Day 6: Machine Learning

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Introduction to Data Science and Big Data Analytics

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Day 7 Outline

Association rules

Model evaluation in machine learning Fitting v. overfitting Precision, recall, and accuracy

Naive Bayes

k-Nearest Neighbour



Introduction to association rules

- Association rule mining is used to discover objects or attributes that frequently occur together, e.g.
 - movies or music that users prefer
 - baskets of products purchased online or in-store
- Used extensively in recommendation engines
- Terminology:
 - transaction a bundle of associated items, such as a collection of movies watched or items puchased, forming the unit of analysis
 - itemset the items that make up a transaction, such as purchases, web sites visited, movies watched, etc.

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- Many different algorithms, but we will focus on one: the a priori algorithm

The apriori algorithm

Two core notions:

```
support the support of an item X is the number of transactions that contain X divided by the total number of transactions confidence expresses our "confidence" in the relation if X, then Y
```

formally:

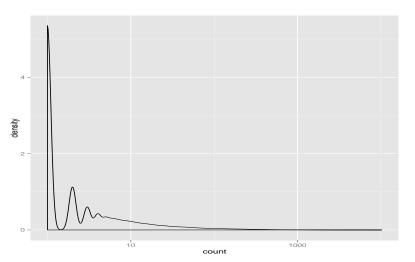
► The goal is to discover the interesting rules in a dataset above some pre-defined thresholds of support and confidence, such as 10% and 60%)

```
## book data can be found from https://qithub.com/WinVector/zmPDSwR/tree/master/
# load in book purchase transactions
require(arules, quietly = TRUE, warn.conflicts = FALSE)
(bookbaskets <- read.transactions("~/Dropbox/Classes/LSE Data Science/Lectures/
                            format = "single", sep = "\t",
                            cols = c("userid", "title"), rm.duplicates = T
## distribution of transactions with duplicates:
## items
     2 3 4 5 6 7 8 9 10 11 12 13 14 15
                                                              18
## 701 222 106 68 43 39 23
                           24 18 18
                                     16
                                         10 7 7
                                                   13
##
  19 20
          21
             22 23 25 26
                           27 28 29
                                     30
                                         31 33 34 35
                                                       38
                                                          39 42
   3 9 4 4 3 2 2 5 4 5 4 4 1 2 1
##
## 44 45 47 48 49 52 56 57 59 61 63 71 73 80 84 86 91
                                                              93
                       2 1 2 1 2 1 1
##
                1
                   1
                                                              1
   95 96 99 103 158 206 260 891
##
      1 1 1 1 2 1 1
## transactions in sparse format with
##
   92108 transactions (rows) and
##
   220447 items (columns)
```

```
# summarize basket sizes
basketSizes <- size(bookbaskets)
summary(basketSizes)

## Min. 1st Qu. Median Mean 3rd Qu. Max.
## 1.0 1.0 1.0 11.1 4.0 10250.0</pre>
```

```
# plot the distribution of basket sizes (log10 scale)
require(ggplot2, quietly = TRUE)
ggplot(data.frame(count = basketSizes)) + scale_x_log10() +
    geom_density(aes(x = count), binwidth = 1)
```

