

$$
Y^{\text {new }}=\operatorname{argmax}_{y_{k}} \widehat{P}\left(Y=y_{k} \mid X_{1}, \ldots, X_{n}\right)=\operatorname{argmax}_{y_{k}} \widehat{P}\left(Y=y_{k}\right) \prod_{i} \widehat{P}\left(X_{i}^{\text {new }} \mid Y=y_{k}\right)
$$

Note: If we never see a certain combination $X_{i}=\mathrm{a}$ and $\mathrm{Y}=\mathrm{b}$ in our training data, then on any new example with $X_{i}=$ a we will predict a zero probability of $\mathrm{Y}=\mathrm{b}$
E.g., if we never see a training instance where $X_{1}=a$ and $Y=b$ ?

$$
\text { e.g., } \mathrm{Y}=\text { SpamEmail, } \mathrm{X}=\text { "Earn" } \quad \widehat{\mathrm{P}}\left(\mathrm{X}_{1}=\mathrm{a} \mid \mathrm{Y}=\mathrm{b}\right)=0
$$

- Thus no matter what the values $X_{2}^{\text {new }}, \ldots, X_{n}^{\text {new }}$ take, we get

$$
\widehat{\mathrm{P}}\left(\mathrm{Y}=\mathrm{b} \mid \mathrm{X}_{1}^{\text {new }}=\mathrm{a}, \mathrm{X}_{2}^{\text {new }}, \ldots, \mathrm{X}_{\mathrm{n}}^{\text {new }}\right)=0
$$

- Solution: use MAP estimate!!!!


## Estimating parameters $\mathrm{Y}, \mathrm{X}_{\mathrm{i}}$ discrete

## Maximum A Posteriori Estimation

- For each value $y_{k}$, get $\widehat{\pi_{k}}=\widehat{P}\left(Y=y_{k}\right)=\frac{\# D\left(Y=y_{k}\right)+1}{|D|+1 K}$

K - number of distinct values label can take; l determines the strength of this smoothing; assume the hallucinated examples are spread evenly over the possible values of Y; so, number of hallucinated examples is 1 K .

- For each value $\mathrm{x}_{\mathrm{ij}}$ of attribute $\mathrm{X}_{\mathrm{i}}$ estimate $\theta_{\mathrm{i}, \mathrm{j}, \mathrm{k}}=\mathrm{P}\left(\mathrm{X}_{\mathrm{i}}=\mathrm{x}_{\mathrm{ij}} \mid Y=\mathrm{y}_{\mathrm{k}}\right)$;

$$
\text { get } \widehat{\theta_{\mathrm{i}, \mathrm{j}, \mathrm{k}}}=\widehat{\mathrm{P}}\left(\mathrm{X}_{\mathrm{i}}=\mathrm{x}_{\mathrm{ij}} \mid Y=\mathrm{y}_{\mathrm{k}}\right)=\frac{\# \mathrm{D}\left(\mathrm{X}_{\mathrm{i}}=\mathrm{x}_{\mathrm{ij}} \wedge \mathrm{Y}=\mathrm{y}_{\mathrm{k}}\right)+\mathrm{l}}{\# \mathrm{D}\left(\mathrm{Y}=\mathrm{y}_{\mathrm{k}}\right)+\mathrm{lj}}
$$

J - number of distinct values that feature i can take; l determines the strength of this smoothing; assume the hallucinated examples are spread evenly over the possible values of $X_{i}$; so, number of hallucinated examples is 1 J .

## Bag of Words Approach



## Case Study: Text Classification

- Classify e-mails
- $\mathrm{Y}=\{$ Spam, NotSpam $\}$
- Classify news articles
- $\mathrm{Y}=$ what is the topic of the article?
- Classify webpages
- $Y=\{$ student, professor, project, ... $\}$
- What about the features X?
- The text!


# Features X are entire document $-\mathrm{X}_{\mathrm{i}}$ for ith word in article 

Article from rec.sport.hockey

```
Path: cantaloupe.srv.cs.cmu.edu!das-news.harvard.\epsilon
From: xxx@yyy.zzz.edu (John Doe)
Subject: Re: This year's biggest and worst (opinic
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
```


## Naïve Bayes for Text Classification

- What are the features: $\mathrm{X}_{\mathrm{i}}$ represents ith word in document.
- the domain of $X_{i}$ is entire vocabulary, e.g., Webster Dictionary, 10,000 words
- E.g., if article has 1000 words, $\mathrm{X}=\left\{\mathrm{X}_{1}, \ldots, \mathrm{X}_{1000}\right\}$, then domain of X has size $10000^{1000}$.
- $\mathrm{P}(\mathrm{X} \mid \mathrm{Y})$ is huge!
- Naïve Bayes assumption helps a lot!
- Meaning of naïve Bayes assumption: the word in position i is independent of all the other words in the document given the label y


