ML Basic

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Linear Regression Essentials in R

load / install the requirement packages

```
library(tidyverse)
```

```
## -- Attaching packages ------------------------------------ tidyverse 1.3.0 --

## v ggplot2 3.3.2     v purrr   0.3.4
## v tibble  3.0.3     v dplyr   1.0.2
## v tidyr   1.1.2     v stringr 1.4.0
## v readr   1.4.0     v forcats 0.5.0

## -- Conflicts --------------------------------------- tidyverse_conflicts() --
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()    masks stats::lag()
```

```
library(caret)
```

```
## Loading required package: lattice

##
## Attaching package: 'caret'

## The following object is masked from 'package:purrr':
##
##     lift
```

```
theme_set(theme_bw())
```

Preparing the data

sample_n(data, sample data), will randomly pick # of sample data

```
data("marketing", package = "datarium")
sample_n(marketing,3)
```

```
##   youtube facebook newspaper sales
## 1   47.40    49.32      6.96 12.96
## 2  261.24    40.20     70.80 23.28
## 3  266.88     4.08     15.72 13.80
```

```
# split the data into training and test set
set.seed(123)

# We'll randomly split the data into training set (80% for building a
# predictive model) and test set (20% for evaluating the model).

training.samples <- marketing$sales %>%
  createDataPartition(p=0.8, list = F)
train.data <- marketing[training.samples, ]
test.data <- marketing[-training.samples, ]

# build model
model <- lm(sales ~., data = train.data)

# summarize the model
summary(model)
```

```
##
## Call:
## lm(formula = sales ~ ., data = train.data)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -10.7142  -0.9939   0.3684   1.4494   3.3619
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 3.594142   0.420815   8.541 1.05e-14 ***
## youtube     0.044636   0.001552  28.758  < 2e-16 ***
## facebook    0.188823   0.009529  19.816  < 2e-16 ***
## newspaper   0.002840   0.006442   0.441     0.66
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.043 on 158 degrees of freedom
## Multiple R-squared:  0.8955, Adjusted R-squared:  0.8935
## F-statistic: 451.2 on 3 and 158 DF,  p-value: < 2.2e-16
```

```
summary(model)$coefficient
```

```
##                Estimate  Std. Error    t value     Pr(>|t|)
## (Intercept) 3.594141778 0.420814685  8.5409134 1.054115e-14
## youtube     0.044635905 0.001552128 28.7578721 1.125356e-64
## facebook    0.188823227 0.009528828 19.8159966 1.090250e-44
## newspaper   0.002839757 0.006441963  0.4408217 6.599447e-01
```

```
# make prediction
predictions <- model %>% predict(test.data)

# model performance
# (a) Prediction error, RMSE
RMSE(predictions, test.data$sales)
```

```
## [1] 1.965508
```

```
# (b) R-square
caret::R2(predictions, test.data$sales)
```

```
## [1] 0.9049049
```

Simple Linear Regression

```
model_you <- lm(sales ~ youtube, data = train.data)
summary(model_you)$coef
```

```
##                 Estimate  Std. Error  t value     Pr(>|t|)
## (Intercept) 8.58914961 0.616044182 13.94242 1.987874e-29
## youtube     0.04671639 0.003003398 15.55451 8.019035e-34
```

Make prediction

```
newdata <- data.frame(youtube = c(0,1000))
model_you %>% predict(newdata)
```

```
##        1        2
##  8.58915 55.30554
```

Multiple Linear Regression

```
model3 <- lm(sales ~ youtube + facebook + newspaper, data = train.data)
summary(model3)$coef
```

```
##                Estimate  Std. Error    t value     Pr(>|t|)
## (Intercept) 3.594141778 0.420814685  8.5409134 1.054115e-14
## youtube     0.044635905 0.001552128 28.7578721 1.125356e-64
## facebook    0.188823227 0.009528828 19.8159966 1.090250e-44
## newspaper   0.002839757 0.006441963  0.4408217 6.599447e-01
```

Quick note, i have a lot of predictor, we can simply use ~. to include all the predictor

```
model3_1 <- lm(sales ~., data = train.data)
summary(model3_1)$coef
```

```
##                Estimate  Std. Error    t value     Pr(>|t|)
## (Intercept) 3.594141778 0.420814685  8.5409134 1.054115e-14
## youtube     0.044635905 0.001552128 28.7578721 1.125356e-64
## facebook    0.188823227 0.009528828 19.8159966 1.090250e-44
## newspaper   0.002839757 0.006441963  0.4408217 6.599447e-01
```

Col1: b0 / y intercept is 3.73546064 Col2: std.error = 0.44062. this represent the accuracy of the coefficients. We always want small value for std.error Col3: T value is the t statistics estimate / std error = t value Col4: P value for the T statistics. The smaller the p value the more significant the estimate is.

Let's make prediction for the values

```
# New advertising budget
newdata <- data.frame( youtube = 2000, facebook = 1000, newspaper = 1000)

# predict sales values
model3_1 %>% predict(newdata)
```

```
##        1
## 284.5289
```

Interpretation.

Before using the model for predictions, i need to access the statsitical significance of the model. We need to apply summary(model_name)

```
summary(model)
```

```
##
## Call:
## lm(formula = sales ~ ., data = train.data)
##
## Residuals:
```

```
##      Min       1Q   Median       3Q      Max
## -10.7142  -0.9939   0.3684   1.4494   3.3619
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 3.594142   0.420815   8.541 1.05e-14 ***
## youtube     0.044636   0.001552  28.758  < 2e-16 ***
## facebook    0.188823   0.009529  19.816  < 2e-16 ***
## newspaper   0.002840   0.006442   0.441     0.66
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.043 on 158 degrees of freedom
## Multiple R-squared:  0.8955, Adjusted R-squared:  0.8935
## F-statistic: 451.2 on 3 and 158 DF,  p-value: < 2.2e-16
```

The residuals, should be normally distributed. Looks like our data is kind of normally distributed. by theory, mean should be zero. Q1 and Q3, min and max should be around the same with + or - sign.

coefficients, shows the paramete values and their significance. If they are significant, it will be shown with starts

RSE / R^2 / F statistics are used to check how well the model fits to our data

First step, always check the F statistics and the associated p value and the bottom of the model summary

Coefficients significance

```r
summary(model)$coef
```

```
##                Estimate  Std. Error    t value     Pr(>|t|)
## (Intercept) 3.594141778 0.420814685  8.5409134 1.054115e-14
## youtube     0.044635905 0.001552128 28.7578721 1.125356e-64
## facebook    0.188823227 0.009528828 19.8159966 1.090250e-44
## newspaper   0.002839757 0.006441963  0.4408217 6.599447e-01
```

Important, from the summary table , we can see that youtube, facebook advertising budget are significantly changing the sales while by newspaper, there is not much of a change.

Also, to interpret the intercept, we can say every 1000 dollar i invest in facebook advertising i will have a return of 1000* 0.19398450 = 193 sale unit. So do youtube, 1000* 0.04516611 = 45.16 sale units

Since newspaper does not affect the outcome much, lets remove it from the model

```r
model4 <- lm(sales ~ youtube + facebook, data = train.data)
summary(model4)
```

```
##
## Call:
## lm(formula = sales ~ youtube + facebook, data = train.data)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -10.8127  -1.0073   0.3236   1.4643   3.3454
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 3.658580   0.393609   9.295   <2e-16 ***
## youtube     0.044650   0.001548  28.846   <2e-16 ***
## facebook    0.190165   0.009006  21.114   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.038 on 159 degrees of freedom
## Multiple R-squared:  0.8954, Adjusted R-squared:  0.894
## F-statistic: 680.2 on 2 and 159 DF,  p-value: < 2.2e-16
```

now our equation can be written as sales = 3.577663 + 0.045287(youtube) + 0.190299(facebook)

Model accuracy

Well, after knowing it is significant, we would like to know how well the model fits our data. This process will be referred to as the goodness of fit The overall quality of the linear regression fit can be shown by model summary RSE, R^2, adjusted R^2, F statistics

RSE / model sigma -> prediction error. it is the observed out come - predicted value (Y_i - Y bar). small rse is the best the model fits to the data. dividing the RSE by the average value of the outcome variable will give me the prediction error rate. Which should be as small as possible.

in our example, we have 1.853 for RSE.

```
(1.853/(mean(train.data$sales)))*100
```

```
## [1] 10.99196
```

It is 10.90% which is low.

R-squared and adjusted R squared R^2 is ranges between 0 and 1. Higher the R square the better the model. High R square = observed data is very close to the prediction data. So the quality of the regression line is pretty good.R^2 = pearson ^2. Here is the trick tho, if i have a lot of parameters, R^2 will increase along with it.

However, the adjusted R^2 is the correction of the for the number of parameters in the predictive model.Therefore, I should always read adjusted R^2 because it will make the correction according the to incorrect R^2

When adjusted R^2 = 0 thats mean the model did not explain much about the variability in the outcome. In our outcome, adjusted R^2 is 0.9112 so it is pretty good.

Lastly, F statistics gives the overall significance of the model. it tells us whether at least one predictor variables has non zero coefficient. In a simple linear regression (one parameter), it wont be interesting because it is just a duplicated info given by the t test from the coef table.

The F statistic becomes more important once we start using multiple predictors as in multiple linear regression.

So according to what we have, our F statistics equal 825.4 with 2 parameters and 159 df, with a p-value of 2.2e^-16. which is highly significant. In order to read the p value, $p < 0.05$ will be significant.

Making predictions

Procedure to make predictions 1) predict the sales values based on new advertising budgets in the test data 2) Assess the model performance by computing: the prediction error RMSE (Root Mean Squared Error), representing the average difference between the observed known outcome values in the test data and the predicted outcome values by the model. The lower the RMSE, the better the model. The R^2, representing the correlation between the observed outcome values and the predicted outcome values. the higher the r^2, the better the model.

```
# make predictions
predictions <- model %>% predict(test.data)

# model performance
```

```r
# (a) compute the prediction error, RMSE
RMSE(predictions, test.data$sales)
```

```
## [1] 1.965508
```

```r
caret::R2(predictions, test.data$sales)
```

```
## [1] 0.9049049
```

```r
(RMSE(predictions, test.data$sales)/ mean(test.data$sales))*100
```

```
## [1] 11.77248
```

The % error is 16.39% is alright

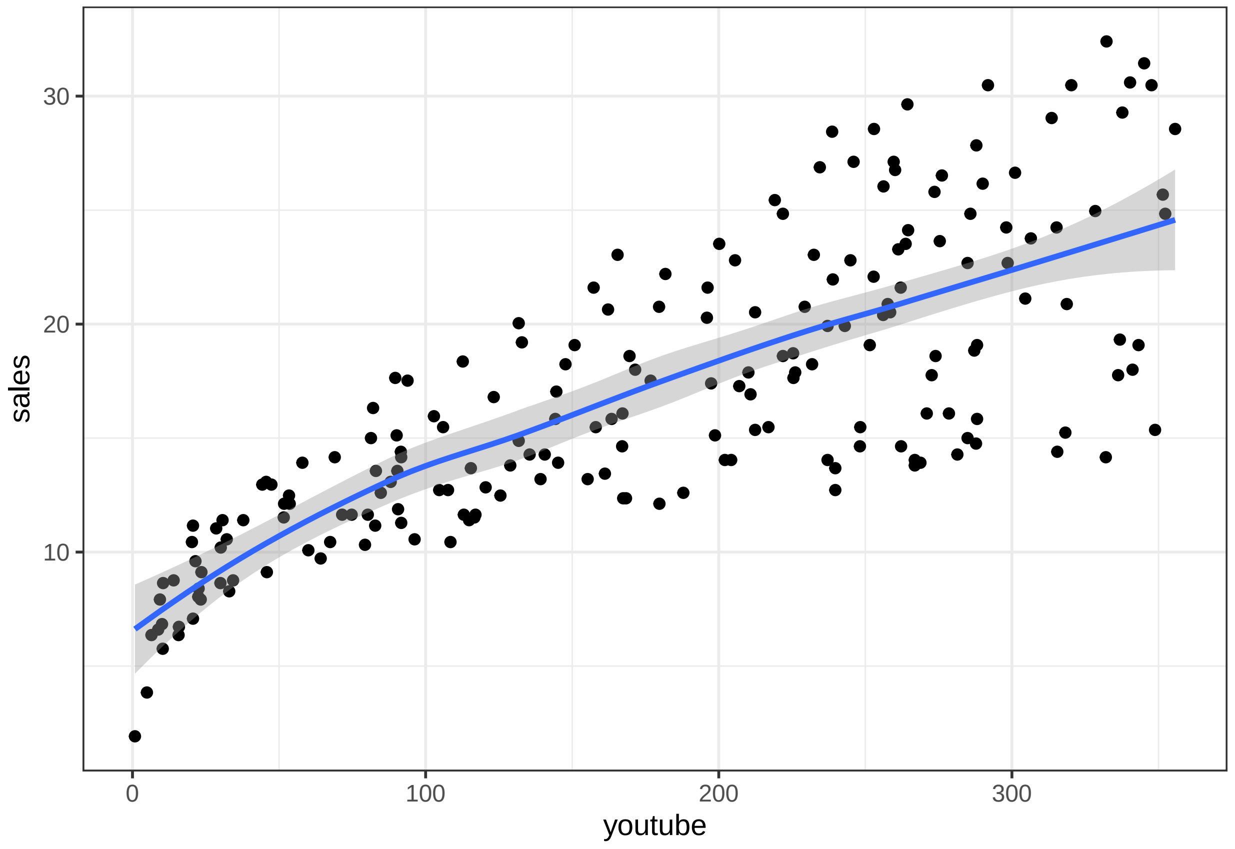
Discussion

This section discuss basic linear regression and provides practical examples in R for computing simple and multiple linear regression model. Also, we have learnt how the accuracy of the model.

The idea of linear regression is to see the predictor relationship with the response. It can be easily be visualized by a basic plot without working a lot on lm() summary and more.

```r
ggplot(marketing, aes(youtube, sales)) +
  geom_point() +
  stat_smooth()
```

```
## 'geom_smooth()' using method = 'loess' and formula 'y ~ x'
```



As we can expected, since we know that the Beta_1 is positive from what we have done before, we can expect that the slope is positive and the scatter dots are following the positive slope.

Interaction Effect in Multiple Regression: Essentials

Considering our example, the additive model assumes that, the effect on sales of youtube advertising is independent of the effect of facebook advertising.

This assumption might not be true. For example, spending money on facebook advertising may increase the effectiveness of youtube advertising on sales. In marketing, this is known as a synergy effect, and in statistics it is referred to as an interaction effect (James et al. 2014).

Interaction effects

```
# build the model
# use this:
model12 <- lm(sales ~ youtube*facebook, data = train.data)
summary(model12)
```

```
##
## Call:
## lm(formula = sales ~ youtube * facebook, data = train.data)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -7.6325 -0.5051  0.2666  0.7425  1.8109
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)      8.179e+00  3.306e-01  24.741  < 2e-16 ***
## youtube          1.859e-02  1.660e-03  11.196  < 2e-16 ***
## facebook         2.781e-02  1.016e-02   2.739  0.00687 **
## youtube:facebook 9.145e-04  4.952e-05  18.467  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.15 on 158 degrees of freedom
## Multiple R-squared:  0.9669, Adjusted R-squared:  0.9662
## F-statistic:  1537 on 3 and 158 DF,  p-value: < 2.2e-16
```

Make predictions

```
predictions12 <- model12 %>% predict(test.data)
# model performance
# (a) prediction error, RMSE
RMSE(predictions12, test.data$sales)
```

```
## [1] 1.055644
```

```
# (b) R-square
caret::R2(predictions12, test.data$sales)
```

```
## [1] 0.9716356
```

```
# % error
(RMSE(predictions12, test.data$sales) / mean(test.data$sales))*100
```

```
## [1] 6.322813
```

Those values are pretty good. high R^2 and 10.67% error

```
summary(model12)$coef
```

```
##                     Estimate   Std. Error   t value     Pr(>|t|)
## (Intercept)      8.1786320203 3.305698e-01 24.741018 3.213476e-56
## youtube          0.0185856131 1.659981e-03 11.196278 8.614530e-22
## facebook         0.0278145861 1.015569e-02  2.738818 6.874607e-03
## youtube:facebook 0.0009145105 4.952241e-05 18.466598 2.668477e-41
```

As you can see that all of them are significant (Pr(>|t|)). so it means there is an interaction relationship between the two predictor variables (youtube and facebook advertising)

our model will be like sales = 7.89 + 0.0189949052(youtube) + 0.0330506939(facebook) + 0.0008751096 (youtube*facebook)

comparing the additive and the interaction models.

The prediction error RMESE of the interaction model is 1.721177 compared with the prediction error of the addictive model 2.642146, interaction model is lower.

R^2 of the interaction model is 0.9373706, and for the addictive model has 0.8322611. Interaction model has a better R^2

Lastly, these result suggest that the model with the interaction term is better than the model that contains only main effects.

So for this specific data, we should go for the model with the interaction model.

Discussion, after finding addictive model which is significant, we should also check if the interaction model is also significant. If they do, we should adapt the interaction model.

Regression with Categorical Variables: Dummy Coding Essentials in R

```r
library(car)
```

```
## Loading required package: carData
```

```
##
## Attaching package: 'car'
```

```
## The following object is masked from 'package:dplyr':
##
##     recode
```

```
## The following object is masked from 'package:purrr':
##
##     some
```

```r
# load data
data("Salaries", package = "car")
```

```
## Warning in data("Salaries", package = "car"): data set 'Salaries' not found
```

```r
# Inspect the data
sample_n(Salaries, 3)
```

```
##       rank discipline yrs.since.phd yrs.service    sex salary
## 1     Prof          A            22          15   Male 166800
## 2     Prof          A            39          36 Female 137000
## 3 AsstProf          A            11           4   Male  78785
```

Categorical variables with two levels From our data set, we would like to investigate differences in salaries between males and females. Based on the gender, we can say m = 1, female = 0 b0 + b1 if person is male bo if person is female. B0 is average salary among females B0 + B1 = average salary among males B1 is average difference in salary between males and females

```
mwage <- lm(salary ~ sex, data = Salaries)
summary(mwage)$coef
```

```
##               Estimate Std. Error   t value     Pr(>|t|)
## (Intercept) 101002.41   4809.386 21.001103 2.683482e-66
## sexMale      14088.01   5064.579  2.781674 5.667107e-03
```

From the above result, average salary for female is 101002.41. Male = B0 + B1 = 101002.41 + 14088.01 = 115090.40

the P value for both sex is very significant, which is suggesting that there is a statistical evidence of a difference in average salary between the genders.

```
contrasts(Salaries$sex)
```

```
##        Male
## Female    0
## Male      1
```

I can use the function relevel() to set the baseline category to males as follow

```
Salaries <- Salaries %>%
  mutate(sex = relevel(sex, ref = "Male"))
```

```
mwage1 <- lm(salary ~ sex , data = Salaries)
summary(mwage1)$coef
```

```
##               Estimate Std. Error   t value      Pr(>|t|)
## (Intercept) 115090.42   1587.378 72.503463 2.459122e-230
## sexFemale   -14088.01   5064.579 -2.781674  5.667107e-03
```

Categorical variables with more than two levels

Generally, categorical variable with n levels will be transformed in to n-1 variables each with two levels. These n-1 new variables contain the same info than the single variable. This recording creates a table called contrast matrix.

In salaries, data has three levels, asstprof, assocprof, and prof. These variables could be dummy coded in to two variables, one called assocprof and one prof.

if rank = assocprof, then the column assocprof would be coded with 1 and prof with 0 if rank = prof, then the col assocprof would be coded with a 0 and prof would be coded with a 1 if rank = asstprof then both cols assocprof and prof would be coded with a 0

```
res <- model.matrix(~rank, data=Salaries)
head(res[,-1])
```

```
##   rankAssocProf rankProf
## 1             0        1
## 2             0        1
## 3             0        0
## 4             0        1
## 5             0        1
## 6             1        0
```

```
head(res)
```

```
##   (Intercept) rankAssocProf rankProf
## 1           1             0        1
## 2           1             0        1
## 3           1             0        0
## 4           1             0        1
## 5           1             0        1
## 6           1             1        0
```

R will always use the first level as a reference and interpret the remaining levels relative to the first level

The following code will give you the level

```
levels(Salaries$rank)
```

```
## [1] "AsstProf"  "AssocProf" "Prof"
```

Indeed, AsstProf will be the reference level.

Also ANOVA(analysis of variance) is just a special case of linear model where the predictors are categorical variables. R understands the fact that ANOVA and regression are both examples of linear models, it lets you extract the classic ANOVA table from the regression model using the R base anova() function or the Anova() function. We generally use Anova() function because it automatically takes care of unbalanced designs.

Lets predict the salary from using a multiple regression procedure

```
mwage2 <- lm(salary ~ yrs.service + rank + discipline + sex, data = Salaries)
Anova(mwage2)
```

```
## Anova Table (Type II tests)
##
## Response: salary
##                Sum Sq  Df  F value    Pr(>F)
## yrs.service 3.2448e+08   1   0.6324    0.4270
## rank        1.0288e+11   2 100.2572 < 2.2e-16 ***
## discipline  1.7373e+10   1  33.8582 1.235e-08 ***
## sex         7.7669e+08   1   1.5137    0.2193
## Residuals   2.0062e+11 391
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
Anova(mwage1)
```

```
## Anova Table (Type II tests)
##
## Response: salary
##               Sum Sq  Df F value   Pr(>F)
## sex       6.9800e+09   1  7.7377 0.005667 **
## Residuals 3.5632e+11 395
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

When we take rank, discipline, yrs of service in to consideration, the variable sex is no longer significant combined with the variation in salary between individuals.

