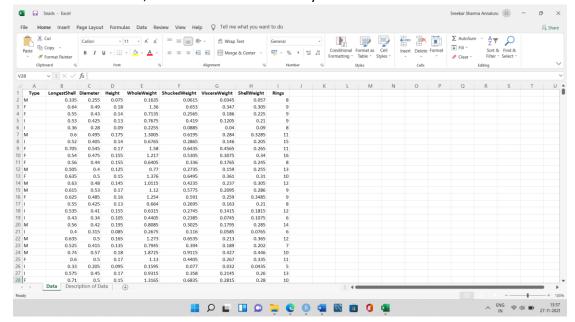
# Home Work Assignment-5

Note: First 17 pages of this assignment are detailed analysis of the work I have done. The labelled answers to the questions (in the assignment) will start from page 18. Also, I am attaching the models to the headings of corresponding regression technique. Though I have answered everything in these 17 pages, I want to be clear. Hence, I answered them separately, with labels. Please note this!!!

❖ Before going into the actual assignment (predicting the age of snails), have a look at the Snails.xlsx data, and summarize the key features or trends in the data set.



All the units are in MMGS system. It looks like most of the data is less than 1, except for the Rings. The description is given in the next page, which is not that important for prediction (for interpreting-yes).

Target: Predicting the Age (Rings) of Snails.

Applied Techniques: Linear Regression, Random Forest Regression, and KNN Regression.

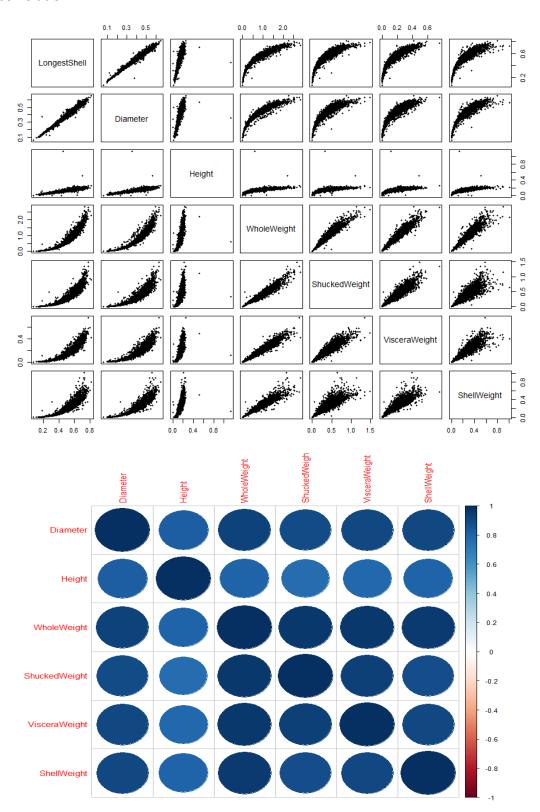
Supporting Methods/Tools: 10-Fold Cross Validation, Standardization of Parameters (For KNN), Validation Set, Subset Selection, and many built-in libraries! (I will explain everything in detail).

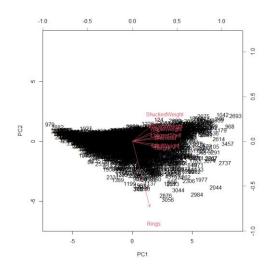
# "Predicting the Age of Snails using Regression"

❖ After importing the Snails data set from my system into R. There are no "NA" values in the data set. Using the methods view (Snails), and summary (Snails), we can see the data in R. The key takeaway from these two methods is that Whole Weight is a linear function of other weight predictors (Shell, Shucked, and Viscera) with unknown

- mass of water/blood. Also, I have observed that the minimum value for predictor "Height" is 0. Practically, this is not possible I will investigate into it!
- Now let's see how the predictors are related using scatter plot using pairs (Snails).

  I have used the correlation plot as well corrplot(), from corrrplot library. I have performed Principal Component Analysis on the same just to cross check the correlation.





