Introduction to Machine Learning

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Part 1: Theoretical Machine Learning

Machine learning: * Takes knowledge as input * Receives parameter settings * ??? (Magic) * Produces knowledge as output

> A machine learning system is a function L that, given some input knowledge $I \in \mathcal{I}$ and parameter settings $p \in P$, produces an output called a model or hypothesis $O \in \mathcal{O}$:
>
> $$\mathcal{L} : \mathcal{I} \times \mathcal{P} \rightarrow \mathcal{O}$$

BUT FIRST… Get to know your data!

It is bad practice to apply machine learning on a dataset you don't know!

Before Machine Learning

Generally, these are the steps you should take:

1. Get data
2. Clean and/or anonymize data
3. Explore data:
   - What is in it?
   - What is useful? (Any of it? Anonymized beyond recognition?)
   - Does it need more cleaning?
4. Apply statistical methods:
   - What are the trends in your data?
   - What is normal behaviour and what is outlier behaviour?
5. Fit simple models, eg. regression model
6. Finally: **apply machine learning algorithms!**
7. Evaluate, repeat if needed

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Steps 1-2: Getting and Cleaning Data

Often, *useful* data is hard to come by * **Option 1:** work with what you have * Problem: garbage in, garbage out * **Option 2:** get better data * Problem: not always possible *** =left Maybe, we can salvage something from the provided dataset: * Data manipulation - [**R package**] **dplyr** * Data grouping and chaining - [**R package**] **dplyr** * Tidying data - [**R package**] **tidyr** * Assemble dates and times - [**R package**] **lubridate**

*** =right

```
<img height='10' src='R.png' />
```

— &twocoltopbottom8020 ## R Package: dplyr *** =left * Data manipulation: * *select():* take out some columns * *filter():* take out some rows * *arrange():* order rows by column value * *mutate():* create column from other column value * *summarize():* collapse data using a function, eg. mean() *** =right

```
<img height='300' src='dplyr.png' />
```

*** =bottom * Data grouping and chaining: * *group_by():* break dataset into groups based on column value * *summarize()* on data grouped by *group_by()* * *%>%*: chaining operator to chain execution of dplyr commands

---

Data Manipulation with dplyr: *select()* Example

Example dataset (R package download logs from CRAN for 1 day, ± 225,000 rows):

```
##   X       date     time   size r_version r_arch      r_os   package version country ip_i
## 1 1 2014-07-08 00:54:41  80589     3.1.0 x86_64   mingw32 htmltools   0.2.4      US     1
## 2 2 2014-07-08 00:59:53 321767     3.1.0 x86_64   mingw32   tseries 0.10-32      US     2
## 3 3 2014-07-08 00:47:13 748063     3.1.0 x86_64 linux-gnu     party  1.0-15      US     3
```

- Load into dplyr, *select()* some of the columns we're interested in:

```
cranShort <- select(cran, size:version) # Select columns size through version
```

```
##     size r_version r_arch      r_os   package version
## 1  80589     3.1.0 x86_64   mingw32 htmltools   0.2.4
## 2 321767     3.1.0 x86_64   mingw32   tseries 0.10-32
## 3 748063     3.1.0 x86_64 linux-gnu     party  1.0-15
## 4 606104     3.1.0 x86_64 linux-gnu     Hmisc  3.14-4
```

Data Manipulation with dplyr: *filter()* Example

- *filter()* is like *select()*, but it takes rows instead of columns
- Let's take the rows for the *'dplyr'* package downloads:

```
filter(cranShort, package =='dplyr') # Retain only rows for package dplyr
```

```
##     size r_version r_arch        r_os package version
## 1 591176     3.0.3 x86_64     mingw32   dplyr     0.2
## 2 591176     3.1.0 x86_64   linux-gnu   dplyr     0.2
## 3 591178     3.1.0 x86_64     mingw32   dplyr     0.2
## 4 591179     3.1.0   i386     mingw32   dplyr     0.2
## 5 591176     3.0.2 x86_64   linux-gnu   dplyr     0.2
## 6 591178     3.0.2 x86_64 darwin10.8.0  dplyr     0.2
```

- Useful *filter()* trick: remove rows with NA's (= missing values):

```
filter(cranShort, !is.na(r_version)) # Filters out rows where r_version is NA
```

Data Manipulation with dplyr: *arrange()* Example

- Order rows of a dataset by column value: *arrange()*
- Let's use it to order the data by package size:

```
arrange(cranShort, size) # Order dataset by size column
```

```
##   size r_version r_arch r_os package version
## 1  512      <NA>   <NA> <NA> ellipse   0.3-8
## 2  513      <NA>   <NA> <NA>   class  7.3-10
```

- The same in descending order:

```
arrange(cranShort, desc(size)) # Order dataset by size column
```

```
##       size r_version r_arch    r_os               package version
## 1 62559635     3.0.3 x86_64 mingw32 ChemometricsWithRData   0.1.3
## 2 62559246     3.0.3 x86_64 mingw32 ChemometricsWithRData   0.1.3
## 3 62553483     3.1.0   i386 mingw32 ChemometricsWithRData   0.1.3
```

Data Manipulation with dplyr: *mutate()* Example

- Create new columns out of (combinations of) other columns: *mutate()*
- Eg. convert size column, now in bytes, to megabytes and gigabytes:

```
# Create column of size in MB and GB
mutate(cranShort, size_mb = size / 2^20, size_gb = size_mb / 2^10)
```

```
##     size r_version r_arch      r_os     package version    size_mb      size_gb
## 1  80589     3.1.0 x86_64   mingw32   htmltools   0.2.4 0.07685566 7.505435e-05
## 2 321767     3.1.0 x86_64   mingw32     tseries 0.10-32 0.30686092 2.996689e-04
## 3 748063     3.1.0 x86_64 linux-gnu       party  1.0-15 0.71340847 6.966880e-04
## 4 606104     3.1.0 x86_64 linux-gnu       Hmisc  3.14-4 0.57802582 5.644783e-04
## 5  79825     3.0.2 x86_64 linux-gnu      digest   0.6.4 0.07612705 7.434282e-05
## 6  77681     3.1.0 x86_64 linux-gnu randomForest   4.6-7 0.07408237 7.234607e-05
## 7 393754     3.1.0 x86_64 linux-gnu        plyr   1.8.1 0.37551308 3.667120e-04
```

Data Manipulation with dplyr: *summarize()* Example

- *summarize()* can be used to collapse the dataset using a function
- Let's do this using the mean package size:

```
summarize(cran, avg_bytes = mean(size)) # Show the mean of the size column
```

```
##   avg_bytes
## 1  844086.5
```

- Not very interesting ... yet

Data Grouping with dplyr: *group_by()* Example

- Break the dataset into groups based on column value: *group_by()*
- Eg. grouping on the *'package'* column:

```
group_by(cranShort, package)
```

```
## Source: local data frame [3 x 6]
## Groups: package [3]
##
##     size r_version r_arch      r_os   package version
##    (int)     (chr)  (chr)     (chr)     (chr)   (chr)
## 1  80589     3.1.0 x86_64   mingw32 htmltools   0.2.4
## 2 321767     3.1.0 x86_64   mingw32   tseries 0.10-32
## 3 748063     3.1.0 x86_64 linux-gnu     party  1.0-15
```

- 'Groups: package' implies a grouping by package occurred, all else is unchanged
- **Any operation we apply to the grouped data will take place on a per package basis!**

Data Grouping with dplyr: *summarize()* Example

- Any operation applied to grouped data takes place on a per group basis
- Let's try *summarize()* again, but on grouped data:

```
summarize(group_by(cranShort, package), avg_bytes = mean(size))
```

```
##       package  avg_bytes
## 1          A3   62194.96
## 2         abc 4826665.00
## 3    abcdeFBA  455979.87
## 4 ABCExtremes   22904.33
## 5     ABCoptim   17807.25
## 6       ABCp2   30473.33
```

Instead of a single value, *summarize()* now returned the mean size for each package!

