

Lecture 5: Classification and Naive Bayes classifier

Statistical Methods for Data Science

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November 16, 2020

Today

1 Classification

- Modeling for classification
- Training, validation and test
- Performance evaluation

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, annotation, training, validation and testing, etc
- Be able to calculate and interpret TP, TN, FP, FN, accuracy, precision, recall, specificity, F1 score
- Understand basic concepts of performance evaluation and comparison of different classifiers
- Be able to explain the Bayes' rule for both multinomial and Gaussian naive Bayes classifiers
- Be able to explain the differences between the multinomial naive Bayes classifier and the Gaussian naive Bayes classifier
- For a given problem, be able to formulate and implement a naive Bayes classifier

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Modeling for classification

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

Note: if you are a "bottom-up" kind of thinker and have a hard time interpreting g , just imagine it as

$$y = g(x) = \begin{cases} 1, & \text{if } x > 0 \\ 0, & \text{if } x \leq 0 \end{cases}, \text{ for two classes 0 and 1}$$

Parameter estimation

- Classification models are **supervised learning** algorithms
- Parameter estimation is called **training**
- Given an estimate $\hat{\theta}$, $g(\mathbf{x}; \hat{\theta} | h)$ is a (trained) **classifier**
- In supervised learning, 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**

Training, validation and test

Problem solving in data science

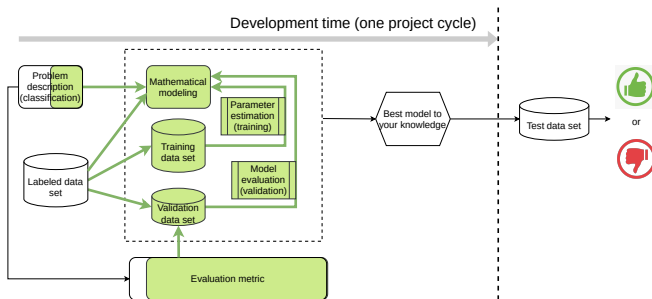


Figure: The (green) shadowed boxes are the actions performed by the data scientist.

During development: training and validation

During development: split the available data set into a training data set and a validation data set

- **Training data set:** to estimate the parameters
- **Validation data:** to evaluate the performance of one or more classifiers

What is being evaluated:

- g (the selection of a family of models with the functional form g)
Philosophies:
 - **Occam's razor:** if multiple models are showing similar performances, the simplest model is preferred
 - **All models are wrong, but some are useful**
- $\hat{\theta}$ (parameter estimation method)
- h (hyperparameter tuning)

After development: testing

After development:

- **Test data set:** the real deal - you DO NOT have access to it during development

For the project, do not use the “test data set” for development! Don’t even look at it before testing your model!!! 😡 Because in reality, you do not have access to it!

Performance evaluation

How to split the data

Given a labeled data set $\{(x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4), (x_5, y_5), (x_6, y_6)\}$, split the data set into a **training data set** and a **validation data set**

- Training-validation split
 - $\{(x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4)\}, \{(x_5, y_5), (x_6, y_6)\}$
- K-fold cross validation, e.g. 3-fold
 - $\{(x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4)\}, \{(x_5, y_5), (x_6, y_6)\}$
 - $\{(x_1, y_1), (x_2, y_2), (x_5, y_5), (x_6, y_6)\}, \{(x_3, y_3), (x_4, y_4)\}$
 - $\{(x_3, y_3), (x_4, y_4), (x_5, y_5), (x_6, y_6)\}, \{(x_1, y_1), (x_2, y_2)\}$
- Leave-one-out cross validation
 - $\{(x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4), (x_5, y_5)\}, \{(x_6, y_6)\}$
 - $\{(x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4), (x_6, y_6)\}, \{(x_5, y_5)\}$
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 - $\{(x_1, y_1), (x_3, y_3), (x_4, y_4), (x_5, y_5), (x_6, y_6)\}, \{(x_2, y_2)\}$
 - $\{(x_2, y_2), (x_3, y_3), (x_4, y_4), (x_5, y_5), (x_6, y_6)\}, \{(x_1, y_1)\}$

Validation: four outcomes

- Given a **binary classification** problem, a trained classifier $g(x; \hat{\theta} | h)$ and a validation data set containing pairs (x, y)
- Positive: $y = 1$; negative: $y = 0$
- Compute $\hat{y} = g(x; \hat{\theta} | h)$ on the validation data set
 - True Positive (TP)**: count(ground truth $y = 1$, classifier output $\hat{y} = 1$)
 - False Positive (FP)**: count(ground truth $y = 0$; classifier output $\hat{y} = 1$)
 - True Negative (TN)**: count(ground truth $y = 0$; classifier output $\hat{y} = 0$)
 - False Negative (FN)**: count(ground truth $y = 1$; classifier output $\hat{y} = 0$)

