# **Applied Machine Learning**

Naive Bayes

**Oumar Kaba** 



## Admin

- Second to last class
- Exam post mortem
- Assignments
- Attendance bonus points

### Learning objectives

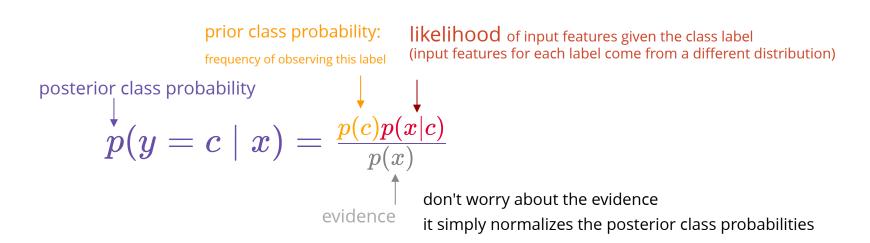
- the assumption of Naive Bayes classifier
- what does learning and prediction steps involve?
- different likelihood functions
- Bayesian parameter learning in Naive Bayes
- practical considerations

## Bayes rule for classification

#### given

- the prior probability of each class
- likelihood of observations given the class

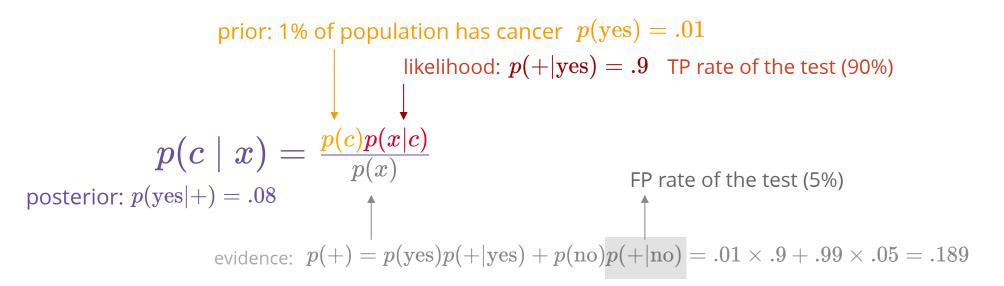
use Bayes rule for classification



### Bayes rule for classification

example

```
x \in \{-, +\} input: test results, a single binary feature y \in \{\mathrm{yes}, \mathrm{no}\} label: patient has cancer
```



### **Generative classification**

training learn the following distributions from the data  $\,\mathcal{D} = \{(x^{(1)}, y^{(1)}), \dots, (x^{(N)}, y^{(N)})\}$ 

**prior** probability of each class  $p(y=c) orall c \in \{1,\ldots,C\}$ 

**likelihood** of data for each class p(x|y=c)

prediction use

use the Bayes rule to get the posterior class probability

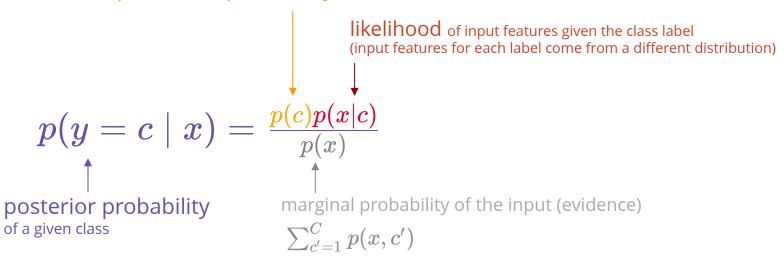
$$p(y = c \mid x) \propto p(c)p(x|c)$$

generative classifier because we are learning the joint data distribution p(x,y)=p(y)p(x|y) we can generate new data from this joint distribution

in a **discriminative classifier** we directly learn p(y|x)

### Generative classification

prior class probability: frequency of observing this label



#### Some generative classifiers:

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



## Naive Bayes model

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

when is this assumption correct?

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

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

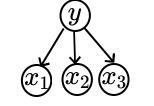
How is the likelihood derived from this independence assumption?

