

Center for Artificial Intelligence Foundations & Scientific Applications Artificial Intelligence Research Laboratory





Data Science for Researchers and Scholars

Vasant G. Honavar

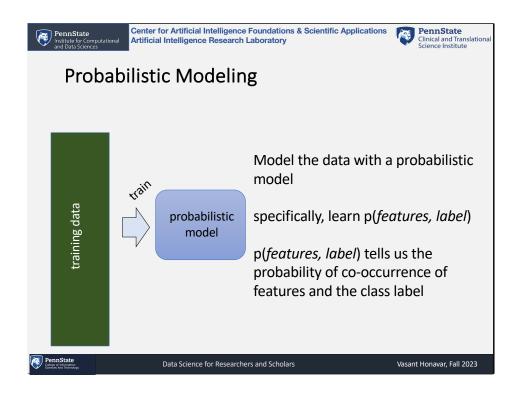
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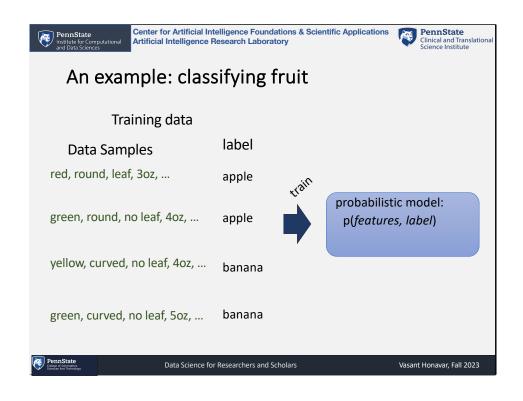
Director, Center for Artificial Intelligence Foundations and Scientific Applications Associate Director, Institute for Computational and Data Sciences Pennsylvania State University

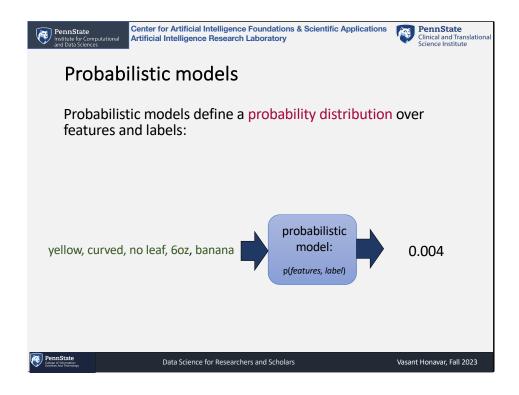
vhonavar@psu.edu http://faculty.ist.psu.edu/vhonavar http://ailab.ist.psu.edu

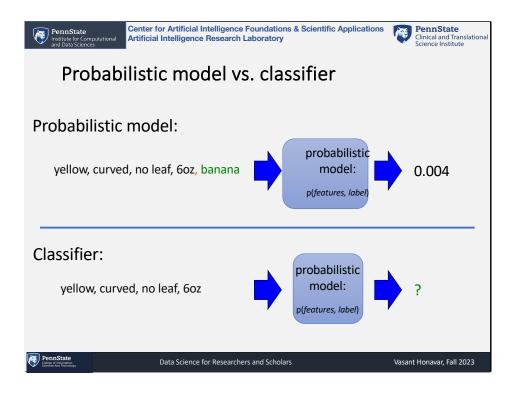


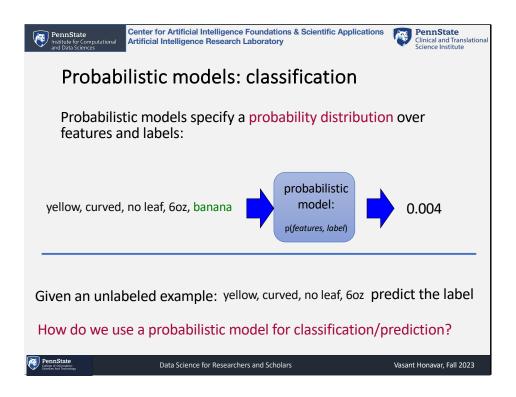
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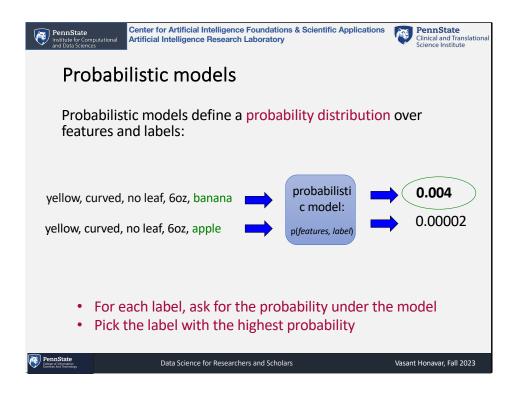


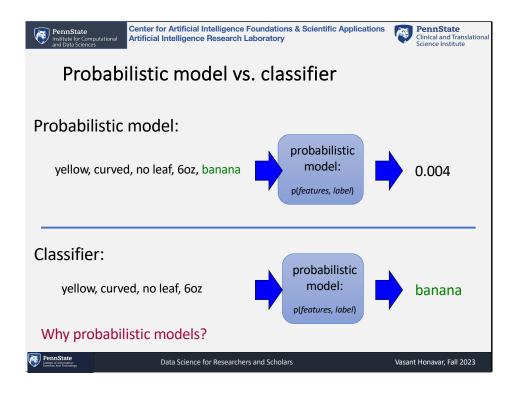


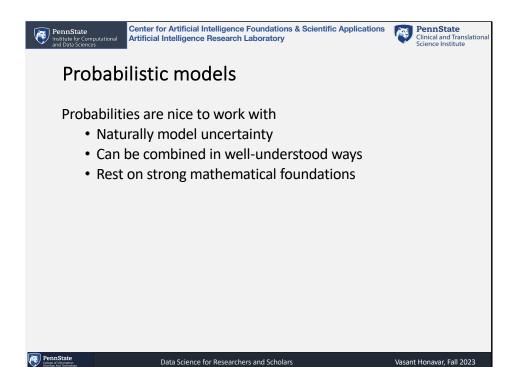


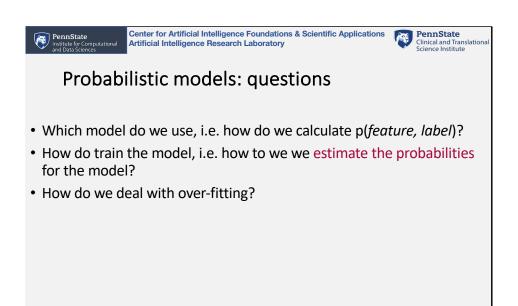












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Probabilistic models are a special class of ML models

Probabilistic models

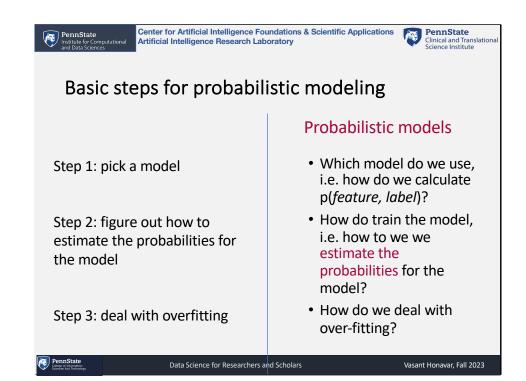
- Which model do we use, i.e. how do we obtain p(feature, label)?
- How do train the model, i.e. how to we we estimate the probabilities for the model?
- How do we deal with over-fitting?