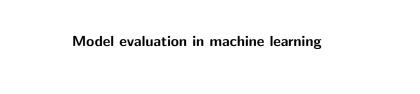


```
# which books are people reading?
bookFreq <- itemFrequency(bookbaskets)</pre>
bookCount <- (bookFreq / sum(bookFreq)) * sum(basketSizes)</pre>
orderedBooks <- sort(bookCount, decreasing = TRUE)</pre>
head(orderedBooks, 10)
##
                                          Wild Animus
##
                                                 2502
                           The Lovely Bones: A Novel
##
##
                                                 1295
##
                                   She's Come Undone
                                                  934
##
##
                                   The Da Vinci Code
##
                                                  905
##
             Harry Potter and the Sorcerer's Stone
##
                                                  832
##
                         The Nanny Diaries: A Novel
                                                  821
##
##
                                     A Painted House
                                                  819
##
##
                               Bridget Jones's Diary
##
                                                  772
##
                             The Secret Life of Bees
##
                                                  762
## Divine Secrets of the Ya-Ya Sisterhood: A Novel
```

```
# mine the rules using the apriori algorithm
rules <- apriori(bookbaskets_use,
                parameter = list(support = 0.002, confidence = 0.75))
##
## Parameter specification:
   confidence minval smax arem aval original Support support minlen maxlen
##
         0.75 0.1 1 none FALSE
                                             TRUE 0.002 1
                                                                       10
##
   target ext
##
   rules FALSE
##
## Algorithmic control:
## filter tree heap memopt load sort verbose
      0.1 TRUE TRUE FALSE TRUE 2
##
                                       TRUE.
##
## apriori - find association rules with the apriori algorithm
## version 4.21 (2004.05.09) (c) 1996-2004 Christian Borgelt
## set item appearances ...[0 item(s)] done [0.00s].
## set transactions ...[216031 item(s), 40822 transaction(s)] done [0.60s].
## sorting and recoding items ... [1256 item(s)] done [0.03s].
## creating transaction tree ... done [0.02s].
## checking subsets of size 1 2 3 4 5 done [0.06s].
## writing ... [191 rule(s)] done [0.00s].
## creating S4 object ... done [0.05s].
```

```
summary(rules)
## set of 191 rules
##
## rule length distribution (lhs + rhs):sizes
##
   2 3 4 5
  11 100 66 14
##
##
## Min. 1st Qu. Median Mean 3rd Qu. Max.
##
  2.000 3.000 3.000 3.435 4.000 5.000
##
  summary of quality measures:
##
      support confidence lift
##
   Min. :0.002009 Min. :0.7500 Min. :40.89
  1st Qu.:0.002131 1st Qu.:0.8113 1st Qu.: 86.44
##
##
  Median: 0.002278 Median: 0.8468 Median: 131.36
  Mean :0.002593 Mean :0.8569 Mean :129.68
##
   3rd Qu.:0.002695
                   3rd Qu.:0.9065 3rd Qu.:158.77
##
##
   Max. :0.005830 Max. :0.9882 Max. :321.89
##
  mining info:
##
             data ntransactions support confidence
   bookbaskets use
                       40822 0.002
##
                                         0.75
```

```
inspect(head((sort(rules, by = "confidence")), n = 5))
##
    lhs
                                                     rhs
## 1 {Four to Score,
##
    High Five,
## Seven Up.
## Two for the Dough}
                                                  => {Three To Get Deadly : A
## 2 {Harry Potter and the Order of the Phoenix,
##
     Harry Potter and the Prisoner of Azkaban,
##
     Harry Potter and the Sorcerer's Stone => {Harry Potter and the Ch
## 3 {Four to Score.
##
    High Five,
##
     One for the Money,
## Two for the Dough}
                                                  => {Three To Get Deadly : A
## 4 {Four to Score.
##
     Seven Up,
##
     Three To Get Deadly : A Stephanie Plum Novel,
##
     Two for the Dough}
                                                   => {High Five}
## 5 {High Five,
##
     Seven Up,
     Three To Get Deadly : A Stephanie Plum Novel,
##
    Two for the Dough}
                                                  => {Four to Score}
##
```



Generalization and overfitting

- Generalization: A classifier or a regression algorithm learns to correctly predict output from given inputs not only in previously seen samples but also in previously unseen samples
- ▶ Overfitting: A classifier or a regression algorithm learns to correctly predict output from given inputs in previously seen samples but fails to do so in previously unseen samples. This causes poor prediction/generalization

How model fit is evaluated

- ► For discretely-valued outcomes (class prediction): Goal is to maximize the frontier of precise identification of true condition with accurate recall, defined in terms of false positives and false negatives
 - will define formally later
- For continuously-valued outcomes: minimize Root Mean Squared Error (RMSE)

Precision and recall

► Illustration framework

		True condition	
		Positive	Negative
Dradiation	Positive	True Positive	False Positive (Type I error)
Prediction	Negative	False Negative (Type II error)	True Negative

