# Lecture 6: Classification and Naive Bayes classifier Statistical Methods for Data Science

#### Yinan Yu

Department of Computer Science and Engineering

November 16, 2023

#### Today,

- Classification
- 2 Naive Bayes classifier
  - Multinomial naive Bayes classifier
  - Gaussian naive Bayes classifier
- Summary





#### Learning outcome

- Be able to explain classification related terminology: classification, binary/multi-class classification
- Be able to explain the Bayes' rule for both multinomial and Gaussian naive Bayes classifiers
- Be able to explain the differences between multinomial naive Bayes classifier and Gaussian naive Bayes classifier
- For a given problem, be able to formulate and implement a naive Bayes classifier



# Today

- Classification





#### Classification

 Recall (cf. lecture 4): modeling is to describe a system using mathematics in order to solve a range of problems. The description has this form:

$$y = g(x; \theta \mid h)$$

- Classification:
  - y: categorical (nominal), scalar each category is called a class; when there are only two classes, i.e.  $y \in \{0,1\}$ , the classification problem is called binary classification; if there are more than two classes, i.e.  $y \in \{1, \dots, C\}$  for C > 2, the classification problem is called multi-class classification
  - x: categorical or numerical
    - Typically, x is a vector denoted by  $x = [x_1, \cdots, x_d]$ ; sometimes the notations x and x are used interchangeably
    - x is called a feature vector
  - g: classification model, e.g. naive Bayes classifiers, support vector machines, decision trees, etc
  - $\bullet$   $\theta$  (parameters) and h (hyperparameters) depend on g





#### Parameter estimation

- In a classification model, parameter estimation process is called training, where the parameters are estimated from a data set called the training data set
- The training data set contains paired data  $\{(x_1, y_1), \dots, (x_N, y_N)\}$ , e.g.

$$\{(i, scoter), (i, goldeneye), \cdots, (i, scoter)\}$$

where  $x_i$  = pixel values in a picture,  $y_i \in \{scoter, goldeneye\}$  is called the ground truth labels; the data set is called a labeled data set

- The targets y<sub>i</sub>'s in the training set are typically created by humans;
   the process of creating the ground truth labels is called annotation or labeling
- Given  $\hat{\theta}$  (estimated parameters),  $g(x; \hat{\theta} \mid h)$  is called a (trained) classifier





#### Today

- Naive Bayes classifier
  - Multinomial naive Bayes classifier
  - Gaussian naive Bayes classifier





### Naive Bayes classifier

- Multinomial naive Bayes classifier (categorical y, categorical x)
- Gaussian naive Bayes classifier (categorical y, continuous x)





### Bayes' rule and MAP for parameter estimation

• Recall (cf. lecture 5), in parameter estimation:

$$f_{\Theta\mid data}(\theta\mid data) = \underbrace{\frac{f_{data\mid \Theta}(data\mid \theta)}{f_{data}(data)}}_{\text{normalization constant}} f_{\Theta\mid data}(\theta\mid data)$$

$$\hat{\theta}_{MAP} = \arg\max_{\theta} \, f_{data\mid\Theta}(data\mid\theta) f_{\Theta}(\theta)$$





### Bayes' rule and MAP for naive Bayes classifier

Let x be the input variables and y the target,

In multinomial naive Bayes classifier (categorical y, categorical x):

$$P(Y = y \mid X = x) = \underbrace{P(X = x \mid Y = y)}_{\text{likelihood}} \underbrace{P(Y = y)}_{\text{prior}}$$

normalization constant

$$\hat{y}_{MAP} = \arg \max_{y} P(X = x \mid Y = y)P(Y = y)$$

In Gaussian naive Bayes classifier (categorical y, continuous x):

$$P(Y = y \mid X = x) = \underbrace{\frac{f_{X|Y=y}(x \mid Y = y)}{f_{X}(x)} \underbrace{P(Y = y)}_{f_{X}(x)}}_{\text{likelihood}}$$

normalization constant

$$\hat{y}_{MAP} = \arg\max_{y} f_{X\mid Y=y}(x\mid Y=y)P(Y=y)$$





# Multinomial naive Bayes classifier





# Example 1: spam filter

An email server would like to build a spam filter for its clients

- Input variables x: the content of an email
- Training data: there are 1000 emails labeled either "spam" or "not spam"
- Prediction task: for a new email, the server would like to identify
  if it is a spam
- Model g: multinomial naive Bayes classifier