Data Chaining with dplyr: Chaining Operator *%>%*

- Chaining operator is syntactic sugar - no added value apart from cleaner code
- Format: *dataset %>% function(args) %>% morefunctions(args)*

```
cran %>% select(ip_id, country, package, size) %>% # select some columns
     mutate(size_mb = size / 2^20) %>% # create the size in MB column
     filter(size_mb <= 0.5) %>% # filter on the created column
     arrange(desc(size_mb)) %>% # order in descending order
     head(3) # take only first 3 rows
```

```
## Source: local data frame [3 x 5]
##
##   ip_id country package   size   size_mb
##   (int)   (chr)   (chr)  (int)     (dbl)
## 1 11034      DE    phia 524232 0.4999466
## 2  9643      US     tis 524152 0.4998703
## 3  1542      IN RcppSMC 524060 0.4997826
```

Tidying Data with tidyr: fixing #1 with *gather()*

#1: Column headers are values, not variable names, eg.:

```
##   grade male female
## 1     A    1      6
## 2     B    5      2
```

Column names should be: grade, gender, count

```
gather(students,gender,count,-grade) # gather all columns except grade (already exists)
```

```
##   grade gender count
## 1     A   male     1
## 2     B   male     5
## 3     A female     6
## 4     B female     2
```

Tidying Data with tidyr: fixing #2 with *separate()*

#2: Multiple variables are stored in one column, eg.:

```
##   grade gender_class count
## 1     A       male_1     1
## 2     A     female_1     2
## 3     A       male_2     3
## 4     A     female_2     4
```

Data from two classes listed in one columns, need to be separated:

```
separate(students2,col=gender_class,into=c("gender","class")) # separate into two columns
```

```
##   grade gender class count
## 1     A   male     1     1
## 2     A female     1     2
## 3     A   male     2     3
## 4     A female     2     4
```

Tidying Data with tidyr: fixing #3 with *spread()*

#3: Variables are stored in both rows and columns, eg.:

```
##    name    test grade
## 1 Sally midterm     A
## 2 Sally   final     C
## 3  Jeff midterm     B
## 4  Jeff   final     A
```

The test column values should be columns:

```
spread(students3,test,grade) # turn test column values into column names containing grade
```

```
##    name final midterm
## 1  Jeff     A       B
## 2 Sally     C       A
```

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Tidying Data with tidyr: fixing #4 with *select()*

#4: Multiple types of observational units are stored in the same table, eg.:

```
##    id  name gender class midterm final
## 1 588 Sally      F CS101       A     B
## 2 588 Sally      F CS201       C     B
## 3 710  Jeff      M CS101       B     A
```

This looks ok? … But id, name and gender are repeated - redundancy is bad.
→ Split into two tables with select - keep id column in both as primary key:

*** =left

```r
select(s4,id,class,midterm,final)
```

```
##    id class midterm final
## 1 588 CS101       A     B
## 2 588 CS201       C     B
## 3 710 CS101       B     A
```

*** =right

```r
unique(select(s4,id,name,gender))
```

```
##    id  name gender
## 1 588 Sally      F
## 3 710  Jeff      M
```

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Tidying Data with tidyr: fixing #5 with *bind_rows()*

#5: A single observational unit is stored in multiple tables, eg. tables "passed" and "failed":

*** =left

```
##    name class grade
## 1 Sally CS101     A
## 2  Jeff CS201     A
```

*** =right

```
##    name class grade
## 1 Brian CS101     E
## 2 Kathy CS201     D
```

*** =bottom We really want to combine "passed" and "failed" into a single table, with the name of the original table as a new variable:

```
passed <- mutate(passed,status='passed'); failed <- mutate(failed,status='failed')
data.frame(bind_rows(passed,failed)) # combine the tables into a single table
```

```
##    name class grade status
## 1 Sally CS101     A passed
## 2  Jeff CS201     A passed
## 3 Brian CS101     E failed
## 4 Kathy CS201     D failed
```

— &twocoltopbottom8020 ## R Package: lubridate *** =left * Date functions: * *today()*: current date * *year()*, *month()*, *day()* * Time functions: * *now()*: current date and time * *hour()*, *minute()*, *second()*

*** =right

```
<img height='300' src='lubridate.png' />
```

*** =bottom * Datetime functions: * Parsing datetimes: *ymd()*, *dmy()*, *hms()*, *ymd_hms()*, etc. * Allows use of arithmetic operators on dates and times, eg. *now() + days(2)* * *with_tz():* timezone conversion * *interval(time1,time2):* returns how much time there is between given datetimes * *stopwatch():* start timer until the next use of *stopwatch()*

Recall.. Before Machine Learning

Recall the steps you should take:

1. ~~Get data~~
2. ~~Clean and/or anonymize data~~
3. **Explore data:**
    - **What is in it?**
    - **What is useful? (Any of it? Anonymized beyond recognition?)**
    - **Does it need more cleaning?**
4. Apply statistical methods:
    - What are the trends in your data?
    - What is normal behaviour and what is outlier behaviour?
5. Fit simple models, eg. regression model
6. Apply machine learning algorithms
7. Evaluate, repeat if needed

— &twocoltopbottom ## Step 3: Exploratory Data Analysis (EDA)

*** =left

`<img height='560' src='datavis.png' />`

*** =right

> "Exploratory data analysis is an approach to analyzing data sets to summarize their main characteristics, often with visual methods."

- Arguably one of the most important aspects of data analysis!
- Often, but not always, through visualizations
- No true "best practice"
- Try things out, look at it, change it
- R is excellent for it

Exploratory Data Analysis with qplot()

Very simple scatterplot:

```
qplot(displ,hwy,data=mpg)
```

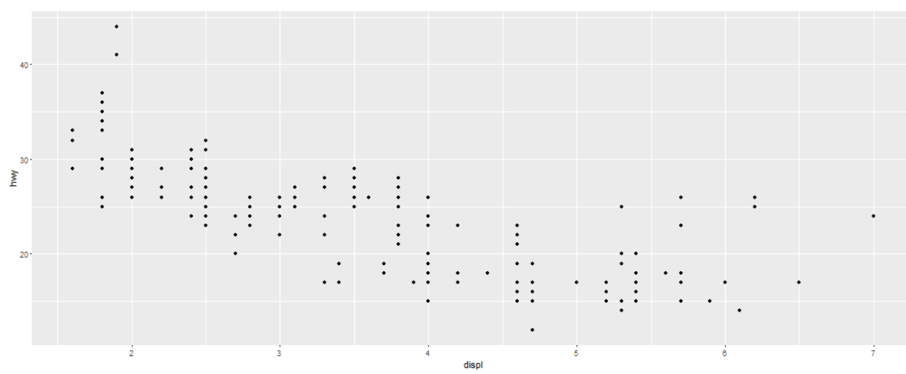


Figure 1: plot of chunk unnamed-chunk-35

Exploratory Data Analysis with qplot()

Add a smoothing function:

```
qplot(displ,hwy,data=mpg,color=drv,geom=c("point","smooth"))
```

Exploratory Data Analysis with qplot()

Add a colour based on a factor variable:

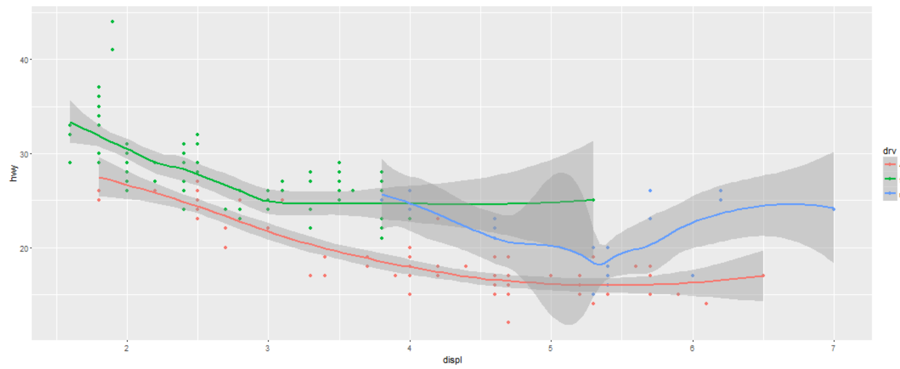


Figure 2: plot of chunk unnamed-chunk-37

```
qplot(drv,hwy,data=mpg,geom="boxplot",color=manufacturer)
```

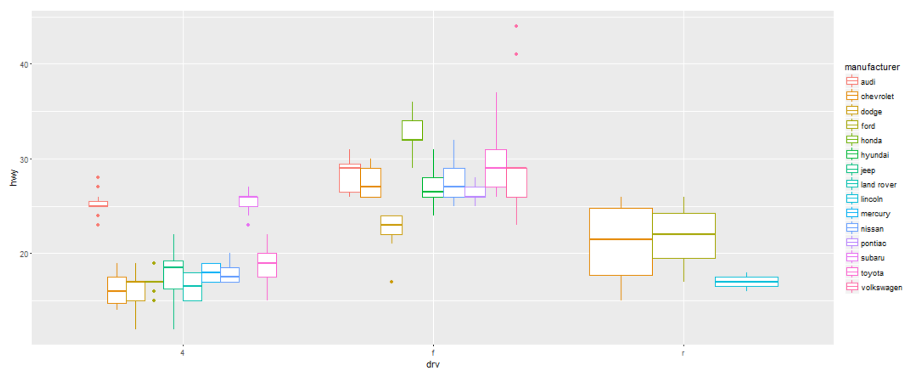


Figure 3: plot of chunk unnamed-chunk-39

Exploratory Data Analysis with qplot()

To get a faceted plot, add argument facets with the desired formula as *rows ~ columns*:

```
qplot(displ,hwy,data=mpg,facets=.~drv)
```

Exploratory Data Analysis with qplot()

Final example combining all of the above:

```
qplot(displ,hwy,data=mpg,geom=c("point","smooth"),facets=.~drv)
```