```
summary(mwage2)
```

```
##
## Call:
## lm(formula = salary ~ yrs.service + rank + discipline + sex,
##     data = Salaries)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -64202 -14255  -1533  10571  99163
```

```
##
## Coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept)   73122.92    3245.27  22.532  < 2e-16 ***
## yrs.service     -88.78     111.64  -0.795 0.426958
## rankAssocProf 14560.40    4098.32   3.553 0.000428 ***
## rankProf      49159.64    3834.49  12.820  < 2e-16 ***
## disciplineB   13473.38    2315.50   5.819 1.24e-08 ***
## sexFemale     -4771.25    3878.00  -1.230 0.219311
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 22650 on 391 degrees of freedom
## Multiple R-squared:  0.4478, Adjusted R-squared:  0.4407
## F-statistic: 63.41 on 5 and 391 DF,  p-value: < 2.2e-16
```

```r
levels(Salaries$discipline)
```

```
## [1] "A" "B"
```

apply ??salaries and check discipline a and b is corresponding to what field from the documentation, dis A is theoretical, dis B is applied department.

For example, from dicipline B (applied departments) is significantly associated with an average increase of 13473.38 in salary compared (there is a difference) to discipline theoretical departments. So that is the reason why discipline B is significant

Nonlinear Regression Essentials in R: Polynomial and Spline Regression Models

http://www.sthda.com/english/articles/40-regression-analysis/162-nonlinear-regression-essentials-in-r-polynomial-and-spline-regression-models/

In this section, you'll learn how to compute non-linear regression models and how to compare the different models in order to choose the one that fits the best your data.

Will also be using RMSE and R2 metric to compare the different models' accuracy Recall, RMSE -> model prediction error. Thats the average difference of the observed outcome values and predicted outcome values.

R2 represents the squared correlation. How accurate is the data, if it is exactly on the regression line, that the R^2 will be 1

The best model is the model with the lowest RMSE and the highest R2

```r
library(tidyverse)
library(caret)
theme_set(theme_classic())
```

Prepare the data

we will use the boston data from MASS package

```r
# Load the data, if the package is not installed, instal it now and load the library
if(!require("MASS")){
  install.packages("MASS")
  library(MASS)
}
```

```
## Loading required package: MASS
```

```
##
## Attaching package: 'MASS'
## The following object is masked from 'package:dplyr':
##
##     select
```

```r
data("Boston", package = "MASS")
str(Boston)
```

```
## 'data.frame':    506 obs. of  14 variables:
##  $ crim   : num  0.00632 0.02731 0.02729 0.03237 0.06905 ...
##  $ zn     : num  18 0 0 0 0 0 12.5 12.5 12.5 12.5 ...
##  $ indus  : num  2.31 7.07 7.07 2.18 2.18 2.18 7.87 7.87 7.87 7.87 ...
##  $ chas   : int  0 0 0 0 0 0 0 0 0 0 ...
##  $ nox    : num  0.538 0.469 0.469 0.458 0.458 0.458 0.524 0.524 0.524 0.524 ...
##  $ rm     : num  6.58 6.42 7.18 7 7.15 ...
##  $ age    : num  65.2 78.9 61.1 45.8 54.2 58.7 66.6 96.1 100 85.9 ...
##  $ dis    : num  4.09 4.97 4.97 6.06 6.06 ...
##  $ rad    : int  1 2 2 3 3 3 5 5 5 5 ...
##  $ tax    : num  296 242 242 222 222 222 311 311 311 311 ...
##  $ ptratio: num  15.3 17.8 17.8 18.7 18.7 18.7 15.2 15.2 15.2 15.2 ...
##  $ black  : num  397 397 393 395 397 ...
##  $ lstat  : num  4.98 9.14 4.03 2.94 5.33 ...
##  $ medv   : num  24 21.6 34.7 33.4 36.2 28.7 22.9 27.1 16.5 18.9 ...
```

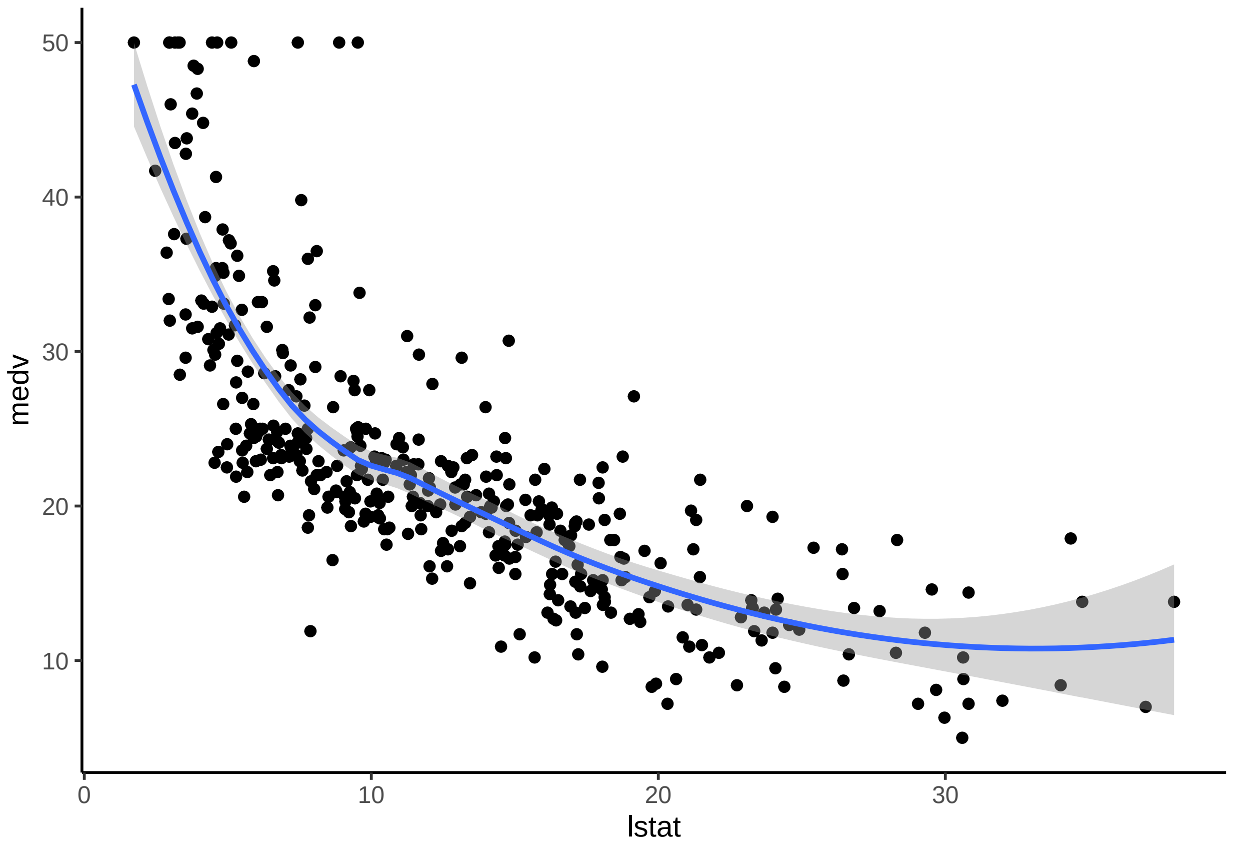
```r
# Split the data in to training and test set
set.seed(123)
ts <- Boston$medv %>%
  createDataPartition(p =0.8, list = F)
trd <- Boston[ts, ]
ted <- Boston[-ts, ]
```

Visualize the scatter plot of the medv vs lstat varaibles, both medv and lstat is from the Boston dataset

use stat_smooth when i want to display the results with non standard geom

```r
ggplot(trd, aes(lstat,medv)) +
  geom_point() +
  stat_smooth()
```

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```



It is obvious to see that the blue line is a curve

Linear Regression

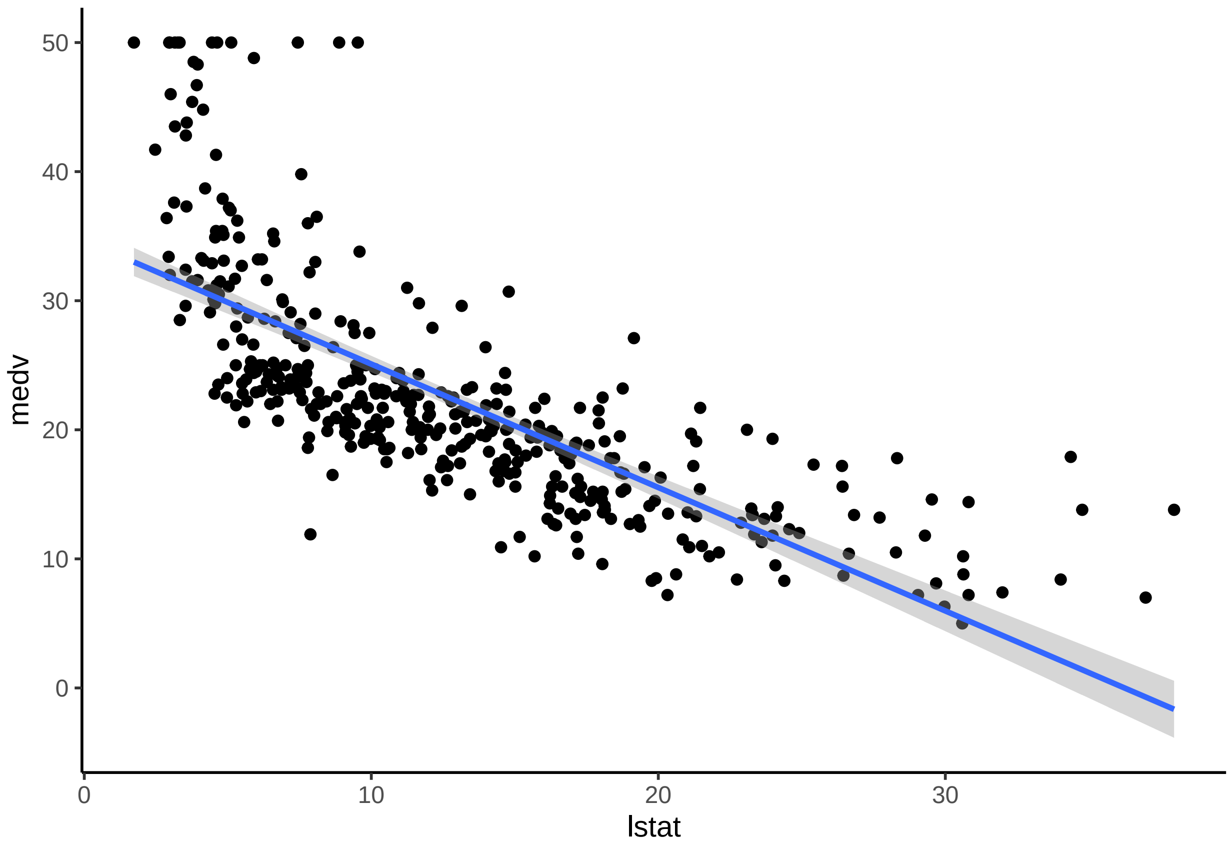
```r
# Build the model
modelc <- lm(medv ~ lstat, data = trd)
# make prediction
pmodelc <- modelc %>% predict(ted)
data.frame(
  rmseL <- RMSE(pmodelc, ted$medv),
  r2L <- caret::R2(pmodelc, ted$medv),
  perrorL <- rmseL / mean(ted$medv)
)
```

```
##   rmseL....RMSE.pmodelc..ted.medv. r2L....caret..R2.pmodelc..ted.medv.
## 1                         6.503817                            0.513163
##   perrorL....rmseL.mean.ted.medv.
## 1                       0.2874712
```

I have a pretty high percent error 26.82%

visualize the data

```r
ggplot(trd, aes(lstat, medv)) +
  geom_point() +
  stat_smooth(method = lm, formula = y ~ x)
```



Polynomial Regression

Lets make it polynomial regression medv is the response.

we should have this following formula medv = b0 + b1 * lstat + b2*lstat^2 in r to make that ^2 we need to apply I(x^2)

```
modelc1 <- lm(medv ~ lstat + I(lstat^2), data = trd)
summary(modelc1)
```

```
##
## Call:
## lm(formula = medv ~ lstat + I(lstat^2), data = trd)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -15.3654  -3.8250  -0.6439   2.2733  25.2922
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 42.573638   0.964887   44.12   <2e-16 ***
## lstat       -2.267309   0.135846  -16.69   <2e-16 ***
## I(lstat^2)   0.041198   0.004095   10.06   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 5.501 on 404 degrees of freedom
## Multiple R-squared:  0.6418, Adjusted R-squared:   0.64
## F-statistic: 361.9 on 2 and 404 DF,  p-value: < 2.2e-16
```

Alternative way to create 2 degree regression model

```r
modelc2<- lm(medv ~ poly(lstat, 2, raw =T), data = trd)
summary(modelc2)
```

```
##
## Call:
## lm(formula = medv ~ poly(lstat, 2, raw = T), data = trd)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -15.3654  -3.8250  -0.6439   2.2733  25.2922
##
## Coefficients:
##                           Estimate Std. Error t value Pr(>|t|)
## (Intercept)              42.573638   0.964887   44.12   <2e-16 ***
## poly(lstat, 2, raw = T)1 -2.267309   0.135846  -16.69   <2e-16 ***
## poly(lstat, 2, raw = T)2  0.041198   0.004095   10.06   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 5.501 on 404 degrees of freedom
## Multiple R-squared:  0.6418, Adjusted R-squared:   0.64
## F-statistic: 361.9 on 2 and 404 DF,  p-value: < 2.2e-16
```

```r
modelc2p <- modelc2 %>% predict(ted)
p2 <- c(RMSE(modelc2p,ted$medv), caret::R2(modelc2p, ted$medv),
        RMSE(modelc2p, ted$medv) / mean(ted$medv))
```

As you can see they are the same. intercepts and the coefficient of beta1 and beta2^2 are all significant. as well as the F statistic P value is also small. Indeed, we have an Adjusted R^2 0.6329 which is ok.

The following is the 6th order

```r
modelc6 <- lm(medv ~ poly(lstat, 6, raw = T), data = trd)
summary(modelc6)
```

```
##
## Call:
## lm(formula = medv ~ poly(lstat, 6, raw = T), data = trd)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -13.1962  -3.1527  -0.7655   2.0404  26.7661
##
## Coefficients:
##                            Estimate Std. Error t value Pr(>|t|)
## (Intercept)               7.788e+01  6.844e+00  11.379  < 2e-16 ***
## poly(lstat, 6, raw = T)1 -1.767e+01  3.569e+00  -4.952 1.08e-06 ***
## poly(lstat, 6, raw = T)2  2.417e+00  6.779e-01   3.566 0.000407 ***
## poly(lstat, 6, raw = T)3 -1.761e-01  6.105e-02  -2.885 0.004121 **
## poly(lstat, 6, raw = T)4  6.845e-03  2.799e-03   2.446 0.014883 *
## poly(lstat, 6, raw = T)5 -1.343e-04  6.290e-05  -2.136 0.033323 *
## poly(lstat, 6, raw = T)6  1.047e-06  5.481e-07   1.910 0.056910 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
```

```
## Residual standard error: 5.188 on 400 degrees of freedom
## Multiple R-squared:  0.6845, Adjusted R-squared:  0.6798
## F-statistic: 144.6 on 6 and 400 DF,  p-value: < 2.2e-16
```

```
modelc6p <- modelc6 %>% predict(ted)
p6 <- c(RMSE(modelc6p,ted$medv), caret::R2(modelc6p, ted$medv),
        RMSE(modelc6p, ted$medv) / mean(ted$medv))
```

From this point we can see that after degree 3 it is no longer significant. Then we will just simply use degree 3 for our model

```
modelc5 <- lm(medv ~ poly(lstat, 5, raw = T), data = trd)
summary(modelc5)
```

```
##
## Call:
## lm(formula = medv ~ poly(lstat, 5, raw = T), data = trd)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -13.1519  -3.1235  -0.5927   2.0962  27.1286
##
## Coefficients:
##                            Estimate Std. Error t value Pr(>|t|)
## (Intercept)               6.765e+01  4.273e+00  15.831  < 2e-16 ***
## poly(lstat, 5, raw = T)1 -1.177e+01  1.786e+00  -6.588 1.40e-10 ***
## poly(lstat, 5, raw = T)2  1.220e+00  2.580e-01   4.727 3.16e-06 ***
## poly(lstat, 5, raw = T)3 -6.385e-02  1.644e-02  -3.884 0.000120 ***
## poly(lstat, 5, raw = T)4  1.577e-03  4.714e-04   3.345 0.000901 ***
## poly(lstat, 5, raw = T)5 -1.459e-05  4.954e-06  -2.945 0.003421 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 5.205 on 401 degrees of freedom
## Multiple R-squared:  0.6816, Adjusted R-squared:  0.6777
## F-statistic: 171.7 on 5 and 401 DF,  p-value: < 2.2e-16
```

```
modelc5p <- modelc5 %>% predict(ted)
p5 <- c(RMSE(modelc5p,ted$medv), caret::R2(modelc5p, ted$medv), RMSE(modelc5p, ted$medv) / mean(ted$med
modelc3 <- lm(medv ~ poly(lstat, 3, raw = T), data = trd)
modelc3p <- modelc3 %>% predict(ted)
p3 <- c(RMSE(modelc3p,ted$medv), caret::R2(modelc3p, ted$medv), RMSE(modelc3p, ted$medv) / mean(ted$med
modelc4 <- lm(medv ~ poly(lstat, 4, raw = T), data = trd)
modelc4p <- modelc4 %>% predict(ted)
p4 <- c(RMSE(modelc4p,ted$medv), caret::R2(modelc4p, ted$medv), RMSE(modelc4p, ted$medv) / mean(ted$med
perrorp4 <- RMSE(modelc4p, ted$medv) / mean(ted$medv)
modelc7 <- lm(medv ~ poly(lstat, 7, raw = T), data = trd)
modelc7p <- modelc7 %>% predict(ted)
p7 <- c(RMSE(modelc7p,ted$medv), caret::R2(modelc7p, ted$medv), RMSE(modelc7p, ted$medv) / mean(ted$med
```

Lets see the RMSE, R2 and percent error p2, p3,p4, p5, p6

```
temp <- cbind(p2,p3,p4,p5,p6,p7)
row.names(temp) <-c("RMSE", "R2", "% error")
temp
```

```
##                 p2        p3        p4        p5        p6        p7
## RMSE    5.6307274 5.5007142 5.3929523 5.2703735 5.3495124 5.3569154
## R2      0.6351934 0.6521415 0.6664867 0.6829474 0.6759031 0.6753441
## % error 0.2488803 0.2431336 0.2383705 0.2329525 0.2364505 0.2367777
```

There are couple patterns are going on. First im looking at the table above, we can see that p5 is the dip of the % error. after that it bounces back and has a small changes at p7. Also, if we look at the anova(p1 : p7) the significance level stops at 4.