**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

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



number of input features

## Naive Bayes: objective

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

a generative classifier maximizes the joint likelihood (or log-likelihood)

$$L(\pi,\theta;\mathcal{D}) = \prod_{n \in \mathcal{D}} p(x^{(n)},y^{(n)};\pi,\theta)$$

$$\pi,\theta \text{ are the model parameters}$$

$$\ell(\pi,\theta) = \sum_n \log p(x^{(n)},y^{(n)};\pi,\theta)$$

$$= \sum_n \left[\log p(y^{(n)};\pi) + \log p(x^{(n)}|y^{(n)};\theta)\right]$$

$$= \sum_n \log p(y^{(n)};\pi) + \sum_n \log p(x^{(n)}|y^{(n)};\theta)$$

$$= \sum_n \log p(y^{(n)};\pi) + \sum_n \log \prod_d p(x^{(n)}_d|y^{(n)};\theta_d) \qquad \text{using Naive Bayes assumption here}$$

$$= \sum_n \log p(y^{(n)};\pi) + \sum_d \sum_n \log p(x^{(n)}_d|y^{(n)};\theta_d) \qquad p(x|y) = \prod_{d=1}^D p(x_d|y)$$

separate max-likelihood problems for prior and each feature  $x_d$  given the label as we will see, training the Naive Bayes classifier has an **analytical solution** 

### **Prior class probabilities**

class probabilities prior to looking at the features

for binary classification, class probability is given by Bernoulli  $\;p(y;\pi)=\pi^y(1-\pi)^{1-y}\;$ 

recall the max-likelihood estimate for Bernoulli

$$rg \max_{\pi} \sum_n \log p(y^{(n)};\pi) = rac{1}{N} \sum_n y^{(n)}$$

for multi-class classification, class probability is given by categorical distribution

$$p(y;\pi) = \prod_{c=1}^C \pi_c{}^{\mathbb{I}(y=c)} = \pi_y$$
 note that in this case  $\pi$  is a vector

max-likelihood estimate is again given by empirical frequencies

$$rg \max_{\pi_c} \sum_n \log p(y^{(n)};\pi) = rac{N(y=c)}{N}$$
 frequency of class c in our dataset  $\pi^* = [rac{N_1}{N}, \dots, rac{N_C}{N}]$ 

In both cases we learn the prior simply as the class frequencies in the training data

## Naive Bayes: objective

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

a generative classifier maximizes the joint likelihood (or log-likelihood)

$$\begin{split} \ell(\pi,\theta) &= \sum_{n} \log p(x^{(n)},y^{(n)};\pi,\theta) \\ &= \sum_{n} \log p(y^{(n)};\pi) + \log p(x^{(n)}|y^{(n)};\theta) \\ &= \sum_{n} \log p(y^{(n)};\pi) + \sum_{n} \log p(x^{(n)}|y^{(n)};\theta) \\ &= \sum_{n} \log p(y^{(n)};\pi) + \sum_{n} \log \prod_{d} p(x^{(n)}_{d}|y^{(n)};\theta_{d}) \\ &\text{to} \\ &= \sum_{n} \log p(y^{(n)};\pi) + \sum_{d} \sum_{n} \log p(x^{(n)}_{d}|y^{(n)};\theta_{d}) \end{split}$$

so far we know how to maximize this part

Next, how to maximize this part

### Likelihood terms

likelihood terms  $p(x_d|y; heta_d)$ 

- encode our assumption about the *generative process*
- different types of features require different forms of likelihood
  - Bernoulli for binary features
  - Categorical for categorical features
  - Multinomial for "count" features
  - Gaussian is one option for continuous feature
- ullet each feature  $x_d$  may use a different likelihood form
- separate maximum conditional likelihood estimate for each feature

$$rg \max_{ heta_d} \sum_{n=1}^N \log p(x_d^{(n)} \mid y^{(n)}; heta_d)$$

### **Bernoulli Naive Bayes**

for a binary **feature** likelihood is Bernoulli

$$\left\{egin{aligned} p(x_d \mid y=0; heta_d) &= ext{Bernoulli}(x_d; heta_{d,0}) \ p(x_d \mid y=1; heta_d) &= ext{Bernoulli}(x_d; heta_{d,1}) \end{aligned}
ight.$$
 one parameter per label

short form:  $p(x_d \mid y; \theta_d) = \text{Bernoulli}(x_d; \theta_{d, y})$ 

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

closed form solution of MLE 
$$hinspace{0.05cm} hinspace{0.05cm} hinspace{0.05cm}$$

