# Exercise 6 - Cross Validation of Models

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# Setup

```
Set random seed.
```

```
set.seed(12208157)
Import libraries
library(ggplot2)
library(ISLR)
library(splines)
library(dplyr)
##
## Attache Paket: 'dplyr'
## Die folgenden Objekte sind maskiert von 'package:stats':
##
##
       filter, lag
## Die folgenden Objekte sind maskiert von 'package:base':
##
##
       intersect, setdiff, setequal, union
library(boot)
```

# Task 1.

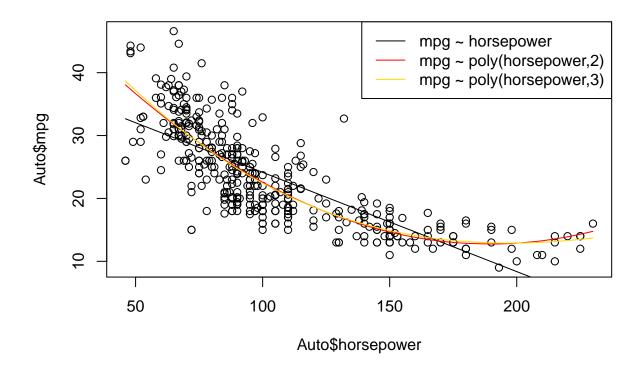
Import data

```
data(Auto)
#?Auto
#pairs(Auto)
```

**a**)

```
Auto <- arrange(Auto, horsepower)
dfs <- 1:3
FITS <- apply(t(dfs), 2, function(df) lm(mpg ~ poly(horsepower, df=df), data=Auto))

plot(Auto$horsepower, Auto$mpg)
lines(Auto$horsepower, fitted(FITS[[1]]), col="black")
lines(Auto$horsepower, fitted(FITS[[2]]), col="red")
lines(Auto$horsepower, fitted(FITS[[3]]), col="gold")
legend("topright",legend=c("mpg ~ horsepower", "mpg ~ poly(horsepower, 2)", "mpg ~ poly(horsepower, 3)"),col</pre>
```



# **b**)

Use the validation set approach to compare the models. Use once a train/test split of 50%/50% and once 70%/30%. Choose the best model based on Root Mean Squared Error, Mean Squared Error and Median Absolute Deviation.

```
dfs <- 1:3
set.seed(12208157)

n <- nrow(Auto)

train_sample_50 <- sample(1:n,n*0.5)
train_sample_70 <- sample(1:n,n*0.7)

TRAIN_50 <- Auto[train_sample_50,]
TEST_50 <- Auto[-train_sample_50,]
TRAIN_70 <- Auto[train_sample_70,]
TEST_70 <- Auto[-train_sample_70,]

FITS <- apply(t(dfs), 2, function(df) lm(mpg ~ poly(horsepower, df=df), data=TRAIN_50))
FITS2 <- apply(t(dfs), 2, function(df) lm(mpg ~ poly(horsepower, df=df), data=TRAIN_70))

PREDS <- lapply(FITS, predict, TEST_50)
PREDS2 <- lapply(FITS2, predict, TEST_70)</pre>
```

Calculate Mean Squared Error values for three models

```
MSE <- function(yhat, y) mean((yhat-y)^2)
MSES <- lapply(PREDS, MSE, y=TEST_50$y)
MSES2 <- lapply(PREDS2, MSE, y=TEST_70$y)

#print("50/50 split:")
#print(paste0("MSE for Model 1: ",round(unlist(MSES)[1],1)))
#print(paste0("MSE for Model 2: ",round(unlist(MSES)[2],1)))
#print(paste0("MSE for Model 3: ",round(unlist(MSES)[3],1)))

#print("70/30 split:")
#print(paste0("MSE for Model 1: ",round(unlist(MSES2)[1],1)))
#print(paste0("MSE for Model 2: ",round(unlist(MSES2)[2],1)))
#print(paste0("MSE for Model 3: ",round(unlist(MSES2)[3],1)))</pre>
```

