

5th)

- Modeling and Prediction

by Kumaran Ponnambalam, Dedicated to Data Science Education Follow

This course focuses on **Modeling** and **Prediction**. Different algorithms for supervised and unsupervised learning are explored. Use cases are presented for the major types of algorithms.

20 Lessons (4h 40m)

URL: https://www.skillshare.com/classes/Applied-Data-Science-5-Modeling-and-Prediction/543485717?via=similar-classes

1. About Applied Data Science Series

8:12

Course goal

- Train students to be full-fledged data science practitioners who could execute end-to-end data science projects to achieve business results
- The course is oriented towards existing software professionals
 - · Heavily focused on programming and solution building
 - · Limited, as-required exposure to math and statistics
 - Overview of ML concepts, with focus on using existing tools to develop solutions

Achievements

- · Understand the concepts and life cycle of Data Science
- Develop proficiency to use R for all stages of analytics
- Learn Data Engineering tools and techniques
- Acquire knowledge of different machine learning techniques and know when and how to use them.
- Become a full-fledged Data Science Practitioner who can immediately contribute to real-life Data Science projects

Course structure

- · Concepts of Data Science
- Data Science Life Cycle
- Statistics for Data Science
- R Programming
 - Examples
- Data Engineering
- Modeling and Predictive Analytics
 - Use cases
- Advanced Topics
- Resource Bundle

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Nom	Modifié le	Type	Taille
AdvancedMethodsBreastCancer.pdf	16-02-15 17:45	Adobe Acrobat D	5.575 Ko
AssociationRulesAccidents.pdf	12-02-15 00:09	Adobe Acrobat D	215 Ko
▶ DecisionTreesIris.pdf	10-02-15 19:19	Adobe Acrobat D	312 Ko
KMeansClusteringAutoData.pdf	11-02-15 19:22	Adobe Acrobat D	232 Ko
LinearRegressionAutoMpg.pdf	09-02-15 20:23	Adobe Acrobat D	732 Ko
NaiveBayesSpamFiltering.pdf	11-02-15 00:35	Adobe Acrobat D	274 Ko
RandomForestBankCustomer.pdf	17-02-15 07:22	Adobe Acrobat D	7.079 Kd
accidents.csv	11-02-15 23:50	Fichier CSV	46 Ke
auto-data.csv	11-02-15 19:10	Fichier CSV	12 Ko
auto-miles-per-gallon.csv	09-02-15 18:39	Fichier CSV	17 Ko
ank.csv	14-02-12 23:38	Fichier CSV	451 Kd
breast_cancer.csv	01-09-13 00:35	Fichier CSV	123 Kd
apoi.csv	19-11-14 21:24	Fichier CSV	2.774 K
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sms_spam_short.csv	31-10-14 06:25	Fichier CSV	44 Ko
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Data Engineering Examples.R	05-02-15 23:03	Fichier R	4 Ka
R-Programming-Examples.R	15-02-15 09:34	Fichier R	12 Ko
Applied Data Science_ADSR-Resources.zip	06-10-20 15:31	zip Archive	14.714 Kd

Analytics and Predictions

2. Types of Analytics

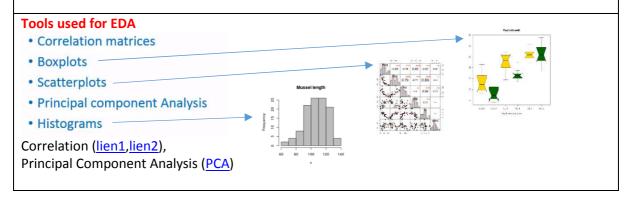
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Types of Analyt	ics
Descriptive	Understand what happened
Exploratory	Find out why something is happening
Inferential	Understand a population from a sample
Predictive	Forecast what is going to happen
Causal	What happens to one variable when you change another
Deep	Use of advanced techniques to understand large and multisource datasets

#6 types : descriptive, exploratory, inferential, predictive, causal, deep Reminder: a <u>subset</u> of a population is called a sample.

Exploratory Data Analysis (EDA)

- Understand the predictors and targets in the data set
 - Spreads
 - Correlations
- Uncover the patterns and trends
- Find key variables and eliminate unwanted variables
- Detect outliers
- Validate previous data ingestion processes for possible mistakes
- Test assumptions and hypothesis



17:16

Machine Learning

- Data contains attributes
- Attributes show relationships (correlation) between entities
- Learning understanding relationships between entities
- Machine Learning a computer analyzing the data and learning about relationships
- · Machine Learning results in a model built using the data
- · Models can be used for grouping and prediction

Data for Machine Learning

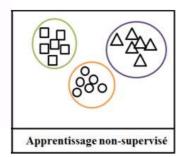
- Machines only understand numbers
- Text Data need to be converted to equivalent numerical representations for ML algorithms to work.
- Number representation
 - (Excellent, Good, Bad can be converted to 1,2,3)
- Boolean variables
 - 3 new Indicator variables called Rating-Excellent, Rating-Good, Rating-Bad with values 0/1
- Document Term matrix

DTM => https://www.tidytextmining.com/tidytext.html

Unsupervised Learning (UL)

- Finding hidden structure / similarity / grouping in data
- Observations grouped based on similarity exhibited by entities
- · Similarity between entities could be by
 - Distance between values
 - Presence / Absence
- Types
 - Clustering
 - Association Rules Mining
 - Collaborative Filtering

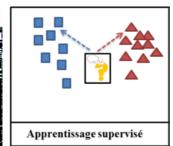
UL: https://fr.wikipedia.org/wiki/Apprentissage_non_supervis%C3%A9



Supervised Learning (SL)

• Trying to predict unknown data attributes (outcomes) based on

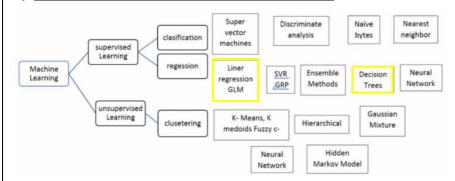




SL: https://fr.wikipedia.org/wiki/Apprentissage non supervis%C3%A9

Machine Learning tree: SL vs. UL

Ref. https://www.educba.com/what-is-supervised-learning/

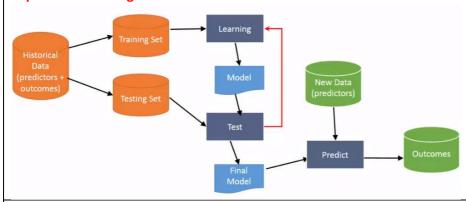


ML > SL > regression > LM, DT

ML > SL > classification

ML > UL > ...

Supervised Learning Process



Training Data

- Historical Data contains both predictors and outcomes
- · Split as training and testing data
- Training data is used to build the model
- Testing data is used to test the model
 - · Apply model on training data
 - · Predict the outcome
 - . Compare the outcome with the actual value
 - Measure accuracy
- Training and Test fit best practices
 - 70-30 split
 - · Random selection of records. Should maintain data spread in both datasets
- + Evaluate machine learning models using the train-test split (tutorial)

Reinforcement learning:

https://mc.ai/understanding-supervised-unsupervised-and-reinforcement-learning/

Comparing Results

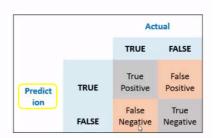
Confusion Matrix

- · Plots the predictions against the actuals for the test data
- · Helps understand the accuracy of the predictions
- · Predictions can be Boolean or classes

Confusion Matrix is a tool to determine the performance of classifier. It contains information about actual and predicted classifications.

Prediction Types

- The importance of prediction types vary by the domain
- True Positive (TP) and True Negative (TN) are the correct predictions
- False Negative (FN) can be critical in medical field
- False Positive (FP) can be critical in judicial field



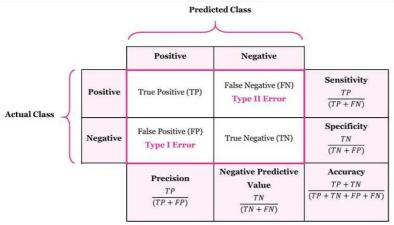
False Negative are not acceptable in <u>medical field</u> (incorrect detection of a disease: patient is positive (ill), but you detect as negative i.e. not ill!

False Positive are not acceptable in <u>judicial field</u> (incorrect detection of a criminal: client is negative (innocent), but you detect as positive i.e. a criminal!

Confusion Matrix metrics

- Accuracy
 - · Measures the accuracy of the prediction
 - Accuracy = (TP + TN) / (TP + TN + FP + FN)
- Sensitivity
 - · Hit rate or recall
 - Sensitivity = TP / (TP + FN)
- Specificity
 - · True negative rate
 - Specificity = TN / (TN + FP)
- Precision
 - Precision = TP / (TP + FP)

#5 metrics: accuracy, sensitivity, specificity, precision, negative predictive value



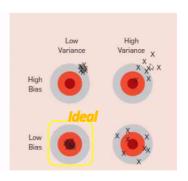
Ref. https://manisha-sirsat.blogspot.com/2019/04/confusion-matrix.html

Prediction Errors

Bias and Variance

- Bias happens when the model "skews" itself to certain aspects of the predictors, while ignoring others. It is the error between prediction and actuals.
- Variance refers to the stability of a model

 Keep predicting consistently for new data sets. It is the variance between predictions for different data sets.

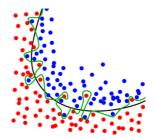


<u>bias vs. variance</u> (tutorial, trade-off)

- 1) Low-bias ML algo: Decision Trees, k-Nearest Neighbours and Support Vector Machines.
- 2) High-bias ML algo: Linear Regression, Linear Discriminant Analysis, and Logistic Regression.
- 3) Low-variance ML algo: Linear Regression, Linear Discriminant Analysis, and Logistic Regression.
- 4) High-variance ML algo: Decision Trees, k-Nearest Neighbours and Support Vector Machines.

Type of errors

- [n-Sample] error is the prediction error when the model is used to predict on the training data set it is built upon.
- Out-of-sample error is the prediction error when the model is used to predict on a new data set.
- Over fitting refers to the situation where the model has very low insample error, but very high out-of-sample error. The model has "over fit" itself to the training data.



<u>Under vs. Over-fitting</u>, <u>In-sample vs. Out-of-sample</u>

Sur-ajustement (overfitting): https://fr.wikipedia.org/wiki/Surapprentissage

Sous-ajustement (underfitting): https://www.statsoft.fr/concepts-

statistiques/glossaire/s/surajustement.html

Ex. https://towardsdatascience.com/overfitting-vs-underfitting-a-complete-example-d05dd7e19765

Regression Analysis

- Method of investigating functional relationship between variables
- Estimate the value of dependent variables from the values of independent variables using a relationship equation
- Used when the dependent and independent variables are continuous and have some correlation.
- · Goodness of Fit analysis is important.

