Applied Machine Learning

Naive Bayes

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Learning objectives

generative vs. discriminative classifier

Naive Bayes classifier

- assumption
- different design choices

Discreminative vs generative classification

discriminative — so far we modeled the ***conditional*** *distribution*: $p(y \mid x)$

generative — learn the ***joint*** *distribution* $p(y, x) = p(y)p(x \mid y)$

prior class probability: frequency of observing this label

likelihood of input features given the class label
(input features for each label come from a different distribution)

how to classify new input x?

Bayes rule

$$p(y = c \mid x) = \frac{p(c)p(x|c)}{p(x)}$$

posterior probability
of a given class

marginal probability of the input (evidence)
$\sum_{c'=1}^{C} p(x, c')$

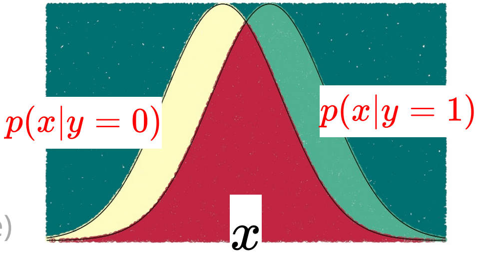


image: https://rpsychologist.com

Example: Bayes rule for classification

$y \in \{\text{yes}, \text{no}\}$ patient having cancer?

$x \in \{-, +\}$ test results, a single binary feature

prior: 1% of population has cancer $p(\text{yes}) = .01$

likelihood: $p(+|\text{yes}) = .9$ TP rate of the test (90%)

$$p(c \mid x) = \frac{p(c)p(x|c)}{p(x)}$$

posterior: $p(\text{yes}|+) = .08$

FP rate of the test (5%)

evidence: $p(+) = p(\text{yes})p(+|\text{yes}) + p(\text{no})p(+|\text{no}) = .01 \times .9 + .99 \times .05 = .189$

in a generative classifier likelihood & prior class probabilities are **learned from data**

Generative classification

prior class probability: frequency of observing this label

likelihood of input features given the class label
(input features for each label come from a different distribution)

$$p(y=c \mid x) = \frac{p(c)p(x|c)}{p(x)}$$

posterior probability
of a given class

marginal probability of the input (evidence)
$\sum_{c'=1}^{C} p(x, c')$

Some generative classifiers:

- Gaussian Discriminant Analysis: the likelihood is multivariate Gaussian
- Naive Bayes: decomposed likelihood

image: https://rpsychologist.com

Naive Bayes: model

number of input features

assumption about the likelihood $p(x|y) = \prod_{d=1}^{D} p(x_d|y)$

when is this assumption correct?

when features are **conditionally independent** given the label $x_i \perp\!\!\!\perp x_j \mid y$

knowing the label, the value of one input feature gives us no information about the other input features

chain rule of probability (true for any distribution)

$$p(x|y) = p(x_1|y)p(x_2|y,x_1)p(x_3|y,x_1,x_2)\dots p(x_D|y,x_1,\dots,x_{D-1})$$

conditional independence assumption

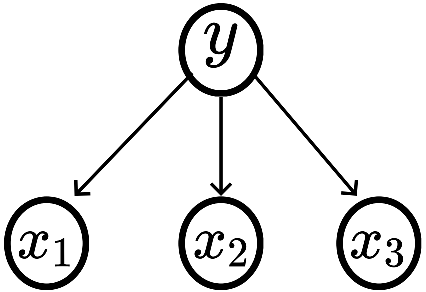
x1, x2 give no extra information, so $p(x_3|y,x_1,x_2) = p(x_3|y)$