Confusion matrix (contingency table)

	$y = 1$	$y = 0$
$\hat{y} = 1$	TP	FP (Type I error)
$\hat{y} = 0$	FN (Type II error)	TN

- What is count($y = 1$)? (15 sec) **TP+FN**
- What is count($y = 0$)? (15 sec) **TN+FP**
- What is size of the entire data set, i.e. count($y = 1$)+count($y = 0$)? (15 sec) **TP+FN+TN+FP**

Evaluation metric

- Accuracy:

$$accuracy = \frac{TP + TN}{count(y = 1) + count(y = 0)} = \frac{TP + TN}{TP + TN + FP + FN}$$

- True Positive Rate (recall, sensitivity):

$$TPR = \frac{TP}{count(y = 1)} = \frac{TP}{TP + FN}$$

- True Negative Rate (specificity):

$$TNR = \frac{TN}{count(y = 0)} = \frac{TN}{TN + FP}$$

- Precision:

$$precision = \frac{TP}{count(\hat{y} = 1)} = \frac{TP}{TP + FP}$$

- F1 score:

$$F = 2 \times \frac{precision \times recall}{precision + recall}$$

- More from scikit-learn:

www.scikit-learn.org/stable/modules/classes.html#module-sklearn.metrics

Evaluation metric (cont.)

- **Use with caution** especially for **imbalanced** data set, e.g. data from medical measurements typically contains more negative data (90% healthy volunteers) than positive data (10% patients); the data set is then imbalanced
 - Terrible metric: accuracy
 - Okay metric:
 - Precision vs recall
 - Sensitivity vs specificity
 - F1 score

Reference: read the data science design manual, section 7.4.1

- In this lecture, we only consider **binary classification** $c \in \{0, 1\}$
- In the multi-class case $c \in \{1, \dots, C\}$:
 - **Macro**: the metrics are computed for each class c and then the average is calculated
 - **Micro**: the metrics are computed globally for all classes

Finding a good classifier

- **Given:** a labeled data set with $y_i \in \{0, 1\}$

$$\{(x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4), (x_5, y_5), (x_6, y_6)\}$$

- **Task:** use this data set to build a good classifier

- **Method:**

- 1) Come up with M models g_m , $m = 1, \dots, M$. Let $\hat{y}_i^m = g_m(x_i; \theta | h)$

For the sake of simplicity (not to overwhelm you with complex notations), we neglect the different choices of h . In practice, when you choose a different set of hyperparameters h , the model needs to be evaluated as a different model.

- 2) Split the data set (cf. page 13) into a **training data set** and a **validation data set**

- Training-validation split
- K-fold cross validation
- Leave-one-out cross validation

- 3) Estimate parameters $\hat{\theta}$ using the **training data set**

- Similar to the choice of h , different parameter estimation techniques will give a different $\hat{\theta}$, which in turn needs to be evaluated.

- 4) **Evaluate** $g_m(x; \hat{\theta} | h)$ on the **validation data set**

- $M = 1$: evaluation of one classifier
- $M > 1$: comparison of multiple classifiers

How to evaluate a classifier?

Given a classifier $g(x; \hat{\theta} | h)$,

- **Goal:** to evaluate the performance of the classifier $g(x; \hat{\theta} | h)$
- **Steps:**
 - Step 1: compute $\hat{y}_i = g(x_i; \hat{\theta} | h)$ on the validation data set $\{(x_1, y_1), \dots, (x_n, y_n)\}$
 - Step 2: compute an evaluation metric (e.g. page 16), denoted by s
- **Interpretation:**
 - Case 1: one validation data set (e.g. training-validation split, leave-one-out cross validation) - only one s , e.g. $s = 0.92$
 - Case 2: multiple validation data sets (e.g. K-fold cross validation) - a set of s , e.g. for 3-fold cross validation, we have 3 validation datasets, which gives us 3 results $\{s_1, s_2, s_3\}$. We can then compute sample statistics (e.g. sample mean, sample standard deviation) from this set.

How to compare two classifiers?

Given two classifiers $g_1(x; \hat{\theta} | h)$ and $g_2(x; \hat{\xi} | t)$ (note: I use different symbols $\hat{\theta}$ and $\hat{\xi}$ to indicate that they might have different parameters; likewise, h and t for different hyperparameters)