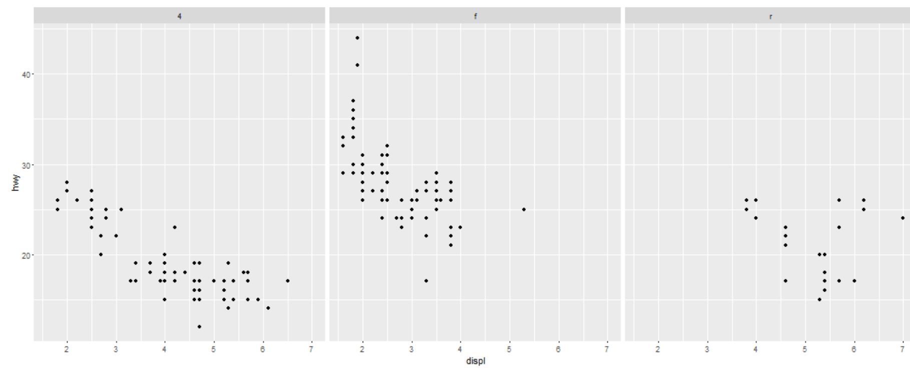


Figure 4: plot of chunk unnamed-chunk-41

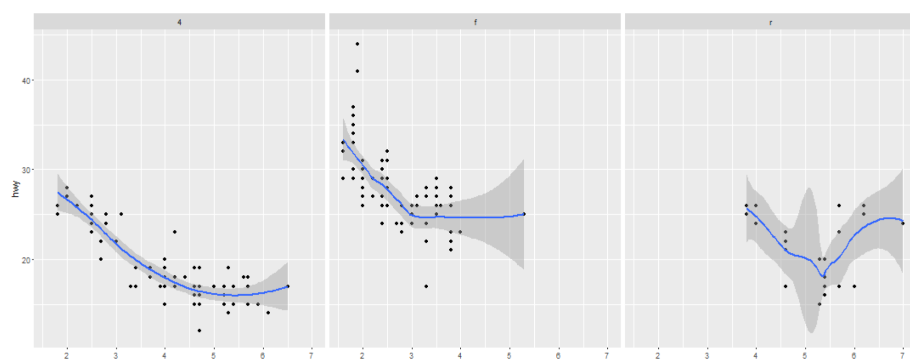


Figure 5: plot of chunk unnamed-chunk-43

Exploratory Data Analysis with ggplot()

Just a quick ggplot example (as you see, more verbose):

```
ggplot(mtcars,aes(factor(am),mpg)) +
     geom_boxplot(width=.6,aes(fill=factor(am,labels=c("Automatic","Manual")))) +
     labs(title="Boxplot of Miles per Gallon vs. Transmission Type") +
     ylab("Miles per Gallon (MPG)") + xlab("Transmission\nType\n") +
     scale_x_discrete(labels=c("0" = "Automatic", "1" = "Manual")) +
     scale_fill_manual("Transmission Type",values=c("Darkblue","steelblue")) +
     coord_flip()
```

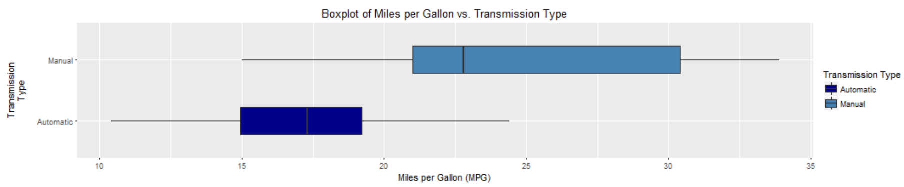


Figure 6: plot of chunk unnamed-chunk-44

Recall.. Before Machine Learning

Recall the steps you should take:

1. ~~Get data~~
2. ~~Clean and/or anonymize data~~
3. ~~Explore data~~
4. ~~Apply statistical methods~~
5. ~~Fit simple models, eg. regression model~~
6. **Apply machine learning algorithms**
7. Evaluate, repeat if needed

Training, Testing and Validation Set

- **Training set:** A machine learning algorithm needs *training data* to create a model
  - Supervised: all data must be labeled
  - Unsupervised: labels not needed, allowed but not used
  - Semi-supervised: some labeled data needed
- **Validation set:**
  - Repeated tests with the same data leads to overfitting

  - Overfitting = tuning our model too much towards the data, not generalizable
  - Thus, intermediate testing is done with *validation data*
  - Label requirements are as above for evaluation purposes
- **Testing set:** To evaluate a finished model, we need *testing data*
  - Label requirements are as above for evaluation purposes
  - In competitions, you will NOT have these labels - they are used for scoring!

Types of Learning Tasks

Machine learning algorithms have many uses, but mainly: * **Classification:** assigning a category to a given observation * Eg. classify email as "spam" or "non-spam" * Output: the assigned class * **Regression:** model the continuous phenomenon that generated the input data * Eg. model the relation between gas-mileage and transmission type * Output: the model, evaluated in a given point * **Forecasting:** generate various predictions, representing what might happen over non-specific time-periods in the future * Eg. model the weather for the coming week * Output: multiple predicted possibilities

Before We Start… R Package: caret

Very useful R package for machine learning: *caret*, contains tools for: * Data splitting * Pre-processing * Feature selection * Model tuning using resampling * Variable importance estimation * etc.

```
<img height='300' src='carrot.png' />
```

— &twocoltopbottom ## Decision Trees

*** =left * Supervised learning, labels needed * Very popular * Tree-shaped flowchart structure * Good prediction accuracy * High interpretability

> **Usage**: Starting at the root of the tree, a path is constructed to a leaf by computing in each internal node the outcome of its associated test for input x, and following the outgoing edge labeled with that outcome, until a leaf is reached. The value y stored in that leaf is the value to which x is mapped by the tree.

*** =right **Example decision tree: rain tomorrow?**

—&twocoltopbottom ## Decision Trees in R with caret

- Train a model using "rpart" (the original decision tree package)
- First argument is of form $y \sim x$, here: predict "Species" using all other variables, written "."

```
model <- train(Species ~ ., data = iris, method = "rpart")
```

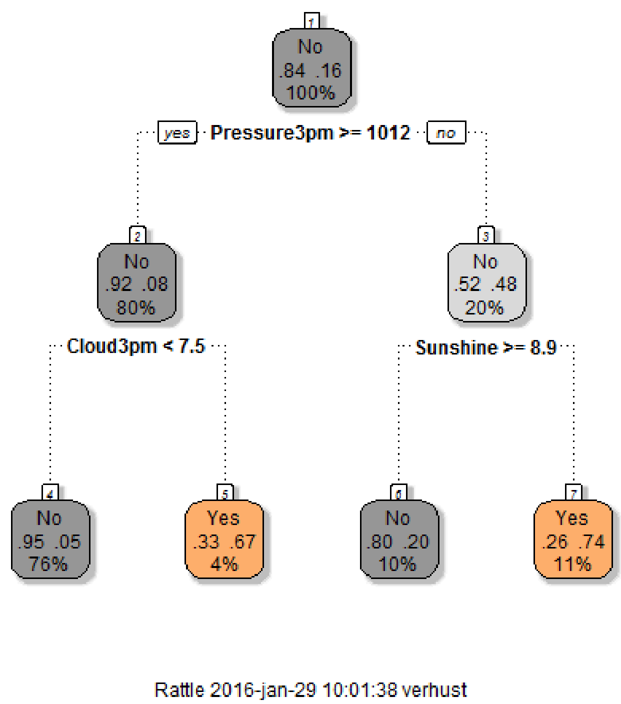


Figure 7: plot of chunk unnamed-chunk-46

*** =left

```
plot(model$finalModel)
text(model$finalModel)
```

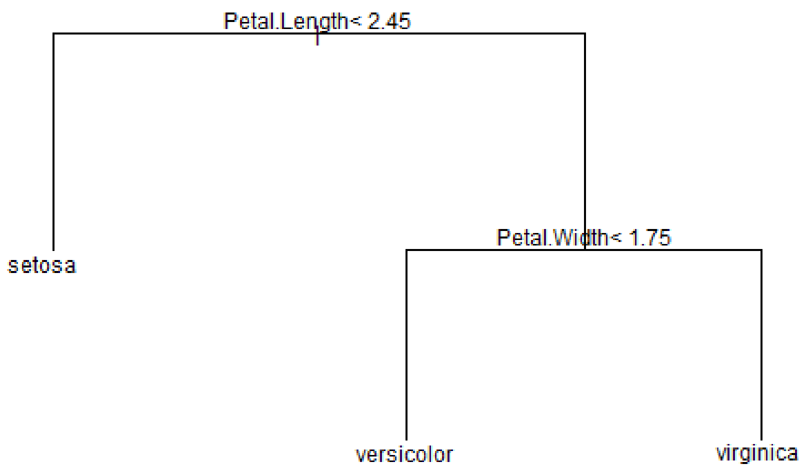


Figure 8: plot of chunk unnamed-chunk-50

*** =right

```
fancyRpartPlot(model$finalModel,
               palettes=c('Greys','Oranges'))
```

— &twocoltopbottom ## Support Vector Machines (SVMs)

*** =left * Supervised learning, labels needed * Models represent data as points in space * Different labels should be separated by a gap * Which side of gap new points are on is used to predict category

Example SVM for linearly separable features:

*** =right

If not separable in linear space, map to higher dimension:

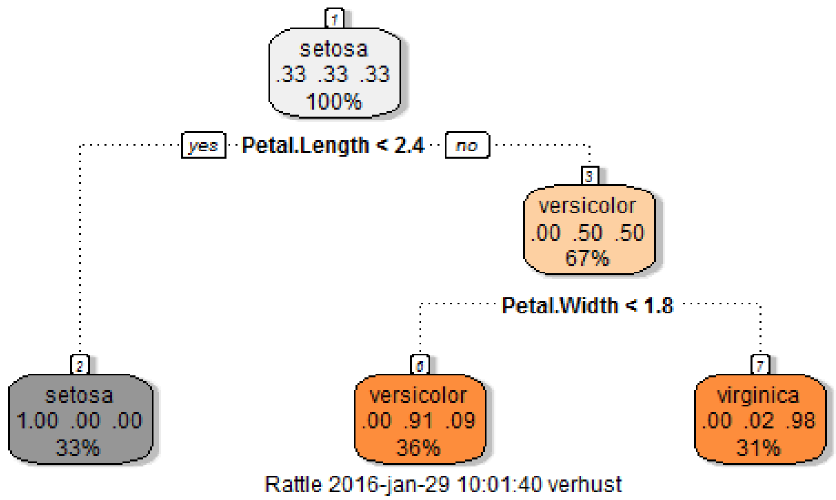


Figure 9: plot of chunk unnamed-chunk-52

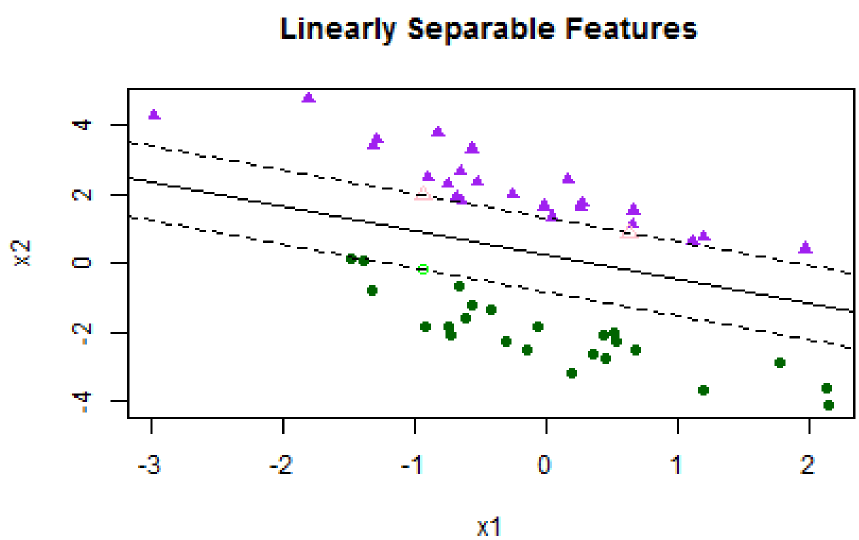
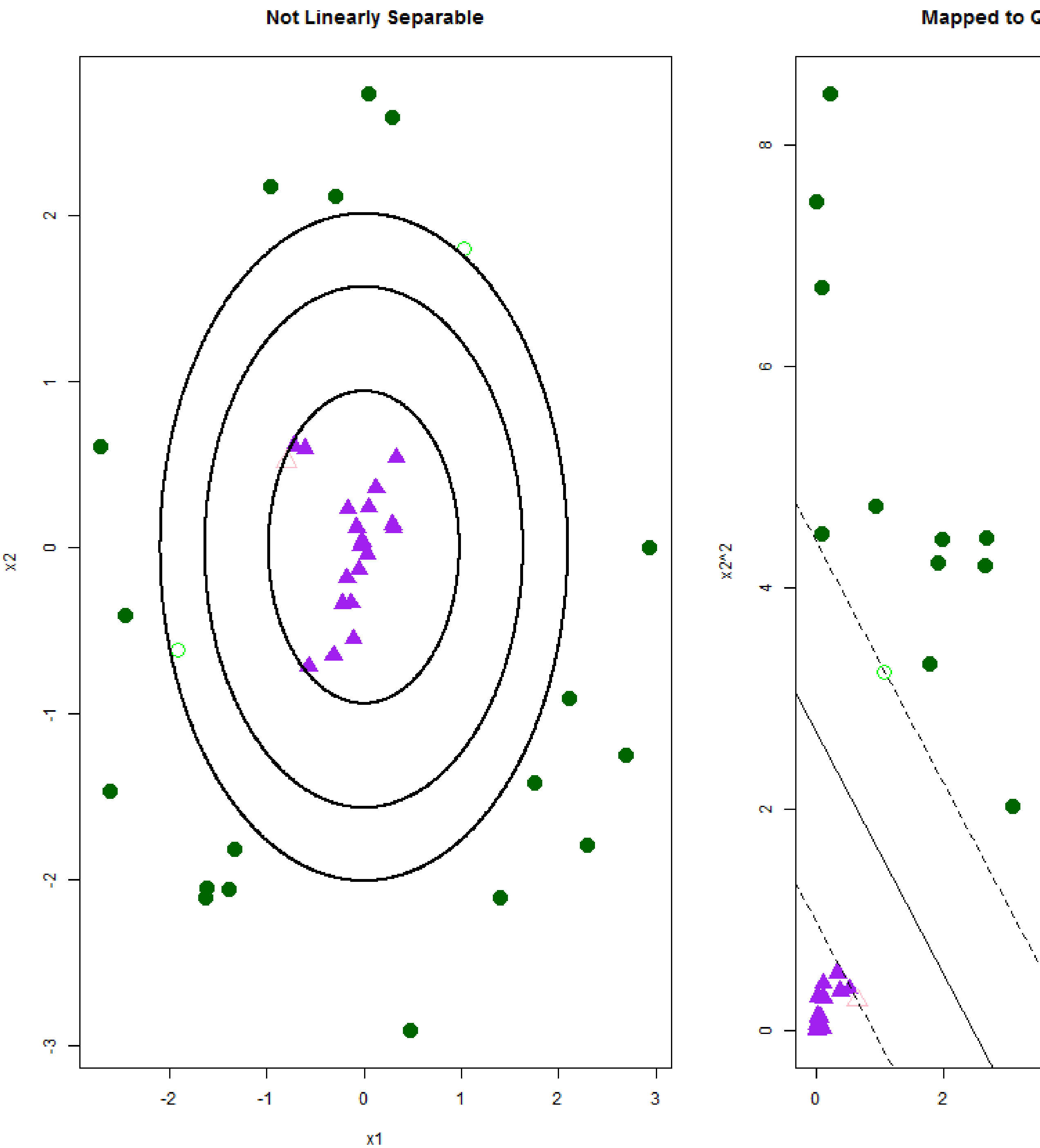


Figure 10: plot of chunk unnamed-chunk-53


Not Linearly Separable
x2
x1
2
1
0
-1
-2
-3
-2
-1
0
1
2
3
Mapped to Q
x2^2
8
6
4
2
0
0
2

— &twocoltopbottom ## More Examples: What Type of Flower?

*** =left **Predicted class:** * Predict class of iris flower

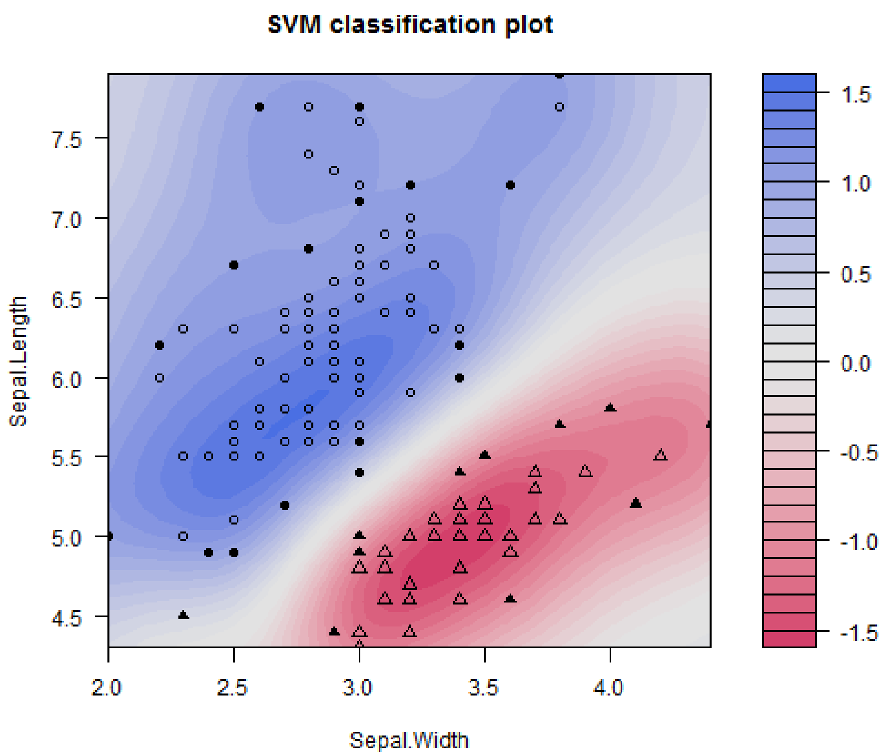


Figure 11: plot of chunk unnamed-chunk-56

*** =right **Prediction confidence:** * How certain are these predictions?

— &twocol ## SVMs in R with caret *** =left Given this randomly generated data: * Train a model using "svmLinear", "svmPoly" or "svmRadial", … * First argument is of form $y \sim x$ * Here we use: $y \sim .$ where "." represents "all available x"