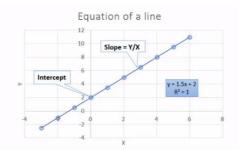
Linear Equation

- X is the independent variable
- Y is the dependent variable
- · Compute Y from X using

$$Y = \alpha X + \beta$$

Coefficients:

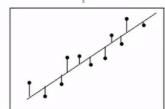
- $\alpha = Slope = Y/X$
- $\beta^{\mathbb{Q}}$ Intercept = value of Y when X=0



Fitting a line

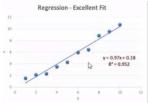
- Given a scatter plot of Y vs X, fit a straight line through the points so that the sum of square of vertical distances between the points and the line (called residuals) is minimized
- Best line = least residuals
- A line can always be fitted for any set of points

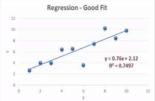


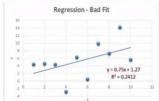


Goodness of Fit

- R-squared measures how close the data is to the fitted line
- R-squared varies from 0 to 1. The higher the value, the better the fit
- You can always fit a line. Use R-squared to see how good the fit is
- · Higher correlation usually leads to better fit







Multiple Regression

- When there are more than one independent variable that is used to predict the dependent variable.
- The equation $Y = \beta + \alpha_1^* X_1 + \alpha_2^* X_2 + ... + \alpha_p^* X_p$
- Same process used for prediction as a single independent variable
- Different predictors have different levels of impact on the dependent variable

Using Linear Regression for ML

- ML Technique to predict continuous data supervised learning
- · Predictors and outcomes provided as input
- Data analyzed (training) to come up with a linear equation
 - Coefficients
 - Intercept
 - R-squared
- Linear equation represents to model.
- · Model used for prediction
- · Typically fast for model building and prediction

Linear Regression - Summary

Advantages

- Fast
- Low cost
- Excellent for linear relationships
- Relatively accurate Continuous variables

Shortcomings

- Only numeric/ continuous variables
- Cannot model nonlinear / fuzzy relationships
- Sensitive to outliers

Used in

 Oldest predictive model used in a wide variety of applications to predict continuous values

Linear Regression exercise - predicting miles per gallon

Problem statement

The input data set contains data about details of various car models. Based on the information provided, the goal is to come up with a model to predict Miles-per-gallon of a given model.

Techniques Used

- 1. Linear Regression (multi-variate)
- 2. Data Imputation
- Variable Reduction

Data Engineering & Analysis

```
R program => C:/Users/User/Workspace/RprogProjects/AppliedDataScience_5
```

str(), summary(), head(), tail()

Data Cleansing

- 1. The ranges of values in each of the variables (columns) look ok without any kind of outliers
- 2. Horsepower is a number and R should have shown the quartiles like other numeric variables. It is being recognized as factor. Also, str() shows "?" as one of the values. So this means, the ? values should be imputed. We will replace the "?" with the mean value for Horsepower.

```
auto_data <- read.csv("auto-miles-per-gallon.csv", stringsAsFactors =
TRUE)</pre>
```

=>

```
$ HORSEPOWER : Factor w/ 94 levels "?", "100", "102",...: 17 35 29 29 24 42 47
```

aucc	_uatalat	ıco_uacaşnı	OKOFFOMFK	:	,]		
Α	В	С	D	E	F	G	Н
MPG	▼ CYLINDERS ▼	DISPLACEMENT *	HORSEPOWER -T	WEIGHT ▼	ACCELERATION	MODELYEAR ▼	NAME
25	4	98	?	2046	19	71	ford pinto
21	6	200	?	2875	17	74	ford maverick
40.9	4	85	?	1835	17.3	80	renault lecar deluxe
23.6	4	140	?	2905	14.3	80	ford mustang cobra
34.5	4	100	?	2320	15.8	81	renault 18i
23	4	151	?	3035	20.5	82	amc concord dl

Cleansing

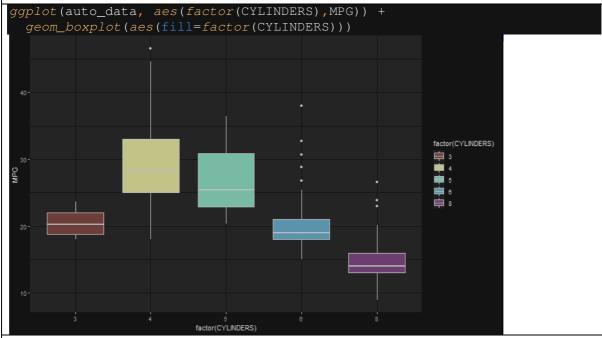
=> replacing ? (NA) by mean of HP

```
# except in column HORSEPOWER where we found some '?'
(33,127,331,337,355,375)
auto_data[auto_data$HORSEPOWER == '?',]
# convert ? to 1 via as.numeric !!!
auto_data$HORSEPOWER <- as.numeric(auto_data$HORSEPOWER)
auto_data[auto_data$HORSEPOWER == 82,]
print(auto_data$HORSEPOWER) # NA values are displayed</pre>
```

```
for (i in c(33,127,331,337,355,375)) {
   print(auto_data[i,]) # HORSEPOWER is NA
}
# now, we will replace NA value with the mean of all the HP !
hp_mean <- mean(auto_data$HORSEPOWER,na.rm="TRUE")
hp_mean # i.e. 104.4694 ok - Mean:104.5 computed by summary
auto_data$HORSEPOWER[is.na(auto_data$HORSEPOWER)] <- hp_mean
for (i in c(33,127,331,337,355,375)) {
   print(auto_data[i,]) # HORSEPOWER is now 104.4694
}
summary(auto_data)</pre>
```

Exploratory Data Analysis

```
library(ggplot2)
ggplot(auto_data, aes(factor(CYLINDERS), MPG)) +
    geom_boxplot( aes(fill=factor(CYLINDERS)))
```



So, when the nbr. of cyclinders increase, MPG decrease (pattern).

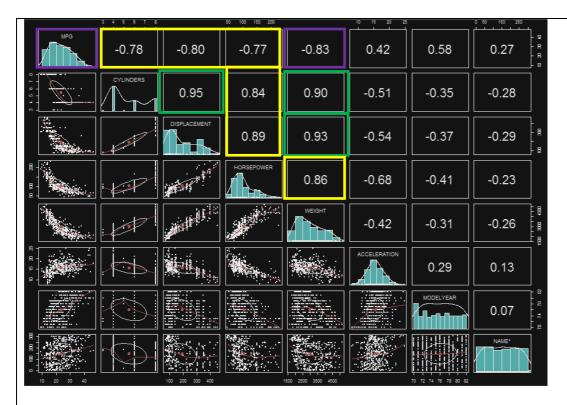
Dots in white are outliers ⇔ BoxPlot − Check for outliers

Correlation

```
library(psych)
pairs.panels(auto_data)
```

Once you do correlations, it is important to find out domain (automobiles in this case) as to why they exist. In this example, we are trying to predict miles-per-gallon. The chart shows the Pearson correlation co-efficient (range -1 to + 1).

MPG CYLINDERS DISPLACEMENT HORSEPOWER WEIGHT ACCELERATION MODELYEAR NAME



Ref. https://www.rdocumentation.org/packages/ggplot2/versions/3.3.2/topics/aes

High correlation between CYLINDERS and WEIGHT

High correlation between CYLINDERS and DISPLACEMENT

High correlation between WEIGHT and DISPLACEMENT

Good correlation between WEIGHT/CYLINDERS/DISPLACEMENT and HORSEPOWER

- Number of Cylinders has a high negative correlation to MPG (As Cylinders increase, MPG decreases).
 This is as expected.
- · Same is the case with Displacement.
- The more the weight the less the acceleration. This also has a logical explanation
- · Name has little correlation to MPG. True. This can be ignored.

Cylinders, Displacement and Weight have high correlation amongst themselves and hence one is a proxy of the other two. To limit the number of variables, we will eliminate displacement and cylinders and just keep Weight alone

```
auto_data$DISPLACEMENT <- NULL
auto_data$CYLINDERS <- NULL
```

Reduce from 3 variables to 1 => just keep one (Weight)

Modelling & Predicting

lm() => https://www.rdocumentation.org/packages/stats/versions/3.6.2/topics/lm

```
lm_model <- lm(MPG ~ . ,auto_data[1:5])
summary(lm_model, TRUE, TRUE, TRUE)
summary.lm(lm_model)</pre>
```

```
lm(formula = MPG ~ ., data = auto_data[1:5])
              10 Median
                              30
                                        Max
-8.7152 -2.3362 -0.1052 2.0100 14.2742
Coefficients:
                Estimate Std. Error t value Pr(>|t|)
(Intercept) -15.599843 4.587024 -3.401 0.000741 ***
HORSEPOWER
                0.005231 0.012873 0.406 0.684677
WEIGHT -0.006757 0.000454 -14.884 < 2e-16 ***
ACCELERATION 0.083131 0.096857 0.858 0.391257
MODELYEAR 0.754431 0.051552 14.634 < 2e-16 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 3.44 on 393 degrees of freedom
Multiple R-squared: 0.8083, Adjusted R-squared: 0.8063
F-statistic: 414.1 on 4 and 393 DF, \, p-value: < 2.2e-16
The model gives the Intercept and co-efficients required for the linear regression equation. The R-Squared
```

value is .8, which is a very good fit for the problem.

summary.lm

mathematical equation can be generalized as follows:

```
Y = \theta 1 + \theta 2X + \epsilon
```

where, 61 is the intercept and 62 is the slope (2 regression coefficients).

 ϵ is the error term, the part of Y the regression model is unable to explain.

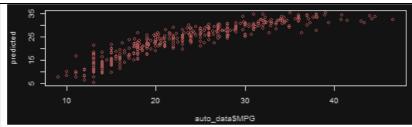
Ref. http://r-statistics.co/Linear-Regression.html

Testing

To test the accuracy of the equation, let us apply the equation on the same data set and predict the MPG for each record. Since we already know the actual value, let us compare the predicted value with the actual value and see the conformance/ error in the prediction.

```
predicted <- predict.lm(lm_model, auto_data)</pre>
summary(predicted)
```

```
> summary(auto_data[1])
     MPG
Min.
      : 9.00
1st Qu.:17.50
Median :23.00
Mean
       :23.51
3rd Qu.:29.00
Max.
       :46.60
> summary(predicted)
  Min. 1st Qu. Median
                          Mean 3rd Qu.
                                          Max.
 5.148 18.451 24.592 23.515 29.142 35.359
```



Ref. https://www.rdocumentation.org/packages/graphics/versions/3.6.2/topics/plot

```
# linear model
lm_model <- lm(MPG ~ . ,auto_data[1:5])
# prediction based on the model and actual data
predicted <- predict.lm(lm_model, auto_data)
summary(predicted)

plot(auto_data$MPG, predicted, col = "red")
# correlation
cor(auto_data$MPG, predicted)
[1] 0.8990293</pre>
```

The plot of prediction vs actual follows a diagnal straight line, which means this is very good prediction. The correlation co-efficient is also very high, which again means very good prediction.

Conclusions

The model built can predict MPG with an accuracy of about 90% (based on the correlation co-efficient)

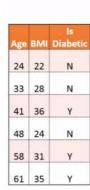
Decision Trees (DT) - Overview

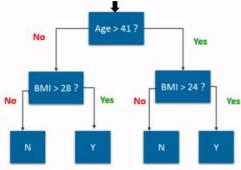
- The simplest, easy to understand and easy to explain ML technique.
- Predictor variables are used to build a tree that would progressively predict the target variable
 - · Trees start with a root node that start the decision making process
 - · Branch nodes refine the decision process
 - · Leaf nodes provide the decisions
- · Training data is used to build a decision tree to predict the target
- The tree becomes the model that is used to predict on new data

More about decision tree >> <u>link</u>
DT algorithms >> <u>link1</u> <u>link2</u>

Ref. https://fr.wikipedia.org/wiki/Arbre de d%C3%A9cision

Decision Trees - Example to predict "diabetic"





Predicting "Is Diabetic?"

Decision Trees - Choosing the right predictors

- The depth of trees are highly influenced by the sequence in which the predictors are chosen for decisions
- · Using predictors with high selectivity gives faster results
- ML implementations automatically make decisions on the sequence /preference of predictors

Decision Trees - Summary

Advantages

- Easy to interpret and explain
- Works with missing data
- Sensitive to local variations
- Fast

Shortcomings

- Limited Accuracy
- Bias builds up pretty quickly
- Not good with large predictors

Used in

- Credit approvals
- Situations with legal needs to explain decisions
- Preliminary categorization

19:36

Decision Trees exercise - Predicting Flower types

Problem Statement

The input data is the iris dataset. It contains recordings of information about flower samples. For each sample, the petal and sepal length and width are recorded along with the type of the flower. We need to use this dataset to build a decision tree model that can predict the type of flower based on the petal and sepal information.

