Machine Learning with R

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Prerequisites

This book is basically a record of my journey in data analysis. So often, I spend time reading articles, blog posts, etc. and wish I could put all the great things I'm learning in a central location.

So this book is a compilation of all the great techniques I've learned along the way. Most of what I have learned is through blog posts, stack overflow questions, etc. I am not taking any credit for all the great ideas, examples, graphs, etc. in this web book. I do take responsability for all mistakes, typos, unclear explanations, poor labeling / presentation of graphs. If you find anything that require improvement, I would be grateful if you would let me know: f.deryckel@gmail.com

I am assuming that you are already somehow familiar with:

- the math behind most algorithms. This is not a math book.
- the basics of how to use R. This is not a computer science book nor a R book.

I wish you great fun in your data science journey, and I hope that this book can contribute positively to your journey.

As much as it makes sense, we will use the tidyverse and the conventions of tidy data throughout our journey. Besides the hype surrounding the tidyverse, there is a couple reasons for us to stick with it:

- learning a language is hard on itself, if we can be proficient and creative with one, it will be much better. All the packages from the tidyverse, might not always be the best ones (more efficient, more elegant), but I'am happy to learn inside out one opiniated framework in order to be able to apply it effortlessly and creatively.
- Because many of the tidyverse packages do their background work in C++, they are usually pretty efficient in the way they work.

library(tidyverse)

Here are some conventions we will be using throughout the book.

- df denotes a data frame. Usually the data frame from a raw set of data
- We'll use df2, df3, etc. for other, "cleaner" versions of that raw data set
- model_pca_xxxx, model_lr_xxxxx denotes models. The second part denotes the algorithm.
- predict_svm_xxxx or predict_mlr_xxxx denotes the outcome of applying a model on a set of indepedent variables.

Tests and inferences

Definetly the first thing to be familiar with while doing machine learning works is the basic of statistical inferences.

In this chapter, we go over some of the few important topics and r-ways to do them.

Let's get started.

You can label chapter and section titles using {#label} after them, e.g., we can reference Chapter 3. If you do not manually label them, there will be automatic labels anyway, e.g., Chapter ??.

Figures and tables with captions will be placed in figure and table environments, respectively.

```
par(mar = c(4, 4, .1, .1))
plot(pressure, type = 'b', pch = 19)
```

Reference a figure by its code chunk label with the fig: prefix, e.g., see Figure 2.1. Similarly, you can reference tables generated from knitr::kable(), e.g., see Table 2.1.

```
knitr::kable(
  head(iris, 10), caption = 'Here is a nice table!',
  booktabs = TRUE
)
```

You can write citations, too. For example, we are using the **bookdown** package (Xie, 2016) in this sample book, which was built on top of R Markdown and **knitr** (Xie, 2015).

Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
5.1	3.5	1.4	0.2	setosa
4.9	3.0	1.4	0.2	setosa
4.7	3.2	1.3	0.2	setosa
4.6	3.1	1.5	0.2	setosa
5.0	3.6	1.4	0.2	setosa
5.4	3.9	1.7	0.4	setosa
4.6	3.4	1.4	0.3	setosa
5.0	3.4	1.5	0.2	setosa
4.4	2.9	1.4	0.2	setosa
4.9	3.1	1.5	0.1	setosa

Table 2.1: Here is a nice table!

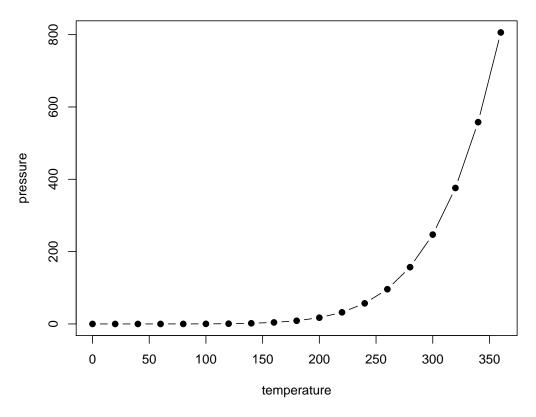


Figure 2.1: Here is a nice figure!

Multiple Linear Regression

Logistic Regressions

4.1 Introduction

Logistic Regression is a classification algorithm. It is used to predict a binary outcome (1 / 0, Yes / No, True / False) given a set of independent variables. To represent binary / categorical outcome, we use dummy variables. You can also think of logistic regression as a special case of linear regression when the outcome variable is categorical, where we are using log of odds as dependent variable. In simple words, it predicts the probability of occurrence of an event by fitting data to a logit function.

Logistic Regression is part of a larger class of algorithms known as Generalized Linear Model (glm).

Although most logisite regression should be called **binomial logistic regression**, since the variable to predict is binary, however, logistic regression can also be used to predict a dependent variable which can assume more than 2 values. In this second case we call the model **multinomial logistic regression**. A typical example for instance, would be classifying films between "Entertaining", "borderline" or "boring".

4.2 The logistic equation.

The general equation of the logit model

$$\mathbf{Y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n$$

where \mathbf{Y} is the variable to predict.

 β is the coefficients of the predictors and the x_i are the predictors (aka independent variables). In logistic regression, we are only concerned about the probability of outcome dependent variable (success or failure). We should then rewrite our function

$$n = e^{(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n)}$$

This however does not garantee to have p between 0 and 1.

Let's then have

$$p = \frac{e^{(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n)}}{e^{(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n)} + 1}$$

or

$$p = \frac{e^Y}{e^Y + 1}$$

where p is the probability of success. With little further manipulations, we have

$$\frac{p}{1-p} = e^Y$$

and

$$\log \frac{p}{1-p} = Y$$

If we remember what was \mathbf{Y} , we get

$$\log \frac{p}{1-p} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n$$

This is the equation used in Logistic Regression. Here (p/1-p) is the odd ratio. Whenever the log of odd ratio is found to be positive, the probability of success is always more than 50%.

4.3 Performance of Logistic Regression Model

To evaluate the performance of a logistic regression model, we can consider a few metrics.

- AIC (Akaike Information Criteria) The analogous metric of adjusted R-squared in logistic regression is AIC. AIC is the measure of fit which penalizes model for the number of model coefficients. Therefore, we always prefer model with minimum AIC value.
- Null Deviance and Residual Deviance Null Deviance indicates the response predicted by a model with nothing but an intercept. Lower the value, better the model. Residual deviance indicates the response predicted by a model on adding independent variables. Lower the value, better the model.
- Confusion Matrix It is nothing but a tabular representation of Actual vs Predicted values. This helps us to find the accuracy of the model and avoid overfitting.
- We can calculate the accuracy of our model by

$$\frac{True Positives + True Negatives}{True Positives + True Negatives + False Positives + False Negatives}$$

• From confusion matrix, Specificity and Sensitivity can be derived as

$$Specificity = \frac{TrueNegatives}{TrueNegative + FalsePositive}$$

and

$$Sensitivity = \frac{TruePositive}{TruePositive + FalseNegative}$$

• ROC Curve Receiver Operating Characteristic(ROC) summarizes the model's performance by evaluating the trade offs between true positive rate (sensitivity) and false positive rate(1- specificity). For plotting ROC, it is advisable to assume p > 0.5 since we are more concerned about success rate. ROC summarizes the predictive power for all possible values of p > 0.5. The area under curve (AUC), referred to as index of accuracy(A) or concordance index, is a perfect performance metric for ROC curve. Higher the area under curve, better the prediction power of the model. The ROC of a perfect predictive model has TP equals 1 and FP equals 0. This curve will touch the top left corner of the graph.

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4.4 Setting up

As usual we will use the tidyverse and caret package

```
library(ROCR) # For confusion matrix
library(ROCR) # For the ROC curve
library(tidyverse)
```

We can now get straight to business and see how to model logisite regression with R and then have the more interesting discussion on its performance.

4.5 Example 1

We use a dataset about factors influencing graduate admission that can be downloaded from the UCLA Institute for Digital Research and Education

The dataset has 4 variables

- admit is the response variable
- gre is the result of a standardized test
- gpa is the result of the student GPA (school reported)
- rank is the type of university the student apply for (4 = Ivy League, 1 = lower level entry U.)

Let's have a quick look at the data and their summary. The goal is to get familiar with the data, type of predictors (continuous, discrete, categorical, etc.)

```
df <- read_csv("dataset/grad_admission.csv")</pre>
glimpse(df)
## Observations: 400
## Variables: 4
## $ admit <int> 0, 1, 1, 1, 0, 1, 1, 0, 1, 0, 0, 0, 1, 0, 1, 0, 0, 0, 0, ...
           <int> 380, 660, 800, 640, 520, 760, 560, 400, 540, 700, 800, 4...
## $ gpa
           <dbl> 3.61, 3.67, 4.00, 3.19, 2.93, 3.00, 2.98, 3.08, 3.39, 3....
## $ rank <int> 3, 3, 1, 4, 4, 2, 1, 2, 3, 2, 4, 1, 1, 2, 1, 3, 4, 3, 2,...
#Quick check to see if our response variable is balanced-ish
table(df$admit)
##
##
     0
         1
## 273 127
```

Well that's not a very balanced response variable, although it is not hugely unbalanced either as it can be the cases sometimes in medical research.

```
## Two-way contingency table of categorical outcome and predictors
round(prop.table(table(df$admit, df$rank), 2), 2)
```

It seems about right ... most students applying to Ivy Leagues graduate programs are not being admitted.

Before we can run our model, let's transform the rank explanatory variable to a factor.

```
df2 <- df
df2$rank <- factor(df2$rank)
# Run the model
model_lr_admission <- glm(admit ~ ., data = df2, family = "binomial")
summary(model_lr_admission)
##
## Call:
## glm(formula = admit ~ ., family = "binomial", data = df2)
##
## Deviance Residuals:
##
       Min
                 1Q
                      Median
                                   30
                                           Max
## -1.6268 -0.8662 -0.6388
                                        2.0790
                               1.1490
##
## Coefficients:
##
                Estimate Std. Error z value Pr(>|z|)
                           1.139951 -3.500 0.000465 ***
## (Intercept) -3.989979
## gre
                0.002264
                           0.001094
                                      2.070 0.038465 *
                0.804038
                           0.331819
                                      2.423 0.015388 *
## gpa
               -0.675443
                           0.316490
                                    -2.134 0.032829 *
## rank2
               -1.340204
                                    -3.881 0.000104 ***
## rank3
                           0.345306
## rank4
               -1.551464
                           0.417832 -3.713 0.000205 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##
       Null deviance: 499.98
                             on 399
                                      degrees of freedom
## Residual deviance: 458.52 on 394 degrees of freedom
## AIC: 470.52
##
## Number of Fisher Scoring iterations: 4
```

The next part of the output shows the coefficients, their standard errors, the z-statistic (sometimes called a Wald z-statistic), and the associated p-values. Both gre and gpa are statistically significant, as are the three terms for rank. The logistic regression coefficients give the change in the log odds of the outcome for a one unit increase in the predictor variable.

For every one unit change in gre, the log odds of admission (versus non-admission) increases by 0.002. For a one unit increase in gpa, the log odds of being admitted to graduate school increases by 0.804. The indicator variables for rank have a slightly different interpretation. For example, having attended an undergraduate institution with rank of 2, versus an institution with a rank of 1, changes the log odds of admission by -0.675.

To see how the variables in the model participates in the decrease of *Residual Deviance*, we can use the ANOVA function on our model.

```
anova(model_lr_admission)

## Analysis of Deviance Table

##
## Model: binomial, link: logit

##
## Response: admit
```

4.5. EXAMPLE 1

```
##
## Terms added sequentially (first to last)
##
##
##
        Df Deviance Resid. Df Resid. Dev
## NULL
                                    499.98
                            399
             13.9204
                            398
                                    486.06
## gre
         1
## gpa
         1
             5.7122
                            397
                                    480.34
         3
            21.8265
                            394
                                    458.52
## rank
```

We can test for an overall effect of rank (its significance) using the wald.test function of the aod library. The order in which the coefficients are given in the table of coefficients is the same as the order of the terms in the model. This is important because the wald.test function refers to the coefficients by their order in the model. We use the wald.test function. b supplies the coefficients, while Sigma supplies the variance covariance matrix of the error terms, finally Terms tells R which terms in the model are to be tested, in this case, terms 4, 5, and 6, are the three terms for the levels of rank.

```
library(aod)
wald.test(Sigma = vcov(model_lr_admission), b = coef(model_lr_admission), Terms = 4:6)

## Wald test:
## -----
##
## Chi-squared test:
## X2 = 20.9, df = 3, P(> X2) = 0.00011
```

The chi-squared test statistic of 20.9, with three degrees of freedom is associated with a p-value of 0.00011 indicating that the overall effect of rank is statistically significant.

Let's check how our model is performing. As mentioned earlier, we need to make a choice on the cutoff value (returned probability) to check our accuracy. In this first example, let's just stick with the usual 0.5 cutoff value.

As it stands, the **predict** function gives us the probability that the observation has a response of 1; in our case, the probability that a student is being admitted into the graduate program.

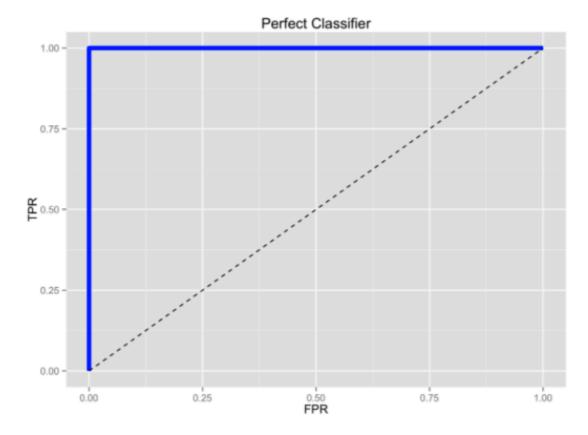
To check the accuracy of the model, we need a confusion matrix with a cut off value. So let's clean that vector of probability.

```
Confusion Matrix and Statistics
##
##
             Reference
## Prediction
                 0
                     1
                    97
##
             0 254
##
             1 19
                    30
##
##
                   Accuracy: 0.71
```

```
95% CI: (0.6628, 0.754)
##
##
       No Information Rate: 0.6825
       P-Value [Acc > NIR] : 0.1293
##
##
##
                     Kappa: 0.1994
   Mcnemar's Test P-Value: 8.724e-13
##
##
##
               Sensitivity: 0.2362
##
               Specificity: 0.9304
            Pos Pred Value: 0.6122
##
##
            Neg Pred Value: 0.7236
                Prevalence: 0.3175
##
##
            Detection Rate: 0.0750
      Detection Prevalence: 0.1225
##
##
         Balanced Accuracy: 0.5833
##
##
          'Positive' Class : 1
##
```

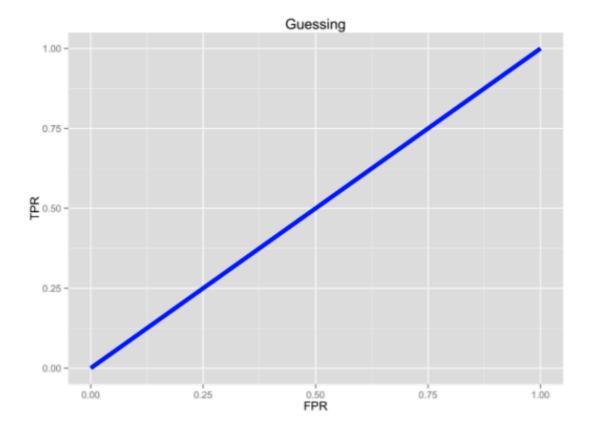
We have an interesting situation here. Although all our variables were significant in our model, the accuracy of our model, 71% is just a little bit higher than the basic benchmark which is the no-information model (ie. we just predict the highest class) in this case 68.25%.

Before we do a ROC curve, let's have a quick reminder on ROC. ROC are plotting the proprotion of TP to FP. So ideally we want to have 100% TP and 0% FP.



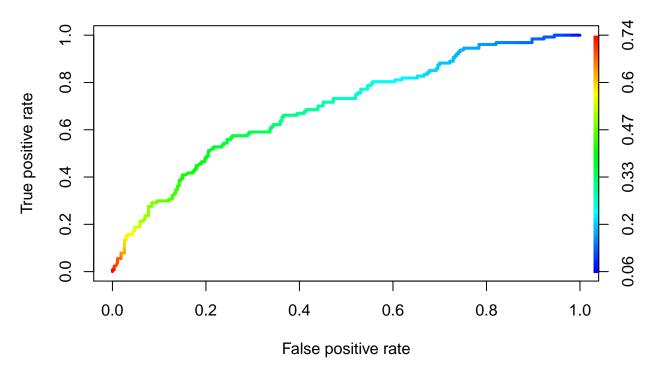
Pure Random guessing should lead to this curve

4.5. EXAMPLE 1



With that in mind, let's do a ROC curve on out model

```
prediction_lr_admission <- predict(model_lr_admission, data = df2, type="response")
pr_admission <- prediction(prediction_lr_admission, df2$admit)
prf_admission <- preformance(pr_admission, measure = "tpr", x.measure = "fpr")
plot(prf_admission, colorize = TRUE, lwd=3)</pre>
```



At least it is better than just random guessing.