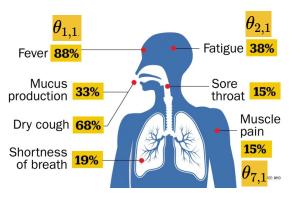
#### Covid-19 classification example

each patient has seven binary features  $x \in \{0,1\}^7$ we have a dataset of N=1000 patients, where 200 had covid-19

#### learning:

learn the prior: 
$$\pi = \frac{N(y=1)}{N} = .2$$
 Bernoulli $(y;\pi)$ 

for each symptom d:



$$\operatorname{Bernoulli}(x_d|y=1; heta_{d,1})$$

$$\mathrm{Bernoulli}(x_d|y=0; heta_{d,0})$$

#### prediction:

for a new patient x calculate unnormalized posterior

$$\left\{egin{aligned} & ilde{p}(y=0|x) = ext{Bernoulli}(0;\pi) \prod_d ext{Bernoulli}(x_d; heta_{d,0}) \ & ilde{p}(y=1|x) = ext{Bernoulli}(1;\pi) \prod_d ext{Bernoulli}(x_d; heta_{d,1}) \end{aligned}
ight.$$

normalize it 
$$\,p(y=1|x)=rac{ ilde{p}(y=1|x)}{ ilde{p}(y=0|x)+ ilde{p}(y=1|x)}$$

### Disease diagnosis example

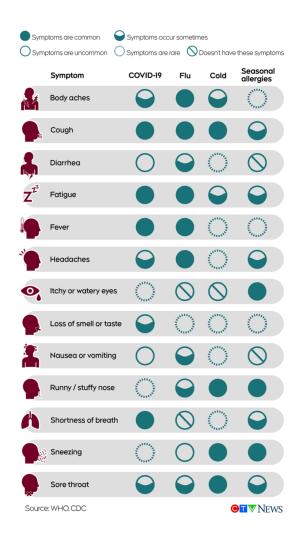
what changes in **multi-class** setting?

$$p(y;\pi)$$
 learn the prior:  $\pi_{m{c}}=rac{N(y=c)}{N}$ 

for each symptom d:

how many parameters in our model?

binary classification, binary features 1+2D multi-class classification, binary features C+CD



### Document classification

example

e.g., spam filtering

# words in our vocabulary

 $x^{(n)} \in \{0,1\}^D$ each document (email) is one instance

 $x_{\scriptscriptstyle J}^{(n)}=1$  if the word d appears in document n

classify the documents based on this bag of words representation

	D-1						
	it	is	puppy	cat	pen	a	this
it is a puppy	1	1	1	0	0	1	0
it is a kitten	1	1	0	0	0	1	0
N=5 it is a cat	1	1	0	1	0	1	0
that is a dog and this is a pen	0	1	0	0	1	1	1
it is a matrix	1	1	0	0	0	1	0

D=7

document-term matrix

#### learning:

MLE for the prior Bernoulli(y;  $\pi$ ) (spam frequency in our dataset)

MLE for the likelihood terms Bernoulli(x;  $\theta_{d,y}$ ) (frequency of word (d) in spam/non-spam documents)

#### prediction:

calculate the posterior  $p(y|x) \propto \text{Bernoulli}(y;\pi) \prod_d \text{Bernoulli}(x_d;\theta_{d,u})$ 