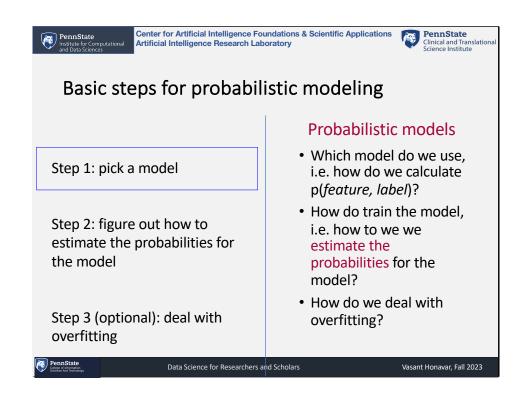
ML in general

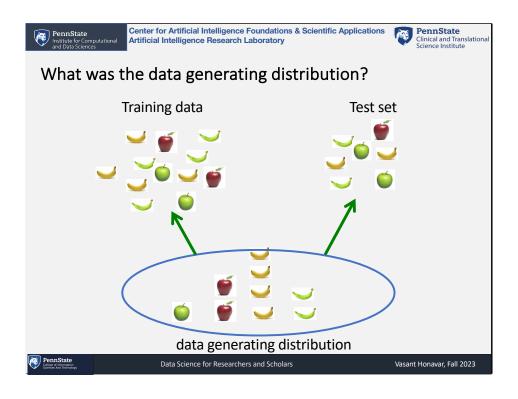
- Which model do we use (linear model, nonparametric)
- How do train the model?
- How do we deal with over-fitting?

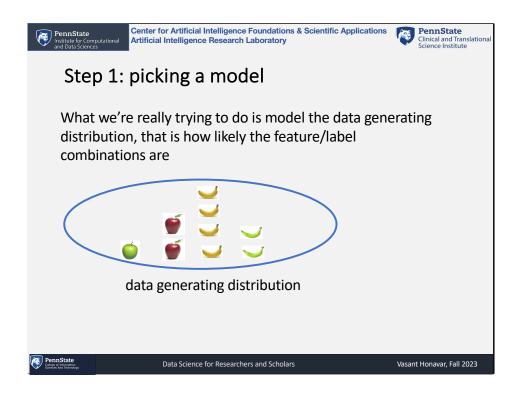
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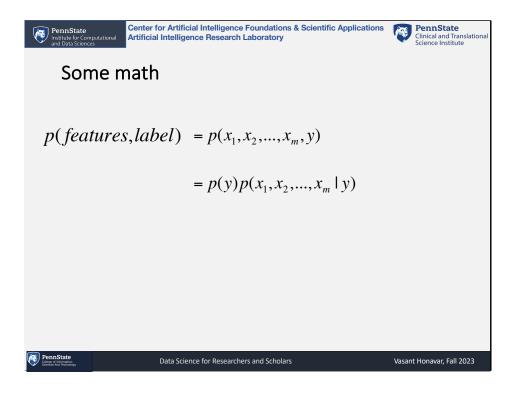
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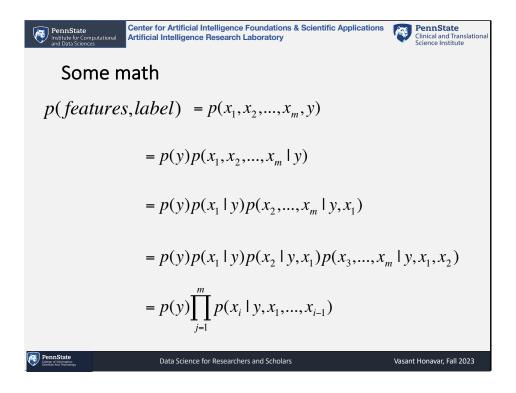




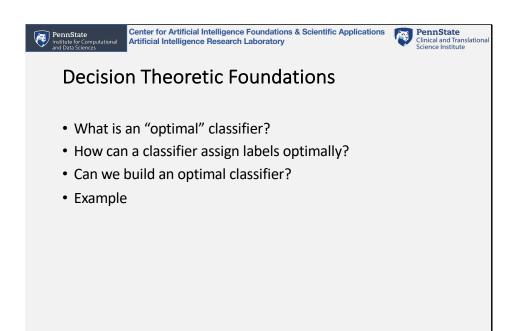




- chain rule!



- chain rule!



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Decision theoretic foundations of classification

Consider the problem of classifying an instance X into one of two mutually exclusive classes ω_1 or ω_2

 $P(\boldsymbol{\omega}_1 | X)$ = probability of class $\boldsymbol{\omega}_1$ given the evidence X

 $P(\boldsymbol{\omega}_2|X)$ = probability of class $\boldsymbol{\omega}_2$ given the evidence X

What is the probability of error?

 $P(error \mid X) = P(\omega_1 \mid X)$ if we choose ω_2

= $P(\omega_2|X)$ if we choose ω_1



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Minimum Error Classification

To minimize classification error

Choose ω_1 if $P(\omega_1|X) > P(\omega_2|X)$

Choose ω_2 if $P(\omega_2|X) > P(\omega_1|X)$

which yields

$$P(error \mid X) = \min[P(\omega_1 \mid X), P(\omega_2 \mid X)]$$

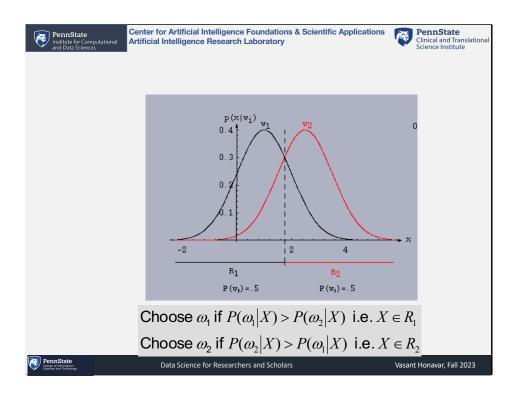
We have:

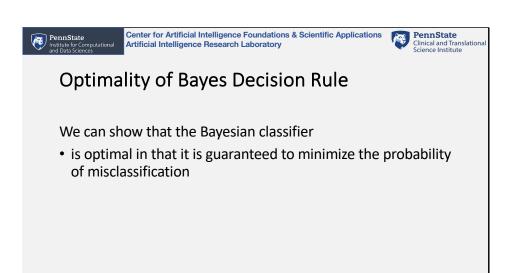
$$P(\omega_1|X) = P(X \mid \omega_1)P(\omega_1);$$

$$P(\omega_2|X) = P(X \mid \omega_2)P(\omega_2)$$



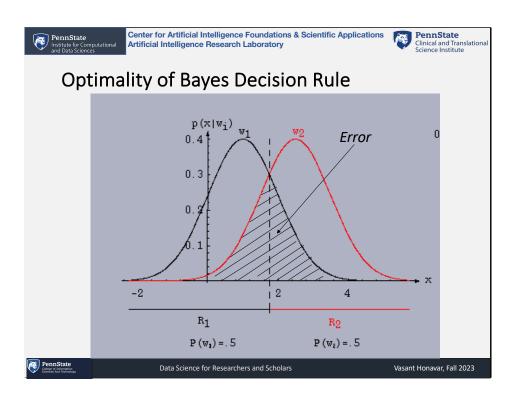
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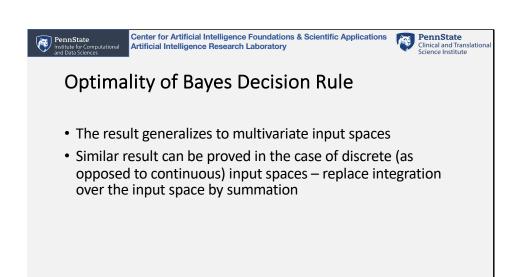




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Bayes Decision Rule yields Minimum Error Classification

To minimize classification error

Choose ω_1 if $P(\omega_1|X) > P(\omega_2|X)$

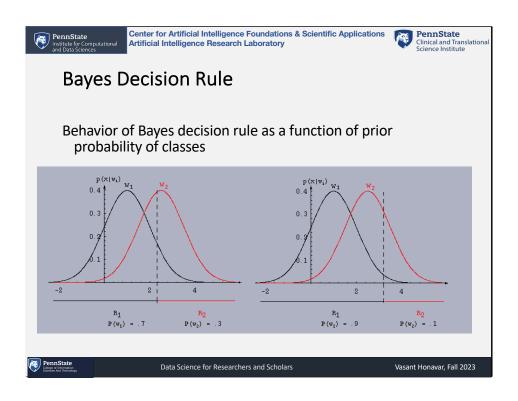
Choose ω_2 if $P(\omega_2|X) > P(\omega_1|X)$

which yields

 $P(error \mid X) = \min[P(\omega_1 \mid X), P(\omega_2 \mid X)]$



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Bayes Optimal Classifier

Classification rule that guarantees minimum error:

Choose
$$\omega_1$$
 if $P(X \mid \omega_1)P(\omega_1) > P(X \mid \omega_2)P(\omega_2)$

Choose
$$\omega_2$$
 if $P(X \mid \omega_2)P(\omega_2) > P(X \mid \omega_1)P(\omega_1)$

If
$$P(X \mid \omega_1) = P(X \mid \omega_2)$$

classification depends entirely on $P(\omega_1)$ and $P(\omega_2)$

If
$$P(\omega_1) = P(\omega_2)$$
,

classification depends entirely on $P(X \mid \omega_1)$ and $P(X \mid \omega_2)$

Bayes classification rule combines the effect of the two terms optimally - so as to yield minimum error classification.

Generalization to multiple classes $c(X) = \arg \max P(\omega_j \mid X)$





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Minimum Risk Classification

Let λ_{ij} = risk or cost associated with assigning an instance to class ω_i when the correct classification is ω_i

 $R(\omega_i \mid X) =$ expected loss incurred in assigning X to class ω_i

$$R(\omega_1 \mid X) = \lambda_{11} P(\omega_1 \mid X) + \lambda_{21} P(\omega_2 \mid X)$$

$$R(\omega_2 \mid X) = \lambda_{12} P(\omega_1 \mid X) + \lambda_{22} P(\omega_2 \mid X)$$

Classification rule that guarantees minimum risk:

Choose
$$\omega_1$$
 if $R(\omega_1 \mid X) < R(\omega_2 \mid X)$

Choose
$$\omega_2$$
 if $R(\omega_2 \mid X) < R(\omega_1 \mid X)$

Flip a coin otherwise



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Minimum Risk Classification

 λ_{ij} = risk or cost associated with assigning an instance to class ω_j when the correct classification is ω_i

Ordinarily $(\lambda_{21} - \lambda_{22})$ and $(\lambda_{12} - \lambda_{11})$ are positive (cost of being correct is less than the cost of error)

So we choose
$$\omega_1$$
 if $\frac{P(X|\omega_1)}{P(X|\omega_2)} > \frac{(\lambda_{21} - \lambda_{22})}{(\lambda_{12} - \lambda_{11})} \frac{P(\omega_2)}{P(\omega_1)}$

Otherwise choose ω_2

Minimum error classification rule is a special case:

$$\lambda_{ij} = 0$$
 if $i = j$ and $\lambda_{ij} = 1$ if $i \neq j$

This classification rule can be shown to be optimal in that it is guaranteed to minimize the risk of misclassification



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Summary of Bayesian recipe for classification

 $\lambda_{ij} = {
m risk}$ or cost associated with assigning an instance to class ω_i when the correct classification is ω_i

Choose
$$\omega_1$$
 if $\frac{P(X|\omega_1)}{P(X|\omega_2)} > \frac{(\lambda_{21} - \lambda_{22})}{(\lambda_{12} - \lambda_{11})} \frac{P(\omega_2)}{P(\omega_1)}$

Choose
$$\omega_2$$
 if $\frac{P(X|\omega_1)}{P(X|\omega_2)} < \frac{(\lambda_{21} - \lambda_{22})}{(\lambda_{12} - \lambda_{11})} \frac{P(\omega_2)}{P(\omega_1)}$

Minimum error classification rule is a special case:

Choose
$$\omega_1$$
 if $\frac{P(X|\omega_1)}{P(X|\omega_2)} > \frac{P(\omega_2)}{P(\omega_1)}$ Otherwise choose ω_2



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Bayesian recipe for classification

Note that
$$P(\omega_i \mid \mathbf{x}) = \frac{P(\mathbf{x} | \omega_i)P(\omega_i)}{P(\mathbf{x})}$$

Model $P(\mathbf{x} | \omega_1)$, $P(\mathbf{x} | \omega_2)$, $P(\omega_1)$, and $P(\omega_2)$

Using Bayes rule, choose ω_1 if $P(\mathbf{x} \mid \omega_1)P(\omega_1) > P(\mathbf{x} \mid \omega_2)P(\omega_2)$

Otherwise choose ω_2



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Estimate
$$P(\omega_i|X) = \frac{P(X|\omega_i)P(\omega_i)}{P(X)}$$

 $\omega = argmax \ P(\omega_i|X)$

Assign sample to the most probable class!