In some applications of ROC curves, you want the point closest to the TPR of 1 and FPR of 0. This cut point is "optimal" in the sense it weighs both sensitivity and specificity equally. Now, there is a cost measure in the ROCR package that you can use to create a performance object. Use it to find the cutoff with minimum cost.

```
cost_admission_perf = performance(pr_admission, "cost")
pr_admission@cutoffs[[1]][which.min(cost_admission_perf@y.values[[1]])]

## 392
## 0.487194

Using that cutoff value we should get our sensitivity and specificity a bit more in balance. Let's try
```

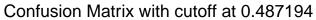
```
## Confusion Matrix and Statistics
##
##
             Reference
##
  Prediction
##
            0 247
                   89
##
               26
                   38
##
##
                  Accuracy: 0.7125
##
                    95% CI: (0.6654, 0.7564)
##
       No Information Rate: 0.6825
       P-Value [Acc > NIR] : 0.1077
##
##
##
                     Kappa: 0.2352
```

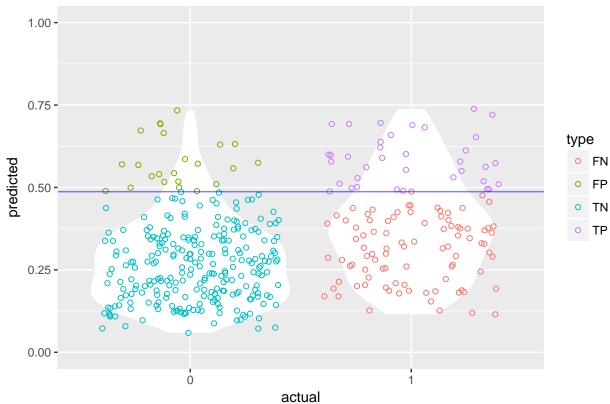
4.5. EXAMPLE 1

```
Mcnemar's Test P-Value: 7.402e-09
##
##
               Sensitivity: 0.2992
##
               Specificity: 0.9048
##
##
            Pos Pred Value: 0.5938
           Neg Pred Value: 0.7351
##
                Prevalence: 0.3175
##
            Detection Rate: 0.0950
##
##
     Detection Prevalence: 0.1600
##
         Balanced Accuracy: 0.6020
##
          'Positive' Class : 1
##
##
```

And bonus, we even gained some accuracy!

I have seen a very cool graph on this website that plots this tradeoff between specificity and sensitivity and shows how this cutoff point can enhance the understanding of the predictive power of our model.



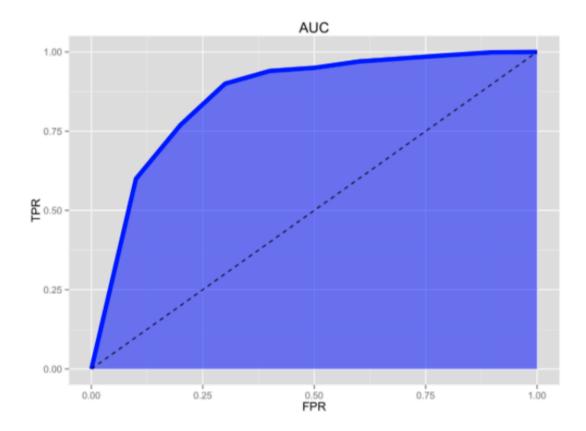


Last thing ... the AUC, aka Area Under the Curve.

The AUC is basically the area under the ROC curve.

You can think of the AUC as sort of a holistic number that represents how well your TP and FP is looking in aggregate.

4.6. EXAMPLE 2 21



AUC=1 -> GOOD

So in the context of an ROC curve, the more "up and left" it looks, the larger the AUC will be and thus, the better your classifier is. Comparing AUC values is also really useful when comparing different models, as we can select the model with the high AUC value, rather than just look at the curves.

In our situation with our model model_admission_lr, we can find our AUC with the ROCR package.

```
prediction_lr_admission <- predict(model_lr_admission, data = df2, type="response")
pr_admission <- prediction(prediction_lr_admission, df2$admit)
auc_admission <- performance(pr_admission, measure = "auc")

# and to get the exact value
auc_admission@y.values[[1]]</pre>
```

[1] 0.6928413

4.6 Example 2

In our second example we will use the *Pima Indians Diabetes Data Set* that can be downloaded on the UCI Machine learning website.

We are also dropping a clean version of the file as .csv on our github dataset folder.

The data set records females patients of at least 21 years old of Pima Indian heritage.

```
df <- read_csv("dataset/diabetes.csv")</pre>
```

The dataset has 768 observations and 9 variables.

Let's rename our variables with the proper names.

```
colnames(df) <- c("pregnant", "glucose", "diastolic",</pre>
                  "triceps", "insulin", "bmi", "diabetes", "age",
                  "test")
glimpse(df)
## Observations: 768
## Variables: 9
## $ pregnant <int> 6, 1, 8, 1, 0, 5, 3, 10, 2, 8, 4, 10, 10, 1, 5, 7, 0...
               <int> 148, 85, 183, 89, 137, 116, 78, 115, 197, 125, 110, ...
## $ glucose
## $ diastolic <int> 72, 66, 64, 66, 40, 74, 50, 0, 70, 96, 92, 74, 80, 6...
## $ triceps
               <int> 35, 29, 0, 23, 35, 0, 32, 0, 45, 0, 0, 0, 0, 23, 19,...
## $ insulin
               <int> 0, 0, 0, 94, 168, 0, 88, 0, 543, 0, 0, 0, 0, 846, 17...
               <dbl> 33.6, 26.6, 23.3, 28.1, 43.1, 25.6, 31.0, 35.3, 30.5...
## $ bmi
## $ diabetes <dbl> 0.627, 0.351, 0.672, 0.167, 2.288, 0.201, 0.248, 0.1...
## $ age
               <int> 50, 31, 32, 21, 33, 30, 26, 29, 53, 54, 30, 34, 57, ...
## $ test
               <int> 1, 0, 1, 0, 1, 0, 1, 0, 1, 1, 0, 1, 0, 1, 1, 1, 1, 1...
All variables seems to have been recorded with the appropriate type in the data frame. Let's just change
the type of the response variable to factor with positive and negative levels.
df$test <- factor(df$test)</pre>
#levels(df$output) <- c("negative", "positive")</pre>
Let's do our regression on the whole dataset.
model_diabetes_lr <- glm(test ~., data = df, family = "binomial")</pre>
summary(model_diabetes_lr)
##
## Call:
## glm(formula = test ~ ., family = "binomial", data = df)
## Deviance Residuals:
                      Median
       Min
                 1Q
                                    3Q
                                            Max
## -2.5566 -0.7274 -0.4159
                               0.7267
                                         2.9297
## Coefficients:
##
                 Estimate Std. Error z value Pr(>|z|)
## (Intercept) -8.4046964 0.7166359 -11.728 < 2e-16 ***
## pregnant
               0.1231823 0.0320776
                                        3.840 0.000123 ***
## glucose
                0.0351637 0.0037087
                                        9.481 < 2e-16 ***
## diastolic -0.0132955 0.0052336 -2.540 0.011072 *
## triceps
               0.0006190 0.0068994
                                      0.090 0.928515
## insulin
               -0.0011917 0.0009012 -1.322 0.186065
## bmi
                0.0897010 0.0150876
                                        5.945 2.76e-09 ***
               0.9451797 0.2991475
                                        3.160 0.001580 **
## diabetes
## age
                0.0148690 0.0093348
                                       1.593 0.111192
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
       Null deviance: 993.48 on 767 degrees of freedom
##
## Residual deviance: 723.45 on 759 degrees of freedom
## AIC: 741.45
##
```

4.6. EXAMPLE 2

```
## Number of Fisher Scoring iterations: 5
```

If we look at the z-statistic and the associated p-values, we can see that the variables triceps, insulin and age are not significant variables.

The logistic regression coefficients give the change in the log odds of the outcome for a one unit increase in the predictor variable. Hence, everything else being equals, any additional pregnancy increase the log odds of having diabetes (class_variable = 1) by another 0.1231.

We can see the confidence interval for each variables using the confint function.

```
confint(model_diabetes_lr)
```

```
## Waiting for profiling to be done...
                     2.5 %
                                  97.5 %
## (Intercept) -9.860319374 -7.0481062619
              0.060918463 0.1868558244
## pregnant
## glucose
               0.028092756 0.0426500736
## diastolic -0.023682464 -0.0031039754
              -0.012849460 0.0142115759
## triceps
## insulin
              -0.002966884 0.0005821426
## bmi
              0.060849478 0.1200608498
               0.365370025 1.5386561742
## diabetes
              -0.003503266 0.0331865712
## age
```

If we want to get the odds, we basically exponentiate the coefficients.

```
exp(coef(model_diabetes_lr))
```

```
## (Intercept) pregnant glucose diastolic triceps
## 0.0002238137 1.1310905981 1.0357892688 0.9867924485 1.0006191560
## insulin bmi diabetes age
## 0.9988090108 1.0938471417 2.5732758592 1.0149800983
```

In this way, for every additional year of age, the odds of getting diabetes (test = positive) is increasing by 1.015.

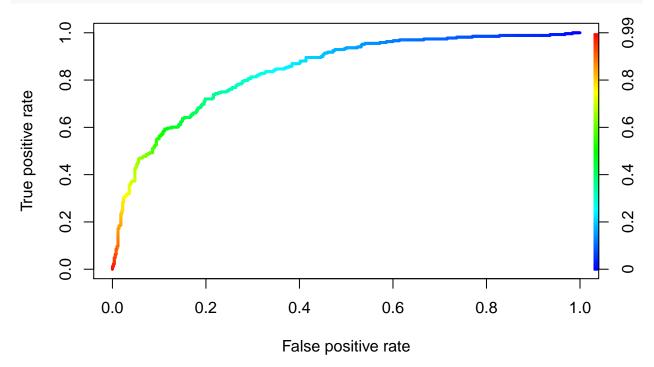
Let's have a first look at how our model perform

```
## Confusion Matrix and Statistics
##
## Reference
## Prediction 0 1
## 0 445 112
```

```
##
            1 55 156
##
                  Accuracy : 0.7826
##
                    95% CI : (0.7517, 0.8112)
##
##
       No Information Rate: 0.651
       P-Value [Acc > NIR] : 1.373e-15
##
##
##
                     Kappa: 0.4966
   Mcnemar's Test P-Value : 1.468e-05
##
##
##
               Sensitivity: 0.5821
##
               Specificity: 0.8900
            Pos Pred Value: 0.7393
##
            Neg Pred Value: 0.7989
##
##
                Prevalence: 0.3490
##
            Detection Rate: 0.2031
##
      Detection Prevalence: 0.2747
##
         Balanced Accuracy: 0.7360
##
          'Positive' Class : 1
##
##
```

Let's create our ROC curve

```
prediction_diabetes_lr <- predict(model_diabetes_lr, data = df, type="response")
pr_diabetes <- prediction(prediction_diabetes_lr, df$test)
prf_diabetes <- performance(pr_diabetes, measure = "tpr", x.measure = "fpr")
plot(prf_diabetes, colorize = TRUE, lwd = 3)</pre>
```



Let's find the best cutoff value for our model.

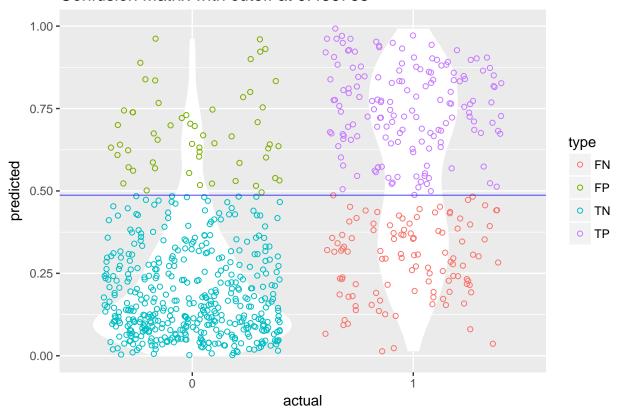
```
cost_diabetes_perf = performance(pr_diabetes, "cost")
pr_diabetes@cutoffs[[1]][which.min(cost_diabetes_perf@y.values[[1]])]
```

4.6. EXAMPLE 2 25

```
## 294
## 0.486768
```

Instead of redoing the whole violin-jitter graph for our model, let's create a function so we can reuse it at a later stage.

Confusion Matrix with cutoff at 0.486768



The accuracy of our model is slightly improved by using that new cutoff value.

4.6.1 Accounting for missing values

The UCI Machine Learning website note that there are no missing values on this dataset. That said, we have to be careful as there are many 0, when it is actually impossible to have such 0. So before we keep going let's fill in these values.

The first thing to to is to change these O into NA.

```
df2 <- df
#TODO Find a way to create a function and use map from purrr to do this
df2$glucose[df2$glucose == 0] <- NA
df2$diastolic[df2$diastolic == 0] <- NA
df2triceps[df2$triceps == 0] <- NA
df2$insulin[df2$insulin == 0] <- NA
df2$bmi[df2$bmi == 0] <- NA
library(visdat)
vis_dat(df2)
   800
   600
                                                                                  Type
Observations
                                                                                      factor
   400
                                                                                      integer
                                                                                      numeric
                                                                                      NA
  200
```

There are a lot of missing values ... too many of them really. If this was really life, it would be important to go back to the drawing board and redisigning the data collection phase.

Variables in Dataset

glm(formula = test ~ ., family = "binomial", data = df2)

```
model_diabetes_lr2 <- glm(test ~., data = df2, family = "binomial")
summary(model_diabetes_lr2)
##
## Call:</pre>
```

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```
##
## Deviance Residuals:
      Min
                1Q Median
                                          Max
## -2.7823 -0.6603 -0.3642 0.6409
                                        2.5612
##
## Coefficients:
                Estimate Std. Error z value Pr(>|z|)
## (Intercept) -1.004e+01 1.218e+00 -8.246 < 2e-16 ***
## pregnant
              8.216e-02 5.543e-02 1.482 0.13825
## glucose
               3.827e-02 5.768e-03 6.635 3.24e-11 ***
## diastolic -1.420e-03 1.183e-02 -0.120 0.90446
               1.122e-02 1.708e-02
## triceps
                                      0.657 0.51128
              -8.253e-04 1.306e-03 -0.632 0.52757
## insulin
              7.054e-02 2.734e-02 2.580 0.00989 **
## bmi
              1.141e+00 4.274e-01 2.669 0.00760 **
## diabetes
               3.395e-02 1.838e-02
                                     1.847 0.06474 .
## age
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## (Dispersion parameter for binomial family taken to be 1)
##
##
      Null deviance: 498.10 on 391 degrees of freedom
## Residual deviance: 344.02 on 383 degrees of freedom
     (376 observations deleted due to missingness)
## AIC: 362.02
## Number of Fisher Scoring iterations: 5
This leads to a very different results than previously.
Let's have a look at this new model performance
prediction_diabetes_lr2 <- predict(model_diabetes_lr2, data = df2, type="response")</pre>
prediction_diabetes_lr2 <- if_else(prediction_diabetes_lr2 > 0.5, 1, 0)
#prediction_diabetes_lr <- factor(prediction_diabetes_lr)</pre>
#levels(prediction_diabetes_lr) <- c("negative", "positive")</pre>
table(df2$test)
##
##
     0
        1
## 500 268
#confusionMatrix(data = prediction_diabetes_lr2,
#
                 reference = df2$test,
                positive = "1")
```

4.6.2 Imputting Missing Values

Now let's impute the missing values using the simputation package. A nice vignette is available here.

```
library(simputation)
df3 <- impute_lm(df2, formula = glucose ~ pregnant + diabetes + age | test)
df3 <- impute_rf(df3, formula = bmi ~ glucose + pregnant + diabetes + age | test)
df3 <- impute_rf(df3, formula = diastolic ~ bmi + glucose + pregnant + diabetes + age | test)
df3 <- impute_en(df3, formula = triceps ~ pregnant + bmi + diabetes + age | test)</pre>
```

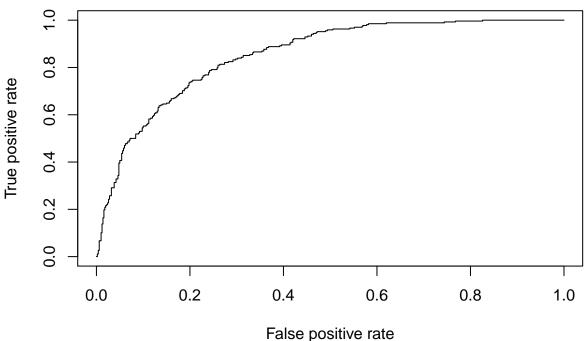
```
df3 <- impute_rf(df3, formula = insulin ~ . | test)</pre>
summary(df3)
##
      pregnant
                       glucose
                                      diastolic
                                                        triceps
   Min. : 0.000
                    Min. : 44.00
                                    Min. : 24.00
                                                     Min. : 7.00
                    1st Qu.: 99.75
  1st Qu.: 1.000
                                    1st Qu.: 64.00
                                                     1st Qu.:22.00
## Median : 3.000
                    Median :117.00
                                   Median : 72.00
                                                     Median :28.98
## Mean : 3.845
                    Mean :121.68
                                    Mean : 72.37
                                                     Mean :28.90
  3rd Qu.: 6.000
                    3rd Qu.:141.00
                                    3rd Qu.: 80.00
                                                     3rd Qu.:35.00
##
## Max.
         :17.000
                    Max. :199.00
                                    Max. :122.00
                                                     Max. :99.00
##
      insulin
                         bmi
                                      diabetes
                                                         age
                                                                    test
## Min.
         : 14.00
                    Min. :18.20
                                   Min.
                                          :0.0780
                                                    Min. :21.00
                                                                    0:500
## 1st Qu.: 92.39
                    1st Qu.:27.50
                                   1st Qu.:0.2437
                                                    1st Qu.:24.00
                                                                    1:268
## Median :135.00
                    Median :32.14
                                   Median :0.3725
                                                    Median :29.00
## Mean
          :155.64
                    Mean
                          :32.43
                                   Mean
                                          :0.4719
                                                    Mean
                                                           :33.24
## 3rd Qu.:190.59
                    3rd Qu.:36.60
                                   3rd Qu.:0.6262
                                                    3rd Qu.:41.00
                           :67.10
                                          :2.4200
## Max.
          :846.00
                    Max.
                                   Max.
                                                    Max.
                                                           :81.00
Ok we managed to get rid of the NAs. Let's run a last time our logistic model.
model_diabetes_lr3 <- glm(test ~ ., data = df3, family = "binomial")</pre>
summary(model_diabetes_lr3)
##
## glm(formula = test ~ ., family = "binomial", data = df3)
##
## Deviance Residuals:
                     Median
                                         Max
      Min
                10
                                  3Q
## -3.2740 -0.7047 -0.3880
                              0.7130
                                      2.3764
##
## Coefficients:
               Estimate Std. Error z value Pr(>|z|)
## (Intercept) -8.659337
                         0.822198 -10.532 < 2e-16 ***
                         0.032256
                                   3.946 7.93e-05 ***
## pregnant
              0.127297
## glucose
               0.031118
                        0.004148
                                   7.502 6.27e-14 ***
## diastolic
              -0.006848
                          0.008684 -0.789
                                            0.4304
               0.004388
                         0.014435
                                   0.304
                                            0.7611
## triceps
                                  2.443
## insulin
               0.003256
                         0.001333
                                            0.0146 *
                         ## bmi
               0.081986
## diabetes
               0.836483
                          0.297978
                                   2.807
                                            0.0050 **
               0.009776
                         0.009708
                                   1.007
## age
                                            0.3139
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
      Null deviance: 993.48 on 767 degrees of freedom
## Residual deviance: 705.44 on 759 degrees of freedom
## AIC: 723.44
## Number of Fisher Scoring iterations: 5
```

4.6. EXAMPLE 2

```
accuracy_model_lr3 <- predict(model_diabetes_lr3, data = df3, type="response")</pre>
accuracy_model_lr3 <- if_else(accuracy_model_lr3 > 0.5, "positive", "negative")
accuracy_model_lr3 <- factor(accuracy_model_lr3)</pre>
levels(accuracy_model_lr3) <- c("negative", "positive")</pre>
table(df3$test, accuracy_model_lr3)
##
      accuracy_model_lr3
##
       negative positive
##
            442
                       58
            112
                      156
##
     1
table(df3$test)
##
##
     0
## 500 268
#######
#confusionMatrix(data = accuracy_model_lr3,
#
                  reference = df3$test,
#
                  positive = "positive")
```

4.6.3 ROC and AUC

```
accuracy_model_lr3 <- predict(model_diabetes_lr3, data = df3, type="response")
pr <- prediction(accuracy_model_lr3, df3$test)
prf <- performance(pr, measure = "tpr", x.measure = "fpr")
plot(prf)</pre>
```



Let's go back to the ideal cut off point that would balance the sensitivity and specificity.