- **Goal:** to check which classifier is better, $g_1(x; \hat{\theta} | h)$ or $g_2(x; \hat{\xi} | t)$
 - **Steps:**
 - Step 1: compute $\hat{y}_i^1 = g_1(x_i; \hat{\theta} | h)$ and $\hat{y}_i^2 = g_2(x_i; \hat{\xi} | t)$ on the validation data set $\{(x_1, y_1), \dots, (x_n, y_n)\}$
 - Step 2: compute an evaluation metric (e.g. page 16) for each classifier, denoted by s^j for $j = 1, 2$
 - Step 3: compare s^1 and s^2 to choose which classifier is better, $g_1(x; \hat{\theta} | h)$ or $g_2(x; \hat{\xi} | t)$
- Example: say we choose the accuracy as the metric
- Question: if $s^1 = 0.92$ and $s^2 = 0.52$, which classifier is better, $g_1(x; \hat{\theta} | h)$ or $g_2(x; \hat{\xi} | t)$?
 - Answer: probably $g_1(x; \hat{\theta} | h)$ since $s^1 \gg s^2$
 - Question: if $s^1 = 0.92$ and $s^2 = 0.91$, now which classifier is better?
 - Still $g_1(x; \hat{\theta} | h)$ with $s^1 \approx s^2$?

We need to use **hypothesis testing** (lecture 7) to determine which classifier is better.

- Case 1: one validation data set (e.g. training-validation split, leave-one-out cross validation) - **McNemar's test**
- Case 2: multiple validation data sets (e.g. K-fold cross validation) - **paired t-test**

Summary

- Classification, binary/multi-class classification
- Training, validation and test data set
- TP, TN, FP, FN
- Evaluation metrics
- Basic concepts of performance evaluation and comparison of different classifiers

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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

- 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):

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

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

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

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

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

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 body 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 naïve Bayes classifier**

Modeling for spam filter

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

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

where $P(c)$ is the prior and $\prod_{i=1}^n P(x_i | c)$ is the likelihood under the 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 $P(\text{word} | c)$ for all words in the vocabulary

Parameter estimation (training)

In this demo, we only consider 7 training emails for illustration purposes

- **Training data:** there are 7 emails labeled either “spam” or “not spam”
 - Email 1 (not spam): “Hi see you at dinner.”
 - Email 2 (spam): “Buy lottery!”
 - Email 3 (not spam): “Hi, wanna have dinner?”
 - Email 4 (not spam): “Hi you, nice dinner today!”
 - Email 5 (spam): “Wanna get rich today?”
 - Email 6 (not spam): “Lottery dinner?”
 - Email 7 (spam): “Win lottery; get rich today!”

Parameter estimation (training) (cont.)

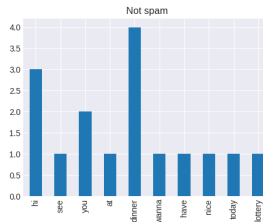
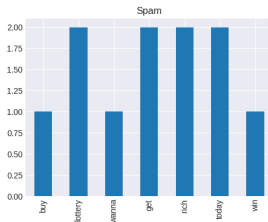
- Step 1: Estimate the likelihood $P(\text{word}_i \mid \text{spam})$ and $P(\text{word}_i \mid \text{not spam})$

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 both spams and not spams:

	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:

- 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

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

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 31),

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

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

	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 $\alpha = 1$,

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

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 4).

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, x_2 = money (k dollar) spent on games, x_3 = active time (hour)
- **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

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

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 classes 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

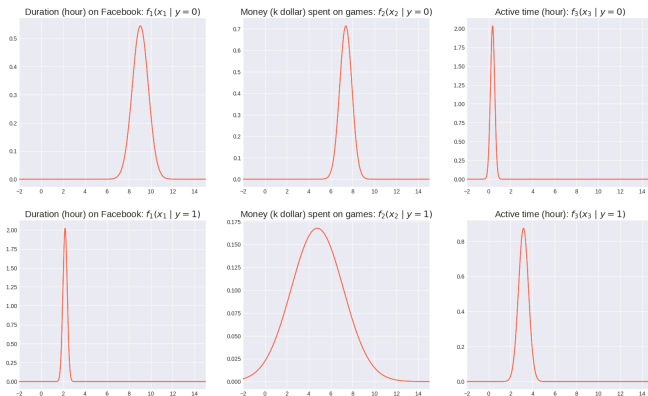
$$f_i(x_i | c) = \frac{1}{\sqrt{2\pi\sigma_{c,i}^2}} e^{-\frac{(x_i - \mu_{c,i})^2}{2\sigma_{c,i}^2}}$$

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

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

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

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

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

- 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:

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

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

- $S_{complete} < S_{drop\ out}$: 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, 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 4 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

- 1 Classification
- 2 Naive Bayes classifier
- 3 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)
- Modeling
- Parameter estimation: maximum likelihood estimation (MLE) and maximum a posteriori estimation (MAP)
- Classification, multinomial naive Bayes classifier, Gaussian naive Bayes classifier

Not yet:

- Evaluation of parameter estimation

Next:

- Interval estimation, confidence interval

Before next lecture:

- Gaussian distribution, sample mean, CDF, quantiles





Only in this one lecture! Sorry!