Exploring Regression Techniques - Diamonds Dataset

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Set Up

Need to read the dataset, reclassify categorical variables, sample the data, and check that everything has been done correctly.

```
diamonds <- read.csv('Diamonds Prices2022.csv')</pre>
head(diamonds)
##
     X carat
                    cut color clarity depth table price
                                                             X
## 1 1
        0.23
                 Ideal
                                  SI2
                                       61.5
                                                      326 3.95 3.98 2.43
## 2 2
        0.21
               Premium
                            Ε
                                  SI1
                                        59.8
                                                61
                                                      326 3.89 3.84 2.31
## 3 3
        0.23
                            Ε
                                        56.9
                                                      327 4.05 4.07 2.31
                  Good
                                  VS1
                                                65
## 4 4
        0.29
               Premium
                            Ι
                                  VS2
                                        62.4
                                                58
                                                     334 4.20 4.23 2.63
## 5 5 0.31
                  Good
                            J
                                  SI2
                                        63.3
                                                58
                                                      335 4.34 4.35 2.75
## 6 6 0.24 Very Good
                            J
                                 VVS2
                                       62.8
                                                57
                                                      336 3.94 3.96 2.48
```

summary(diamonds)

```
##
                         carat
                                           cut
                                                               color
##
                             :0.2000
                                       Length: 53943
                 1
                     Min.
                                                           Length: 53943
                     1st Qu.:0.4000
    1st Qu.:13486
                                       Class : character
                                                           Class : character
   Median :26972
                     Median :0.7000
                                       Mode :character
                                                           Mode :character
           :26972
                            :0.7979
##
    Mean
                     Mean
##
    3rd Qu.:40458
                     3rd Qu.:1.0400
    Max.
           :53943
                     Max.
                            :5.0100
##
      clarity
                            depth
                                             table
                                                               price
##
   Length: 53943
                                :43.00
                                                 :43.00
                                                                     326
                        Min.
                                         Min.
                                                          Min.
   Class : character
                        1st Qu.:61.00
                                         1st Qu.:56.00
                                                          1st Qu.:
                                                                     950
   Mode :character
                        Median :61.80
                                         Median :57.00
                                                          Median: 2401
##
                        Mean
                                :61.75
                                         Mean
                                                 :57.46
                                                          Mean
                                                                  : 3933
##
                        3rd Qu.:62.50
                                         3rd Qu.:59.00
                                                          3rd Qu.: 5324
##
                        Max.
                                :79.00
                                         Max.
                                                 :95.00
                                                                  :18823
##
                                               z
          Х
                                                : 0.000
           : 0.000
                             : 0.000
    Min.
                      Min.
                                        Min.
                      1st Qu.: 4.720
    1st Qu.: 4.710
                                        1st Qu.: 2.910
   Median : 5.700
                      Median : 5.710
                                        Median : 3.530
    Mean
           : 5.731
                              : 5.735
                                        Mean
                                                : 3.539
                      Mean
    3rd Qu.: 6.540
                      3rd Qu.: 6.540
                                        3rd Qu.: 4.040
##
           :10.740
                              :58.900
    Max.
                      Max.
                                        Max.
                                                :31.800
```

```
diamonds$color = factor(diamonds$color,
                        levels = c('D', 'E', 'F', 'G', 'H', 'I', 'J'))
diamonds$clarity = factor(diamonds$clarity,
                          levels = c('I1', 'SI2', 'SI1', 'VS2', 'VS1', 'VVS2', 'VVS1', 'IF'))
set.seed(101)
sample diamonds <- diamonds[sample(1:nrow(diamonds), size = 500, replace = FALSE), ]</pre>
str(sample diamonds)
## 'data.frame':
                    500 obs. of 11 variables:
          : int 2873 43103 19665 21855 35772 46326 38688 14688 2531 43324 ...
## $ carat : num 1 0.5 1.41 1.24 0.4 0.6 0.37 1.25 0.7 0.51 ...
            : Factor w/ 5 levels "Fair", "Good", ...: 3 5 5 4 3 2 5 4 5 3 ...
## $ cut
## $ color : Factor w/ 7 levels "D", "E", "F", "G", ...: 6 5 7 1 2 4 2 6 4 1 ...
## $ clarity: Factor w/ 8 levels "I1", "SI2", "SI1", ...: 2 5 5 4 4 5 4 4 6 3 ...
## $ depth : num 62.4 61.6 61.6 59.3 61.2 60.1 61.6 62.2 61 61.7 ...
## $ table : num 63 58 56 58 60 61 57 57 56 58 ...
## $ price : int 3276 1384 8275 9916 912 1757 1041 5925 3205 1403 ...
           : num 6.44 5.08 7.19 7.09 4.79 5.44 4.65 6.92 5.74 5.09 ...
            : num 6.35 5.11 7.22 7.03 4.68 5.5 4.61 6.84 5.77 5.12 ...
## $ y
            : num 3.99 3.14 4.44 4.19 2.9 3.29 2.85 4.28 3.51 3.15 ...
```

Regression

cutPremium

cutIdeal

carat

colorE

Now we look to fit a linear regression model removing x, y, and z variables due to high correlation with carat variable.