# Modeling for spam filter

- Prediction y: spam or not spam
- Variables  $x_i$ ,  $i = 1, \dots, n$ : the content of an email with n words
  - Assumptions:
    - the words are independent a bag of words (the order does not matter) NAIVE!
    - the words are generated from a categorical distribution; each category is a word from a vocabulary
- Model g: multinomial naive Bayes classifier

$$\hat{y} = g(x_1, \dots, x_n) = \underset{c \in \{spam, \text{ not } spam\}}{\arg \max} P(c) \prod_{i=1}^n P(x_i \mid c)$$

where P(c) is the prior and  $\prod_{i=1}^{n} P(x_i \mid c)$  is the likelihood under the aforementioned assumptions

Note: it is the maximum a posteriori estimation of the label (spam or not spam)

- Hyperparameters h: smoothing factor  $\alpha$  (explained soon)
- Parameters  $\theta$ : P(c), a vocabulary (if not given) and  $P(word \mid c)$  for all words in the vocabulary





# Parameter estimation (training)

#### A small example

- Training data (x, y): there are 7 emails labeled either "spam" or "not spam"
  - Email 1: ("Hi see you at dinner.", not spam)
  - Email 2: ("Buy lottery!", spam)
  - Email 3: ("Hi, wanna have dinner?", not spam)
  - Email 4: ("Hi you, nice dinner today!", not spam)
  - Email 5: ("Wanna get rich today?", spam)
  - Email 6: ("Lottery dinner?", not spam)
  - Email 7: ("Win lottery; get rich today!", spam)
- Multinomial naive Bayes classifier: e.g., y = 1 (spam)

likelihood of x being a spam probability of spams (prior)

$$P \underbrace{(Y=1 \mid X=x)}_{\text{the given email } x \text{ is a spam}} = \underbrace{P(X=x \mid Y=1)}_{P(X=x)} \underbrace{P(Y=1)}_{P(X=x)}$$

normalization constant

$$\hat{y}_{MAP} = \arg \max_{y} P(X = x \mid Y = y)P(Y = y)$$



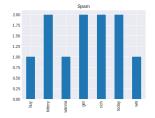


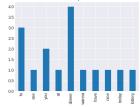
- Step 1: Estimate the likelihood  $P(word_i \mid spam)$  and  $P(word_i \mid not spam)$ 
  - 1.1 Build a vocabulary containing all unique words from the 7 emails:

 $V = \{$ buy, lottery, wanna, get, rich, today, win, hi, see, you, at, dinner, have, nice $\}$ 

1.2 Count how many times each word appears in spam emails and not spam emails:

	buy	lottery	wanna	 dinner	have	nice
Spam	1	2	1	 0	0	0
Not spam	0	1	1	 4	1	1





Not spam





- Step 1 (cont.):
  - 1.3 Count how many words in total for each class in the training data:
    - Spam: 11 wordsNot spam: 16 words
  - 1.4 Estimate the **likelihood**  $P(word_i \mid spam)$  and
    - $P(word_i \mid not \ spam)$  for all  $word_i \in V$ :

	buy	lottery	 you	at	dinner	have	nice
Spam $P(word_i \mid spam)$	$\frac{1}{11}$	$\frac{2}{11}$	 $\frac{0}{11}$	$\frac{0}{11}$	$\frac{0}{11}$	$\frac{0}{11}$	$\frac{0}{11}$
Not spam $P(word_i \mid not spam)$	$\frac{0}{16}$	$\frac{1}{16}$	 $\frac{2}{16}$	$\frac{1}{16}$	$\frac{4}{16}$	$\frac{1}{16}$	$\frac{1}{16}$

- Step 2: Estimate the **prior** P(spam) **and** P(not spam)
  - Spam P(spam):  $\frac{\# \text{ of spams}}{\# \text{ of total emails}} = \frac{3}{7}$
  - Not spam P(not spam):  $\frac{\# \text{ of not spams}}{\# \text{ of total emails}} = \frac{4}{7}$