Naive Bayes: model

$$p(x_3|y, x_1, x_2) = p(x_3|y)$$

A graphical representation of the 'naive Bayes' model

This shows that conditioned on the class label, the input features are independent



$$p(x|y) = \prod_{d=1}^{D} p(x_d|y)$$

This reduces the model parameters to *D*

Useful when dimensionality of input space is high

Naive Bayes: objective

given the training dataset $\mathcal{D} = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(N)}, y^{(N)})\}$

maximize the joint likelihood (contrast with logistic regression)

$$\ell(w, u) = \sum_n \log p_{u,w}(x^{(n)}, y^{(n)})$$

$$= \sum_n \left[\log p_u(y^{(n)}) + \log p_w(x^{(n)}|y^{(n)})\right]$$

$$= \sum_n \log p_u(y^{(n)}) + \sum_n \log p_w(x^{(n)}|y^{(n)})$$

using Naive Bayes assumption

$p(x|y) = \prod_{d=1}^{D} p(x_d|y)$

$\log p(x|y) = \sum_{d=1}^{D} \log p(x_d|y)$

$$= \sum_n \log p_u(y^{(n)}) + \sum_d \sum_n \log p_{w_{[d]}}(x_d^{(n)}|y^{(n)})$$

separate MLE estimates for each part

Naive Bayes: train-test

given the training dataset $\mathcal{D} = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(N)}, y^{(N)})\}$

training time

learn the prior class probabilities $p_u(y)$

learn the likelihood components $p_{w_{[d]}}(x_d|y) \quad \forall d$

test time find posterior class probabilities

$$\arg\max_c p(c|x) = \arg\max_c \frac{p_u(c) \overbrace{\boxed{\prod_{d=1}^{D} p_{w_{[d]}}(x_d|c)}}^{p(x|c)}}{\sum_{c'=1}^{C} p_u(c') \prod_{d=1}^{D} p_{w_{[d]}}(x_d|c')}$$

$$= \arg\max_c p_u(c) \prod_{d=1}^{D} p_{w_{[d]}}(x_d|c)$$

Class prior

$$p(c|x) = \frac{p_u(c)\prod_{d=1}^{D} p_{w_{[d]}}(x_d|c)}{\sum_{c'=1}^{C} p_u(c)\prod_{d=1}^{D} p_{w_{[d]}}(x_d|c')}$$

binary classification

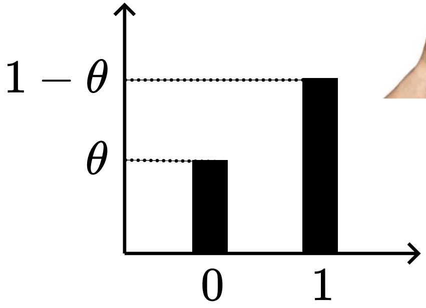
Bernoulli distribution $p_u(y) = u^y(1-u)^{1-y}$

Bernoulli random variable takes values of 0 or 1

$$p(y|\theta) = \begin{cases} \theta & y = 1 \\ 1-\theta & y = 0 \end{cases}$$

can be written as

$$p(y|\theta) = \theta^y(1-\theta)^{1-y}$$



Class prior

$$p(c|x) = \frac{p_u(c) \prod_{d=1}^{D} p_{w_{[d]}}(x_d|c)}{\sum_{c'=1}^{C} p_u(c) \prod_{d=1}^{D} p_{w_{[d]}}(x_d|c')}$$

binary classification

Bernoulli distribution $p_u(y) = u^y(1-u)^{1-y}$

maximizing the log-likelihood

$$\sum_n \log p_u(y^{(n)}) + \sum_d \sum_n \log p_{w_{[d]}}(x_d^{(n)}|y^{(n)})$$

$$\ell(u) = \sum_{n=1}^{N} \left[y^{(n)} \log(u) + (1-y^{(n)}) \log(1-u)\right]$$

$$= N_1 \log(u) + (N - N_1) \log(1-u)$$

frequency of class 1 in the dataset

frequency of class 0 in the dataset

setting its derivative to zero

$$\frac{\mathrm{d}}{\mathrm{d}u}\ell(u) = \frac{N_1}{u} - \frac{N-N_1}{1-u} = 0 \Rightarrow u^* = \frac{N_1}{N}$$