```
cost_diabetes_perf <- performance(pr, "cost")
pr@cutoffs[[1]][which.min(cost_diabetes_perf@y.values[[1]])]</pre>
```

```
## 10
## 0.4525332
```

So for maximum accuracy, the ideal cutoff point is 0.487194.

Let's redo our confusion matrix then and see some improvement.

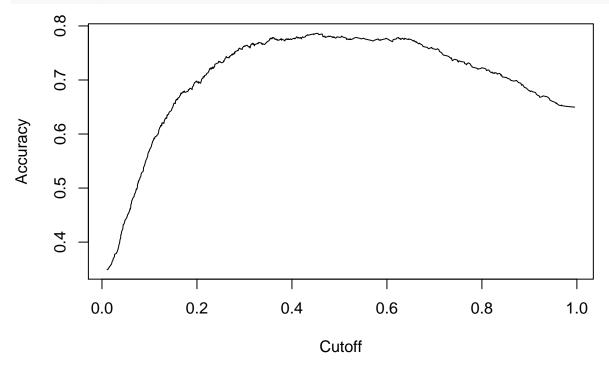
```
accuracy_model_lr3 <- predict(model_diabetes_lr3, data = df3, type="response")
accuracy_model_lr3 <- if_else(accuracy_model_lr3 >= 0.487194, "positive", "negative")

#confusionMatrix(data = accuracy_model_lr3,
# reference = df3$test,
# positive = "positive")
```

Another cost measure that is popular is overall accuracy. This measure optimizes the correct results, but may be skewed if there are many more negatives than positives, or vice versa. Let's get the overall accuracy for the simple predictions and plot it.

Actually the ROCR package can also give us a plot of accuracy for various cutoff points

```
accuracy_diabetes_lr3 <- performance(pr, measure = "acc")
plot(accuracy_diabetes_lr3)</pre>
```



Often in medical research for instance, there is a cost in having false negative is quite higher than a false positive.

Let's say the cost of missing someone having diabetes is 3 times the cost of telling someone that he has diabetes when in reality he/she doesn't.

```
cost_diabetes_perf <- performance(pr, "cost", cost.fp = 1, cost.fn = 3)
pr@cutoffs[[1]][which.min(cost_diabetes_perf@y.values[[1]])]</pre>
```

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0.2271368

Lastly, in regards to AUC

```
auc <- performance(pr, measure = "auc")
auc <- auc@y.values[[1]]
auc</pre>
```

[1] 0.8530075

4.7 References

- The Introduction is from the AV website
- Confusion plot. The webpage and the code
- The UCLA Institute for Digital Research and Education site where we got the dataset for our first example
- The UCI Machine learning site where we got the dataset for our second example
- $\bullet\,$ Function to use ROC with ggplot 2 - The Joy of Data and here as well

Trees and Classification

5.1 Introduction

Classification trees are non-parametric methods to recursively partition the data into more "pure" nodes, based on splitting rules.

Logistic regression vs Decision trees. It is dependent on the type of problem you are solving. Let's look at some key factors which will help you to decide which algorithm to use:

- If the relationship between dependent & independent variable is well approximated by a linear model, linear regression will outperform tree based model.
- If there is a high non-linearity & complex relationship between dependent & independent variables, a tree model will outperform a classical regression method.
- If you need to build a model which is easy to explain to people, a decision tree model will always do better than a linear model. Decision tree models are even simpler to interpret than linear regression!

The 2 main disadventages of Decision trees: **Over fitting**: Over fitting is one of the most practical difficulty for decision tree models. This problem gets solved by setting constraints on model parameters and pruning (discussed in detailed below).

Not fit for continuous variables: While working with continuous numerical variables, decision tree looses information when it categorizes variables in different categories.

Decision trees use multiple algorithms to decide to split a node in two or more sub-nodes. The creation of sub-nodes increases the homogeneity of resultant sub-nodes. In other words, we can say that purity of the node increases with respect to the target variable. Decision tree splits the nodes on all available variables and then selects the split which results in most homogeneous sub-nodes.

5.2 First example.

Let's do a CART on the iris dataset. This is the Hello World! of CART.

```
library(rpart)
library(rpart.plot)
data("iris")
str(iris)
```

```
## '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 0.4 0.3 0.2 0.2 0.1 ...
                  : Factor w/ 3 levels "setosa", "versicolor", ...: 1 1 1 1 1 1 1 1 1 1 ...
table(iris$Species)
##
##
       setosa versicolor virginica
##
           50
                      50
tree <- rpart(Species ~., data = iris, method = "class")</pre>
## n = 150
##
## node), split, n, loss, yval, (yprob)
##
         * denotes terminal node
##
## 1) root 150 100 setosa (0.33333333 0.33333333 0.33333333)
     2) Petal.Length< 2.45 50 0 setosa (1.00000000 0.00000000 0.00000000) *
##
     3) Petal.Length>=2.45 100 50 versicolor (0.00000000 0.50000000 0.50000000)
##
       6) Petal.Width< 1.75 54
                                 5 versicolor (0.00000000 0.90740741 0.09259259) *
##
##
       7) Petal.Width>=1.75 46
                                 1 virginica (0.00000000 0.02173913 0.97826087) *
```

The method-argument can be switched according to the type of the response variable. It is class for categorial, anova for numerical, poisson for count data and 'exp for survival data.

Important Terminology related to Decision Trees

Root Node: It represents entire population or sample and this further gets divided into two or more homogeneous sets.

Splitting: It is a process of dividing a node into two or more sub-nodes.

Decision Node: When a sub-node splits into further sub-nodes, then it is called decision node.

Leaf/ Terminal Node: Nodes do not split is called Leaf or Terminal node.

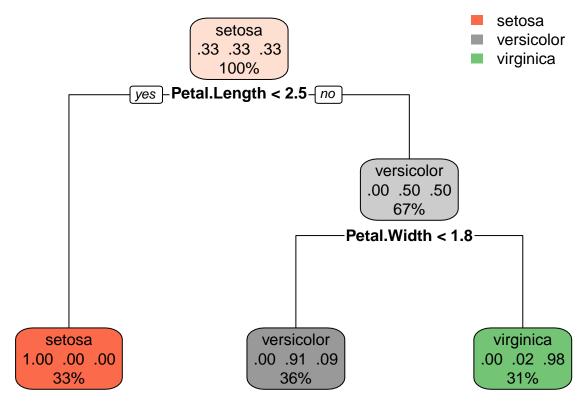
Pruning: When we remove sub-nodes of a decision node, this process is called pruning. You can say opposite process of splitting.

Branch / Sub-Tree: A sub section of entire tree is called branch or sub-tree.

Parent and Child Node: A node, which is divided into sub-nodes is called parent node of sub-nodes where as sub-nodes are the child of parent node.

```
rpart.plot(tree)
```

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This is a model with a **multi-class response**. Each node shows

- the predicted class (setosa, versicolor, virginica),
- the predicted probability of each class,
- the percentage of observations in the node

```
table(iris$Species, predict(tree, type = "class"))
##
##
                 setosa versicolor virginica
##
                     50
                                 0
     setosa
##
     versicolor
                      0
                                49
                                            1
##
     virginica
                      0
                                 5
                                           45
```

5.3 Second Example.

Data set is the titanic. This is a model with a binary response.

```
data("ptitanic")
str(ptitanic)

## 'data.frame': 1309 obs. of 6 variables:
## $ pclass : Factor w/ 3 levels "1st","2nd","3rd": 1 1 1 1 1 1 1 1 1 1 1 1 ...
## $ survived: Factor w/ 2 levels "died","survived": 2 2 1 1 1 2 2 1 2 1 ...
## $ sex : Factor w/ 2 levels "female","male": 1 2 1 2 1 2 1 2 1 2 ...
## $ age :Class 'labelled' atomic [1:1309] 29 0.917 2 30 25 ...
## ...- attr(*, "units")= chr "Year"
## ...- attr(*, "label")= chr "Age"
## $ sibsp :Class 'labelled' atomic [1:1309] 0 1 1 1 1 0 1 0 2 0 ...
## ...- attr(*, "label")= chr "Number of Siblings/Spouses Aboard"
```

```
## $ parch :Class 'labelled' atomic [1:1309] 0 2 2 2 2 0 0 0 0 0 ...
## ...- attr(*, "label") = chr "Number of Parents/Children Aboard"

ptitanic$age <- as.numeric(ptitanic$age)
ptitanic$sibsp <- as.integer(ptitanic$sibsp)
ptitanic$parch <- as.integer(ptitanic$parch)</pre>
```

Actually we can make the table more relevant.

```
round(prop.table(table(ptitanic$sex, ptitanic$survived), 1), 2)
```

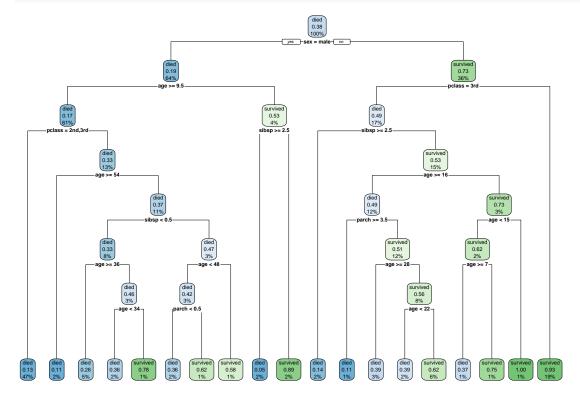
```
## died survived
## female 0.27 0.73
## male 0.81 0.19
```

One can see here that the sum of the percentage add to 1 horizontally. If one want to make it vertically, we use 2.

You can find the default limits by typing ?rpart.control. The first one we want to unleash is the cp parameter, this is the metric that stops splits that aren't deemed important enough. The other one we want to open up is minsplit which governs how many passengers must sit in a bucket before even looking for a split.

By putting a very low cp we are asking to have a very deep tree. The idea is that we prune it later. So in this first regression on ptitanic we'll set a very low cp.

```
library(rpart)
library(rpart.plot)
set.seed(123)
tree <- rpart(survived ~ ., data = ptitanic, cp=0.00001)
rpart.plot(tree)</pre>
```



Each node shows

- the predicted class (died or survived),
- the predicted probability of survival,
- the percentage of observations in the node.

Let's do a confusion matrix based on this tree.

```
conf.matrix <- round(prop.table(table(ptitanic$survived, predict(tree, type="class")), 2),
rownames(conf.matrix) <- c("Actually died", "Actually Survived")
colnames(conf.matrix) <- c("Predicted dead", "Predicted Survived")
conf.matrix
##</pre>
```

Predicted dead Predicted Survived
Actually died 0.83 0.16
Actually Survived 0.17 0.84

Let's learn a bit more about trees. By using the name function, one can see all the object inherent to the tree function.

A few intersting ones. The '\$where component indicates to which leaf the different observations have been assigned.

```
names(tree)
```

```
[1] "frame"
                                "where"
##
                                                        "call"
    [4] "terms"
                                "cptable"
                                                        "method"
##
    [7] "parms"
                                "control"
                                                        "functions"
## [10] "numresp"
                                "splits"
                                                        "csplit"
                                "v"
## [13] "variable.importance"
                                                        "ordered"
```

How to prune a tree? We want the cp value (with a simpler tree) that minimizes the xerror. So you need to find the lowest Cross-Validation Error. 2 ways to do this. Either the plotcp or the printcp functions. The plotcp is a visual representation of printcp function.

The problem with reducing the 'xerror is that the cross-validation error is a random quantity. There is no guarantee that if we were to fit the sequence of trees again using a different random seed that the same tree would minimize the cross-validation error.

A more robust alternative to minimum cross-validation error is to use the one standard deviation rule: choose the smallest tree whose cross-validation error is within one standard error of the minimum. Depending on how we define this there are two possible choices. The first tree whose point estimate of the cross-validation error falls within the \pm 1 xstd of the minimum. On the other hand the standard error lower limit of the tree of size three is within + 1 xstd of the minimum.

Either of these is a reasonable choice, but insisting that the point estimate itself fall within the standard error limits is probably the more robust solution.

As discussed earlier, the technique of setting constraint is a greedy-approach. In other words, it will check for the best split instantaneously and move forward until one of the specified stopping condition is reached. Let's consider the following case when you're driving: There are 2 lanes: A lane with cars moving at 80km/h A lane with trucks moving at 30km/h At this instant, you are a car in the fast lane and you have 2 choices: Take a left and overtake the other 2 cars quickly Keep moving in the present lane Lets analyze these choice. In the former choice, you'll immediately overtake the car ahead and reach behind the truck and start moving at 30 km/h, looking for an opportunity to move back right. All cars originally behind you move ahead in the meanwhile. This would be the optimum choice if your objective is to maximize the distance covered in next say 10 seconds. In the later choice, you sale through at same speed, cross trucks and then overtake maybe depending on situation ahead. Greedy you!

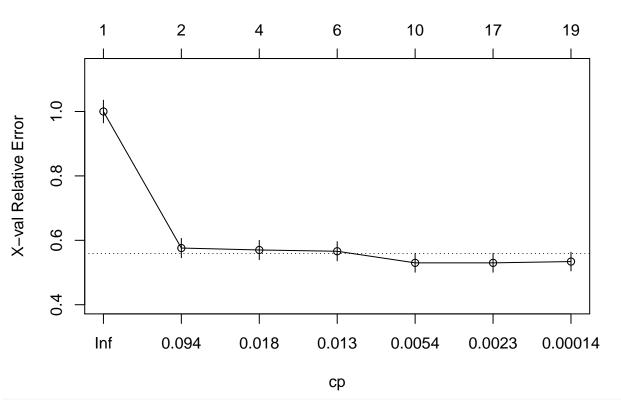
This is exactly the difference between normal decision tree & pruning. A decision tree with constraints won't see the truck ahead and adopt a greedy approach by taking a left. On the other hand if we use pruning, we in effect look at a few steps ahead and make a choice. So we know pruning is better.

printcp(tree)

```
##
## Classification tree:
## rpart(formula = survived \sim ., data = ptitanic, cp = 1e-05)
## Variables actually used in tree construction:
##
  [1] age
              parch pclass sex
                                    sibsp
##
## Root node error: 500/1309 = 0.38197
##
## n= 1309
##
##
            CP nsplit rel error xerror
                                            xstd
## 1 0.4240000
                    0
                          1.000 1.000 0.035158
## 2 0.0210000
                           0.576
                                 0.576 0.029976
                    1
## 3 0.0150000
                    3
                          0.534
                                 0.570 0.029863
                    5
## 4 0.0113333
                          0.504
                                 0.566 0.029787
## 5 0.0025714
                    9
                                  0.530 0.029076
                          0.458
## 6 0.0020000
                           0.440
                                  0.530 0.029076
                   16
## 7 0.0000100
                   18
                           0.436 0.534 0.029157
```

plotcp(tree)

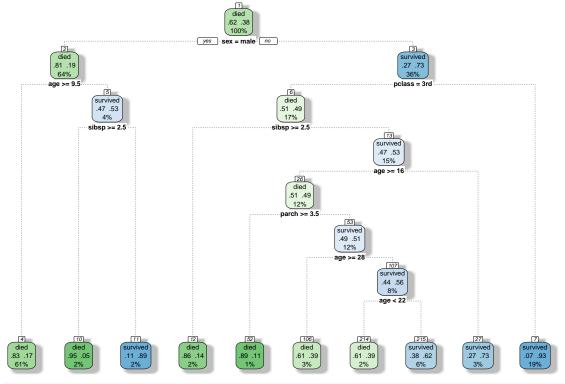
size of tree



tree\$cptable[which.min(tree\$cptable[,"xerror"]),"CP"]

[1] 0.002571429

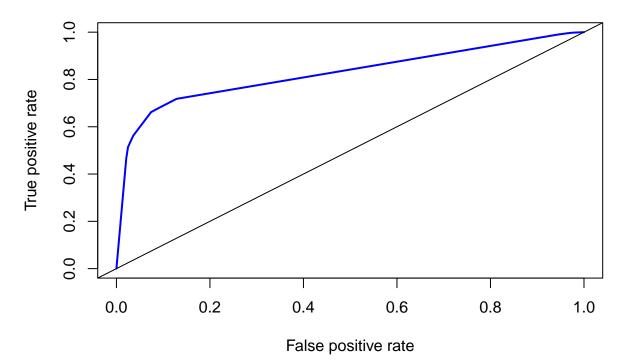
See if we can prune slightly the tree



```
conf.matrix <- round(prop.table(table(ptitanic$survived, predict(tree.pruned, type="class"))), 2)
rownames(conf.matrix) <- c("Actually died", "Actually Survived")
colnames(conf.matrix) <- c("Predicted dead", "Predicted Survived")
conf.matrix</pre>
```