# Classify a new email

• Construct the multinomial naive Bayes classifier

The naive Bayes classifier is a function of a given email. Let  $s_{spam}$ and  $s_{not\ spam}$  be the posterior without the normalization constant

$$s_{spam} = P(spam) \prod_{\forall word \in email} P(word \mid spam)$$

$$s_{not \ spam} = P(not \ spam) \prod_{\forall word \in email} P(word \mid not \ spam)$$

- If  $s_{spam} > s_{not spam}$ : the email is spam
- If  $s_{spam} \leq s_{not spam}$ : the email is not spam





# Classify a new email (cont.)

- Compute the posterior of this email (with the normalization constant)
  - Spam:  $P(spam \mid an \ email) = \frac{s_{spam}}{s_{spam} + s_{not \ spam}}$
  - Not spam:  $P(not spam \mid an email) = \frac{s_{not spam}}{s_{spam} + s_{not spam}}$

These are the probability of the email being a spam and not a spam, respectively.





#### One problemo

Say, the email is "You! Lottery! Lottery! Lottery!!" and it is clearly a spam. But when we compute the likelihood (cf. page 17),

$$s_{spam} = P(spam)P("you" \mid spam)P("lottery" \mid spam)^3$$

 $s_{not \ spam} = P(not \ spam)P("you" \mid not \ spam)P("lottery" \mid not \ spam)^3$ 

	buy	lottery	 you	at	dinner	have	nice
Spam $P(word_i \mid spam)$	$\frac{1}{11}$	$\frac{2}{11}$	 $\frac{0}{11}$	0 11	$\frac{0}{11}$	0 11	0 11
Not spam $P(word_i \mid not spam)$	$\frac{0}{16}$	$\frac{1}{16}$	 $\frac{2}{16}$	$\frac{1}{16}$	$\frac{4}{16}$	$\frac{1}{16}$	$\frac{1}{16}$

• 
$$s_{spam} = \frac{3}{7} \times \frac{0}{11} \times \frac{2}{11}^3 = 0$$

• 
$$s_{not spam} = \frac{4}{7} \times \frac{2}{16} \times \frac{1}{16}^3 > s_{spam}$$

This email will be classified as not a spam simply because the word "you" has never appeared in spam emails.





#### Solution to the problemo

Smoothing or discounting with hyperparameter  $\alpha$ : we need to alter Step 1.4

Let |V| be the size of the vocabulary

	buy	lottery	 you	at	dinner	have	nice
Spam $P(word_i \mid spam)$	$\frac{1+\alpha}{11+\alpha V }$	$\frac{2+\alpha}{11+\alpha V }$	 $\frac{0+\alpha}{11+\alpha V }$	$\frac{0+\alpha}{11+\alpha V }$	$\frac{0+\alpha}{11+\alpha V }$	$\frac{0+\alpha}{11+\alpha V }$	$\frac{0+\alpha}{11+\alpha V }$
Not spam $P(word_i \mid not spam)$	$\frac{0+\alpha}{16+\alpha V }$	$\frac{1+\alpha}{16+\alpha V }$	 $\frac{2+\alpha}{16+\alpha V }$	$\frac{1+\alpha}{16+\alpha V }$	$\frac{4+\alpha}{16+\alpha V }$	$\frac{1+\alpha}{16+\alpha V }$	$\frac{1+\alpha}{16+\alpha V }$

Let  $\alpha = 1$ .

• 
$$s_{spam} = \frac{3}{7} \times \frac{1}{25} \times \frac{3}{25}^3 = 0.0000296$$

• 
$$s_{not \ spam} = \frac{4}{7} \times \frac{3}{30} \times \frac{2}{30}^3 = 0.0000169 < s_{spam}$$

Note: these are very small values due to the product of small values. Typically, we apply the logarithm function to avoid underflow as in MAP and MLE (cf. lecture 5).