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- The Bayesian recipe is simple, optimal, and in principle, straightforward to apply
- To use this recipe in practice, we need to know $P(X | \omega_i)$ the generative model for data for each class and $P(\omega_i)$ the prior probabilities of classes
- Because these probabilities are unknown, we need to estimate them from data – or learn them!
- X is typically high-dimensional or may have complex structure
- Need to estimate $P(X | \omega_i)$ from data

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Step 1: pick a model

$$p(features, label) = p(y) \prod_{j=1}^{m} p(x_i | y, x_1, ..., x_{i-1})$$

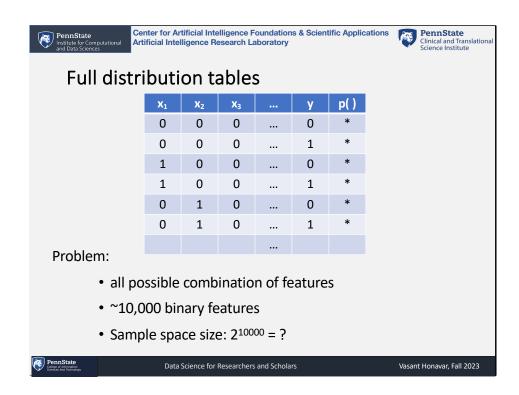
So, far we have made NO assumptions about the data

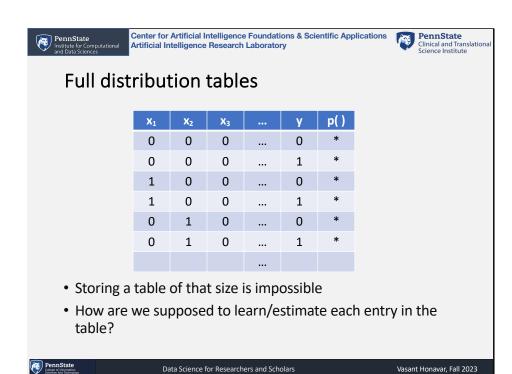
$$p(x_m | y, x_1, x_2, ..., x_{m-1})$$

How many entries would the probability distribution table have if we tried to represent all possible values Suppose we have 10000 binary features?



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Step 1: pick a model

$$p(features, label) = p(y) \prod_{j=1}^{m} p(x_i | y, x_1, ..., x_{i-1})$$

So, far we have made NO assumptions about the data

Model selection involves making assumptions about the data

We did this before, e.g. assume the data is linearly separable

These assumptions allow us to represent the data more compactly and to estimate the parameters of the model



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ndependence

s are independent if one has nothing to do er

pendent variables, knowing the value of one nge the probability distribution of the other he probability of any individual event) of the toss of a coin is independent of a roll of a die of tea in England is independent of the whether or ass DS Methods course

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nt or dependent?

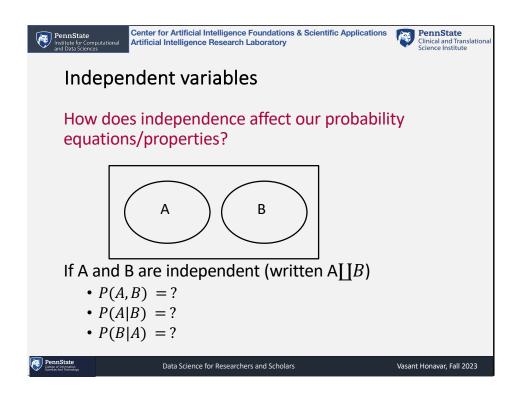
and having a cat-allergy

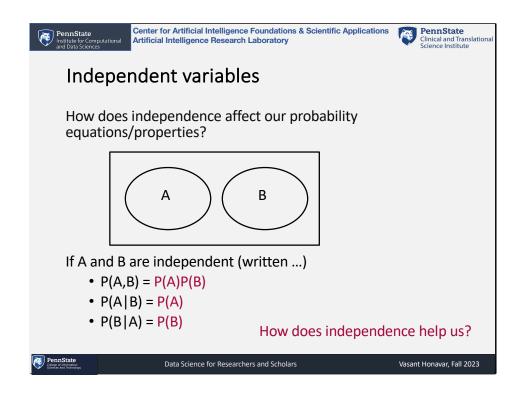
n and driving habits

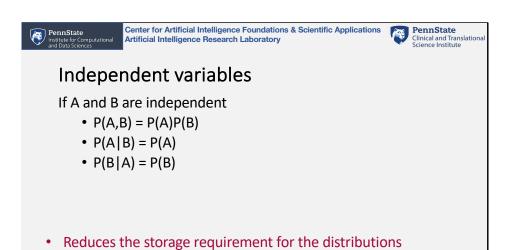
gevity

ity

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• Reduces the number of probabilities we need to estimate

• Reduces the complexity of the distribution



ndependence

nts can become independent given certain other

weight

weight given genetics

onally independent given C

?(A|C)P(B|C)

(A | C)

)(B|C)

: P(A)P(B)

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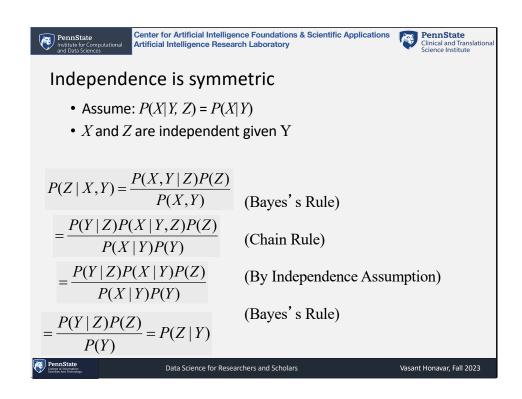
Conditional Independence

- *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*:
- P(X | Y, Z) = P(X | Z) that is,

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



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$$p(features, label) = p(y) \prod_{i=1}^{m} p(x_i | y, x_1, \cdots, x_{i-1})$$

$$\forall i \quad p(x_i \mid y, x_1, x_2, ..., x_{i-1}) = p(x_i \mid y)$$

What does this mean?

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$$p(features, label) = p(y) \prod_{i=1}^{m} p(x_i | y, x_1, \cdots, x_{i-1})$$

$$p(x_i | y, x_1, x_2, ..., x_{i-1}) = p(x_i | y)$$

Assumes *i*th feature is independent of the the other features *given* the label



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$$p(x_i | y, x_1, x_2, ..., x_{i-1}) = p(x_i | y)$$

- We assume that the *i*th feature is independent of the the other features *given the label*
- Example: the probability of a word occurring in a review is independent of the other words *given the label*
- For example, the probability of the word "fish" occurring is independent of whether or not "wine" occurs given that the review is about "chardonnay"

Is this assumption true?



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$$p(x_i | y, x_1, x_2, ..., x_{i-1}) = p(x_i | y)$$

- For most applications, this is not true!
- For example, the fact that "pinot" occurs will probably make it more likely that "noir" occurs (or take a compound phrase like "San Francisco")
- However, this is often a reasonable approximation:

$$p(x_i | y, x_1, x_2, ..., x_{i-1}) \approx p(x_i | y)$$



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Naïve Bayes model

$$p(features, label) = p(y) \prod_{i=1}^{m} p(x_i | y, x_1, \dots, x_{i-1})$$

$$= p(y) \prod_{i=1}^{m} p(x_i \mid y) \qquad \text{Na\"{i}ve bayes assumption}$$

 $p(x_i|y)$ is the probability of a particular feature value given the label

How do we model this?

