Lecture 5: Classification and Naive Bayes classifier Statistical Methods for Data Science

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Today

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

Modeling for classification





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



 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:

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Classification:

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 - \bullet θ (parameters) and h (hyperparameters) depend on g





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 - x: categorical or numerical
 - Typically, x is a vector denoted by $\mathbf{x} = [x_1, \dots, x_d]$; 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
 - 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

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





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- The training data set contains paired data $\{(x_1, y_1), \dots, (x_N, y_N)\}$, e.g.

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in, scoter $),($ in, goldeneye $),\cdots,($ in, 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



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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_i's in the training set are typically created by humans.
 The process of creating the ground truth labels is called annotation or labeling



Modeling for classification Training, validation and test Performance evaluation

Training, validation and test





Problem solving in data science

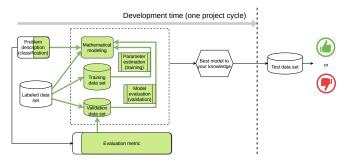


Figure: The (green) shadowed boxes are the actions performed by the data scientist.

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





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!





Modeling for classification Training, validation and test Performance evaluation

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
 - $\bullet \ \{(x_1,y_1),(x_2,y_2),(x_3,y_3),(x_4,y_4)\},\ \{(x_5,y_5),(x_6,y_6)\}$
 - $\{(x_1, y_1), (x_2, y_2), (x_5, y_5), (x_6, y_6)\}, \{(x_3, y_3), (x_4, y_4)\}$
 - $\{(x_3, y_3), (x_4, y_4), (x_5, y_5), (x_6, y_6)\}, \{(x_1, y_1), (x_2, y_2)\}$
- Leave-one-out cross validation
 - $\{(x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4), (x_5, y_5)\}, \{(x_6, y_6)\}$
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- Given a binary classification problem, a trained classifier $g(x; \hat{\theta} \mid h)$ and a validation data set containing pairs (x, y)
- Positive: y = 1; negative: y = 0



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 - True Positive (TP): count(ground truth y = 1, classifier output $\hat{y} = 1$)
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Confusion matrix (contingency table)

	y = 1	y = 0
$\hat{y} = 1$	TP	FP (Type I error)
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Validation: four outcomes

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Confusion matrix (contingency table)

	y = 1	y = 0
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- 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)





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- 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:

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

• True Positive Rate (recall, sensitivity):

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

• 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 $\hat{y}_i^m=g_m(x_i;\theta\mid h)$

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 $g_m(x; \hat{\theta} \mid h)$ 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 $g(x; \hat{\theta} \mid h)$,

- Goal: to evaluate the performance of the classifier $g(x; \hat{\theta} \mid h)$
- Steps:
 - Step 1: compute $\hat{y}_i = g(x_i; \hat{\theta} \mid h)$ on the validation data set $\{(x_1, y_1), \cdots, (x_n, y_n)\}$
 - 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.



- Goal: to check which classifier is better, $g_1(x; \hat{\theta} \mid h)$ or $g_2(x; \hat{\xi} \mid t)$
- Steps:
 - Step 1: compute $\hat{y}_i^1 = g_1(x_i; \hat{\theta} \mid h)$ and $\hat{y}_i^2 = g_2(x_i; \hat{\xi} \mid t)$ on the validation data set $\{(x_1, y_1), \cdots, (x_n, y_n)\}$
 - 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 classier is better, $g_1(x; \hat{\theta} \mid h)$ or $g_2(x; \hat{\xi} \mid t)$





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 - Question: if $s^1 = 0.92$ and $s^2 = 0.52$, which classifier is better, $g_1(x; \hat{\theta} \mid h)$ or $g_2(x; \hat{\xi} \mid t)$?





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 - Answer: probably $g_1(x; \hat{\theta} \mid h)$ since $s^1 \gg s^2$





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 - Answer: probably $g_1(x; \hat{\theta} \mid h)$ since $s^1 \gg s^2$
 - Question: if $s^1 = 0.92$ and $s^2 = 0.91$, now which classifier is better?





- Goal: to check which classifier is better, $g_1(x; \hat{\theta} \mid h)$ or $g_2(x; \hat{\xi} \mid t)$
- Steps:
 - Step 1: compute $\hat{y}_i^1 = g_1(x_i; \hat{\theta} \mid h)$ and $\hat{y}_i^2 = g_2(x_i; \hat{\xi} \mid t)$ on the validation data set $\{(x_1, y_1), \cdots, (x_n, y_n)\}$
 - 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 classier is better, $g_1(x; \hat{\theta} \mid h)$ or $g_2(x; \hat{\xi} \mid t)$ Example: say we choose the accuracy as the metric
 - Question: if $s^1 = 0.92$ and $s^2 = 0.52$, which classifier is better, $g_1(x; \hat{\theta} \mid h)$ or $g_2(x; \hat{\xi} \mid t)$?
 - Answer: probably $g_1(x; \hat{\theta} \mid h)$ since $s^1 \gg s^2$
 - Question: if $s^1 = 0.92$ and $s^2 = 0.91$, now which classifier is better?
 - Still $g_1(x; \hat{\theta} \mid h)$ with $s^1 \approx s^2$?





Given two classifiers $g_1(x; \hat{\theta} \mid h)$ and $g_2(x; \hat{\xi} \mid t)$ (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, $g_1(x; \hat{\theta} \mid h)$ or $g_2(x; \hat{\xi} \mid t)$
- Steps:
 - Step 1: compute $\hat{y}_i^1 = g_1(x_i; \hat{\theta} \mid h)$ and $\hat{y}_i^2 = g_2(x_i; \hat{\xi} \mid t)$ on the validation data set $\{(x_1, y_1), \dots, (x_p, y_p)\}$
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 - Question: if $s^1 = 0.92$ and $s^2 = 0.91$, now which classifier is better?
 - Still $g_1(x; \hat{\theta} \mid h)$ with $s^1 \approx s^2$?

