

Chapter 18 Interactive Notebook for Students

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Load packages

```
library(caret)
```

```
## Loading required package: ggplot2
```

```
## Loading required package: lattice
```

```
library(rattle)
```

```
## Loading required package: tibble
```

```
## Loading required package: bitops
```

```
## Rattle: A free graphical interface for data science with R.
## Version 5.5.1 Copyright (c) 2006-2021 Togaware Pty Ltd.
## Type 'rattle()' to shake, rattle, and roll your data.
```

Get the data and pre-process

Read data

```
dataset <- read.csv('diabetes.csv', header = TRUE)
dim(dataset)
```

```
## [1] 442 11
```

Partition Data

- Note the use of `sample()` function to create training, validation, and test datasets. Another interesting function is `sapply()`. This is part of a list of so-called `apply()` functions in R. They essentially allow you to run a function on multiple different inputs. In the case below, we want to get the number of rows (which is done through a function) for three different dataframes. Instead of writing three different lines of code, `sapply()` makes the coding simpler and more elegant.

```
set.seed(123456)
N = nrow(dataset)
cut1 = floor(0.6*N)
cut2 = floor(0.8*N)
index = sample(1:N)
train_index = index[1:cut1]
val_index = index[(cut1+1):cut2]
test_index = index[(cut2+1):N]
df_train = dataset[train_index,]
df_val = dataset[val_index,]
df_test = dataset[test_index,]
sapply(list(df_train,df_val,df_test),nrow)
```

```
## [1] 265 88 89
```

Linear Regression Model

- For this and the subsequent chapter, we will make use of the `caret` package that provides a uniform approach to work with a variety of predictive models. Also note the use of `::` notation. This is used to indicate the package that contains the function that follows. This is helpful as often different packages may use the same function names.

```
df_train[-11] = scale(df_train[-11])
lr = caret::train(target ~ ., method='lm',data = df_train)
train_pred = predict(lr,newdata = df_train)
val_pred = predict(lr,newdata = scale(df_val[-11]))
test_pred = predict(lr,newdata = scale(df_test[-11]))
```

Compute functions for Residual Mean,MSE, RMSE and R₂

```
rm <- function(actual,pred) {
  return(mean(abs(actual-pred)))
}
mse <- function(actual,pred) {
  return(mean((pred-actual)^2))
}
rmse <- function(actual,pred) {
  return(mse(pred,actual)^0.5)
}
R_2 <- function(actual,pred){
```

```

mean_v = rep(mean(actual),length(actual))
SST = sum((actual-mean_v)^2)
SSE = sum((actual-pred)^2)
return(1-(SSE/SST))
}

```

Performance of the Linear Regression Model

- In the code below, we want to assess the performance of the model on training, validation, and test datasets. To make it easier to read and compare, we will put the results in a dataframe. Also note the use of `lapply()` function - in this case we want to change the data type of all the variables, except the first column, to numeric. Again, this function makes it easier to code.

```

res = data.frame()
w = rm(df_train$target,train_pred)
x = mse(df_train$target,train_pred)
y = rmse(df_train$target,train_pred)
z = R_2(df_train$target,train_pred)
res = rbind(res,c("Train",w,x,y,z))
w = rm(df_val$target,val_pred)
x = mse(df_val$target,val_pred)
y = rmse(df_val$target,val_pred)
z = R_2(df_val$target,val_pred)
res = rbind(res,c("Validation",w,x,y,z))
w = rm(df_test$target,test_pred)
x = mse(df_test$target,test_pred)
y = rmse(df_test$target,test_pred)
z = R_2(df_test$target,test_pred)
res = rbind(res,c("Test",w,x,y,z))
colnames(res) = c("Data","Residual Mean","MSE","RMSE","R_2")
# Following converts appropriate columns to numeric type
res[-1] = lapply(res[-1], FUN = function(y){as.numeric(y)})
# Following rounds numeric values to 4 digits
res[,sapply(res, is.numeric)] <-round(res[,sapply(res, is.numeric)],4)
knitr::kable(res)

```

Data	Residual Mean	MSE	RMSE	R_2
Train	41.73	2655	51.52	0.5749
Validation	47.85	3548	59.57	0.3137
Test	43.83	3023	54.98	0.4676