```r
anova(modelc2,modelc3,modelc4,modelc5, modelc6, modelc7)
```

```
## Analysis of Variance Table
##
## Model 1: medv ~ poly(lstat, 2, raw = T)
## Model 2: medv ~ poly(lstat, 3, raw = T)
## Model 3: medv ~ poly(lstat, 4, raw = T)
## Model 4: medv ~ poly(lstat, 5, raw = T)
## Model 5: medv ~ poly(lstat, 6, raw = T)
## Model 6: medv ~ poly(lstat, 7, raw = T)
##   Res.Df   RSS Df Sum of Sq       F    Pr(>F)
## 1    404 12224
## 2    403 11624  1    599.27 22.2105 3.381e-06 ***
## 3    402 11100  1    524.61 19.4432 1.334e-05 ***
## 4    401 10865  1    234.93  8.7072  0.003356 **
## 5    400 10767  1     98.14  3.6375  0.057210 .
## 6    399 10766  1      1.00  0.0372  0.847094
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

So i would say degree 4 is the best option.

```r
modelc4 <- lm(medv ~ poly(lstat, 4, raw = T), data = trd)
modelc4p <- modelc4 %>% predict(ted)
p4 <- c(RMSE(modelc4p,ted$medv), caret::R2(modelc4p, ted$medv), RMSE(modelc4p, ted$medv) / mean(ted$medv
p4
```

```
## [1] 5.3929523 0.6664867 0.2383705
```

```r
summary(modelc4)
```

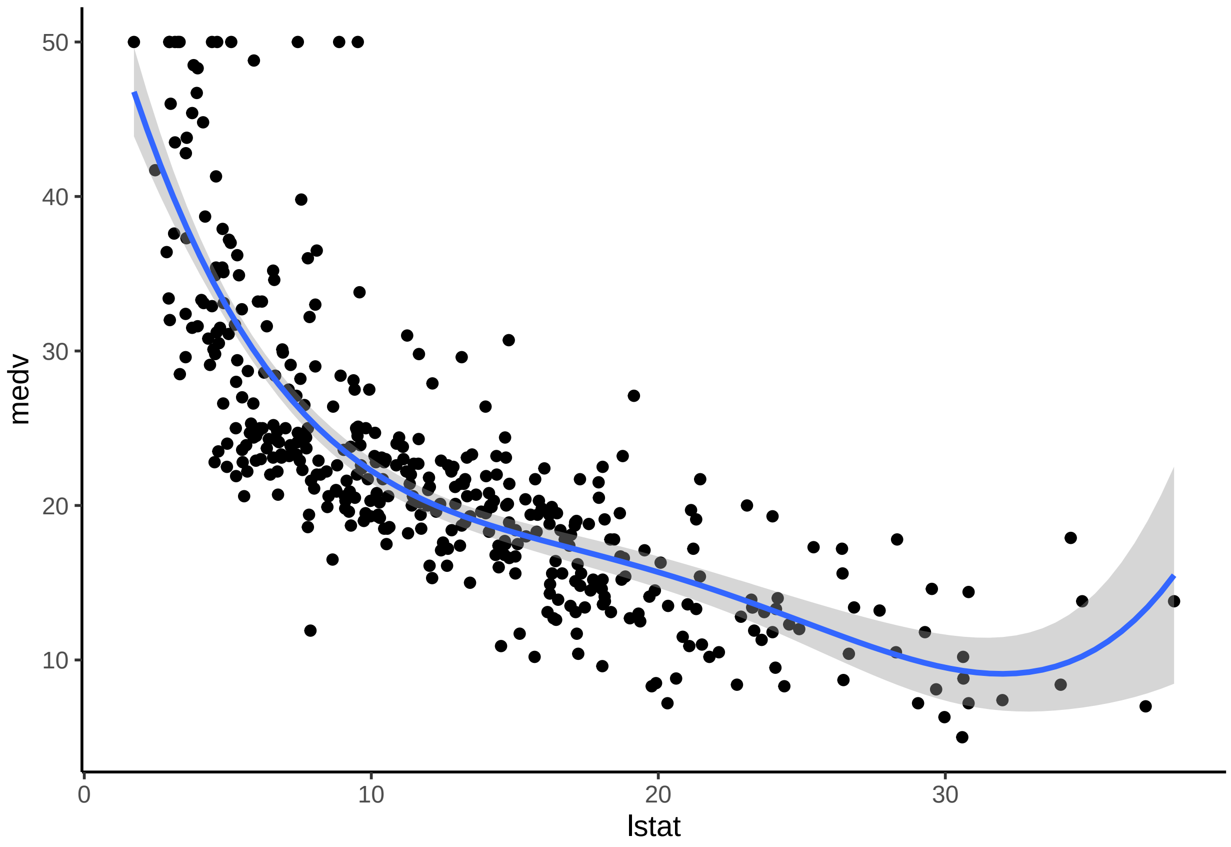
```
##
## Call:
## lm(formula = medv ~ poly(lstat, 4, raw = T), data = trd)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -13.6093  -3.1719  -0.6806   2.2075  27.1453
##
## Coefficients:
##                            Estimate Std. Error t value Pr(>|t|)
## (Intercept)               5.764e+01  2.615e+00  22.047  < 2e-16 ***
## poly(lstat, 4, raw = T)1 -7.098e+00  8.303e-01  -8.549 2.62e-16 ***
## poly(lstat, 4, raw = T)2  5.007e-01  8.419e-02   5.947 5.94e-09 ***
## poly(lstat, 4, raw = T)3 -1.643e-02  3.336e-03  -4.925 1.24e-06 ***
## poly(lstat, 4, raw = T)4  1.948e-04  4.468e-05   4.359 1.66e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
```

```
## Residual standard error: 5.255 on 402 degrees of freedom
## Multiple R-squared:  0.6747, Adjusted R-squared:  0.6715
## F-statistic: 208.5 on 4 and 402 DF,  p-value: < 2.2e-16
```

The residuals distribution is alright. By theory, the median should be 0 and 1Q, 3Q, and min max should be balanced. so this is not the best model but thats all we have.

Let's visualize the data

```r
ggplot(trd, aes(lstat, medv)) +
  geom_point() +
  stat_smooth(method = lm, formula = y ~ poly(x, 4, raw = T))
```



Log Transformation When i have a non linear relationship, i can also try a log transformation of the predictor variables.

```r
# build the model
modelcLog <- lm(medv ~ log(lstat), data = trd)

# make predictions
pmodelcLog <- modelcLog %>% predict(ted)

# model performance
(rmseLog <- RMSE(pmodelcLog, ted$medv))
```

```
## [1] 5.467124
```

```r
(r2Log <-  caret::R2(pmodelcLog, ted$medv))
```

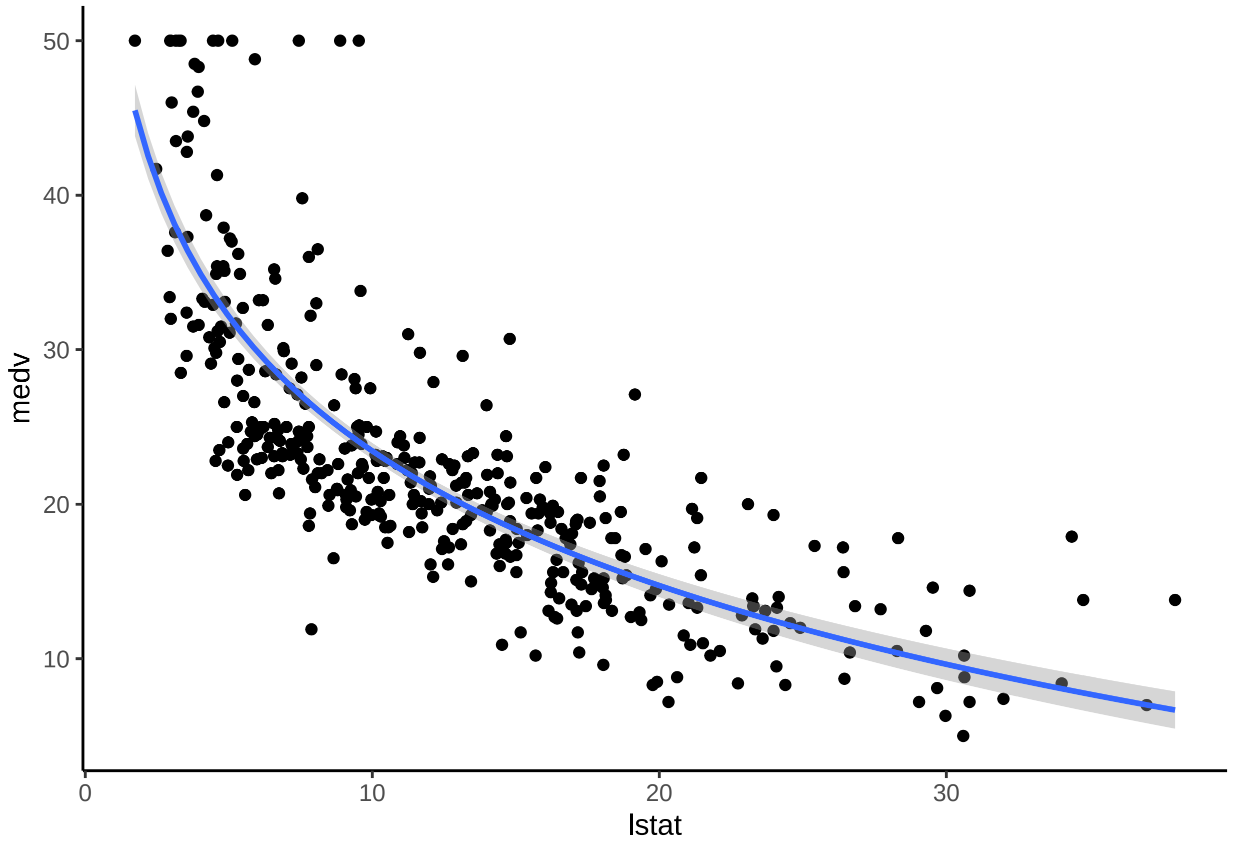
```
## [1] 0.6570091
```

```
(perrorLog <- rmseLog/ mean(ted$medv))
```

```
## [1] 0.2416489
```

visualize the data

```
ggplot(trd, aes(lstat, medv)) +
  geom_point() +
  stat_smooth(method = lm, formula = y ~ log(x))
```



Spline regression

```
library(splines)
# splines becomes a base package so you shouldnt be install
# it if you are using R version 4.0.2
knots <- quantile(trd$lstat, p = c(.25,.5,.75))
# build model
modelcSp <- lm(medv ~ bs(lstat, knots = knots), data = trd)
# make prediction
pmodelcSp <- modelcSp %>% predict(ted)

# model performance
(rmseSp <- RMSE(pmodelcSp, ted$medv))
```

```
## [1] 5.317372
```

```
(r2Sp <-  caret::R2(pmodelcSp, ted$medv))
```

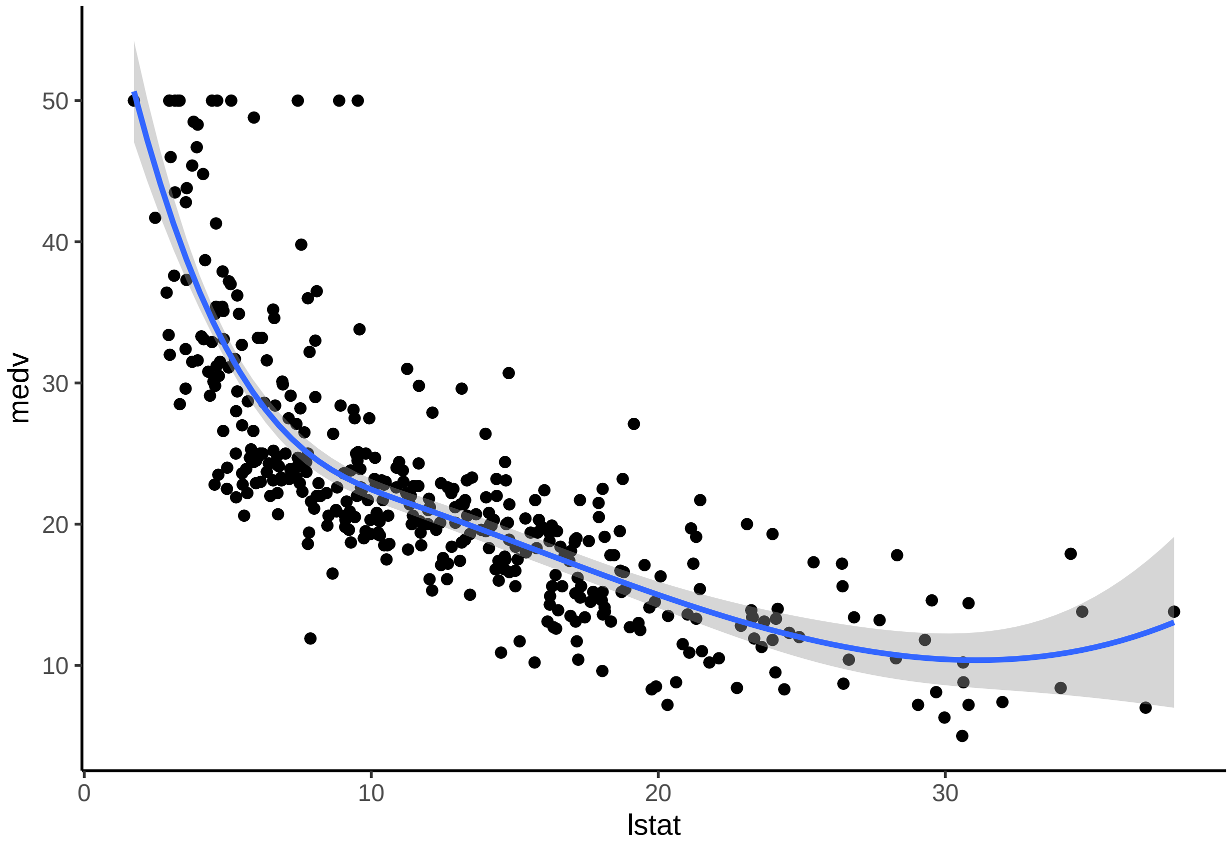
```
## [1] 0.6786367
```

```
(perrorSp <- rmseSp/ mean(ted$medv))
```

```
## [1] 0.2350299
```

Lets visualize the data

```
ggplot(trd, aes(lstat, medv)) +
  geom_point() +
  stat_smooth(method = lm, formula = y ~ splines::bs(x, df =4))
```



Generalized additive models

Here is another problem. Once I know that the model is non linear relationship in my data, the polynomial terms might not be flexible enough to capture the relationship, and the spline terms require specifying the knots. Therefore, we have Generalized additive models, GAM, are a technique to automatically fit a spline regression. We need mgcv package

```
library(mgcv)
```

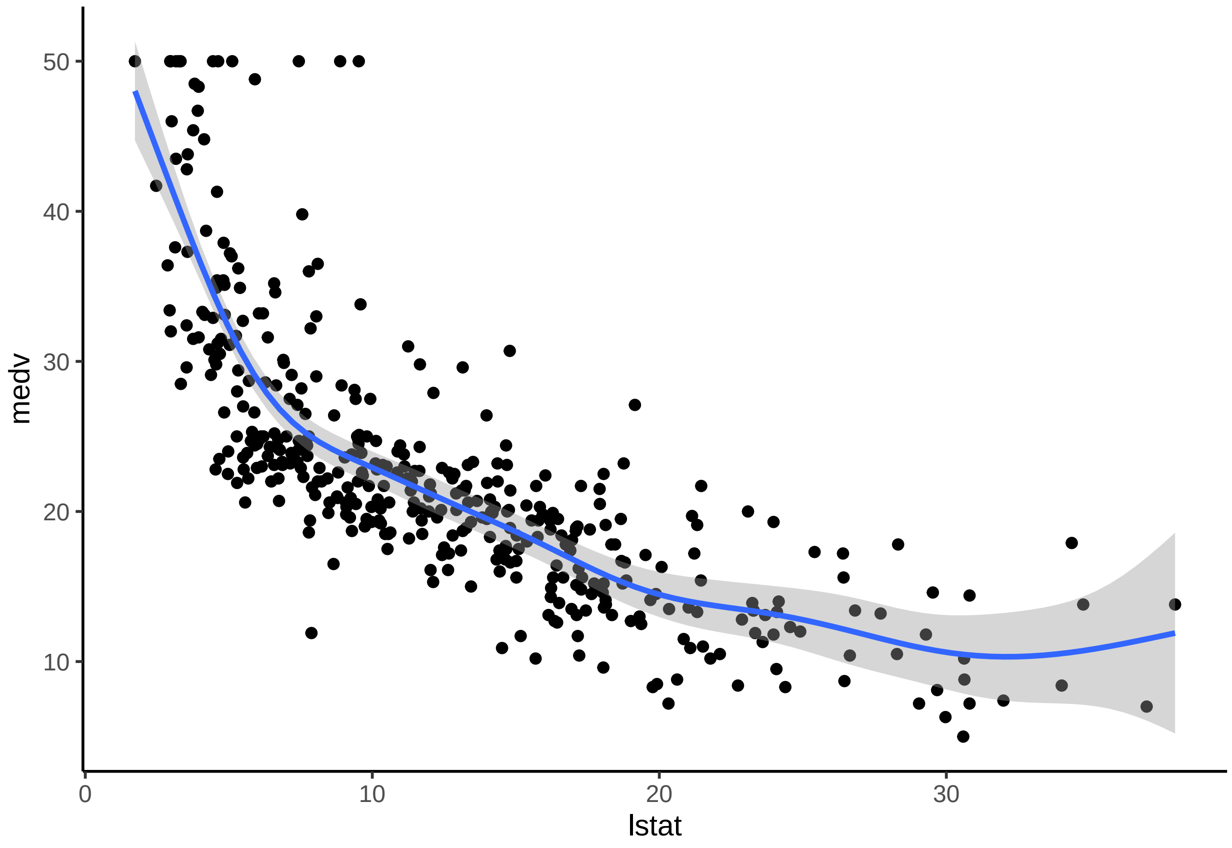
```
## Loading required package: nlme

##
## Attaching package: 'nlme'

## The following object is masked from 'package:dplyr':
##
##     collapse

## This is mgcv 1.8-31. For overview type 'help("mgcv-package")'.
```

```
# build the model
modelcGam <- gam(medv ~s(lstat), data = trd)
# make predictions
pmodelcGam <- modelcGam %>% predict(ted)
# Model performance
data.frame(
  rmsegam <- RMSE(pmodelcGam, ted$medv),
  r2gam <- caret::R2(pmodelcGam, ted$medv),
  perrorGam <- rmsegam / mean(ted$medv))
```

```
##   rmsegam....RMSE.pmodelcGam..ted.medv.
## 1                              5.318856
##   r2gam....caret..R2.pmodelcGam..ted.medv. perrorGam....rmsegam.mean.ted.medv.
## 1                                0.6760512                           0.2350954
```

Visualize the plot

```
ggplot(trd, aes(lstat, medv)) +
  geom_point() +
  stat_smooth(method = gam, formula = y ~ s(x))
```



Lets compare all the models linear, p^4, log, splines, and GAM

```
(fourmodelsPercentError <- rbind(perrorL, perrorp4, perrorLog, perrorSp, perrorGam))
```

```
##                [,1]
## perrorL   0.2874712
## perrorp4  0.2383705
## perrorLog 0.2416489
## perrorSp  0.2350299
## perrorGam 0.2350954
```

Among all 5 models, the best model we have is splines. why? think of how it works. it's like integral, it breaks in to small little part and find the slope thats why the stat_smooth fits the best of the data. Therefore Sp is the best model

Multiple Linear Regression in R

A little bit duplicated with the first section, however, in this section we are dealing with more than one variables.

With three predictor variables (x), the prediction of y is expressed by the following equation:

y = b0 + b1*x1 + b2*x2 + b3*x3

Outcome: 1) build and interpret a multiple linear regression model in R 2) Check the overall quality of the model

```r
data("marketing", package = "datarium")
modelLS <- lm(sales ~ youtube + facebook + newspaper, data = marketing)
summary(modelLS)
```

```
##
## Call:
## lm(formula = sales ~ youtube + facebook + newspaper, data = marketing)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -10.5932  -1.0690   0.2902   1.4272   3.3951
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  3.526667   0.374290   9.422   <2e-16 ***
## youtube      0.045765   0.001395  32.809   <2e-16 ***
## facebook     0.188530   0.008611  21.893   <2e-16 ***
## newspaper   -0.001037   0.005871  -0.177     0.86
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.023 on 196 degrees of freedom
## Multiple R-squared:  0.8972, Adjusted R-squared:  0.8956
## F-statistic: 570.3 on 3 and 196 DF,  p-value: < 2.2e-16
```

Let's interpret the data

First we might want to look at the F statistics' p value We have a pretty high significant value. This mean that, at least one of the variable is significantly related to the outcome. You can think of it is true that the parameter (youtube / facebook / newspaper) has the relationship with the response variable

You should have this question, so which one has the relationship with the response variable?

let's take a look with the following code

```r
summary(modelLS)$coef
```

```
##                 Estimate  Std. Error    t value     Pr(>|t|)
## (Intercept)  3.526667243 0.374289884  9.4222884 1.267295e-17
## youtube      0.045764645 0.001394897 32.8086244 1.509960e-81
## facebook     0.188530017 0.008611234 21.8934961 1.505339e-54
## newspaper   -0.001037493 0.005871010 -0.1767146 8.599151e-01
```

Look at the T statistics is checking if the b0, b1, b2, b3 is 0 or not. Look at the newspaper, we have -0.001037493 as the beta3 right? and look at the t value, -0.1767146.

The T value for the newspaper is pretty close to 0 and look at B3, we have -0.001037493, it simply no use at all so we can simply create another model without the news paper.

But the rest, youtube, facebook have a high impact for the sales. There is a relationship with the sales. So more money to put in to youtube and facebook, we have more feedback from the sales.

Lets create another model

```r
modelLSyf <- lm(sales ~ youtube + facebook, data = marketing)
summary(modelLSyf)
```

```
##
## Call:
## lm(formula = sales ~ youtube + facebook, data = marketing)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -10.5572  -1.0502   0.2906   1.4049   3.3994
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  3.50532    0.35339   9.919   <2e-16 ***
## youtube      0.04575    0.00139  32.909   <2e-16 ***
## facebook     0.18799    0.00804  23.382   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.018 on 197 degrees of freedom
## Multiple R-squared:  0.8972, Adjusted R-squared:  0.8962
## F-statistic: 859.6 on 2 and 197 DF,  p-value: < 2.2e-16
```

95% confident interval for the coefficient

```r
confint(modelLSyf)
```

```
##                  2.5 %     97.5 %
## (Intercept) 2.80841159 4.20222820
## youtube     0.04301292 0.04849671
## facebook    0.17213877 0.20384969
```

Model accuracy assessment

As we know, simple linear regression, the overall quality is based on R^2 and Residual standard error (RSE)

Remember one thing, the more parameters we have the higher the R^2. Eventhough the parameter does not have much effect on the Y response, it will still in play with the R square. Thats the reason why we have adjusted R^2

Residual standard error (RSE), or sigma

The RSE estimate gives a measure of error of prediction. we want small RSE

```r
sigma(modelLSyf)/mean(marketing$sales)
```

```
## [1] 0.1199045
```

This number is not to bad. so we have approximately 12% error rate.