We can 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





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)



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

• In parameter estimation:

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

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





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 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



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 naive 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 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 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 $P(word \mid c)$ 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!"





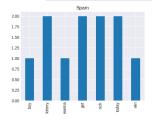
Parameter estimation (training) (cont.)

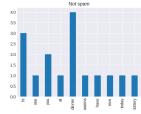
- Step 1: Estimate the likelihood $P(word_i \mid spam)$ and $P(word_i \mid not spam)$
 - 1.1 Build a vocabulary containing all unique words from the 7 emails:

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

1.2 Count how many times each word appears in 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 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 $P(word_i \mid spam)$	$\frac{1}{11}$	$\frac{2}{11}$	 $\frac{0}{11}$	0 11	$\frac{0}{11}$	$\frac{0}{11}$	$\frac{0}{11}$
Not spam $P(word_i \mid not spam)$	<u>0</u> 16	1 16	 2 16	1/16	4 16	1 16	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
 - 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.





Say, the email is "You! Lottery! Lottery! Lottery!!" and it is clearly a spam. But when we compute the likelihood (cf. page 31),

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

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

	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 $P(word_i \mid not spam)$	$\frac{0}{16}$	$\frac{1}{16}$	 $\frac{2}{16}$	$\frac{1}{16}$	$\frac{4}{16}$	1/16	$\frac{1}{16}$





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

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

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





Say, the email is "You! Lottery! Lottery! Lottery!!" and it is clearly a spam. But when we compute the likelihood (cf. page 31),

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

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

	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 $P(word_i \mid not spam)$	$\frac{0}{16}$	$\frac{1}{16}$	 $\frac{2}{16}$	$\frac{1}{16}$	$\frac{4}{16}$	$\frac{1}{16}$	$\frac{1}{16}$

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

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





Say, the email is "You! Lottery! Lottery! Lottery!!" and it is clearly a spam. But when we compute the likelihood (cf. page 31),

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

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

	buy	lottery	 you	at	dinner	have	nice
Spam $P(word_i \mid spam)$	$\frac{1}{11}$	$\frac{2}{11}$	 $\frac{0}{11}$	0 11	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 α : we need to alter Step 1.4

Let |V| be the size of the vocabulary

	buy	lottery	 you	at	dinner	have	nice
Spam $P(word_i \mid spam)$	$\frac{1+\alpha}{11+\alpha V }$	$\frac{2+\alpha}{11+\alpha V }$	 $\frac{0+\alpha}{11+\alpha V }$	$\frac{0+\alpha}{11+\alpha V }$	$\frac{0+\alpha}{11+\alpha V }$	$\frac{0+\alpha}{11+\alpha V }$	$\frac{0+\alpha}{11+\alpha V }$
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 4).





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_i follows a categorical distribution

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

• Model g:

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

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 α
- Parameters θ : 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





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 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)





Example 2: real-time customer insight

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 - 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 $x = [x_1, x_2, x_3]$: $x_1 =$ duration (hour) on Facebook, $x_2 =$ money (k dollar) spent on games, $x_3 =$ active time (hour)
 - Assumptions:
 - x₁, x₂, x₃ are independent NAIVE!
 - \bullet given data from class c, x_i 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

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

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

•
$$\mathbf{x}_1 = [x_1^1, x_2^1, x_3^1] = [2.44, 2.48, 2.64], y_1 = 1 \text{ drop out}$$

•
$$\mathbf{x}_2 = [x_1^2, x_2^2, x_3^2] = [9.77, 6.82, 0.55], y_2 = 0$$
 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



Parameter estimation (training) (cont.)

• 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 $c \in \{complete, drop \ out\}$

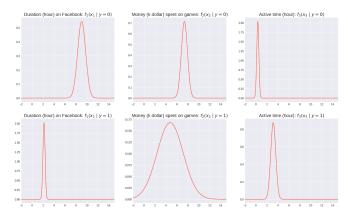
- For each i=1,2,3, collect all x_i^j for $y_j=drop\ out$. Compute the sample mean $\hat{\mu}_{drop\ out,i}$ and the sample standard deviation $\hat{\sigma}_{drop\ out,i}$.
- For each i = 1, 2, 3, collect all x_i^j for $y_j = complete$. Compute the sample mean $\hat{\mu}_{complete,i}$ and the sample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





Parameter estimation (training) (cont.)

Estimated likelihood







Parameter estimation (training) (cont.)

- Step 2: Estimate the **prior** P(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 = [x₁, x₂, x₃]. 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





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.



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:







Compute the scores:

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

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

$$\approx 0$$
 $s_{drop \ out} = P(drop \ out) \prod_{i=1}^{3} f_i(x_i \mid drop \ out)$

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

$$= \frac{3}{5} f_1(2.51 \mid drop \ out) f_2(4.38 \mid drop \ out) f_3(2.51 \mid drop \ out)$$

$$= 0.016$$



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





Compute the scores:

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





Compute the scores:

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

$$= \frac{2}{5} f_1(2.51 \mid complete) f_2(4.38 \mid complete) f_3(2.51 \mid complete)$$
 ≈ 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_i's are independent NAIVE!
 - x_i 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 θ : 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 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

- Classification
- 2 Naive Bayes classifier
- 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

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• Evaluation of parameter estimation





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Next:

• Interval estimation, confidence interval





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Before next lecture:

• Gaussian distribution, sample mean, CDF, quantiles







Only in this one lecture! Sorry!