Techniques Used

- 1. Decision Trees C5.0
- 2. Training and Testing
- 3. Confusion Matrix

Data engineering & Analysis

```
library(datasets)
data(iris)
iris_data <- iris
str(iris)
summary(iris)</pre>
```

```
> str(iris_data)
'data.frame': 150 obs. of 5 variables:
$ Sepal.Length: num 5.1 4.9 4.7 4.6 5 5.4 4.6 5 4.4 4.9 ...
$ Sepal.Width : num 3.5 3 3.2 3.1 3.6 3.9 3.4 3.4 2.9 3.1 ...
$ Petal.Length: num 1.4 1.4 1.3 1.5 1.4 1.7 1.4 1.5 1.4 1.5 ...
$ Petal.Width : num 0.2 0.2 0.2 0.2 0.2 0.4 0.3 0.2 0.2 0.1 ...
$ Species : Factor w/ 3 levels "setosa", "versicolor", ..: 1 1 1 1 1 1 1 1 1 ...
```

```
> summary(iris)
Sepal.Length Sepal.Width Petal.Length Petal.Width Species
Min. :4.300 Min. :2.000 Min. :1.000 Min. :0.100 setosa :50
1st Qu.:5.100 1st Qu.:2.800 1st Qu.:1.600 1st Qu.:0.300 versicolor:50
Median :5.800 Median :3.000 Median :4.350 Median :1.300 virginica :50
Mean :5.843 Mean :3.057 Mean :3.758 Mean :1.199
3rd Qu.:6.400 3rd Qu.:3.300 3rd Qu.:5.100 3rd Qu.:1.800
Max. :7.900 Max. :4.400 Max. :6.900 Max. :2.500
```

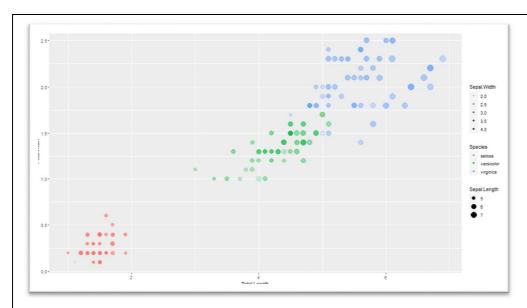
No cleansing required

Data Cleansing

- 1. The ranges of values in each of the variables (columns) look ok without any kind of outliers
- 2. There is equal distribution of the three classes setosa, versicolor and virginia

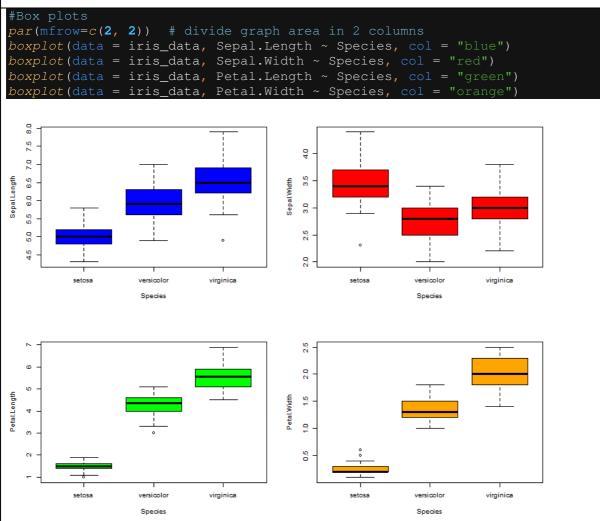
Exploratory Data Analysis

```
library(ggplot2)
ggplot(data = iris_data) +
  geom_point(aes(x = Petal.Length, y = Petal.Width, color = Species, size
= Sepal.Length, alpha = Sepal.Width))
```



So, Petal.Length and Petal.Width are good indicators to distinguish the species.

Ref. https://juba.github.io/tidyverse/08-ggplot2.html

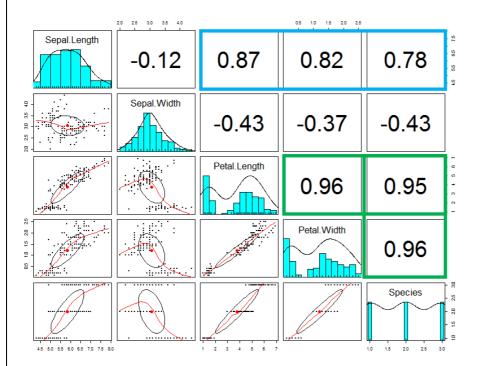


Again, Petal.Length and Petal.Width are very good indicators to distinguish the species. Septal.Length is ok too...

All 3 except Sepal Width seem to bring the significant differenciation between the 3 classes

Correlations

```
library(psych)
pairs.panels(iris_data)
```



All 3 except Sepal Width seem to bring the significant differenciation between the 3 classes

The correlation co-efficients confirm the findings of the Exploratory Data Analysis.

Modelling & Predictions

Split Training and Testing

Split training and testing datasets in the ratio of 70-30

```
library(caret)
# creation of a vector with the training data set (70%)
inTrain <- createDataPartition(y=iris_data$Species, p=0.7, list=FALSE)
class(inTrain); str(inTrain)
# training: 105 obs vs. testing: 45 obs
training <- iris_data[inTrain,]
class(training); str(training); dim(training)
table(training$Species)

testing <- iris_data[-inTrain,]
class(testing); str(testing); dim(testing)
table(testing$Species)</pre>
```

Model building

Build model based on the training data

```
#Ref. https://cran.r-project.org/web/packages/C50/index.html
library(C50)
# build a model based on training datasert (target is Species)
model <- C5.0(training[-5], training$Species)
summary(model)</pre>
```

```
The model clearly shows how the decision tree looks like. This is one of the advantages of decision trees.
 5.0 [Release 2.07 GPL Edition] - Mon Oct 26 11:40:36 2020
 Class specified by attribute `outcome'
 Read 105 cases (5 attributes) from undefined.data
Decision tree:
 Petal.Width <= 0.4: setosa (35)
 Petal.Width > 0.4:
     :... Petal.Length <= 4.8: versicolor (33/1)
        Petal.Length > 4.8: virginica (37/3)
Evaluation on training data (105 cases)
        Decision Tree - Size Errors
                                     (3.8%) <<
           (a) (b) (c) <-classified as
                       (a): class setosa
               32 3 (b): class versicolor
               1 34 (c): class virginica
          Attribute usage:
                              100.00%
                                         Petal.Width,
                                                               66.67% Petal.Length
```

Testing

Now let us predict the class for each sample in the test data. Then compare the prediction with the actual value of the class.

```
predicted <- predict(model, testing)
class(predicted)
str(predicted)
table(predicted)
confusionMatrix(predicted, testing$Species)</pre>
```

Confusion Matrix and Statistics – Reference

```
        Prediction
        setosa versicolor virginica

        setosa
        13
        0
        0

        versicolor
        2
        14
        2

        virginica
        0
        1
        13

        Overall Statistics

        Accuracy: 0.8889

        95% CI: (0.7595, 0.9629)

        No Information Rate: 0.3333

        P-Value [Acc > NIR]: 1.408e-14
```

Kappa: 0.8333

Mcnemar's Test P-	Value : NA		
Statistics by Class:	setosa	versicolor	virginica
Sensitivity	0.8667	0.9333	0.8667
Specificity	1.0000	0.8667	0.9667
Pos Pred Value	1.0000	0.7778	0.9286
Neg Pred Value	0.9375	0.9630	0.9355
Prevalence	0.3333	0.3333	0.3333
Detection Rate	0.2889	0.3111	0.2889
Detection Prevalen	ce 0.2889	0.4000	0.3111
Balanced Accuracy	0.9333	0.9000	0.9167

The model shows very high accuracy. The reason why the accuracy is so high is because, the data itself has very strong signals (seperation between the classes). Sepal.Length and Sepal.Width have very high correlations and they are used in the decision tree. In order to see how the tree will behave if it only had Sepal.Length and Sepal.Width, let us remove that data and see how accurate the tree is.

```
#get only Sepal Length, width and species
sub_data <- iris_data[, c(1,2,5)]</pre>
```

```
# Modelling with a sub-set of data (just Sepal & Species)
sub_data <- iris_data[c(1,2,5)]
sub_inTrain <- createDataPartition(y=sub_data$Species, p=0.7, list=FALSE)
sub_training <- sub_data[sub_inTrain,]
sub_testing <- sub_data[-sub_inTrain,]
model2 <- C5.0(sub_training[-3], sub_training$Species)</pre>
```

summary(model2)

sub_predicted <- predict(model2, sub_testing)
confusionMatrix(sub_predicted, sub_testing\$Species)</pre>

Model2 is less accurate than first model

Decision Tree => Errors 4 25 (23.8%)

(a) (b) (c) <- classified as

33 2 (a): class setosa

15 20 (b): class versicolor

3 32 (c): class virginica

Overall Statistics => Accuracy: 0.6889 ... Kappa: 0.5333

You will notice that the decision tree itself has become more complex and the accuracy dropped significantly

Conclusions

. Irrespective of the algorithm used, we need high correlations between the predictor and target variables for good predictions

9. Naive Bayes Classifier

19:21

Naïves Bayes - theorem (overview)

- Probability of an event A = P(A) is between 0 and 1
- Baves' theorem gives the conditional probability of an event A given event B has already occurred.

$$P(A/B) = P(A \text{ intersect B}) * P(A) / P(B)$$

- Example
 - There are 100 patients
 - Probability of a patient having diabetes is P(A) = .2
 - Probability of patient having diabetes (A) given that the patient's age is > 50
 (B) is P(A/B) = .4

Other Refs.

- 1) https://fr.wikipedia.org/wiki/Classification_na%C3%AFve_bay%C3%A9sienne
- 2) https://le-datascientist.fr/les-algorithmes-de-naives-bayes

Naïves Bayes - Classifications

- · Application of Bayes' theorem to ML
- The target variable becomes event A
- The predictors become events B1 Bn
- We try to find P(A / B1-Bn)

Age	BMI	Is Diabetic	
24	22	N	Probability of Is Diabetic = Y given that Age = 24 and BMI = 22
41	36	Y	Probability of Is Diabetic – Y given that Age = 41 and BMI = 36

Naïves Bayes - Model building and prediction

• The model generated stores the conditional probability of the target for every possible value of the predictor.

	Overall			Gender					
Salary		1 to 20	20 to 30	30 to 40	40 to 50	50 to 60	60 to 100	Female	Male
< 50K	.75	0.1	0.3	0.25	0.17	0.1	0.08	0.39	0.61
> 50K	.25	0.03	0.08	0.3	0.32	0.2	0.07	0.15	0.85
Overall		.08	.24	.26	.21	.12	.08	.33	.67

- When a new prediction needs to be done, the conditional probabilities are applied using Bayes' formula to find the probability
 - To predict for Age = 25
 - P(Salary < 50K / Age=25) = 0.3 * 0.75 / 0.24 = ~ 0.92
 - P(Salary > 50K / Age=25) = 0.08 * 0.25 / 0.24 = ~ 0.08

Naïves Bayes – Summary

Advantages

- Simple and fast
- Works well with noisy
 Expects predictors to and missing data
- Provides probabilities
 Not good with large of the result
- Very good with categorical data

Shortcomings

- Limited Accuracy
- be independent
- numeric features

Used in

- Medical diagnosis
- Spam filtering
- Document classification
- Sports predictions

10. R Use Case: Naive Bayes

19:12

Naïve Bayes exercise – Spam Filtering

Problem Statement

The input data is a set of SMS messages that has been classified as either "ham" or "spam". The goal of the exercise is to build a model to identify messages as either ham or spam.

Ham email is an email that is wanted by the recipient and is not considered spam.