max-likelihood estimate (MLE) is the frequency of class labels

Class prior

$$p(c|x) = \frac{p_u(c) \prod_{d=1}^{D} p_{w_{[d]}}(x_d|c)}{\sum_{c'=1}^{C} p_u(c) \prod_{d=1}^{D} p_{w_{[d]}}(x_d|c')}$$

multiclass classification

categorical distribution $p_u(y) = \prod_{c=1}^{C} u_c^{y_c}$

assuming one-hot coding for labels

$u = [u_1, \ldots, u_C]$ is now a parameter vector

maximizing the log likelihood $\ell(u) = \sum_n \sum_c y_c^{(n)} \log(u_c)$

subject to: $\sum_c u_c = 1$

number of instances in class 1

closed form for the optimal parameter $u^* = [\frac{N_1}{N}, \ldots, \frac{N_C}{N}]$

all instances in the dataset

Likelihood terms

$p(c|x) = \frac{p_u(c) \prod_{d=1}^{D} p_{w_{[d]}}(x_d|c)}{\sum_{c'=1}^{C} p_u(c) \prod_{d=1}^{D} p_{w_{[d]}}(x_d|c')}$

choice of likelihood distribution depends on the type of features

(likelihood encodes our assumption about "generative process")

- Bernoulli: binary features
- Categorical: categorical features
- Gaussian: continuous distribution
- ...

note that these are different from the choice of distribution for class prior

each feature x_d may use a different likelihood

separate max-likelihood estimates for each feature

$$w_{[d]}{}^* = \arg\max_{w_{[d]}} \sum_{n=1}^{N} \log p_{w_{[d]}}(x_d^{(n)} \mid y^{(n)})$$

Bernoulli Naive Bayes

binary **features**: *likelihood is Bernoulli*

$$\begin{cases} p_{w_{[d]}}(x_d \mid y=0) = \mathrm{Bernoulli}(x_d; w_{[d],0}) \\ p_{w_{[d]}}(x_d \mid y=1) = \mathrm{Bernoulli}(x_d; w_{[d],1}) \end{cases}$$

$$p(x_d|w_{[d],0}) = \begin{cases} w_{[d],0} & x_d = 1\{y=0\} \\ 1-w_{[d],0} & x_d = 0\{y=0\} \end{cases}$$

short form: $p_{w_{[d]}}(x_d \mid y) = \mathrm{Bernoulli}(x_d; w_{[d],y})$

$$\sum_n \log p_u(y^{(n)}) + \sum_d \sum_n \log p_{w_{[d]}}(x_d^{(n)}|y^{(n)})$$

$$\ell(w_{[d]}) = \sum_{n\in\mathcal{D}_{y=0}} \log p_{w_{[d]}}(x_d^{(n)}|y=0) + \sum_{n\in\mathcal{D}_{y=1}} p_{w_{[d]}}(x_d^{(n)}|y=1)$$

$$\sum_{n\in\mathcal{D}_{y=0}} \left(x_d^{(n)} \log w_{[d],0} + (1-x_d^{(n)})\log(1-w_{[d],0})\right)$$

$$N_{\{y=0,x_d=1\}} \log w_{[d],0} + N_{\{y=0,x_d=0\}} \log(1-w_{[d],0})$$

$$N_{\{y=0,x_d=1\}} \log w_{[d],0} + (N_{\{y=0\}} - N_{\{y=0,x_d=1\}}) \log(1-w_{[d],0})$$

$$\frac{\mathrm{d}}{\mathrm{d}w_{[d],0}}\ell(w_{[d],0}) = \frac{N_{\{y=0,x_d=1\}}}{w_{[d],0}} - \frac{N_{\{y=0\}}-N_{\{y=0,x_d=1\}}}{1-w_{[d],0}} = 0 \Rightarrow w^*_{[d],0} = \frac{N\{y=0,x_d=1\}}{N\{y=0\}}$$