```
##
## Predicted dead Predicted Survived
## Actually died 0.57 0.05
## Actually Survived 0.13 0.25
```

Another way to check the output of the classifier is with a ROC (Receiver Operating Characteristics) Curve. This plots the true positive rate against the false positive rate, and gives us a visual feedback as to how well our model is performing. The package we will use for this is ROCR.



ROC: Classification Trees on Titanic Dataset

Ordinarily, using the confusion matrix for creating the ROC curve would give us a single point (as it is based off True positive rate vs false positive rate). What we do here is ask the prediction algorithm to give class probabilities to each observation, and then we plot the performance of the prediction using class probability as a cutoff. This gives us the "smooth" ROC curve.

5.4 How does a tree decide where to split?

A bit more theory, before we go further. This part has been taken from this great tutorial.

5.5 Third example.

The dataset I will be using for this third example is the "Adult" dataset hosted on UCI's Machine Learning Repository. It contains approximately 32000 observations, with 15 variables. The dependent variable that in all cases we will be trying to predict is whether or not an "individual" has an income greater than \$50,000 a year.

Here is the set of variables contained in the data.

- age The age of the individual
- type_employer The type of employer the individual has. Whether they are government, military, private, an d so on.
- fnlwgt The # of people the census takers believe that observation represents. We will be ignoring this variable
- education The highest level of education achieved for that individual
- education_num Highest level of education in numerical form
- marital Marital status of the individual
- occupation The occupation of the individual

5.6. REFERENCES 41

• relationship – A bit more difficult to explain. Contains family relationship values like husband, father, and so on, but only contains one per observation. I'm not sure what this is supposed to represent

- race descriptions of the individuals race. Black, White, Eskimo, and so on
- sex Biological Sex
- capital_gain Capital gains recorded
- capital_loss Capital Losses recorded
- hr per week Hours worked per week
- country Country of origin for person
- income Boolean Variable. Whether or not the person makes more than \$50,000 per annum income.

5.6 References

- Trees with the rpart package
- Wholesale customers Data Set Origin of the data set of first example.
- Titanic: Getting Started With R Part 3: Decision Trees. First understanding on how to read the graph of a tree.
- Classification and Regression Trees (CART) with rpart and rpart.plot. Got the Titanic example from there as well as a first understanding on pruning.
- Statistical Consulting Group. We learn here how to use the ROC curve. And we got out of it the adultdataset.
- A Complete Tutorial on Tree Based Modeling from Scratch (in R & Python). This website is a real gems as always.
- Stephen Milborrow. rpart.plot: Plot rpart Models. An Enhanced Version of plot.rpart., 2016. R Package. It is important to cite the very generous people who dedicates so much of their time to offer us great tool.

Chapter 6

Principal Component Analysis

To create a predictive model based on regression we like to have as many relevant predictors as possible. The whole difficulty resides in finding *relevant* predictors. For predictors to be relevant, they should explain the variance of the dependent variable.

Too many predictors (high dimensionality) and we take the risk of over-fitting.

The intuition of Principal Component Analysis is to find new combination of variables which form larger variances. Why are larger variances important? This is a similar concept of entropy in information theory. Let's say you have two variables. One of them (Var 1) forms N(1, 0.01) and the other (Var 2) forms N(1, 1). Which variable do you think has more information? Var 1 is always pretty much 1 whereas Var 2 can take a wider range of values, like 0 or 2. Thus, Var 2 has more chances to have various values than Var 1, which means Var 2's entropy is larger than Var 1's. Thus, we can say Var 2 contains more information than Var 1.

PCA tries to find linear combination of the variables which contain much information by looking at the variance. This is why the standard deviation is one of the important metrics to determine the number of new variables in PCA. Another interesting aspect of the new variables derived by PCA is that all new variables are orthogonal. You can think that PCA is rotating and translating the data such that the first axis contains the most information, and the second has the second most information, and so forth.

Principal Component Analysis (PCA) is a feature extraction methods that use orthogonal linear projections to capture the underlying variance of the data. When PCR compute the principle components is not looking at the response but only at the predictors (by looking for a linear combination of the predictors that has the highest variance). It makes the assumption that the linear combination of the predictors that has the highest variance is associated with the response.

The algorithm when applied linearly transforms m-dimensional input space to n-dimensional (n < m) output space, with the objective to minimize the amount of information/variance lost by discarding (m-n) dimensions. PCA allows us to discard the variables/features that have less variance.

When choosing the principal component, we assume that the regression plane varies along the line and doesn't vary in the other orthogonal direction. By choosing one component and not the other, we're ignoring the second direction.

PCR looks in the direction of variation of the predictors to find the places where the responses is most likely to vary.

Some of the most notable advantages of performing PCA are the following:

- Dimensionality reduction
- Avoidance of multicollinearity between predictors. Variables are orthogonal, so including, say, PC9 in the model has no bearing on, say, PC3
- Variables are ordered in terms of standard error. Thus, they also tend to be ordered in terms of statistical significance

• Overfitting mitigation

The primary disadvantage is that this model is far more difficult to interpret than a regular logistic regression model

With principal components regression, the new transformed variables (the principal components) are calculated in a totally **unsupervised** way:

- the response Y is not used to help determine the principal component directions).
- the response does not supervise the identification of the principal components.
- PCR just looks at the x variables

The PCA method can dramatically improve estimation and insight in problems where multicollinearity is a large problem – as well as aid in detecting it.

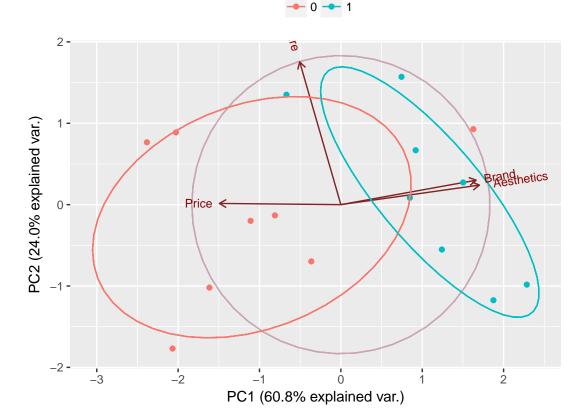
6.1 PCA on an easy example.

OS $\leftarrow c(0,0,0,0,1,0,0,0,1,1,0,1,1,1,1,1)$

library(ggbiplot)

Let's say we asked 16 participants four questions (on a 7 scale) about what they care about when choosing a new computer, and got the results like this.

```
Price \leftarrow c(6,7,6,5,7,6,5,6,3,1,2,5,2,3,1,2)
Software \leftarrow c(5,3,4,7,7,4,7,5,5,3,6,7,4,5,6,3)
Aesthetics \leftarrow c(3,2,4,1,5,2,2,4,6,7,6,7,5,6,5,7)
Brand \leftarrow c(4,2,5,3,5,3,1,4,7,5,7,6,6,5,5,7)
buy_computer <- tibble(Price, Software, Aesthetics, Brand)</pre>
Let's go on with the PCA. princomp is part of the stats package.
pca_buycomputer <- prcomp(buy_computer, scale = TRUE, center = TRUE)</pre>
names(pca_buycomputer)
## [1] "sdev"
                   "rotation" "center"
                                                      "x"
                                          "scale"
print(pca_buycomputer)
## Standard deviations:
## [1] 1.5589391 0.9804092 0.6816673 0.3792578
##
## Rotation:
                                 PC2
                                             PC3
                                                          PC4
##
                      PC1
## Price
              -0.5229138 0.00807487 -0.8483525 0.08242604
## Software -0.1771390 0.97675554 0.1198660 0.01423081
## Aesthetics 0.5965260 0.13369503 -0.2950727 0.73431229
## Brand
               0.5825287 0.16735905 -0.4229212 -0.67363855
summary(pca_buycomputer, loadings = TRUE)
## Warning: In summary.prcomp(pca_buycomputer, loadings = TRUE) :
    extra argument 'loadings' will be disregarded
## Importance of components:
##
                              PC1
                                      PC2
                                             PC3
                                                      PC4
## Standard deviation
                           1.5589 0.9804 0.6817 0.37926
## Proportion of Variance 0.6076 0.2403 0.1162 0.03596
## Cumulative Proportion 0.6076 0.8479 0.9640 1.00000
```



Remember that one of the disadventage of PCA is how difficult it is to interpret the model (ie. what does the PC1 is representing, what does PC2 is representing, etc.). The **biplot** graph help somehow to overcome that.

In the above graph, one can see that Brandand Aesthetic explain most of the variance in the new predictor PC1 while Software explain most of the variance in the new predictor PC2. It is also to be noted that Brand and Aesthetic are quite highly correlated.

Once you have done the analysis with PCA, you may want to look into whether the new variables can predict some phenomena well. This is kinda like machine learning: Whether features can classify the data well. Let's say you have asked the participants one more thing, which OS they are using (Windows or Mac) in your survey, and the results are like this.

```
OS <- c(0,0,0,0,1,0,0,0,1,1,0,1,1,1,1,1)
# Let's test our model
model1 <- glm(OS ~ pca_buycomputer$x[,1] + pca_buycomputer$x[,2], family = binomial)
summary(model1)
##
## Call:</pre>
```

glm(formula = OS ~ pca_buycomputer\$x[, 1] + pca_buycomputer\$x[,

2], family = binomial)

##

fitted(model1)

```
## Deviance Residuals:
##
       Min
                 1Q
                      Median
                                     30
                                             Max
                      0.1258
                                          1.2814
##
   -2.4485
            -0.4003
                                0.5652
##
##
  Coefficients:
##
                           Estimate Std. Error z value Pr(>|z|)
## (Intercept)
                            -0.2138
                                         0.7993
                                                 -0.268
                                                           0.7891
   pca_buycomputer$x[, 1]
                             1.5227
                                         0.6621
                                                  2.300
                                                           0.0215 *
  pca_buycomputer$x[, 2]
                             0.7337
                                         0.9234
                                                  0.795
                                                           0.4269
                   0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
  Signif. codes:
##
   (Dispersion parameter for binomial family taken to be 1)
##
##
##
       Null deviance: 22.181
                               on 15
                                      degrees of freedom
## Residual deviance: 11.338
                                      degrees of freedom
                               on 13
## AIC: 17.338
## Number of Fisher Scoring iterations: 5
```

Let's see how well this model predicts the kind of OS. You can use fitted() function to see the prediction.

```
## 1 2 3 4 5 6
## 0.114201733 0.009372181 0.217716320 0.066009817 0.440016243 0.031640529
## 7 8 9 10 11 12
```

0.036189119 0.175766013 0.906761064 0.855587371 0.950088045 0.888272270 ## 13 14 15 16 ## 0.781098710 0.757499202 0.842557931 0.927223453

These values represent the probabilities of being 1. For example, we can expect 11% chance that Participant 1 is using OS 1 based on the variable derived by PCA. Thus, in this case, Participant 1 is more likely to be using OS 0, which agrees with the survey response. In this way, PCA can be used with regression models for calculating the probability of a phenomenon or making a prediction.

I have tried to do the same with scaling the data using scale(x) and it changed absolutely nothing.

6.2 Attempt of PCA on technical indicators.

For this purpose, we have taken a random stock, added a lots of variables and have one dependent variable.

```
# Read the file
library(readr)
stock_data <- read_csv("AugmentedStockData/CVX.csv")</pre>
```

Now onto create our dependent variable and stipping down the data frame to just the columns that interest us, and only get rows and columns without NA.

```
library(dplyr)
binary = if_else(stock_data$ret3days[25:4150] > 0.03, 1, 0)
depend_var <- stock_data[25:4150,8:34]</pre>
```

The base R function prcomp() is used to perform PCA. PCA only works with normalized data. So we need to center the variable to have mean equals to zero. With parameter scale. = T, we normalize the

variables to have standard deviation equals to 1. Normalized predictors have mean equals to zero and standard deviation equals to one.

```
prin_comp <- prcomp(depend_var, scale. = TRUE, center = TRUE)</pre>
```

Let's have a closer look at that 'prcomp' function.

##

wma3

wma5

wma7

wma9

wma11

Center and scale refers to respective mean and standard deviation of the variables that are used for normalization prior to implementing PCA.

```
names(prin_comp)
## [1] "sdev"
                  "rotation" "center"
                                                    "x"
                                         "scale"
summary(prin_comp)
## Importance of components:
                             PC1
                                            PC3
                                                            PC5
##
                                     PC2
                                                    PC4
                                                                     PC6
## Standard deviation
                          3.3007 2.5311 1.6647 1.58184 1.12216 0.89194
## Proportion of Variance 0.4035 0.2373 0.1026 0.09268 0.04664 0.02947
## Cumulative Proportion 0.4035 0.6408 0.7434 0.83609 0.88273 0.91220
##
                              PC7
                                      PC8
                                               PC9
                                                      PC10
                                                              PC11
                          0.80601 0.63478 0.59745 0.53196 0.42057 0.39748
## Standard deviation
## Proportion of Variance 0.02406 0.01492 0.01322 0.01048 0.00655 0.00585
## Cumulative Proportion 0.93626 0.95118 0.96440 0.97488 0.98143 0.98728
                                              PC15
##
                             PC13
                                      PC14
                                                      PC16
## Standard deviation
                          0.36869 0.33376 0.18342 0.17136 0.14502 0.08488
## Proportion of Variance 0.00503 0.00413 0.00125 0.00109 0.00078 0.00027
## Cumulative Proportion 0.99232 0.99644 0.99769 0.99878 0.99956 0.99982
                             PC19
                                      PC20
                                              PC21
                                                      PC22
                                                               PC23
##
## Standard deviation
                          0.05953 0.02347 0.01988 0.01569 0.003083 0.002066
## Proportion of Variance 0.00013 0.00002 0.00001 0.00001 0.000000 0.000000
## Cumulative Proportion 0.99996 0.99998 0.99999 1.00000 1.000000 1.000000
##
                               PC25
                                          PC26
                                                    PC27
## Standard deviation
                          2.065e-15 1.629e-15 1.194e-15
## Proportion of Variance 0.000e+00 0.000e+00 0.000e+00
## Cumulative Proportion 1.000e+00 1.000e+00 1.000e+00
#outputs the mean of variables
prin_comp$center
##
                        wma5
                                                   wma9
                                                               wma11
           wma3
                                      wma7
## 2.621433e-05 7.849430e-05 1.321253e-04 1.852866e-04 2.367136e-04
       rsi 3val
                    rsi_3dir
                                 rsi_5val
                                               rsi 5dir
                                                            rsi 7val
## 5.249290e-01 2.259665e-01 5.219632e-01 5.112341e-02 5.198979e-01
##
       rsi_7dir
                    rsi_9val
                                 rsi_9dir
                                              rsi_11val
                                                           rsi_11dir
## 2.280991e-02 5.183530e-01 1.295840e-02 5.171323e-01 8.388109e-03
##
         11arup
                     11ardow
                                  11arosci
                                                 19arup
                                                             19ardow
## 5.318600e-01 4.556251e-01 7.623496e-02 5.355895e-01 4.540398e-01
##
       19arosci
                                   23ardow
                                               23arosci ave_vol3days
                      23arup
## 8.154961e-02 5.418344e-01 4.505785e-01 9.125587e-02 1.393280e-03
## ave_vol5days ave_vol7days
## 3.236529e-03 4.388667e-03
#outputs the standard deviation of variables
prin_comp$scale
```

```
0.01014433
                  0.01488609
                               0.01842084
                                            0.02129883
                                                         0.02378999
##
      rsi_3val
                  rsi_3dir
                                              rsi_5dir
##
                                 rsi_5val
                                                           rsi_7val
                 1.55382629
##
     0.25196379
                               0.19466505
                                            0.40810579
                                                         0.16395437
##
                                 rsi_9dir
      rsi_7dir
                   rsi_9val
                                             rsi_11val
                                                          rsi_11dir
##
     0.23886699
                  0.14412998
                              0.17015563
                                            0.13002831
                                                         0.13287362
##
                                                            19ardow
         11arup
                     11ardow
                                 11arosci
                                                19arup
##
     0.37456507
                  0.36908431
                               0.65809034
                                            0.36982907
                                                         0.36010315
                                              23arosci ave_vol3days
##
       19arosci
                      23arup
                                  23ardow
##
     0.64812635
                  0.36425219
                               0.35741487
                                            0.63505784
                                                         0.18659298
## ave_vol5days ave_vol7days
     0.22564569
                  0.24793982
```

The rotation measure provides the principal component loading. Each column of rotation matrix contains the principal component loading vector. This is the most important measure we should be interested in.

```
#because it can be a huge matrix, let's only check the first few rows and columns.
prin_comp$rotation[1:5, 1:5]
```

```
## PC1 PC2 PC3 PC4 PC5
## wma3 0.1788016 0.2543854 -0.00981180 -0.08087736 0.2431686
## wma5 0.2086344 0.2209183 0.02753808 -0.18315739 0.2465858
## wma7 0.2252186 0.1839885 0.04507260 -0.23309018 0.2168579
## wma9 0.2360512 0.1499467 0.05369872 -0.25316224 0.1770487
## wma11 0.2437448 0.1198431 0.05604151 -0.25599437 0.1376221
```

Let's plot the resultant principal components.

The prcomp() function also provides the facility to compute standard deviation of each principal component. sdev refers to the standard deviation of principal components.