Some cool trick, we dont have to type all the parameters. we can simply do

model <- lm(sales ~. data = marketing) that ~ means all

now if we would like to drop the newspaper from the parameter list model <- lm(sales ~. - newspaper, data = marketing)

Alternative model <- update(model, ~. - newspaper)

Predict in R: Model Predictions and Confidence Intervals

Outcome: predict outcome for new observations data, display confidence intervals and the prediction intervals.

```
# load the data
data("cars", package = "datasets")
# build the model
modelcar <- lm(dist ~ speed, data = cars)
modelcar
```

```
##
## Call:
## lm(formula = dist ~ speed, data = cars)
##
## Coefficients:
## (Intercept)        speed
##     -17.579        3.932
```

Prediction for new data set

```
# create data
cardata <- data.frame(speed <- c(12,19,24))
# predict data
predict(modelcar, newdata = cardata)
```

```
##        1        2        3
## 29.60981 57.13667 76.79872
```

Confidence interval

by default the confidence interval is 95%

```
predict(modelcar, newdata = cardata, interval = "confidence")
```

```
##        fit      lwr      upr
## 1 29.60981 24.39514 34.82448
## 2 57.13667 51.82913 62.44421
## 3 76.79872 68.38765 85.20978
```

From our newly created data. Lets take 19 miles per hr as our example. Distance is in ft we can say that 19 miles per hr has an average stopping dist between 51.82913 to 62.44421. the regression line has predict the value for 19mph with a stopping dist @ 57.13667

Prediction interval prediction interval gives an uncertainty around a single value.

```
predict(modelcar, newdata = cardata, interval = "prediction")
```

```
##        fit       lwr       upr
## 1 29.60981 -1.749529  60.96915
## 2 57.13667 25.761756  88.51159
## 3 76.79872 44.752478 108.84495
```

From the table above, we can say that 95% prediction intervals tell us that with a speed of 19 mph with the stopping distance is 25.76 to 88.51. This means that, based on our model 95% of the cars with a speed of 19 mph have a stopping distance between 25.76 and 88.51

Now you should have at least one question in your mind at this point. WTH? what is the difference between prediction interval and confidence interval?

The key word for both interpreting is average.

prediction interval is predicting a single future value at that point.

confidence interval is predicting the mean.

https://stats.stackexchange.com/questions/16493/difference-between-confidence-intervals-and-prediction-intervals

More on prediction interval or confidence interval

A prediction interval reflects the uncertainty around a single value, while a confidence interval reflects the uncertainty around the mean prediction values. Thus, a prediction interval will be generally much wider than a confidence interval for the same value.

Generally, we are interested in specific individual predictions. So a prediction interval would be more appropriate. Using a confidence interval when you should be using a prediction interval will be underestimate the uncertainty in a given predicted value

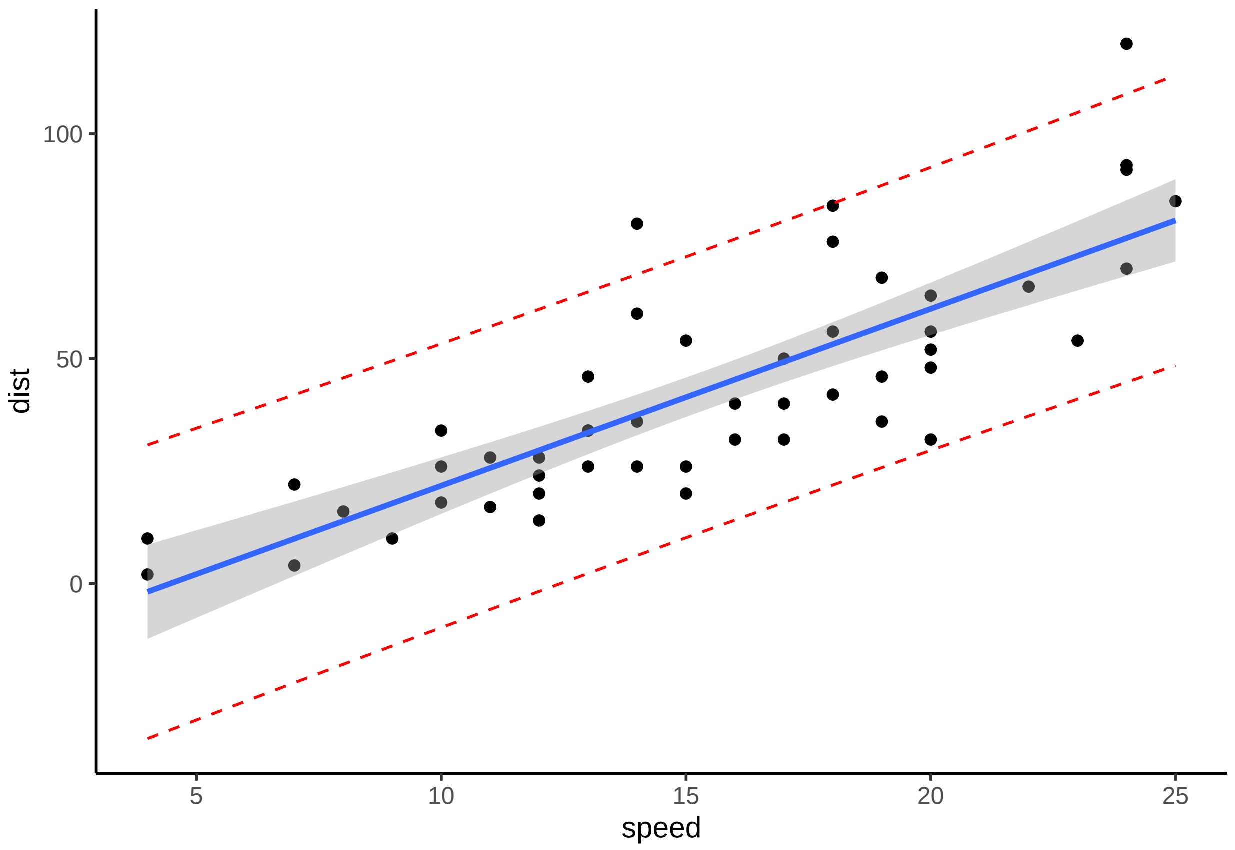
lets build the prediction band and confidence inteval

```r
# build the model
data("cars", package = "datasets")
modelcar1 <- lm(dist~speed, data =cars)
# add the predictions
p.int <- predict(modelcar1, interval = "prediction")
```

```
## Warning in predict.lm(modelcar1, interval = "prediction"): predictions on current data refer to _futu
```

```r
carD <- cbind(cars, p.int)
# Regression line + confidence intervals
p <- ggplot(carD, aes(speed, dist)) +
  geom_point() +
  stat_smooth(method = lm) +
  geom_line(aes(y = lwr), color = "red", linetype = "dashed") + #prediction interval
  geom_line(aes(y = upr), color = "red", linetype = "dashed") # prediction interval
p
```

```
## `geom_smooth()` using formula 'y ~ x'
```



Section 2 - Regression Model Diagnostics - 3 Sub Sections

Intro This section is focusing in making diagnostics to detect potential problems in the data.

Sub-Section 1

Linear Regression Assumptions and Diagnostics in R: Essentials

By the title, you can tell we are going to check if the model works well for the data.

1) inspect the significance of the regression beta coefficients
2) R^2

Those are what we have learnt from the previous sections

This section, we will learn the additional steps to evaluate how well the model fits the data.

For example, linear regression model makes the assumption that the relationship between x and y are linear. but that might not be true. The relationship could be polynomial or logarithmic

the data might contain outlines which will affect the result.

Thats why we need to diagnose the regression model and detect potential problems and check the assumptions is met by the linear regression model

in order to do so, we will check the distribution of residuals errors, which will tell us more about my data.

Main idea for this section. - explaining residuals errors and fitted values. - present linear regression assumptions, as well as potential problems you can will tackles while performing regression analysis - We will talk about some built in diagnostic plots in R to test the assumptions about our linear regression model.

Lets get started

```r
if(!require("broom")){
  install.packages("broom")
  library(tidyverse)
library(broom)
}
```

```
## Loading required package: broom
```

```r
theme_set(theme_classic())
```

```r
# load the data
data("marketing", package = "datarium")
# inspect the data
sample_n(marketing, 3)
```

```
##   youtube facebook newspaper sales
## 1   10.44    58.68     90.00  8.64
## 2  345.12    51.60     86.16 31.44
## 3  195.96    37.92     63.48 20.28
```

Build the regression model

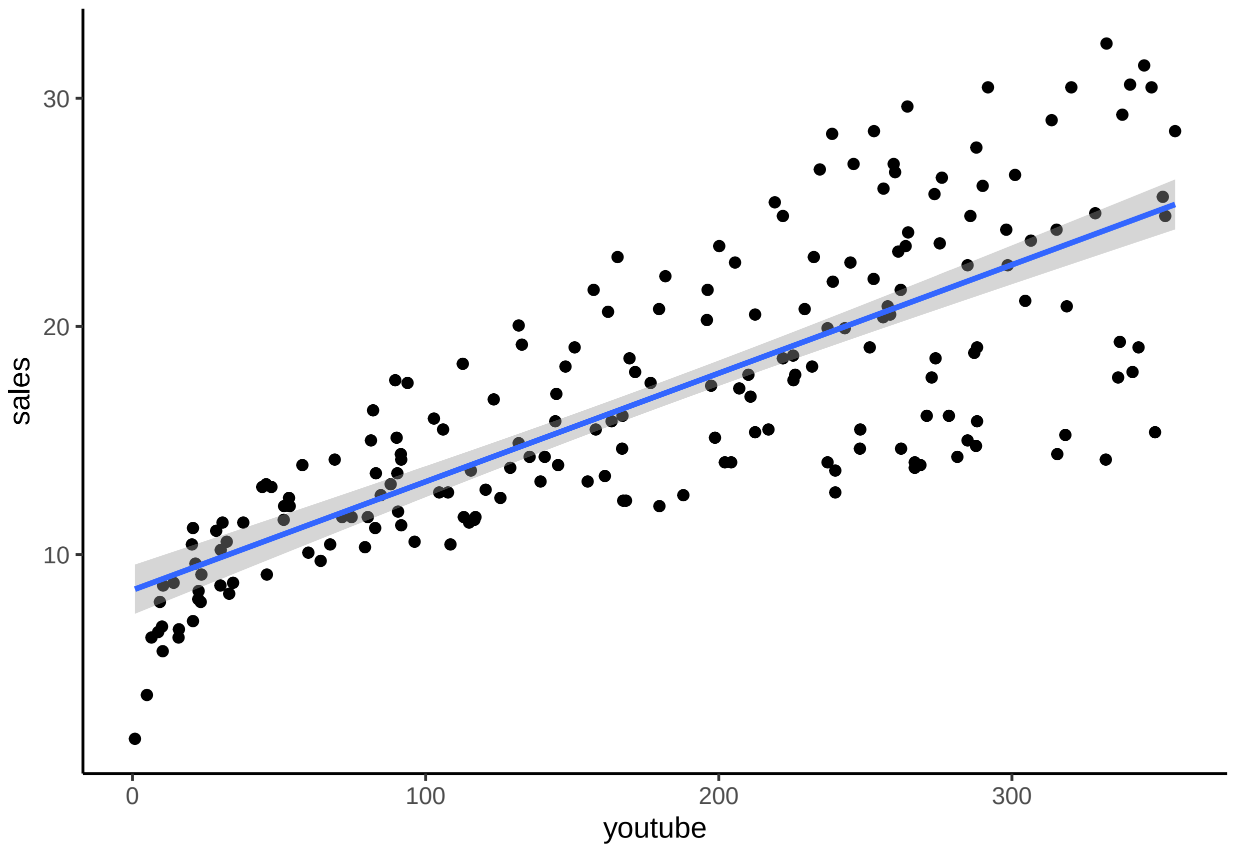
```r
modelm <- lm(sales ~ youtube, data = marketing)
modelm
```

```
##
## Call:
## lm(formula = sales ~ youtube, data = marketing)
##
## Coefficients:
## (Intercept)      youtube
##     8.43911      0.04754
```

Fitted value (predicted value) is the value that is predicted from the regression line.

```r
ggplot(marketing, aes(youtube, sales)) +
  geom_point() +
  stat_smooth(method = lm)
```

```
## ‘geom_smooth()‘ using formula ’y ~ x’
```



augment is from broom package

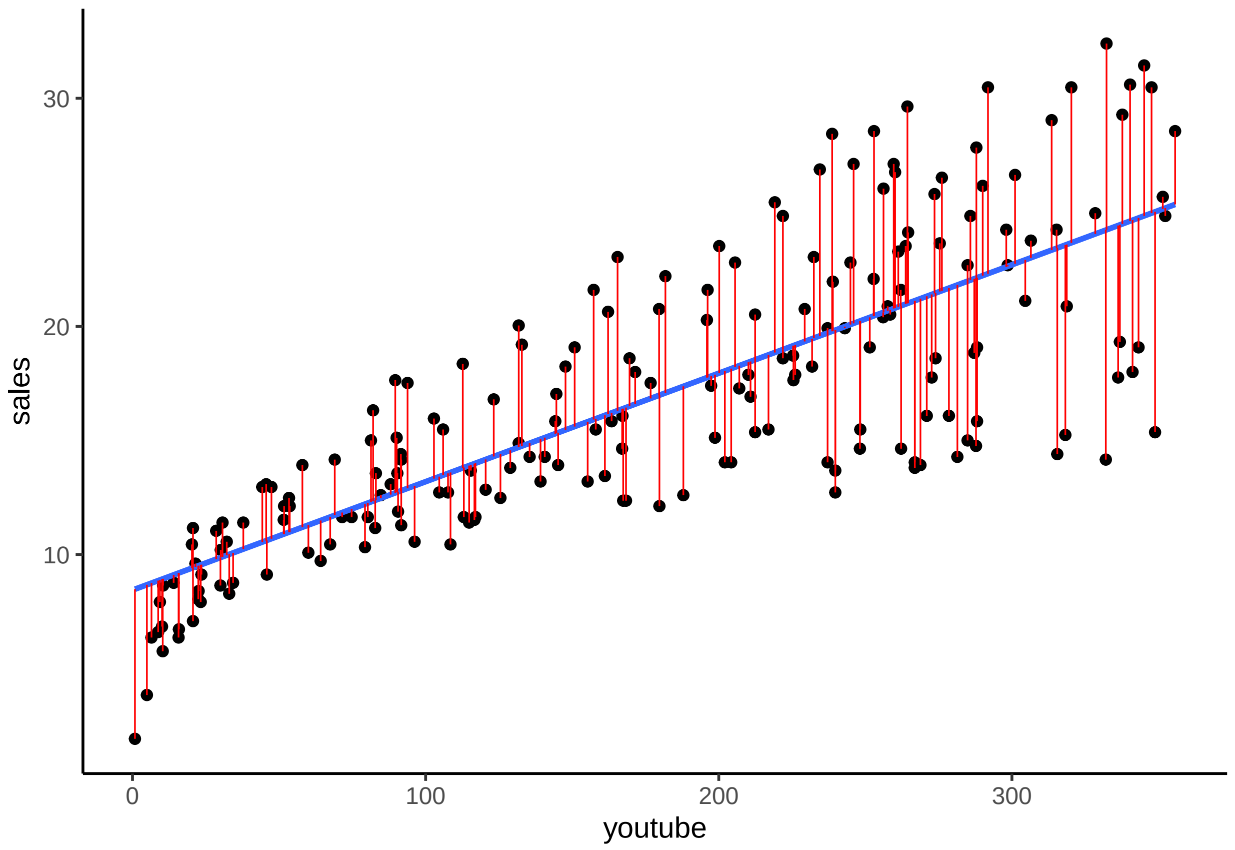
```r
model.diag.metrics <- augment(modelm)
head(model.diag.metrics)
```

```
## # A tibble: 6 x 8
##   sales youtube .fitted .resid .std.resid    .hat .sigma   .cooksd
##   <dbl>   <dbl>   <dbl>  <dbl>      <dbl>   <dbl>  <dbl>     <dbl>
## 1 26.5    276.     21.6   4.96      1.27   0.00970   3.90 0.00794
## 2 12.5     53.4    11.0   1.50      0.387  0.0122    3.92 0.000920
## 3 11.2     20.6     9.42  1.74      0.449  0.0165    3.92 0.00169
## 4 22.2    182.     17.1   5.12      1.31   0.00501   3.90 0.00434
## 5 15.5    217.     18.8  -3.27     -0.839  0.00578   3.91 0.00205
## 6  8.64    10.4     8.94 -0.295    -0.0762 0.0180    3.92 0.0000534
```

Lets plot the residuals error in red

```r
ggplot(model.diag.metrics, aes(youtube, sales)) +
  geom_point() +
  stat_smooth(method = lm, se = F) +
  geom_segment(aes(xend = youtube, yend = .fitted), color = "red", size =0.3)
```

```
## `geom_smooth()` using formula 'y ~ x'
```



In order to check the regression assumption, we need to see the distribution of the residuals

Linear regression makes several assumptions about the data, such as :

Linearity of the data. The relationship between the predictor (x) and the outcome (y) is assumed to be linear.

Normality of residuals. The residual errors are assumed to be normally distributed.

Homogeneity of residuals variance. The residuals are assumed to have a constant variance (homoscedasticity)

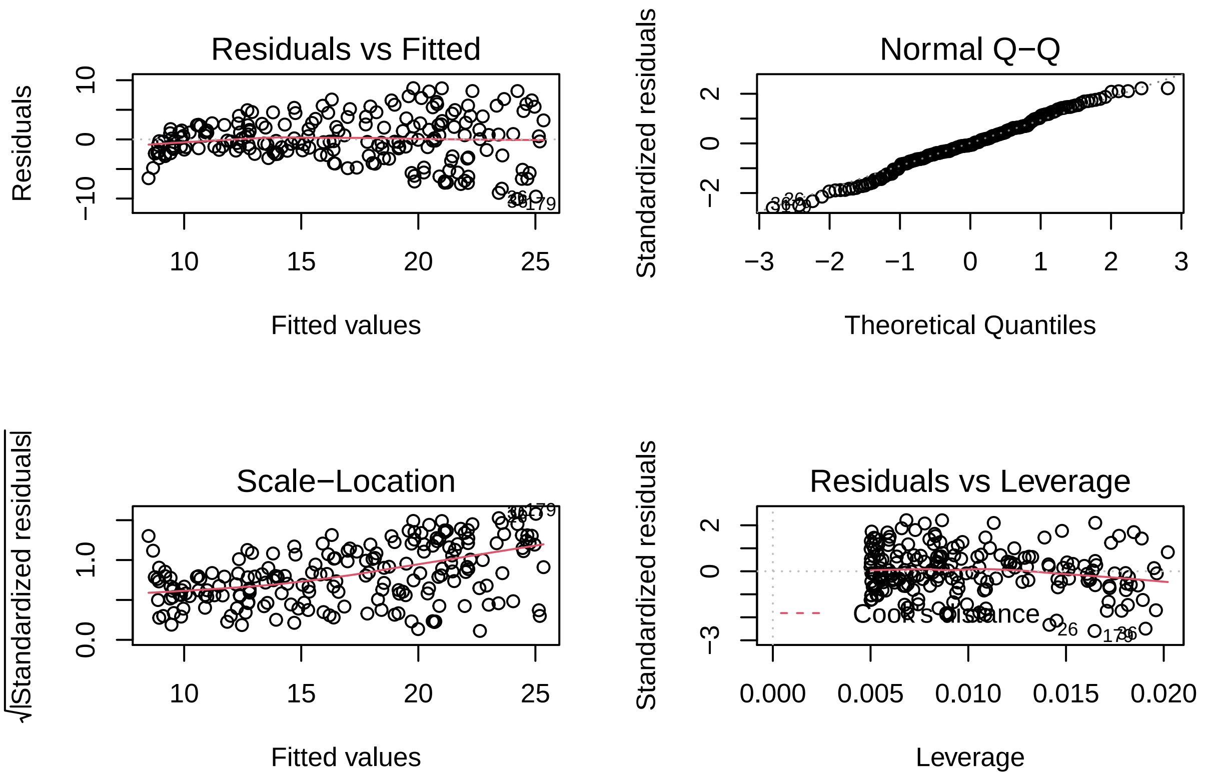
Independence of residuals error terms.

You should check whether or not these assumptions hold true. Potential problems include:

Non-linearity of the outcome - predictor relationships Heteroscedasticity: Non-constant variance of error terms. Presence of influential values in the data that can be: Outliers: extreme values in the outcome (y) variable High-leverage points: extreme values in the predictors (x) variable

Those problems can be solved by diagnostic plot

```r
par(mfrow = c(2,2))
plot(modelm)
```



How to read it?

https://data.library.virginia.edu/diagnostic-plots/

Residuals vs Fitted. Used to check the linear relationship assumptions. A horizontal line, without distinct patterns is an indication for a linear relationship, what is good.

Normal Q-Q. Used to examine whether the residuals are normally distributed. It's good if residuals points follow the straight dashed line.

Scale-Location (or Spread-Location). Used to check the homogeneity of variance of the residuals (homoscedasticity). Horizontal line with equally spread points is a good indication of homoscedasticity. This is not the case in our example, where we have a heteroscedasticity problem.

Residuals vs Leverage. Used to identify influential cases, that is extreme values that might influence the regression results when included or excluded from the analysis. This plot will be described further in the next sections.