Polynomial Regression Model

- Column names of the original data set.

```
colnames(df_train)
```

```
## [1] "age"    "sex"    "bmi"    "bp"     "s1"     "s2"     "s3"     "s4"
## [9] "s5"     "s6"     "target"
```

Generate the dataset

- The strategy is to write a formula for squared and interaction terms, and use the formula to generate a new dataset that contains the polynomial terms.

```
# Degree 2 polynomial feature generation function

pf2_transform <- function(df, target_name='target') {
  formula_pf2 <- as.formula(paste(target_name, '~ .^2 +',
                                paste('poly(',
                                      colnames(df)[-c(1)],
                                      ',2, raw=TRUE)[, 2]',
                                      collapse = ' + ')
                                )
  )
  output <- model.matrix(formula_pf2, data = df)
  # Rewrite column names for readability
  colnames_pf2 <- c("1",
                    colnames(df)[-1], # exclude target
                    paste0(colnames(df)[-1], "^2"), # include squares
                    colnames(output)[-1:(length(df)*2-1)]) # include interactions
  colnames(output) <- colnames_pf2
  # Convert to dataframe
  output_df <- data.frame(output)
  # Exclude intercept column
  output_df[,1] <- NULL
  return(output_df)
}
```

Create training, validation and test sets

- Create the training data set

```
train_sc_pf2 <- pf2_transform(df_train, target_name = "target")
train_sc_pf2$target = df_train$target
train_sc_pf2 = train_sc_pf2[-20]
print(colnames(train_sc_pf2))
```

```
## [1] "sex"      "bmi"      "bp"       "s1"       "s2"       "s3"       "s4"
## [8] "s5"       "s6"       "target"   "sex.2"    "bmi.2"    "bp.2"     "s1.2"
## [15] "s2.2"     "s3.2"     "s4.2"     "s5.2"     "s6.2"     "age.sex"  "age.bmi"
## [22] "age.bp"   "age.s1"   "age.s2"   "age.s3"   "age.s4"   "age.s5"   "age.s6"
## [29] "sex.bmi"  "sex.bp"   "sex.s1"   "sex.s2"   "sex.s3"   "sex.s4"   "sex.s5"
## [36] "sex.s6"   "bmi.bp"   "bmi.s1"   "bmi.s2"   "bmi.s3"   "bmi.s4"   "bmi.s5"
## [43] "bmi.s6"   "bp.s1"    "bp.s2"    "bp.s3"    "bp.s4"    "bp.s5"    "bp.s6"
## [50] "s1.s2"    "s1.s3"    "s1.s4"    "s1.s5"    "s1.s6"    "s2.s3"    "s2.s4"
## [57] "s2.s5"    "s2.s6"    "s3.s4"    "s3.s5"    "s3.s6"    "s4.s5"    "s4.s6"
## [64] "s5.s6"
```

```
dim(df_train[-10])
```

```
## [1] 265 10
```

```
dim(train_sc_pf2)
```

```
## [1] 265 64
```

- Prepare the validation and test sets

```
df_val[-11]= scale(df_val[-11])
val_sc_pf2 <- pf2_transform(df_val,target_name = "target")
val_sc_pf2$target = df_val$target
val_sc_pf2 = val_sc_pf2[-20]

df_test[-11]= scale(df_test[-11])
test_sc_pf2 <- pf2_transform(df_test,target_name = "target")
test_sc_pf2$target = df_test$target
test_sc_pf2 = test_sc_pf2[-20]
```

Run the Polynomial Regression

```
lr = caret::train(target ~ ., method='lm',data = train_sc_pf2)
train_pred = predict(lr,newdata = train_sc_pf2)
val_pred = predict(lr,newdata = val_sc_pf2)
test_pred = predict(lr,newdata = test_sc_pf2)
```

Evaluate the results

```
res = data.frame()
y = rmse(df_train$target,train_pred)
res = rbind(res,c("Train",y))
y = rmse(df_val$target,val_pred)
res = rbind(res,c("Validation",y))
y = rmse(df_test$target,test_pred)
res = rbind(res,c("Test",y))
colnames(res) = c("Data","RMSE")
# Following converts appropriate columns to numeric type
res[-1] = lapply(res[-1], FUN = function(y){as.numeric(y)})
# Following rounds numeric values to 4 digits
res[,sapply(res, is.numeric)] <-round(res[,sapply(res, is.numeric)],4)
knitr::kable(res)
```