```
#compute standard deviation of each principal component
std_dev <- prin_comp$sdev

#compute variance
pr_var <- std_dev^2

#check variance of first 10 components
pr_var[1:10]</pre>
```

```
## [1] 10.8943784 6.4065586 2.7713407 2.5022255 1.2592331 0.7955608
## [7] 0.6496465 0.4029457 0.3569417 0.2829776
```

We aim to find the components which explain the maximum variance. This is because, we want to retain as much information as possible using these components. So, higher is the explained variance, higher will be the information contained in those components.

To compute the proportion of variance explained by each component, we simply divide the variance by sum of total variance. This results in:

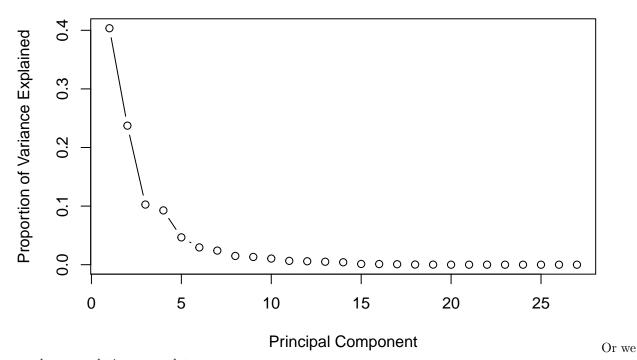
```
#proportion of variance explained
prop_varex <- pr_var/sum(pr_var)
prop_varex[1:20]</pre>
```

```
## [1] 4.034955e-01 2.372799e-01 1.026422e-01 9.267502e-02 4.663826e-02 ## [6] 2.946522e-02 2.406098e-02 1.492391e-02 1.322006e-02 1.048065e-02 ## [11] 6.550995e-03 5.851611e-03 5.034607e-03 4.125722e-03 1.246026e-03 ## [16] 1.087586e-03 7.789197e-04 2.668137e-04 1.312590e-04 2.039572e-05
```

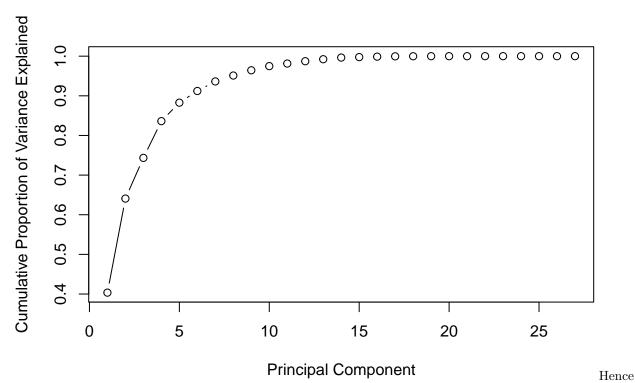
This shows that first principal component explains 41.7% variance. Second component explains 23.8%

variance. Third component explains 10.4% variance and so on. So, how do we decide how many components should we select for modeling stage?

The answer to this question is provided by a scree plot. A scree plot is used to access components or factors which explains the most of variability in the data. It represents values in descending order.



can do a cumulative scree plot



in this case the first 6 Principal Components explain over 90% of the variance of the data. That is we can use these first 6 PC as predictor in our next model.

Let's apply this now on a logisite regression model. For this, we need to create our binary dependent variable. So we'll put a 1 for every ret3days > 3%, 0 otherwise.

```
mydata <- cbind(binary, prin_comp$x)
mydata <- as.data.frame(mydata)
model1 <- glm(binary ~ PC1 + PC2 + PC5 + PC6 + PC7, data = mydata, family=binomial)
summary(model1)</pre>
```

```
##
## Call:
##
  glm(formula = binary ~ PC1 + PC2 + PC5 + PC6 + PC7, family = binomial,
##
       data = mydata)
##
## Deviance Residuals:
##
       Min
                 10
                      Median
                                    3Q
                                            Max
##
  -1.5159
           -0.5197
                     -0.4511
                              -0.3740
                                         2.4644
##
## Coefficients:
##
               Estimate Std. Error z value Pr(>|z|)
## (Intercept) -2.15924
                           0.05268 -40.989
                                            < 2e-16 ***
               -0.11636
                                     -7.685 1.53e-14 ***
## PC1
                           0.01514
## PC2
                0.03253
                           0.01815
                                      1.793
                                              0.0731
## PC5
               -0.05541
                           0.04094
                                     -1.353
                                              0.1760
## PC6
               -0.08353
                           0.05546
                                     -1.506
                                              0.1320
               -0.04292
## PC7
                           0.05665
                                     -0.758
                                              0.4486
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## (Dispersion parameter for binomial family taken to be 1)
```

```
##
##
       Null deviance: 2851.7 on 4125 degrees of freedom
## Residual deviance: 2784.3 on 4120 degrees of freedom
## AIC: 2796.3
## Number of Fisher Scoring iterations: 5
mydata <- cbind(binary, prin_comp$x)</pre>
mydata <- as.data.frame(mydata)</pre>
checkit <- fitted(model1)</pre>
checkit <- cbind(binary, checkit)</pre>
checkit <- as.data.frame(checkit)</pre>
head(checkit %>% filter(binary == 1), 20)
##
      binary
                checkit
## 1
           1 0.18260120
## 2
           1 0.18252003
## 3
          1 0.21606180
## 4
           1 0.21251118
## 5
           1 0.11869114
## 6
           1 0.14243678
## 7
           1 0.15250266
## 8
           1 0.08137055
## 9
           1 0.09081918
## 10
           1 0.07178808
## 11
           1 0.08675686
## 12
           1 0.08601504
## 13
           1 0.05538413
## 14
           1 0.13325771
## 15
           1 0.11428528
## 16
           1 0.13216528
## 17
           1 0.08095967
## 18
           1 0.07966423
## 19
           1 0.09559465
## 20
           1 0.16822463
head(checkit %>% filter(checkit > 0.2), 20)
      binary checkit
## 1
           0 0.2199392
## 2
           1 0.2160618
## 3
           1 0.2125112
```

```
0 0.2136409
## 5
           1 0.2187997
## 6
           1 0.2116685
## 7
           0 0.2070526
## 8
           0 0.2038604
## 9
           0 0.2097841
## 10
           0 0.2034205
## 11
           0 0.2187273
## 12
           1 0.2275500
## 13
           1 0.2281150
## 14
           0 0.2183669
## 15
           0 0.2060439
## 16
           0 0.2201554
```

```
## 17
           0 0.2692442
## 18
           1 0.2772148
## 19
           1 0.2574167
## 20
           1 0.2005783
```

Really not very successful model.

6.3 Doing PCA and PCR with the PLS package

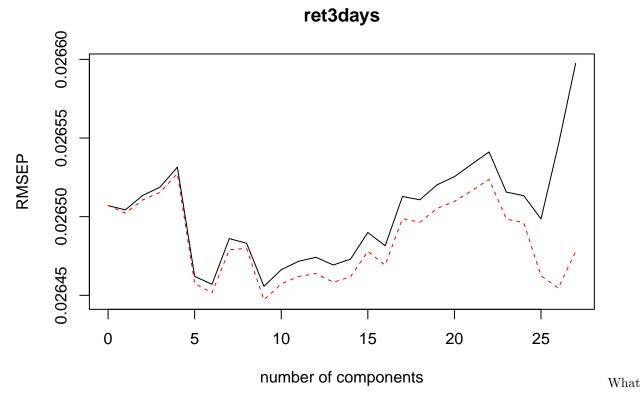
Same as before we can not have NA data in our set.

```
library(pls)
##
## Attaching package: 'pls'
## The following object is masked from 'package:caret':
##
##
       R2
## The following object is masked from 'package:stats':
##
##
       loadings
depend_var <- stock_data[25:4150,8:35]</pre>
pcr_model <- pcr(ret3days~., data = depend_var, scale = TRUE, validation = "CV")</pre>
In oder to print out the results, simply use the summary function as below
summary(pcr_model)
## Data:
            X dimension: 4126 27
## Y dimension: 4126 1
## Fit method: svdpc
## Number of components considered: 27
## VALIDATION: RMSEP
## Cross-validated using 10 random segments.
##
          (Intercept) 1 comps 2 comps 3 comps 4 comps 5 comps 6 comps
## CV
             0.02651
                       0.0265 0.02651 0.02652 0.02653 0.02646
             0.02651
                        0.0265 0.02651 0.02652 0.02653 0.02646
## adjCV
                                                                    0.02645
##
         7 comps 8 comps 9 comps 10 comps 11 comps 12 comps 13 comps
## CV
         0.02649 0.02648 0.02646
                                    0.02647
                                                0.02647
                                                          0.02647
                                                                    0.02647
## adjCV 0.02648 0.02648 0.02645
                                      0.02646
                                                0.02646
                                                          0.02646
                                                                    0.02646
##
          14 comps 15 comps 16 comps 17 comps 18 comps 19 comps
## CV
          0.02647
                     0.02649
                             0.02648
                                       0.02651
                                                   0.02651
                                                             0.02652
## adjCV
         0.02646
                     0.02648
                              0.02647
                                        0.02650
                                                   0.02650
                                                             0.02651
                             22 comps 23 comps 24 comps 25 comps
##
         20 comps 21 comps
## CV
          0.02653
                     0.02653
                              0.02654
                                       0.02652
                                                  0.02651
                                                             0.02650
                              0.02652
                                                  0.02650
## adjCV
          0.02651
                     0.02652
                                       0.02650
                                                             0.02646
##
          26 comps 27 comps
## CV
          0.02655
                     0.02660
## adjCV
          0.02645
                     0.02648
##
## TRAINING: % variance explained
            1 comps 2 comps 3 comps 4 comps 5 comps 6 comps 7 comps
##
```

##	X	40.3495	64.0775	74.3418	83.609 88	8.2731	91.22 93.626
##	ret3days	0.2797	0.3122	0.3381	0.359	0.9058	1.09 1.103
##		8 comps	9 comps	10 comps	11 comps	12 comps	13 comps
##	X	95.118	96.440	97.488	98.14	98.728	99.232
##	ret3days	1.122	1.521	1.523	1.56	1.685	1.738
##		14 comps	15 comps	16 compa	s 17 compa	s 18 comp	s 19 comps
##	X	99.644	99.769	99.87	99.95	6 99.98	2 99.996
##	ret3days	1.745	1.746	1.79	6 1.79	7 1.84	7 1.865
##		20 comps	21 comps	22 compa	s 23 compa	s 24 comp	s 25 comps
##	X	100.0	99.999	100.00	0 100.000	0 100.00	0 100.000
##	ret3days	1.9	1.997	2.01	7 2.16	6 2.21	5 2.268
##		26 comps	27 comps				
##	X	100.000	100.000				
##	ret3days	2.594	2.632				

As you can see, two main results are printed, namely the validation error and the cumulative percentage of variance explained using n components. The cross validation results are computed for each number of components used so that you can easily check the score with a particular number of components without trying each combination on your own. The pls package provides also a set of methods to plot the results of PCR. For example you can plot the results of cross validation using the validationplot function. By default, the pcr function computes the root mean squared error and the validationplot function plots this statistic, however you can choose to plot the usual mean squared error or the R2 by setting the val.type argument equal to "MSEP" or "R2" respectively

Plot the root mean squared error
validationplot(pcr_model)



you would like to see is a low cross validation error with a lower number of components than the number of variables in your dataset. If this is not the case or if the smalles cross validation error occurs with a number of components close to the number of variables in the original data, then no dimensionality reduction occurs. In the example above, it looks like 3 components are enough to explain more than 90% of the variability

in the data. Now you can try to use PCR on a traning-test set and evaluate its performance using, for example, using only 6 components

```
# Train-test split
train <- stock_data[25:3000,8:35]
y_test <- stock_data[3001:4150,35]
test <- stock_data[3001:4150,8:34]

pcr_model <- pcr(ret3days~., data = train,scale =TRUE, validation = "CV")

pcr_pred <- predict(pcr_model, test, ncomp = 6)
mean((pcr_pred - y_test)^2)</pre>
```

[1] 0.0005600123

6.4 References.

Here are the articles I have consulted for this research.

- Principal Component Analysis (PCA)
- Principal Component Analysis using R
- Computing and visualizing PCA in R This is where we learned about the 'ggbiplot
- Practical Guide to Principal Component Analysis (PCA) in R & Python
- Performing Principal Components Regression (PCR) in R
- Data Mining Principal Component (Analysis|Regression) (PCA)
- PRINCIPAL COMPONENT ANALYSIS IN R A really nice explanation on the difference between the main packages doing PCA such as svd, princompand prcomp. In R there are two general methods to perform PCA without any missing values: The spectral decomposition method of analysis examines the covariances and correlations between variables, whereas the singular value decomposition method looks at the covariances and correlations among the samples. While both methods can easily be performed within R, the singular value decomposition method is the preferred analysis for numerical accuracy.

Although principal component analysis assumes multivariate normality, this is not a very strict assumption, especially when the procedure is used for data reduction or exploratory purposes. Undoubtedly, the correlation and covariance matrices are better measures of similarity if the data is normal, and yet, PCA is often unaffected by mild violations. However, if the new components are to be used in further analyses, such as regression analysis, normality of the data might be more important.

Chapter 7

Case Study - Mushrooms Classification

This chapter demonstrates how to classify multiprooms as edible or not. It also answers the question: what are the main characteristics of an edible mushroom?

This blog post gave us first the idea and we followed most of it. We also noticed that Kaggle has put online the same data set and classification exercise. We have taken inspiration from some posts here and here

The data set is available on the Machine Learning Repository of the UC Irvine website.

7.1 Import the data

The data set is given to us in a rough form and quite a bit of editing is necessary.

```
# Load the data - we downloaded the data from the website and saved it into a .csv file
library(readr)
library(dplyr)

mushroom <- read_csv("dataset/Mushroom.csv", col_names = FALSE)
glimpse(mushroom)</pre>
```

```
## Observations: 8,124
## Variables: 23
"p",
                          "x",
      <chr> "x", "x", "b", "x",
                              "x", "b", "b",
                                          "x",
                                              "b",
## $ X2
               "s",
                  "s", "y", "s",
                              "v",
                                  "s",
                                              "s"
## $ X3
      <chr> "s",
                                  "w", "w",
      <chr> "n", "y", "w", "w", "g", "y",
                                          "w",
      <chr> "t", "t", "t", "t", "f",
                              "t",
                                  "t",
                                      "t",
                                          "t",
## $ X5
              "a", "l", "p",
                                  "a",
                          "n",
                              "a",
                                      "1",
## $ X6
                   "f",
      <chr> "f",
               "f",
                      "f",
                          "f".
                              "f".
                                  "f",
                                      "f".
                                          "f".
## $ X7
                  "c",
                                  "c",
                      "c",
               "c",
                   "b", "n",
                          "b",
                                      "b",
                                          "n",
## $ X9 <chr> "n", "b",
                              "b", "b",
                                                 "b",
                                              "b".
                  "n",
                      "n", "k",
                              "n",
                                  "g",
                                     "n"
## $ X10 <chr> "k",
              "k",
                                          "p",
## $ X11 <chr> "e", "e", "e", "e", "t",
                              "e", "e", "e", "e",
                                             "e",
                                                 "e", "e"...
```

```
"w",
       "w",
        "w", "w",
             "w",
## $ X15 <chr> "w", "w",
              "w".
                "w".
                  "w"
                   "w".
## $ X22 <chr> "s", "n", "n", "s", "a", "n", "n", "s", "v", "s",
                   "n".
## $ X23 <chr> "u", "g", "m", "u", "g", "g", "m", "m", "g", "m", "g", "m"...
```

Basically we have 8124 mushrooms in the dataset. And each observation consists of 23 variables. As it stands, the data frame doesn't look very meaningfull. We have to go back to the source to bring meaning to each of the variables and to the various levels of the categorical variables.

7.2 Tidy the data

This is the least fun part of the workflow.

We'll start by giving names to each of the variables, then we specify the category for each variable. It is not necessary to do so but it does add meaning to what we do.

```
# Rename the variables
colnames(mushroom) <- c("edibility", "cap shape", "cap surface",</pre>
                         "cap_color", "bruises", "odor",
                         "gill_attachement", "gill_spacing", "gill_size",
                         "gill_color", "stalk_shape", "stalk_root",
                         "stalk_surface_above_ring", "stalk_surface_below_ring", "stalk_color_above_ring
                         "stalk_color_below_ring", "veil_type", "veil_color",
                         "ring_number", "ring_type", "spore_print_color",
                         "population", "habitat")
# Defining the levels for the categorical variables
## We make each variable as a factor
library(purrr)
mushroom <- mushroom %>% map df(function(.x) as.factor(.x))
## We redefine each of the category for each of the variables
levels(mushroom$edibility) <- c("edible", "poisonous")</pre>
levels(mushroom$cap_shape) <- c("bell", "conical", "flat", "knobbed", "sunken", "convex")</pre>
levels(mushroom$cap_color) <- c("buff", "cinnamon", "red", "gray", "brown", "pink",</pre>
                                  "green", "purple", "white", "yellow")
levels(mushroom$cap_surface) <- c("fibrous", "grooves", "scaly", "smooth")</pre>
levels(mushroom$bruises) <- c("no", "yes")</pre>
levels(mushroom$odor) <- c("almond", "creosote", "foul", "anise", "musty", "none", "pungent", "spicy",</pre>
levels(mushroom$gill_attachement) <- c("attached", "free")</pre>
levels(mushroom$gill_spacing) <- c("close", "crowded")</pre>
levels(mushroom$gill_size) <- c("broad", "narrow")</pre>
levels(mushroom$gill_color) <- c("buff", "red", "gray", "chocolate", "black", "brown", "orange",</pre>
                                   "pink", "green", "purple", "white", "yellow")
levels(mushroom$stalk_shape) <- c("enlarging", "tapering")</pre>
levels(mushroom$stalk_root) <- c("missing", "bulbous", "club", "equal", "rooted")</pre>
levels(mushroom$stalk_surface_above_ring) <- c("fibrous", "silky", "smooth", "scaly")</pre>
levels(mushroom$stalk_surface_below_ring) <- c("fibrous", "silky", "smooth", "scaly")</pre>
```

7.2. TIDY THE DATA 57

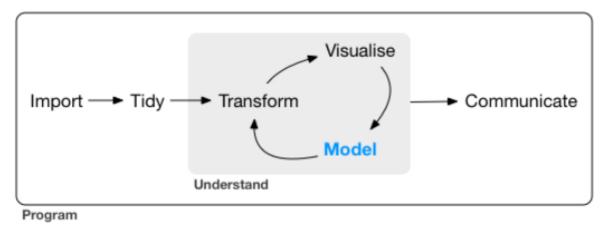
```
levels(mushroom$stalk_color_above_ring) <- c("buff", "cinnamon", "red", "gray", "brown", "pink",</pre>
                                 "green", "purple", "white", "yellow")
levels(mushroom$stalk_color_below_ring) <- c("buff", "cinnamon", "red", "gray", "brown", "pink",</pre>
                                 "green", "purple", "white", "yellow")
levels(mushroom$veil_type) <- "partial"</pre>
levels(mushroom$veil_color) <- c("brown", "orange", "white", "yellow")</pre>
levels(mushroom$ring_number) <- c("none", "one", "two")</pre>
levels(mushroom$ring type) <- c("evanescent", "flaring", "large", "none", "pendant")</pre>
levels(mushroom$spore_print_color) <- c("buff", "chocolate", "black", "brown", "orange",</pre>
                                         "green", "purple", "white", "yellow")
levels(mushroom$population) <- c("abundant", "clustered", "numerous", "scattered", "several", "solitary</pre>
levels(mushroom$habitat) <- c("wood", "grasses", "leaves", "meadows", "paths", "urban", "waste")</pre>
glimpse(mushroom)
## Observations: 8,124
## Variables: 23
## $ edibility
                               <fctr> poisonous, edible, edible, poisonous...
## $ cap_shape
                               <fctr> convex, convex, bell, convex, convex...
## $ cap_surface
                              <fctr> scaly, scaly, scaly, smooth, scaly, ...
## $ cap_color
                               <fctr> brown, yellow, white, white, gray, y...
## $ bruises
                               <fctr> yes, yes, yes, no, yes, yes, ye...
## $ odor
                               <fctr> pungent, almond, anise, pungent, non...
## $ gill_attachement
                              <fctr> free, free, free, free, free, free, ...
## $ gill spacing
                              <fctr> close, close, close, crowded,...
## $ gill_size
                              <fctr> narrow, broad, broad, narrow, broad,...
## $ gill_color
                              <fctr> black, black, brown, brown, black, b...
## $ stalk_shape
                               <fctr> enlarging, enlarging, enlarging, enl...
## $ stalk_root
                               <fctr> equal, club, club, equal, equal, clu...
## $ stalk_surface_above_ring <fctr> smooth, smooth, smooth, smooth, smooth, smoo...
## $ stalk_surface_below_ring <fctr> smooth, smooth, smooth, smooth, smooth, smoo...
## $ stalk_color_above_ring
                               <fctr> purple, purple, purple, purple, purp...
## $ stalk_color_below_ring
                               <fctr> purple, purple, purple, purple, purp...
## $ veil_type
                               <fctr> partial, partial, partial, ...
## $ veil color
                               <fctr> white, white, white, white, w...
## $ ring_number
                               <fctr> one, one, one, one, one, one, o...
## $ ring_type
                               <fctr> pendant, pendant, pendant, ...
## $ spore_print_color
                               <fctr> black, brown, brown, black, brown, b...
## $ population
                               <fctr> scattered, numerous, numerous, scatt...
## $ habitat
                               <fctr> urban, grasses, meadows, urban, gras...
As each variables is categorical, let's see how many categories are we speaking about?
library(tibble)
number_class <- function(x){</pre>
 x <- length(levels(x))
}
x <- mushroom %>% map_dbl(function(.x) number_class(.x)) %>% as_tibble() %>%
       rownames_to_column() %>% arrange(desc(value))
colnames(x) <- c("Variable name", "Number of levels")</pre>
print(x)
```

A tibble: 23×2

