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	
<pre>## 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.</pre>	

Get the data and pre-process

Read data

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

[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,]
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.

```
means = apply(df_train[-11],2,mean)
sds = apply(df_train[-11],2,sd)
scalefum = function(x){
    return((x-means)/sds)
}
df_train[-11] = data.frame(sapply(df_train[-11],scalefun))
df_val[-11] = data.frame(sapply(df_val[-11],scalefun))
df_test[-11] = data.frame(sapply(df_test[-11],scalefun))
printfun = function(x){
    means = apply(x[-11],2,mean)
    sds = apply(x[-11],2,sd)
    print(paste(mean(means),mean(sds)))
}
printfun(df_train)
```

[1] "0.000554657253475731 1.00044597757519"

```
printfun(df_val)
```

[1] "-0.0182503268108164 0.980026441948433"

```
printfun(df_test)

## [1] "0.0533555353079712 0.987301726800513"

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 R_2

```
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))
}</pre>
```

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)</pre>
```

Data	Residual Mean	MSE	RMSE	R_2
Train Validation Test	41.79 47.58 43.69	2659 3497 3014	51.56 59.13 54.90	0.0

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') {</pre>
  formula_pf2 <- as.formula(paste(target_name, '~ .^2 +',</pre>
                                    paste('poly(',
                                           colnames(df)[-c(1)],
                                          ',2, raw=TRUE)[, 2]',
                                           collapse = ' + ')
                                    )
   output <- model.matrix(formula_pf2, data = df)</pre>
  # Rewrite column names for readability
   colnames_pf2 <- c("1",</pre>
                                                      # exclude target
                     colnames(df)[-1],
                     paste0(colnames(df)[-1],"^2"), # include squares
                     colnames(output)[-(1:(length(df)*2-1))]) # include interactions
    colnames(output) <- colnames pf2</pre>
  # Convert to dataframe
  output df <- data.frame(output)</pre>
  # Exclude intercept column
```

```
output_df[,1] <- NULL
return(output_df)
}</pre>
```

Create training, validation and test sets

• Create the training data set

```
train_sc_pf2 <- pf2_transform(df_train, target_name = "target")</pre>
train_sc_pf2$target= df_train$target
train_sc_pf2 = train_sc_pf2[-20]
print(colnames(train_sc_pf2))
                            "bp"
                                                         "s3"
                                                                   "s4"
   [1] "sex"
                  "bmi"
                                      "s1"
                                               "s2"
##
## [8] "s5"
                  "s6"
                            "target"
                                     "sex.2"
                                               "bmi.2"
                                                         "bp.2"
                                                                   "s1.2"
                 "s3.2"
                            "s4.2"
                                     "s5.2"
                                               "s6.2"
                                                         "age.sex" "age.bmi"
## [15] "s2.2"
## [22] "age.bp" "age.s1"
                           "age.s2" "age.s3"
                                               "age.s4"
                                                         "age.s5"
                                                                   "age.s6"
                           "sex.s1" "sex.s2"
## [29] "sex.bmi" "sex.bp"
                                               "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"
                                                         "s2.s3"
                                                                   "s2.s4"
                                     "s1.s5"
                                               "s1.s6"
## [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]</pre>
```

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)</pre>
```

Data	RMSE
Train Validation Test	44.95 71.05 77.25

Ridge Regression

Basic Model

```
# 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)</pre>
```

Data	RMSE
Train Validation Test	46.66 59.19 57.10

Hyper-parameter tuning

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

Run the Optimized Ridge Regression

```
ridge_best<-caret::train(y = train_sc_pf2$target,</pre>
     x = train_sc_pf2[-10],
      method = 'glmnet',
      tuneGrid = expand.grid(alpha = 0, lambda = ridge$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)</pre>
knitr::kable(res)
```

Data	RMSE
Train	49.03
Validation Test	57.48 55.76

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)</pre>
```

Data	R_2
Train	0.6275
Validation	0.3794
Test	0.4754

Lasso Regression

Basic Model

```
lasso<-caret::train(y = train_sc_pf2$target,</pre>
      x = train_sc_pf2[-10],
      method = 'glmnet',
      tuneGrid = expand.grid(alpha = 1, lambda = 0))
train_pred = predict(lasso,newdata = train_sc_pf2)
val_pred = predict(lasso,newdata = val_sc_pf2)
test_pred = predict(lasso,newdata = test_sc_pf2)
res = data.frame()
y = rmse(df_train$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)</pre>
```

Data	RMSE
Train Validation Test	45.42 62.98 65.22

Hyper-parameter tuning

• Find the best hyper parameter lambda

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

Run the Optimized Lasso Regression

```
lasso_best<-caret::train(y = train_sc_pf2$target,</pre>
      x = train_sc_pf2[-10],
      method = 'glmnet',
      tuneGrid = expand.grid(alpha = 1, lambda = lasso$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)</pre>
knitr::kable(res)
```

Data	RMSE
Train Validation Test	52.63 57.74 53.41

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)</pre>
```

Data	R_2
Train	0.5663
Validation	0.3677
Test	0.5078

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)	153.1769
bp	25.3203
s6	19.9792
s1	13.1870
bmi.s6	3.7814
sex.s3	2.0960
age.s6	1.1315
s6.2	0.2655
bmi.bp	0.2125

Neural Network

Large network

```
mlp <- caret::train(target ~ .,data = train_sc_pf2,method='mlp',size=1000)</pre>
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)</pre>
knitr::kable(res)
```

Data	RMSE
Train Validation	102.7 100.9
Test	107.1

Smaller network

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

Data	RMSE
Train Validation Test	86.42 83.83 86.49

Regression Tree

Basic Tree

```
dtr <- caret::train(target ~ .,data = train_sc_pf2,method='rpart')</pre>
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)</pre>
knitr::kable(res)
```

Data	RMSE
Train Validation	59.71 66.82
Test	60.15

Tree with a maximum depth of 2

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)</pre>
knitr::kable(res)
```

Data	RMSE
Train Validation Test	59.71 66.82 60.15

Harder problem

Data preparation

• Read data

```
df <- read.csv("../../data/ENB2012_data.csv")</pre>
```

• 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],</pre>
                 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],</pre>
                 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],</pre>
                 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)</pre>
```

Model	Train	Validation	Test
Linear Regression	1.921	2.140	1.992
Ridge Regression	2.308	2.241	2.540
Lasso Regression	1.923	2.139	1.993
Neural Net	3.228	3.547	3.324
Regression Tree	3.006	3.101	3.301