We will use price as our dependent variable.

1229.85

1620.29

-87.95

```
diamonds_model <- lm(price ~ depth + cut + carat + color + table, data = sample_diamonds)
summary(diamonds model)
##
## lm(formula = price ~ depth + cut + carat + color + table, data = sample_diamonds)
##
## Residuals:
##
       Min
                 1Q
                      Median
                                   30
                                           Max
## -10582.0 -654.7
                       -50.7
                                457.3
                                        9114.2
##
## Coefficients:
               Estimate Std. Error t value Pr(>|t|)
##
## (Intercept) -2905.72
                           4758.01 -0.611 0.541683
## depth
                 -28.85
                             52.78 -0.547 0.584896
## cutGood
                 920.52
                            442.43 2.081 0.037993 *
                            426.94 3.630 0.000313 ***
## cutVery Good 1549.96
```

431.90 2.848 0.004593 **

440.68 3.677 0.000263 ***

259.33 -0.339 0.734635

7557.20 153.80 49.136 < 2e-16 ***

```
## colorF
                -196.31
                             262.70 -0.747 0.455257
                                    -0.431 0.666571
                -104.83
## colorG
                             243.15
                                    -3.008 0.002767 **
## colorH
                -796.27
                             264.72
                             290.32
                                    -3.261 0.001189 **
## colorI
                -946.71
## colorJ
                -1497.65
                             353.88
                                    -4.232 2.77e-05 ***
                              38.96
                                     0.654 0.513534
## table
                   25.47
## ---
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
##
## Residual standard error: 1454 on 486 degrees of freedom
## Multiple R-squared: 0.841, Adjusted R-squared: 0.8367
## F-statistic: 197.7 on 13 and 486 DF, p-value: < 2.2e-16
```

Checking for multicollinearity (VIF & Condition Index)

Now that we have fit a model we need to check and adjust the model as need to find the best regression line.

First, we will check for multicollinearity. One way we can explore this is by calculating the Variance inflation factor (VIF).

Calculating VIF using R, we will use the vif function in the faraway library.

```
vif_data <- faraway::vif(diamonds_model)
vif_values <- data.frame(
   Coefficient=names(vif_data),
   VIF=as.numeric(vif_data)
)
kable(vif_values)</pre>
```

Coefficient	VIF
depth	1.327361
${\it cutGood}$	4.385521
cutVery Good	8.080182
$\operatorname{cutPremium}$	7.810604
$\operatorname{cutIdeal}$	10.860483
carat	1.121647
colorE	2.243471
colorF	2.215037
colorG	2.648693
colorH	2.135606
colorI	1.888445
colorJ	1.512476
table	1.722300

We can see that the VIF of cutIdeal has a value over 10, which suggests that there could exist multicollinearity. However, this variable is a dummy variable, so this is not a cause for concern.

We will now look at other ways to explore multicollinearity in our model.

Another way is using condition index. The square root of the largest eigen value divided by the smallest eigen value gives us the condition number. When this number is larger than 30, there could be multicollinearity.

For this we will to use the correlation matrix from our regression equation.

```
diamonds_matrix <- model.matrix(diamonds_model)[,-1]
diamonds_corr <- cor(diamonds_matrix)
eigenvalue <- eigen(diamonds_corr)$values
coefficient_names <- colnames(diamonds_matrix)
condition_index <- sqrt(max(eigenvalue)/eigenvalue)
CI_df <- data.frame(Coefficiant=coefficient_names, CI=condition_index)
kable(CI_df)</pre>
```

Coefficient	CI
depth	1.000000
${\it cut}{\it Good}$	1.196043
cutVery Good	1.269965
cutPremium	1.286559
${\it cutIdeal}$	1.323254
carat	1.335179
colorE	1.353269
colorF	1.422821
colorG	1.496735
colorH	1.693845
colorI	2.175808
colorJ	4.151526
table	7.795474

We can see here that there are no values over 30, so we will explore other options for testing our model.