Bernoulli Naive Bayes

binary **features**: *likelihood is Bernoulli*

$$\begin{cases} p_{w_{[d]}}(x_d \mid y = 0) = \mathrm{Bernoulli}(x_d; w_{[d],0}) \\ p_{w_{[d]}}(x_d \mid y = 1) = \mathrm{Bernoulli}(x_d; w_{[d],1}) \end{cases}$$

short form: $p_{w_{[d]}}(x_d \mid y) = \mathrm{Bernoulli}(x_d; w_{[d],y})$

max-likelihood estimation is similar to what we saw for the prior

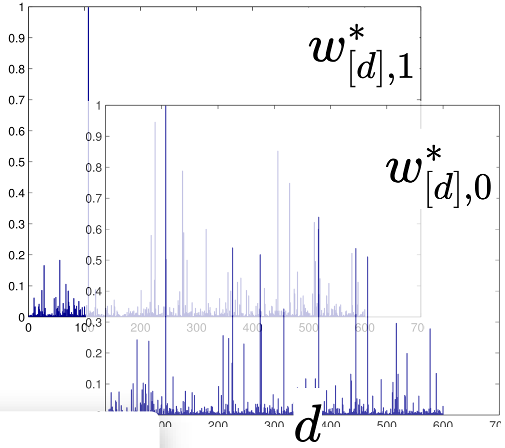
closed form solution of MLE → $w^*_{[d],c} = \frac{N(y=c, x_d=1)}{N(y=c)}$ number of training instances satisfying this condition

Bernoulli Naive Bayes: Example

using naive Bayes for **document classification**:

- 2 classes (documents types)
- 600 binary features
  - $x_d^{(n)} = 1$ iff word d is present in the document n (vocabulary of 600)

likelihood of words in two document types $\xrightarrow{\quad w^*_{[d],c} = \frac{N(y=c, x_d=1)}{N(y=c)} \quad}$




```python
def BernoulliNaiveBayes(prior,# vector of size 2 for class prior
                        likelihood, #600 x 2: likelihood of each word under each class
                        x, #vector of size 600: binary features for a new document
                       ):
  logp = np.log(prior) + np.sum(np.log(likelihood) * x[:,None], 0) + \
                np.sum(np.log(1-likelihood) * (1 - x[:,None]), 0)
  log_p -= np.max(log_p) #numerical stability
  posterior = np.exp(log_p) # vector of size 2
  posterior /= np.sum(posterior) # normalize
  return posterior # posterior class probability
```

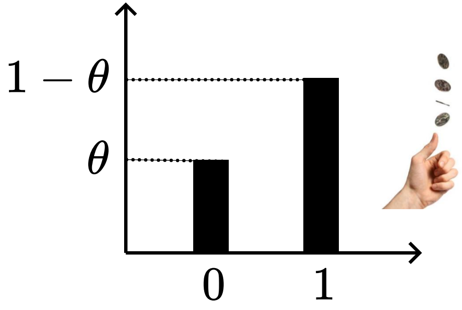
$$\log p_{w_{[d]}}(x_d|c) = x_d \log w_{[d],c} + (1-x_d)\log(1-w_{[d],c})$$

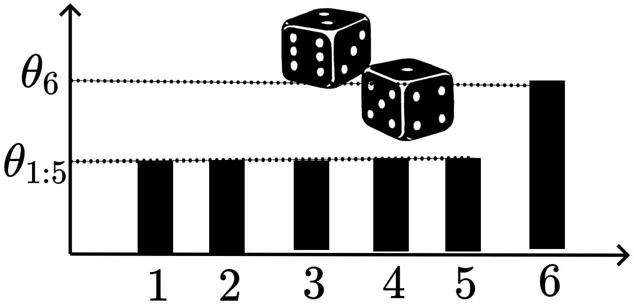
$$p(c|x) = \frac{p_u(c)\prod_{d=1}^{D} p_{w_{[d]}}(x_d|c)}{\sum_{c'=1}^{C} p_u(c')\prod_{d=1}^{D} p_{w_{[d]}}(x_d|c')}$$