```
##
              `Variable name` `Number of levels`
##
                         <chr>
                                             <dbl>
## 1
                   gill_color
                                                12
##
  2
                                                10
                    cap_color
##
  3
      stalk_color_above_ring
                                                10
      stalk_color_below_ring
## 4
                                                10
                                                 9
## 5
## 6
           spore_print_color
                                                 9
## 7
                      habitat
                                                 7
## 8
                    cap_shape
                                                 6
## 9
                   population
                                                 6
## 10
                                                 5
                   stalk_root
## # ... with 13 more rows
```

7.3 Understand the data

This is the circular phase of our dealing with data. This is where each of the transforming, visualizing and modeling stage reinforce each other to create a better understanding.



7.3.1 A. Transform the data

map dbl(mushroom, function(.x) {sum(is.na(.x))})

We noticed from the previous section an issue with the veil_type variable. It has only one factor. So basically, it does not bring any information. Furthermore, factor variable with only one level do create issues later on at the modeling stage. R will throw out an error for the categorical variable that has only one level. So let's take away that column.

```
mushroom <- mushroom %>% select(- veil_type)
```

Do we have any missing data? Most ML algorithms won't work if we have missing data.

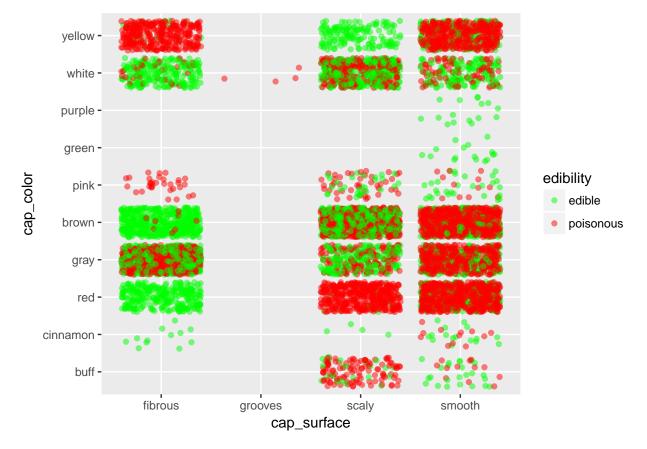
```
##
                                               cap_shape
                   edibility
                                                                         cap_surface
##
                             0
                                                        0
                                                                                    0
##
                                                                                 odor
                   cap_color
                                                  bruises
##
                                                        0
                                                                                    0
##
            gill attachement
                                            gill_spacing
                                                                           gill_size
##
                                                                                    0
```

##	gill_color	stalk_shape	stalk_root
##	0	0	0
##	stalk_surface_above_ring	stalk_surface_below_ring	stalk_color_above_ring
##	0	0	0
##	stalk_color_below_ring	veil_color	ring_number
##	0	0	0
##	ring_type	spore_print_color	population
##	0	0	0
##	habitat		
##	0		

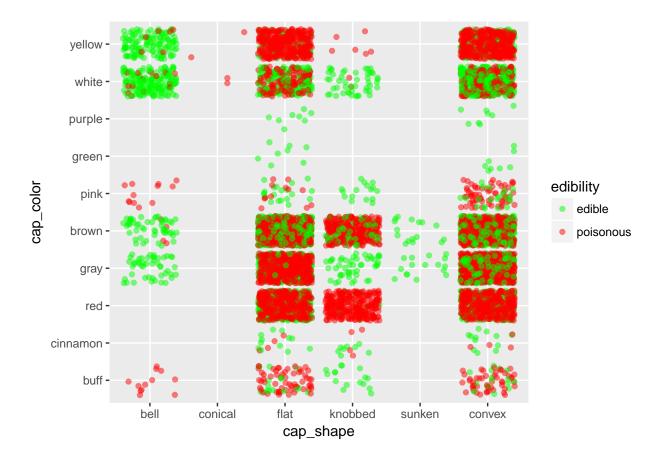
Lucky us! We have no missing data.

7.3.2 A. Visualize the data

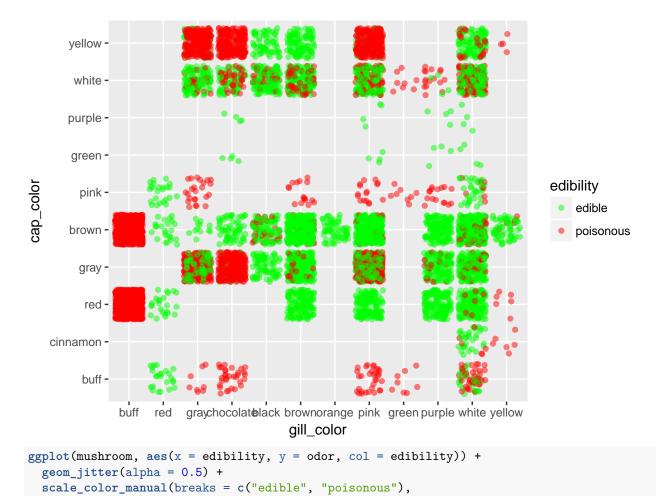
This is one of the most important step in the DS process. This stage can gives us unexpected insights and often allows us to ask the right questions.



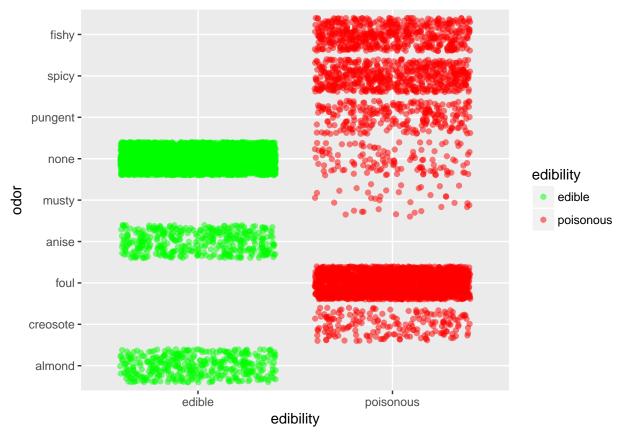
If we want to stay safe, better bet on fibrous surface. Stay especially away from smooth surface, except if they are purple or green.



Again, in case one don't know about mushroom, it is better to stay away from all shapes except maybe for bell shape mushrooms.



values = c("green", "red"))



Odor is defintely quite an informative predictor. Basically, if it smells fishy, spicy or pungent just stay away. If it smells like anise or almond you can go ahead. If it doesn't smell anything, you have better chance that it is edible than not.

TO DO: put a comment on what we see TO DO: put a mosaic graph

7.3.3 A. Modeling

At this stage, we should have gathered enough information and insights on our data to choose appropriate modeling techniques.

Before we go ahead, we need to split the data into a training and testing set

```
set.seed(1810)
mushsample <- caret::createDataPartition(y = mushroom$edibility, times = 1, p = 0.8, list = FALSE)
train_mushroom <- mushroom[mushsample, ]
test_mushroom <- mushroom[-mushsample, ]

We can check the quality of the splits in regards to our predicted (dependent) variable.
round(prop.table(table(mushroom$edibility)), 2)</pre>
```

```
##
## edible poisonous
## 0.52 0.48
round(prop.table(train_mushroom$edibility)), 2)
```

```
##
      edible poisonous
##
        0.52
                   0.48
round(prop.table(table(test_mushroom$edibility)), 2)
##
##
      edible poisonous
##
        0.52
                   0.48
It seems like we have the right splits.
```

7.3.3.1 A. Use of Regression Tree

As we have many categorical variables, regression tree is an ideal classification tools for such situation.

```
We'll use the rpart package. Let's give it a try without any customization.
library(rpart)
library(rpart.plot)
set.seed(1810)
model_tree <- rpart(edibility ~ ., data = train_mushroom, method = "class")</pre>
model_tree
## n= 6500
##
## node), split, n, loss, yval, (yprob)
##
         * denotes terminal node
##
## 1) root 6500 3133 edible (0.51800000 0.48200000)
     2) odor=almond,anise,none 3468 101 edible (0.97087659 0.02912341)
##
     4) spore_print_color=buff,chocolate,black,brown,orange,purple,white,yellow 3408 41 edible (0.98796
##
##
       5) spore_print_color=green 60
                                         0 poisonous (0.00000000 1.00000000) *
    3) odor=creosote, foul, musty, pungent, spicy, fishy 3032 0 poisonous (0.00000000 1.00000000) *
caret::confusionMatrix(data=predict(model_tree, type = "class"),
                        reference = train_mushroom$edibility,
                        positive="edible")
## Confusion Matrix and Statistics
##
##
              Reference
## Prediction edible poisonous
##
     edible
                 3367
                              41
##
     poisonous
                    0
                            3092
##
                  Accuracy: 0.9937
##
##
                    95% CI: (0.9915, 0.9955)
##
       No Information Rate: 0.518
       P-Value [Acc > NIR] : < 2.2e-16
##
```

Kappa: 0.9874 Mcnemar's Test P-Value: 4.185e-10 ## ## Sensitivity: 1.0000 ## ## Specificity: 0.9869 Pos Pred Value: 0.9880 ## Neg Pred Value: 1.0000

```
## Prevalence : 0.5180
## Detection Rate : 0.5180
## Detection Prevalence : 0.5243
## Balanced Accuracy : 0.9935
##
## 'Positive' Class : edible
##
```

We have quite an issue here. 40 mushrooms have been predicted as edible but were actually poisonous. That should not be happening. So we'll set up a penalty for wrongly predicting a mushroom as edible when in reality it is poisonous. A mistake the other way is not as bad. At worst we miss on a good recipe! So let's redo our tree with a penalty for wrongly predicting poisonous. To do this, we introduce a penalty matrix that we'll use as a parameter in our rpart function.

```
## Confusion Matrix and Statistics
##
##
              Reference
## Prediction edible poisonous
##
     edible
                 3367
##
     poisonous
                    0
                           3133
##
##
                  Accuracy: 1
                    95% CI: (0.9994, 1)
##
##
       No Information Rate: 0.518
##
       P-Value [Acc > NIR] : < 2.2e-16
##
##
                     Kappa: 1
    Mcnemar's Test P-Value : NA
##
##
##
               Sensitivity: 1.000
##
               Specificity: 1.000
##
            Pos Pred Value: 1.000
##
            Neg Pred Value: 1.000
                Prevalence: 0.518
##
##
            Detection Rate: 0.518
##
      Detection Prevalence: 0.518
##
         Balanced Accuracy: 1.000
##
##
          'Positive' Class : edible
##
```

So introducing a penalty did the job; it gave us a perfect prediction and saves us from a jounrey at the hospital.

Another way to increase the accuracy of our tree model is to play on the cp parameter.

We start to build a tree with a very low cp (that is we'll have a deep tree). The idea is that we then prune it later.

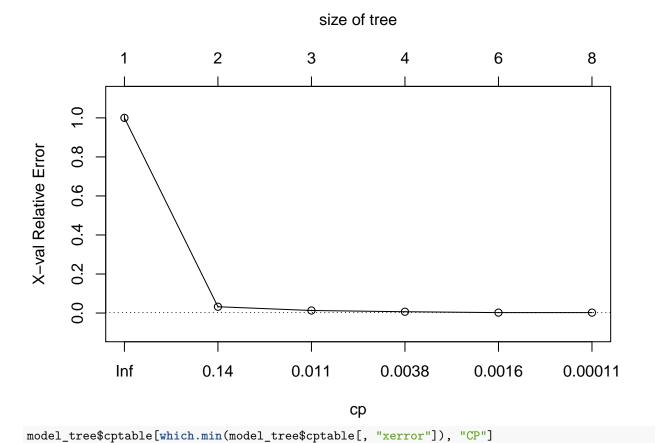
To prune a tree, we first have to find the cp that gives the lowest xerror or cross-validation error. We can find the lowest xerror using either the printcp or plotcp function.

```
printcp(model_tree)
```

```
##
## Classification tree:
## rpart(formula = edibility ~ ., data = train_mushroom, method = "class",
      cp = 1e-05)
##
## Variables actually used in tree construction:
## [1] cap_surface
                           habitat
                                                odor
## [4] spore_print_color
                           stalk_color_below_ring stalk_root
##
## Root node error: 3133/6500 = 0.482
##
## n = 6500
##
##
           CP nsplit rel error
                               xerror
## 1 0.9677625       0 1.0000000 1.0000000 0.01285833
## 2 0.0191510
                  1 0.0322375 0.0322375 0.00318273
                2 0.0130865 0.0130865 0.00203731
## 3 0.0063837
```

We can see here that that the lowest xerror happen at the 5th split.

```
plotcp(model_tree)
```

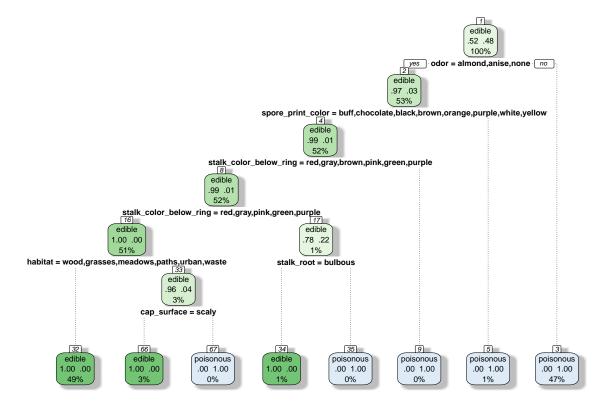


[1] 0.00111714

So now we can start pruning our tree with the cp that gives the lowest cross-validation error.

```
bestcp <- round(model_tree$cptable[which.min(model_tree$cptable[, "xerror"]), "CP"], 4)
model_tree_pruned <- prune(model_tree, cp = bestcp)</pre>
```

Let's have a quick look at the tree as it stands



How does the model perform on the train data?

```
##
  Confusion Matrix and Statistics
##
##
              Reference
## Prediction edible poisonous
     edible
                 3367
##
##
                           3133
     poisonous
##
##
                  Accuracy: 1
##
                    95% CI: (0.9994, 1)
##
       No Information Rate: 0.518
       P-Value [Acc > NIR] : < 2.2e-16
##
##
##
                     Kappa: 1
##
    Mcnemar's Test P-Value : NA
##
##
               Sensitivity: 1.000
##
               Specificity: 1.000
            Pos Pred Value : 1.000
##
##
            Neg Pred Value: 1.000
##
                Prevalence: 0.518
##
            Detection Rate: 0.518
      Detection Prevalence: 0.518
##
```

```
## Balanced Accuracy : 1.000
##
## 'Positive' Class : edible
##
```

It seems like we have a perfect accuracy on our training set. It is quite rare to have such perfect accuracy.

Let's check how it fares on the testing set.

```
## Confusion Matrix and Statistics
##
##
              Reference
## Prediction edible poisonous
                  841
##
     edible
                    0
##
     poisonous
                            783
##
                  Accuracy: 1
##
##
                    95% CI: (0.9977, 1)
##
       No Information Rate: 0.5179
       P-Value [Acc > NIR] : < 2.2e-16
##
##
##
                     Kappa: 1
##
    Mcnemar's Test P-Value : NA
##
##
               Sensitivity: 1.0000
##
               Specificity: 1.0000
            Pos Pred Value: 1.0000
##
            Neg Pred Value: 1.0000
##
##
                Prevalence: 0.5179
            Detection Rate: 0.5179
##
      Detection Prevalence: 0.5179
##
##
         Balanced Accuracy: 1.0000
##
          'Positive' Class : edible
##
##
```

Perfect prediction here as well.

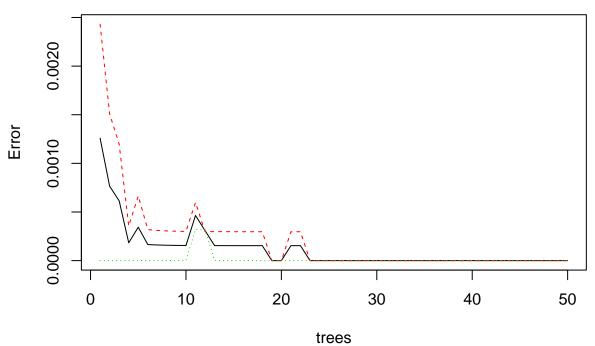
7.3.3.2 A. Use of Random Forest

We usually use random forest if a tree is not enough. In this case, as we have perfect prediction using a single tree, it is not really necessary to use a Random Forest algorithm. We just use for learning sake without tuning any of the parameters.