# Summary: Bayes' rule for multinomial naive Bayes classifier

- Data: categorical y, categorical x
- Random variable: discrete Y, discrete X

$$P(Y = y \mid X = x) = \frac{P(X = x \mid Y = y)P(Y = y)}{P(X = x)}$$

$$\hat{y}_{MAP} = \arg\max_{y} P(X = x \mid Y = y)P(Y = y)$$





### Summary: multinomial naive Bayes classifier

- Prediction y: categorical data  $y \in \{1, \dots, C\}$
- Variables  $x_i$ ,  $i = 1, \dots, n$ : categorical data  $x_i \in V$ , where V is the vocabulary  $V = \{w_1, \dots, w_K\}$  given K unique categories
  - Assumptions:
    - xi's are independent NAIVE!
    - x<sub>i</sub> follows a categorical distribution

Note: here n is the size of the input data, e.g. the length of a document

• Model g:

$$\hat{y} = g(x_1, \dots, x_n) = \underset{c \in \{1, \dots, C\}}{\operatorname{arg max}} P(c) \prod_{i=1}^n P(x_i \mid c)$$

where P(c) is the prior and  $\prod_{i=1}^{n} P(x_i \mid c)$  is the likelihood under the assumptions

- Hyperparameters h: smoothing factor  $\alpha$
- Parameters  $\theta$ : P(c), V (if not given) and  $P(w_i \mid c)$  for all  $w_i \in V$





# Summary: multinomial naive Bayes classifier (cont.)

- Parameter estimation (training):
  - Given the vocabulary  $V = \{w_k\}_{k=1}^K$  and a training data set  $\{(b_1, y_1), \cdots, (b_N, y_N)\}$ , where each  $b_j$  contains a list of words. Let  $N_c = count(y_i = c)$ .
    - Likelihood  $P(w_i \mid c)$  for each  $w_i$ :

$$P(w_i \mid c) = \frac{count(occurrences of w_i in all b_j for y_j = c) + \alpha}{count(all words from class c) + \alpha K}$$

• Prior *P*(*c*):

$$P(c) = \frac{N_c}{N}$$





# Gaussian naive Bayes classifier





# Example 2: real-time customer insight

An online shop is selling a new gaming computer

- Prediction task y: for a customer browsing this computer, the shop would like to predict if
  the customer will complete the transaction. If the prediction says no, the shop will perform
  certain actions, such as
  - proposing a discount to the customer
  - threatening the customer by showing an irritating message, e.g. "there are 20 people looking at this item right now"
  - offering a free item to encourage the transaction
- Input variables x: the shop has the following information about the customers who are browsing this computer:
  - All kinds of personal information from different sources (Google, Facebook, via e.g. cookies, IP address, the version of your browser, etc)
  - In this example, they choose the following features as the input variables: 1) average time
    they stay on Facebook everyday; 2) how much money they spend on games (yes they have
    access to their Steam account); 3) daily active time on average (and yes they have access to
    their smart watch)
- Training data:
  - The aforementioned personal information recorded from 1000 customers
  - If they have completed the transaction of purchasing the computer or not





### Modeling for real-time customer insight

- Prediction y: complete transaction or drop out before paying
- Variables  $x = [x_1, x_2, x_3]$ :
  - x1: duration (hour) on Facebook per day
  - x2: money (dollar) spent on games
  - x3: active time (hour) per day
  - Assumptions:
    - x<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub> are independent NAIVE!
    - given data from class c, xi is generated from a Gaussian distribution with PDF

$$f_i(x_i \mid c) = \frac{1}{\sqrt{2\pi\sigma_{c,i}^2}} e^{-\frac{(x_i - \mu_{c,i})^2}{2\sigma_{c,i}^2}}$$

Model g: Gaussian naive Bayes classifier

$$\hat{y} = \underset{c \in \{complete, \ drop \ out\}}{\text{arg max}} P(c) \prod_{i=1}^{d} f_i(x_i \mid c)$$

where P(c) is the prior and  $\prod_{i=1}^{d} f_i(x_i \mid c)$  is the likelihood under the assumptions Note: it is the maximum a posteriori estimation of the label (complete or drop out).