Calculate Root Mean Squared Error values for three models

```
RMSE <- function(yhat, y) sqrt(mean((yhat-y)^2))
RMSES <- lapply(PREDS, RMSE, y=TEST_50$y)
RMSES2 <- lapply(PREDS2, RMSE, y=TEST_70$y)

#print("50/50 split:")
#print(paste0("RMSE for Model 1: ",round(unlist(RMSES)[1],2)))
#print(paste0("RMSE for Model 2: ",round(unlist(RMSES)[2],2)))
#print(paste0("RMSE for Model 3: ",round(unlist(RMSES)[3],2)))

#print("70/30 split:")
#print(paste0("RMSE for Model 1: ",round(unlist(RMSES2)[1],2)))
#print(paste0("RMSE for Model 2: ",round(unlist(RMSES2)[2],2)))
#print(paste0("RMSE for Model 3: ",round(unlist(RMSES2)[3],2)))</pre>
```

Calculate Median Absolute Deviation values for three models

```
MAD <- function(yhat, y) median(abs(yhat-y))
MADS <- lapply(PREDS, MAD, y=TEST_50$y)
MADS2 <- lapply(PREDS2, MAD, y=TEST_70$y)

#print("50/50 split:")
#print(paste0("MAD for Model 1: ",round(unlist(MADS)[1],2)))
#print(paste0("MAD for Model 2: ",round(unlist(MADS)[2],2)))
#print(paste0("MAD for Model 3: ",round(unlist(MADS)[3],2)))

#print("70/30 split:")
#print(paste0("MAD for Model 1: ",round(unlist(MADS2)[1],2)))
#print(paste0("MAD for Model 2: ",round(unlist(MADS2)[2],2)))
#print(paste0("MAD for Model 3: ",round(unlist(MADS2)[3],2)))</pre>
```

**c**)

Use the cv.glm function in the boot package for the following steps.

1. Use cv.glm for Leave-one-out Cross Validation to compare the models above.

```
dfs <- 1:3
FITS <- apply(t(dfs), 2, function(df) lm(mpg ~ poly(horsepower, df=df), data=Auto))

cv.mod1.1 <- cv.glm(Auto, glm(FITS[[1]]))
cv.mod2.1 <- cv.glm(Auto, glm(FITS[[2]]))
cv.mod3.1 <- cv.glm(Auto, glm(FITS[[3]]))</pre>
```

2. Use cv.glm for 5-fold and 10-fold Cross Validation to compare the models above.

5-fold cross validation:

```
cv.mod1.2 <- cv.glm(Auto, glm(FITS[[1]]), K=5)
cv.mod2.2 <- cv.glm(Auto, glm(FITS[[2]]), K=5)
cv.mod3.2 <- cv.glm(Auto, glm(FITS[[3]]), K=5)</pre>
```

10-fold cross validation:

```
cv.mod1.3 <- cv.glm(Auto, glm(FITS[[1]]), K=10)
cv.mod2.3 <- cv.glm(Auto, glm(FITS[[2]]), K=10)
cv.mod3.3 <- cv.glm(Auto, glm(FITS[[3]]), K=10)</pre>
```

d)

Compare all results from 2 and 3. in a table and draw your conclusions.

Results: MSE, RMSE, MDA for each model and both train/test splits

```
data.frame(
   "Split" = c("50/50 split","50/50 split","50/50 split","70/30 split","70/30 split","70/30 split"),
   "Model" = c("model1", "model2", "model3","model1", "model2", "model3"),

"MSE" = c(round(unlist(MSES)[1],1),round(unlist(MSES)[2],1),round(unlist(MSES)[3],1),round(unlist(MSES)[2],1),round(unlist(MSES)[3],1)),

"RMSE" = c(round(unlist(RMSES)[1],1),round(unlist(RMSES)[2],1),round(unlist(RMSES)[3],1)),

"RMSE" = c(round(unlist(RMSES)[2],1),round(unlist(RMSES)[3],1)),

"MAD" = c(round(unlist(MADS)[1],1),round(unlist(MADS)[2],1),round(unlist(MADS)[3],1),round(unlist(MADS),round(unlist(MADS)[2],1),round(unlist(MADS)[3],1)))
```

#### Conclusions:

For the 50/50 train/test split the second model performs best if you look at MAD values but the first model has a lower MSE value. The models perform overall very similar.

For the 70/30 train/test split first model performs better than the other ones for all metrics.