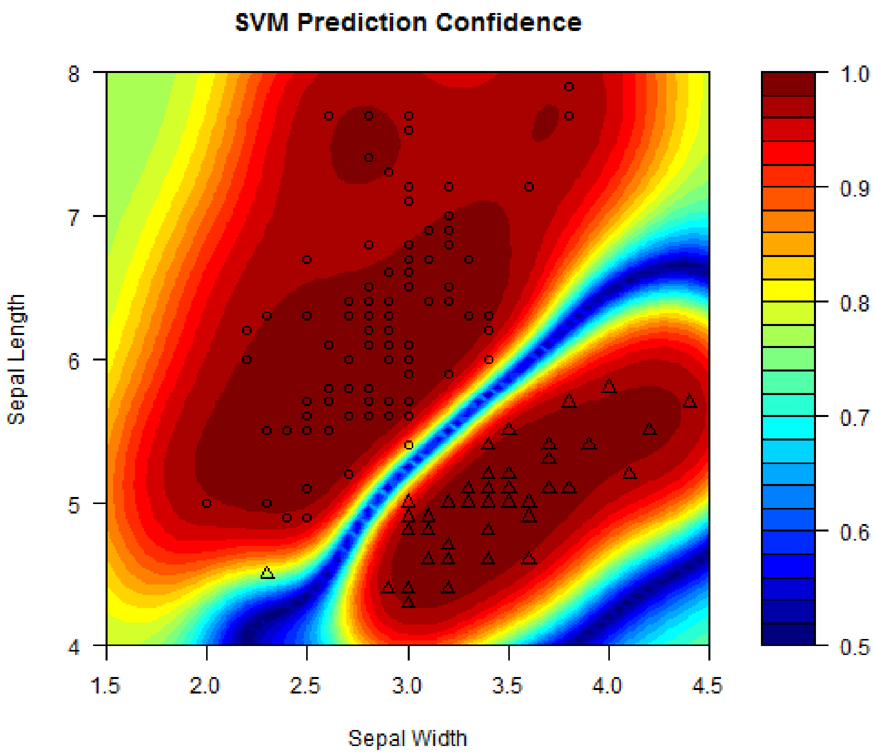
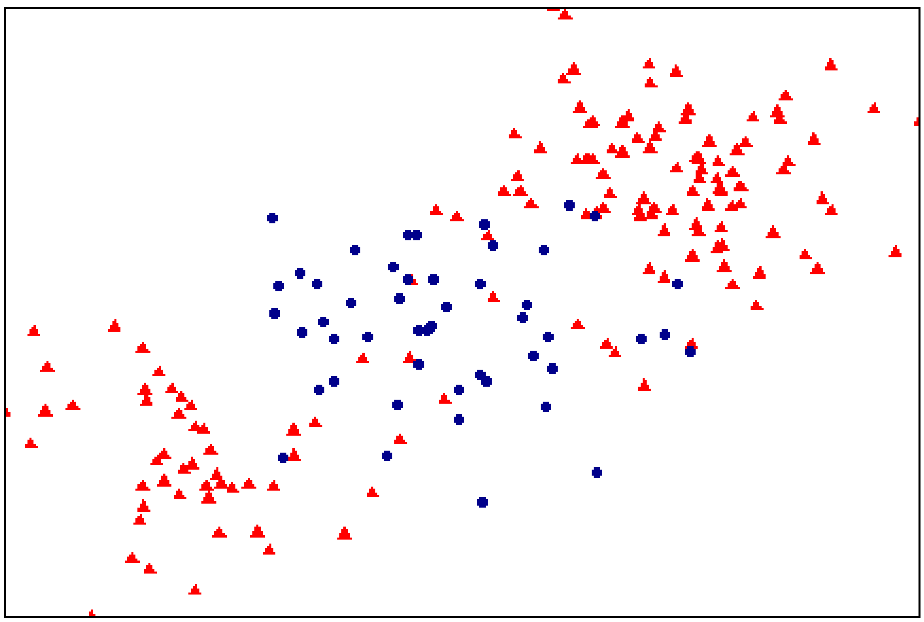


Figure 12: plot of chunk unnamed-chunk-57



*** =right **Linear SVM attempt**

```
mL <- train(y~.,data=dat,method="svmLinear")
plot(mL$finalModel)
```

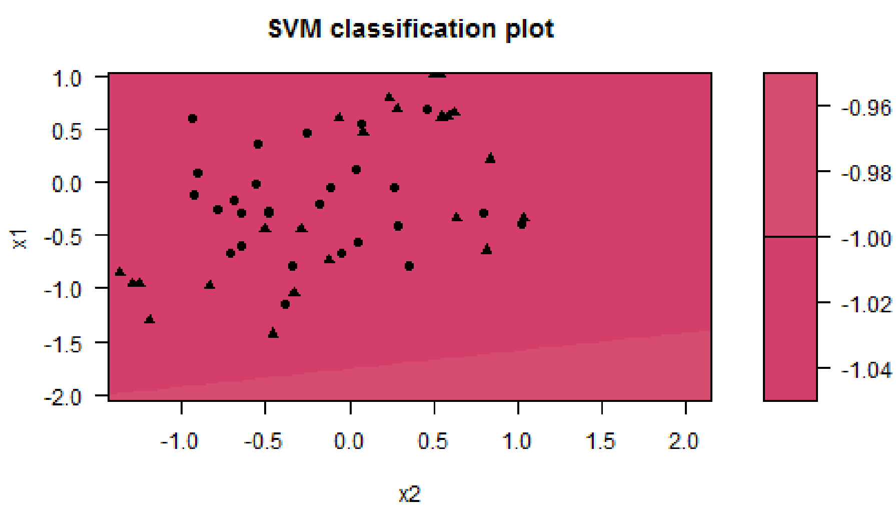


Figure 13: plot of chunk unnamed-chunk-61

- **Accuracy:** 0.8
- Reason: more red than blue - **Beware!**

— &twocoltopbottom ## SVMs in R with caret

*** =left **Polynomial SVM attempt**

```
mP <- train(y~.,data=dat,method="svmPoly")
plot(mP$finalModel)
```

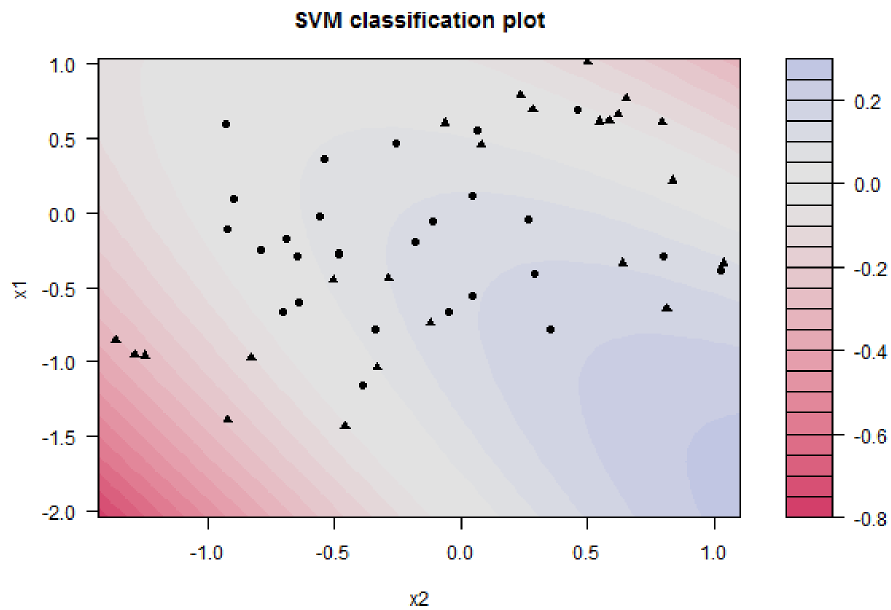


Figure 14: plot of chunk unnamed-chunk-64

Accuracy: 0.9272727 *** =right **Radial SVM attempt**

```
mR <- train(y~.,data=dat,method="svmRadial")
plot(mR$finalModel)
```

Accuracy: 0.9454545

— &twocoltopbottom ## Clustering

*** =left * Unsupervised learning, NO labels needed * Grouping data into categories based on some measure of distance or similarity * Two famous types: * K-means clustering * Hierarchical clustering * Visualization #1: **dendrogram**