Lets create a better table for model.diag.metrics

```
names(model.diag.metrics)
```

```
## [1] "sales"      "youtube"    ".fitted"    ".resid"     ".std.resid"
## [6] ".hat"       ".sigma"     ".cooksd"
```

Before and after

```
index <- c(1:nrow(model.diag.metrics))
model.diag.metrics1 <- data.frame(index,model.diag.metrics[ , c(-7)])
names(model.diag.metrics1)
```

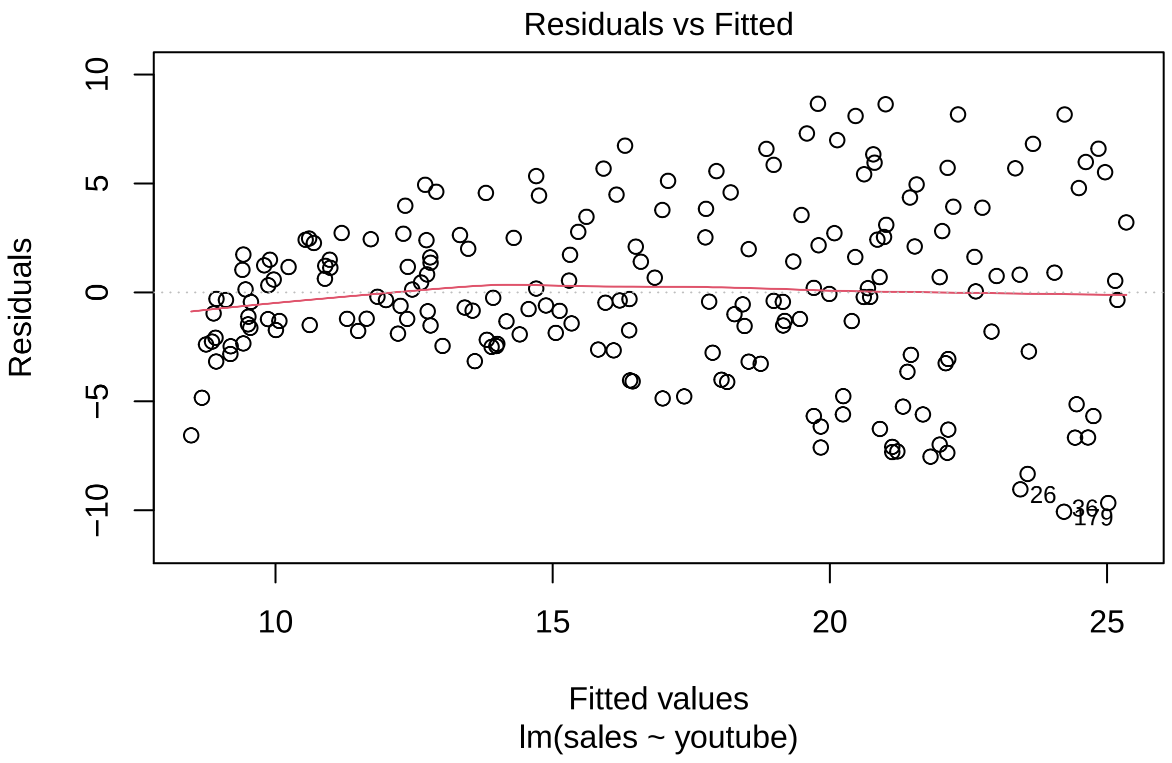
```
## [1] "index"      "sales"      "youtube"    ".fitted"    ".resid"
## [6] ".std.resid" ".hat"       ".cooksd"
```

fitted values = predicted value from the regression line .resid = residual errors .hat = outliers .std.resid =

detect outliers, extreme values -> standardized residuals = residuals / standard errors .cooksd = Cook's distance -> detect influential values outliers or high leverage point

Let's look at the plot one by one

```
plot(modelm,1)
```



Good plot would be show no fitted pattern, which means the red line should be a horizontal line at 0. If the red line is not at 0 or around 0 there might be a problem with our linear model, which means we need to use non linear model. In our example, plot 1 residuals vs fitted, there is no pattern in the residual plot, so we can assume it is a linear relationship sales ~ youtube.

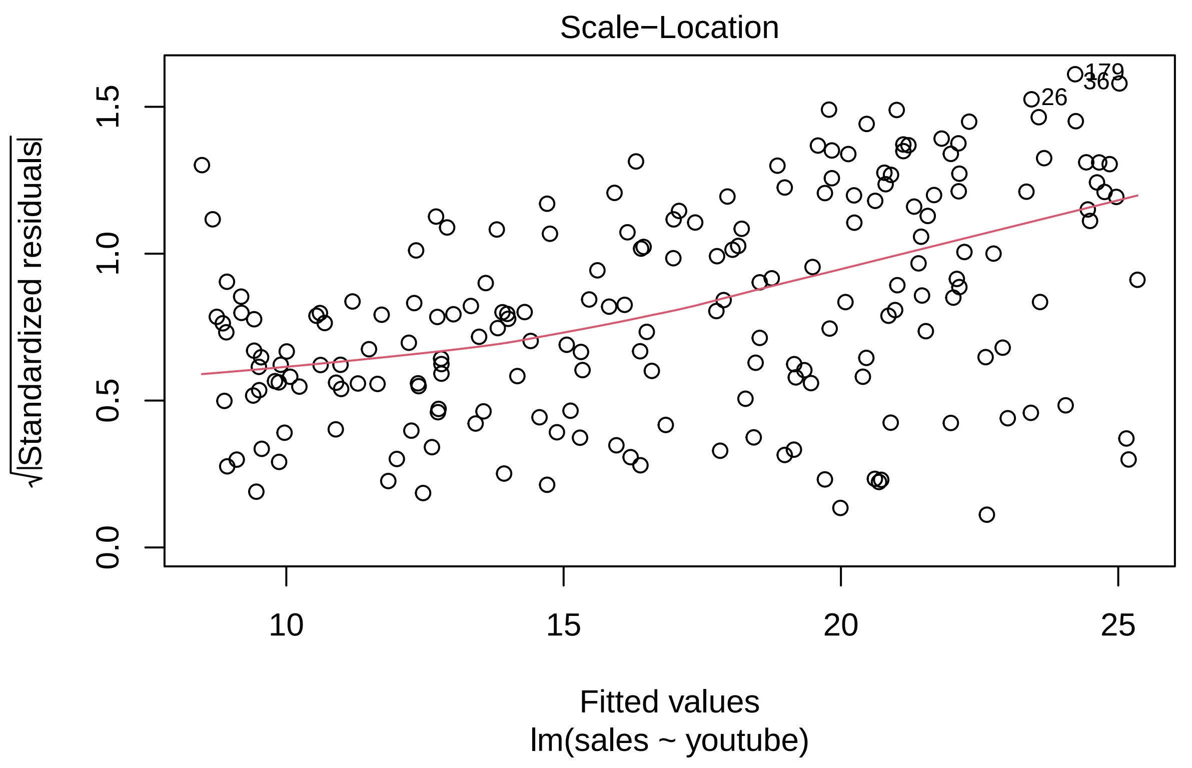
if the residual plot is non linear relationship, you need to transform your data ith log(x), sqrt(x), x^2 in the regression and so on.

You might ask how do you know if it is non linear? well it will be obvious that red line is something else like quadratic or something. reference link: non linear https://i0.wp.com/blogs.sas.com/content/iml/files/2019/06/residsmooth1.png?ssl=1

Homogeneity of variance

This assumption can be checked by examining the scale - location plot, also known as the spread- location plot

```
plot(modelm,3)
```



Good plot for scale - location is the data set is close together and close the the line. since this plot is spreading wider when x increases, so this is not a good plot.

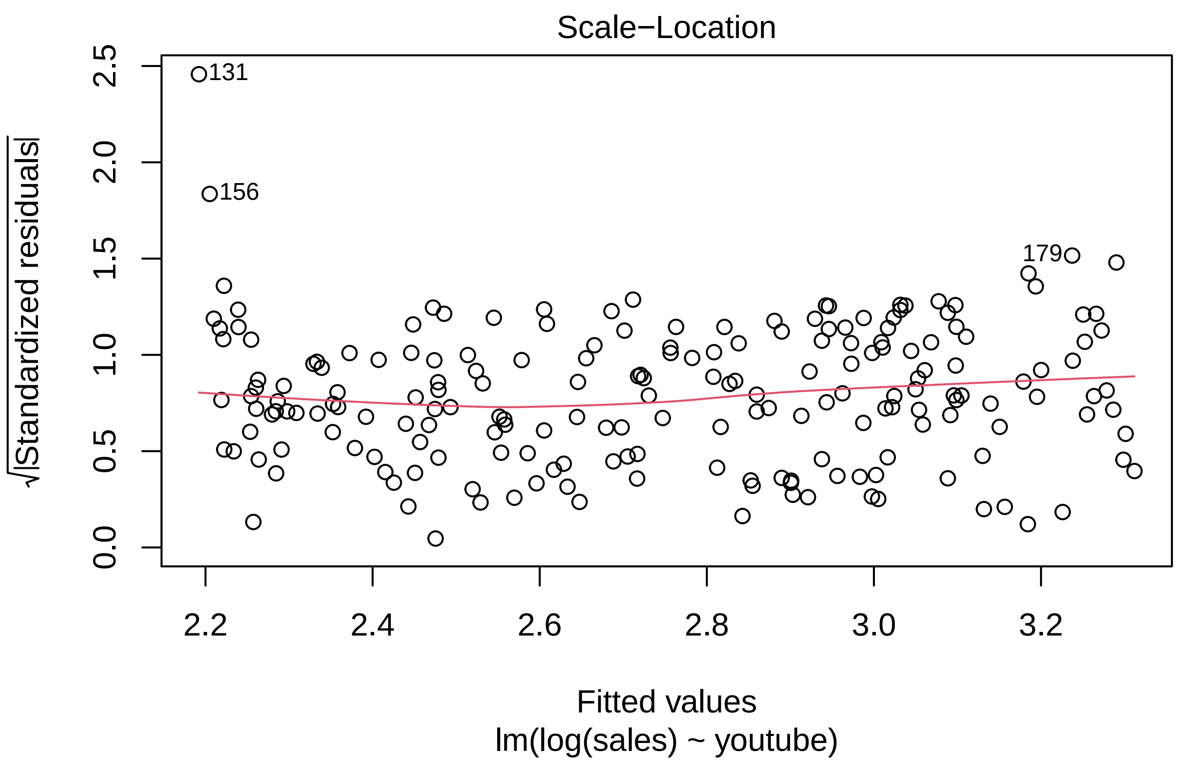
So i can say not a constant variances in the residuals error (heterosedasticity)

Remember, by theory epsilon has mean zero and the variance is constant.

a possible solution to reduce the variance is to use log or square root transformation for variable y

lets try again by transforming the plot

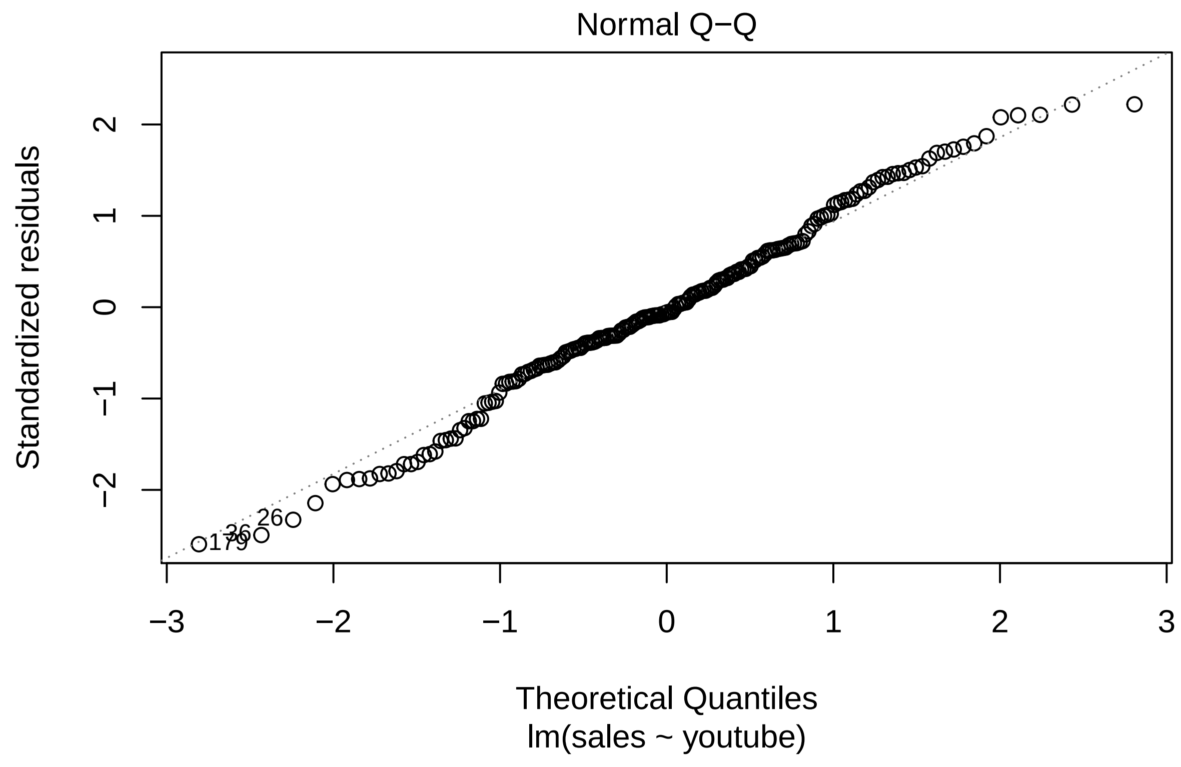
```
modelmLog <- lm(log(sales) ~ youtube, data = marketing)
plot(modelmLog,3)
```



This plot looks a lot better

Normality of Residuals this is also called QQ plot. This plot can check the normality assumption. The normal probability plot of residuals should approximately follow a straight line like below.

```r
plot(modelm, 2)
```



Outliers and high Leverage points

The outliers will directly affect the RSE because it is so far away from the regression line. Outliers can be identified by examining the standardized residual (or studentized residual), which is the residual divided by the estimated standard error.

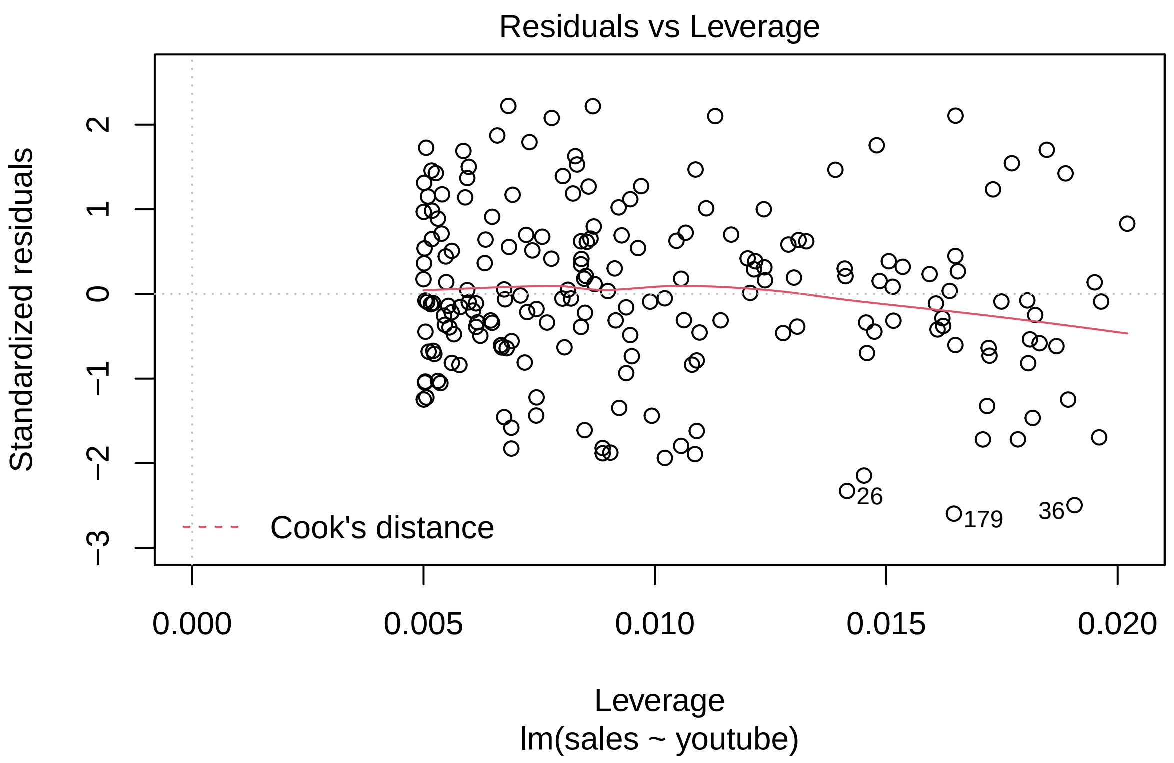
Observations whose standardized residuals are greater than 3 in absolute value are possible outliers (James et al. 2014).

High leverage points (hat value)

A value of this statistic above 2(p + 1)/n indicates an observation with high leverage (P. Bruce and Bruce 2017); where, p is the number of predictors and n is the number of observations.

Residuals vs Leverage plot

```r
plot(modelm, 5)
```



The plot will highlight the most extreme points. 26, 179, 36. as you can see no outliers that have exceed 3 standard deviations, which is a good plot.

Influential values

Not all outliers (extreme data points) are influential in linear regression analysis

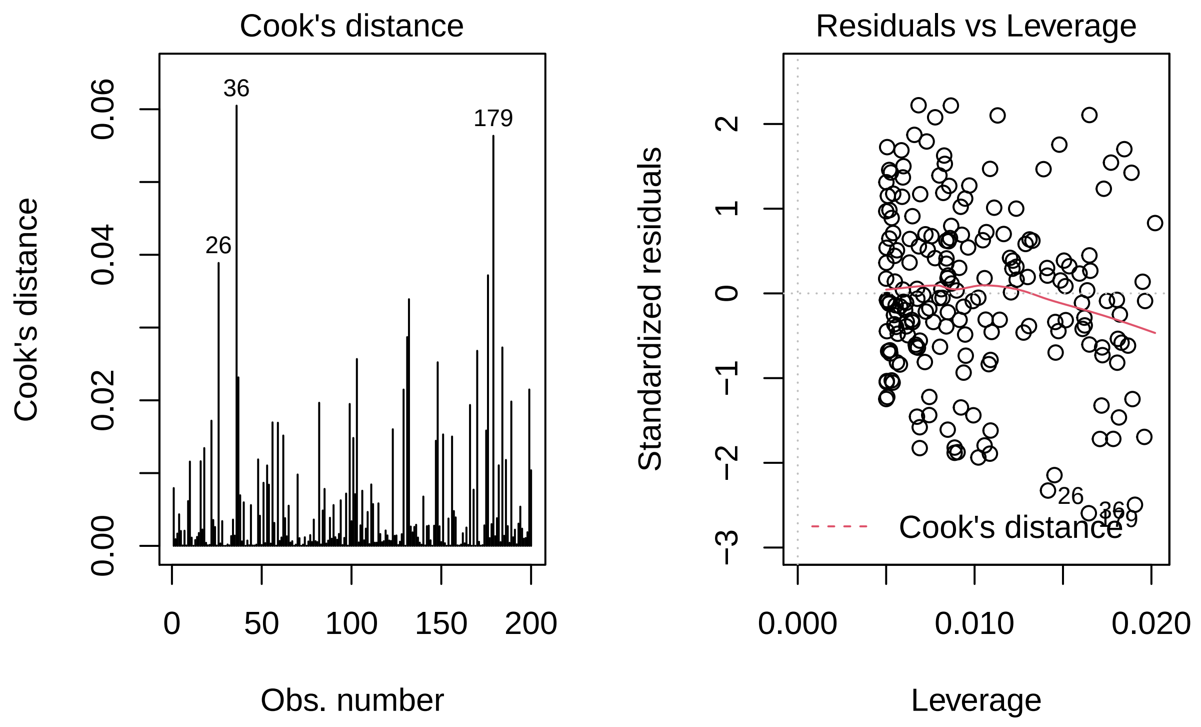
We use Cook's distance to determine the influence of a value. This metric defines influence as a combination of leverage and residual size.

High influence if Cook's distance exceeds 4/ (n - p - 1) n = # of observations p = number of predictor variables.

again residuals vs leverage plot can help us to find influential observations. outlying values are generally located at the upper right corner or lower right corner.

Those corners will have direct influential against a regression line.

```r
par(mfrow=c(1,2))
# Cook's distance
plot(modelm, 4)
# Residuals vs Leverage
plot(modelm, 5)
```



Now we have been talking about Cook's distance for the last 10 mins, so how do I know if the outliers are influencing the regression line?

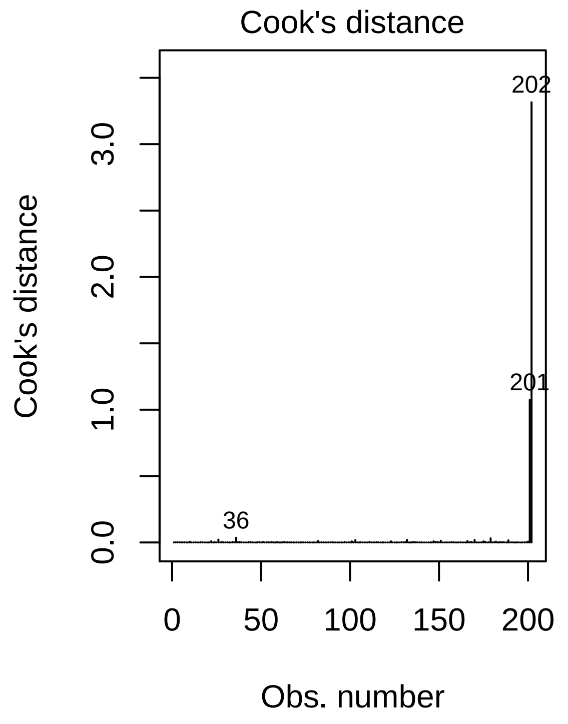
First from the Residuals vs Leverage plot, i am not seeing any red dashed line, so that means my outliers is not affecting the regression line a lot. If we see the dashed line that's mean we are close to the Cook's distance line which means it is some how affecting the regression line seriously. but usually if the outliers are within the Cook's distance we are all good.