Results: MSE for each model with 5-fold 10-fold and LOO CV

```
data.frame(
   "Model" = c("model1", "model2", "model3"),
   "5-folf CV MSE" = c(round(cv.mod1.2$delta[1],2),round(cv.mod2.2$delta[1],2),round(cv.mod3.2$delta[1],
   "10-folf CV MSE" = c(round(cv.mod1.3$delta[1],2),round(cv.mod2.3$delta[1],2),round(cv.mod3.3$delta[1]
   "LOOCV MSE" = c(round(cv.mod1.1$delta[1],2),round(cv.mod2.1$delta[1],2),round(cv.mod3.1$delta[1],2)))
```

```
## Model X5.folf.CV.MSE X10.folf.CV.MSE LOOCV.MSE
## 1 model1 24.27 24.26 24.23
## 2 model2 19.21 19.33 19.25
## 3 model3 19.53 19.38 19.33
```

#### Conclusions:

The second model performs best. It is only slightly better than the third model but much better than the first model.

The results are very similar for 5-fold, 10-fold and LOO CV.

#### Task 2.

```
data(economics)
```

**a**)

Fit the following models to explain the number of unemployed persons 'unemploy' by the median number of days unemployed 'uempmed' and vice versa

#### 1. Linear Model

```
lm_unemploy <- glm(unemploy ~ uempmed, data = economics)
summary(lm_unemploy)</pre>
```

```
##
## glm(formula = unemploy ~ uempmed, data = economics)
##
## Deviance Residuals:
      Min 1Q Median
                                  3Q
                                          Max
## -3005.2 -792.9
                    -109.8
                                       3600.7
                               931.1
##
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
##
## (Intercept)
                2956.8
                            126.8
                                    23.32
                                            <2e-16 ***
                 559.3
                             13.3
                                    42.06
                                            <2e-16 ***
## uempmed
## ---
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for gaussian family taken to be 1708187)
##
##
      Null deviance: 3999510381 on 573 degrees of freedom
```

```
## Residual deviance: 977082779 on 572 degrees of freedom
## AIC: 9870.4
##
## Number of Fisher Scoring iterations: 2
lm_uempmed <- glm(uempmed ~ unemploy, data = economics)</pre>
summary(lm_uempmed)
##
## Call:
## glm(formula = uempmed ~ unemploy, data = economics)
## Deviance Residuals:
##
      Min
                 1Q
                      Median
                                   3Q
                                           Max
## -4.2674 -1.5802
                     0.0181
                               1.0254
                                        7.5343
##
## Coefficients:
                Estimate Std. Error t value Pr(>|t|)
## (Intercept) -1.892e+00 2.637e-01 -7.177 2.22e-12 ***
## unemploy
              1.351e-03 3.212e-05 42.064 < 2e-16 ***
## ---
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
##
## (Dispersion parameter for gaussian family taken to be 4.127218)
##
##
      Null deviance: 9663.4 on 573 degrees of freedom
## Residual deviance: 2360.8 on 572 degrees of freedom
## AIC: 2446.6
## Number of Fisher Scoring iterations: 2
  2. exponential or logarithmic model
log_unemploy <- glm(unemploy ~ log(uempmed), data = economics)</pre>
summary(log_unemploy)
##
## glm(formula = unemploy ~ log(uempmed), data = economics)
##
## Deviance Residuals:
##
      Min
            1Q
                    Median
                                           Max
                                   3Q
## -2280.5 -891.0
                     -252.0
                                878.5
                                        3133.5
##
## Coefficients:
##
                Estimate Std. Error t value Pr(>|t|)
                -4935.7
## (Intercept)
                              261.8 -18.85
                                             <2e-16 ***
                              124.4
                                              <2e-16 ***
## log(uempmed)
                 6143.9
                                    49.37
## ---
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
## (Dispersion parameter for gaussian family taken to be 1328910)
```

```
##
##
       Null deviance: 3999510381 on 573 degrees of freedom
## Residual deviance: 760136476 on 572 degrees of freedom
## AIC: 9726.3
## Number of Fisher Scoring iterations: 2
exp_uempmed <- glm(uempmed ~ log(unemploy), data = economics)</pre>
summary(exp_uempmed)
##
## Call:
## glm(formula = uempmed ~ log(unemploy), data = economics)
## Deviance Residuals:
##
       Min
                 1Q
                      Median
                                    3Q
  -3.7856 -1.9608 -0.4871
                               0.7934
                                       10.5946
## Coefficients:
##
                 Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                 -69.6121 2.7317 -25.48
                                               <2e-16 ***
## log(unemploy)
                   8.7909
                              0.3068
                                        28.66
                                                <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## (Dispersion parameter for gaussian family taken to be 6.935919)
##
##
       Null deviance: 9663.4 on 573 degrees of freedom
## Residual deviance: 3967.3 on 572 degrees of freedom
## AIC: 2744.6
##
## Number of Fisher Scoring iterations: 2
3.polynomial model of 2nd, 3rd and 10th degree
poly.2_unemploy <- glm(unemploy ~ poly(uempmed,2), data = economics)</pre>
poly.3_unemploy <- glm(unemploy ~ poly(uempmed,3), data = economics)</pre>
poly.10_unemploy <- glm(unemploy ~ poly(uempmed,10), data = economics)</pre>
poly.2_uempmed <- glm(uempmed ~ poly(unemploy,2), data = economics)</pre>
poly.3_uempmed <- glm(uempmed ~ poly(unemploy,3), data = economics)</pre>
poly.10_uempmed <- glm(uempmed ~ poly(unemploy,10), data = economics)</pre>
```