Precision and recall and related statistics

- ► Precision: true positives / true positives + false positives
- ► Recall: true positives / false negatives
- Accuracy: Correctly classified Total number of cases
- $F1 = 2 \; \frac{\text{Precision} \; \times \; \text{Recall}}{\text{Precision} \; + \; \text{Recall}}$ (the harmonic mean of precision and recall)

Example: Computing precision/recall

Assume:

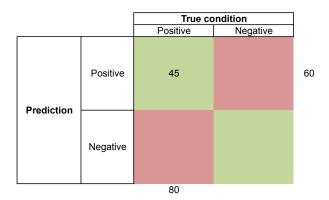
- We have a sample in which 80 outcomes are really positive (as opposed to negative, as in sentiment)
- Our method declares that 60 are positive
- ▶ Of the 60 declared positive, 45 are actually positive

Solution:

Precision =
$$(45/(45+15)) = 45/60 = 0.75$$

Recall = $(45/(45+35)) = 45/80 = 0.56$

Accuracy?



add in the cells we can compute

		True condition		1
		Positive	Negative	
Prodiction	Positive	45	15	60
Prediction	Negative	35		
		80		

How do we get "true" condition?

- ▶ In some domains: through more expensive or extensive tests
- ▶ In social sciences: typically by expert annotation or coding
- A scheme should be tested and reported for its reliability



Naive Bayes classification

- ► The following examples refer to "words" and "documents" but can be thought of as generic "features" and "cases"
- We will being with a discrete case, and then cover continuous feature values
- Objective is typically MAP: identification of the maximum a posteriori class probability

Multinomial Bayes model of Class given a Word

Consider J word types distributed across I documents, each assigned one of K classes.

At the word level, Bayes Theorem tells us that:

$$P(c_k|w_j) = \frac{P(w_j|c_k)P(c_k)}{P(w_j)}$$

For two classes, this can be expressed as

$$= \frac{P(w_j|c_k)P(c_k)}{P(w_j|c_k)P(c_k) + P(w_j|c_{\neg k})P(c_{\neg k})}$$
(1)

Multinomial Bayes model of Class given a Word Class-conditional word likelihoods

$$P(c_k|w_j) = \frac{P(w_j|c_k)P(c_k)}{P(w_j|c_k)P(c_k) + P(w_j|c_{\neg k})P(c_{\neg k})}$$

- The word likelihood within class
- ▶ The maximum likelihood estimate is simply the proportion of times that word *j* occurs in class *k*, but it is more common to use Laplace smoothing by adding 1 to each observed count within class

Multinomial Bayes model of Class given a Word Word probabilities

$$P(c_k|w_j) = \frac{P(w_j|c_k)P(c_k)}{P(w_j)}$$

- ► This represents the word probability from the training corpus
- Usually uninteresting, since it is constant for the training data, but needed to compute posteriors on a probability scale

Multinomial Bayes model of Class given a Word Class prior probabilities

$$P(c_k|w_j) = \frac{P(w_j|c_k)P(c_k)}{P(w_j|c_k)P(c_k) + P(w_j|c_{\neg k})P(c_{\neg k})}$$

- ► This represents the class prior probability
- Machine learning typically takes this as the document frequency in the training set
- ➤ This approach is flawed for scaling, however, since we are scaling the latent class-ness of an unknown document, not predicting class uniform priors are more appropriate

Multinomial Bayes model of Class given a Word Class posterior probabilities

$$P(c_k|w_j) = \frac{P(w_j|c_k)P(c_k)}{P(w_j|c_k)P(c_k) + P(w_j|c_{\neg k})P(c_{\neg k})}$$

► This represents the posterior probability of membership in class *k* for word *j*

Moving to the document level

The "Naive" Bayes model of a joint document-level class posterior assumes conditional independence, to multiply the word likelihoods from a "test" document, to produce:

$$P(c|d) = P(c) \prod_{j} \frac{P(w_{j}|c)}{P(w_{j})}$$

- ▶ This is why we call it "naive": because it (wrongly) assumes:
 - conditional independence of word counts
 - positional independence of word counts

Naive Bayes Classification Example

(From Manning, Raghavan and Schütze, *Introduction to Information Retrieval*)

► Table 13.1 Data for parameter estimation examples.

	docID	words in document	in $c = China$?
training set	1	Chinese Beijing Chinese	yes
_	2	Chinese Chinese Shanghai	yes
	3	Chinese Macao	yes
	4	Tokyo Japan Chinese	no
test set	5	Chinese Chinese Tokyo Japan	?