Techniques Used

- 1. Naive Bayes Classifier
- 2. Training and Testing
- 3. Confusion Matrix
- 4. Text Pre-Processing

Data Engineering & Analysis

Loading and understanding the dataset

```
sms_data <- read.csv("sms_spam_short.csv", stringsAsFactors = FALSE)</pre>
class(sms_data); dim(sms_data); str(sms_data)
head(sms_data[1]); head(sms_data[2])
sms_type_factors <- as.factor(sms_data$type)</pre>
class(sms_type_factors)
```

```
str(sms_type_factors)
sms_data$type <- sms_type_factors
str(sms_data) # type are now seen as factor (2 levels)
summary(sms_data) # 437 ham / 63 spam</pre>
```

Data Cleansing

The dataset contains raw text. The text need to be pre-processed and converted into a Document Term Matrix before it can be used for classification purposes. The steps required are documented as comments below

```
# data cleansing on email messages via Corpus
library(tm)
email_msg_corpus <- Corpus(VectorSource(sms_data$text))</pre>
class(email_msg_corpus)
inspect(email_msg_corpus) # [1:3]) # inspect first 3 on 500 documents
refined_msg_corpus <- tm_map(email_msg_corpus,</pre>
content_transformer(tolower))
# removing punctuation, white space, numbers, stop and specific words
refined_msg_corpus <- tm_map(refined_msg_corpus, removePunctuation)
refined_msg_corpus <- tm_map(refined_msg_corpus, removeNumbers)
refined_msg_corpus <- tm_map(refined_msg_corpus, stripWhitespace)
refined_msg_corpus <- tm_map(refined_msg_corpus, removeWords,
stopwords())
refined_msg_corpus <- tm_map(refined_msg_corpus, removeWords,
c("else", "the", "are", "for"))
refined_msg_corpus <- tm_map(refined_msg_corpus, removeWords,</pre>
refined_msg_corpus <- tm_map(refined_msg_corpus, removeWords,
inspect (refined_msg_corpus)
# creation of a document-term sparse matrix
dtm <- DocumentTermMatrix(refined_msg_corpus)</pre>
str(dtm)
dim(dtm)
filtered_dtm <- DocumentTermMatrix(refined_msg_corpus,
list(dictionary=findFreqTerms(dtm, 10)))
filtered_dtm
dim(filtered_dtm)
t(inspect(filtered_dtm)[1:5,])
```

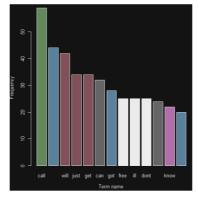
Exploratory Data Analysis

The following example shows a word cloud for both ham and spam message. The size of words shown in the word cloud is based on the frequency of occurance. It will clearly show that there is a difference in the most common occuring words between these types

```
# Build a matrix 'm' from 'filtered_dtm'
# rem. in a matrix all the elements are the same type of data
# ref. http://www.sthda.com/french/wiki/text-mining-et-nuage-de-mots-
avec-le-logiciel-r-5-etapes-simples-a-savoir
# https://www.datamentor.io/r-programming/matrix/
m <- as.matrix(filtered_dtm)
class(m); attributes(m) # $dim 500 59, $dimnames$Docs , $dimnames$Terms</pre>
```

```
head(colnames(m)) # Terms
head(rownames(m)) # Docs ids
print(head(m))
v <- sort(colSums(m), decreasing=TRUE)</pre>
head(v); class(v[1]); str(v); names(v)
# rem. in a data frame the columns contain different types of data
head(d, 5) # top five term occurences
       horiz = FALSE)
# Ref. https://www.rdocumentation.org/packages/tm/versions/0.7-
7/topics/findFreqTerms
findFreqTerms(dtm, lowfreq = 40, highfreq = Inf)
findAssocs(dtm, terms = "call", corlimit = 0.3)
# world cloud
https://www.rdocumentation.org/packages/wordcloud/versions/2.6/topics/wor
https://www.rdocumentation.org/packages/RColorBrewer/versions/1.1-
2/topics/RColorBrewer
library(wordcloud)
pal_colors <- brewer.pal(9, "Dark2")</pre>
display.brewer.pal(9, "Dark2")
wordcloud(refined_msg_corpus, min.freq = 5, colors = pal_colors,
random.order=FALSE)
wordcloud(refined_msg_corpus[sms_data$type == "ham"], min.freq = 5,
colors = pal_colors, random.order=FALSE)
wordcloud(refined_msg_corpus[sms_data$type == "spam"], min.freq = 5,
colors = pal_colors, random.order=FALSE, scale = 2)
```







Modeling & Prediction

Split Training and Testing

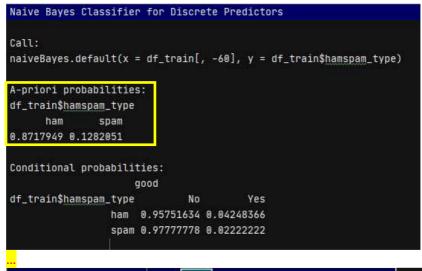
Split training and testing datasets in the ratio of 70-30

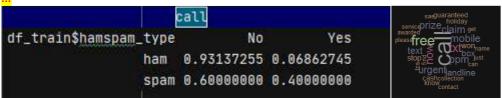
```
# Ref. http://topepo.github.io/caret/index.html (lattice, ggplot2)
library(caret)
# ref. https://www.rdocumentation.org/packages/caret/versions/6.0-
inTrain <- createDataPartition(y=sms_data$type, p=0.7, list=FALSE)
#matrix
dim(inTrain); inTrain[1:8,1]
train_rawdata <- sms_data[inTrain,]
test_rawdata <- sms_data[-inTrain,]
dim(raw_data_train); dim(raw_data_test)
str(raw_data_train); str(raw_data_test)
raw_data_train[1:3,1:2]
# splitting the corpus between training and testing
train_corpus <- refined_msg_corpus[inTrain]</pre>
test_corpus <- refined_msg_corpus[-inTrain]</pre>
train_dtm <- filtered_dtm[inTrain,]
test_dtm <- filtered_dtm[-inTrain,]
in a doc)
conv_counts <- function(x) {</pre>
  x \leftarrow factor(y, levels = c(0,1), labels = c("No", "Yes"))
https://www.rdocumentation.org/packages/base/versions/3.6.2/topics/apply
train <- apply(train_dtm, MARGIN = 2, FUN = conv_counts)</pre>
test <- apply(test_dtm, MARGIN = 2, FUN = conv_counts)</pre>
df_train <- as.data.frame(train)</pre>
df_test <- as.data.frame(test)</pre>
df_train[1:5,1:6]
str(df_train) # 351 obs of 59 var
str(df_test)
  _train$hamspam_type <- train_rawdata$type
df_test$hamspam_type <- test_rawdata$type</pre>
str(df_train) # 351 obs of 60 var
str(df_test)
               # 149 obs of 60 var
```

		dont	day	home	new	great	hamspam_type
	470	No	No	No	No	No	ham
	473	No	No	No	No	No	ham
	477	No	No	No	No	No	ham
	482	No	No	No	No	No	ham
						No	ham
df test	490	No	No	No	No	No	spam

Model Building

```
Build model based on the training data
library(e1071)
nb_model <- naiveBayes (df_train[,-60], df_train$hamspam_type)</pre>
filename <- "my_naive_bayes_log.txt"</pre>
sink(filename) # prepare to write into output file
nb_model
sink() # return to R Console
 AppliedDataScience_5 \ 🕡 naive_bayes.R
   ■ Project ▼
                          ⊕ ÷
     AppliedDataScience_5 C:\Us
       auto-miles-per-gallon.csv
       @ Billard.R
       @ decision_tree.R
       👰 linear_regression.R
       my_naive_bayes_log.txt
       naive_bayes.R
       sms_spam_short.csv
Naive Bayes Classifier for Discrete Predictors
```





Testing

Now let us predict the class for each sample in the test data. Then compare the prediction with the actual

```
predicted <- predict(nb_model, df_test)</pre>
confusionMatrix(predicted, df_test$hamspam_type)
sink(filename, append=TRUE) # prepare to write into output file
confusionMatrix(predicted, df_test$hamspam_type)
sink() # return to R Console
```

```
Reference
Prediction ham spam
ham 127 3
spam 4 15

Accuracy: 0.953
95% CI: (0.9056, 0.9809)
No Information Rate: 0.8792
P-Value [Acc > NIR]: 0.001811

Kappa: 0.784

Mcnemar's Test P-Value: 1.000000
```

Total Observations in Table: 149					
	actual				
predicted	ham	spam	Row Total		
ham	127] 3	130		
	0.977	0.023	0.872		
	0.969	0.167	1 1		
spam	4	15	19		
	0.211	0.789	0.128		
	0.031	0.833	1 1		
Column Total	131	18	149		
	0.879	0.121	1		

How to test the model on real message???

10:31

Random Forest - Overview

- Random Forest is one of the most popular and accurate algorithms
- It is an Ensemble method based on decision trees
 - Builds multiple models each model a decision tree
 - · For prediction each tree is used to predict an individual result
 - · A vote is taken on all the results to find the best answer

Random Forest - How it works?

- Lets say the dataset contains m samples (rows) and n predictors (columns)
- · x trees are built, each with a subset of data
- For each tree, a subset of m rows and n columns are chosen randomly.
- For example, if the data has 1000 rows and 5 columns, each tree is built using 700 rows and 3 columns
- · The data subset is used to build a tree
- For prediction, new data is passed to each of the x trees and x possible results obtained
- For example, if we are predicting buy=Y/N and there are 500 trees, we might get 350 Y and 150 N results
- The most found result is the aggregate prediction.

Ref. https://fr.wikipedia.org/wiki/For%C3%AAt d%27arbres d%C3%A9cisionnels https://cran.r-project.org/web/packages/randomForest/index.html

Random Forest – Summary

Advantages

- · Highly accurate
- Efficient on large number of predictors
- · Fully parallelizable
- Very good with missing data

Shortcomings

- Time and Resource consuming
- For categorical variables, bias might exist if levels are disproportionate

Used in

- Scientific Research
- Competitions
- Medical Diagnosis

Random Forest - Prospective customers of a bank

Problem Statement

D

The input data contains surveyed information about potential customers for a bank. The goal is to build a model that would predict if the prospect would become a customer of a bank, if contacted by a marketing exercise.