Data	RMSE
Train	45.13
Validation	288.66
Test	231.93

Ridge Regression

Basic Model

```
ridge <- caret::train(y = train_sc_pf2$target, x = train_sc_pf2[-10],
                     method = 'glmnet',
                     tuneGrid = expand.grid(alpha = 0, lambda = 1)
                     )
train_pred = predict(ridge, newdata = train_sc_pf2)
val_pred = predict(ridge, newdata = val_sc_pf2)
test_pred = predict(ridge, newdata = test_sc_pf2)

res = data.frame()
y = rmse(df_train$target, train_pred)
res = rbind(res, c("Train", y))
y = rmse(df_val$target, val_pred)
res = rbind(res, c("Validation", y))
y = rmse(df_test$target, test_pred)
res = rbind(res, c("Test", y))
colnames(res) = c("Data", "RMSE")
# Following converts appropriate columns to numeric type
res[-1] = lapply(res[-1], FUN = function(y){as.numeric(y)})
# Following rounds numeric values to 4 digits
res[, sapply(res, is.numeric)] <- round(res[, sapply(res, is.numeric)], 4)
knitr::kable(res)
```

Data	RMSE
Train	46.67
Validation	59.98
Test	58.11

Hyper-parameter tuning

```
parameters <- c(seq(0.1, 2, by = 0.1) , seq(2, 5, 0.5) , seq(5, 25, 1))

ridge <- caret::train(y = train_sc_pf2$target,
                     x = train_sc_pf2[-10],
                     method = 'glmnet',
                     tuneGrid = expand.grid(alpha = 0, lambda = parameters) ,
                     metric = "Rsquared"
                     )
paste(" Ridge Best lambda = ", ridge$finalModel$lambdaOpt)
```

```
## [1] " Ridge Best lambda = 25"
```

Run the Optimized Ridge Regression

```

ridge_best<-caret::train(y = train_sc_pf2$target,
  x = train_sc_pf2[-10],
  method = 'glmnet',
  tuneGrid = expand.grid(alpha = 0, lambda = ridge$finalModel$lambdaOpt))
train_pred = predict(ridge_best,newdata = train_sc_pf2)
val_pred = predict(ridge_best,newdata = val_sc_pf2)
test_pred = predict(ridge_best,newdata = test_sc_pf2)
res = data.frame()
y = rmse(df_train$target,train_pred)
res = rbind(res,c("Train",y))
y = rmse(df_val$target,val_pred)
res = rbind(res,c("Validation",y))
y = rmse(df_test$target,test_pred)
res = rbind(res,c("Test",y))
colnames(res) = c("Data","RMSE")
# Following converts appropriate columns to numeric type
res[-1] = lapply(res[-1], FUN = function(y){as.numeric(y)})
# Following rounds numeric values to 4 digits
res[,sapply(res, is.numeric)] <-round(res[,sapply(res, is.numeric)],4)
knitr::kable(res)

```

Data	RMSE
Train	48.93
Validation	57.66
Test	56.02

Evaluate Performance of the optimized Ridge Regression

```

res = data.frame()
y = R2(train_pred,df_train$target)
res = rbind(res,c("Train",y))
y = R2(val_pred,df_val$target)
res = rbind(res,c("Validation",y))
y = R2(test_pred,df_test$target)
res = rbind(res,c("Test",y))
colnames(res) = c("Data","R_2")
# Following converts appropriate columns to numeric type
res[-1] = lapply(res[-1], FUN = function(y){as.numeric(y)})
# Following rounds numeric values to 4 digits
res[,sapply(res, is.numeric)] <-round(res[,sapply(res, is.numeric)],4)
knitr::kable(res)