Naive Bayes Classification Example

Example 13.1: For the example in Table 13.1, the multinomial parameters we need to classify the test document are the priors $\hat{P}(c) = 3/4$ and $\hat{P}(\overline{c}) = 1/4$ and the following conditional probabilities:

$$\begin{array}{rcl} \hat{P}(\mathsf{Chinese}|c) & = & (5+1)/(8+6) = 6/14 = 3/7 \\ \hat{P}(\mathsf{Tokyo}|c) = \hat{P}(\mathsf{Japan}|c) & = & (0+1)/(8+6) = 1/14 \\ & \hat{P}(\mathsf{Chinese}|\overline{c}) & = & (1+1)/(3+6) = 2/9 \\ \hat{P}(\mathsf{Tokyo}|\overline{c}) = \hat{P}(\mathsf{Japan}|\overline{c}) & = & (1+1)/(3+6) = 2/9 \end{array}$$

The denominators are (8+6) and (3+6) because the lengths of $text_c$ and $text_{\overline{c}}$ are 8 and 3, respectively, and because the constant B in Equation (13.7) is 6 as the vocabulary consists of six terms.

We then get:

$$\hat{P}(c|d_5) \propto 3/4 \cdot (3/7)^3 \cdot 1/14 \cdot 1/14 \approx 0.0003.$$

$$\hat{P}(\overline{c}|d_5) \propto 1/4 \cdot (2/9)^3 \cdot 2/9 \cdot 2/9 \approx 0.0001.$$

Thus, the classifier assigns the test document to c = China. The reason for this classification decision is that the three occurrences of the positive indicator Chinese in d_5 outweigh the occurrences of the two negative indicators Japan and Tokyo.

Naive Bayes with continuous covariates

```
library(e1071) # has a normal distribution Naive Bayes
## Error in library(e1071): there is no package called 'e1071'
# Congressional Voting Records of 1984 (abstentions treated as missing)
data(HouseVotes84, package = "mlbench")
## Error in find.package(package, lib.loc, verbose = verbose): there is
no package called 'mlbench'
model <- naiveBayes(Class ~ ., data = HouseVotes84)</pre>
## Error in eval(expr, envir, enclos): could not find function
"naiveBayes"
# predict the first 10 Congresspeople
data.frame(Predicted = predict(model, HouseVotes84[1:10,-1]),
           Actual = HouseVotes84[1:10,1],
           postPr = predict(model, HouseVotes84[1:10, -1], type = "raw"))
## Error in predict(model, HouseVotes84[1:10, -1]): error in evaluating
the argument 'object' in selecting a method for function 'predict':
Error: object 'model' not found
```

Overall prediction performance

```
# now all of them: this is the resubstitution error
(mytable <- table(predict(model, HouseVotes84[,-1]), HouseVotes84$Class))
## Error in predict(model, HouseVotes84[, -1]): error in evaluating the argument 'object' in selecting a method for function 'predict': Error: object 'model' not found
prop.table(mytable, margin=1)
## Error in sweep(x, margin, margin.table(x, margin), "/", check.margin = FALSE): object 'mytable' not found</pre>
```