- · for binary features
- for count features
- · for real valued features



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Naïve Bayes Classifier

- How to learn $P(X|\omega_i)$?
- Naïve Bayes solution: Assume that the random variables in X are conditionally independent given the class.
- Result: Naïve Bayes classifier which performs optimally under certain assumptions
- A simple, practical learning algorithm grounded in Probability Theory

When to use

- Attributes that describe instances are likely to be conditionally independent given classification
- The data is insufficient to estimate all the probabilities reliably if we do not assume independence



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Implications of Independence

- Suppose we have 5 Binary attributes and a binary class label
- Without independence, in order to specify the joint distribution, we need to specify a probability for each possible assignment of values to each variable resulting in a table of size 2⁶=64
- Suppose the features are independent given the class label we only need $5(2\times2)=20$ entries
- The reduction in the number of probabilities to be estimated is even more striking when N, the number of attributes is large from $O(2^N)$ to O(N)



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Naive Bayes Classifier

Consider a discrete valued target function $f: \chi \to \Omega$ where an instance $X = (X_1, X_2 ... X_n) \in \chi$ is described in terms of attribute values $X_1 = x_1, \ X_2 = x_2, \ ... \ X_n = x_n$ where $x_i \in Domain(X_i)$

$$\begin{split} \omega_{MAP} &= \arg\max_{\omega_{j} \in \Omega} P(\omega_{j} \mid X_{1} = x_{1}, X_{2} = x_{2}... X_{n} = x_{n}) \\ &= \arg\max_{\omega_{j} \in \Omega} \frac{P(X_{1} = x_{1}, X_{2} = x_{2},..., X_{n} = x_{n} \mid \omega_{j}) P(\omega_{j})}{P(X_{1} = x_{1}, X_{2} = x_{2},..., X_{n} = x_{n})} \\ &= \arg\max_{\omega_{j} \in \Omega} P(X_{1} = x_{1}, X_{2} = x_{2},..., X_{n} = x_{n} \mid \omega_{j}) P(\omega_{j}) \end{split}$$

 ω_{MAP} is called the $\mathit{maximum}\ a\ posteriori$ classification



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Naive Bayes Classifier

$$\begin{aligned} \omega_{MAP} &= \arg \max_{\omega_{j} \in \Omega} P(\omega_{j} \mid X_{1} = x_{1}, X_{2} = x_{2}... X_{n} = x_{n}) \\ &= \arg \max_{\omega_{j} \in \Omega} P(X_{1} = x_{1}, X_{2} = x_{2},..., X_{n} = x_{n} \mid \omega_{j}) P(\omega_{j}) \end{aligned}$$

If the attributes are independent given the class, we have

$$\omega_{MAP} = \arg \max_{\omega_j \in \Omega} \prod_{i=1}^n P(X_i = x_i \mid \omega_j) P(\omega_j)$$

 $=\omega_{NB}$

$$= \arg \max_{\omega_j \in \Omega} P(\omega_j) \prod_{i=1}^n P(X_i = x_i \mid \omega_j)$$



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Naive Bayes Learner

For each possible value ω_i of Ω ,

$$\hat{P}(\Omega = \omega_i) \leftarrow Estimate(P(\Omega = \omega_i), D)$$

For each possible value $a_{i_{\iota}}$ of X_{i}

$$\hat{P}(X_i = a_{i_k} \mid \omega_j) \leftarrow Estimate\left(P(X_i = a_{i_k} \mid \Omega = \omega_j), D\right)$$

Classify a new instance $X = (x_1, x_2, ... x_N)$

$$c(X) = \arg \max_{\omega_j \in \Omega} P(\omega_j) \prod_{i=1}^n P(X_i = x_i \mid \omega_j)$$

Estimate is a procedure for estimating the relevant probabilities from set of training examples



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Learning Dating Preferences

Data samples – ordered 3-tuples of
attribute values corresponding to

Height (tall, short) Hair (dark, blonde, red) Eye (blue, brown) Classes +, -

Training Data

Insta	ince Class lab	el
I_1	(t, d, l)	+
I_2	(s, d, l)	+
I_3	(t, b, l)	_
I_4	(t, r, l)	_
I_5	(s, b, l)	_
I_6	(t, b, w)	+
I_7	(t, d, w)	+
I_8	(s, b, w)	+

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Probabilities to estimate

$$P(+) = 5/8$$
 $P(-) = 3/8$ $P(Height | c) | t | s $+ | 3/5 | 2/5$
 $- | 2/3 | 1/3$$

$P(Hair \mid c)$	d	b	r
+	3/5	2/5	0
_	0	2/3	1/3

$P(Eye \mid c)$	l	w
+	2/5	3/5
_	1	0

Classify (Height=t, Hair=b, eye=l)

 $P(X \mid +) = (3/5)(2/5)(2/5) = (12/125)$ $P(X \mid -) = (2/3)(2/3)(1) = (4/9)$

 $P(+|X) \propto P(+)P(X|+)=(5/8)(12/125)=0.06$

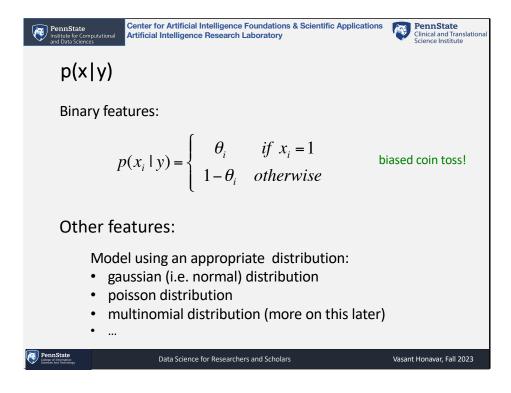
 $P(-|X) \propto P(-)P(X|-)=(3/8)(4/9)=0.1667$

Classify (Height=t, Hair=r, eye=w)

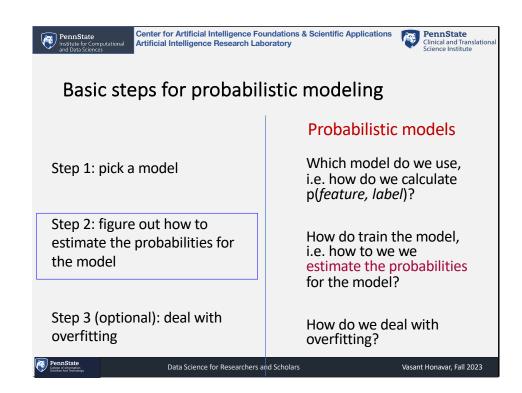
Note the problem with zero probabilities Solution – Use Laplacian correction

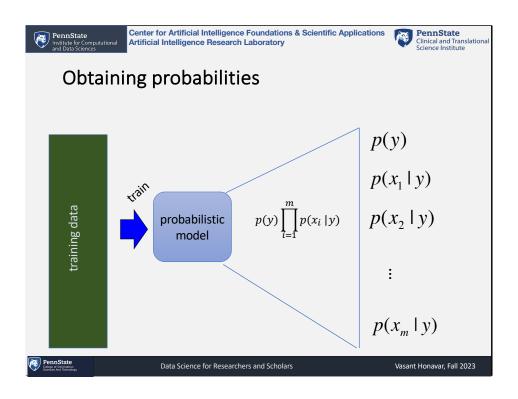


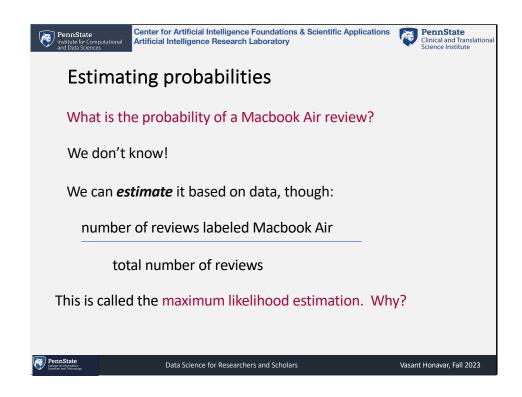
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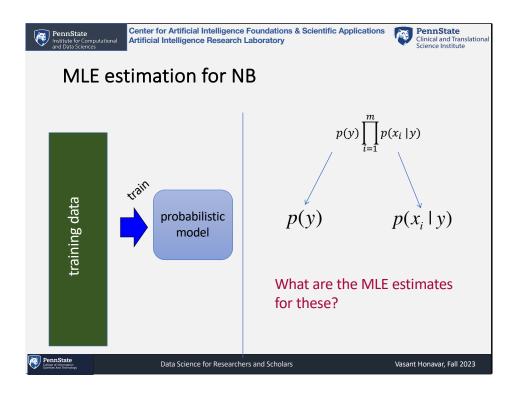