• Parameters  $\theta$ : P(c) and  $\mu_{c,i}$ ,  $\sigma_{c,i}$  in the likelihood  $f_i(x_i \mid c)$  for all variable i and all class c





### Parameter estimation (training)

In this demo, we only consider 5 customers in the training data for illustration purposes

- Training data: there are 5 customers:
  - $\mathbf{x}_1 = [x_1^1, x_2^1, x_3^1] = [2.44, 2.48, 2.64], y_1 = 1 \text{ drop out}$
  - $\mathbf{x}_2 = [x_1^2, x_2^2, x_3^2] = [9.77, 6.82, 0.55], y_2 = 0$  complete
  - $\mathbf{x}_3 = [x_1^3, x_2^3, x_3^3] = [2.15, 8.05, 3.11], y_3 = 1 \text{ drop out}$
  - $\mathbf{x}_4 = [x_1^4, x_2^4, x_3^4] = [1.96, 3.78, 3.75], y_4 = 1 \text{ drop out}$
  - $\mathbf{x}_5 = [x_1^5, x_2^5, x_3^5] = [8.31, 7.93, 0.16], y_5 = 0$  complete





• Step 1: Estimate  $\mu_{c,i}$ ,  $\sigma_{c,i}$  in the likelihood

$$f_i(x_i \mid c) = \frac{1}{\sqrt{2\pi\sigma_{c,i}^2}} e^{-\frac{(x_i - \mu_{c,i})^2}{2\sigma_{c,i}^2}}$$

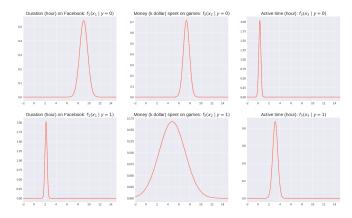
for all variable i and  $c \in \{complete, drop \ out\}$ 

- For each i=1,2,3 and  $j=1,\cdots,5$ , collect all  $x_i^j$  for  $y_j=drop\ out$ . Compute the sample mean  $\hat{\mu}_{drop\ out,i}$  and the sample standard deviation  $\hat{\sigma}_{drop\ out,i}$ .
- For each i=1,2,3 and  $j=1,\cdots,5$ , collect all  $x_i^J$  for  $y_j=complete$ . Compute the sample mean  $\hat{\mu}_{complete,i}$  and the sample standard deviation  $\hat{\sigma}_{complete,i}$ .





#### Estimated likelihood







- Step 2: Estimate the **prior** P(complete) and P(drop out)
  - Customers who have completed transaction *P*(*complete*):

$$P(complete) = \frac{\# \text{ of complete}}{\# \text{ of customers}} = \frac{2}{5}$$

• Customers who have dropped out before paying  $P(drop \ out)$ :

$$P(drop \ out) = \frac{\# \ of \ drop \ out}{\# \ of \ customers} = \frac{3}{5}$$





# Classify a new customer

Construct the Gaussian naive Bayes classifier
 The Gaussian naive Bayes classifier is a function of a given customer,
 i.e. x = [x<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub>]. Let s<sub>complete</sub> and s<sub>drop out</sub> be the posterior
 without the normalization constant

$$s_{complete} = P(complete) \prod_{i=1}^{3} f_i(x_i \mid complete)$$

$$s_{drop\ out} = P(drop\ out) \prod_{i=1}^{3} f_i(x_i \mid drop\ out)$$

- If  $s_{complete} > s_{drop,out}$ : the customer will complete the transaction
- If  $s_{complete} \leq s_{drop\ out}$ : the customer will drop out





# Classify a new customer (cont.)

Compute the posterior of this customer

```
• Complete: P(complete \mid a \ customer) = \frac{s_{complete}}{s_{complete} + s_{drop \ out}}
• Drop out: P(drop \ out \mid a \ customer) = \frac{s_{complete} + s_{drop \ out}}{s_{complete} + s_{drop \ out}}
```

These are the probability of the customer completing the transaction and dropping out, respectively.



# Classify a new customer (cont.)

For a new customer: hours spent on Facebook  $x_1 = 2.51$ ; money spent on games  $x_2 = 4.38$ ; active time  $x_3 = 2.51$ 

• The likelihood of this customer completing a transaction:



• The likelihood of this customer dropping out before paying:







# Classify a new customer (cont.)

Compute the scores:

$$s_{complete} = P(complete) \prod_{i=1}^{3} f_i(x_i \mid complete)$$

$$= \frac{2}{5} f_1(2.51 \mid complete) f_2(4.38 \mid complete) f_3(2.51 \mid complete)$$
 $\approx 0$ 

$$s_{drop \ out} = P(drop \ out) \prod_{i=1}^{3} f_i(x_i \mid drop \ out)$$
  
=  $\frac{3}{5} f_1(2.51 \mid drop \ out) f_2(4.38 \mid drop \ out) f_3(2.51 \mid drop \ out)$   
= 0.016

- $s_{complete} < s_{drop\ out}$ : the customer will drop out before paying
- Therefore, the online shop will send a message to threaten this customer.