*** =right * Visualization #2: **Heatmap** (with/without the added dendrogram)

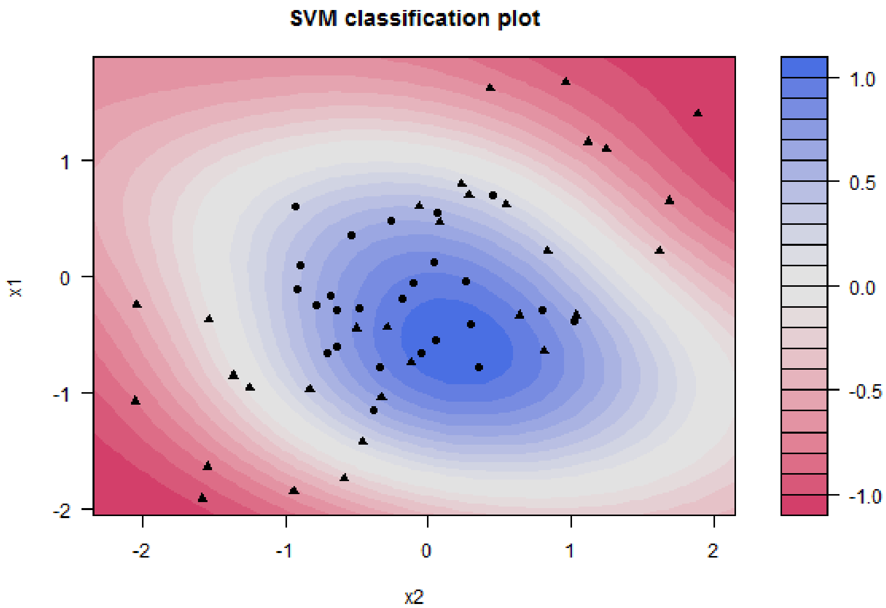


Figure 15: plot of chunk unnamed-chunk-67

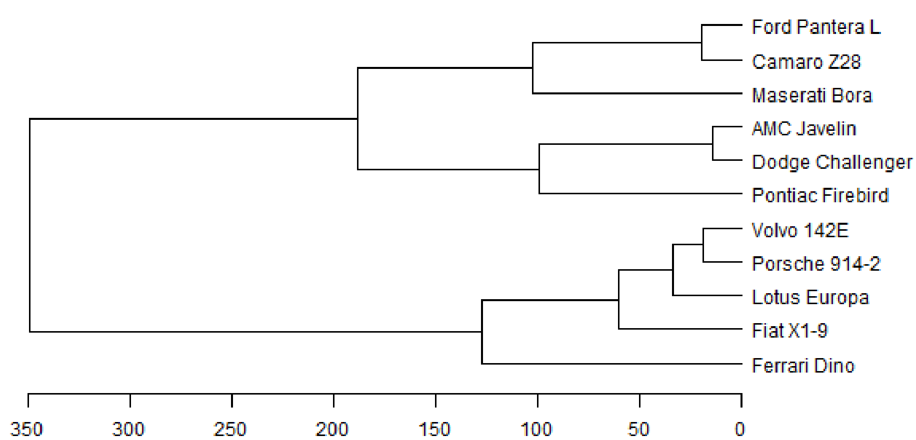


Figure 16: plot of chunk unnamed-chunk-69

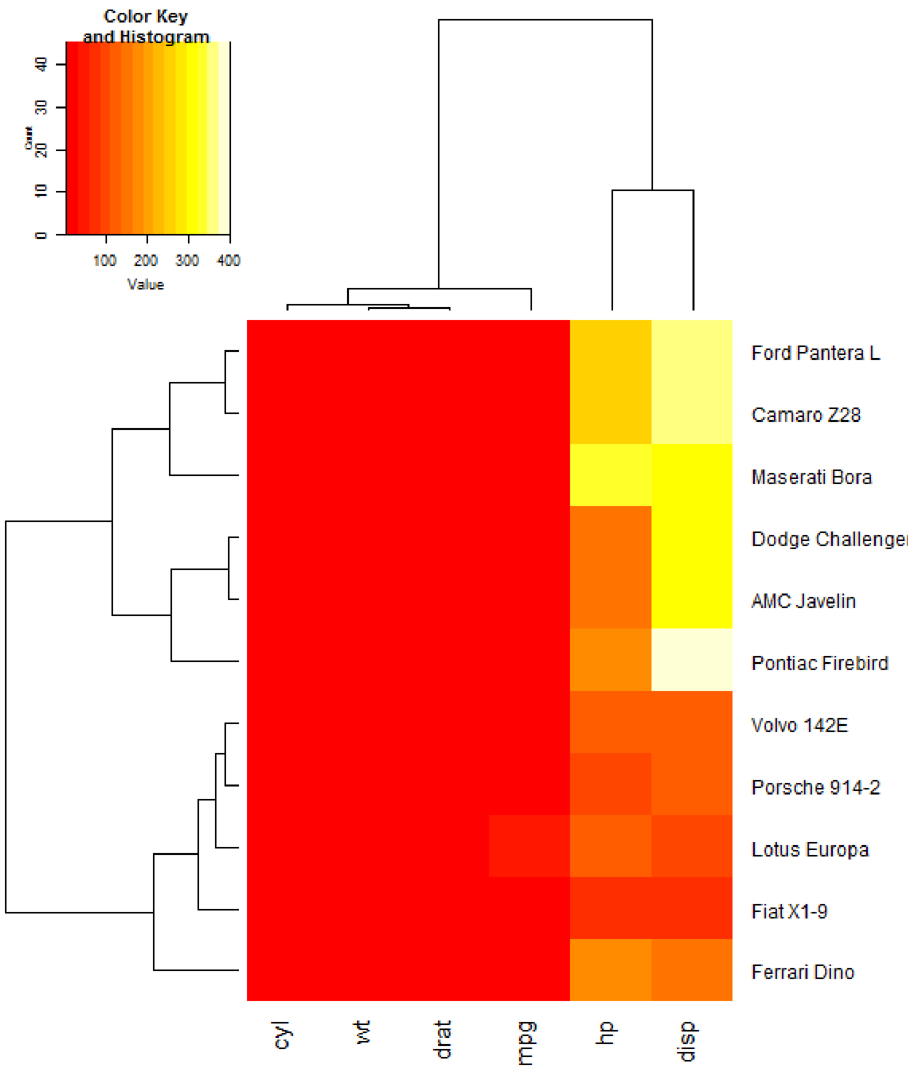
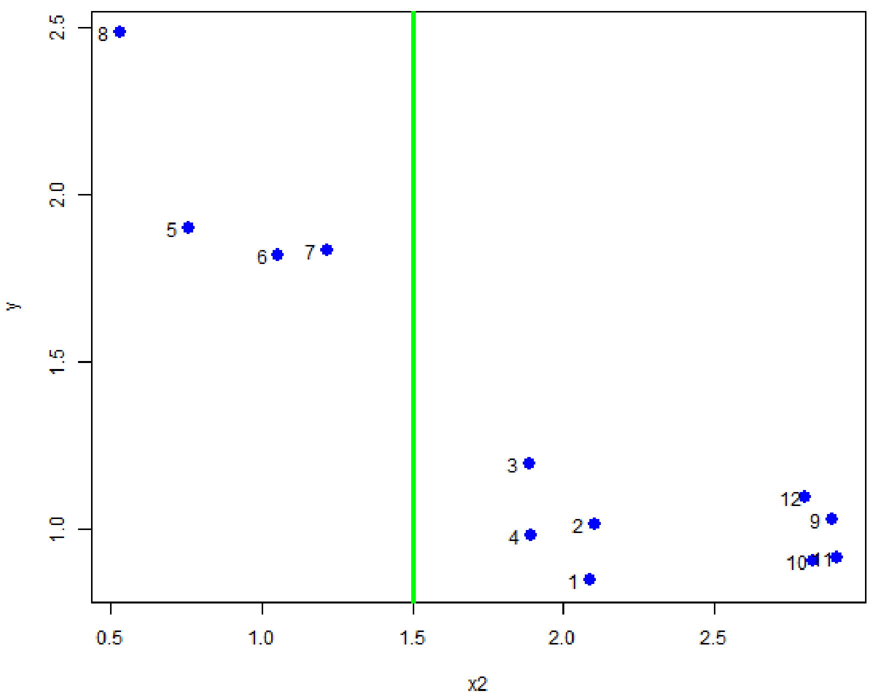
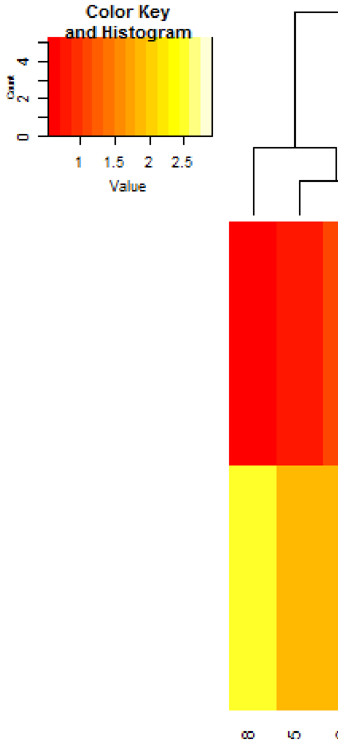