Stepwise Elemination

We will now use stepwise elimination to identify the most relevant predictors for the model.

These methods help to avoid overfitting leaving out predictors that are not significantly increasing the accuracy of the model.

We will check both forward and backward stepwise elimination to see if we get the same result. We will use a k value of 2, because this is the standard k value for minimizing prediction error in models.

```
#backwards stepwise
diamonds_stepB <- stepAIC(diamonds_model, direction="backward", k = 2, trace = 0)
summary(diamonds_stepB)</pre>
```

```
##
## Call:
## lm(formula = price ~ cut + carat + color, data = sample_diamonds)
##
## Residuals:
##
       Min
                 1Q
                                   3Q
                     Median
                                           Max
## -10706.3 -677.3
                       -68.6
                                467.0
                                        9056.6
##
## Coefficients:
##
               Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                -3251.7
                             429.8 -7.566 1.94e-13 ***
## cutGood
                  981.9
                             427.2 2.299 0.02194 *
```

```
## cutVery Good
                  1593.9
                              401.5
                                      3.970 8.27e-05 ***
## cutPremium
                  1301.4
                              402.2
                                      3.235 0.00130 **
## cutIdeal
                  1611.6
                              395.6
                                     4.074 5.40e-05 ***
## carat
                  7568.4
                              152.8
                                    49.521
                                            < 2e-16 ***
## colorE
                  -103.9
                              258.7
                                     -0.402
                                            0.68805
## colorF
                  -199.4
                              262.3
                                    -0.760 0.44766
## colorG
                  -119.3
                              242.6
                                    -0.492
                                            0.62310
## colorH
                  -807.0
                              264.1
                                     -3.055
                                            0.00237 **
## colorI
                  -954.8
                              289.9
                                    -3.294 0.00106 **
## colorJ
                 -1508.5
                              353.4 -4.269 2.36e-05 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 1453 on 488 degrees of freedom
## Multiple R-squared: 0.8406, Adjusted R-squared: 0.837
## F-statistic:
                  234 on 11 and 488 DF, p-value: < 2.2e-16
```

Backwards stepwise elimination yields a final model includes only the variables cut, carat, and color.

This model appears to be slightly better than our original diamonds_model because the Adjusted R-squared value is slightly higher, with a value of 0.837 rather than 0.8367. This is a minor improvement, but an improvement nonetheless.

We will now confirm this adjusted model with forward stepwise elimination to see if we get the same result.

```
#forward stepwise
diamonds_stepF <- stepAIC(diamonds_model, direction="forward", k = 2, trace = 0)
summary(diamonds_stepF)
##
## Call:
## lm(formula = price ~ depth + cut + carat + color + table, data = sample_diamonds)
##
## Residuals:
##
                  1Q
                       Median
                                     3Q
        Min
                                             Max
##
  -10582.0
              -654.7
                        -50.7
                                  457.3
                                          9114.2
##
## Coefficients:
                Estimate Std. Error t value Pr(>|t|)
##
                            4758.01
                                     -0.611 0.541683
## (Intercept)
                -2905.72
                  -28.85
                                     -0.547 0.584896
## depth
                              52.78
## cutGood
                  920.52
                             442.43
                                      2.081 0.037993 *
## cutVery Good 1549.96
                             426.94
                                      3.630 0.000313 ***
## cutPremium
                             431.90
                 1229.85
                                      2.848 0.004593 **
## cutIdeal
                 1620.29
                             440.68
                                      3.677 0.000263 ***
## carat
                 7557.20
                             153.80 49.136
                                             < 2e-16 ***
## colorE
                  -87.95
                             259.33
                                     -0.339 0.734635
## colorF
                 -196.31
                             262.70
                                     -0.747 0.455257
## colorG
                 -104.83
                             243.15
                                     -0.431 0.666571
## colorH
                 -796.27
                              264.72
                                     -3.008 0.002767 **
                             290.32 -3.261 0.001189 **
## colorI
                 -946.71
## colorJ
                -1497.65
                             353.88 -4.232 2.77e-05 ***
## table
                   25.47
                              38.96
                                     0.654 0.513534
## ---
```

```
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1454 on 486 degrees of freedom
## Multiple R-squared: 0.841, Adjusted R-squared: 0.8367
## F-statistic: 197.7 on 13 and 486 DF, p-value: < 2.2e-16</pre>
```