- 1. The most important point is the data is hugely correlated! For instance, Diameter and Whole Weight is 92% correlated! Fun Fact: The least correlated pair is (Shucked Weight, Height). Even these two are 76.5% correlated! This is excluding rings.
  - Note: I have included rings in a separate scatter plot (it will be in my R file), according to that with rings all the predictors are 50-60% correlated!
- 2. As I have mentioned earlier, the Whole Weight seems to be highly correlated with the other weight predictors.
- 3. Principal Component Analysis is validating the first statement. You can see all the predictors are pretty close on both the principal components. Shucked Weight is slightly away from the rest.
- 4. Most of the Rings are between 5 and 15.
- Investigating the Zero Height case. There are two points with Height = 0. Have a look at those 2 points.

```
Investigating Height =0
> Snails[Snails$Height :
            Longestshell Diameter Height WholeWeight
0.430 0.34 0 0.428
                                                                 shuckedweight visceraweight shellweight Rings
1597
                                                                          0.2065
                                                                                            0.0860
                                                                                                            0.1150
                     0.315
                                  0.23
                                                         0.134
                                                                          0.0575
                                                                                            0.0285
                                                                                                           0.3505
> summary(snails)
 Type
Length: 3500
                          LongestShell
                                                                        Height
:0.0000
                                                                                           who leweight
                                                                                                               ShuckedWeight
                         Min.
                                                      :0.0550
                                  :0.075
                                              Min.
                                                                    Min.
                                                                                         Min.
                                                                                                  :0.0020
                                                                                                               Min.
                                                                                                                        :0.0010
                         1st Qu.:0.450
Median :0.545
 class :character
                                              1st Qu.: 0.3500
                                                                        Qu.:0.1150
                                                                                              Qu.: 0.4404
                                                                                                                   Qu.:0.1850
        :character
                                             Median :0.4250
Mean :0.4078
                                                                   Median :0.1400
Mean :0.1396
 Mode
                                                                                         Median :0.7985
                                                                                                              Median :0.3355
                         Mean :0.524
3rd Qu.:0.615
                                                                                                  :0.8292
                                                                   Mean
                                                                                         Mean
                                                                                                              Mean
                                              3rd Qu.: 0,4800
                                                                   3rd Qu.:0.1650
                                                                                         3rd Qu.:1.1566
                                                                                                              3rd ou.: 0.5015
                         Max
                                   :0.815
                                                       :0.6500
                                              Max.
                                                                   Max.
                                             Min. : 1.

Min. : 1.

1st Qu.: 8.000

Median : 9.000

Median : 9.949
 visceraweight
                         shellweight
 Min. :0.00050
1st Qu.:0.09287
                        Min. :0.0015
1st Qu.:0.1300
 Median :0.17125
                        Median :0.2328
                        Mean
                                 :0.2393
 3rd ou.: 0.25362
                        3rd Qu.: 0.3300
                        Max.
```

The other values seem valid. Also, for the predictor Whole Weight, we see that these values are really small compared to rest of observation and they are below first quantile (Q1). This tells us that this **might not be a data error** and we cannot exclude it from the dataset.

Checking for the Linearity with respect to Whole Weight. By intuition the Whole Weight has to be the summation of the remaining weight, or in worst case less than

the sum of weights (because of losses). However, it cannot be greater than the Whole Weight. In our date we have 127 observations are violating this rule. Let's have a look.

```
# Investigating Height =0
Snails[Snails$Height == 0,]
# Including Weight Difference
Snails.wDiff < 0,snails$WholeWeight - (Snails$ShuckedWeight + Snails$VisceraWeight + Snails$ShellWeight)
dim(Snails[Snails.wDiff < 0,])
dim(Snails[Snails.wDiff == 0,])
Snails[Snails.wDiff < 0,]</pre>
   27:1 (Top Level) $
 Console Terminal ×
                                                Jobs ×
 R 4.1.0 · C:/Users/sharm/OneDrive/Desktop/Sharma/Industrial Engineering/ISEN 613/
arls[Snails.wDiff < 0,]

Type LongestShell Diameter Height Wholeweight
F 0.560 0.440 0.155 0.6405 0.3360 0.1765 0.2450 8
I 0.480 0.390 0.145 0.5825 0.2315 0.1210 0.2550 15
M 0.260 0.200 0.065 0.9860 0.0440 0.0270 0.0300 6
I 0.270 0.195 0.080 0.0730 0.0285 0.0235 0.0300 5
F 0.580 0.460 0.175 1.1650 0.6500 0.2205 0.3055 9
I 0.215 0.155 0.060 0.0525 0.0210 0.0165 0.0150 5
M 0.540 0.420 0.190 0.6855 0.2930 0.1630 0.3800 10
I 0.380 0.390 0.090 0.2770 0.1655 0.0625 0.0820 6
142
154
156
161
                                                                                                                                                                                                    0.1630
0.0625
0.3060
0.1600
                                                                                                                                                                                                                                                                13
 188
                                                                                                                                                                                                                                     0.0820
0.4355
0.1750
0.1400
0.3240
0.1100
0.2130
                                                                                          0.205
0.110
0.120
0.165
                                                                                                                                                               0.6900
0.3050
0.2220
 202
212
                                               0.650
                                                                                                                         1.4275
0.6250
                                               0.505
                                                                       0.405
                                                                                                                                                                                                   0.1600
0.1190
0.4365
0.0775
0.1545
0.0055
0.0390
 213
227
                                               0.465
                                              0.465
0.620
0.455
0.540
0.180
0.280
                                                                                                                        0.4/10
1.0125
0.3720
0.6860
0.0230
0.1270
                                                                       0.480
                                                                       0.330
0.425
0.125
0.205
```