Multinomial Naive Bayes

what if we wanted to use *word frequencies* in document classification

$x_d^{(n)}$ is the number of times word d appears in document n





once:	Bernoulli distribution	categorical distribution
n times:	binomial distribution	multinomial distribution

$$p_\theta(x) = \frac{n!}{\prod_{d=1}^{D} x_d!} \prod_{d=1}^{D} \theta_d^{x_d}$$

Multinomial Naive Bayes

what if we wanted to use *word frequencies* in document classification

$x_d^{(n)}$ is the number of times word d appears in document n

Multinomial likelihood: $p_w(x|c) = \frac{(\sum_d x_d)!}{\prod_{d=1}^{D} x_d!} \prod_{d=1}^{D} w_{d,c}^{x_d}$

we have a vector of size D for each class $C \times D$ (parameters)

MLE estimates: $w^*_{d,c} = \frac{\sum x_d^{(n)} y_c^{(n)}}{\sum_n \sum_{d'} x_{d'}^{(n)} y_c^{(n)}}$

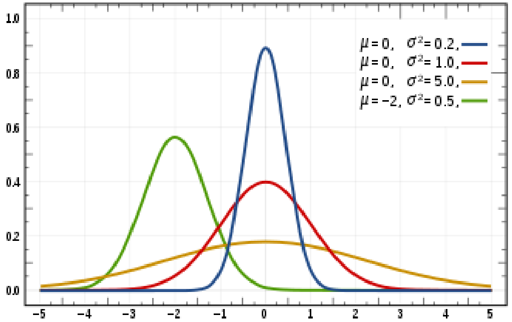
count of word d in all documents labelled **y**

total word count in all documents labelled **y**

Gaussian Naive Bayes

Gaussian likelihood terms

$$p_{w_{[d]}}(x_d \mid y) = \mathcal{N}(x_d; \mu_{d,y}, \sigma^2_{d,y}) = \frac{1}{\sqrt{2\pi\sigma_{d,y}{}^2}} e^{-\frac{(x_d - \mu_{d,y})^2}{2\sigma_{d,y}{}^2}}$$



$w_{[d]} = (\mu_{d,1}, \sigma_{d,1}, \ldots, \mu_{d,C}, \sigma_{d,C})$

one mean and std. parameter for each class-feature pair

writing log-likelihood and setting derivative to zero we get maximum likelihood estimate:

$$\mu_{d,y} = \frac{1}{N_c} \sum_{n=1}^{N} x_d^{(n)} y_c^{(n)}$$

$$\sigma^2_{d,y} = \frac{1}{N_c} \sum_{n=1}^{N} y_c^{(n)} (x_d^{(n)} - \mu_{d,y})^2$$

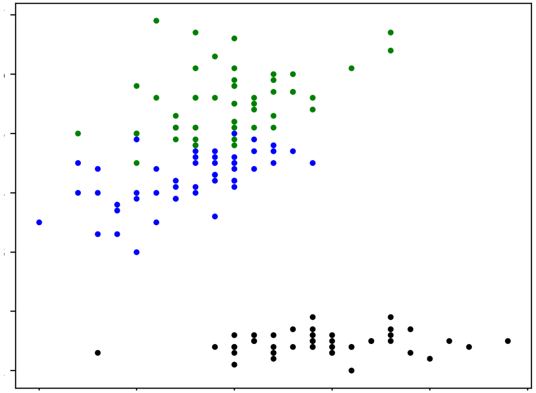
empirical mean & std of feature x_d
across instances with label y