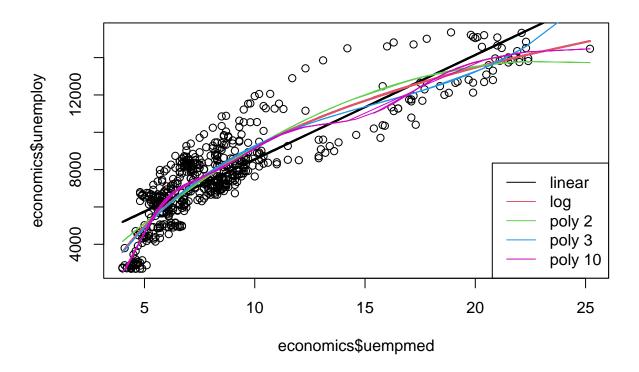
b)

Plot the corresponding data and add all the models for comparison.

Plot models to predict umemploy:

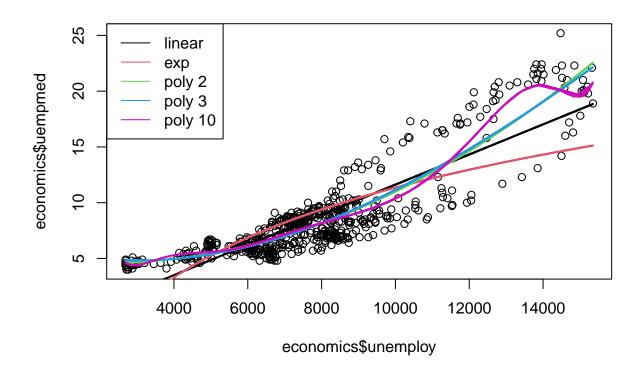
```
plot(economics$uempmed, economics$unemploy)
lines(economics$uempmed, fitted(lm_unemploy), col=1, lwd=2)
lines(economics$uempmed, fitted(log_unemploy), col=2, lwd=2)
```

```
lines(economics$uempmed, fitted(poly.2_unemploy), col=3, lwd=1)
lines(economics$uempmed, fitted(poly.3_unemploy), col=4, lwd=1)
lines(economics$uempmed, fitted(poly.10_unemploy), col=6, lwd=1)
legend("bottomright",legend=c("linear","log","poly 2","poly 3","poly 10"),col=c(1,2,3,4,6), lty=1)
```



Plot models to predict uempmed:

```
plot(economics$unemploy, economics$uempmed)
lines(economics$unemploy, fitted(lm_uempmed), col=1, lwd=2)
lines(economics$unemploy, fitted(exp_uempmed), col=2, lwd=2)
lines(economics$unemploy, fitted(poly.2_uempmed), col=3, lwd=2)
lines(economics$unemploy, fitted(poly.3_uempmed), col=4, lwd=2)
lines(economics$unemploy, fitted(poly.10_uempmed), col=6, lwd=2)
legend("topleft",legend=c("linear","exp","poly 2","poly 3","poly 10"),col=c(1,2,3,4,6), lty=1)
```



**c**)

Use the cv.glm function in the boot package for the following steps. Compare the Root Mean Squared Error and Mean Squared Error.