```

Data	R_2
Train	0.6295
Validation	0.3788
Test	0.4761

Lasso Regression

Basic Model

```
lasso<-caret::train(y = train_sc_pf2$target,
  x = train_sc_pf2[-10],
  method = 'glmnet',
  tuneGrid = expand.grid(alpha = 1, lambda = 0))
train_pred = predict(lasso,newdata = train_sc_pf2)
val_pred = predict(lasso,newdata = val_sc_pf2)
test_pred = predict(lasso,newdata = test_sc_pf2)
res = data.frame()
y = rmse(df_train$target,train_pred)
res = rbind(res,c("Train",y))
y = rmse(df_val$target,val_pred)
res = rbind(res,c("Validation",y))
y = rmse(df_test$target,test_pred)
res = rbind(res,c("Test",y))
colnames(res) = c("Data","RMSE")
# Following converts appropriate columns to numeric type
res[-1] = lapply(res[-1], FUN = function(y){as.numeric(y)})
# Following rounds numeric values to 4 digits
res[,sapply(res, is.numeric)] <-round(res[,sapply(res, is.numeric)],4)
knitr::kable(res)
```

Data	RMSE
Train	45.51
Validation	63.96
Test	59.27

Hyper-parameter tuning

- Find the best hyper parameter lambda

```
parameters <- c(seq(0.1, 2, by =0.1) , seq(2, 5, 0.5) , seq(5, 25, 1))
lasso<-caret::train(y = train_sc_pf2$target,
  x = train_sc_pf2[-10],
  method = 'glmnet',
  tuneGrid = expand.grid(alpha = 1, lambda = parameters) ,
  metric = "Rsquared"
)
paste(" Lasso Best lambda = ",lasso$finalModel$lambdaOpt)
```

```
## [1] " Lasso Best lambda = 5"
```

Run the Optimized Lasso Regression

```

lasso_best<-caret::train(y = train_sc_pf2$target,
  x = train_sc_pf2[-10],
  method = 'glmnet',
  tuneGrid = expand.grid(alpha = 1, lambda = lasso$finalModel$lambdaOpt))
train_pred = predict(lasso_best,newdata = train_sc_pf2)
val_pred = predict(lasso_best,newdata = val_sc_pf2)
test_pred = predict(lasso_best,newdata = test_sc_pf2)
res = data.frame()
y = rmse(df_train$target,train_pred)
res = rbind(res,c("Train",y))
y = rmse(df_val$target,val_pred)
res = rbind(res,c("Validation",y))
y = rmse(df_test$target,test_pred)
res = rbind(res,c("Test",y))
colnames(res) = c("Data","RMSE")
# Following converts appropriate columns to numeric type
res[-1] = lapply(res[-1], FUN = function(y){as.numeric(y)})
# Following rounds numeric values to 4 digits
res[,sapply(res, is.numeric)] <-round(res[,sapply(res, is.numeric)],4)
knitr::kable(res)

```

Data	RMSE
Train	52.57
Validation	58.00
Test	53.24

Performance of the Optimized Lasso Regression

```

res = data.frame()
y = R2(train_pred,df_train$target)
res = rbind(res,c("Train",y))
y = R2(val_pred,df_val$target)
res = rbind(res,c("Validation",y))
y = R2(test_pred,df_test$target)
res = rbind(res,c("Test",y))
colnames(res) = c("Data","R_2")
# Following converts appropriate columns to numeric type
res[-1] = lapply(res[-1], FUN = function(y){as.numeric(y)})
# Following rounds numeric values to 4 digits
res[,sapply(res, is.numeric)] <-round(res[,sapply(res, is.numeric)],4)
knitr::kable(res)

```

Data	R_2
Train	0.5673
Validation	0.3646
Test	0.5117

Determine non-zero coefficients

```
df = data.frame(  
  lasso = as.data.frame.matrix(coef(lasso$finalModel, lasso$finalModel$lambdaOpt))  
)  
df = subset(df, s1 > 0.1)  
df$var = row.names(df)  
knitr::kable(df[order(-df$s1), c(2, 1)] [2])
```

	s1
(Intercept)	154.3001
bp	25.3282
s6	20.6368
s1	13.4184
bmi.s6	3.9376
sex.s3	2.2168
age.s6	0.7353
bmi.bp	0.4412
age.sex	0.1728
s6.2	0.1407