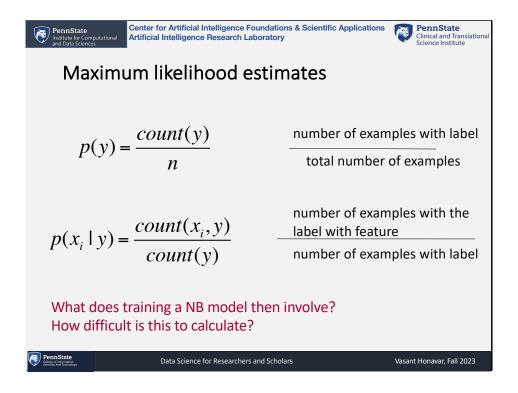
- for discrete, we could simply do a much larger table, but often that doesn't capture everything we want



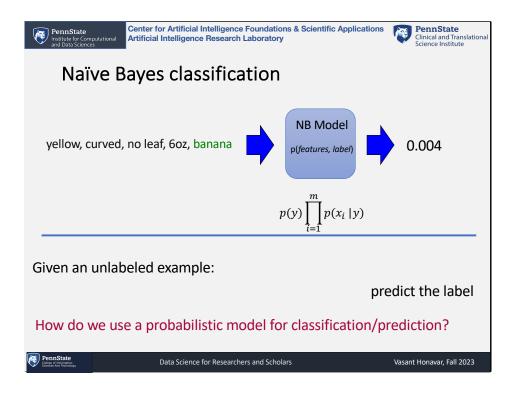


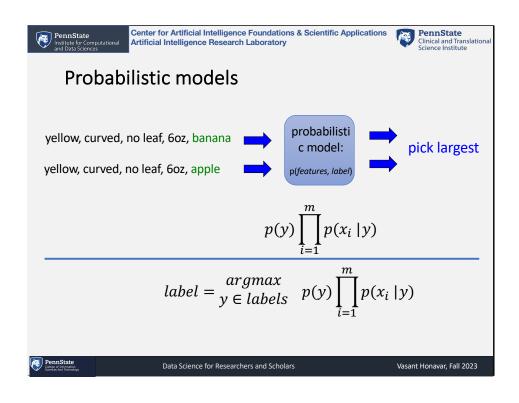


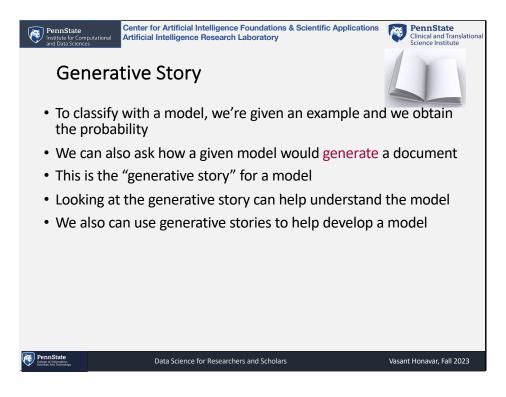




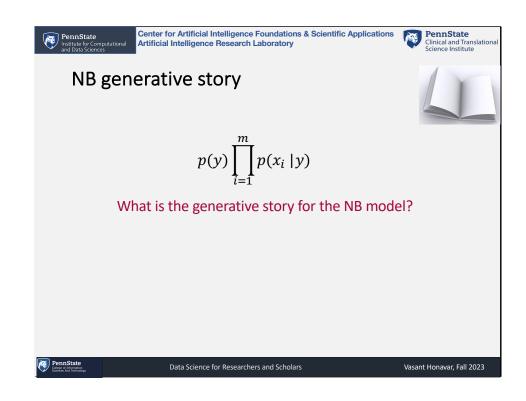
- just involves iterating over the data and aggregating these counts!







- although we don't generally "generate" a document from a model, it's often useful to look at the generative story of a model (i.e. how the model says a document was generate) to help us understand why the model assigns certain probabilities





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NB generative story

$$p(y)\prod_{i=1}^m p(x_i\mid y)$$

- 1. Pick a label according to p(y)
 - roll a biased, m sided die
- 2. For each binart feature:
 - Flip a biased coin:
 - if heads, include the feature (value 1)
 - if tails, don't include the feature (value 0)



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Sample Applications of Naïve Bayes Classifier

Naive Bayes is among the most useful algorithms

- Learning dating preferences
- Learn which news articles are of interest
- Learn to classify web pages by topic
- Learn to classify SPAM
- Learn to assign proteins to functional families

What attributes shall we use to represent text?



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Learning to Classify Text

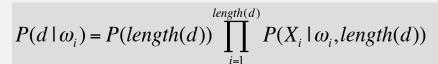
- Target function *Interesting*: Documents → {+,-}
- Learning: Use training examples to estimate
 P(+), P(-), P(d|+), P(d|-)

Alternative generative models for documents:

- Represent each document as a sequence of words
 - In the most general case, we need a probability for each word occurrence in each position in the document, for each possible document length



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This would require estimating for each document,

$$\left| \textit{Vocabulary} \right|^{\textit{length(d)}} \times \left| \Omega \right|$$

probabilities for each possible document length!

To simplify matters, assume that probability of encountering a specific word in a particular position is independent of the position, and of document length

Treat each document as a bag of words!



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Vasant Honavar, Fall 2023

PennState Clinical and Translational Science Institute





Bag of Words Representation

So we estimate one position-independent class-conditional probability $P(w_k \mid \boldsymbol{\omega}_j)$ for each word instead of the set of position-specific word occurrence probabilities $P(X_1 = w_k \mid \boldsymbol{\omega}_j)$... $P(X_{length(d)} = w_k \mid \boldsymbol{\omega}_j)$ The number of probabilities to be estimated drops to $|Vocabulary| \times |\Omega|$

The result is a generative model for documents that treats each document as an ordered tuple of word frequencies

More sophisticated models can consider dependencies between adjacent word positions



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Learning to Classify Text

With the bag of words representation, we have

$$P(d \mid \omega_j)$$
 is proportional to $\left\{ \frac{\left(\sum_k n_{kd}\right)!}{\prod_k n_{kd}!} \right\} \prod_k \left(P(w_k \mid \omega_j)\right)^{n_{kd}}$

where n_{kd} is the number of occurences of w_k in document d (ignoring dependence on length of the document) We can estimate $P(w_k \mid \omega_i)$ from the labeled bags of words we have.