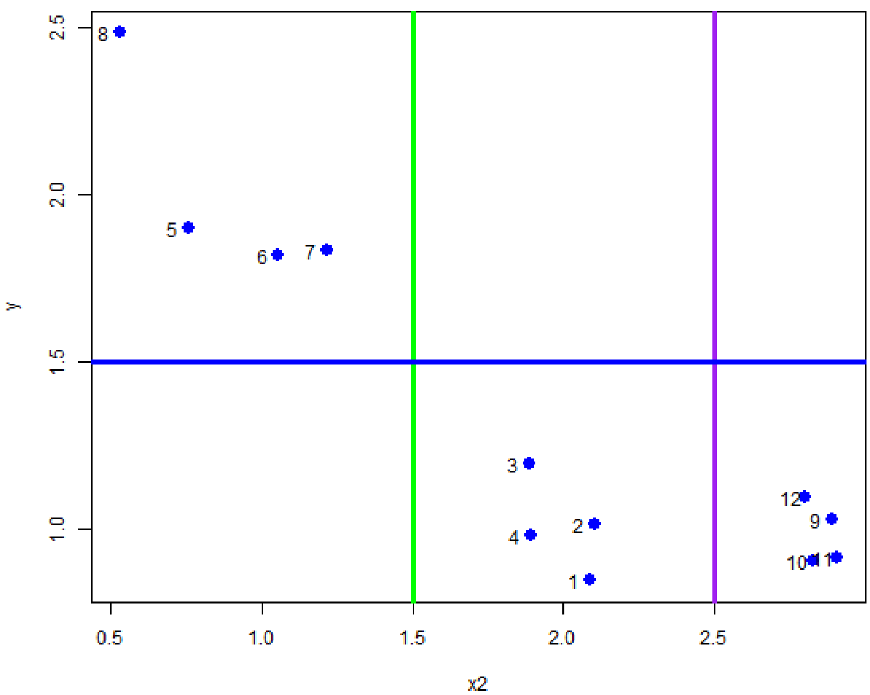
Figure 17: plot of chunk unnamed-chunk-70

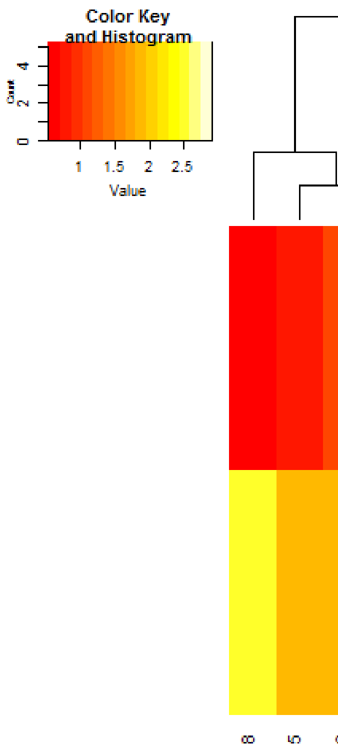
Clustering Heatmap Explanation





Clustering Heatmap Explanation





K-Means Clustering Example

- Assumed number of clusters: 3
- Calculate cluster centroids (= element representing center)

K-Means Clustering Example

- **Next:** recalculate cluster centroids

K-Means Clustering Example

- **Next:** recalculate cluster centroids

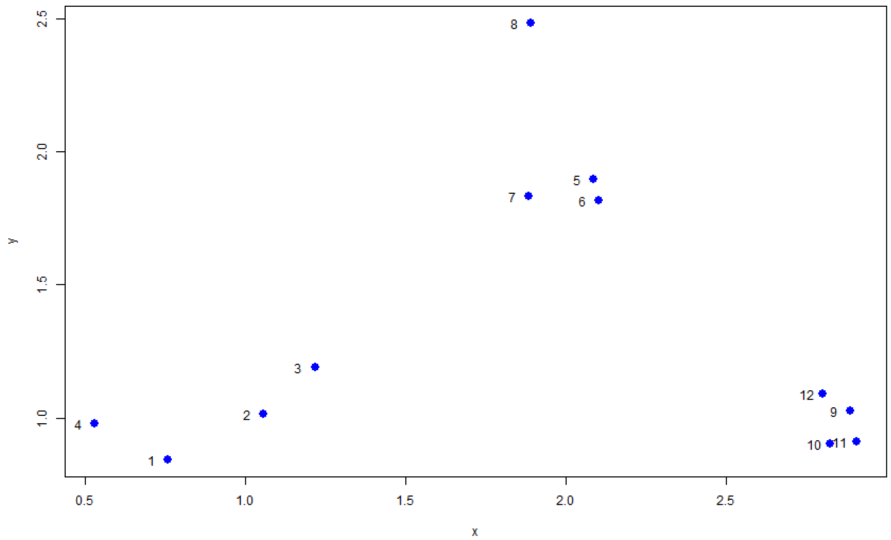


Figure 18: plot of chunk unnamed-chunk-89

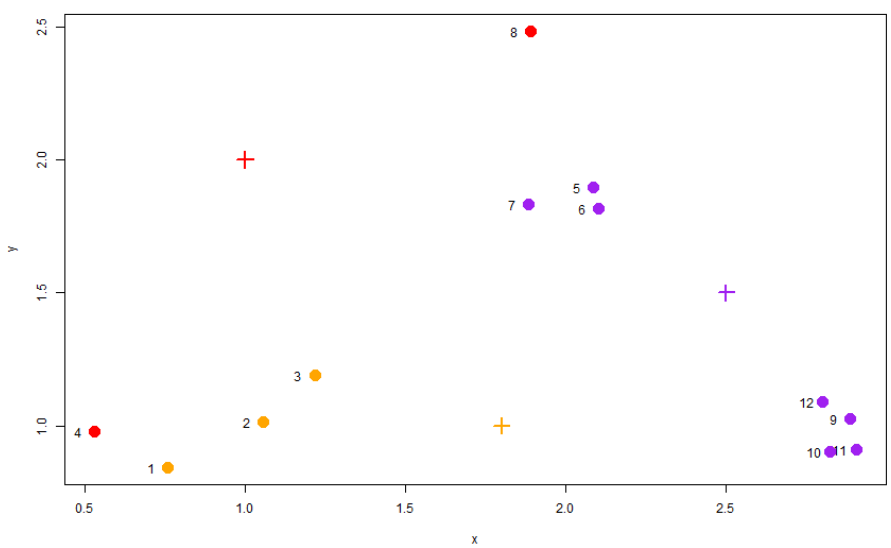


Figure 19: plot of chunk unnamed-chunk-93

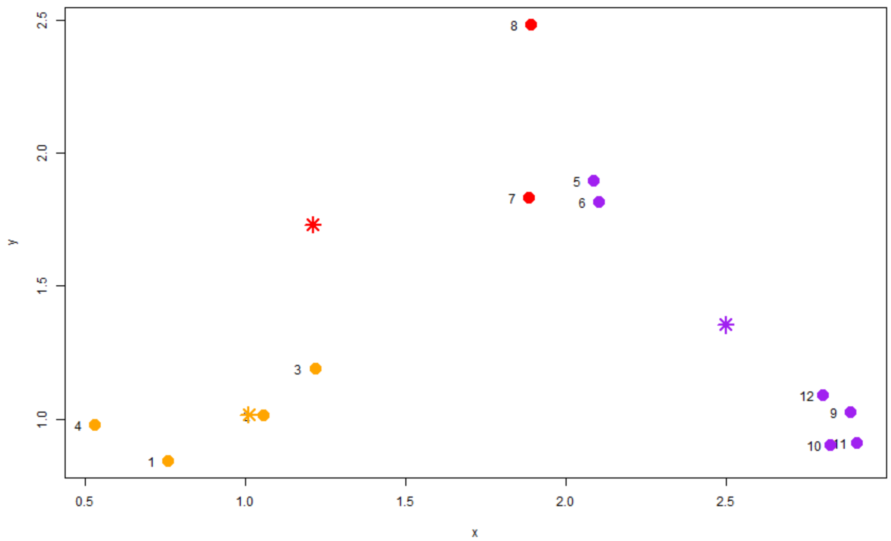


Figure 20: plot of chunk unnamed-chunk-97

K-Means Clustering Example

No more points would change cluster: we are done!