Neural Network

Large network

```
mlp <- caret::train(target ~ ., data = train_sc_pf2, method='mlp', size=1000)  
  
train_pred = predict(mlp, newdata = train_sc_pf2)  
val_pred = predict(mlp, newdata = val_sc_pf2)  
test_pred = predict(mlp, newdata = test_sc_pf2)  
res = data.frame()  
y = rmse(df_train$target, train_pred)  
res = rbind(res, c("Train", y))  
y = rmse(df_val$target, val_pred)  
res = rbind(res, c("Validation", y))  
y = rmse(df_test$target, test_pred)  
res = rbind(res, c("Test", y))  
colnames(res) = c("Data", "RMSE")  
# Following converts appropriate columns to numeric type  
res[-1] = lapply(res[-1], FUN = function(y){as.numeric(y)})  
# Following rounds numeric values to 4 digits  
res[, sapply(res, is.numeric)] <- round(res[, sapply(res, is.numeric)], 4)  
knitr::kable(res)
```

Data	RMSE
Train	104.5
Validation	103.7

Data	RMSE
Test	107.5

Smaller network

```
mlp <- caret::train(target ~ ., data = train_sc_pf2, method='mlp', size=50)

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

train_pred = predict(mlp, newdata = train_sc_pf2)
val_pred = predict(mlp, newdata = val_sc_pf2)
test_pred = predict(mlp, newdata = test_sc_pf2)
res = data.frame()
y = rmse(df_train$target, train_pred)
res = rbind(res, c("Train", y))
y = rmse(df_val$target, val_pred)
res = rbind(res, c("Validation", y))
y = rmse(df_test$target, test_pred)
res = rbind(res, c("Test", y))
colnames(res) = c("Data", "RMSE")
# Following converts appropriate columns to numeric type
res[-1] = lapply(res[-1], FUN = function(y){as.numeric(y)})
# Following rounds numeric values to 4 digits
res[,sapply(res, is.numeric)] <- round(res[,sapply(res, is.numeric)], 4)
knitr::kable(res)
```

Data	RMSE
Train	83.34
Validation	74.52
Test	77.62

Regression Tree

Basic Tree

```
dtr <- caret::train(target ~ ., data = train_sc_pf2, method='rpart')

train_pred = predict(dtr, newdata = train_sc_pf2)
val_pred = predict(dtr, newdata = val_sc_pf2)
test_pred = predict(dtr, newdata = test_sc_pf2)
res = data.frame()
y = rmse(df_train$target, train_pred)
res = rbind(res, c("Train", y))
y = rmse(df_val$target, val_pred)
```

```

res = rbind(res,c("Validation",y))
y = rmse(df_test$target,test_pred)
res = rbind(res,c("Test",y))
colnames(res) = c("Data","RMSE")
# Following converts appropriate columns to numeric type
res[-1] = lapply(res[-1], FUN = function(y){as.numeric(y)})
# Following rounds numeric values to 4 digits
res[,sapply(res, is.numeric)] <-round(res[,sapply(res, is.numeric)],4)
knitr::kable(res)

```

Data	RMSE
Train	60.28
Validation	66.73
Test	60.40

Tree with a maximum depth of 2

```

dtr <- caret::train(target ~ .,data = train_sc_pf2,method='rpart',
                    control = list(max_depth=2))

```

```

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

```

```

train_pred = predict(dtr,newdata = train_sc_pf2)
val_pred = predict(dtr,newdata = val_sc_pf2)
test_pred = predict(dtr,newdata = test_sc_pf2)
res = data.frame()
y = rmse(df_train$target,train_pred)
res = rbind(res,c("Train",y))
y = rmse(df_val$target,val_pred)
res = rbind(res,c("Validation",y))
y = rmse(df_test$target,test_pred)
res = rbind(res,c("Test",y))
colnames(res) = c("Data","RMSE")
# Following converts appropriate columns to numeric type
res[-1] = lapply(res[-1], FUN = function(y){as.numeric(y)})
# Following rounds numeric values to 4 digits
res[,sapply(res, is.numeric)] <-round(res[,sapply(res, is.numeric)],4)
knitr::kable(res)