This yields a different result than backwards stepwise elimination. We will now perform bidirectional stepwise elimination.

```
#bidirectional stepwise
diamonds_step <- stepAIC(diamonds_model, direction="both", k = 2, trace = 0)
summary(diamonds_step)
##
## Call:
## lm(formula = price ~ cut + carat + color, data = sample_diamonds)
## Residuals:
        Min
                  1Q
                       Median
                                    3Q
                                            Max
##
  -10706.3
              -677.3
                        -68.6
                                 467.0
                                         9056.6
##
## Coefficients:
                Estimate Std. Error t value Pr(>|t|)
##
## (Intercept)
                 -3251.7
                              429.8
                                    -7.566 1.94e-13 ***
## cutGood
                   981.9
                              427.2
                                      2.299 0.02194 *
## cutVery Good
                  1593.9
                              401.5
                                      3.970 8.27e-05 ***
## cutPremium
                  1301.4
                              402.2
                                      3.235 0.00130 **
## cutIdeal
                  1611.6
                              395.6
                                      4.074 5.40e-05 ***
                  7568.4
                              152.8 49.521
                                             < 2e-16 ***
## carat
## colorE
                  -103.9
                              258.7
                                     -0.402
                                             0.68805
## colorF
                  -199.4
                              262.3
                                     -0.760
                                             0.44766
## colorG
                  -119.3
                              242.6
                                    -0.492
                                             0.62310
                  -807.0
                                     -3.055
## colorH
                              264.1
                                             0.00237 **
## colorI
                  -954.8
                              289.9
                                     -3.294 0.00106 **
## colorJ
                 -1508.5
                              353.4 -4.269 2.36e-05 ***
## ---
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
## Residual standard error: 1453 on 488 degrees of freedom
## Multiple R-squared: 0.8406, Adjusted R-squared: 0.837
## F-statistic:
                  234 on 11 and 488 DF, p-value: < 2.2e-16
```

Performing bidirectional stepwise elimination returns the same result as backwards stepwise elimination. This suggests that a better model includes only predictors cut, carat, and color. Forward stepwise elimination returns the best model to include only predictors cut, carat, color, and table.

The inclusion of the table predictor in this model could be due to forward stepwise's inability to remove predictors after adding them. If when table was added to the model, it improved the fit then after other predictors are added it weakened the fit, it cannot remove table.

Backward and bidirectional stepwise elimination are more computationally taxing then forward stepwise elimination, but they generally return better results.

Cross Validation

We can check if our new model results in less Mean Squared Error using Cross Validation.

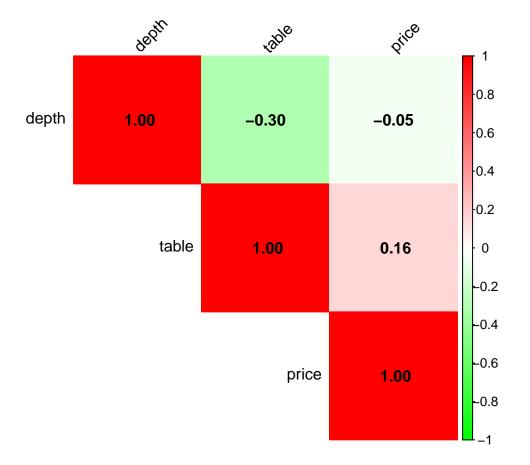
We will do so by creating a CV function, then applying it to our two models to check each models MSE.

```
#CV function
kFoldCV <- function(data, response, formula, k, seed = FALSE, seed num, shuffle = FALSE) {
  if (seed == TRUE) {
    set.seed(seed num)
  if(shuffle == TRUE) {
    shuffle index = sample(1:nrow(data), replace = FALSE)
    data = data[shuffle_index,]
    response = response[shuffle_index]
  folds <- cut(seq(1,nrow(data)),breaks=k,labels=FALSE)</pre>
  mse = numeric()
  for(i in 1:k){
    testIndexes <- which(folds == i, arr.ind=TRUE)</pre>
    testData <- data[testIndexes, ]</pre>
    trainData <- data[-testIndexes, ]</pre>
    diamonds_model.train = lm(formula, data = trainData)
    mse[i] = (1/length(testIndexes))*sum((response[testIndexes]
                                           - predict(diamonds_model.train, newdata = testData))^2)
  }
 rmse = sqrt(mse)
  cv_k_mse = sum(mse)/k
  cv k rmse = sum(rmse)/k
  return(list(CV_MSE = cv_k_mse, CV_RMSE = cv_k_rmse))
}
#CV on original model
kFoldCV(response = diamonds$price, formula =price ~ depth + cut + carat + color + table,
        data = diamonds, k = 10, shuffle = TRUE, seed = TRUE, seed_num = 1)
## $CV_MSE
## [1] 2045164
##
## $CV_RMSE
## [1] 1429.692
#CV on new model
kFoldCV(response = diamonds$price, formula = price ~ cut + carat + color, data = diamonds,
        k = 10, shuffle = TRUE, seed = TRUE, seed_num = 1)
## $CV_MSE
## [1] 2051609
##
## $CV_RMSE
## [1] 1431.963
```