Data Science Step-by-Step

Recall the steps you should take:

1. ~~Get data~~
2. ~~Clean and/or anonymize data~~
3. ~~Explore data~~
4. ~~Apply statistical methods~~
5. ~~Fit simple models, eg. regression model~~
6. ~~Apply machine learning algorithms~~
7. **Evaluate, repeat if needed**

— &twocoltopbottom ## Evaluation and Comparison of ML Models *** =left **Classification output: class label** * Either correct or incorrect * Common evaluation metrics: * Accuracy: % correct * Confidence intervals * P-values * True/False Positive/Negative Rate * Confidence matrix * Visual: * Heatmap of confidence matrix * Variable importance plots * ROC curves

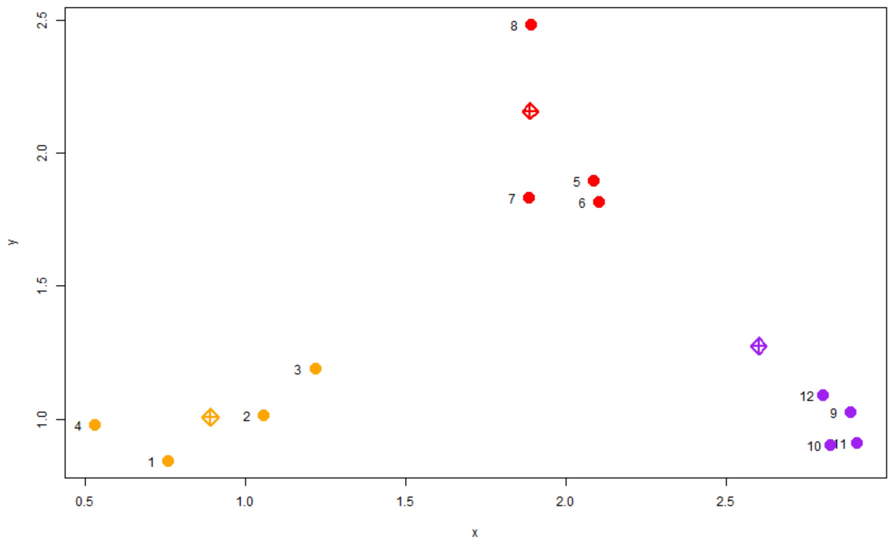


Figure 21: plot of chunk unnamed-chunk-101

*** =right **Regression output: continuous number** * Closer to real value = better * Common evaluation metrics: * Residuals: what model doesn't explain * (Adjusted) R-squared: goodness-of-fit * Standard Error * Correlation with real value * Visual: * Residual plots * Variable importance plots

Evaluating Classification in R: Variable Importance

- Variable Importance Plot "VarImpPlot"
- To evaluate model features' importance
  - Top right: most important - bottom left: least important
- In R: *randomForest* package, *varImpPlot()* function

```
varImpPlot(classModel)
```

— &twocoltopbottom7030 ## Evaluating Classification in R: Evaluation Metrics *** =left

```
<img height='5' src='ROC.png' />
```

*** =right **Evaluation metrics:** * True positive rate (TPR), aka "Sensitivity", "Recall" * True negative rate (TNR), aka "Specificity" * False positive rate (FPR), aka "Fall-out", "Type I Error Rate" * False negative rate (FNR), aka "Miss Rate", "Type II Error Rate"

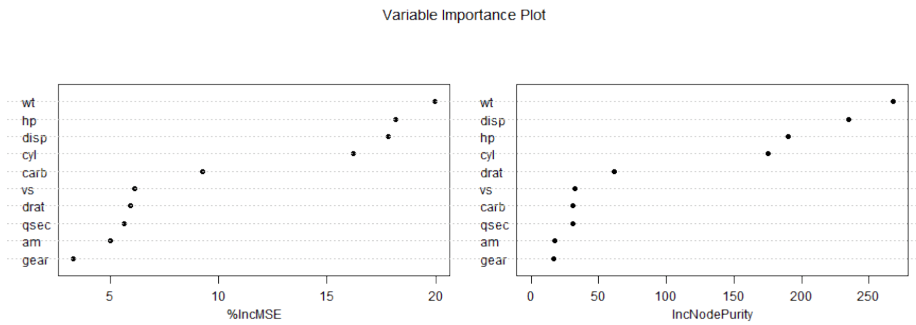


Figure 22: plot of chunk unnamed-chunk-107

— &twocol ## Comparing Classification in R: ROC Curves *** =left * Receiver Operating Characteristic (ROC) * Evaluate performance of classifier * Y-axis: true positive rate (TPR) * X-axis: false positive rate (FPR) * Bigger area under curve (AUC) = better

*** =right * ROC curves also excellent for visual model comparison * Example:

Sources

Code and information adapted from: * H. Blockeel. Machine Learning and Inductive Inference. Acco, Leuven, 2010. * http://swirlstats.com/ * http://www.r-bloggers.com/learning-kernels-svm/ * http://coreynoone.com/archives/182 * https://rpubs.com/ryankelly/svm * http://machinelearningmastery.com/

— { tpl: thankyou, social: [{title: Website, href: "http://www.archimiddle.com"}, {title: LinkedIn, href: "https://www.linkedin.com/company/archimiddle"}] }

Thank You

For more information:

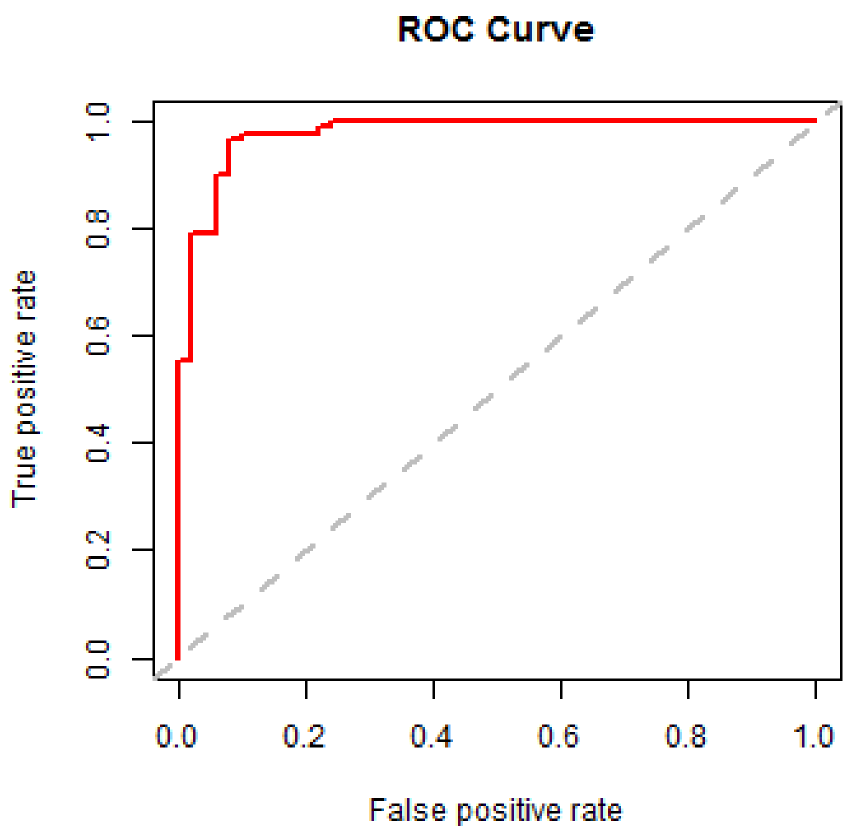


Figure 23: plot of chunk unnamed-chunk-108

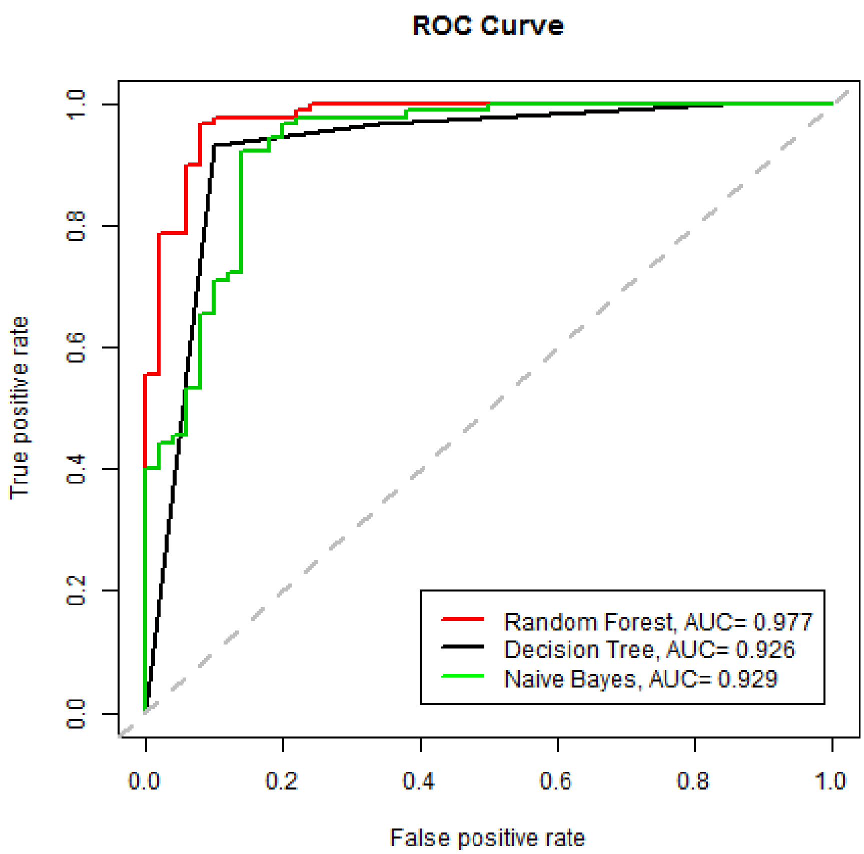


Figure 24: plot of chunk unnamed-chunk-109