```

Data	RMSE
Train	60.28
Validation	66.73
Test	60.40

Harder problem

Data preparation

- Read data

```
df <- read.csv("ENB2012_data.csv")
```

- Create training, validation and test datasets.

```
dataset = df[-c(11,12)]
N = nrow(dataset)
cut1 = floor(0.6*N)
cut2 = floor(0.8*N)
index = sample(1:N)
train_index = index[1:cut1]
val_index = index[(cut1+1):cut2]
test_index = index[(cut2+1):N]
df_train = dataset[train_index,]
df_val = dataset[val_index,]
df_test = dataset[test_index,]
sapply(list(df_train,df_val,df_test),nrow)
```

```
## [1] 460 154 154
```

```
df_train[-10] = scale(df_train[-10])
```

Build and Evaluate Models

```
res = data.frame()
# Linear Regression
lr = caret::train(Y2 ~ ., method='lm', data = df_train)
train_pred = predict(lr, newdata = df_train)
val_pred = predict(lr, newdata = scale(df_val[-10]))
test_pred = predict(lr, newdata = scale(df_test[-10]))
y1 = rmse(df_train$Y2, train_pred)
y2 = rmse(df_val$Y2, val_pred)
y3 = rmse(df_test$Y2, test_pred)
res = rbind(res, c("Linear Regression", y1, y2, y3))
# Ridge Regression
ridge <- caret::train(y = df_train$Y2, x = df_train[-10],
                      method = 'glmnet',
                      tuneGrid = expand.grid(alpha = 0, lambda = 1)
)
train_pred = predict(ridge, newdata = df_train)
val_pred = predict(ridge, newdata = scale(df_val[-10]))
test_pred = predict(ridge, newdata = scale(df_test[-10]))
y1 = rmse(df_train$Y2, train_pred)
y2 = rmse(df_val$Y2, val_pred)
```

```

y3 = rmse(df_test$Y2,test_pred)
res = rbind(res,c("Ridge Regression",y1,y2,y3))
# Lasso Regression
lasso <- caret::train(y = df_train$Y2,x = df_train[-10],
                      method = 'glmnet',
                      tuneGrid = expand.grid(alpha = 1, lambda = 0)
                      )
train_pred = predict(lasso,newdata = df_train)
val_pred = predict(lasso,newdata = scale(df_val[-10]))
test_pred = predict(lasso,newdata = scale(df_test[-10]))
y1 = rmse(df_train$Y2,train_pred)
y2 = rmse(df_val$Y2,val_pred)
y3 = rmse(df_test$Y2,test_pred)
res = rbind(res,c("Lasso Regression",y1,y2,y3))
# Neural Net
nn <- caret::train(y = df_train$Y2,x = df_train[-10],
                   method = 'mlp')
train_pred = predict(nn,newdata = df_train)
val_pred = predict(nn,newdata = scale(df_val[-10]))
test_pred = predict(nn,newdata = scale(df_test[-10]))
y1 = rmse(df_train$Y2,train_pred)
y2 = rmse(df_val$Y2,val_pred)
y3 = rmse(df_test$Y2,test_pred)
res = rbind(res,c("Neural Net",y1,y2,y3))
# Regression Tree
dt <- caret::train(y = df_train$Y2,x = df_train[-10],
                   method = 'rpart')
train_pred = predict(dt,newdata = df_train)
val_pred = predict(dt,newdata = scale(df_val[-10]))
test_pred = predict(dt,newdata = scale(df_test[-10]))
y1 = rmse(df_train$Y2,train_pred)
y2 = rmse(df_val$Y2,val_pred)
y3 = rmse(df_test$Y2,test_pred)
res = rbind(res,c("Regression Tree",y1,y2,y3))

colnames(res) = c("Model","Train","Validation","Test")
# Following converts appropriate columns to numeric type
res[-1] = lapply(res[-1], FUN = function(y){as.numeric(y)})
# Following rounds numeric values to 4 digits
res[,sapply(res, is.numeric)] <-round(res[,sapply(res, is.numeric)],4)
knitr::kable(res)

```

Model	Train	Validation	Test
Linear Regression	1.901	2.014	2.026
Ridge Regression	2.223	2.453	2.481
Lasso Regression	1.903	2.015	2.022
Neural Net	2.506	2.529	2.574
Regression Tree	2.989	3.219	3.325