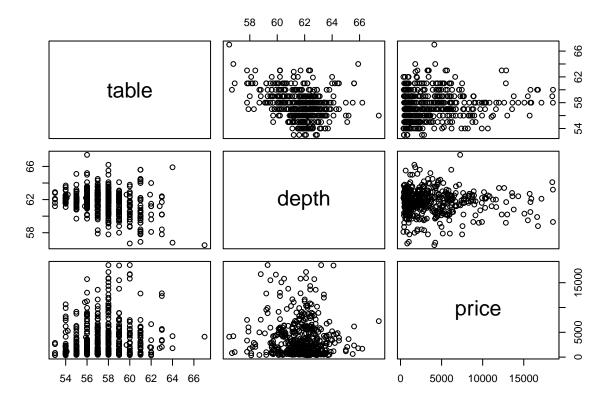
Cross validation is giving us an interesting result. We can see that MSE for our simplified model is higher than the MSE for our original model.

The results of cross validation pose need for a look into the correlation between depth and price and table and price.

For this we can use a corr plot.



```
#pairs plot
pairs(sample_diamonds[, c('table', 'depth', 'price')])
```



It appears that neither table, depth, or price are significantly correlated. It seems strange that MSE increases when they are removed from the model.

It is possible the seed used is giving an unlucky result. Since the MSE increase is strange, let's explore other seeds.

```
kFoldCV(response = diamonds$price, formula =price ~ depth + cut + carat + color + table,
        data = diamonds, k = 10, shuffle = TRUE, seed = TRUE, seed_num = 713)
## $CV_MSE
## [1] 2045273
## $CV_RMSE
## [1] 1429.948
kFoldCV(response = diamonds$price, formula =price ~ cut + carat + color,
        data = diamonds, k = 10, shuffle = TRUE, seed = TRUE, seed_num = 713)
## $CV_MSE
## [1] 2051743
##
## $CV_RMSE
## [1] 1432.203
kFoldCV(response = diamonds$price, formula =price ~ depth + cut + carat + color + table,
        data = diamonds, k = 10, shuffle = TRUE, seed = TRUE, seed_num = 123)
## $CV_MSE
## [1] 2045532
##
## $CV RMSE
## [1] 1429.976
kFoldCV(response = diamonds$price, formula =price ~ cut + carat + color,
        data = diamonds, k = 10, shuffle = TRUE, seed = TRUE, seed_num = 123)
## $CV_MSE
## [1] 2051922
## $CV_RMSE
## [1] 1432.201
kFoldCV(response = diamonds$price, formula =price ~ depth + cut + carat + color + table,
        data = diamonds, k = 10, shuffle = TRUE, seed = TRUE, seed_num = 600493)
## $CV_MSE
## [1] 2045483
## $CV_RMSE
## [1] 1429.728
kFoldCV(response = diamonds$price, formula =price ~ cut + carat + color,
        data = diamonds, k = 10, shuffle = TRUE, seed = TRUE, seed_num = 600493)
## $CV_MSE
## [1] 2051736
##
## $CV_RMSE
## [1] 1431.936
```

Conclusion

After trying multiple seeds, the result is showing the same. This suggests that increase in MSE with the reduced model is likely not resulting from an unlucky seed number. The adjusted R^2 value only increases by a very marginal amount (0.0003) when removing the predictor table from the model suggesting the reduced model does not substantially improve variance explanation. Additionally, the reduced model has a greater MSE than our original model suggesting the reduced model sacrifices prediction accuracy and the does not generalize to new data as well as the original model. Therefore, we conclude that the original model (with predictors cut, carat, color, and table) performs better than the reduced model.

We could further our model selection using alternative strategies such as LASSO Regression and Cross-Validation-Based Feature Selection (i.e. Recursive Feature Elimination). LASSO Regression would reduce our risk of overfitting through regularization and automatically performs feature selection to find the best model, although it is more computationally expensive than Stepwise Elimination. Cross-Validation-Based Feature Selection would select the best model based on the test error of the model, however, it is computationally expensive which would not be optimal for data this size. Both of these model selection strategies would provide more consistent results than the Stepwise Elimination we used previously.

It would be worth considering the results of LASSO Regression and comparing them to the results of the Stepwise Elimination performed on our Linear Regression Model.