There are only 4 observations with Whole Weight = Sum (Viscera Weight + Shell Weight + Shucked Weight). Those 127 observations seem to be counterintuitive they might be error while loading

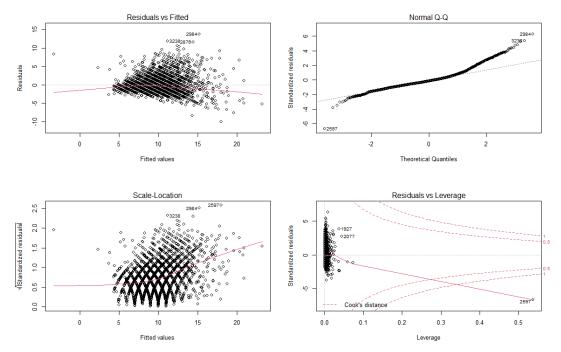
Note that these 127 observations have a combined weight greater than Whole Weight. When we look at 10 such observations, it seems that the other values are correct and there is no similarity and hence we are sure this might be a **data entry error**.

Conclusion: The main reason behind doing this is to check the status of the data. It looks like there are some errors. Somewhat similar to "Exploratory Data Analysis", not entirely though. We can do something about this but for this assignment it is not required. As the data is highly correlated this data entry error is not a huge worry.

Check the attached R-file for more details.

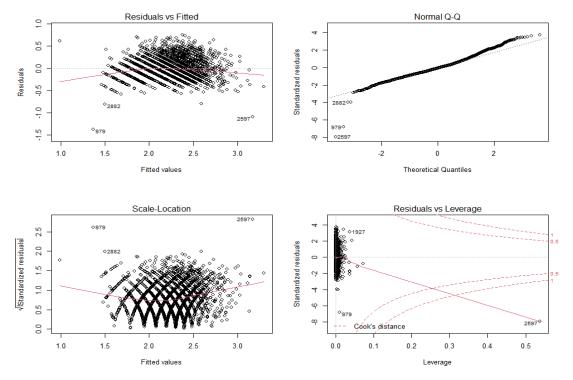
## "Linear Regression Model"

- ❖ Before going to the Linear Regression, I would like to comment on Ridge Regression and Lasso, and the reason why I didn't choose them. I have performed both those techniques in my R file. I got a test R-squared of around 54% (with best lambda using 10-fold cross validation), which is less than my FinalModel\_LR, which I have submitted as my final model. You can refer to the R code for more details.
- ❖ First things first, I have built a simple multiple regression using all the predictors, without any interactions and transformations. Have a look at the plot.



As you can see the there are "Non-Constant Variance Terms". Hence, I have applied logarithm to the Rings (to remove **Heteroscedasticity**) and there is a huge improvement. Also, the data is hugely deviated from the Normal. High Leverage Points and Outliers are not a huge problem of concern for this data, as they are only a couple.