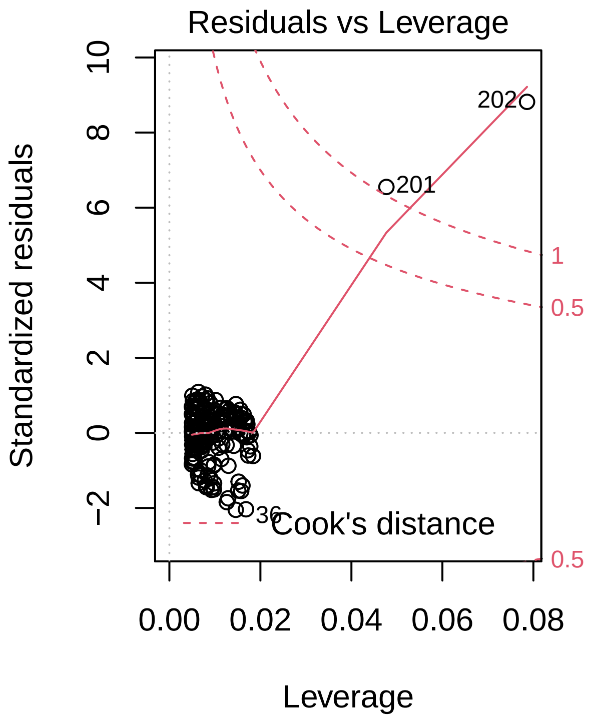
By default, only top 3 most extreme values are labeled on Cook's distance plot, if I want to add more i can use the following code plot(modelm, 4, id.n = 5)

if i would like to access those distance later, i can use the following code model.diag.metrics %?% top_n(3, wt = .cooksd)

Lets create something that is outside the Cook's distance

```r
dfcook <- data.frame(
  x <- c(marketing$youtube, 500,600),
  y <- c(marketing$sales, 80,100)
)
modelm2 <- lm(y~x, dfcook)
par(mfrow = c(1,2))
# Cook's distance
plot(modelm2, 4)
# Residuals vs Leverage
plot(modelm2, 5)
```





As you can see from the Residuals vs Leverage, you can see there are 2 outliers are outside of the dashed line (Cook's distance) those are the outliers that are affecting the regression line directly. In the other words, those data are outside of the cook's distance would simply mean they have a high cook's value.

The plot identified the influential observation as #201 and #202. If you exclude these points from the analysis, the slope coefficient changes from 0.06 to 0.04 and R2 from 0.5 to 0.6. Pretty big impact!

There are a lot of concepts that must be understood, so take your time to go thru it again.

Discussion. This section describes linear regression assumptions and how to diagnose the potential problems in the model You must visualizing the residuals and the patterns in residuals is not a stop signal. your current regression model might not be the best way to understand your data.

Here are the potential problems: non - linear relationships between the outcome and the predictor variables. When facing to this problem, one solution is to include a quadratic term, such as polynomial terms or log transformation. See Chapter

Existence of important variables that you left out from your model. Other variables you didn't include (e.g., age or gender) may play an important role in your model and data.

Presence of outliers. If you believe that an outliers have occurred due to an error in data collection and entry, then one solution is to simply remove the concerned observation.

Sub-Section 2

Multi-collinearity Essentials and VIF in R

In multiple regression, 2 or more parameters might be correlated with each other is called collinearity.

There is an extreme situation, called multicollinearity, which collinearity exists between three or more variables, even if no pair of variables have a particularly high correlation. To simplify that, there is redundancy between parameter variables.

If we have multicollinearity in our model, it will become unstable.

VIF (variance inflation factor) measures how much the variance of a regression coefficient is inflated due to multicollinearity.

“The smallest possible value of VIF is one (absence of multicollinearity). As a rule of thumb, a VIF value that exceeds 5 or 10 indicates a problematic amount of collinearity (James et al. 2014).”

So in this section, we will be detecting the multicollinearity in a regression model using R

Required R packages tidyverse, caret

```
library("tidyverse")
library("caret")
```

Data Preparation

```
# load the data
data("boston", package = "MASS")
```

```
## Warning in data("boston", package = "MASS"): data set 'boston' not found
```

```
# split the data into training and test set
set.seed(123)
btr.samples <- Boston$medv %>%
  createDataPartition(p=0.8, list = F)
btrd <- Boston[btr.samples, ]
bted <- Boston[-btr.samples,]
```

Build a regression model

```
# build the model
modelbos <- lm(medv ~., data = btrd)

# make predictions
bpred <- modelbos %>% predict(bted)

# model performance
brmse <- RMSE(bpred, bted$medv)
br2 <- caret::R2(bpred, bted$medv)
brmse
```

```
## [1] 4.588948
```

```
br2
```

```
## [1] 0.761126
```

Detecting multicollinearity need to install car package for vif()

```
car::vif(modelbos)
```

```
##     crim       zn    indus     chas      nox       rm      age      dis
## 1.844585 2.323334 3.956419 1.066866 4.447852 1.911905 3.213786 4.065420
##      rad      tax  ptratio    black    lstat
## 8.152643 9.660128 1.851645 1.364539 3.131835
```

From there we can see that tax has a 9.660128 score, which is a problem.

Dealing with multicollinearity

```
# build a model excluding the tax variable
modelbos.cleaned <- lm(medv ~. -tax, data = btrd)

# make predictions
modelbos.cleaned.pred <- modelbos.cleaned %>% predict(bted)
```

```r
#  performance
brmse.cleaned <- RMSE(modelbos.cleaned.pred, bted$medv)
br2.cleaned <- caret::R2(modelbos.cleaned.pred, bted$medv)
brmse.cleaned
```

```
## [1] 4.644396
```

```r
br2.cleaned
```

```
## [1] 0.7558647
```

Now we have a lower R2 and a higher RMSE

This section is simply detecting and how to deal with multicollinearity in regression models. anything that is above 5 or 10, those parameters must be removed.

Note that, in a large data set presenting multiple correlated predictor variables, you can perform principal component regression and partial least square regression strategies.

Sub-Section 3 Confounding Variable Essentials

library required gapminder

```r
library(gapminder)
lm(lifeExp ~ gdpPercap, data = gapminder)
```

```
##
## Call:
## lm(formula = lifeExp ~ gdpPercap, data = gapminder)
##
## Coefficients:
## (Intercept)    gdpPercap
##   5.396e+01    7.649e-04
```

So obviously the continent is an important variable like countries in Europe are estimated to have a higher life expectancy compared to countries in Africa. So by adding continent as a confounding variable will increase the accuracy of our model.

```r
lm(lifeExp ~ gdpPercap + continent, data = gapminder)
```

```
##
## Call:
## lm(formula = lifeExp ~ gdpPercap + continent, data = gapminder)
##
## Coefficients:
##       (Intercept)          gdpPercap  continentAmericas      continentAsia
##         4.789e+01          4.453e-04          1.359e+01          8.658e+00
##   continentEurope   continentOceania
##         1.757e+01          1.815e+01
```

Regression Model Validation - 3 sections

Info

In this big section, we will talk about goodness of the model, how well the model fits the training data used to build the model and how accurate is the model in predicting the outcome for new unseen test observations.

In this part, you will learn techniques for assessing regression model accuracy and for validating the performance of the model.

Sub section 1

Regression Model Accuracy Metrics: R-square, AIC, BIC, Cp and more

This section, we will be discussing different statistical regression metrics for measuring the performance of the regression model

Model Performance metrics

R-Squared: interval -> +/ - 1 +- 1 is the max or min. Closer to 1 the better it is. It measures how close the actual data to the regression line. If we have 1 that means all the actual data are on exactly lies on the regression line.

Root mean squared error RMSE: We want a small RMSE. RMSE is simply the square root of MSE. MSE is exactly the epsilon term from the regression model. Formula = MSE = actual - theoretical value) ˆ2

Residual Standard Error (RSE): it is the same as model sigma. We want small RSE. In real world practice, the difference between RMSE and RSE is very small, specifically when we are working on large scale multivariate data.

Mean Absolute error (MAE): it is similar with RMSE. It's measures the prediction error. formula = MAE = mean(abs(actual - theoretical))

Recall that, the more variable we add, Rˆ2 will increase as well. So, we need another method to measure the accuracy of the model

Concerning R2, we have adjusted R- Squared, which adjusts the R2 for having too many variables. Additionally, we have AIC, AICc, BIC, and Mallows Cp, that are commonly used for model evaluation and selection. Those are unbiased estimate of the model prediction error MSE. We want small # from those result.

AIC (Akaike's information Criteria): this is developed by the Japanese Statistician. The idea of AIC is to penalize the inclusion of additional variables to a model. it adds a penalty that increase the error when including additional terms. The lower the AIC, the better the model.

AICc: is a version of AIC corrected for a small sample sizes.

BIC (Bayesian information criteria): is derived from AIC with a stronger penalty for including additional variables to the model.

Mallows Cp: is derived from AIC developed by Colin Mallows.

Generally speaking, we use Adjusted R2, AIC, BIC, and Cp to measure the regression model quality and for comparing models.

Lets get in to the code

```r
if(!require("modelr")){
  install.packages("modelr")
  library(tidyverse)
  library(modelr)
  library(broom)
}
```

```
## Loading required package: modelr
```

```
##
## Attaching package: 'modelr'
```

```
## The following object is masked from 'package:broom':
##
##     bootstrap
```

Example of data

```r
# load data
data("swiss")
# inspect the data
sample_n(swiss,3)
```

```
##            Fertility Agriculture Examination Education Catholic
## Porrentruy      76.1        35.3           9         7    90.57
## Entremont       69.3        84.9           7         6    99.68
## Aigle           64.1        62.0          21        12     8.52
##            Infant.Mortality
## Porrentruy             26.6
## Entremont              19.8
## Aigle                  16.5
```

Build the regression models model1 all parameters model2 except examination

```r
models1 <- lm(Fertility ~., data = swiss)
models2 <- lm(Fertility ~., -Examination, data = swiss)
```

Now, lets check the model quality, the following code will look like duplicate because im showing how to find those result in different ways.

summary() will return Rsquared and adjusted R squared and the RSE AIC() and BIC() computes the AIC and BIC repsectively.

```r
summary(models1)
```

```
##
## Call:
## lm(formula = Fertility ~ ., data = swiss)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -15.2743  -5.2617   0.5032   4.1198  15.3213
##
## Coefficients:
##                  Estimate Std. Error t value Pr(>|t|)
## (Intercept)      66.91518   10.70604   6.250 1.91e-07 ***
## Agriculture      -0.17211    0.07030  -2.448  0.01873 *
## Examination      -0.25801    0.25388  -1.016  0.31546
## Education        -0.87094    0.18303  -4.758 2.43e-05 ***
## Catholic          0.10412    0.03526   2.953  0.00519 **
## Infant.Mortality  1.07705    0.38172   2.822  0.00734 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 7.165 on 41 degrees of freedom
## Multiple R-squared:  0.7067, Adjusted R-squared:  0.671
## F-statistic: 19.76 on 5 and 41 DF,  p-value: 5.594e-10
```

```r
AIC(models1)
```

```
## [1] 326.0716
```

```r
BIC(models1)
```

```
## [1] 339.0226
```

rsquare(), rmse() and mae() [modelr package], computes, respectively, the R2, RMSE and the MAE.

```r
models1.r2 <- rsquare(models1, data =swiss)
models1.rmse <- rmse(models1, data = swiss)
models1.mae <- mae(models1, data = swiss)
```

R2(), RMSE() and MAE() [caret package], computes, respectively, the R2, RMSE and the MAE.

```r
library(caret)
models1.pred <- models1 %>% predict(swiss)
models1.R2 <- caret::R2(models1.pred, swiss$Fertility)
models1.RMSE <- RMSE(models1.pred, swiss$Fertility)
models1.MAE <- MAE(models1.pred, swiss$Fertility)
```

glance() [broom package], computes the R2, adjusted R2, sigma (RSE), AIC, BIC.

```r
library(broom)
glance(models1)
```

```
## # A tibble: 1 x 12
##   r.squared adj.r.squared sigma statistic  p.value    df logLik   AIC   BIC
##       <dbl>         <dbl> <dbl>     <dbl>    <dbl> <dbl>  <dbl> <dbl> <dbl>
## 1     0.707         0.671  7.17      19.8 5.59e-10     5  -156.  326.  339.
## # ... with 3 more variables: deviance <dbl>, df.residual <int>, nobs <int>
```

Now lets compare the performance

```r
name <- c("adj.r.squared", "sigma", "AIC" , "BIC", "p.value")
models1.temp <- c(glance(models1))
models1.performance <- models1.temp[c(2,3,8,9,5)]
models2.temp <- c(glance(models2))
models2.performance <- models2.temp[c(2,3,8,9,5)]
models.performance <- rbind(models1.performance, models2.performance)
models.performance
```

```
##                     adj.r.squared sigma    AIC      BIC      p.value
## models1.performance 0.670971      7.165369 326.0716 339.0226 5.593799e-10
## models2.performance 0.7630908     6.888644 174.5797 183.1118 2.493363e-06
```

From the above table we can see couple things

We have a better R^2 from model2.performance, which means models2 explain better for the predicted value, the model from models2 has a better accuracy.

RSE: models1 = 7.165369, models2 = 6.888644 RSE = sigma. So from models2 we have a smaller sigma which is a good thing. so models2 wins in this case.

Now, AIC and BIC. it is obvious that models2 has a better numbers than models1. remember we want small number from AIC and BIC. so models2 wins again

F statistics p value.

```r
5.593799e-10 > 2.493363e-06
```

```
## [1] FALSE
```

if you can compare it by looking at it, just calculate it with R. so models1 has a smaller F statistics. However, imo, i would take models2.performance as my model because of all those numbers compared with models1, models2 has a better accuracy.

```r
sigma(models1)/mean(swiss$Fertility)
```

```
## [1] 0.1021544
```

```r
sigma(models2)/mean(swiss$Fertility)
```

```
## [1] 0.0982092
```

Lastly, as you can see, models2 has a better prediction error.

Discussion

We have gone thru the overall performance of a regression model

The most important metrics are the Adjusted R^2, RMSE, AIC, and BIC. These metrics are also used as the basis of model comparison and optimal model selection.

Note that regression metrics are all internal measures. They tell you how well the model fits to the data in hand, training data set.

In general, we don't care how well the method works on the training data. Rater, we are interested in the accuracy of the predictions that we obtain when we apply our method to previously unseen test data. However, the test data is not always available making the test error very difficult to estimate. Because of this situation, we have cross-validation and bootstrap that are applied for estimating the test error (the prediction error rate) using training data.

sub section 2

Cross-Validation Essentials in R

intro
Cross validation refers to a set of methods for measuring the performance of a given predictive model on new test data set

Idea of Cross validation:
1) Training set to build the model
2) Testing set to see the prediction error

Cross validation is also known as re-sampling method

In this section you will learn:
1) most commonly used statistical metrics that measure the performance of a regression model in predicting the outcome of new test data

2) validation set approach (data split)
   Leave one out cross validation
   K - fold Cross validation
   Repeated K fold cross validation

   Those 4 methods have their advantages and drawbacks. Use it that fit the best of your problem. Mostly, K fold cross validation is recommended

required R packages

```r
library(tidyverse)
library(caret)
```

Preper the data

```r
# load the data
data("swiss")
```

```
# inspect the data
sample_n(swiss,3)
```

```
##              Fertility Agriculture Examination Education Catholic
## La Vallee         54.3        15.2          31        20     2.15
## Paysd'enhaut      72.0        63.5           6         3     2.56
## Entremont         69.3        84.9           7         6    99.68
##              Infant.Mortality
## La Vallee                10.8
## Paysd'enhaut             18.0
## Entremont                19.8
```

To see the accuracy of the model on predicting the outcome. simply we want to estimate the prediction error.

1) R^2
2) RMSE: square root the MSE
3) compute the prediction errors

R^2, RMSE, MAE are used to measure the regression model performance during the cross-validation.

Cross validation method 1) reserve a small sample of data set 2) build (or train) the model using the remaining part of the data set (unseen data) 3) test the effectiveness of the model on the reserved sample data set. If the model works well on the test data set, then it is good. (MSE)

The Validation set Approach

We split the data in to two part 80% for the training and 20% for the testing

```
# split the data in to two part
set.seed(1234)
training.samples.swiss <- swiss$Fertility %>%
  createDataPartition(p =0.8, list =F)
train.data.swiss <- swiss[training.samples.swiss, ]
test.data.swiss <- swiss[-training.samples.swiss, ]
# build the model
model.swiss <- lm(Fertility ~., data = train.data.swiss)
# make predictions and compute the R2, RMSE, MAE
swiss.pred <- model.swiss %>%
  predict(test.data.swiss)
swiss.performance <- c(caret::R2(swiss.pred, test.data.swiss$Fertility),
                       RMSE(swiss.pred, test.data.swiss$Fertility),
                       MAE(swiss.pred, test.data.swiss$Fertility))
swiss.prediction.percent.error <- RMSE(swiss.pred, test.data.swiss$Fertility) / mean(test.data.swiss$Fe
swiss.performance
```

```
## [1] 0.7845619 7.2493973 5.8573987
```

```
(swiss.prediction.percent.error*100)
```

```
## [1] 10.44394
```

When building the model, we always want to use the lowest test sample RMSE. RMSE and MAE are measured in the same scale as the outcome variable.

Note that, the validation set method is only useful if you have a lot of data. Disadvantage is that, we build a model on a fraction of the data set only. We might have leaving out some interesting information about data, leading to higher bias. So the test error rate can be highly variable, depending on which observations are included in the training set and which observations are included in the validation set.

LOOCV (leave one out cross validation)

Process 1) leave out one data point and build the model on the rest of the data 2) Test the model against the data point that is left out at step 1 and record the test error associated with the prediction 3) repeat the process for all data points 4) get the overall prediction error by taking the average of all these test error estimates recorded at step 2

code:

```r
# define training control
train.control <- trainControl(method = "LOOCV")

# Train the model
loocv.model <- train(Fertility ~., data = swiss, method = "lm", trControl = train.control)

# Summarize the result
print(loocv.model)
```

```
## Linear Regression
##
## 47 samples
##  5 predictor
##
## No pre-processing
## Resampling: Leave-One-Out Cross-Validation
## Summary of sample sizes: 46, 46, 46, 46, 46, 46, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
##   7.738618  0.6128307  6.116021
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

Good thing about LOOCV is that we reduce the potential bias. However, the process is repeated a lot of time, so it will take a long time if we have a large data set. Because the model will be tested each data point at each iteration, which might yield a higher variation in the prediction error, if some data points are outliers. So we need a good ratio of testing data points, thats why we have k fold cross validation method.

K Fold Cross Validation

1) Randomly split the data set into k-subsets (or k-fold)(for example 5 subsets)
2) Reserve one subset and train the model on all other subsets
3) Test the model on the reserved subset and record the prediction error
4) Repeat this process until each of the k subsets has served as the test set.
5) Compute the average of the k recorded errors. This is called the cross-validation error serving as the performance metric for the model.

KFCV is a powerful method to estimate the accuracy of a model.

"The most obvious advantage of k-fold CV compared to LOOCV is computational. A less obvious but potentially more important advantage of k-fold CV is that it often gives more accurate estimates of the test error rate than does LOOCV (James et al. 2014)."

the question will become, how to choose the right value of K

small k -> more biased and undesirable. high K = less biased but suffer from large variability.

high value will lead us to LOOCV approach. small K will take use to validation set approach

Most often, we use K= 5 / k = 10. These values have been shown empirically to yield test error rate estimates that suffer neither from excessively high bias nor form very high variance.

The following we use k = 10

```r
# define training control
set.seed(321)
train.control.k <- trainControl(method = "cv", number = 10)

# train the model
k.model <- train(Fertility ~., data = swiss, method = "lm", trControl = train.control.k)

# summarize the results
print(k.model)
```

```
## Linear Regression
##
## 47 samples
##  5 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 42, 41, 43, 42, 43, 42, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
##   7.462458  0.6749535  6.07299
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

If you check both model, k.model has a better R squared MAE and RMSE.

```r
print(loocv.model)
```

```
## Linear Regression
##
## 47 samples
##  5 predictor
##
## No pre-processing
## Resampling: Leave-One-Out Cross-Validation
## Summary of sample sizes: 46, 46, 46, 46, 46, 46, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
##   7.738618  0.6128307  6.116021
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

Lets go for repeated K fold cross validation

```r
set.seed(432)
# Define training control
train.control.k.repeat <- trainControl(method = "repeatedcv", number = 10,
                                       repeats = 3)
# train the model
model.k.repeat <- train(Fertility ~., data = swiss, method = "lm",
                        trControl = train.control)

# summarize the results
```

```r
print(model.k.repeat)
```

```
## Linear Regression
##
## 47 samples
##  5 predictor
##
## No pre-processing
## Resampling: Leave-One-Out Cross-Validation
## Summary of sample sizes: 46, 46, 46, 46, 46, 46, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
##   7.738618  0.6128307  6.116021
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

Non repeat K fold RMSE Squared MAE
7.462458 0.6749535 6.07299 if you compared non repeat K fold, the non repeat k fold is a better model because it has a higher R squared and lower RMSE MAE,

In this section, we have go thru 4 different methods for assessing the performance of a model on unseen test data. 1) validation set approach, 2) leave-one-out cross-validation, 3) k-fold cross-validation 4) repeated k fold cross-validation

We generally recommend the repeated K fold cross-validation to estimate the prediction error rate. It can be used in regression and classification settings.

another method is using bootstrap re-sampling methods, which consists of repeatedly and randomly selecting a sample of n observations from the original data set, and to evaluate the model performance on each copy.

