

Lecture 6: Classification and Naive Bayes classifier

Statistical Methods for Data Science

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Today

- 1 Classification
- 2 Naive Bayes classifier
 - Multinomial naive Bayes classifier
 - Gaussian naive Bayes classifier
- 3 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 naïve Bayes classifiers
- Be able to explain the differences between multinomial naïve Bayes classifier and Gaussian naïve Bayes classifier
- For a given problem, be able to formulate and implement a naïve Bayes classifier

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Classification

- Recall (cf. lecture 3): 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 $x = [x_1, \dots, x_d]$; sometimes the notations x and \mathbf{x} are used interchangeably
 - x is called a **feature vector**
 - g : **classification model**, e.g. naive Bayes classifiers, support vector machines, decision trees, etc
 - θ (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 $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\}$, e.g.

$$\{(\text{scoter}, \text{scoter}), (\text{goldeneye}, \text{goldeneye}), \dots, (\text{scoter}, \text{scoter})\}$$

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

- The targets y_i '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), $g(\mathbf{x}; \hat{\theta} \mid h)$ is called a (trained) **classifier**

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Naive Bayes classifier

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



Bayes' rule and MAP for **parameter estimation**

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

$$f_{\Theta|data}(\theta | data) = \frac{\overbrace{f_{data|\Theta}(data | \theta)}^{\text{likelihood}} \overbrace{f_{\Theta}(\theta)}^{\text{prior}}}{\underbrace{f_{data}(data)}_{\text{normalization constant}}}$$

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

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):

$$P(Y = y | X = x) = \frac{\overbrace{P(X = x | Y = y)}^{\text{likelihood}} \overbrace{P(Y = y)}^{\text{prior}}}{\underbrace{P(X = x)}_{\text{normalization constant}}}$$

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

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

$$P(Y = y | X = x) = \frac{\overbrace{f_{X|Y=y}(x | Y = y)}^{\text{likelihood}} \overbrace{P(Y = y)}^{\text{prior}}}{\underbrace{f_X(x)}_{\text{normalization constant}}}$$

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

Multinomial naïve 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 naïve Bayes classifier**

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

where $P(c)$ is the prior and $\prod_{i=1}^n P(x_i | c)$ 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 α (explained soon)
- **Parameters** θ : $P(c)$, a vocabulary (if not given) and $P(word | c)$ 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 naïve Bayes classifier**: e.g., $y = 1$ (spam)

$$P(\underbrace{Y = 1 | X = x}_{\text{the given email } x \text{ is a spam}}) = \frac{\overbrace{P(X = x | Y = 1)}^{\text{likelihood of } x \text{ being a spam}} \overbrace{P(Y = 1)}^{\text{probability of spams (prior)}}}{\underbrace{P(X = x)}_{\text{normalization constant}}}$$

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

Parameter estimation (training) (cont.)

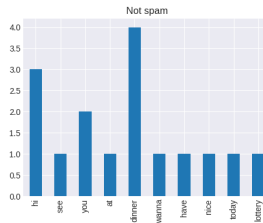
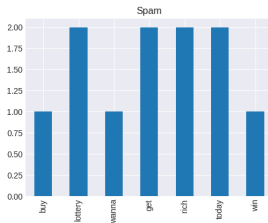
- Step 1: Estimate the likelihood $P(\text{word}_i \mid \text{spam})$ and $P(\text{word}_i \mid \text{not spam})$

1.1 Build a vocabulary containing all unique words from the 7 emails:

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

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



Parameter estimation (training) (cont.)

- Step 1 (cont.):

1.3 Count how many words in total for each class in the training data:

- Spam: 11 words
- Not spam: 16 words

1.4 Estimate the **likelihood** $P(\text{word}_i | \text{spam})$ and $P(\text{word}_i | \text{not spam})$ for all $\text{word}_i \in V$:

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

- Step 2: Estimate the **prior** $P(\text{spam})$ and $P(\text{not spam})$

- Spam $P(\text{spam})$: $\frac{\# \text{ of spams}}{\# \text{ of total emails}} = \frac{3}{7}$
- Not spam $P(\text{not spam})$: $\frac{\# \text{ of not spams}}{\# \text{ of total emails}} = \frac{4}{7}$

Classify a new email

- Construct the multinomial naïve Bayes classifier

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

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

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

- 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: $P(spam \mid \text{an email}) = \frac{s_{spam}}{s_{spam} + s_{not \text{ spam}}}$
- Not spam: $P(not \text{ spam} \mid \text{an email}) = \frac{s_{not \text{ spam}}}{s_{spam} + s_{not \text{ spam}}}$

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),

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

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

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

- $s_{spam} = \frac{3}{7} \times \frac{0}{11} \times \frac{2}{11}^3 = 0$
- $s_{not\ spam} = \frac{4}{7} \times \frac{2}{16} \times \frac{1}{16}^3 > s_{spam}$

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** α : we need to alter Step 1.4

Let $|V|$ be the size of the vocabulary

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

Let $\alpha = 1$,

- $S_{\text{spam}} = \frac{3}{7} \times \frac{1}{25} \times \frac{3}{25} = 0.0000296$
- $S_{\text{not spam}} = \frac{4}{7} \times \frac{3}{30} \times \frac{2}{30} = 0.0000169 < S_{\text{spam}}$

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 naïve 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 naïve 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:**
 - x_i 's are independent - **NAIVE!**
 - x_i follows a categorical distribution

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

- **Model g :**

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

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

- **Hyperparameters h :** smoothing factor α
- **Parameters θ :** $P(c)$, V (if not given) and $P(w_i | c)$ for all $w_i \in V$

Summary: multinomial naïve Bayes classifier (cont.)