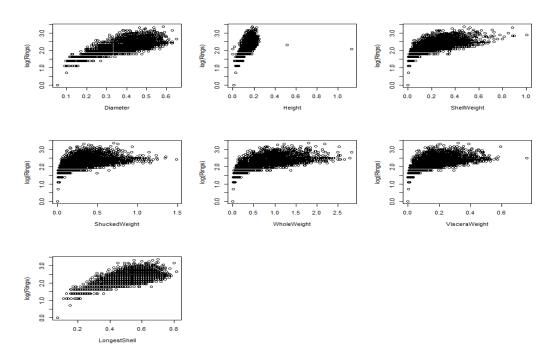
After removing heteroscedasticity, the training R-Squared has increased to 0.6 from 0.54. Updated model plot {This is the only instance where I have used training-Squared}. Everywhere else I have used test R-Squared. That's because I didn't split the data yet!



Now the residuals look a lot better. Also, you can see the deviation from normality in Q-Q plot has improved. Hence applying logarithm to Rings is very useful, in fact mandatory.

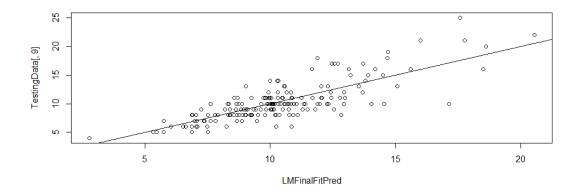
Note that the relation is slightly non-linear which I will address as I go ahead!!

Now let's split the data into Training and Testing. I have gone with 95:5 split. "I will explain my logic behind this in a few minutes". Before going to the Test R-Squared. Let's see how the plots of predictors vs Rings look like. This will give the reason behind my split.

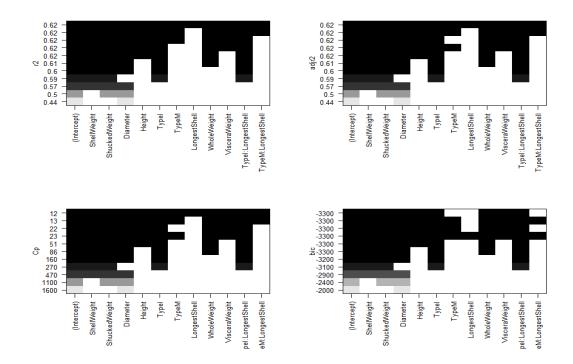


The predictors are almost linearly related to log (Rings). As soon as I see this plot, I am very confidant that Linear Model will perform well on this data. Hence, I have given very few test data (5%). One important point to note is that predictors like, Whole Weight, Viscera Weight, Shucked Weight, Shell Weight, and Diameter are slightly non-linear. I have performed 10-fold Cross Validation and solved that problem. By transforming the predictors my Linear Regression test R-Squared is 64% (Don't forget seed 1.

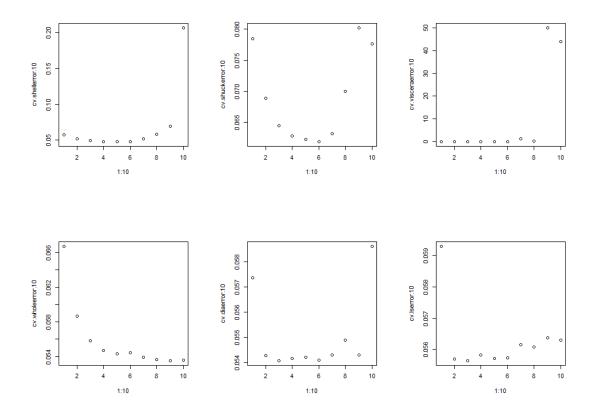
Here is the plot of fitted values vs actual values.



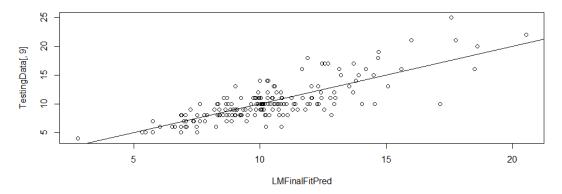
Now I have performed best subset selection to choose the best subsets. I have used the argument nymax as 15. If you observe the plot the values of Adjusted R2, Cp, and BIC have reached a **saturation limit after 8 variables**. In fact, the minimum value of BIC is exactly at 8. The minimum values of Adjusted R2 and Cp are 11. The key point is "**Minimum number of predictors in the model should be at least 8!**" If we are interested in interpretability, we can stick to 8/9. But we are worried about predictability hence we can go as far as we can, provided it should increase test R-Squared.