Techniques Used

- 1. Random Forests
- 4. Indicator Variables
- 2. Training and Testing
- 5. Binning
- 3. Confusion Matrix
- 6. Variable Reduction

Data Engineering & A 4. Indicator Variables

Loading and understandil 5. Binning

```
bank_data <- read.

sep = ";" + convert to factors
```

header = TRUE, as.is = FALSE)

```
# i.e.
```

str(bank_data)
summary(bank_data)
head(bank_data)

```
> head(bank_data)
```

```
job marital education default balance housing loan co
1 30 unemployed married
                         primary
                                     no
                                            1787
                                                     no
                                                         no cel
                                            4789
2 33
        services married secondary
                                      no
                                                    yes yes cel
3 35 management single tertiary
                                            1350
                                      no
                                                    yes
                                                         no cel
      management married tertiary
```

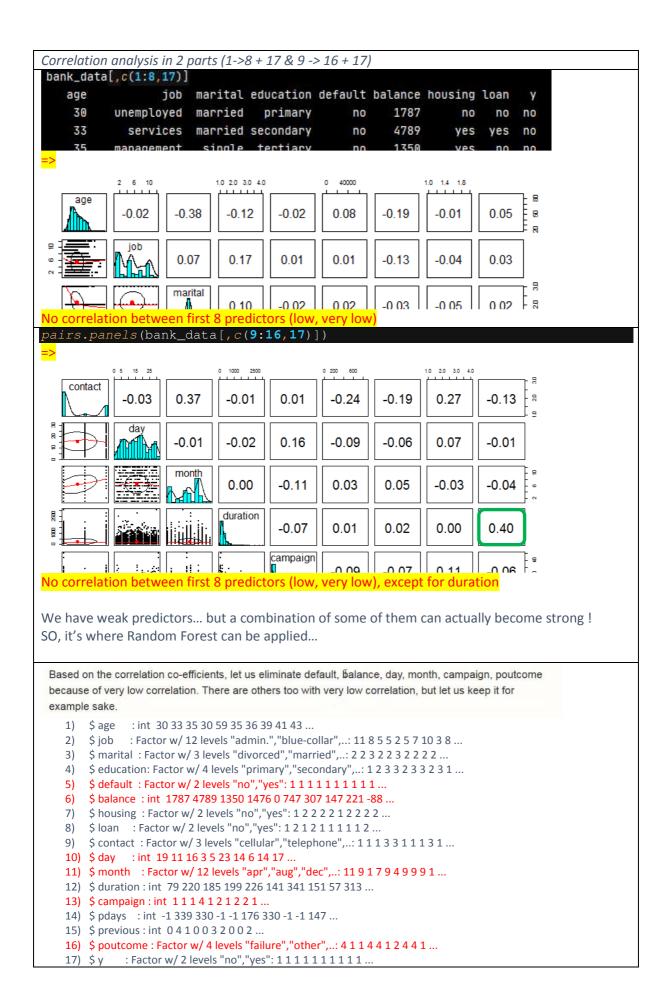
No cleansing required

Correlations

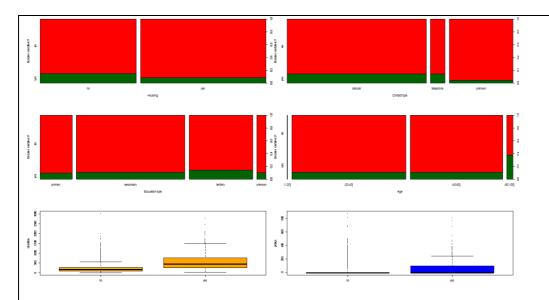
Given the large number of predictors, we would like to start with a correlation analysis to see if some variables can be dropped

'data.frame': 4521 obs. of 17 variables:

- 1) \$ age : int 30 33 35 30 59 35 36 39 41 43 ...
- 2) \$ job : Factor w/ 12 levels "admin.","blue-collar",..: 11 8 5 5 2 5 7 10 3 8 ...
- 3) \$ marital : Factor w/ 3 levels "divorced", "married",..: 2 2 3 2 2 3 2 2 2 2 ...
- 4) \$ education: Factor w/ 4 levels "primary", "secondary", ..: 1 2 3 3 2 3 3 2 3 1 ...
- 5) \$ default : Factor w/ 2 levels "no", "yes": 1 1 1 1 1 1 1 1 1 1 ...
- 6) \$ balance : int 1787 4789 1350 1476 0 747 307 147 221 -88 ...
- 7) \$ housing : Factor w/ 2 levels "no","yes": 1 2 2 2 2 1 2 2 2 2 ...
- 8) \$ loan : Factor w/ 2 levels "no", "yes": 1 2 1 2 1 1 1 1 1 2 ...
- 9) \$ contact : Factor w/ 3 levels "cellular", "telephone", ..: 1 1 1 3 3 1 1 1 3 1 ...
- 10) \$ day : int 19 11 16 3 5 23 14 6 14 17 ...
- 11) \$ month : Factor w/ 12 levels "apr", "aug", "dec", ...: 11 9 1 7 9 4 9 9 9 1 ...
- 12) \$ duration: int 79 220 185 199 226 141 341 151 57 313 ...
- 13) \$ campaign: int 1114121221...
- 14) \$ pdays : int -1 339 330 -1 -1 176 330 -1 -1 147 ...
- 15) \$ previous: int 0410032002...
- 16) \$ poutcome : Factor w/ 4 levels "failure", "other",..: 4 1 1 4 4 1 2 4 4 1 ...
- 17) \$ y : Factor w/ 2 levels "no", "yes": 1 1 1 1 1 1 1 1 1 1 ...



```
Eliminate variables with very low coeff < 0.1 (below 10%)
new data <-bank_data[, c(1:4,7:9,12,14,15,17)]
library(psych)
pairs.panels(bank_data[,c(1:8,17)])
pairs.panels(bank_data[,c(9:16,17)])
newbank_data <- bank_data[c(1:4,7:9,12,14,15,17)]
pairs.panels(newbank_data)
Do some transforamtions...
create bins on the age
https://www.rdocumentation.org/packages/base/versions/3.6.2/topics/cut
Levels: (1,20] (20,40] (40,60] (60,100]
Do some transforamtions...
split mariage into three categories (is divorced, is single, is married)
newbank_data$is_divorced <- ifelse(newbank_data$marital == "divorced")</pre>
newbank_data$is_single <- ifelse(newbank_data$marital == "single" , 1, 0)
newbank_data$is_married <- ifelse(newbank_data$marital == "married", 1, 0)</pre>
newbank_data$marital <- NULL # to delete</pre>
str(newbank data)
'data.frame': 4521 obs. of 13 variables:
        : Factor w/ 4 levels "(1,20]","(20,40]",..: 2 2 2 2 3 2 2 2 3 3 ...
$ job
        : Factor w/ 12 levels "admin.", "blue-collar", ..: 11 8 5 5 2 5 7 10 3 8 ...
$ education: Factor w/ 4 levels "primary", "secondary", ..: 1 2 3 3 2 3 3 2 3 1 ...
$ housing : Factor w/ 2 levels "no", "yes": 1 2 2 2 2 1 2 2 2 2 ...
        : Factor w/ 2 levels "no", "yes": 1 2 1 2 1 1 1 1 1 2 ...
$ contact : Factor w/ 3 levels "cellular", "telephone", ..: 1113311...
$ duration: int 79 220 185 199 226 141 341 151 57 313 ...
$ pdays : int -1 339 330 -1 -1 176 330 -1 -1 147 ...
$ previous : int 0410032002...
       : Factor w/ 2 levels "no", "yes": 1 1 1 1 1 1 1 1 1 1 ...
$ v
$ is divorced: num 000000000...
$ is single : num 0010010000...
$ is married: num 1101101111...
Exploratory Data Analysis
par(mfrow=c(3,2), las=0)
plot(newbank_data$housing, newbank_data$y, xlab="Housing" , ylab="Become")
plot(newbank_data$contact, newbank_data$y, xlab="Contact type" , ylab="Become
plot(newbank_data$education, newbank_data$y, xlab="Contact type", ylab="Become
plot(newbank_data$age, newbank_data$y, xlab="Contact type" , ylab="Become
customer?" , col=c("darkgreen","red"))
boxplot(duration ~ y, data = newbank_data, col="orange")
boxplot(pdays ~ y, data = newbank_data, col="blue")
```



We can see few insights:

- having no house gives a better chance to become a new customer
- telephone and mobile contact increase the chance to get a new customer
- being educate (tertiary) gives more chance to become a new customer
- boxplots shown many outliers

... no great confidence

Model building

```
library(caret)
inTrain <- createDataPartition(y=newbank_data$y, p=0.7, list=FALSE)
training_data <- newbank_data[inTrain,]
testing_data <- newbank_data[-inTrain,]
dim(training_data); dim(testing_data)</pre>
```

3165 13 1356 13

table(training_data\$y);table(testing_data\$y);

no yes no yes 2800 365 1200 156

Radom Forest model

```
# Random forest
# ref. https://www.rdocumentation.org/packages/randomForest/versions/4.6-
14/topics/randomForest
# see example with 'iris' data set
library(randomForest)
model <- randomForest( y ~ . , data=training_data)
print(model)</pre>
```

randomForest(formula = y ~ . , data = training_data)

Type of random forest: classification

Number of trees: 500

No. of variables tried at each split: 3
OOB estimate of error rate: 10.49%

Confusion matrix: no yes class.error

no 2719 81 0.02892857 (2%) yes 251 114 0.68767123 (68%)

If the client is already a customer, then it's difficult to know if he will remains... (68% errors)

```
ref. https://www.rdocumentation.org/packages/randomForest/versions/4.6-
14/topics/importance
# Extract Variable Importance Measure - extractor function for variable
importance measures as
importance(model)
round(importance(model),2)
```

MeanDecreaseGini

age	25.94
job	61.40
education	25.79
housing	<u> 18.35</u>
loan	9.02
<mark>contact</mark>	17.95
duration	220.49
pdays	49.97
previous	27.49
is_divorced	7.49
is_single	8.10
is_married	<u> 10.83</u>

Testing

Now let us predict the class for each sample in the test data. Then compare the prediction with the actual value of the class.

Radom Forest test

```
predicted <- predict(model, testing_data)</pre>
str(predicted)
table(predicted)
cm <- confusionMatrix(predicted, testing_data$y)</pre>
print(cm)
cm$byClass
cm$overall
cm$positive
cm$table
```

predicted no yes 1272 84

confusionMatrix(predicted, testing_data\$y)

Reference - Prediction no no 1162 **110**

yes 38 46

Accuracy: 0.8909 95% CI: (0.873, 0.907) No Information Rate: 0.885 P-Value [Acc > NIR] : 0.2638

Kappa: 0.3293

Mcnemar's Test P-Value: 5.342e-09

Sensitivity: 0.9683 Specificity: 0.2949 Pos Pred Value: 0.9135 Neg Pred Value: 0.5476 Prevalence: 0.8850 Detection Rate: 0.8569 Detection Prevalence: 0.9381 Balanced Accuracy: 0.6316

'Positive' Class: no

It's still difficult to predict the YES because in our data set the proportion of the No is much higher than the Yes :

table(training_data\$y);table(testing_data\$y);

no yes no yes 2800 365 1200 156

Inspite of the correlations being not so high, the accuracy is high because of the combined effect of predictors as well as the power of building multiple trees.

cm\$overali

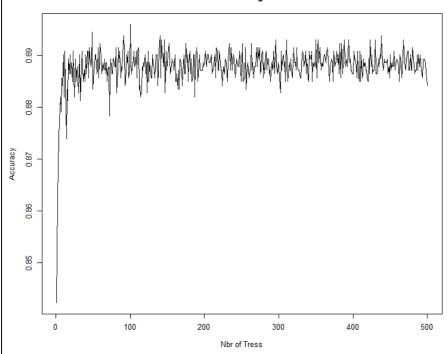
 Accuracy
 Kappa
 AccuracyLower
 AccuracyUpper
 AccuracyNull
 AccuracyPValue
 McnemarPValue

 8.901180e-01
 3.271390e-01
 8.722508e-01
 9.062734e-01
 8.849558e-01
 2.926765e-01
 9.772923e-09

Effect of increasing tree count

Let us try to build different number of trees and see the effect of that on the accuracy of the prediction

Effect of increasing tree size



Conclusions

Random forests provide better accuracy than plain decision trees because of the power of the number of trees built. The example shows that as we increase the number of trees, accuracy also increases. But that comes at a cost of increased time and resource usage.