Gaussian Naive Bayes: example

classification on **Iris flowers dataset**:

(a classic dataset originally used by Fisher)

$N_c = 50$ samples with D=4 features, for each of C=3 species of Iris flower

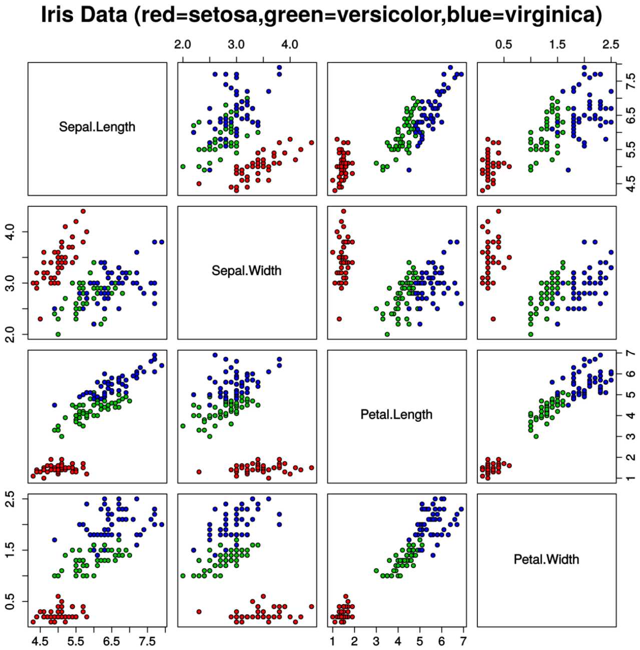


our setting

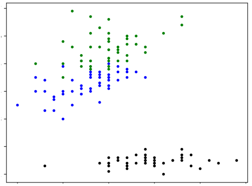
3 classes

2 features

(septal width, petal length)



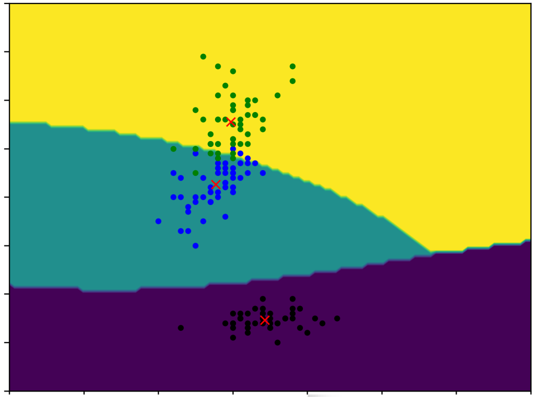
Gaussian Naive Bayes: example



categorical class prior & Gaussian likelihood

```python
def GaussianNaiveBayes(
                X, # N x D
                y, # N x C
                Xtest,# N_test x D
               ):
    N,C = y.shape
    D = X.shape[1]
    mu, s = np.zeros((C,D)), np.zeros((C,D))
    for c in range(C): #calculate mean and std
        inds = np.nonzero(y[:,c])[0]
        mu[c,:] = np.mean(X[inds,:], 0)
        s[c,:] = np.std(X[inds,:], 0)
    log_prior = np.log(np.mean(y, 0))[:,None]
    log_likelihood = - np.sum( np.log(s[:,None,:]) +.5*(((Xt[None,:,:] - mu[:,None,:])/s[:,None,:])**2), 2)
    return log_prior + log_likelihood #N_text x C
```

decision boundaries are not linear!