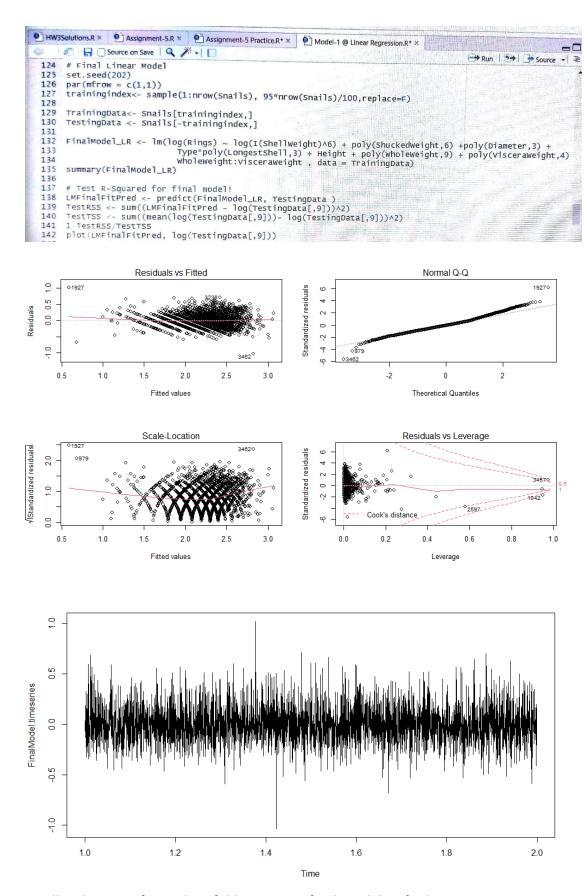
Now I have performed cross validation on the predictors. As we have seen some of them are slightly non-linear. Before going to that, I would like to explain why I have gone with 10-fold CV. The one-word answer is "Bias-Variance Tradeoff". LOOCV gives the least bias, however, but it tends to have higher variance compared to k-fold CV. The reason is LOOCV makes the output highly correlated hence it has higher variance. Remember that out date is already correlated. Keeping this point in mind I didn't perform LOOCV. Why 10 over 5? Well, there is no strong answer. We can go with 5 as well but I have read, in ISLR textbook, that 10 is more preferred as it gives results close to the true test results. There are a lot of 10-fold CV's in text book but very few 5-fold. Let's have a look at the plots. The minimum values of test errors for the predictors are: {Shell Weight - 6, Shucked Weight - 6, Viscera Weight - 4, Whole Weight - 9, Longest Shell - 3, and Diameter- 3}. As we are not worried about interpretability, I have transformed all these predictors. There is a good improvement in test R-Squared, which is very crucial for predictability.



After all these techniques I got a **training Adjusted R-Squared of 0.6637**. Corresponding **testing R-Squared is 0.64**, which is a good improvement from previous model. As you can see, we cannot improve the R-Squared, irrespective of the number of parameters, recollect the BIC and Adj R2 graphs. They have saturated after a certain limit. Finally, lets have a look at the plot between Final Fitted Values and Testing data.



You can see the relation is "Linear". It is very clear. Hence this is my first model. The pic of the model is:



Finally, I have performed 10-fold CV on my final model to find out test error. I got an error of **0.0369** for this model.

```
Null deviance: 360.48 on 3499 degrees of freedom
Residual deviance: 121.40 on 3463 degrees of freedom
AIC: -1756.5

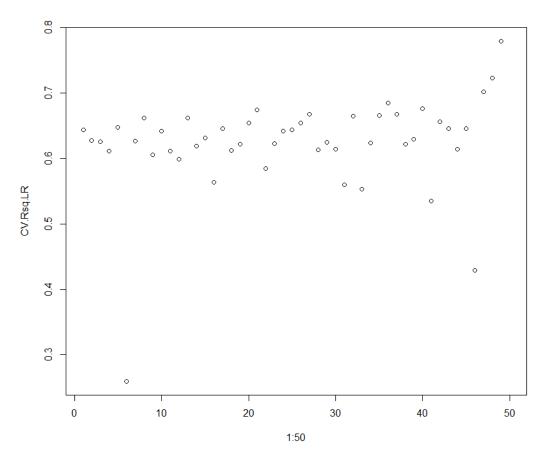
Number of Fisher Scoring iterations: 2

> library(boot)
> set.seed(1)
> cv.error.10 <- cv.glm(Snails, glm.fit, K=10)$delta[1]
> cv.error.10
[1] 0.03699901
```