## Naïve Bayes for Text Classification

- Naïve Bayes assumption helps a lot!
- $P\left(X_{i}=x_{i} \mid Y=y\right)$ is just the probability of observing word $x_{i}$ at the ith position in a document on topic $y$.
- Assume $X_{i}$ is independent of all other words in document given the label $y$ : $P\left(X_{i}=x_{i} \mid Y=y, X_{-i}\right)=P\left(X_{i}=x_{i} \mid Y=y\right)$.

$$
\mathrm{h}_{\mathrm{NB}}(\mathrm{x})=\arg \max _{\mathrm{y}} \mathrm{P}(\mathrm{y}) \prod_{\mathrm{i}=1}^{\text {lengthDoc }} \mathrm{P}\left(\mathrm{X}_{\mathrm{i}}=\mathrm{x}_{\mathrm{i}} \mid \mathrm{y}\right)
$$

- For each label y, have 1000 distributions of size 10000 to estimate.
- This is $10000 \times 1000$ items, which is big but much less than $10000^{1000}$.


## Bag of Words Model

- Typical additional assumption - Position in document doesn't matter:

$$
P\left(X_{i}=x_{i} \mid Y=y\right)=P\left(X_{k}=x_{i} \mid Y=y\right)
$$

the probability distributions of words are the same at each position: $P_{i}=P_{j}$ for all $i, j$.

- "Bag of Words" model - order of words in the document is ignored
- Now, only 10000 quantities $\mathrm{P}\left(\mathrm{x}_{\mathrm{i}} \mid \mathrm{y}\right)$ to estimate for each label y (the 10000 possible values that $x_{i}$ can be) plus the prior.

$$
\mathrm{h}_{\mathrm{NB}}(\mathrm{x})=\arg \max _{\mathrm{y}} \mathrm{P}(\mathrm{y}) \prod_{\mathrm{i}=1}^{1000} \mathrm{P}\left(\mathrm{x}_{\mathrm{i}} \mid \mathrm{y}\right)
$$

## Bag of Words model

- Typical additional assumption - Position in document doesn't matter:

$$
P\left(X_{i}=x_{i} \mid Y=y\right)=P\left(X_{k}=x_{i} \mid Y=y\right)
$$

- "Bag of Words" model - order of words on the page ignored
- Sounds silly but often works very well

A piece of text like "When the lecture is over, remember to take your bag" would look to this algorithm the same as if we just sorted the words alphabetically"bag is lecture over remember take the to When your"

## Bag of Words model

- Typical additional assumption - Position in document doesn't matter:

$$
P\left(X_{i}=x_{i} \mid Y=y\right)=P\left(X_{k}=x_{i} \mid Y=y\right)
$$

- "Bag of Words" model - order of words on the page ignored

Can simplify further:

$$
\prod_{\mathrm{i}=1}^{\text {lengthDoc }} \mathrm{P}\left(\mathrm{x}_{\mathrm{i}} \mid \mathrm{y}\right)=\prod_{\mathrm{w}=1}^{\mathrm{W}} \mathrm{P}(\mathrm{w} \mid \mathrm{y})^{\text {count }(\mathrm{w})}
$$

## Bag of Words representation

- Since we are assuming the order of words doesn't matter, an alternative representation of document is as vector of counts:
- $\mathrm{x}^{(\mathrm{j})}=$ number of occurrences of word j in document x .
- Typical document: [0010030001000100200 ...]
- Called "bag of words" or "term vector" or "vector space model" representation


## Naïve Bayes with Bag of Words for text classification

- Learning phase
- Class Prior $\mathrm{P}(\mathrm{Y})$
- $\mathrm{P}\left(\mathrm{X}_{\mathrm{i}} \mid \mathrm{Y}\right)$
- Test phase:
- For each document
- Use naïve Bayes decision rule

$$
\mathrm{h}_{\mathrm{NB}}(\mathrm{x})=\arg \max _{\mathrm{y}} \mathrm{P}(\mathrm{y}) \prod_{\mathrm{i}=1}^{1000} \mathrm{P}\left(\mathrm{x}_{\mathrm{i}} \mid \mathrm{y}\right)
$$

## Twenty news groups results

- Given 1000 training documents from each group, learn to classify new documents according to which newsgroup it came from
comp.graphics, comp.os.ms-windows.misc, comp.sys.ibm.pc.hardware, comp.sys.max.hardware, comp.windows.x, misc.forsale, rec.autos, rec.motorcycles, rec.sport.baseball, rec.sport.hockey
alt.atheism, soc.religion.christian, talk.religion.misc, talk.politics.mideast, talk.politics.misc, talk.politics.guns,
sci.space, sci.crypt, sci.electronics, sci.med
- Naïve Bayes: $89 \%$ classification accuracy