```
library(randomForest)
model_rf <- randomForest(edibility ~ ., ntree = 50, data = train_mushroom)
plot(model_rf)</pre>
```

The

model_rf



default number of trees for the random forest is 500; we just use 50 here. As we can see on the plot, above 20 trees, the error isn't decreasing anymore. And actually, the error seems to be 0 or almost 0. The next step can tell us this more accurately.

```
print(model_rf)
```

```
##
## Call:
    randomForest(formula = edibility ~ ., data = train_mushroom,
                                                                        ntree = 50)
##
                  Type of random forest: classification
##
                        Number of trees: 50
## No. of variables tried at each split: 4
##
           OOB estimate of error rate: 0%
##
##
  Confusion matrix:
##
             edible poisonous class.error
               3367
                             0
                                         0
## edible
## poisonous
                          3133
                                         0
```

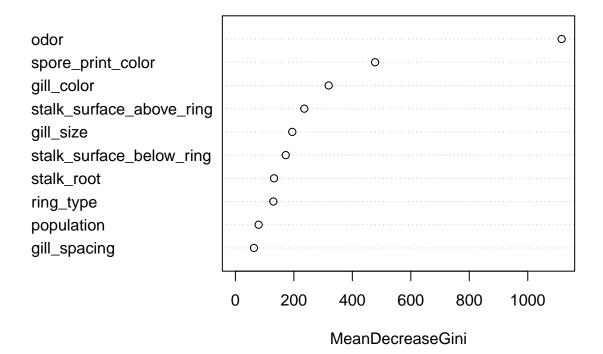
Altough it is not really necessary to this here as we have a perfect prediction, we can use the confusionMatrix function from the caret pacakge.

```
## Confusion Matrix and Statistics
##
## Reference
## Prediction edible poisonous
## edible 3367 0
## poisonous 0 3133
##
```

```
##
                  Accuracy: 1
                    95% CI: (0.9994, 1)
##
##
       No Information Rate: 0.518
       P-Value [Acc > NIR] : < 2.2e-16
##
##
##
                     Kappa: 1
   Mcnemar's Test P-Value : NA
##
##
##
               Sensitivity: 1.000
##
               Specificity: 1.000
##
            Pos Pred Value: 1.000
            Neg Pred Value: 1.000
##
##
                Prevalence: 0.518
##
            Detection Rate: 0.518
##
      Detection Prevalence: 0.518
##
         Balanced Accuracy: 1.000
##
##
          'Positive' Class : edible
##
```

If we want to look at the most important variable in terms of predicting edibility in our model, we can do that using the *Mean Decreasing Gini*

The 10 variables with the most predictive power



Another way to look at the predictible power of the variables is to use the importance extractor function.

```
library(tibble)
importance(model_rf) %>% data.frame() %>%
  rownames_to_column(var = "Variable") %>%
```

arrange(desc(MeanDecreaseGini)) %>% head(10)

```
##
                       Variable MeanDecreaseGini
## 1
                           odor
                                      1115.85522
             spore_print_color
## 2
                                       477.71557
## 3
                     gill_color
                                        319.02467
## 4
      stalk_surface_above_ring
                                        235.59574
## 5
                                       194.56155
                      gill_size
## 6
                                        172.26749
      stalk_surface_below_ring
## 7
                     stalk_root
                                        132.26045
## 8
                     ring_type
                                        129.88445
## 9
                     population
                                        79.42030
## 10
                                        63.42436
                  gill_spacing
```

We could compare that with the important variables from the classification tree obtained above.

```
model_tree_penalty$variable.importance %>%
  as_tibble() %>% rownames_to_column(var = "variable") %>%
  arrange(desc(value)) %>% head(10)
```

```
## # A tibble: 10 × 2
##
                       variable
                                    value
##
                                    <dbl>
                          <chr>>
## 1
                           odor 848.00494
## 2
             spore_print_color 804.39831
                    gill_color 503.71270
## 3
## 4
      stalk_surface_above_ring 501.28385
      stalk_surface_below_ring 453.92877
## 5
## 6
                     ring_type 450.29286
                   ring number 170.56141
## 7
## 8
                    stalk root 117.78800
## 9
                       habitat 98.22176
        stalk_color_below_ring 74.72602
## 10
```

Interestingly gill_size which is the 5th most important predictor in the random forest does not appear in the top 10 of our classification tree.

Now we apply our model to our testing set.

```
test_rf <- predict(model_rf, newdata = test_mushroom)

# Quick check on our prediction
table(test_rf, test_mushroom$edibility)

##
## test_rf edible poisonous
## edible 841 0
## poisonous 0 783
Perfect Prediction!</pre>
```

7.3.3.3 A. Use of SVM

```
library(e1071)
model_svm <- svm(edibility ~. , data=train_mushroom, cost = 1000, gamma = 0.01)</pre>
```

Check the prediction

```
test_svm <- predict(model_svm, newdata = test_mushroom)
table(test_svm, test_mushroom$edibility)
##</pre>
```

```
## test_svm edible poisonous
## edible 841 0
## poisonous 0 783
```

And perfect prediction again!

7.4 Communication

With some fine tuning, a regression tree managed to predict accurately the edibility of mushroom. They were 2 parameters to look at: the cpand the penalty matrix. Random Forest and SVM achieved similar results out of the box.

The regression tree approach has to be prefered as it is a lot easier to grasp the results from a tree than from a SVM algorithm.

For sure I will take my little tree picture next time I go shrooming. That said, I will still only go with a good mycologist.

We would love to hear from you. Give us feedback below.

7.5 Example one

7.6 Example two

Chapter 8

Case Study - Predicting Survicalship on the Titanic

This chapter demonstrates another example of classification with machine learning. Kaggle made this exercise quite popular.

In this study, the training and test sets have already been defined, so we

8.1 Import the data.

\$ Cabin
\$ Embarked

We have put our data into our google drive here and here. You can find them on Kaggle if need be.

```
library(tidyverse)
train_set <- read_csv("~/Google Drive/Software/R projects/datasets/Kaggle_Titanic_train.csv")</pre>
test_set <- read_csv("~/Google Drive/Software/R projects/datasets/Kaggle_Titanic_test.csv")
## Let's bind both set of data for our exploratory analysis.
mydata <- bind_rows(train_set, test_set)</pre>
## Let's have a first glimpse to our data
glimpse(mydata)
## Observations: 1,309
## Variables: 12
## $ PassengerId <int> 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15,...
                 <int> 0, 1, 1, 1, 0, 0, 0, 0, 1, 1, 1, 1, 0, 0, 0, 1, 0,...
## $ Survived
## $ Pclass
                 <int> 3, 1, 3, 1, 3, 3, 1, 3, 3, 2, 3, 1, 3, 3, 3, 2, 3,...
## $ Name
                 <chr> "Braund, Mr. Owen Harris", "Cumings, Mrs. John Bra...
                 <chr> "male", "female", "female", "female", "male", "mal...
## $ Sex
                 <dbl> 22, 38, 26, 35, 35, NA, 54, 2, 27, 14, 4, 58, 20, ...
## $ Age
## $ SibSp
                 <int> 1, 1, 0, 1, 0, 0, 0, 3, 0, 1, 1, 0, 0, 1, 0, 0, 4,...
## $ Parch
                 <int> 0, 0, 0, 0, 0, 0, 0, 1, 2, 0, 1, 0, 0, 5, 0, 0, 1,...
## $ Ticket
                 <chr> "A/5 21171", "PC 17599", "STON/O2. 3101282", "1138...
## $ Fare
                 <dbl> 7.2500, 71.2833, 7.9250, 53.1000, 8.0500, 8.4583, ...
```

<chr> NA, "C85", NA, "C123", NA, NA, "E46", NA, NA, NA, ...

<chr> "S", "C", "S", "S", "Q", "S", "S", "S", "C", ...

8.2 Tidy the data

One can already see that we should put Survived, Sex and Embarked as factor.

```
mydata$Survived <- factor(mydata$Survived)
mydata$Sex <- factor(mydata$Sex)
mydata$Embarked <- factor(mydata$Embarked)</pre>
```

8.3 Understand the data

This step consists in massaging our variables to see if we can construct new ones or create additional meaning from what we have. This step require some additional knowledge related to the data and getting familiar with the topics at hand.

8.3.1 A. Transform the data

The great thing about this data set is all the features engineering one can do to increase the predictibilty power of our model.

8.3.1.1 Dealing with names.

One of the thing one can notice is the title associated with the name. The full names on their own might have little predictibility power, but the *title* in the name might have some value and can be used as an additional variables.

```
glimpse(mydata$Name)
## chr [1:1309] "Braund, Mr. Owen Harris" ...
## gsub is never fun to use. But we need to strip the cell up to the comma,
## then everything after the point of the title.
mydata\$title \leftarrow gsub('(.*,)|()..*)', "", mydata\$Name)
table(mydata$Sex,mydata$title)
##
##
                     Col
                          Don
                                Dona
                                       \mathtt{Dr}
                                           Jonkheer
                                                      Lady
                                                             Major
                                                                     Master
                                                                              Miss
              Capt
                                                                  0
                                                                           0
                                                                               260
##
                       0
                             0
                                        1
                                                   0
     female
                  0
                                   1
                                                          1
                                        7
                                                          0
                                                                  2
##
     male
                                   0
                                                                          61
                                                                                  0
##
##
              Mlle
                     Mme
                          Mr
                               Mrs
                                    Ms
                                         R.ev
                                               Sir
                                                    the Countess
##
                  2
                            0
                               197
                                      2
                                           0
     female
                       1
                                                 0
     male
                  0
                       0 757
                                           8
                                                                 0
##
```

Some titles are just translations from other languages. Let's regroup those. Some other titles aren't occuring often and would not justify to have a category on their own. We have regroup some titles under common category. There is some arbitraire in here.

```
mydata$title <- gsub("Mlle", "Miss", mydata$title)
mydata$title <- gsub("Mme", "Mrs", mydata$title)
mydata$title <- gsub("Ms", "Miss", mydata$title)
mydata$title <- gsub("Jonkheer", "Mr", mydata$title)
mydata$title <- gsub("Capt|Col|Major", "Army", mydata$title)
mydata$title <- gsub("Don|Dona|Lady|Sir|the Countess", "Nobility", mydata$title)</pre>
```

```
##
##
             Mrs Miss Master Mr
                                    Others Army Nobility
##
     female
             198
                   264
                             0
                                 0
                                          1
                                                0
                                                          3
                                                          2
               0
                            61 758
                                         15
##
     male
                     0
```

It would be also interesting in fact to check the proportion of survivors for each type of title.

```
round(prop.table(table(mydata$Survived, mydata$title), 2), 2)
```

```
##
##
        Mrs Miss Master
                            Mr Others
                                       Army
                                             Nobility
##
     0 0.21 0.30
                     0.42 0.84
                                       0.60
                                                  0.25
                                  0.77
                     0.57 0.16
                                                  0.75
     1 0.79 0.70
                                  0.23 0.40
##
```

We can notice that Mrs are more likely to survive than Miss. As expected, our Mr have a very low likelyhood of success. Our Noble title managed mostly to survive.

Our next step is to create a Last_Name variable. This could be helpful as the ways family have escaped the boat might hold some pattens.

```
## To get the last name we strip everything after the first comma.
mydata$last_name <- gsub(",.*", "", mydata$Name)

## We can now put this as factor and check how many families.
mydata$last_name <- factor(mydata$last_name)</pre>
```

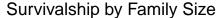
So we have 875 different families on board of the Titanic. Of course, there might have different families with the same last name. If that's the case, we won't know.

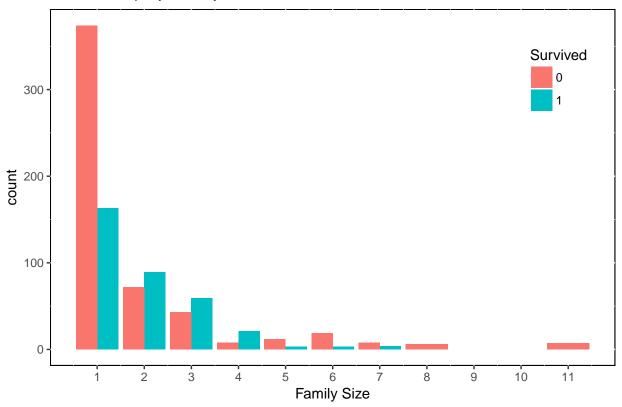
8.3.2 A. Vizualize with families.

We could add a variable about the family size.

```
mydata$family_size <- mydata$SibSp + mydata$Parch + 1</pre>
```

If we plot that to check survivalship in function of family size, one can notice interesting patterns.





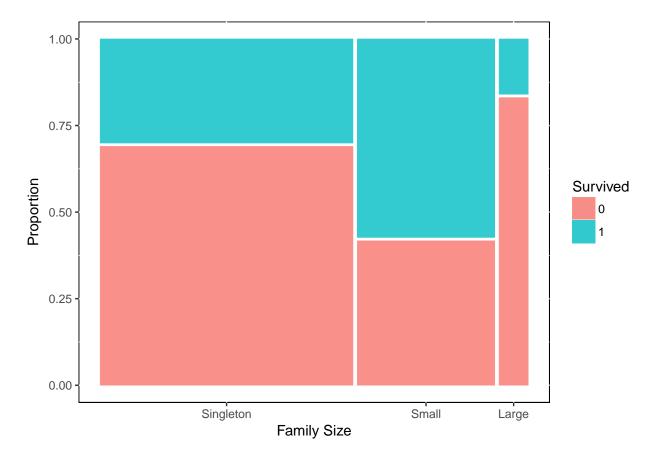
Obviously, we only have the survivalship for the train set of data, as we have to guess the test set of data. So from what we have, there is a clear advantage in being a family of 2, 3 or 4. We could collapse the variable Family_Size into 3 levels.

```
mydata$family_size_type[mydata$family_size == 1] <- "Singleton"
mydata$family_size_type[mydata$family_size <= 4 & mydata$family_size > 1] <- "Small"
mydata$family_size_type[mydata$family_size > 4] <- "Large"
mydata$family_size_type <- factor(mydata$family_size_type, levels = c("Singleton", "Small", "Large"))</pre>
```

We can see how many people in each category, then we plot the proportion of survivers in each category.

```
x <- mydata[1:891,]
table(x$Survived, x$family_size_type)</pre>
```

```
##
##
       Singleton Small Large
##
     0
             374
                   123
                           52
##
             163
                   169
                           10
library(ggmosaic)
ggplot(data = x) + geom_mosaic(aes(x = product(family_size_type), fill = Survived)) +
 labs(x = "Family Size", y = "Proportion") +
  theme(panel.background = NULL)
```

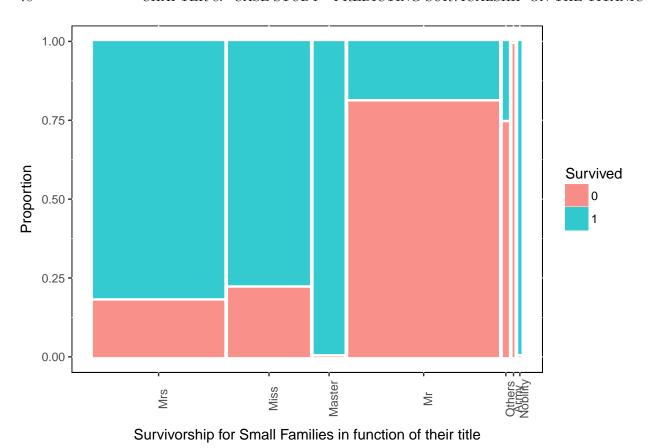


Clearly, there is an advantage in being in a family of size 2, 3 or 4; while there is a disadventage in being part of of a bigger family.

We can try to digg in a bit further with our new family size and titles. For people who are part of a *Small* family size, which *title* are more likely to surived?