### **Document classification**

#### example

let's learn the Naive Bayes for the following data the label y=1 if the sentence is about animals

it is a puppy ata it is a kitten it is a cat that is a dog and this is a pen

it is a matrix

it	is	puppy	cat pen		a	this	
1	1	1	0	0	1	0	
1	1	0	0	0	1	0	
1	1	0	1	0	1	0	
0	1	0	0	1	1	1	
1	1	0	0	0	1	0	

prior parameter:  $\pi = \frac{4}{5}$ 

class conditional parameters:  $\, heta_{d,y}$ 



y = 0	<u>1</u>	<u>1</u>	$\frac{0}{1}$	$\frac{0}{1}$	$\frac{0}{1}$	<u>1</u> 1	$\frac{0}{1}$	,0?
y = 1	$\frac{3}{4}$	$\frac{4}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{4}{4}$	$\frac{1}{4}$	,1?
	d = 1						d = 7	

we get a new sentence: it is a random sentence

$$ilde{p}(y=0|x)=rac{1}{5} imesrac{1}{1} imesrac{1}{1}=.2$$

$$ilde{p}(y=1|x)=rac{4}{5} imesrac{3}{4} imesrac{4}{4} imesrac{3}{4} imesrac{3}{4} imesrac{3}{4} imesrac{3}{4} imesrac{3}{4} imesrac{4}{4} imesrac{3}{4}pprox.19$$

$$x = [1, 1, 0, 0, 0, 1, 0]$$

$$p(y=1|x) = \frac{.19}{.2+.19} \approx .49$$

## Why Naive Bayes assumption?

Naive Bayes assumption  $\;p(x|y)=\prod_d p(x_d|y)\;$ 

#### what if we did not make this assumption?

consider the **spam filtering example**:

- D can be very large
- with the Naive Bayes assumption: learn the frequency of each word (d) in spam/non-spam documents
- without it: learn the frequency of each possible subset of words in spam/non-spam documents

*e.g.*, for 
$$x=[1,1,0,0,0,1,0]$$
 we need to estimate  $p(x|y)$ 

#### problems

- many combinations of words may not appear in even one document
- we need exponentially more parameters
- even for large datasets, this could lead to overfitting

(3)								
		it	is	puppy	cat	pen	a	this
it is a	1 рирру	1	1	1	0	0	1	0
	a kitten	1	1	0	0	0	1	0
ent <sub>it</sub>	is a cat	1	1	0	1	0	1	0
that is a dog and this	is a pen	0	1	0	0	1	1	1
it is a	matrix	1	1	0	0	0	1	0

## **Bayesian Naive Bayes**

using MLE in Naive Bayes can lead to overfitting

example

let's classify this new sentence:

that dog was my puppy

$$ilde{p}(y=1|x)=rac{4}{5} imesrac{1}{4} imesrac{0}{4} imes\ldots=0$$

$$ilde{p}(y=0|x)=rac{1}{5} imesrac{0}{1} imesrac{0}{1} imes\ldots=0$$

the problem is that the word "is" appears in all instances

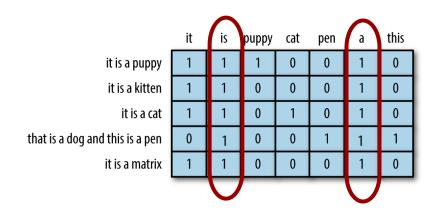
max-likelihood estimate 
$$\theta_{1,1} = \theta_{1,0} = 1$$

we can solve this by being Bayesian in parameter learning:

instead of maintaining a point estimates  $\pi, \theta_{d,y}$  we maintain distributions  $p(\pi), p(\theta_{d,y})$  for  $y \in \{0,1\}, d$ start from separate prior for each parameter  $p(\pi), p(\theta_{d.u})$ 

calculate the likelihood 
$$\prod_n p(y^{(n)}|\pi)$$

update with observed frequencies in the dataset



### **Bayesian Naive Bayes**

start from separate prior for each parameter  $p(\pi) = \text{Beta}(\pi; \alpha^{\pi}, \beta^{\pi})$   $p(\theta_{d,y}) = \text{Beta}(\theta; \alpha^{\theta}, \beta^{\theta})$ 