# Predict unemploy

1. Use cv.glm for Leave-one-out Cross Validation to compare the models above

```
## Model LOOCV.MSE LOOCV.RMSE
## 1 linear 1715211 1309.661
## 2 exponential 1333997 1154.988
## 3 poly 2 1432531 1196.884
## 4 poly 3 1366405 1168.933
## 5 poly 10 4530738 2128.553
```

2. Use cv.glm for 5-fold and 10-fold Cross Validation to compare the models above.

# 5-fold CV

```
cv5.lm_unemploy <- cv.glm(economics, glm(lm_unemploy), K=5)
cv5.log_unemploy <- cv.glm(economics, glm(log_unemploy), K=5)</pre>
cv5.poly.2_unemploy <- cv.glm(economics, glm(poly.2_unemploy), K=5)
cv5.poly.3_unemploy <- cv.glm(economics, glm(poly.3_unemploy), K=5)
cv5.poly.10 unemploy <- cv.glm(economics, glm(poly.10 unemploy), K=5)
data.frame(
  "Model" = c("linear", "exponential", "poly 2", "poly 3", "poly 10"),
  "5-fold CV MSE" = c(cv5.lm_unemploy$delta[1],cv5.log_unemploy$delta[1],cv5.poly.2_unemploy$delta[1],
                  cv5.poly.3_unemploy$delta[1],cv5.poly.10_unemploy$delta[1]),
  "5-fold CV RMSE" = c(sqrt(cv5.lm_unemploy$delta[1]),sqrt(cv5.log_unemploy$delta[1]),sqrt(cv5.poly.2_u
                  sqrt(cv5.poly.3_unemploy$delta[1]),sqrt(cv5.poly.10_unemploy$delta[1])))
##
           Model X5.fold.CV.MSE X5.fold.CV.RMSE
## 1
          linear
                        1718388
                                       1310.873
## 2 exponential
                        1333038
                                       1154.573
                                       1201.186
## 3
         poly 2
                        1442848
## 4
         poly 3
                                       1164.073
                        1355067
```

#### 10-fold CV

poly 10

linear

1774928

1713789

## 5

## 1

```
cv10.lm_unemploy <- cv.glm(economics, glm(lm_unemploy), K=10)
cv10.log_unemploy <- cv.glm(economics, glm(log_unemploy), K=10)
cv10.poly.2_unemploy <- cv.glm(economics, glm(poly.2_unemploy), K=10)
cv10.poly.3_unemploy <- cv.glm(economics, glm(poly.3_unemploy), K=10)
cv10.poly.10_unemploy <- cv.glm(economics, glm(poly.10_unemploy), K=10)

data.frame(
   "Model" = c("linear", "exponential", "poly 2", "poly 3", "poly 10"),
   "10-fold CV MSE" = c(cv10.lm_unemploy$delta[1],cv10.log_unemploy$delta[1],cv10.poly.2_unemploy$delta[cv10.poly.3_unemploy$delta[1]),
   "10-fold CV RMSE" = c(sqrt(cv10.lm_unemploy$delta[1]),sqrt(cv10.log_unemploy$delta[1]),sqrt(cv10.poly.3_unemploy$delta[1]))

### Model X10.fold.CV.MSE X10.fold.CV.RMSE</pre>
```

1309.118

1332.264

```
## 2 exponential 1335553 1155.661

## 3 poly 2 1430499 1196.035

## 4 poly 3 1363996 1167.902

## 5 poly 10 16079526 4009.928
```

#### Conclusions

The results of 5-fold, 10-fold and LOO cross validation are very similar overall. Therefore we can assume that they give a reliable measure of the models performance.

The exponential performs best to predict unemploy. Poly3 and poly4 also perform well. The linear and poly10 models are not suitable.