#### alm.fit is FinalModel LR.

I have performed all the techniques and arrived at this model! I am very confidant that this will perform better on any un seen data! The final model is satisfying all the four primary assumptions of a Linear Model. **Linear Relationship, Homoscedasticity, Independence, Normality**. I am sure "Linear Regression outperform all the techniques" for this dataset.

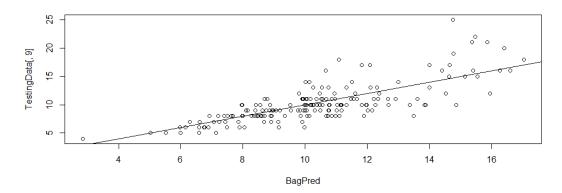
**Fun Fact**: I have done a lot of iterations on splitting the data and plotted how train R-Squared varies with respect to splitting ratio, starting from 50:50. Have a look at the plot. Iterating part of the code is Column = {(50+i)\*nrow/100, for i in 1:50}.



This may not be the technical cross validation but somewhat similar to it. As you can see the trend has a very minute positive slope. After plotting this I have finalized my splitting ratio- 95:5.

## "Random Forest Regression"

- ❖ I have chosen Random Forest as my second model. We know that decision trees do not have same level of prediction accuracy compared to other regression techniques. Hence, we should aggregate many decision trees to improve the prediction capacity. Note: In my R file I have performed all the three ensemble methods (Bagging, Random Forest, and Boosting). RF is performing slightly better than Bagging. Hence, it is my third model. This seems quite logical. We know that Bagging predicts outputs which are highly correlated. Adding to that, our date is highly correlated. As a result, it might not perform well on new un seen data. On the other hand, Random Forest decorrelates the data. Because of this it will tend to perform better on a new unseen data set! Again "Bias-Variance Tradeoff". Coming to Boosting, it might be over fitting the data, which is already correlated, hence, it is performing slightly worse compared to Bagging and Random Forest.
- ❖ I have installed package "randomForest". I have split the data in the ratio of 95:5. Then I have performed Bagging, Random Forest and Boosting respectively. I have set a seed of 1. I have performed Bagging, using mtry = 8 all predictors. The plot of the Bagging fit is shown below.



As you can see the predictions are very accurate. Let's have a look at the code used.

```
# Performing Bagging.
install.packages("randomForest")
library(randomForest)

trainingindex-- sample(1:nrow(Snails), 95*nrow(Snails)/100,replace=F)

Trainingbata<- snails[trainingindex,]

Testingbata <- snails[-trainingindex,]

bag.Snails <- randomForest(log(Rings) - Shellweight + Shuckedweight + Diameter +

Type + LongestShell + Height + Wholeweight+visceraweight ,

data = Snails, mtry = 8, importance = TRUE, subset = trainingindex )

BagPred <- exp(predict(bag.Snails, newdata = Snails[-trainingindex,]))

TestRSS <- sum((BagPred - Testingbata[,9])^2)

TestRSS <- sum((mean(Testingbata[,9])^2)

TestRSS/TestTSS

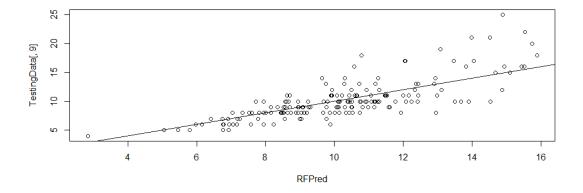
# 59.7% variability explained!!!

I
```

I am not worried about Training R-Squared! In the entire assignment I never mentioned that parameter. All the percentages are corresponding to testing data, as our target is to predict.

Now Let's see random forest results!