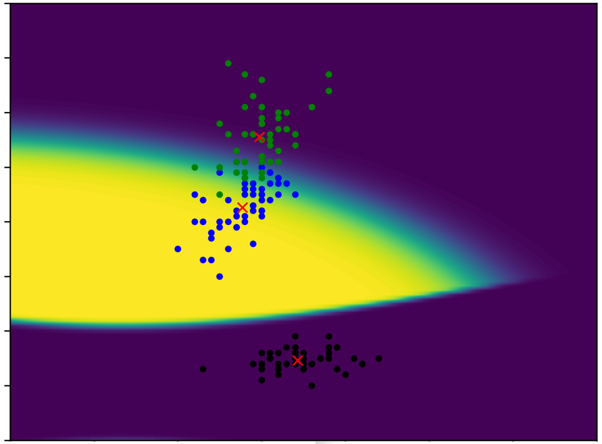
$$p_{w_{[d]}}(x_d \mid y) = \frac{1}{\sqrt{2\pi{\sigma_{d,y}}^2}} e^{-\boxed{\frac{(x_d-\mu_{d,y})^2}{2{\sigma_{d,y}}^2}}}$$

Gaussian Naive Bayes: example

categorical class prior & Gaussian likelihood

```
def GaussianNaiveBayes(
                X, # N x D
                y, # N x C
                Xtest,# N_test x D
               ):
    N,C = y.shape
    D = X.shape[1]
    mu, s = np.zeros((C,D)), np.zeros((C,D))
    for c in range(C): #calculate mean and std
        inds = np.nonzero(y[:,c])[0]
        mu[c,:] = np.mean(X[inds,:], 0)
        s[c,:] = np.std(X[inds,:], 0)
    log_prior = np.log(np.mean(y, 0))[:,None]
    log_likelihood = - np.sum( np.log(s[:,None,:]) +.
- mu[:,None,:])/s[:,None,:])**2), 2)
    return log_prior + log_likelihood #N_text x C
```