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Naïve Bayes Text Classifier

- Given 1000 training documents from each group, learn to classify new documents according to the newsgroup where it belongs
- Naive Bayes achieves 89% classification accuracy

comp.graphics

 $comp.os.ms\hbox{-}windows.misc$

comp.sys.ibm.pc.hardware

comp.sys.mac.hardware comp.windows.x

alt.atheism

soc.religion.christian talk.religion.misc talk.politics.mideast

talk.politics.misc talk.politics.guns

misc.forsale rec.autos

rec.motorcycles rec.sport.baseball rec.sport.hockey

> sci.space sci.crypt sci.electronics sci.med



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Naïve Bayes Text Classifier

Representative article from rec.sport.hockey

Path: cantaloupe.srv.cs.cmu.edu!das-news.harvard.edu!ogicse!uwm.edu

From: xxx@yyy.zzz.edu (John Doe)

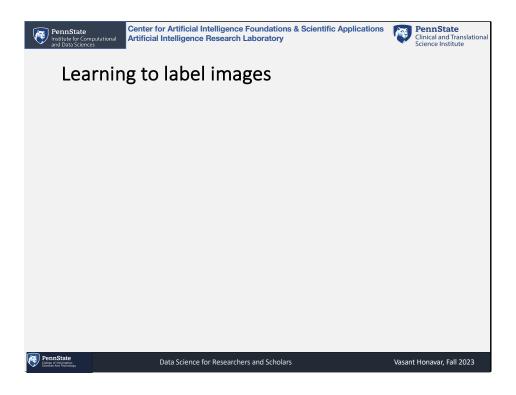
Subject: Re: This year's biggest and worst (opinion)...

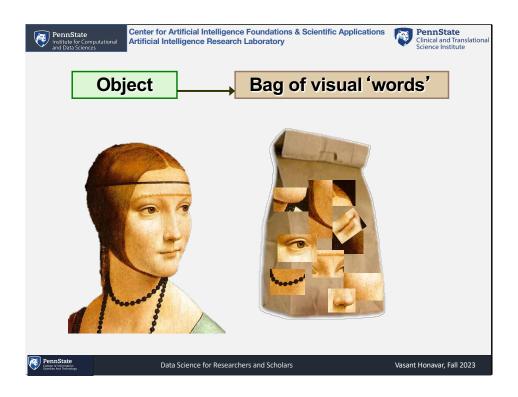
Date: 5 Apr 93 09:53:39 GMT

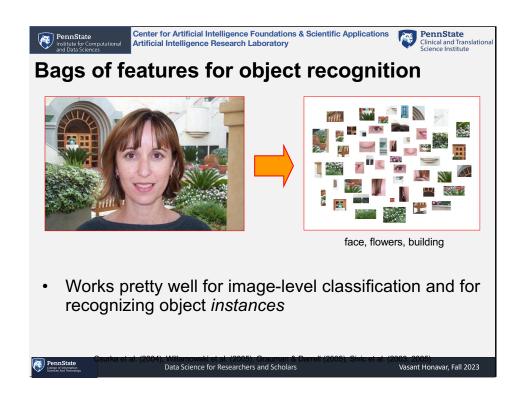
I can only comment on the Kings, but the most obvious candidate for pleasant surprise is Alex Zhitnik. He came highly touted as a defensive defenseman, but he's clearly much more than that. Great skater and hard shot (though wish he were more accurate). In fact, he pretty much allowed the Kings to trade 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

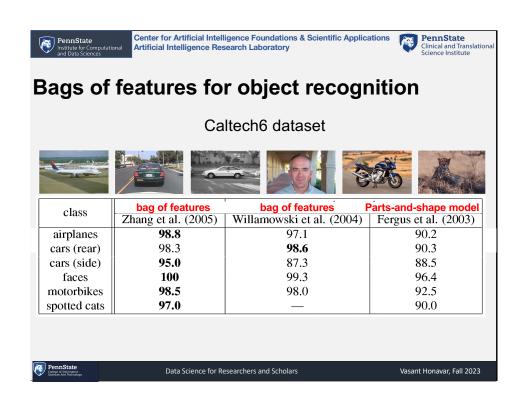


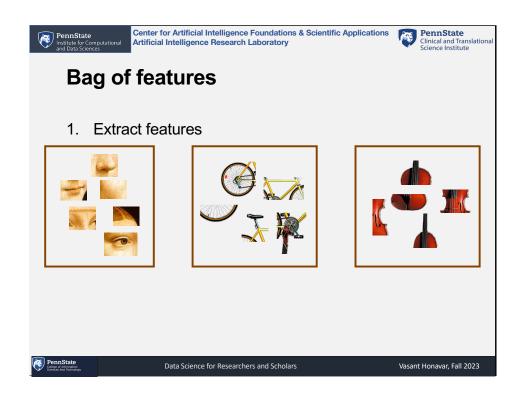
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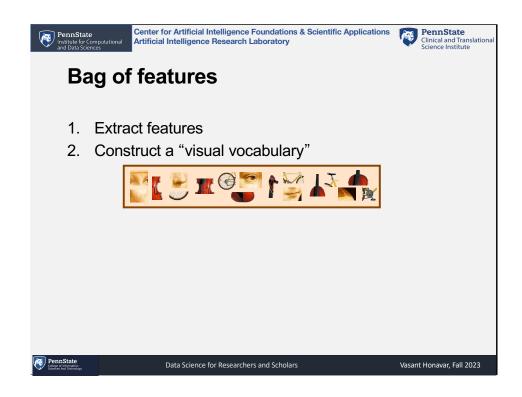


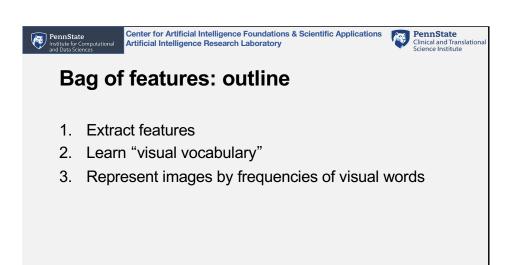






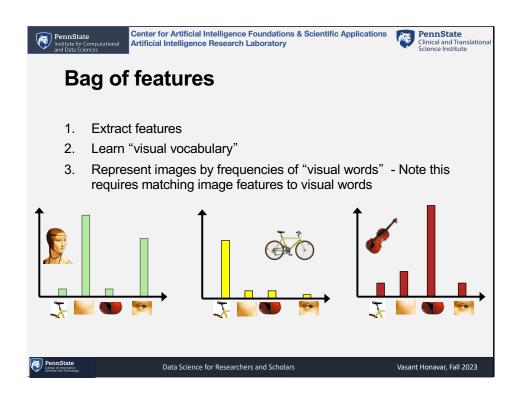






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Naïve Bayes Learner – Summary