Sub-Section 3

Bootstrap Re-sampling Essentials in R

bootstrap re-sampling method can be used to measure the accuracy of a predictive model. Also, it can measure the uncertainty associated with any statistical estimator.

Bootstrap re-sampling consist of repeatedly selecting a sample of n observations from the original data set and evaluate the model on each copy. An average standard error is then calculated with the results provide an indication of the overall variance of the model performance.

```r
library(tidyverse)
library(caret)
```

Load the data from swiss

```r
# load the data
data("swiss")
# inspect the data
sample_n(swiss, 3)
```

```
##            Fertility Agriculture Examination Education Catholic
## Courtelary      80.2        17.0          15        12     9.96
## Grandson        71.7        34.0          17         8     3.30
## Boudry          70.4        38.4          26        12     5.62
##            Infant.Mortality
## Courtelary             22.2
## Grandson               20.0
## Boudry                   20.3
```

Bootstrap procedure

The bootstrap method is used to quantify the uncertainty associated with a given statistical estimator or with a predictive model.

It consists of randomly selecting a sample of n observations from the original data set. This subset, called bootstrap data set is then used to evaluate the model.

This procedure is repeated a large number of times and the standard error of the bootstrap estimate is then calculated. The results provide an indication of the variance of the models performance.

Note that, the sampling is performed with replacement, which means that the same observation can occur more than once in the bootstrap data set.

Evaluating a predictive model performance

sample size 100

```r
# define training control
train.control.bs <- trainControl(method = "boot", number = 100)

# train the model
model.bs <- train(Fertility ~., data = swiss, method = "lm", trControl = train.control.bs)

# summarize the results
print(model.bs)
```

```
## Linear Regression
##
## 47 samples
##  5 predictor
##
## No pre-processing
## Resampling: Bootstrapped (100 reps)
## Summary of sample sizes: 47, 47, 47, 47, 47, 47, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
##   8.127003  0.6189821  6.531412
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

the model is alright. not too bad RMSE and MAE, Rsquare is .609 is okay

Lets talk about quantifying an estimator uncertainty and confidence intervals

Simply saying, we want to estimate the accuracy of the linear regression beta coefficient using bootstrap method. 1) Create a simple function, model_coef(), that takes the swiss data set as well as the indices for the observations, and returns the regression coefficients. 2) apply the function boot_fun() to the full data set of 47 observations in order to compute the coefficients

```r
model_coef <- function(data, index){
  coef(lm(Fertility ~., data = data, subset = index))
}
model_coef(swiss, 1:47)
```

```
##      (Intercept)      Agriculture      Examination        Education
##       66.9151817       -0.1721140       -0.2580082       -0.8709401
##         Catholic Infant.Mortality
##        0.1041153        1.0770481
```

Let use boot() function to compute the standard error of 500 bootstrap estimates for the coefficients

```r
library(boot)
```

```
##
## Attaching package: 'boot'

## The following object is masked from 'package:car':
##
##     logit

## The following object is masked from 'package:lattice':
##
##     melanoma
```

```r
boot(swiss, model_coef, 500)
```

```
##
## ORDINARY NONPARAMETRIC BOOTSTRAP
##
##
## Call:
## boot(data = swiss, statistic = model_coef, R = 500)
##
##
## Bootstrap Statistics :
##       original        bias    std. error
## t1* 66.9151817 -0.2277779630 10.93143313
## t2* -0.1721140 -0.0029933680  0.06556137
## t3* -0.2580082 -0.0232585784  0.26616110
## t4* -0.8709401  0.0202862351  0.23240613
## t5*  0.1041153 -0.0004434766  0.03281364
## t6*  1.0770481  0.0332737829  0.44912907
```

The original column corresponds to the regression coef, with the associated standard errors t1 corresponds to the intercept, t2 corresponds to agriculture and so on

```r
names(swiss)
```

```
## [1] "Fertility"        "Agriculture"      "Examination"      "Education"
## [5] "Catholic"         "Infant.Mortality"
```

the standard error of the regression coefficient associated with Agriculture is 0.07. The standard errors measure the variability / accuracy of the beta coef. it can be used to compute the confidence intervals of the coefficients.

```r
summary(lm(Fertility ~., data = swiss))$coef
```

```
##                    Estimate  Std. Error   t value     Pr(>|t|)
## (Intercept)      66.9151817 10.70603759  6.250229 1.906051e-07
## Agriculture      -0.1721140  0.07030392 -2.448142 1.872715e-02
## Examination      -0.2580082  0.25387820 -1.016268 3.154617e-01
## Education        -0.8709401  0.18302860 -4.758492 2.430605e-05
## Catholic          0.1041153  0.03525785  2.952969 5.190079e-03
## Infant.Mortality  1.0770481  0.38171965  2.821568 7.335715e-03
```

The bootstrap approach does not rely on any of these assumptions made by the linear model, and so it is likely giving a more accurate estimate of the coefficients and standard errors than the summary function.

Section 4

Model Selection Essentials in R

Best subsets regression means test all possible combination of the predictors, and then select the best model.

Stepwise regression means adding and deleting predictors in order to find the best performing model with a reduced set of variables.

Penalized Regression (ridge and lasso regression) and Principal components based regression method.

This this section we will talk about 1) Best subsets selection 2) Stepwise Selection 3) penalized Regression 4) Dimension Reduction Methods

load libraries and data Quick guide, lapply will simply load all the libraries from the vector

```
lib <- c("tidyverse", "caret", "leaps")
lapply(lib, require, character.only = T)
```

```
## Loading required package: leaps
```

```
## [[1]]
## [1] TRUE
##
## [[2]]
## [1] TRUE
##
## [[3]]
## [1] TRUE
```

```
data("swiss")
sample_n(swiss, 3)
```

```
##                Fertility Agriculture Examination Education Catholic
## Vevey               58.3        26.8          25        19    18.46
## Orbe                57.4        54.1          20         6     4.20
## V. De Geneve        35.0         1.2          37        53    42.34
##                Infant.Mortality
## Vevey                      20.9
## Orbe                       15.3
## V. De Geneve               18.0
```

Computing the best subset regression nvmax = 5 is because we only have 5 variables

```
modelsub <- regsubsets(Fertility ~., data = swiss, nvmax =5)
summary(modelsub)
```

```
## Subset selection object
## Call: regsubsets.formula(Fertility ~ ., data = swiss, nvmax = 5)
## 5 Variables  (and intercept)
##                  Forced in Forced out
## Agriculture          FALSE      FALSE
## Examination          FALSE      FALSE
## Education            FALSE      FALSE
## Catholic             FALSE      FALSE
## Infant.Mortality     FALSE      FALSE
## 1 subsets of each size up to 5
## Selection Algorithm: exhaustive
##          Agriculture Examination Education Catholic Infant.Mortality
## 1  ( 1 ) " "         " "         "*"       " "      " "
## 2  ( 1 ) " "         " "         "*"       "*"      " "
## 3  ( 1 ) " "         " "         "*"       "*"      "*"
## 4  ( 1 ) "*"         " "         "*"       "*"      "*"
## 5  ( 1 ) "*"         "*"         "*"       "*"      "*"
```

Now, at the bottom of the table, row 1 to 5. It simply means the best 1, 2, . . . , 5 variables model is what.

The best alone model is simply include education. Best 2 variables model is include education and catholic and so on for the next 3 models.

Now the problem is, which one to choose. Now, we need some statistical metrics or strategies to compare all the performance, and pick the best one, which means low BIC, cp, and high Adj R2.

```r
perf.modelsub <- summary(modelsub)
df.performance.modelsub <- data.frame(
  Adj.R2 = which.max(perf.modelsub$adjr2),
  CP = which.min(perf.modelsub$cp),
  BIC = which.min(perf.modelsub$bic)
)
df.performance.modelsub
```

```
##   Adj.R2 CP BIC
## 1      5  4   4
```

As we can see from the table above, Adj.R2 is the best with model 5, however; if we are looking at the CP and BIC, we should shift to model 4 instead.

here is a important question, are those metrics from a test data or training data? You might need to sleep on it if you are having trouble to identify what is training data and testing data.

Another approach is to select a models based on prediction error computed on a new test data using k fold cross validation techniques.

K fold cross-validation

Remember, we either set k to 5 or 10.

Lets make a function

```r
#       id: model id
#   object: regsubsets object
#     data: data used to fit regsubsets
#  outcome: outcome varaible
get_model_formula <- function(id, object, outcome){
  # get model data
  getModelData <- summary(object)$which[id,-1]
  # get outcome varaible
  form <- as.formula(object$call[[2]])
  outcome <- all.vars(form)[1]
  # get model predictors
  predictors.a <- names(which(getModelData == T))
  predictors.a <- paste(predictors.a, collapse = "+")
  # build model formula
  as.formula(paste0(outcome, "~", predictors.a))
}
```

lets get the best 3 variable model formula,

```
get_model_formula(3, modelsub, "Fertility")
```

```
## Fertility ~ Education + Catholic + Infant.Mortality
## <environment: 0x7f9c8c9970e8>
```

let's build the get_cv_error() function for cross-validation error for a given model

```
get_cv_error <- function(model.formula, data){
  set.seed(3)
  train.controlsub <- trainControl(method = "cv", number = 5)
  cv <- train(model.formula, data = data,
              method = "lm", trControl = train.control)
  cv$results$RMSE
}
```

lets get the error

```
# compute cross-validation error
model.ids <- 1:5
cv.errors <- map(model.ids, get_model_formula, modelsub, "Fertility") %>%
  map(get_cv_error, data = swiss) %>%
  unlist()
cv.errors
```

```
## [1] 9.591367 8.617911 7.857175 7.614933 7.738618
```

Now, get the smallest RMSE

```
which.min(cv.errors)
```

```
## [1] 4
```

```
coef(modelsub, 4)
```

```
##      (Intercept)      Agriculture        Education         Catholic
##       62.1013116       -0.1546175       -0.9802638        0.1246664
## Infant.Mortality
##        1.0784422
```

This entire section has gone thru how to find the best model out of multiple variables.

Sub-Section 2

Stepwise Regression Essentials in R

Stepwise Regression is constantly adding and removing predictor variables and see who has the best performance, which implies lowers prediction error.

There are three methods.

Forward selection, starts with no predictors and then stop when there is no longer statistically significant.

Backward selection (or backward elimination), starts from all possible predictors, and removes the least contribute predictors and stop when all predictors are statistically significant.

Stepwise selection (sequential replacement), which is a combination of forward and backward selections. start with no predictors, and sequentially adding the most contributing predictors (like forward selection). After adding each new variable, remove any variables that are no longer provide an improvement in the model fit (like backward selection).

Restriction Forward selection and stepwise selection can be applied in the high dimensional configuration, where the number of sample n is inferior to the number of predictors p, such as in genomic fields.

Backward selection requires that the number of samples n is larger than the number of variables p, so that the full model can be fit.

library tidyverse, caret, leaps, MASS

```
libsteps <- c("tidyverse", "caret", "leaps", "MASS")
lapply(libsteps, require, character.only = T)
```

```
## [[1]]
## [1] TRUE
##
## [[2]]
## [1] TRUE
##
## [[3]]
## [1] TRUE
##
## [[4]]
## [1] TRUE
```

```
# fit the full model
full.model <- lm(Fertility ~., data = swiss)
# stepwise regression model
step.model <- stepAIC(full.model, direction = "both", trace = F)
```

regsubsets() from leaps package, which has the tuning parameter nvmax. please see the previous section where i have initially introduced you this parameter. It returns multiple models with different size up to nvmax. you need to compare the performance of those models for picking the best one. regsubsets() has the option method for you to specify which selection you would like to make. backward, forward, seqrep

```
modelselection <- regsubsets(Fertility ~., data = swiss, nvmax =5, method = "seqrep")
summary(modelselection)
```

```
## Subset selection object
## Call: regsubsets.formula(Fertility ~ ., data = swiss, nvmax = 5, method = "seqrep")
## 5 Variables  (and intercept)
##                  Forced in Forced out
## Agriculture          FALSE      FALSE
## Examination          FALSE      FALSE
## Education            FALSE      FALSE
## Catholic             FALSE      FALSE
## Infant.Mortality     FALSE      FALSE
## 1 subsets of each size up to 5
## Selection Algorithm: 'sequential replacement'
##          Agriculture Examination Education Catholic Infant.Mortality
## 1  ( 1 ) " "         " "         "*"       " "      " "
## 2  ( 1 ) " "         " "         "*"       "*"      " "
## 3  ( 1 ) " "         " "         "*"       "*"      "*"
## 4  ( 1 ) "*"         "*"         "*"       "*"      " "
## 5  ( 1 ) "*"         "*"         "*"       "*"      "*"
```

train() from caret package also has a easier work flow to perform stepwise selection using the leaps and mass package. It has an option named method, with the following values “leapBackward”, “leapForward”, “leapSeq”

Following code will also apply 10 k fold cv to estimate the average prediction error.

```r
set.seed(999)
train.control.selection <- trainControl(method = "cv", number =10)
step.model.selection <- train(Fertility ~., data = swiss,
                              method = "leapBackward",
                              tuneGrid = data.frame(nvmax = 1:5),
                              trControl = train.control)
step.model.selection
```

```
## Linear Regression with Backwards Selection
##
## 47 samples
##  5 predictor
##
## No pre-processing
## Resampling: Leave-One-Out Cross-Validation
## Summary of sample sizes: 46, 46, 46, 46, 46, 46, ...
## Resampling results across tuning parameters:
##
##   nvmax  RMSE      Rsquared   MAE
##   1      9.591367  0.3991715  8.107915
##   2      9.930877  0.3740050  8.283843
##   3      8.059676  0.5771867  6.506707
##   4      7.614933  0.6236409  6.071138
##   5      7.738618  0.6128307  6.116021
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was nvmax = 4.
```

Again, we want small # for RMSE and MAE, also we want as close to 1 as possible for r^2

```r
step.model.selection$bestTune
```

```
##   nvmax
## 4     4
```

the bestTune wil give us the best model to select

```r
summary(step.model.selection$finalModel)
```

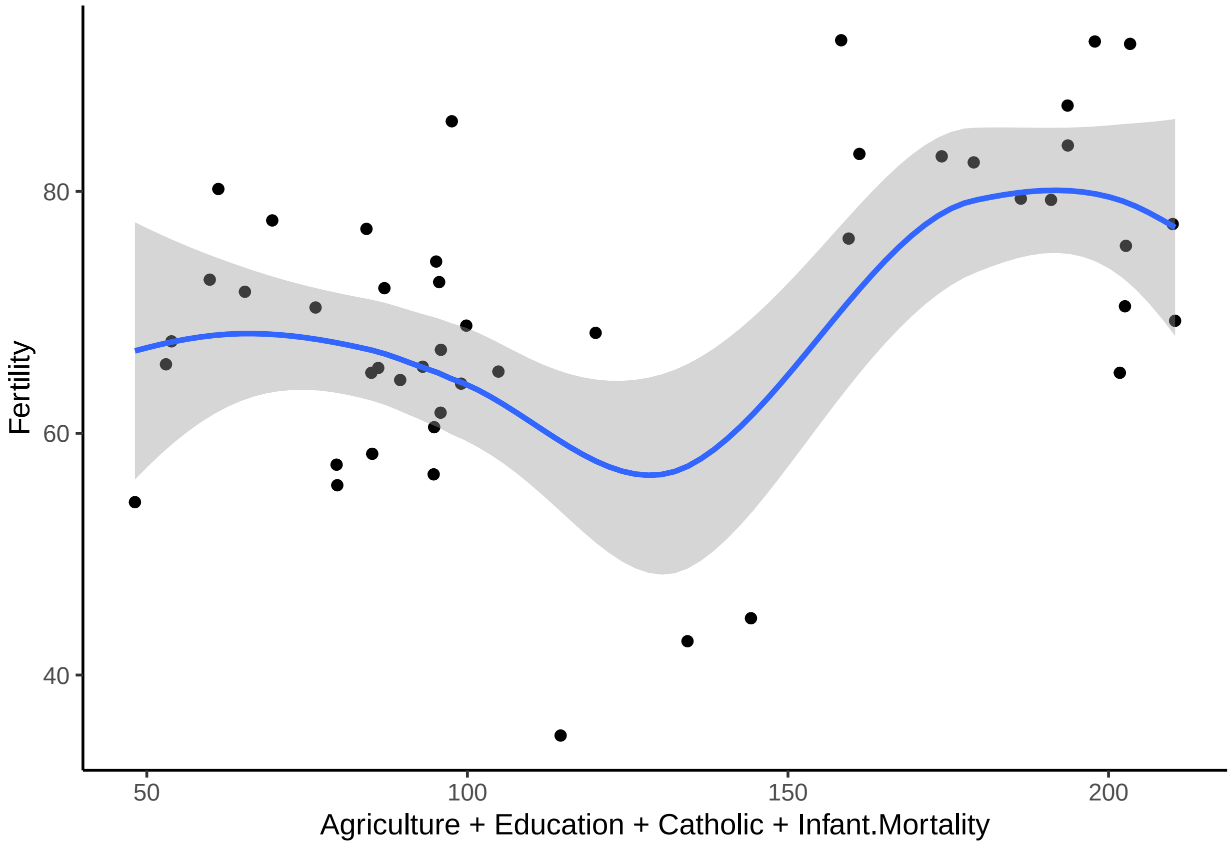
```
## Subset selection object
## 5 Variables  (and intercept)
##                    Forced in Forced out
## Agriculture            FALSE      FALSE
## Examination            FALSE      FALSE
## Education              FALSE      FALSE
## Catholic               FALSE      FALSE
## Infant.Mortality       FALSE      FALSE
## 1 subsets of each size up to 4
## Selection Algorithm: backward
##          Agriculture Examination Education Catholic Infant.Mortality
## 1  ( 1 ) " "         " "         "*"       " "      " "
## 2  ( 1 ) " "         " "         "*"       "*"      " "
## 3  ( 1 ) " "         " "         "*"       "*"      "*"
## 4  ( 1 ) "*"         " "         "*"       "*"      "*"
```

```r
coef(step.model.selection$finalModel, 4)
```

```
##      (Intercept)      Agriculture        Education         Catholic
##       62.1013116       -0.1546175       -0.9802638        0.1246664
## Infant.Mortality
##        1.0784422
```

```
step.model.selection.lm <- lm(Fertility ~ Agriculture + Education + Catholic + Infant.Mortality, data =
ggplot(step.model.selection.lm, aes(x = Agriculture + Education + Catholic + Infant.Mortality, Fertilit
  geom_point() +
  stat_smooth()
```

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```



In MASS library, it has a function called stepAIC. you can use the direction parameter and set the value to both, forward, and backward for the selection.

In addition, caret package has method to compute stepwise regression using the MASS package, with method = "lmStepAIC"

please read the documentation on how to apply selection method.

Conclusion,

Stepwise regression is very useful and important for high - dimensional data that has multiple predictor variables. Other alternatives are the penalized regression (ridge and lasso regression) and the principal components based regression method (PCR and PLS)

Sub-Section 3

Penalized Regression Essentials: Ridge, Lasso & Elastic Net

The standard linear model doesn't work well when we have a lot of parameters. So we have alternative method which is penalized regression. This will add a constraint in the equation, which is known as shrinkage or regularization methods.

what the penalty does is to reduce the coefficient values towards zero. This will eliminate those less contribution variables to the regression model, down to zero or at least close to zero.

In the mean time, the reduction requires the tuning parameter (lambda) to determines the amount of shrinkage.

In this section we will discuss the most commonly used penalized regression methods, including ridge regression, lasso regression and elastic net regression.

Library tidyverse, caret, glmnet (computing penalized regression)

```r
libpen <- c("tidyverse", "caret", "glmnet")
lapply(libpen, require, character.only = T)
```

```
## Loading required package: glmnet

## Loading required package: Matrix

##
## Attaching package: 'Matrix'

## The following objects are masked from 'package:tidyr':
##
##     expand, pack, unpack

## Loaded glmnet 4.0-2

## [[1]]
## [1] TRUE
##
## [[2]]
## [1] TRUE
##
## [[3]]
## [1] TRUE
```

```r
data("Boston", package = "MASS")
# By now i hope you are already familiar wit the next 5 lines of code
set.seed(323)
training.samples.pen <- Boston$medv %>%
  createDataPartition(p = 0.8, list = F)
train.data.pen <- Boston[training.samples.pen, ]
test.data.pen <- Boston[-training.samples.pen, ]
# Predictor variables
x.pen <- model.matrix(medv~., train.data.pen)[, -1]
y.pen <- train.data.pen$medv
```

glmnet() is for computing penalized linear regression models. glmnet(x.pen, y.pen, alpha =1, lambda = NULL)

x: matrix of predictor variables y: the response or outcome variable, which is a binary variable. alpha: the elasticnet mixing parameter. Allowed values include: "1": for lasso regression "0": for ridge regression a value between 0 and 1 (say 0.3) for elastic net regression. lambda: a numeric value defining the amount of shrinkage. Should be specify by analyst.

In penalized regression, you need to specify a constant lambda to adjust the amount of the coefficient shrinkage. The best lambda for your data, can be defined as the lambda that minimize the cross-validation prediction error rate. This can be determined automatically using the function cv.glmnet().

Lets dig into the real code

Computing Ridge Regression

```
# find the best lambda using cross- validation
set.seed(32423)
cv.pen <- cv.glmnet(x.pen, y.pen, alpha = 0)
cv.pen$lambda.min
```

```
## [1] 0.6619773
```

Let's use this lambda

```
model.pen <- glmnet(x.pen, y.pen, alpha = 0, lambda = cv.pen$lambda.min)
# Display regression coefficients
coef(model.pen)
```