posterior class probability for c=1

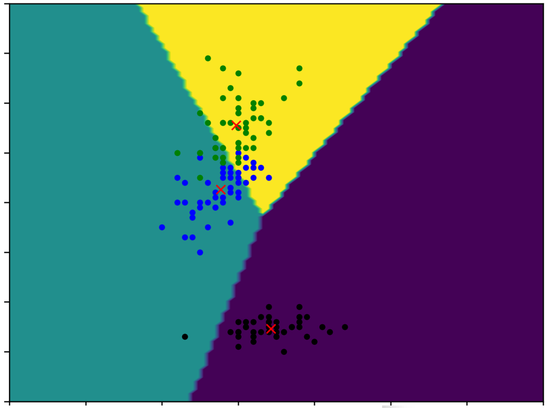


Gaussian Naive Bayes: example

using the **same variance** for all classes

its value does not make a difference

decision boundaries **are linear**



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                y, # N x C
                Xtest,# N_test x D
               ):
    N,C = y.shape
    D = X.shape[1]
    mu, s = np.zeros((C,D)), np.zeros((C,D))
    for c in range(C): #calculate mean and std
        inds = np.nonzero(y[:,c])[0]
        mu[c,:] = np.mean(X[inds,:], 0)
    log_prior = np.log(np.mean(y, 0))[:,None]
    log_likelihood = - np.sum(.5*(((Xt[None,:,:] - mu[:,None,:]))**2), 2)
    return log_prior + log_likelihood #N_text x C
```

Decision boundary in generative classifiers

decision boundaries: two classes have the same probability $p(y|x) = p(y'|x)$

which means $$\log \frac{p(y{=}c|x)}{p(y{=}c'|x)} = \log \frac{p(c)p(x|c)}{p(c')p(x|c')} = \underbrace{\log \frac{p(c)}{p(c')}}_{\text{not a function of x (ignore)}} + \log \frac{p(x|c)}{p(x|c')} = 0$$

this ratio is linear (in some bases) for a large family of probabilities

(called linear exponential family)

$$p(x|c) = \frac{e^{w_{y,c}^T \phi(x)}}{Z(w_{y,c})} \rightarrow \log \frac{p(x|c)}{p(x|c')} = \underbrace{(w_{y,c} - w_{y,c'})^T \phi(x)}_{\text{linear using some bases}} + \underbrace{g(w_{y,c}, w_{y,c'})}_{\text{not a function of x}}$$

e.g., Bernoulli is a member of this family with $\phi(x) = x$

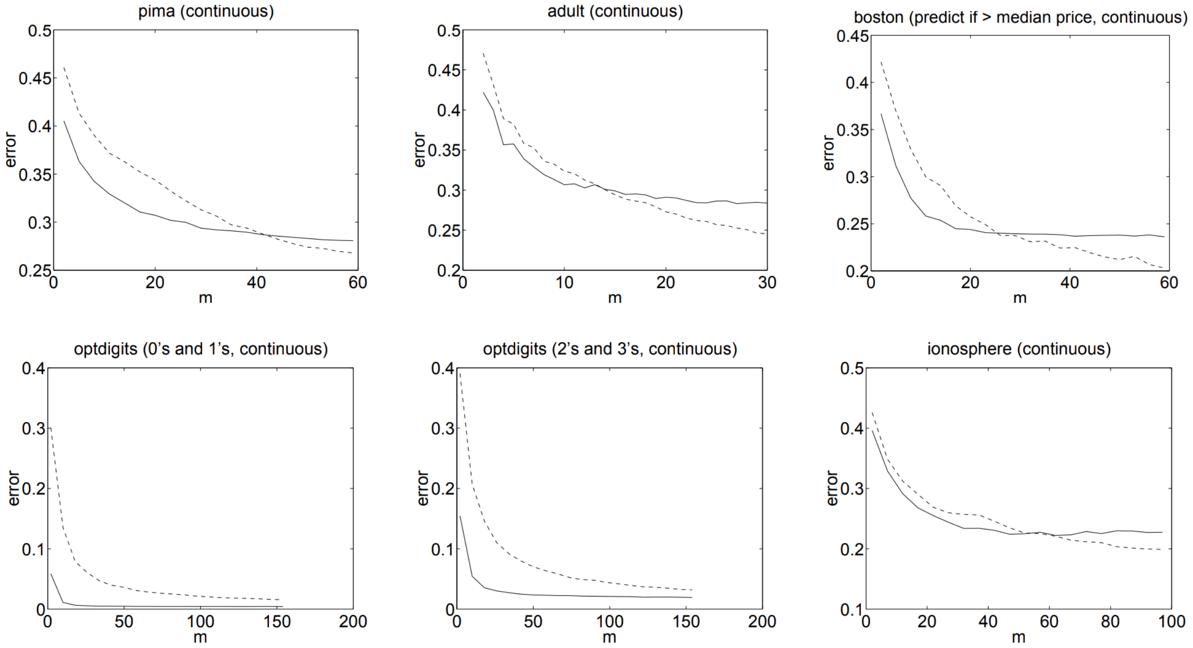
→ *Bernoulli Naive Bayes has a linear decision boundary*

Discreminative vs generative classification

$p(y, x) = p(y)p(x \mid y)$ **generative**	**discriminative** $p(y \mid x)$
maximize **joint** likelihood	maximize ***conditional*** *likelihood*
it makes assumptions about $p(x)$	makes no assumption about $p(x)$
can deal with missing values	often works better on larger datasets
can learn from unlabelled data	
often works better on smaller datasets	

Discriminative vs generative classification

Example naive Bayes vs logistic regression on UCI datasets



naive Bayes

logistic regression

m is #instances

from: Ng & Jordan 2001

Summary

- generative classification
  - learn the class prior and likelihood
  - Bayes rule for conditional class probability
- Naive Bayes
  - assumes conditional independence
    - *e.g., word appearances indep. of each other given document type*
  - class prior: Bernoulli or Categorical
  - likelihood: Bernoulli, Gaussian, Categorical...
  - MLE has closed form (in contrast to logistic regression)
  - estimated separately for each feature and each label