calculate the posterior 
$$p(\pi|\mathcal{D}) = \mathrm{Beta}(\pi; lpha^\pi + N(y=1), eta^\pi + N(y=0))$$
 
$$p( heta_{d\,ar{u}}|\mathcal{D}) = \mathrm{Beta}( heta_{d\,ar{u}}; lpha^\theta + N(y=ar{y}, x_d=1), eta^\theta + N(y=ar{y}, x_d=0))$$

use posterior predictive for a new instance (x)  $p(y=1|x,\mathcal{D})=\int_{\theta} p(y=1|\pi)p(\pi|\mathcal{D})\prod_{d}p(x_{d}|\theta_{d,1})p(\theta_{d,1}|\mathcal{D})\mathrm{d}\theta\mathrm{d}\pi$ 



individual posterior predictives 
$$lacksquare$$
  $= \left(\int_{\pi} p(y=1|\pi)p(\pi|\mathcal{D})\mathrm{d}\pi\right)\prod_{d}\left(\int_{\theta_{d,1}} p(x_{d}|\theta_{d,1})p(\theta_{d,1}|\mathcal{D})\mathrm{d}\theta\right)$ 

for Beta distribution, we simply used the posterior mean (and dropped the integral)

$$ilde{p}(y=1|x,\mathcal{D}) = rac{lpha^\pi + N(y=1)}{lpha^\pi + eta^\pi + N} \prod_d \left(rac{lpha^ heta + N(y=1,x_d=1)}{lpha^ heta + eta^ heta + N(y=1)}
ight)^{x_d} \left(rac{eta^ heta + N(y=1,x_d=0)}{lpha^ heta + eta^ heta + N(y=1)}
ight)^{(1-x_d)}$$
 recall: Laplace smoothing

compare with our previous prediction (using MLE)

$$ilde{p}(y=1|x,\mathcal{D}) = rac{N(y=1)}{N} \prod_d \left(rac{N(y=1,x_d=1)}{N(y=1)}
ight)^{x_d} \left(rac{N(y=1,x_d=0)}{N(y=1)}
ight)^{(1-x_d)}$$
 we are simply adding a constant to various frequencies

### **Bayesian Naive Bayes**

example

is this puppy cat pen it is a puppy it is a kitten it is a cat that is a dog and this is a pen it is a matrix

y = 0  $\frac{1}{1}$   $\frac{1}{1}$   $\frac{0}{1}$   $\frac{0}{1}$   $\frac{0}{1}$   $\frac{1}{1}$   $\frac{0}{1}$ 

let's classify this new sentence using Laplace smoothing:

$$lpha^\pi=eta^\pi=lpha^ heta=eta^ heta=1$$

$$ilde{p}(y=1|x) = rac{4+1}{5+2} imes rac{1+1}{4+2} imes rac{0+1}{4+2} imes rac{1+1}{4+2} imes rac{3+1}{4+2} imes rac{3+1}{4+2} imes rac{0+1}{4+2} imes rac{1+1}{4+2} pprox .00032$$

$$ilde{p}(y=0|x) = rac{1+1}{5+2} imes rac{0+1}{1+2} imes rac{0+1}{1+2} imes rac{0+1}{1+2} imes rac{1+1}{1+2} imes rac{1+1}{1+2} imes rac{1+1}{1+2} imes rac{0+1}{1+2} imes rac{0+1}{1+2} pprox .00052$$

$$p(y=0|x) = \frac{.00052}{.00032 + .00052} \approx .62$$

note that if D is large we have to calculate the product of many terms



numerical problems!