## Learning curve for twenty news groups



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

## What if features are continuous?

- E.g., character recognition: $\mathrm{X}_{\mathrm{i}}$ is intensity at ith pixel
- Gaussian Naïve Bayes (GNB):

$$
P\left(X_{i}=x \mid Y=y_{k}\right)=\frac{1}{\sigma_{\mathrm{ik}} \sqrt{2 \pi}} e^{-\frac{\left(\mathrm{x}-\mu_{\mathrm{ik}}\right)^{2}}{2 \sigma_{\mathrm{ik}}^{2}}}
$$


distribution of feature $X_{i}$ is Gaussian with a mean and variance that can depend on the label $y_{k}$ and which feature $X_{i}$ it is

## What if features are continuous?

- E.g., character recognition: $\mathrm{X}_{\mathrm{i}}$ is intensity at ith pixel
- Gaussian Naïve Bayes (GNB):

$$
P\left(X_{i}=x \mid Y=y_{k}\right)=\frac{1}{\sigma_{\mathrm{ik}} \sqrt{2 \pi}} e^{-\frac{\left(x-\mu_{\mathrm{ik}}\right)^{2}}{2 \sigma_{\mathrm{ik}}^{2}}}
$$



- Different mean and variance for each class k and each pixel i .
- Sometimes assume variance:
- Is independent of $Y$ (i.e., just have $\sigma_{i}$ )
- Or independent of $X$ (i.e., just have $\sigma_{k}$ )
- Or both (i.e., just have $\sigma$ )


## Estimating parameters: $Y$ discrete, $X_{i}$ continuous

- Maximum likelihood estimates:

$$
\hat{\mu}_{\mathrm{MLE}}=\frac{1}{\mathrm{~N}} \sum_{\mathrm{j}=1}^{\mathrm{N}} \mathrm{x}_{\mathrm{j}}
$$

$$
\hat{\mu}_{\mathrm{ik}}=\frac{1}{\sum_{\mathrm{j}} \delta\left(\mathrm{Y}^{\mathrm{j}}=\mathrm{y}_{\mathrm{k}}\right)} \sum_{\mathrm{j}} \mathrm{X}_{\mathrm{i}}^{\mathrm{j}} \delta\left(\mathrm{Y}^{\mathrm{j}}=\mathrm{y}_{\mathrm{k}}\right) \underset{\text { kth class }}{\substack{\text { jthaining image }}}
$$

ith pixel in jth training image

$$
\widehat{\sigma}_{\text {unbiased }}^{2}=\frac{1}{\mathrm{~N}-1} \sum_{\mathrm{j}=1}^{\mathrm{N}}\left(\mathrm{x}_{\mathrm{j}}-\hat{\mu}\right)^{2}
$$

$$
\widehat{\sigma}_{i k}^{2}=\frac{1}{\sum_{\mathrm{j}} \delta\left(\mathrm{Y}^{j}=\mathrm{y}_{\mathrm{k}}\right)-1} \sum_{\mathrm{j}}\left(\mathrm{X}_{\mathrm{i}}^{\mathrm{j}}-\hat{\mu}_{\mathrm{ik}}\right)^{2} \delta\left(\mathrm{Y}^{\mathrm{j}}=\mathrm{y}_{\mathrm{k}}\right)
$$

## Example: GNB for classifying mental states



- Classify a person's cognitive state, based on brain image
- reading a sentence or viewing a picture?
- reading the word describing a "Tool" or "Building"?
- reading the word describing a "Person" or an "Animal"?
- Training: Patients were shown words of different categories and then a measurement was done to see what parts of the brain responded.



## Example: GNB for classifying mental states


~1mm resolution
~2 images per sec.
15,000 voxels/image
Non-invasive, save
Measures Blood Oxygen Level Dependent response (BOLD)


## Gaussian Naïve Bayes: Learned $\mu_{\text {voxel,word }}$


[Mitchell et al.]

15,000 voxels or features


10 training examples or subjects per class

# Learned Naïve Bayes Models Means for P(BrainActivity | WordCategory) 

Pairwise classification accuracy: 85\%
[Mitchell et al.]
People words
-5 o ts Animal words


## What you should know

- Naïve Bayes classifier
- What's the assumption
- Why we use it
- How do we learn it
- Why is Bayesian estimation important
- Text classification
- Bag of words model
- Gaussian NB
- Features are still conditionally independent
- Each feature has a Gaussian distribution given class