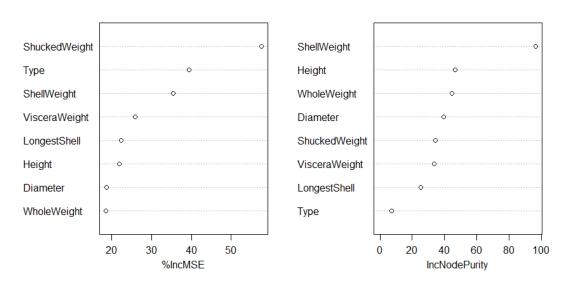
For this I have used mtry = 2. I want to decorrelate the model as much as possible. Hence, I have picked 2 as my mtry argument.



You can see the plots are almost similar, so do the testing R-Squared. As RF is performing better and it tends to decorrelates the output, I feel it will outperform Bagging on the new unseen data. Hence, Random Forest is my second model.

Let's look at the importance of variables. The lefthand side is corresponds to the MSE, and the righthand side is corresponds to the Node Purity, that means how confidant you can be predicting using that predictor.

rf Snails

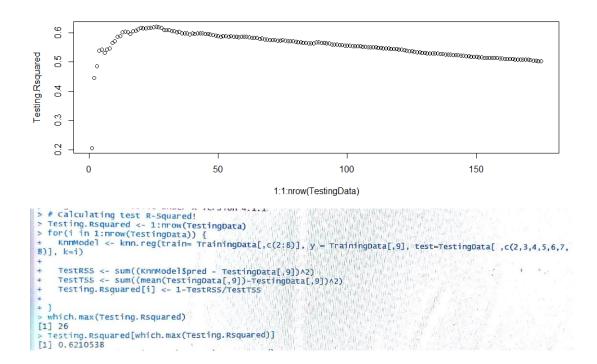


I am not summarizing boosting, BART here. It is in my R code for the second model. The results are worse than Bagging and Random Forest. Hence, I just dropped those!

# "KNN Regression"

- The third model I have chosen is K Nearest Neighbours Regression. Before diving into the detailed analysis from scratch I would like to comment on "Curse of Dimensionality". As we all know KNN Regression suffers from the curse of dimensionality. But we have to keep in mind that this curse of dimensionality is more profound if the sample size is too small compared to the predictors (higher dimension). In our case, the model is higher dimensional (p=7), however, the sample size (n) = 3500, this implies the curse is not that profound in this case. Also, we know that if n is large KNN performs better and it is very useful for predicting, which is exactly what we want.
- ❖ 1)- Let's perform the KNN Regression, without Type predictor. I didn't worry about training r-squared as I got K = 1 and R-Squared =1. Hence, I have directly calculated

test R-Squared and found the corresponding value of K. Let's have a look at the picture. I have set a seed of 1.



As you can see with K=26, I got the maximum testing R-Squared, which is 62.1%.

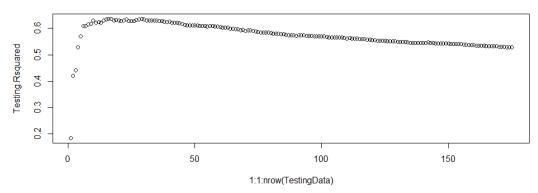
Now I have performed the KNN again with the same seed but by including the numeric version of Type variable, using strtoi(). Have a look at the plot and result.

The testing R-Squared is 61.5%, the prediction accuracy has decreased. Hence, I would like to stick to the previous model as my third model. This might be wrong but I just tried converting the Type predictor into a numeric.

❖ What is the probability that KNN might give more weightage to bigger points, despite the fact that all are in MMGS system. Though normalizing is not required I have done it to see what might change. Indeed, there is a change, the testing R-Squared went down to 52% from 61%. Note that, I have converted the predictor "Type" into numeric

before performing KNN. I have performed KNN without using "TYPE" and the model has performed better.

❖ I have standardized the predictors and performed the KNN regression again with same seed. Let's have a look at the results. You can see the inverted U shape.



KNN is explaining 63% variability. However, Linear Regression should perform better as the true relationship is almost linear and number of predictors are more, higher dimensionality.

**Conclusion**: I have executed all methods and techniques that have been discussed in the class and finalized the above three models. For more information please do check the corresponding R file. I have used the Testing R-Squared as the metric to compare all the techniques. Also, I used 95:5 splitting ratio to all the models.

After performing all the techniques, Linear Regression seems to outperform all the methods for this Snails dataset. Hence, I am suggesting that as my final model. I have attached all my codes to the titles and in the question 4.