# Summary: Bayes' rule for Gaussian naive Bayes classifier

- Data: categorical y, continuous x
- Random variable: discrete Y, continuous X

$$P(Y = y \mid X = x) = \frac{f_{X|Y=y}(x \mid Y = y)P(Y = y)}{f_X(x)}$$

$$\hat{y}_{MAP} = \arg\max_{y} f_{X|Y=y}(x \mid Y=y)P(Y=y)$$





# Summary: Gaussian naive Bayes classifier

- Prediction y: categorical data  $y \in \{1, \dots, C\}$
- Variables  $x_i$ ,  $i = 1, \dots, d$ : continuous numerical data  $x_i \in \mathbb{R}$ 
  - Assumption:
    - x<sub>i</sub>'s are independent NAIVE!
    - x<sub>i</sub> follows a Gaussian distribution
- Model g:

$$\hat{y} = g(x_1, \dots, x_d)$$

$$= \underset{c \in \{1, \dots, C\}}{\arg \max} P(c) \prod_{i=1}^d f_i(x_i \mid y = c)$$

where P(c) is the prior and  $\prod_{i=1}^d f_i(x_i \mid y=c)$  is the likelihood under the assumptions with  $f_i(x_i \mid y=c) = \frac{1}{\sqrt{2\pi\sigma_{c,i}^2}} e^{-\frac{(x_i-\mu_{c,i})^2}{2\sigma_{c,i}^2}}$ 

• Parameters  $\theta$ : P(c),  $\mu_{c,i}$ ,  $\sigma_{c,i}$  in  $f_i(x_i \mid y=c)$  for all c and i





# Summary: Gaussian naive Bayes classifier (cont.)

- Parameter estimation (training):
  - Given a training data set  $\{(x_1, y_1), \cdots, (x_N, y_N)\}$ , where each  $x_j = [x_1^j, \cdots, x_d^j]$  is a vector containing all the features for one data point. Let  $N_c = count(y_j = c)$ .
    - $\mu_{c,i}$ ,  $\sigma_{c,i}$  in the likelihood  $f_i(x_i \mid y = c)$  for all variable i and all classes c:

$$\hat{\mu}_{c,i} = \frac{1}{N_c} \sum_{t=1}^{N_c} x_i^t$$

$$\hat{\sigma}_{c,i} = \sqrt{\frac{1}{N_c - 1} \sum_{t=1}^{N_c} (x_i^t - \hat{\mu}_{c,i})^2}$$

for all  $t \in \text{class c}$ 

Prior P(c):

$$P(c) = \frac{N_c}{N}$$





# Naive Bayes: pros and cons

- Pros:
  - Highly scalable
  - Simple
  - Interpretable
  - Easy to implement
  - Working fine for some use cases (e.g. spam filter)
- Cons:
  - Too simple for most use cases
  - Assumptions are too naive





# A word on model complexity

- Models with high complexity:
  - Smart-ass models: they usually suffer from overfitting when the training data set is "small", i.e. working well on the training data set, but generalizing poorly on unseen data
  - Low bias (good)
  - High variance (bad)
  - Regularization is needed during training (cf. lecture 5 MLE vs MAP)
- Simple models:
  - They usually suffer less from overfitting, i.e. they might not work very well on the training data set; they are not performing much worse on unseen data
  - High bias (bad)
  - Low variance (good)





# Today

- Classification
- Naive Bayes classifier
- Summary





### Summary

#### So far:

- Data types and data containers
- Descriptive data analysis: descriptive statistics, visualization
- Probability distributions, events, random variables, PMF, PDF, parameters
- CDF, Q-Q plot, how to compare two distributions (data vs theoretical, data vs data)
- Mathematical modeling and probabilistic models
- Parameter estimation: maximum likelihood estimation (MLE) and maximum a posteriori estimation (MAP)
- Classification, multinomial naive Bayes classifier, Gaussian naive Bayes classifier

#### Next:

- Evaluation of a classifier
- Other applications

#### Before next lecture:

Bayes' rule







Only in this one lecture! Sorry!