d = 1

## Log-Sum-Exp trick

In estimating unnormalized posteriors we could get numerical problems (underflow) when calculating the posterior for new instances, we work with in the **log-domain**:

$$\log ilde{p}(y|x;\pi, heta) = \log p(y;\pi) + \sum_d \log p(x_d|y; heta_d)$$

to get the final probabilities we need to normalize  $ilde{\mathcal{p}}$ 

$$p(y|x;\pi, heta) = rac{ ilde{p}(y|x;\pi, heta)}{\sum_{c=1}^{C} ilde{p}(c|x;\pi, heta)}$$

we can do this **normalization in the log domain** as well:

$$\log p(y|x;\pi, heta) = \log ilde{p}(y|x;\pi, heta) - \log \sum_{c=1}^{C} \exp(\log ilde{p}(c|x;\pi, heta))$$

we could run into very large or small numbers inside the exponential

## Log-Sum-Exp trick

we can do this **normalization in the log domain** as well:

$$\log p(y|x;\pi, heta) = \log ilde{p}(y|x;\pi, heta) - \log \sum_{c=1}^{C} \exp(\log ilde{p}(c|x;\pi, heta))$$

observation

$$\log \sum_c \exp a_c = \log \left( \exp(a_0) (\sum_c \exp(a_c - a_0)) = a_0 + \log \sum_c \exp(a_c - a_0) 
ight)$$

to make log-sum-exp numerically stable, bring the numbers  $\ a_c$  close to zero

for example choose  $a_0 \leftarrow \max_c a_c$ 

### Multinomial likelihood

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

	it	is	puppy	cat	pen	a	this
it is a puppy	1	1	1	0	0	1	0
it is a kitten	1	1	0	0	0	1	0
it is a cat	1	1	0	1	0	1	0
that is a dog and this is a pen	0	2	0	0	1	2	1
it is a matrix	1	1	0	0	0	1	0

#### Multinomial likelihood

$$p(x|y) = ext{Mult}(x; heta_y) = rac{(\sum_d x_d)!}{\prod_{d=1}^D x_d!} \prod_{d=1}^D heta_{d,y}^{x_d}$$
 probability of word d appearing  $x_d$  time

the max-likelihood estimate is again given by the relative frequency

$$heta_{d,c}^{MLE} = rac{\sum_n x_d^{(n)} \mathbb{I}(y^{(n)} = c)}{\sum_n \sum_{d'} x_{d'}^{(n)} \mathbb{I}(y^{(n)} = c)}$$
 counts of word d in all documents labelled count in al

total word count in all documents labelled c

## **Univariate Gaussian density**

Gaussian probability density function (pdf)

$$\mathcal{N}(x;\mu,\sigma^2) = rac{1}{\sqrt{2\pi\sigma^2}}e^{-rac{(x-\mu)^2}{2\sigma^2}}$$

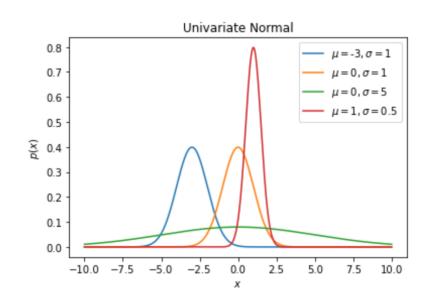
two parameters are  $\mu, \sigma^2$ 

turn out to be the mean and variance

$$\mathbb{E}[x] = \mu$$

$$\mathbb{E}[(x-\mu)^2] = \sigma^2$$

this is a random variable; we are using the same notation for a random variable and a particular value of that variable



### **Univariate Gaussian density**

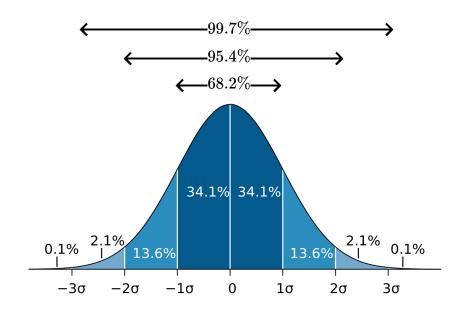
Gaussian probability density function (pdf)

$$\mathcal{N}(x;\mu,\sigma) = rac{1}{\sqrt{2\pi\sigma^2}} e^{-rac{(x-\mu)^2}{2\sigma^2}}$$

given a dataset  $\mathcal{D} = \{x^{(1)}, \dots, x^{(N)}\}$ 

maximum likelihood estimate of  $\mu, \sigma^2$  are empirical mean and variance

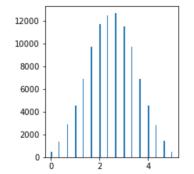
$$\mu^{MLE} = rac{1}{N} \sum_n x^{(n)}$$
  $\sigma^{2^{MLE}} = rac{1}{N} \sum_n (x^{(n)} - \mu^{MLE})^2$ 



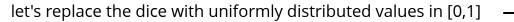
### **Univariate Gaussian density**

two reasons why Gaussian is an important dist.