- **Parameter estimation (training):**

Given the vocabulary $V = \{w_k\}_{k=1}^K$ and a training data set $\{(b_1, y_1), \dots, (b_N, y_N)\}$, where each b_j contains a list of words. Let $N_c = \text{count}(y_j = c)$.

- Likelihood $P(w_i | c)$ for each w_i :

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

- Prior $P(c)$:

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

Gaussian naïve 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 $\mathbf{x} = [x_1, x_2, x_3]$:**
 - x_1 : duration (hour) on Facebook per day
 - x_2 : money (dollar) spent on games
 - x_3 : active time (hour) per day
- **Assumptions:**
 - x_1, x_2, x_3 are independent - **NAIVE!**
 - given data from class c , x_i is generated from a Gaussian distribution with PDF

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

- **Model g :** Gaussian naïve Bayes classifier

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

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

- **Parameters θ :** $P(c)$ and $\mu_{c,i}, \sigma_{c,i}$ in the likelihood $f_i(x_i | c)$ 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:

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

Parameter estimation (training) (cont.)

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

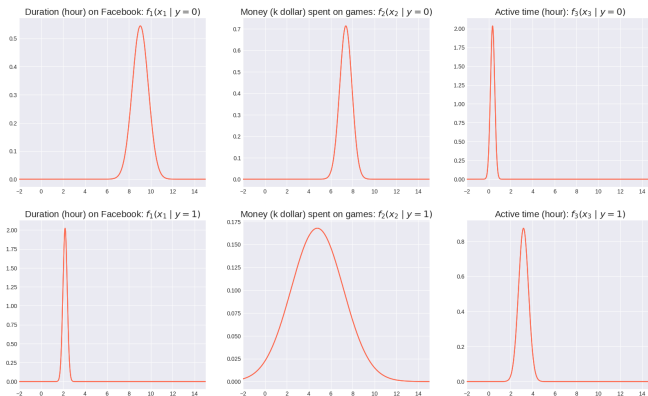
$$f_i(x_i | c) = \frac{1}{\sqrt{2\pi\sigma_{c,i}^2}} e^{-\frac{(x_i - \mu_{c,i})^2}{2\sigma_{c,i}^2}}$$

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

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

Parameter estimation (training) (cont.)

Estimated likelihood



Parameter estimation (training) (cont.)

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

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

- Customers who have dropped out before paying $P(\text{drop out})$:

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

Classify a new customer

- Construct the Gaussian naïve Bayes classifier

The Gaussian naïve Bayes classifier is a function of a given customer, i.e. $\mathbf{x} = [x_1, x_2, x_3]$. Let $s_{complete}$ and $s_{drop\ out}$ 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: $P(\text{complete} \mid a \text{ customer}) = \frac{s_{\text{complete}}}{s_{\text{complete}} + s_{\text{drop out}}}$
 - Drop out: $P(\text{drop out} \mid a \text{ customer}) = \frac{s_{\text{drop out}}}{s_{\text{complete}} + s_{\text{drop out}}}$

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:

$$\begin{aligned} s_{\text{complete}} &= P(\text{complete}) \prod_{i=1}^3 f_i(x_i \mid \text{complete}) \\ &= \frac{2}{5} f_1(2.51 \mid \text{complete}) f_2(4.38 \mid \text{complete}) f_3(2.51 \mid \text{complete}) \\ &\approx 0 \end{aligned}$$

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

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

THE END

Summary: Bayes' rule for Gaussian naïve 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 naïve 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_i 's are independent - **NAIVE!**
 - x_i follows a Gaussian distribution
- **Model** g :

$$\begin{aligned}\hat{y} &= g(x_1, \dots, x_d) \\ &= \arg \max_{c \in \{1, \dots, C\}} P(c) \prod_{i=1}^d f_i(x_i | y = c)\end{aligned}$$

where $P(c)$ is the prior and $\prod_{i=1}^d f_i(x_i | y = c)$ is the likelihood under the

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

- **Parameters** θ : $P(c), \mu_{c,i}, \sigma_{c,i}$ in $f_i(x_i | y = c)$ for all c and i

Summary: Gaussian naïve Bayes classifier (cont.)

- **Parameter estimation (training):**

Given a training data set $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\}$, where each $\mathbf{x}_j = [x_1^j, \dots, x_d^j]$ is a vector containing all the features for one data point. Let $N_c = \text{count}(y_j = c)$.

- $\mu_{c,i}, \sigma_{c,i}$ in the likelihood $f_i(x_i | y = c)$ 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

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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!