```
y <- x %>% dplyr::filter(family_size_type == "Small")
table(y$Survived, y$title)
```

```
##
##
                                Others
                                        Army
                                              Nobility
##
     0
         17
               13
                         0
                           89
                                     3
                                           1
                                                      0
         78
               46
                        22
                           20
                                     1
                                                      2
ggplot(data = y) + geom_mosaic(aes(x = product(title), fill = Survived)) +
  labs(x = "Survivorship for Small Families in function of their title",
       y = "Proportion") +
  theme(panel.background = NULL, axis.text.x = element_text(angle=90, vjust=1))
```

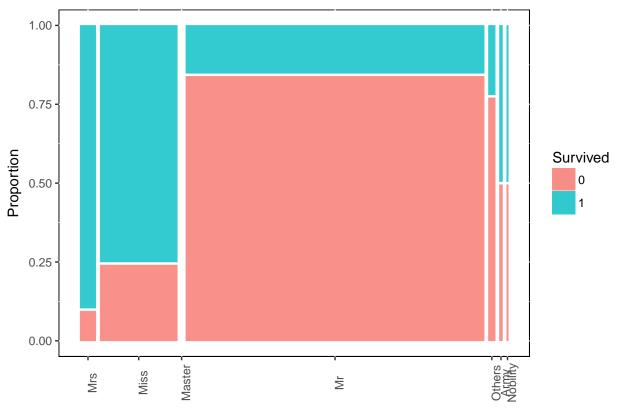


All masters in small families have survived. Miss & Mrs in small family size have also lots of chane of survival.

Similarly, for people who embarked alone (Singleton), which title are more likely to survived?

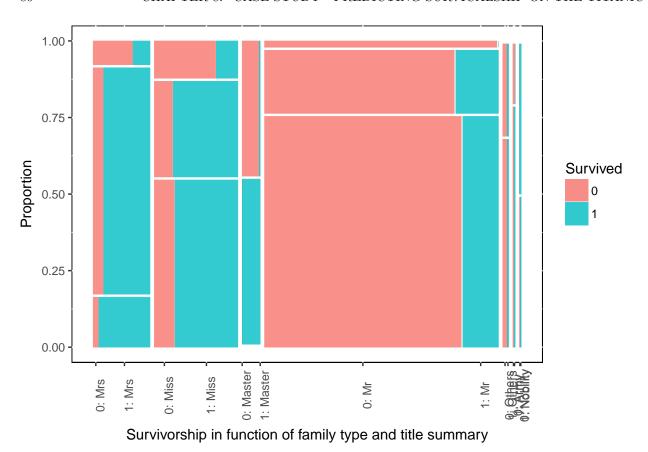
```
y <- x %>% filter(family_size_type == "Singleton")
table(y$Survived, y$title)
```

```
##
##
                                Others
                                              Nobility
##
     0
          2
               25
                        0 337
                                     7
                                           2
                                                     1
               78
         19
                        0 61
                                     2
                                                     1
ggplot(data = y) + geom_mosaic(aes(x = product(title), fill = Survived)) +
  labs(x = "Survivorship for people who boarded alone in function of their title",
       y = "Proportion") +
 theme(panel.background = NULL, axis.text.x = element_text(angle=90, vjust=1))
```



Survivorship for people who boarded alone in function of their title

It might not comes as clear, but we could do the same for title and gender. Vertically the stacks are ordered as Singleton then Small then Large.



8.4 A. Visualize with cabins.

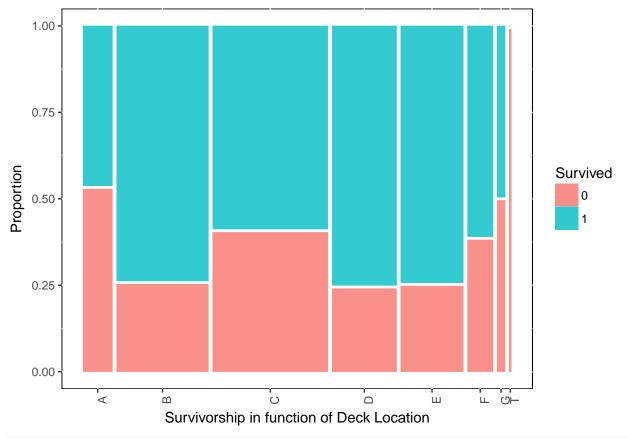
Although there are many missing data there, we can use the cabin number given to passengers. The first letter of the cabin number correspond to the deck on the boat. So let's strip that deck location from the cabin number.

```
x$deck <- gsub("([A-Z]+).*", "\\1", x$Cabin)
y <- x %>% filter(!is.na(deck))

table(x$Survived, x$deck)
```

```
##
## A B C D E F G T
## 0 8 12 24 8 8 5 2 1
## 1 7 35 35 25 24 8 2 0

ggplot(data = y) + geom_mosaic(aes(x = product(deck), fill = Survived)) +
    labs(x = "Survivorship in function of Deck Location", y = "Proportion") +
    theme(panel.background = NULL, axis.text.x = element_text(angle=90, vjust=1))
```



detach("package:ggmosaic", unload=TRUE)

There is a bit of an anomaly here as it almost as if most people survived. Now let's keep in mind, that this is only for people which we have their cabin data.

Let's have a look at how the Passenger Class are distributed on the decks. As we are also finishing this first round of feature engineering, let's just mention also how the Passenger Class is affecting survivalship.

table(x\$Pclass, x\$deck)

```
##
## A B C D E F G T
## 1 15 47 59 29 25 0 0 1
## 2 0 0 0 4 4 8 0 0
## 3 0 0 0 0 3 5 4 0

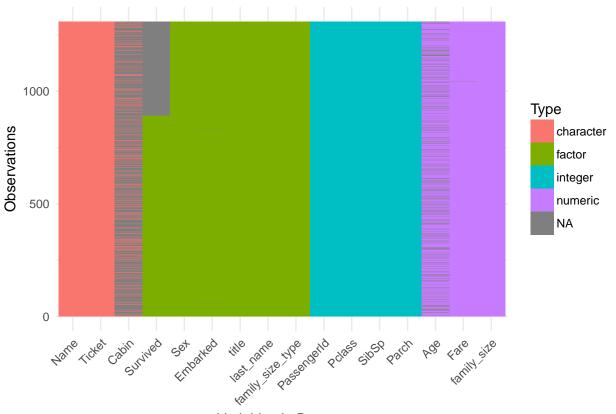
round(prop.table(table(x$Survived, x$Pclass), 2), 2)
```

More first class people have survived than other classes.

8.5 B. Transform Dealing with missing data.

8.5.1 Overview.

I found this very cool package called visdat based on ggplot2 that help us visualize easily missing data. visdat::vis_dat(mydata)



Variables in Dataset

Straight away one can see that the variables cabin and and Age have quite a lot of missing data. For more accuracy one could check

fun1 <- function(x){sum(is.na(x))}
map_dbl(mydata, fun1)</pre>

##	PassengerId	Survived	Pclass	Name
##	0	418	0	0
##	Sex	Age	SibSp	Parch
##	0	263	0	0
##	Ticket	Fare	Cabin	Embarked
##	0	1	1014	2
##	title	last_name	<pre>family_size</pre>	<pre>family_size_type</pre>
##	0	0	0	0

So we can see some missing data in Fare and in Embarked as well. Let's deal with these last 2 variables first.

8.5.1.1 Basic Replacement.

We first start with the dessert and the variables that have few missing data. For those, one can take the median of similar data.

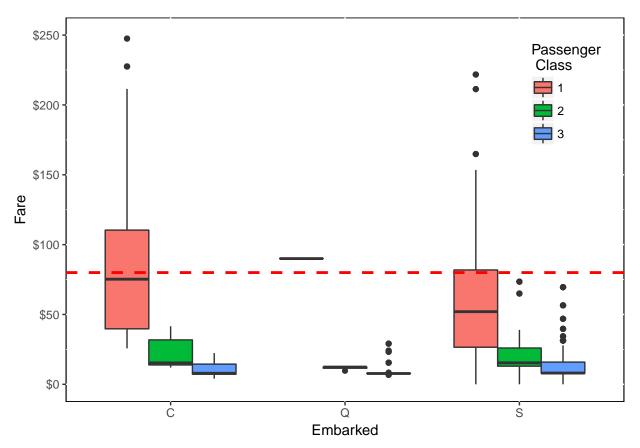
```
y <- which(is.na(mydata$Embarked))
glimpse(mydata[y, ])</pre>
```

```
## Observations: 2
## Variables: 16
## $ PassengerId
                     <int> 62, 830
                     <fctr> 1, 1
## $ Survived
## $ Pclass
                     <int> 1, 1
## $ Name
                     <chr> "Icard, Miss. Amelie", "Stone, Mrs. George Ne...
## $ Sex
                    <fctr> female, female
## $ Age
                     <dbl> 38, 62
## $ SibSp
                    <int> 0, 0
## $ Parch
                     <int> 0, 0
                    <chr> "113572", "113572"
## $ Ticket
## $ Fare
                     <dbl> 80, 80
                     <chr> "B28", "B28"
## $ Cabin
## $ Embarked
                    <fctr> NA, NA
## $ title
                     <fctr> Miss, Mrs
                     <fctr> Icard, Stone
## $ last name
## $ family_size
                     <dbl> 1, 1
## $ family_size_type <fctr> Singleton, Singleton
```

So the 2 passengers that have no data on the origin of their embarqument are 2 ladies that boarded alone and that shared the same room in first class and that paid \$80.

Let's see who might have paid \$80 for a fare.

```
y <- mydata %>% filter(!is.na(Embarked))
ggplot(y, aes(x = Embarked, y = Fare, fill = factor(Pclass))) +
  geom_boxplot() +
  scale_y_continuous(labels = scales::dollar, limits = c(0, 250)) +
  labs(fill = "Passenger \n Class") +
  geom_hline(aes(yintercept = 80), color = "red", linetype = "dashed", lwd = 1) +
  theme(legend.position = c(0.9, 0.8), panel.background = NULL)
```



Following this graph, the 2 passengers without origin of embarcation are most likely from "C". That said, one can argue that the 2 ladies should have embarked from "S" as this is where most people embarked as shown in this table.

table(mydata\$Embarked)

```
## C Q S
## 270 123 914
```

That said, if we filter our data for the demographics of these 2 ladies, the likelhood of coming from "S" decreased quite a bit.

```
x <- mydata %>% filter(Sex == "female", Pclass == 1, family_size == 1)
table(x$Embarked)
```

```
##
## C Q S
## 30 0 20
```

So if we go with median price and with the demographics of the ladies, it would be more likely that they come from "C". So let's input that.

```
mydata$Embarked[c(62, 830)] <- "C"
```

Now onto that missing Fare data

```
y <- which(is.na(mydata$Fare))
glimpse(mydata[y, ])</pre>
```

```
## Observations: 1
```

```
## Variables: 16
                     <int> 1044
## $ PassengerId
## $ Survived
                     <fctr> NA
## $ Pclass
                     <int> 3
## $ Name
                     <chr> "Storey, Mr. Thomas"
## $ Sex
                     <fctr> male
## $ Age
                     <dbl> 60.5
                     <int> 0
## $ SibSp
## $ Parch
                     <int> 0
                     <chr> "3701"
## $ Ticket
## $ Fare
                     <dbl> NA
## $ Cabin
                     <chr> NA
## $ Embarked
                     <fctr> S
## $ title
                     <fctr> Mr
## $ last_name
                     <fctr> Storey
## $ family_size
                     <dbl> 1
## $ family_size_type <fctr> Singleton
```

That passenger is a male that boarded in Southampton in third class. So let's take the median price for similar passagers.

8.5.1.2 Predictive modeling replacement.

First, we'll focus on the Age variable.

There are several methods to input missing data. We'll try 2 different ones in here.

But before we can go forward, we have to factorise some variables.

Let's do the same with Sibsp and Parch

```
mydata$Pclass <- factor(mydata$Pclass)</pre>
```

The first method we'll be using is with the missForest package.

```
y <- mydata %>% select(Pclass, Sex, Fare, Embarked, title, family_size, SibSp, Parch, Age)
y <- data.frame(y)

library(missForest)
z1 <- missForest(y, maxiter = 50, ntree = 500)
z1 <- z1[[1]]

# To view the new ages
# View(z1[[1]])

detach("package:missForest", unload=TRUE)</pre>
```

The process is fairly rapid on my computer (around 10~15 seconds)

Our second method takes slightly more time.

This time we are using the mice package.

```
y <- mydata %>% select(Pclass, Sex, Fare, Embarked, title, family_size, SibSp, Parch, Age)
y$Pclass <- factor(y$Pclass)
y$family_size <- factor(y$family_size)
y <- data.frame(y)

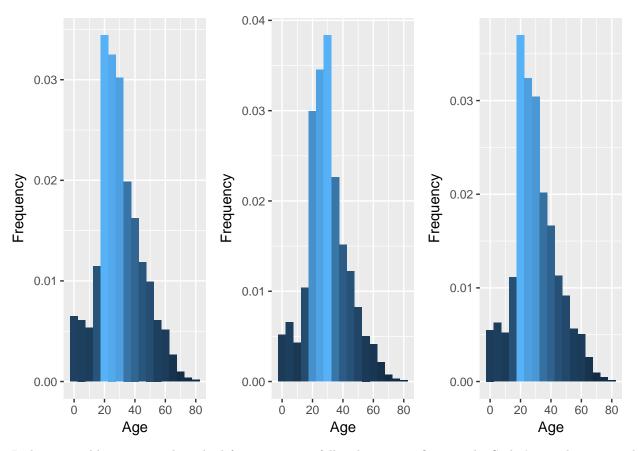
library(mice)
mice_mod <- mice(y, method = 'rf')
z2 <- complete(mice_mod)

# To view the new ages
#View(z2[[1]])

detach("package:mice", unload=TRUE)</pre>
```

let's compare both type of imputations.

8.6. REFERENCES. 87



It does seem like our second method for imputation follow better our first graph. So let's use that one and input our predicted age into our main dataframe.

mydata\$Age <- z2\$Age

8.5.2 C. Transform More feature engineering with the ages and others.

Now that we have filled the NA for the age variable. we can massage a bit more that variable. We can create 3 more variables: Infant from 0 to 5 years old. Child from 5 to 15 years old. Mothers if it is a woman with the variable Parch which is greater than one.

```
mydata$infant <- factor(if_else(mydata$Age <= 5, 1, 0))
mydata$child <- factor(if_else((mydata$Age > 5 & mydata$Age < 15), 1, 0))

mydata$mother <- factor(if_else((mydata$Sex == "female" & mydata$Parch != 0), 1, 0))
mydata$single <- factor(if_else((mydata$SibSp + mydata$Parch + 1 == 1), 1, 0))</pre>
```

8.6 References.

- Exploring the titanic dataset from Megan Risdal. here
- The visdat package. here
- The ggmosaic package. here

Chapter 9

Case Study - Text classification: Spam and Ham.

This chapter has been inspired by the Coursera course on Machine Learning Foundations: A Case Study Approach given by Carlos Guestrin and by Emily Fox from Washington University. This course is part of the Machine Learning Specialization

The task was to apply classification on an Amazon review dataset. Given a review, we create a model that will decide if the review is *positive* (associated with a rating of 4 or 5) or *negative* (associate with a rating of 1 or 2). This is a supervised learning task as the grading associated with the reviews is used as the response variable.

As usual, let's first start by loading our libraries

```
library(tidyverse)
```

Let's have a quick look at our data.

```
##
## | name
                                                                | rating
## | Philips Avent 3 Pack 9oz | If I had not been given a ton |
## | Bottles
                              | of Avent bottles, I would have |
## |
                              | chosen some other system. The |
## |
                              | leaking is terrible!!! You
## |
                              | have to buy the disks
                              | separately, you should get
## I
                              | them for free because they are |
## |
                              | absolutely essential. The
## |
                              | only way to mix formula in the |
                              | bottle or transport liquid is |
                              | to use the disks in the ring,
## |
```

```
## |
                               | then switch to the nipple when |
## |
                               | you are ready to feed. The
## |
                               | only reason I give it a two is |
                               | because I do like that you can |
## |
## |
                               | pump directly into the bottle |
                               | with the ISIS breast pump.
## |
                               | And, I like the sippy cups.
## | Philips Avent 3 Pack 9oz | Leaks! Especially difficult to |
## | Bottles
                              | get a tight seal if you use
## |
                               | one hand (while holding baby). |
## |
                               A much better design is the
## |
                               | Breast Flow Learning Curve
## |
                               | First Years bottles. Instead
## |
                               | buy The First Years 3pk.
## |
                               | Breastflow 5oz. Bottles These
## |
                               | worked much better for me.
## | Philips Avent 3 Pack 9oz | I have been using the Avent
                                                                      5
## | Bottles
                               | bottle system for six months
## |
                               | and have been completely
## |
                               | satisfied. I introduced an
## |
                               | Avent bottle to my daughter at |
                               | four weeks old and she
## |
## |
                               | transitioned easily between
                               | breast and bottle. She is
                               | still breastfed in the morning |
## |
## |
                               | and evenings but receives an
## |
                               | Avent bottle at daycare and
## |
                               | has never had a problem. I
## |
                               | have never had a bottle leak
## |
                               | of which other consumers have
## |
                               | complained. I would recommend
## |
                               | this system to any parent,
## |
                               | especially those of part-time
## |
                               | breastfed babies.
```

```
#Let's see the table of ratings.
table(product_review$rating)
```

```
##
## 1 2 3 4 5
## 45 33 17 30 66
```

Interestingly the ratings on the Avent Bottles are quite spread on the extreme. It might be that people only write reviews if they are super excited or very frustrated with a product. Because we want this to be a binary classification exercise, we'll do some transformation on these ratings.

Now we create our corpus, then tokenize it, then make it back to a data frame.

```
library(tm)
corpus_toy <- Corpus(VectorSource(product_review_training$review))</pre>
tdm_toy <- DocumentTermMatrix(corpus_toy, list(removePunctuation = TRUE,</pre>
                                                 removeNumbers = TRUE))
training_set_toy <- as.matrix(tdm_toy)</pre>
training_set_toy <- cbind(training_set_toy, product_review_training$rating_new)
colnames(training set toy)[ncol(training set toy)] <- "y"</pre>
training_set_toy <- as.data.frame(training_set_toy)</pre>
training_set_toy$y <- as.factor(training_set_toy$y)</pre>
Now that we have our data frame ready, let's create our model using the symLinear3 method.
review_toy_model <- caret::train(y ~., data = training_set_toy, method = 'svmLinear3')</pre>
Now we try our model on new review data
test_review_data <- product_review[151:174, ]</pre>
test_corpus <- Corpus(VectorSource(test_review_data$review))</pre>
test_tdm <- DocumentTermMatrix(test_corpus, control=list(dictionary = Terms(tdm_toy)))</pre>
test_tdm <- as.matrix(test_tdm)</pre>
#Build the prediction
model_toy_result <- predict(review_toy_model, newdata = test_tdm)</pre>
check_accuracy <- as.data.frame(cbind(prediction = model_toy_result,</pre>
                                        rating = test_review_data$rating_new))
check_accuracy <- check_accuracy %>% mutate(prediction = as.integer(prediction) - 1)
check_accuracy$accuracy$accuracy$rating, 1, 0)
round(prop.table(table(check_accuracy$accuracy)), 3)
##
##
       0
             1
## 0.458 0.542
Another way to deal with text classification is to use the RtextTool library.
We can use the same dataframe that we used in our previous method. Like before we "DocumentTermMatrix",
we create a matrix of terms
library(RTextTools)
## Loading required package: SparseM
##
## Attaching package: 'SparseM'
## The following object is masked from 'package:base':
##
##
       backsolve
product_review_matrix <- create_matrix(product_review[,2], language = "English",</pre>
                                         removeNumbers = TRUE,
```

Chapter 10

Final Words

We have finished a nice book.

Bibliography

Xie, Y. (2015). Dynamic Documents with R and knitr. Chapman and Hall/CRC, Boca Raton, Florida, 2nd edition. ISBN 978-1498716963.

Xie, Y. (2016). bookdown: Authoring Books and Technical Documents with R Markdown. R package version 0.3.9.