- maximum entropy dist. with a fixed variance
- central limit theorem

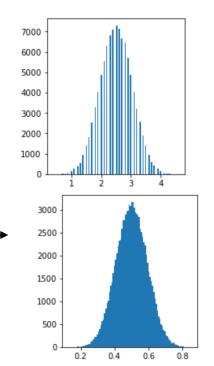


let's throw three dice, repeatedly plot the histogram of the average outcome looks familiar?



the average (and sum) of IID random variables has a Gaussian distribution

justifies use of Gaussian for observations that are mean or sum of some random values



## **Gaussian Naive Bayes**

for continuous features one option is the Gaussian conditional likelihood

$$p(x_d \mid y) = \mathcal{N}(x_d; \mu_{d,y}, \sigma_{d,y}^2) = rac{1}{\sqrt{2\pi\sigma_{d,y}^2}} e^{-rac{(x_d - \mu_{d,y})^2}{2\sigma_{d,y}^2}}$$
 corresponds to what we previously called  $heta_{d,y}$ 

Maximum likelihood estimates:

empirical mean & variance of feature  $\,x_d\,$  across instances with label  $\,y\,$ 

$$egin{align} \mu_{d,c} &= rac{1}{N(y=c)} \sum_{n=1}^N x_d^{(n)} \mathbb{I}(y^{(n)} = c) \ & \ \sigma_{d,c}^2 &= rac{1}{N(y=c)} \sum_{n=1}^N \mathbb{I}(y^{(n)} = c) (x_d^{(n)} - \mu_{d,y})^2 \ & \ \end{array}$$

### Gaussian Naive Bayes

example





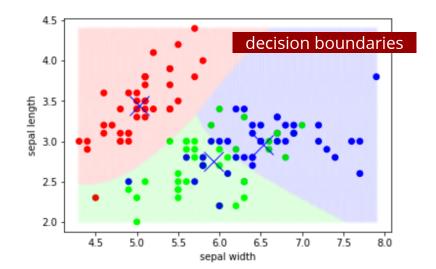


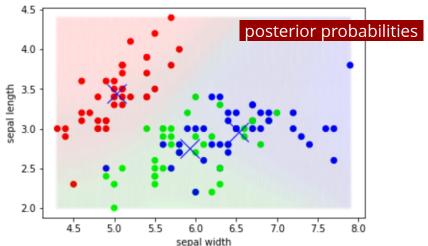
classification on **Iris flowers dataset**:

- we use categorical class prior (3 classes)
- Gaussian likelihood since the features are continuous (we use D=2 features)

the **decision boundary** found by Gaussian NB three means are identified using X

- note that we have a mean \(\mu\_{d,c}\) and variance \(\sigma\_{d,c}^2\) for each class-feature combination
  in the plot each X is showing the *combined* mean of two features, sepal length and sepal width.





### Generative vs. discriminative classification

#### naive Bayes

learns the **joint** distribution

$$p(y,x) = p(y)p(x \mid y)$$

the max-likelihood estimate of prior and likelihood has closed-form solution

(using empirical frequencies)

makes stronger assumptions

usually works better with smaller datasets

linear decision boundary for Gaussian naive Bayes only **if** the variance is fixed

#### logistic regression

learns the **conditional** distribution

$$p(y \mid x)$$

no closed-form solution

(use numerical optimization)

weaker assumptions, since it doesn't model the distribution of input (x)

usually works better with larger datasets

linear decision boundary

### 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, Multinomial...
  - MLE has closed-form, estimated separately for each feature and each label
  - Bayesian Naive Bayes helps with overfitting
    - with frequent or rare feature values