Linear Regression	Random Forest	KNN Regression
Performed better than techniques like Ridge and Lasso and Ridge	Performed better than Bagging and Boosting	Easy to compute and used for predicting
Applied log to the Rings to remove Heteroscedasticity.	Used m value of 2	Performed with and without standardizing
10-Fold CV has been used on all the predictors	No transformations & validations performed on the predictors	No transformation has been performed on predictors/rings
Seed = 1	Seed = 1	Seed = 1
Training R-Squared = 66%	Training R-Squared = 64.5%	Training R-Squared = 100%
Testing R-Squared = 64%	Testing R-Squared = 59%	Testing R-Squared = 62%
Validation Set Approach with 95:5 ratio.	Validation Set Approach with 95:5 ratio	Validation Set Approach with 95:5 ratio
Cross Validation Error of 0.0369 on the final model.	No Cross Validation required	Cross Validation not performed.
Best Regression for this dataset.	Almost a tie up with Linear Regression. Second best.	Not good compared to LR, and RF. But can be used
True relation is almost linear.	Decorrelating the Output. Hence performing better.	A trustworthy regression for prediction.

# "Assignment 5 Answers"

1. The single model which I would be suggesting is Linear Model. My final model is:

```
Final Model\_LR <- Im(log(Rings) \sim log(I(Shell Weight)^6) + poly(Shucked Weight,6) + poly(Diameter,3) + Type*poly(Longest Shell,3) + Height + poly(Whole Weight,9) + poly(Viscera Weight, 4) + Whole Weight: Viscera Weight, data = Training Data)
```

I have selected this model because the true relation is almost linear. As you can see in my analysis, the graph of FinalModel\_LR has a very clear linear trend. Adding to that, I got a very good Testing R-Squared (around 64%). Finally, the final fit model has solved all the deviations of the initial model (Heteroscedasticity, Independence, Normality, and Linearity). I believe in all the methods I have done. Hence, I recommend this transformed "Linear Model" will yield accurate results, even on the un seen testing data.

- 2. First things first, as prediction is our primary goal, I was not at all worried about the complexity of predictors. I have started with a simple multiple regression with all the predictors. That model is clearly having Heteroscedasticity, and hugely deviating from Normality, also, the residuals are not Linear. Hence, I have addressed these points. My second model solves the first 2 points. Now for solving the Linearity I have performed 10-fold Cross Validation on each predictor to minimize test error. Before that, I have performed best subset selection and found out the number of minimum predictors required to yield accurate results. Had our target been interpreting, I would have dig deep into it and make the more interpretable. Going back to CV, after performing 10-fold Cross Validation, I got this complicated model. It looks complicated but very accurate. I suggest this model for testing on the un seen data!
- 3. **Linear Regression**: The testing R-Squared for this model is 64%. It explains about 64% variability on the test data. The relation between predicted values and test values is close to linear. The logarithm transformation has been applied to remove heteroscedasticity. The polynomial function has been used to remove the non-linearity of residuals. Time Series plot has been used to check independence.

**Random Forest**: The testing R-Squared for this model is 59%. I have used 2 variables (m = 2) for Random Forest Regression. In total 500 trees were created. As our target is prediction, I neglected it. Had it been interpretability, I would have reduced the number of trees. According to RF, the important predictors are Shucked Weight, Type

and Shell Weight. Predictors with higher node purity are Shell Weight, Whole Weight, Diameter, and Height.

**KNN Regression**: Firstly, I have performed KNN without standardizing the data. I got maximum testing R-Squared as 62.1% at K = 26. The testing R-Squared is not a perfectly inverted 'U' – inverted hockey stick (NIKE logo), nevertheless it is an inverted U! Then I thought what is the probability that KNN is giving more weightage to the points which are higher. Adding to that, we are dealing with higher dimensions. Hence, I have decided to standardize the data and re-iterated the whole process. Now, the maximum testing R-Squared is 64% at K = 17. It is an inverted hockey stick shape.

4. Click the links to open the corresponding R files.

Model-1 (Suggested Model) – <u>Linear Regression</u>.

Model-2 – Random Forest Regression.

Model-3 – KNN Regression.

5. This is the R code containing my suggested model. Set your directly and run this code then you will get testing R-Squared as an output. <u>Testing.R</u>.