```
## 14 x 1 sparse Matrix of class "dgCMatrix"
##                        s0
## (Intercept)  28.232030472
## crim         -0.089534050
## zn            0.036242574
## indus        -0.031221170
## chas          2.134380075
## nox         -12.039681211
## rm            3.920996982
## age          -0.006864208
## dis          -1.083784241
## rad           0.163168176
## tax          -0.005723189
## ptratio      -0.845413054
## black         0.008149447
## lstat        -0.444799608
```

Make predictions on the test data

```
x.pen.test <- model.matrix(medv ~., test.data.pen)[,-1]
pred.pen <- model.pen %>% predict(x.pen.test) %>% as.vector()
# model performance metrics
pen.performance <- data.frame(
  RMSE = RMSE(pred.pen, test.data.pen$medv),
  R2 = caret::R2(pred.pen, test.data.pen$medv),
  perError = RMSE(pred.pen, test.data.pen$medv) / mean(test.data.pen$medv)
)
pen.performance
```

```
##       RMSE        R2 perError
## 1 5.223382 0.7698707 0.226606
```

Computing Lasso Regression

```
# find the best lambda using cross- validation
set.seed(222)
cv.lasso <- cv.glmnet(x.pen,y.pen, alpha =1)
# display the best lambda value
cv.lasso$lambda.min
```

```
## [1] 0.03001987
```

build the model with training data

```r
model.lasso <- glmnet(x.pen, y.pen, alpha = 1, lambda = cv.lasso$lambda.min)
# display regression coefficients
coef(model.lasso)
```

```
## 14 x 1 sparse Matrix of class "dgCMatrix"
##                        s0
## (Intercept)  34.945127094
## crim         -0.102476332
## zn            0.046148759
## indus         .
## chas          1.869352924
## nox         -16.237862317
## rm            3.733797896
## age          -0.001125746
## dis          -1.357155920
## rad           0.267631419
## tax          -0.009948424
## ptratio      -0.932842063
## black         0.008107730
## lstat        -0.492879263
```

Make prediction

```r
x.test.lasso <- model.matrix(medv ~., test.data.pen)[, -1]
pred.lasso <- model.lasso %>% predict(x.test.lasso) %>% as.vector()
# model performance metrics
lasso.perf <- data.frame(
  RMSE = RMSE(pred.lasso, test.data.pen$medv),
  R2 = caret::R2(pred.lasso, test.data.pen$medv),
  perError = RMSE(pred.lasso, test.data.pen$medv) / mean(test.data.pen$medv)
)
lasso.perf
```

```
##       RMSE        R2  perError
## 1 5.123271 0.7727101 0.2222628
```

Last one, elastic net regression

Build the model, it is more simple then the previous twos. We can use caret work flow to implement everything. caret will automatically select the best tuning parameters alpha and lambda. Why? because it will tests a range of possible alpha and lambda values, and select the best #.

Lets dive in to the code

```r
set.seed(32132)
model.elastic <- train(
  medv ~., data = train.data.pen, method = "glmnet",
  trControl = trainControl("cv", number = 10),
  tuneLength = 10
)
# Best tuning parameter
model.elastic$bestTune
```

```
##    alpha     lambda
## 15   0.2 0.08710736
```

Coefficient of the final model. You need to specify the best lambda

```
coef(model.elastic$finalModel, model.elastic$bestTune$lambda)
```

```
## 14 x 1 sparse Matrix of class "dgCMatrix"
##                         1
## (Intercept)  34.470824042
## crim         -0.102830127
## zn            0.045773890
## indus         .
## chas          1.916667364
## nox         -15.961162078
## rm            3.760890396
## age          -0.002868719
## dis          -1.348319420
## rad           0.263050842
## tax          -0.009777302
## ptratio      -0.928301292
## black         0.008226864
## lstat        -0.486022274
```

Make Prediction

```
x.test.elastic <-model.matrix(medv ~., test.data.pen)[, -1]
pred.elastic <- model.elastic %>% predict(test.data.pen)
# model performance metrics
elastic.perf <- data.frame(
  RMSE = RMSE(pred.elastic, test.data.pen$medv),
  R2 = caret::R2(pred.elastic, test.data.pen$medv),
  perError = RMSE(pred.elastic,test.data.pen$medv) / mean(test.data.pen$medv)
)
elastic.perf
```

```
##       RMSE       R2  perError
## 1 5.127825 0.772687 0.2224604
```

```
penalized.performance <- rbind.data.frame(pen.performance , lasso.perf, elastic.perf)
Pen.Test.Name <- c("Ridge", "Lasso", "Elastic")
penalized.performance <- cbind.data.frame(Pen.Test.Name, penalized.performance)
penalized.performance
```

```
##   Pen.Test.Name     RMSE        R2  perError
## 1         Ridge 5.223382 0.7698707 0.2266060
## 2         Lasso 5.123271 0.7727101 0.2222628
## 3       Elastic 5.127825 0.7726870 0.2224604
```

As you can see the table above, we can either use Lasso model or Elastic. Imo, i would use Lasso, because of smaller RMSE, slightly higher R2, but more importantly, i have smaller percent error. If i have huge data set, 0.1% does make a different.

The following code is repeating the process above, but when we use caret package, it will be simpler.

Setup a grid range of lambda values

```
lambda <-  10^seq(-3,3, length = 100)
# Ridge Regression
# Build the model
set.seed(123)
model.ridge <- train(
  medv ~., data = train.data.pen, method = "glmnet",
```

```r
  trControl = trainControl("cv", number = 10),
  tuneGrid = expand.grid(alpha = 0, lambda = lambda)
  )
# Model coefficients
coef(model.ridge$finalModel, model.ridge$bestTune$lambda)
```

```
## 14 x 1 sparse Matrix of class "dgCMatrix"
##                        1
## (Intercept)  28.191064926
## crim         -0.089284990
## zn            0.036328235
## indus        -0.030992288
## chas          2.130837097
## nox         -11.960838032
## rm            3.917523323
## age          -0.006704166
## dis          -1.081966364
## rad           0.162842416
## tax          -0.005741076
## ptratio      -0.844484238
## black         0.008152874
## lstat        -0.445670277
```

```r
# Make predictions
ridge.pred <- model.ridge %>% predict(test.data.pen)
# Model prediction performance
ridge.perf <- data.frame(
  RMSE = RMSE(ridge.pred, test.data.pen$medv),
  R2 = caret::R2(ridge.pred, test.data.pen$medv),
  perError = RMSE(ridge.pred, test.data.pen$medv) / mean(test.data.pen$medv)
)
```

Lasso Regression

```r
# Build the model
set.seed(123)
lasso.model <- train(
  medv ~., data = train.data.pen, method = "glmnet",
  trControl = trainControl("cv", number = 10),
  tuneGrid = expand.grid(alpha = 1, lambda = lambda)
  )
```

```
## Warning in nominalTrainWorkflow(x = x, y = y, wts = weights, info = trainInfo, :
## There were missing values in resampled performance measures.
```

```r
# Model coefficients
coef(lasso.model$finalModel, lasso.model$bestTune$lambda)
```

```
## 14 x 1 sparse Matrix of class "dgCMatrix"
##                        1
## (Intercept)  34.702436000
## crim         -0.101281965
## zn            0.045572769
## indus         .
## chas          1.866717118
## nox         -16.116721558
## rm            3.741896185
## age          -0.000923771
## dis          -1.343836057
## rad           0.262070223
## tax          -0.009718290
## ptratio      -0.930921265
## black         0.008082672
## lstat        -0.493240898
```

```
# Make predictions
lasso.pred <- lasso.model %>% predict(test.data.pen)
# Model prediction performance
lasso.perf <- data.frame(  RMSE = RMSE(lasso.pred, test.data.pen$medv),
                             R2 = caret::R2(lasso.pred, test.data.pen$medv),
                  perError = RMSE(lasso.pred, test.data.pen$medv) / mean(test.data.pen$medv)
)
```

Elastic net regression

```
# Build the model
set.seed(123)
elastic.model <- train(
  medv ~., data = train.data.pen, method = "glmnet",
  trControl = trainControl("cv", number = 10),
  tuneLength = 10
  )
# Model coefficients
coef(elastic.model$finalModel, elastic.model$bestTune$lambda)
```

```
## 14 x 1 sparse Matrix of class "dgCMatrix"
##                         1
## (Intercept)  3.454809e+01
## crim        -1.006986e-01
## zn           4.528772e-02
## indus        .
## chas         1.866481e+00
## nox         -1.604215e+01
## rm           3.746872e+00
## age         -8.610915e-04
## dis         -1.336128e+00
## rad          2.587846e-01
## tax         -9.580351e-03
## ptratio     -9.294301e-01
## black        8.069791e-03
## lstat       -4.931172e-01
```

```
# Make predictions
predictions <- elastic.model %>% predict(test.data.pen)
# Model prediction performance
elastic.perf <- data.frame(
  RMSE = RMSE(predictions, test.data.pen$medv),
  R2 = caret::R2(predictions, test.data.pen$medv),
  perError = RMSE(predictions, test.data.pen$medv) / mean(test.data.pen$medv)
)
```

The performance of the different models - ridge, lasso and elastic net - can be easily compared using caret. The best model is defined as the one that minimizes the prediction error.

```r
modelsss <- list(ridge = model.ridge, lasso = lasso.model, elastic = elastic.model)
resamples(modelsss) %>% summary(metric = "RMSE")
```

```
##
## Call:
## summary.resamples(object = ., metric = "RMSE")
##
## Models: ridge, lasso, elastic
## Number of resamples: 10
##
## RMSE
##             Min.  1st Qu.   Median     Mean  3rd Qu.     Max. NA's
## ridge   2.985268 3.890679 4.468207 4.653439 5.288179 6.996436    0
## lasso   3.010413 3.868703 4.438512 4.621414 5.251428 6.920674    0
## elastic 3.008035 3.865748 4.438152 4.621372 5.251111 6.922004    0
```

Amount all 3 models, elastic has the lowest median RMSE.

However, if we conclude everything together, lasso would be my first option

```r
penalized.performance
```

```
##   Pen.Test.Name     RMSE        R2  perError
## 1         Ridge 5.223382 0.7698707 0.2266060
## 2         Lasso 5.123271 0.7727101 0.2222628
## 3       Elastic 5.127825 0.7726870 0.2224604
```

Sub- section 4

Principal Component and Partial Least Squares Regression Essentials

Intro

This section will be talking about dimension reduction. It is very useful if we have a large data set with multiple correlated predictor variables.

The way how reduction methods work is: First summarizing the original predictors into few new variables called principal components (PCs), which are used as predictors to fit the linear regression model. It will avoid multicollinearity between predictors, which is a big issue in regression setting.

When using dimension reduction methods, it's generally recommended to standardize each predictor to make them comparable. Standardization consists of dividing the predictor by its standard deviation.

Two well known regression methods based on dimension reduction: Principal Component Regression (PCR) Partial Least Squares (PLS)

Principal Component Regression

PCR means summarize the original predictor variables into few new variables also known as principal components (PC), which are a linear combination of the original data.

Those PC are used to build the linear regression model. Those PC are chosen by cross-validation (CV).

Note that, PCR is suitable when the data set contains highly correlated predictors.

Partial Least Squares Regression

Downside of PCR is that, we cant guarantee that the selected principal components are associated with the outcome. The selection of the principal components that are included in the model is not supervised by the outcome variable.

The alternative to PCR is Partial Least Squares (PLS) Regression. PLS identifies new principal components that not only summarizes the original predictors, but also that are related to the outcome. Then those components are used to fit the regression model. Compared to PCR, PLS uses a dimension reduction strategy that is supervised by the outcome.

Like PCR, PLS is convenient for data with highly- correlated predictors. The # of PCs used in PLS is generally chosen by the Cross-Validation. To make variables comparable, predictors and the outcome variables should be generally standardized. Prepare the data

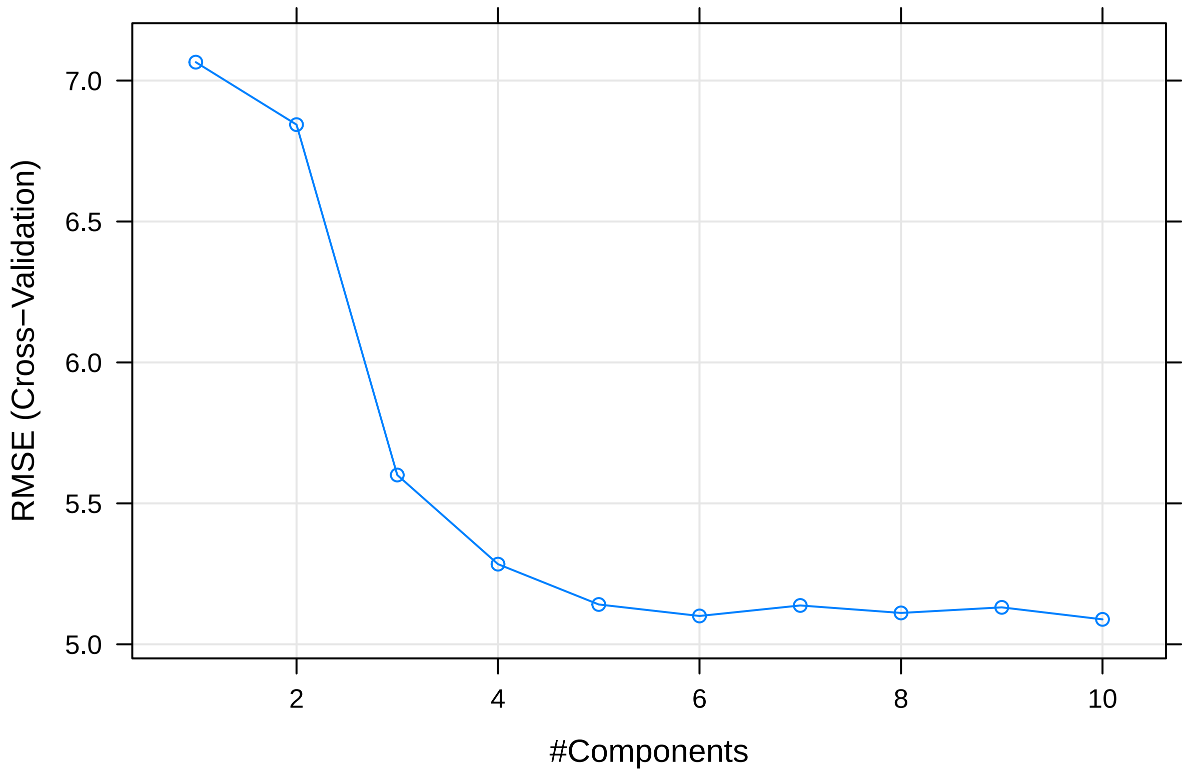
```r
library(tidyverse)
library(caret)
library(pls)
```

```
##
## Attaching package: 'pls'

## The following object is masked from 'package:caret':
##
##     R2

## The following object is masked from 'package:stats':
##
##     loadings
```

```r
# Load the data
data("Boston", package = "MASS")
# Split the data into training and test set
set.seed(123)
training.samples <- Boston$medv %>%
  createDataPartition(p = 0.8, list = FALSE)
train.data  <- Boston[training.samples, ]
test.data <- Boston[-training.samples, ]
```

Computing Principal Component Regression

```r
# Build the model on training set
set.seed(123)
model <- train(
  medv~., data = train.data, method = "pcr",
  scale = TRUE,
  trControl = trainControl("cv", number = 10),
  tuneLength = 10
  )
# Plot model RMSE vs different values of components
plot(model)
```



From the plot, we can see that 6 or 10 is our best principal components number. which also gives the smallest prediction error RMSE.

Without guessing we can use the following code

```
# Print the best tuning parameter ncomp that
# minimize the cross-validation error, RMSE
model$bestTune
```

```
##    ncomp
## 10    10
```

It said, the best model is 10

```
# Summarize the final model
summary(model$finalModel)
```

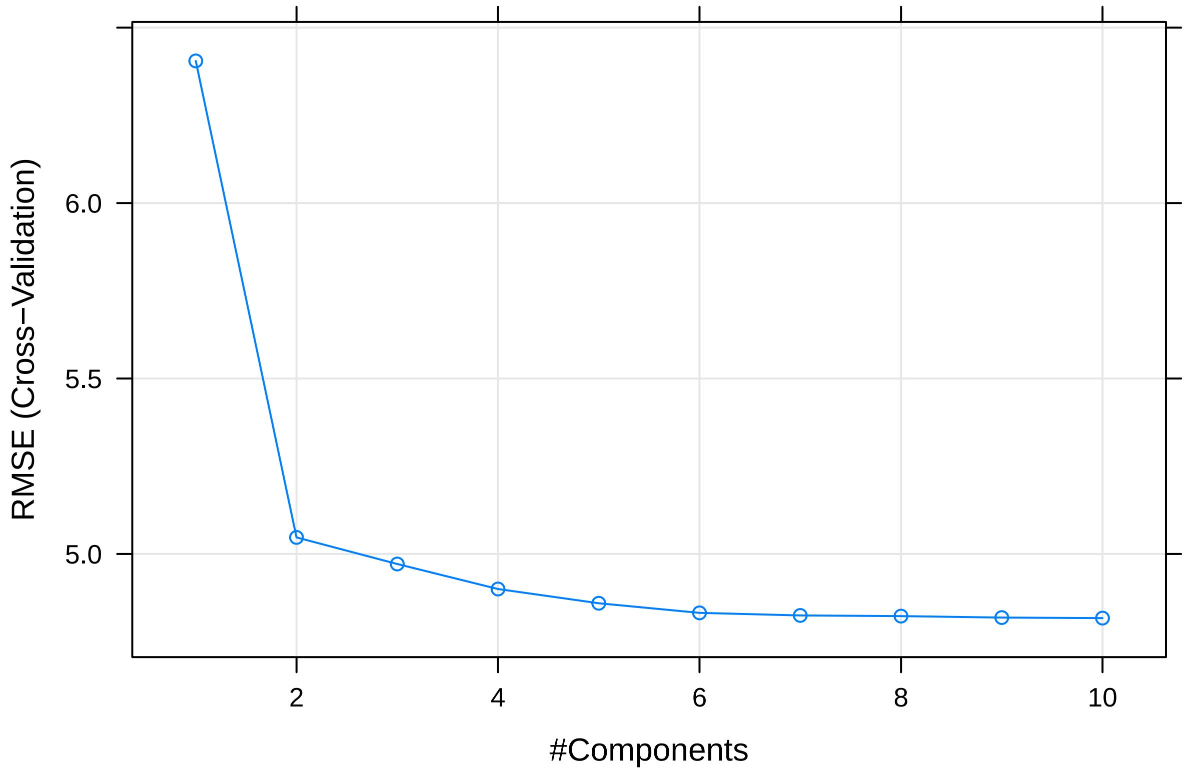
```
## Data:    X dimension: 407 13
##  Y dimension: 407 1
## Fit method: svdpc
## Number of components considered: 10
## TRAINING: % variance explained
##           1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps
## X           48.02    58.82    67.97    74.78    81.04    86.16    90.21
## .outcome    37.80    43.76    62.57    67.24    68.66    69.30    69.31
##           8 comps  9 comps  10 comps
## X           93.21    95.31     96.92
## .outcome    69.87    69.88     70.64
```

From the last two rows, we want big number. For 10 comps, 96.92% of the variation (or information) contained in the predictors are captured by 6 principal components. Also, setting ncomp = 10 will captures 70.64% of the information in the outcome variable, which is pretty good.

```
# Make predictions
predictions <- model %>% predict(test.data)
# Model performance metrics
pcr.performance <-data.frame(
  RMSE = caret::RMSE(predictions, test.data$medv),
  Rsquare = caret::R2(predictions, test.data$medv),
  perError = caret::RMSE(predictions, test.data$medv) / mean(test.data$medv)
)
```

2

```
# Build the model on training set
set.seed(123)
model <- train(
  medv~., data = train.data, method = "pls",
  scale = TRUE,
  trControl = trainControl("cv", number = 10),
  tuneLength = 10
  )
# Plot model RMSE vs different values of components
plot(model)
```



```
# Print the best tuning parameter ncomp that
# minimize the cross-validation error, RMSE
model$bestTune
```

```
##    ncomp
## 10    10
```

```
# Summarize the final model
summary(model$finalModel)
```

```
## Data:    X dimension: 407 13
##  Y dimension: 407 1
## Fit method: oscorespls
## Number of components considered: 10
## TRAINING: % variance explained
##           1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps
## X           46.91    57.21    64.47    69.89    75.76    79.59    83.17
## .outcome    49.21    70.10    71.68    72.72    73.13    73.28    73.38
##           8 comps  9 comps  10 comps
## X           85.82    90.83     92.65
## .outcome    73.45    73.46     73.46
```

```r
# Make predictions
predictions <- model %>% predict(test.data)
# Model performance metrics
pls.performance <- data.frame(
  RMSE = caret::RMSE(predictions, test.data$medv),
  Rsquare = caret::R2(predictions, test.data$medv),
  perError = caret::RMSE(predictions, test.data$medv) / mean(test.data$medv)
)
rbind.data.frame(PCR = pcr.performance, PLS = pls.performance)
```

```
##         RMSE   Rsquare  perError
## PCR 4.935417 0.7270573 0.2181473
## PLS 4.590163 0.7610013 0.2028869
```

Unfortunately, we get exactly the same data, so we can either use both model.

Comment:

I have been suffering from the following error "Error in UseMethod("R2") : no applicable method for 'R2' applied to an object of class"c('double', 'numeric')""

The way I fixed this problem is to add caret::R2()