K Means Clustering - Overview

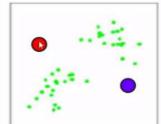
- Unsupervised Learning technique
- Popular method for grouping data into subsets based on the similarity
- Partitions n observations with m variables into k clusters where by each observation belongs to only one cluster
- · How it works
 - · An m dimensional space is created
 - Each observation is plotted based on this space based on the variable values
 - Clustering is done by measuring the distance between points and grouping them
- Multiple types of distance measures available like Euclidian distance and Manhattan distance

Ref. <u>https://fr.wikipedia.org/wiki/K-moyennes</u>, <u>https://dataanalyticspost.com/Lexique/k-means-ou-k-moyennes/...</u> http://mathlasup5.fr/docs/manhattan.pdf

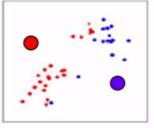
K Means Clustering – Stages



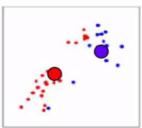
- Dataset contains only m=2 variables. We will create k=2 clusters
- Plot observations on a two dimensional plot



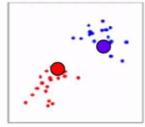
- Choose k=2 centroids at random
- Measure the distance between each observation to each centroid



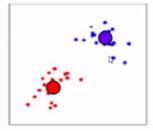
- Assign each observation to the nearest centroid
- This forms the clusters for round 1



- Find the centroid of each of the cluster
- Centroid is the point where the sum of distances between the centroid and each point is minimum



 Repeat the process of finding the distance between each observation to each centroid (the new one) and reassign each point to the nearest one



- Find the centroid for the new clusters
- Repeat the process until the centroids don't move

Iteration => convergence (stable)

K Means Clustering - Summary

Advantages

- Fast
- Efficient with large number of variables
- Explainable

Shortcomings

- The initial centroid position has influence on clusters • General grouping formed

Used in

- K needs to be known
 Preliminary grouping of data before other classification

 - Geographical clustering

14. R Use Case: K Means Clustering 16:24

K Means Clustering - Auto data

Problem Statement

The input data contains samples of cars and technical / price information about them. The goal of this problem is to group these cars into 4 clusters based on their attributes

Techniques Used

- 1. K-Means Clustering
- 2. Centering and Scaling

Data Engineering & Analysis

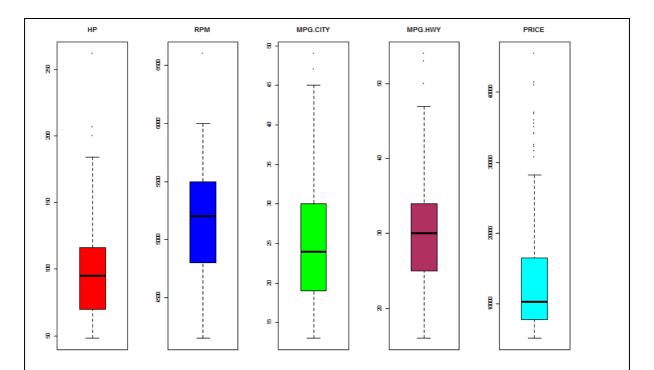
Loading and understanding the dataset

```
car_data <- read.csv("auto-data.csv", as.is=FALSE)</pre>
str(car_data)
head(car_data)
summary(car_data)
head(car_data)
  MAKE FUELTYPE ASPIRE DOORS BODY DRIVE CYLINDERS HP RPM MPG.CITY MPG.HWY PRICE
1 subaru gas std two hatchback fwd four 69 4900 31 36
                                                                 5118
2 chevrolet gas
              std two hatchback fwd three 48 5100 47
                                                                  5151
```

Exploratory Data Analysis

Typically, for Clustering problems, EDA is only required for finding out outliers and errors. If outliers are found, we would want to eliminate them since they might skew the clusters formed by moving the centeroids signficantly.

```
par(mfrow=c(1,5))
boxplot(x = car_data$HP, col = "red", main = "HP")
boxplot(x = car_data$RPM, col = "blue", main = "RPM")
boxplot(x = car_data$MPG.CITY, col = "green", main = "MPG.CITY")
boxplot(x = car_data$MPG.HWY, col = "maroon", main = "MPG.HWY")
boxplot(x = car_data$PRICE, col = "cyan", main = "PRICE")
```



We choose not to remove the outliers (dots in the charts) since they are many (hence may not be outliers

Modeling & prediction

Build Clusters for 2 variables

In order to demonstrate the clusters being formed on a 2-dimensional plot, we will only use 100 samples and 2 attributes - HP and PRICE to create 4 clusters.

```
# classification - https://cran.r-
library(class)
project.org/web/packages/class/class.pdf
set.seed(11111) # to generate the same random (here with ID=11111)
car_subset <- car_data[1:100, c(8,12)] # 100 rows , 2 dim. { #HP ~ PRICE }</pre>
car_subset
```

```
ar_subset
 HP PRICE
 69 5118
  48 5151
 68 5195
```

```
car_clusters <- kmeans(car_subset, 4) # 4 clusters</pre>
car_clusters
```

K-means clustering with 4 clusters of sizes 20, 15, 29, 36

Cluster means:

HP **PRICE** 1 88.05000 8821.600

2 96.60000 9984.667

3 67.24138 6163.690

4 74.00000 7596.083

Clustering vector:

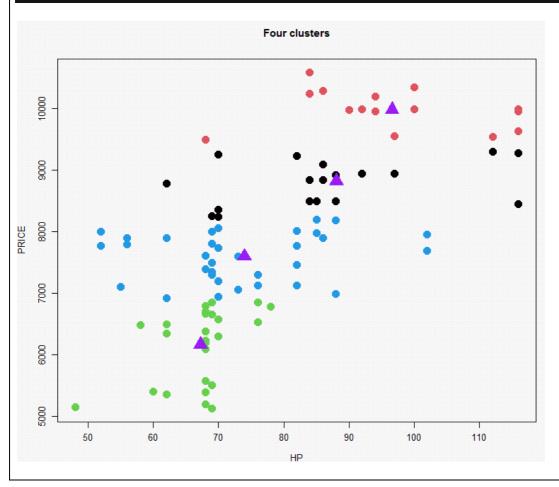
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3

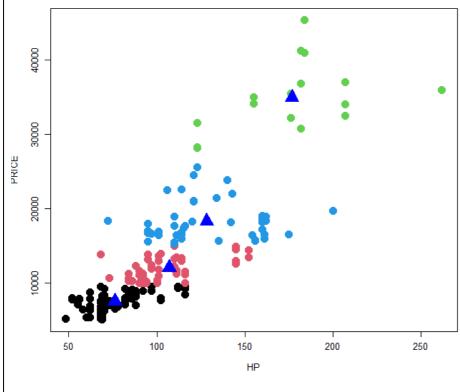
21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40

41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60

```
61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80
81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100
Within cluster sum of squares by cluster:
                                 (between_SS / total_SS = 90.2 %)
[1] 2479534 1464655 9728274 5071069
Available components:
[1] "cluster" "centers"
                     "totss"
                              "withinss" "tot.withinss"
[6] "betweenss" "size"
                      "iter"
                              "ifault"
                     # classification - https://cran.r-
set.seed(11111) # to generate the same random (here with ID=11111)
car_subset <- car_data[1:100, c(8,12)] # 100 rows , 2 dim. { #HP ~ PRICE
car_subset
car_clusters <- kmeans(car_subset, 4) # 4 clusters</pre>
car_clusters; car_clusters$centers; car_clusters$cluster
# plot - https://www.datamentor.io/r-programming/plot-function/
par(mfrow=c(1,1), cex=1, mai=c(1,1,1,1))
plot(car_subset$HP, car_subset$PRICE, col=car_clusters$cluster,pch=20,
cex=3, xlab="HP", ylab="PRICE", main="Four clusters")
points(car_clusters$centers, col="purple", pch=17, cex=3)
# legend("topleft", c(1:4), fill=c("green", "blue", "black", "red"))
```

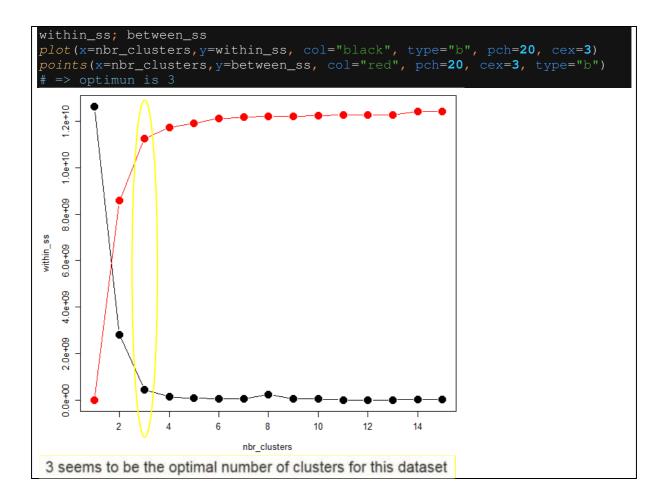


Clustering for all the data Data transformation (from factors to numeric) car data2 <- car data for (columns in 1:8) { car_data2[,columns] <- as.numeric(car_data[,columns])</pre> car_data[1:3,]; car_data2[1:3,] MAKE FUELTYPE ASPIRE DOORS BODY DRIVE CYLINDERS HP RPM MPG.CITY MPG.HWY PRICE two hatchback four 69 4900 subaru gas fwd 36 5118 chevrolet two hatchback fwd three 48 5100 53 5151 gas 30 31 5195 mazda std two hatchback fwd four 68 5000 gas MAKE FUELTYPE ASPIRE DOORS BODY DRIVE CYLINDERS HP RPM MPG.CITY MPG.HWY PRICE 36 5118 18 3 69 4900 31 5 48 5100 53 5151 dim(car_data2) # 197 12 # to generate the same random (here with ID=11111) set.seed(11111) car_clusters2 <- kmeans(car_data2, 4) # 4 clusters</pre> car_clusters2\$centers car_clusters2\$centers[,c(8,12)] par(mfrow=c(1,1), cex=1, mai=c(1,1,1,1)) plot(car_data2\$HP, car_data2\$PRICE, col=car_clusters2\$cluster, pch=20, cex=3, xlab="HP", ylab="PRICE", main="Four clusters on all data") #points - https://www.math.ucla.edu/~anderson/rw1001/library/base/html/points.html points(car_clusters2\$centers[,c(8,12)], col="blue", pch=17, cex=3) Four clusters on all data 0000 30000



K-means clustering with 4 clusters of sizes 89, 47, 16, 45 Cluster means: MAKE FUELTYPE ASPIRE DOORS BODY DRIVE CYLINDERS HP RPM MPG.CITY 1 13.20225 1.932584 1.056180 1.471910 3.617978 2.022472 3.022472 76.04494 5157.865 30.17978 2 14.10638 1.914894 1.255319 1.425532 3.574468 2.276596 3.297872 107.17021 5094.681 22.91489 3 9.43750 1.812500 1.187500 1.500000 3.187500 3.000000 3.000000 176.75000 4996.875 16.68750 4 12.51111 1.866667 1.333333 1.333333 3.777778 2.800000 3.244444 128.37778 5106.667 20.55556 Clustering vector: [185] 3 3 3 3 3 3 3 3 3 3 3 3 3 Within cluster sum of squares by cluster: [1] 140048031 115551241 334439368 302547347 (between_SS / total_SS = 92.9 %) Available components: [1] "cluster" "centers" "totss" "withinss" "tot.withinss" "betweenss" "size" "iter" "ifault" Finding optimum number of clusters wssplot <- function(data, nc=15, seed=1234){ wss <- (nrow(data)-1)*sum(apply(data,2,var)) for (i in 2:nc){ set.seed(seed) wss[i] <- sum(kmeans(data, centers=i)\$withinss)}</pre> plot(1:nc, wss, type="b", xlab="Number of Clusters", ylab="Within groups sum of squares", col="red")} wssplot(auto_data) Within groups sum of squares 9009 4000 2000 8 14 10 12 Number of Clusters 3 seems to be the optimal number of clusters for this dataset set.seed(**11111**) within_ss <- c(); between_ss <- c(); nbr_clusters <- 1:15 for (i in nbr_cluster_range) { cluster_i <- kmeans(car_data2, i)</pre>

within_ss[i] <- cluster_i\$withinss
between_ss[i] <- cluster_i\$betweenss</pre>



15. Association Rules Mining

11:30

Association Rules Mining - Overview of ARM

- ARM shows how frequently sets of items occur together
 - · Find Items frequently brought together
 - Find fraudulent transactions.
 - Frequent Pattern Mining/ Exploratory Data Analysis
 - · Finding the next word
- One of the clustering techniques
- Assumes all data are categorical not applicable for numeric data
- Helps generate association rules that can be then used for business purposes like stocking aisles.