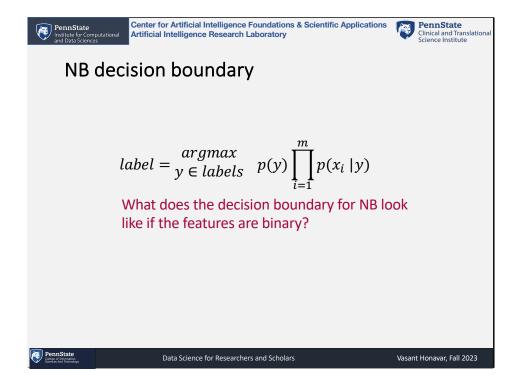
• Produces minimum error classifier if attributes are conditionally independent given the class

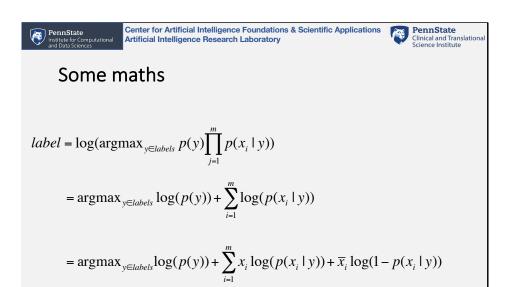
When to use

- Attributes that describe instances are likely to be conditionally independent given classification
- There is not enough data to estimate all the probabilities reliably if we do not assume independence
- Often works well even if when independence assumption is violated (Domigos and Pazzani, 1996)
- Can be used iteratively Kang et al., 2006



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 $p(x_i \mid y) = \begin{cases} \theta_i & \text{if } x_i = 1\\ 1 - \theta_i & \text{otherwise} \end{cases}$

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Some more maths

$$labels = \operatorname{argmax}_{y \in labels} \log(p(y)) + \sum_{i=1}^{m} x_i \log(p(x_i \mid y)) + \overline{x}_i \log(1 - p(x_i \mid y))$$

$$= \operatorname{argmax}_{y \in labels} \log(p(y)) + \sum_{i=1}^{m} x_i \log(p(x_i \mid y)) + (1 - x_i) \log(1 - p(x_i \mid y))$$
(because x_i are binary)

$$= \operatorname{argmax}_{y \in labels} \log(p(y)) + \sum_{i=1}^{m} x_i \log(p(x_i \mid y)) - x_i \log(1 - p(x_i \mid y) + \log(1 - p(x_i \mid y))$$

$$= \operatorname{argmax}_{y \in labels} \log(p(y)) + \sum_{i=1}^{m} x_i \log \left(\frac{p(x_i \mid y)}{1 - p(x_i \mid y)} \right) + \log(1 - p(x_i \mid y))$$

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And...

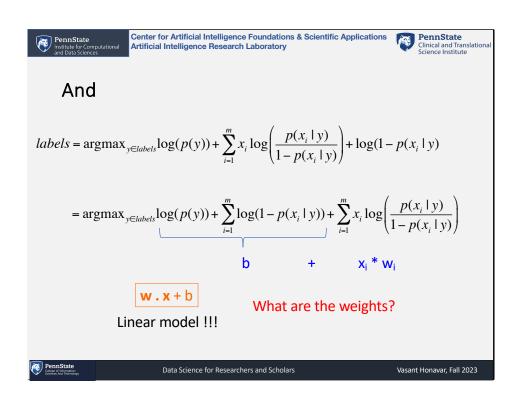
$$labels = \operatorname{argmax}_{y \in labels} \log(p(y)) + \sum_{i=1}^{m} x_i \log \left(\frac{p(x_i \mid y)}{1 - p(x_i \mid y)} \right) + \log(1 - p(x_i \mid y))$$

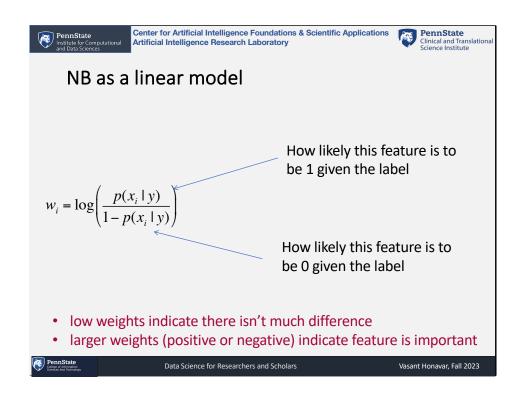
$$= \operatorname{argmax}_{y \in labels} \log(p(y)) + \sum_{i=1}^{m} \log(1 - p(x_i \mid y)) + \sum_{i=1}^{m} x_i \log\left(\frac{p(x_i \mid y)}{1 - p(x_i \mid y)}\right)$$

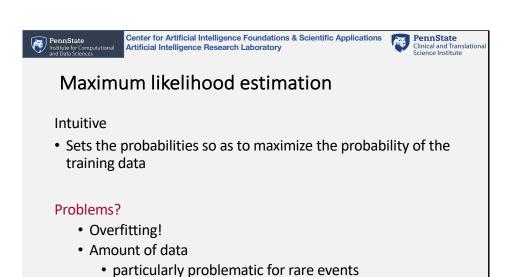
What does this look like?



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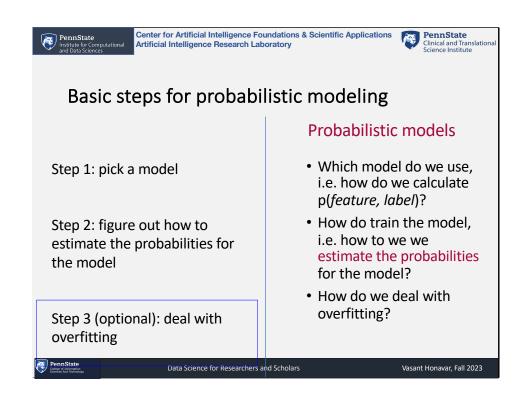


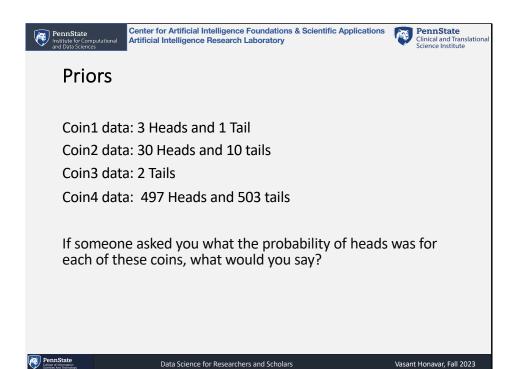


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• Is our training data representative?







Estimation of Probabilities from Small Samples

$$\hat{P}(X_i = a_{i_k} \mid \boldsymbol{\omega}_j) \leftarrow \frac{n_{ji_k} + mp_{ji}}{n_j + m}$$

 n_j is the number of training examples of class ω_j n_{ji_k} = number of training examples of class ω_j which have attribute value a_{i_k} for attribute X_i

 p_{ji} is the prior estimate for $\hat{P}(X_i = a_{i_k} \mid \boldsymbol{\omega}_j)$ m is the weight given to the prior

As
$$n \to \infty$$
, $\hat{P}(X_i = a_{i_k} \mid \boldsymbol{\omega}_j) \to \frac{n_{ji_k}}{n_j}$

This is effectively the same as using Dirichlet priors



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