# Predict uempmed

1. Use cv.glm for Leave-one-out Cross Validation to compare the models above

```
\# cost.MSE \leftarrow function(r, pi = 0) mean((r-pi)^2)
cv.lm_uempmed <- cv.glm(economics, glm(lm_uempmed))</pre>
cv.exp_uempmed <- cv.glm(economics, glm(exp_uempmed))</pre>
cv.poly.2_uempmed <- cv.glm(economics, glm(poly.2_uempmed))</pre>
cv.poly.3_uempmed <- cv.glm(economics, glm(poly.3_uempmed))</pre>
cv.poly.10 uempmed <- cv.glm(economics, glm(poly.10 uempmed))
data.frame(
  "Model" = c("linear", "exponential", "poly 2", "poly 3", "poly 10"),
  "LOOCV MSE" = c(cv.lm_uempmed$delta[1],cv.exp_uempmed$delta[1],cv.poly.2_uempmed$delta[1],
                  cv.poly.3_uempmed$delta[1],cv.poly.10_uempmed$delta[1]),
  "LOOCV RMSE" = c(sqrt(cv.lm_uempmed$delta[1]),sqrt(cv.exp_uempmed$delta[1]),sqrt(cv.poly.2_uempmed$de
                  sqrt(cv.poly.3_uempmed$delta[1]),sqrt(cv.poly.10_uempmed$delta[1])) )
##
           Model LOOCV.MSE LOOCV.RMSE
## 1
          linear 4.159797
                              2.039558
## 2 exponential
                  6.998858
                              2.645536
## 3
          poly 2 3.005112
                              1.733526
```

2. Use cv.glm for 5-fold and 10-fold Cross Validation to compare the models above.

1.734916

1.682945

#### 5-fold CV

poly 3 3.009934

poly 10 2.832303

## 4

## 5

```
cv.lm_uempmed <- cv.glm(economics, glm(lm_uempmed),K=5)
cv.exp_uempmed <- cv.glm(economics, glm(exp_uempmed),K=5)
cv.poly.2_uempmed <- cv.glm(economics, glm(poly.2_uempmed),K=5)
cv.poly.3_uempmed <- cv.glm(economics, glm(poly.3_uempmed),K=5)
cv.poly.10_uempmed <- cv.glm(economics, glm(poly.10_uempmed),K=5)</pre>
```

```
##
           Model LOOCV.MSE LOOCV.RMSE
## 1
          linear 4.132461
                             2.032846
## 2 exponential
                  6.970403
                             2.640152
## 3
          poly 2 3.019736
                             1.737739
## 4
          poly 3 2.996704
                             1.731099
## 5
         poly 10 2.831195
                             1.682616
```

#### 10-fold CV

```
##
           Model LOOCV.MSE LOOCV.RMSE
## 1
          linear 4.151843
                             2.037607
## 2 exponential 7.057241
                             2.656547
## 3
          poly 2
                  3.022632
                             1.738572
## 4
                  3.039117
                             1.743306
          poly 3
## 5
                  2.802345
                             1.674021
         poly 10
```

The polynomial models have the best performance to predict uempmed. The best results are obtained with the poly10 model. However, the poly2 and poly3 models are almost as good.

# d)

Explain based on the CV and graphical model fits the concepts of Underfitting, Overfitting and how to apply cross-validation to determine the appropriate model fit. Also, describe the different variants of cross validation in this context.

### Answer:

The concepts of underfitting and overfitting describe how a model fits a set of data. In unterfitting the model fits the data to rough which results in a prediction bias. An example for underfitting would be the linear model for the economica dataset. The complexity of the linear model is not enough to learn the curved

structure of the data. Overfitting means that the model fits the training data too strongly that it also learn noise resulting in a high variance. An example of overfitting is the polynomial model of degree 10 for the economics data. You can also see in the MSE values from the CV that underfittet and overfittet models perform much worse that optimally fittet models. It is very important to find the right balance to achieve the best possible performance

Computing a cross validation score can give you a good idea of when the model starts to under- or overfit the data. Cross validation withholds a portion of the data for model building and uses this data to evaluate the model. Every data point is used for evaluation one time. The evaluation of the models can be done with a percentage 1/k of the data which is called k-fold cross validation. The dataset is split in k folds in this case. Or it can be done with just one datapoint for evaluation in each iteration which is called leave one out cross validation.

This technique gives a good idea of how the model would perform when confronted with unseen data. To find the appropriate model fit it is important to find a balance between bias and variance. The best model fit can be achieved by selecting the model with the lowest crocc validation error.