Association Rules Mining – Datasets

- Market basket transactions
 - Tran 1 { bread, cheese, milk}
 - Tran 2 { apple, eggs, yogurt}
 - Tran 3 {bread, eggs}
- Text document data set (bag of words)
 - Doc 1 { cricket, sachin, India }
 - Doc 2 { soccer, messi, Barcelona}
 - Doc 3 { sachin, messi, superstars}

Association Rules Mining – Measures

- Let N be the number of transactions
- Let X, Y and Z be individual items
- Support measures how frequently an combination of items occurs in the transactions
 - Support(X) = count(transactions with X)/ N
 - Support(X,Y)= count(transactions with X and Y)/N
- Confidence measures the expected probability that Y would occur when X occurs
 - Confidence(X -> Y) = support(X,Y) / support(X)
- Lift measures how many more times X and Y occurs together than expected
 - Lift(X -> Y) = confidence(X->Y) / support(Y)

Association Rules Mining – Rules and goals

- A rule specifies when one item occurs the other too occurs
 - When bread is brought, milk is brought 33% of the time.
 - When India occurs in the bag of words, sachin occurs 20% of the time.
- Goal is to find all rules that satisfy the user specified minimum support and minimum confidence
- A frequent itemset is an itemset whose support is > the minimum support level specified.
- Apriori algorithm is the most popular ARM algorithm

16. R Use Case: Association Rules Mi... 13:11

Association Rules Mining – Accident conditions

Problem Statement

The input dataset contains information about 1000 fatal accidents. It has different feature variables associated with the accident. The goal is to find patterns in the variables - which accident conditions frequently occur together.

Techniques Used

- 1. Association Rules Mining
- 2. Converting Feature data into Basket Data

Data Engineering & Analysis

Loading and understanding the dataset

```
accident_data <- read.csv("accidents.csv")
str(accident_data); dim(accident_data) # 1000 obs. of 16 variables
accident_data[1:5,]</pre>
```

summary(accident_data)

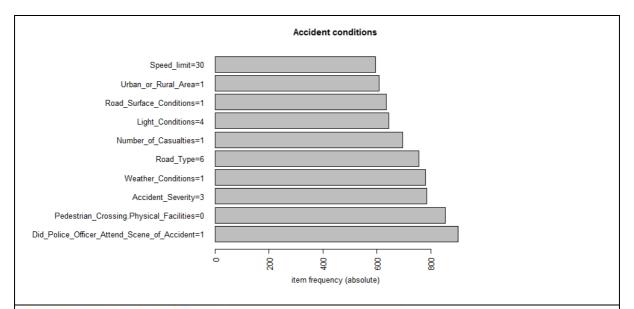
□ 1000 obs. of 16 variables

Data Transformation

The data frame needs to be converted into a Basket form to be loaded by the arules dataset. The following custom code does it.

```
colnames <- names(accident_data)
str(colnames); length(colnames)
# In a basket, every row represents a transaction (Id,<K=V>, ...)
# paste - ref. https://www.math.ucla.edu/~anderson/rw1001/library/base/html/paste.html
# char - ref. https://stat.ethz.ch/R-manual/R-devel/library/base/html/nchar.html
```

```
basket <- list()
 for (n in 1:nrow(accident_data)) {
 kv <- pasteO(n, SEP=",")
 for (c in 2:ncol(accident_data)) { # without column n°2
  transaction <- pasteO(colnames[c], sep = "=", accident_data[n,c], collapse = NULL)
  kv <- pasteO(kv, transaction, SEP=",")
 basket[n] <- substr(kv, 1, nchar(kv) - 1)
write(as.character(basket), "accidents basket.csv")
 ■ Project ▼ ② ★ □ □ association_rules_mining.R × □ accidents_basket.csv ×
     AppliedDataScience_5 C:\User
                             Plugins supporting *.csv files found.
        accidents.csv
                              Data importer supporting *.csv files found
        accidents_basket.csv
                                      1, Police_Force=1, Accident_Severity=3, Number_of_Vehicles=3, Number_
        association_rules_mining.R
                                      2, Police_Force=1, Accident_Severity=3, Number_of_Vehicles=1, Number_
        auto-data.csv
                                      3,Police_Force=1,Accident_Severity=3,Number_of_Vehicles=2,Number
        auto-miles-per-gallon.csv
                                      4, Police_Force=1, Accident_Severity=3, Number_of_Vehicles=2, Number_
        bank.csv
                                      5, Police_Force=1, Accident_Severity=3, Number_of_Vehicles=1, Number_
        @ Billard.R
Exploratory Data Analysis
Typically, for Clustering problems, EDA is only required for finding out outliers and errors. If outliers are
found, we would want to eliminate them since they might skew the clusters formed by moving the
centeroids signficantly.
# arules - ref. https://www.rdocumentation.org/packages/arules/versions/1.6-6
          https://www.rdocumentation.org/packages/arules/versions/1.6-6/topics/read.transactions
library(arules) # load "Mining Association Rules and Frequent Itemsets"
accidents <- read.transactions("accidents basket.csv", format = "basket", sep=",")
summary(accidents)
transactions as itemMatrix in sparse format with
1000 rows (elements/itemsets/transactions) and
1452 columns (items) and a density of 0.01101928
most frequent items (TOP 5):
Did_Police_Officer_Attend_Scene_of_Accident=1 902
Pedestrian_Crossing.Physical_Facilities=0
                                          854
Accident_Severity=3
                                          786
Weather_Conditions=1
                                          781
Road_Type=6
                                         755
(Other)
                                        11922
element (itemset/transaction) length distribution: sizes 16 / 1000
 Min. 1st Qu. Median Mean 3rd Qu. Max.
 16 16
           16
                    16 16
includes extended item information - examples:
labels 1 1 / 2 10 / 3 100
itemFrequencyPlot(accidents, type = "absolute", topN = 10, popCol = "green",
popLwd = 1,
cex.names=graphics::par("cex.axis"),
                         main = "Accident conditions")
```



Modeling & Prediction

```
We discover the frequently occuring patterns with arules.
rules <- apriori(accidents, parameter=list(supp=0.1, conf = 0.3))</pre>
Apriori - Parameter specification:
confidence minval smax arem aval
                                     originalSupport maxtime support minlen maxlen target ext
         0.1 1 none FALSE TRUE
                                                           0.1
                                                                  1
                                                                          10
                                                                                 rules TRUE
    0.3
Algorithmic control:
Filter tree heap memopt load sort verbose
 0.1 TRUE TRUE FALSE
                          TRUE 2
Absolute minimum support count: 100
set item appearances ...[0 item(s)] done [0.00s].
set transactions ...[1452 item(s), 1000 transaction(s)] done [0.02s].
sorting and recoding items ... [29 item(s)] done [0.00s].
creating transaction tree ... done [0.00s].
checking subsets of size 1 2 3 4 5 6 7 8 9 done [0.00s].
writing ... [21772 rule(s)] done [0.02s].
creating S4 object ... done [0.01s].
6/topics/apriori
class(rules) # arules
length(rules) # set of 21772 rules
inspect(rules[1:40])
                                rhs
                                                                         support confidence lift
     Ths
 ## 21 {Weather_Conditions=2} => {Road_Surface_Conditions=2}
                                                                         0.124 0.9841 2.9822
```

```
# Example also here : http://r-statistics.co/Association-Mining-With-
R.html
XXX item was purchased,
rules_conf <- sort (rules, by="confidence", decreasing=TRUE) # 'high-
inspect(head(rules_conf))
and YYY are 18 times more likely to be purchased together compared to the
purchases when they are assumed to be unrelated.
rules_lift <- sort (rules, by="lift", decreasing=TRUE) # 'high-lift'
inspect(head(rules_lift)) # show the support, lift and confidence for all
  inspect(head(rules_conf))
   lhs
                                       rhs
                                                                       support confidence coverage
                                                                                            lift coun
[1] {Junction_Detail=0,
    Number_of_Casualties=2}
                                     => {Pedestrian_Crossing.Physical_Facilities=0} 0.108
                                                                                      0.108 1.17096
                                                                                                 10
[2] {Did_Police_Officer_Attend_Scene_of_Accident=1,
    Junction_Detail=0,
                                                                                      0.100 1.17096
    Number_of_Casualties=2}
                                     => {Pedestrian_Crossing.Physical_Facilities=0} 0.100
   nspect(head(rules_lift))  # show the support, lift and confidence for
   lhs
                                                          support confidence coverage
                                                                                    lift count
                                            rhs
[1] {Light_Conditions=6,
    Road_Type=6,
    Urban_or_Rural_Area=2,
                                          => {Speed_limit=60} 0.118 0.8939394
                                                                           0.132 3.990801
    Weather_Conditions=1}
```

Artifical Neural Networks (ANN) - Overview

- Biologically inspired by how the human brain works.
- A Black box algorithm (a full explanation would require few hours and mathematical prerequisites)
- Used in artificial intelligence domain and of late for machine learning
- Helps discover complex correlations hidden in the data similar to the human brain
- Works well on noisy data and where the relationships between variables is vaguely understood.
- Fast prediction
- Very slow training and easy to over fit

Ref. ANN - https://fr.wikipedia.org/wiki/R%C3%A9seau de neurones artificiels https://en.wikipedia.org/wiki/Artificial neural network

Support Vector Machines (SVM) - Overview

- A Black box method for machine learning inner workings are complex, tricky and difficult to understand.
- One of the kernel methods.
- Algorithm based on vector geometry and statistical learning theory
- Can model highly complex relationships very popular in pattern recognition (face recognition, text recognition etc.)
- Successful applications in many fields like bioinformatics, image recognition etc.
- Used for both classification and regression (discrete and continuous outcomes).

Ref. SVM - https://fr.wikipedia.org/wiki/Machine %C3%A0 vecteurs de support https://en.wikipedia.org/wiki/Support vector machine

No use case... out of scope (too big) topic ...

Bagging = Bootstrap Aggregating - Overview

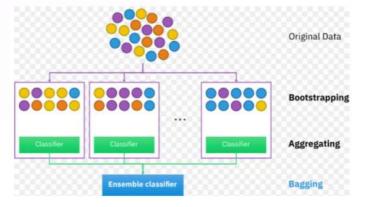
- Bootstrap Aggregating / Ensemble method
- Uses a base classifier <u>Decision trees</u> to train on multiple sample sets and to generate multiple models
- Prediction is done using each model and the most occurring result across all models is selected.
- For each training round a different bootstrap replicate dataset is constructed based on the original dataset.
 - If the original dataset has m examples, then n rounds of sampling is done to get m/n examples each
 - The n samples sets are then added up to for a dataset of m size
 - Examples could be duplicated in the sample sets or might not occur at all.

Bootstrap aggregating, also called **bagging** (from **b**ootstrap **aggregating**), is a <u>machine learning</u> <u>ensemble meta-algorithm</u> designed to improve the stability and accuracy of <u>machine learning</u> algorithms used in <u>statistical classification</u> and <u>regression</u>. It also <u>reduces variance</u> and helps to avoid <u>overfitting</u>. Although it is usually applied to decision tree methods, it can be used with any type of method.

Ref. https://en.wikipedia.org/wiki/Bootstrap_aggregating

Bagging – How it works

- Suppose we want to run training 5 times on a dataset that has 8 records (Record ID 1:8).
- For each round, we do 2 sets of sampling with replacement to build the bootstrap aggregate.
- Training round 1:
 - sample 1: 1,4,5,7
 - sample 2: 2,4,6,7
 - bootstrap replicate: 1,2,4,4,5,6,7,7
- Training round 2:
 - sample 1: 2,3,5,6
 - sample 2:1,2,6,8
 - bootstrap replicate: 1,2,2,3,5,6,6,8



Bagging – Remarks

- May produce improved results than the base classifier if the base classifier produces unstable results.
- High resource requirements and takes longer times to build models
- Various models available difference is the base classifier used (some examples)
 - adaBag
 - Bagged CART
 - Bagged Flexible Discriminant Analysis
 - · Bagged Logic Regression
 - · Model Averaged Neural Network

Boosting – Overview

- · Ensemble method like bagging
- · Creates multiple models.
- Prediction done on multiple models and results aggregated to deliver the final prediction
- Different samples (records /observations) getadifferent weights during learning for each of the training rounds
- Weight determined based on misclassification during previous round.