With Laplace smoothing

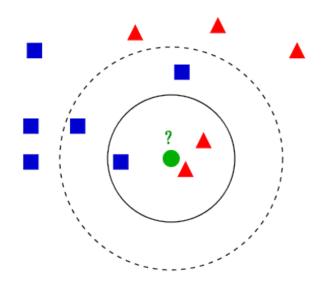
```
model <- naiveBayes(Class ~ ., data = HouseVotes84, laplace = 3)</pre>
## Error in eval(expr, envir, enclos): could not find function
"naiveBaves"
(mytable <- table(predict(model, HouseVotes84[,-1]), HouseVotes84$Class))</pre>
## Error in predict(model, HouseVotes84[, -1]): error in evaluating the
argument 'object' in selecting a method for function 'predict': Error:
object 'model' not found
prop.table(mytable, margin=1)
## Error in sweep(x, margin, margin.table(x, margin), "/", check.margin
= FALSE): object 'mytable' not found
```

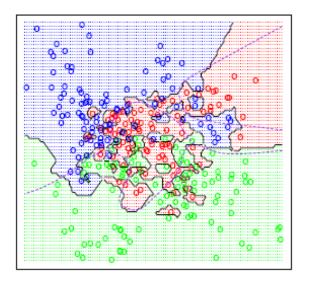
k-Nearest Neighbour

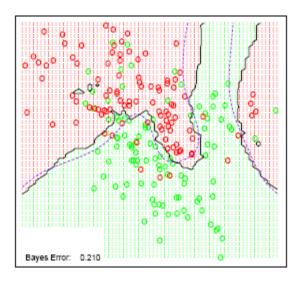
k-nearest neighbour

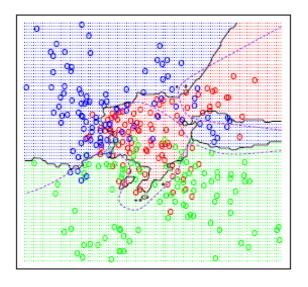
- ► A non-parametric method for classifying objects based on the training examples taht are *closest* in the feature space
- ▶ A type of instance-based learning, or "lazy learning" where the function is only approximated locally and all computation is deferred until classification
- ▶ An object is classified by a majority vote of its neighbors, with the object being assigned to the class most common amongst its *k* nearest neighbors (where *k* is a positive integer, usually small)
- Extremely simple: the only parameter that adjusts is k
 (number of neighbors to be used) increasing k smooths the
 decision boundary

k-NN Example: Red or Blue?









```
## kNN classification
require(class)
## Loading required package: class
require(quantedaData)
## Loading required package:
                              quantedaData
## Loading required package:
                              quanteda
##
## Attaching package: 'quanteda'
##
## The following object is masked from 'package:arules':
##
      sample
##
##
   The following object is masked from 'package:base':
##
##
      sample
data(amicusCorpus)
# create a matrix of documents and features
amicusDfm <- dfm(amicusCorpus, ignoredFeatures=stopwords("english"),</pre>
                 stem=TRUE, verbose=FALSE)
# threshold-based feature selection
```

```
# tf-idf weighting
amicusDfm <- weight(amicusDfm, "tfidf")

## Note: method with signature 'CsparseMatrix#Matrix#missing#replValue'
chosen for function '[<-',
## target signature 'dfmSparse#ngCMatrix#missing#numeric'.
## "Matrix#nsparseMatrix#missing#replValue" would also be valid

# partition the training and test sets
train <- amicusDfm[!is.na(docvars(amicusCorpus, "trainclass")), ]
test <- amicusDfm[!is.na(docvars(amicusCorpus, "testclass")), ]
trainclass <- docvars(amicusCorpus, "trainclass")[1:4]</pre>
```

```
# classifier with k=1
classified <- knn(train, test, trainclass, k=1)
table(classified, docvars(amicusCorpus, "testclass")[-c(1:4)])

##
## classified AP AR
## P 14 5
## R 5 74</pre>
```

```
# classifier with k=2
classified <- knn(train, test, trainclass, k=2)
table(classified, docvars(amicusCorpus, "testclass")[-c(1:4)])

##
## classified AP AR
## P 12 36
## R 7 43</pre>
```

k-nearest neighbour issues: Dimensionality

- ▶ Distance usually relates to all the attributes and assumes all of them have the same effects on distance
- Misclassification may results from attributes not confirming to this assumption (sometimes called the "curse of dimensionality") – solution is to reduce the dimensions
- ▶ There are (many!) different *metrics* of distance