In <u>machine learning</u>, **boosting** is an <u>ensemble meta-algorithm</u> for primarily <u>reducing bias</u>. and also variance in <u>supervised learning</u>, and a family of machine learning algorithms that convert weak learners to strong ones.

Ref. https://en.wikipedia.org/wiki/Boosting (machine learning)

Boosting – How it works

- Multiple rounds of training. Weights of all records equal for the first round
- · For each model building round
 - Build the model
 - Predict on the same training set using the model
 - · Find misclassified records
 - · Increase weights of misclassified records
 - · Repeat model building
- Results in multiple models
- Predictions done using each model. Results aggregated.



Boosting – Remarks

- High resource requirements and takes longer times to build models
- Use a set of weak learners to create a strong learner
- Reduces bias
- Different algorithms available
 - Boosted Classification Trees
 - Boosted Generalized Additive Model
 - · Boosted Generalized Linear Model

Dimensionality Reduction - Overview

Reduce issues when too many predictors...

- Memory requirements
- CPU requirements / time taken for machine learning algorithms
- Correlation between predictors
- · Over fitting
- Some ML algorithms don't work fine with too many predictors

Dimensionality Reduction - How to do

1) Manual selection

- Using domain knowledge
 - · Purely based on hypothesis
 - Risky there could be unknown correlations
- Using Correlation co-efficients
 - Variables with good correlation can only be picked up.
- Using Decision Trees
 - Decision trees are fast and choose variables based on correlation
 - Variables used in the decision trees can be picked for further processing

2) Principal Component Analysis (PCA)

- Used to reduce the number of predictors
- Based on Eigen Vectors and Eigen Values
- Given a set of M predictors, PCA transforms this to a set of N predictors such that N < M
- The new predictors are derived predictors called PC1, PC2, PC3
- The new predictors retain similar levels of correlation and predictability like the original predictors

Ref. <u>https://fr.wikipedia.org/wiki/Analyse_en_composantes_principales_https://en.wikipedia.org/wiki/Principal_component_analysis_https://en.wiki/Principal_component_analysis_https://en.wiki/Principal_component_analysis_https://en.wiki/Principal_component_analysis_https://en.wiki/Principal_component_analysis_https://en.wiki/Principal_component_analysis_https://en.wiki/Principal_component_analysis_https://en.wiki/Principal_component_analysis_https://en.wiki/Principal_component_analysis_https://en.wiki/Principal_component_analysis_https://en.wiki/Principal_component_analysis_https://en.wiki/Principal_component_analysis_https://en.wiki/Principal_component_analysis_https://en.wiki/Principal_component_analysis_https://en.wiki/Principal_compone</u>

20. R Use Case: Advanced Methods 17:18

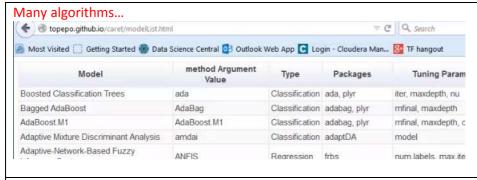
The Caret package - overview

Classification And REgression Training package is a set of functions that attempt to streamline the process for creating predictive models. It contains tools for:

- 1. data splitting
- 2. pre-processing
- 3. feature selection
- 4. model tuning using resampling
- 5. variable importance estimation

There are many different modelling functions in R. Some have different syntax for model training and/or prediction. The package started off as a way to provide a uniform interface the functions themselves, as well as a way to standardize common tasks (such parameter tuning and variable importance).

Ref. http://topepo.github.io/caret/index.html https://github.com/topepo



Breast cancer – predict disease

Problem Statement

The dataset contains diagnosis data about breast cancer patients and whether they are Benign (healthy) or Malignant (possible disease). We need to predict whether new patients are benign or malignant based on model built on this data

Techniques Used

- 1. Principal Component Analysis
- 2. Training and Testing
- 3. Confusion Matrix
- 4 Neural Networks
- 5. Support Vector Machines
- 6. Bagging
- 7. Boosting

Use the caret package to build models for all the datasets provided in the use cases. Use the same algorithm used in the example use case, but with the caret package. Compare the results between the caret package and the output seen in the use cases.

Data Engineering & Analysis

Loading and understanding the dataset

```
cancer_data <- read.csv("breast_cancer.csv")</pre>
cancer_data[1:5,] # breast cancer data frame
  cancer_data[1:5,] # breast cancer data frame
       id diagnosis radius_mean texture_mean perimeter_mean
                               12.39
1 87139402
                     12.32
                                             78.85
              В
  8910251
                В
                       10.60
                                  18.95
                                               69.28
   905520
                В
                       11.04
                                  16.83
                                               70.92
dim(cancer_data)
                          # 569 rows, 32 columns
str(cancer_data)
       many variables (#31)
  str(cancer_data)
 'data.frame': 569 obs. of 32 variables:
                : int 87139402 8910251 905520 868871 9012568 906539 925291 87880 862989 89827 .
 $ id
 $ diagnosis
                : chr "B" "B" "B" "B" ...
: num 12.3 10.6 11 11.3 15.2 ...
 $ radius_mean
 $ texture_mean : num 12.4 18.9 16.8 13.4 13.2 ...
 $ perimeter_mean : num 78.8 69.3 70.9 73 97.7 ...
```

Exploratory Data Analysis Correlation – split into 3 sets (2 ~ 3:10 / 11:21 / 22:32) *library*(psych) pairs.panels(cancer_data[,c(2,3:10)]) # scatter plot of matrices (SPLOM) pairs.panels(cancer_data[,c(2,10:20)]) pairs.panels(cancer_data[,c(2,21:32)]) 10 0.0 0.1 0.2 0.3 0.4 10 15 20 25 100 150 0.06 0.10 0.14 0.73 0.74 0.71 0.36 0.70 0.78 0.42 0.60 0.32 1.00 0.99 0.17 0.51 0.68 0.82 0.32 0.30 0.33 -0.020.24 0.29 0.99 0.56 0.21 0.72 0.85 0.18 0.50 0.69 0.82 0.52 0.55 0.66 0.88 0.83 8 2 0.92 1.0 **Principal Components Analysis (PCA)** https://www.rdocumentation.org/packages/stats/versions/3.6.2/topics/prcomp scale_data <- scale(cancer_data[,3:32])</pre> pca_data <- prcomp(scale_data)</pre> str(pca_data); summary(pca_data) summary(pca data) Importance of components: PC1 PC2 PC3 PC4 PC5 PC6 PC7 PC8 PC9 Standard deviation 3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172 0.69037 0.6457 Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251 0.01589 0.0139 Cumulative Proportion 0.4427 0.6324 0.72636 0.79239 0.84734 0.88759 0.91010 0.92598 0.9399 PC10 PC11 PC12 PC13 PC14 PC15 PC16 PC17 Standard deviation $0.59219 \ 0.5421 \ 0.51104 \ 0.49128 \ 0.39624 \ 0.30681 \ 0.28260 \ 0.24372 \ 0.22939$ Proportion of Variance 0.01169 0.0098 0.00871 0.00805 0.00523 0.00314 0.00266 0.00198 0.00175 Cumulative Proportion 0.95157 0.9614 0.97007 0.97812 0.98335 0.98649 0.98915 0.99113 0.99288 PC19 PC20 PC21 PC22 PC23 PC24 PC25 PC26 PC27 0.22244 0.17652 0.1731 0.16565 0.15602 0.1344 0.12442 0.09043 0.08307 Standard deviation Proportion of Variance 0.00165 0.00104 0.0010 0.00091 0.00081 0.0006 0.00052 0.00027 0.00023 Cumulative Proportion 0.99453 0.99557 0.9966 0.99749 0.99830 0.9989 0.99942 0.99969 0.99992 PC28 PC29 PC30 Standard deviation 0.03987 0.02736 0.01153 Proportion of Variance 0.00005 0.00002 0.00000 With these four (4) first variables, we are covering 79% of the others



The first 3 principal components influences 75% of the target, so we only pick the top 3. A correlation analysis shows that these 3 have very good correlation to the target. Also the 3 PCs don't have any correlation amongst them.

Modelling and predicting library(caret) inTrain <- createDataPartition(y=final_data\$diagnosis, p=0.7, list=FALSE) training_data<- final_data[inTrain,] test_data<- final_data[-inTrain,] dim(training_data); dim(test_data) table(training_data\$diagnosis); table(test_data\$diagnosis) => 399-4 / 170- 4 => table(..._data\$diagnosis): B-M / 250-149 B-M / 107-63

Model Building and Testing

We will build different models based on 4 different algorithms. Then we predict on the test data and measure accuracy. Finally, we compare the algorithms for their accuracy and speed. The "caret" package in R provides a convenient unified interface for using any of the algorithms for modeling and prediction. It has an extensive library of algorithms http://topepo.github.io/caret/modelList.html . This can be used to compare performance of different algorithms for a given dataset.

```
predlist <- c("bagFDA", #Bagging

"LogitBoost", #Boosting

"nnet", #Neural Networks

"svmRadialCost") #Support vector machines</pre>
```

```
algoList <- c("bagFDA", "LogitBoost", "nnet", "svmRadialCost")
results <- data.frame(Algorithm=character(), Duration=numeric(),</pre>
for (i in 1:length(algoList)) {
  algo <- algoList[i]</pre>
  print(paste("Alogrithm:", algo))
  startTime <- as.integer(Sys.time())</pre>
https://www.rdocumentation.org/packages/caret/versions/4.47/topics/train
 model <- train( diagnosis ~ . , data = training_data , method = algo)</pre>
  model
  predicted <- predict(model, test_data)</pre>
  length(predicted); length(test_data$diagnosis)
  comp <- confusionMatrix(predicted, as.factor(test_data$diagnosis))</pre>
  stopTime <- as.integer(Sys.time())</pre>
 result <- c( as.character(algo) , stopTime - startTime ,</pre>
as.numeric(comp$overall[1]) )
  print(result)
  results[i,1] <- as.character(algo)
  results[i,2] <- ( stopTime - startTime )</pre>
  results[i,3] <- round(as.numeric(comp$overall[1]) * 100, 2)</pre>
```

Conclusions

Given that there is one main principal component PC1, most algorithms will perform with excellent accuracy. This example shows how large predictors can be easily compressed using PCA and then used for prediction.

Annex





Terminology

"Predictive modeling" is one of the many names that refers to the process of uncovering relationships within data for predicting some desired outcome.

Since many scientific domains have contributed to this field, there are synonyms for different entities:

- The terms *sample*, *data point*, *observation*, or *instance* refer to a single, independent unit of data, such as a customer, patient, or compound.
- The term *sample* can also refer to a subset of data points, such as the training set sample. The text will clarify the appropriate context when this term is used.
- The *training set* consists of the data used to develop models while the *test* or *validation* sets are used solely for evaluating the performance of a final set of candidate models.
- The *predictors*, *independent variables*, *attributes*, or *descriptors* are the data used as input for the prediction equation.
- *Outcome*, *dependent variable*, *target*, *class*, or *response* refer to the outcome event or quantity that is being predicted.
- *Continuous* data have natural, numeric scales. Blood pressure, the cost of an item, or the number of bathrooms are all continuous. In the last case, the counts cannot be a fractional number, but is still treated as continuous data.
- *Categorical* data, otherwise known as *nominal*, *attribute*, or *discrete* data, take on specific values that have no scale. Credit status ("good" or "bad") or color ("red," "blue," etc.) are examples of these data.
- *Model building, model training*, and *parameter estimation* all refer to the process of using data to determine values of model equations.

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