Statistical Learning Final Report

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Contents

1	Intr	roduction]
2	Dat 2.1	a Data Transformation	1
	2.2	Data Cleaning	2
	2.3	Rename Columns	
3	Cor	relation Analysis	9
4	Dat	a Visualization	4
	4.1	Histograms	4
	4.2	Pairplot	F
	4.3	Barplot	6
		4.3.1 Beverages Barplot	7
	4.4	Boxplot	
	4.5	Scatterplot	
5	Reg	gression Analysis	14
	5.1	Linear Regression	14
	5.2	Lasso Regression	17
	5.3	Ridge Regression	19
	5.4	Model Comparison	
	5.5	Model Evaluation	
	5.6	Cross Validation	21

1 Introduction

Here Eleonora you can write the introduction of the project describing the scope and the data used.

Thank you Albi, I will. What is our project scope though?

I think that we have to analyze the dataset and perform some statistical analysis on it. We can start by calculating the correlation matrix and then we can visualize the data through histograms, pairplots, barplots and boxplots. Finally, we can perform a regression analysis.

2 Data

The dataset we will analyze in this project is *Starbucks Beverage Components* from Kaggle, that you can find at the following link: https://www.kaggle.com/datasets/henryshan/starbucks.

This data provides a comprehensive guide to the nutritional content of the beverages available on the Starbucks menu. We have a total of 242 samples described by 18 variables. These attributes include the name of the beverage, its categorization and preparation method, the total caloric content and the constituents of the beverage.

In the upcoming code lines, we import the dataset and generate a summary visualization. This initial step allows us to gain a better understanding of the data structure and the variables involved.

```
data <- read.csv("Data/starbucks.csv", header = TRUE, sep = ",")</pre>
```

2.1 Data Transformation

Note that several variables in our dataset, namely "Vitamin.A....DV.", "Vitamin.C....DV.", "Calcium....DV." and "Iron....DV.", are represented as percentages. Consequently, the percentage symbol is included in our data. However, when conducting statistical analysis using R, the presence of non-numeric characters such as the percentage symbol can cause complications, interfering with the processing and analysis of the data. Therefore, we proceed to remove it.

Similarly, as R primarily operates on numeric and categorical data, we also convert all the other numerical variables into numeric format.

These preprocessing steps ensure a smooth and efficient analysis, making it easier to explore, visualize, and understand our data.

```
# Remove percentage sign from the data
data$Vitamin.C....DV. <- as.numeric(gsub("%", "", data$Vitamin.C....DV.))
data$Calcium....DV. <- as.numeric(gsub("%", "", data$Calcium....DV.))
data$Iron....DV. <- as.numeric(gsub("%", "", data$Iron....DV.))
data$Vitamin.A....DV. <- as.numeric(gsub("%", "", data$Vitamin.A....DV.))
# Set the other variables as numeric
data$Calories <- as.numeric(data$Calories)
data$Trans.Fat..g. <- as.numeric(data$Trans.Fat..g.)
data$Total.Fat..g. <- as.numeric(data$Total.Fat..g.)
data$Cholesterol..mg. <- as.numeric(data$Cholesterol..mg.)
data$Codium..mg. <- as.numeric(data$Sodium..mg.)
data$Total.Carbohydrates..g. <- as.numeric(data$Total.Carbohydrates..g.)
data$Sugars..g. <- as.numeric(data$Dietary.Fibre..g.)
data$Sugars..g. <- as.numeric(data$Sugars..g.)
data$Caffeine..mg. <- as.numeric(data$Caffeine..mg.)</pre>
```

2.2 Data Cleaning

Another challenge we have to face is the presence of missing data. Indeed, in "Caffeine..mg." column there are some NA values. This is a common issue in data analysis and needs to be addressed appropriately to ensure the validity of our statistical results.

One way to deal with these unwanted NA values is to omit the samples containing them from our study. This guarantees that our analysis is conducted solely on complete and dependable data. Alternatively, we can fill them in with the average or the median of the observed values for that specific attribute. This second method helps to preserve the overall data distribution while addressing the missing data points.

In our work, we opt for the latter approach, replacing NA values with the median. This choice is particularly suitable for our data, which is skewed and contains outliers. Indeed, the median, being a measure of central tendency that is not affected by extreme values, provides a more robust replacement in the presence of outliers.

```
# Summary of the Caffeine column summary(data$Caffeine..mg.)
```

```
##
      Min. 1st Qu. Median
                              Mean 3rd Qu.
                                                       NA's
                                               Max.
##
             50.00
                     75.00
                             89.52 142.50
      0.00
                                            410.00
                                                         23
# Replace NA values with the median
data cleaned <- data
data_cleaned$Caffeine..mg.[is.na(data_cleaned$Caffeine..mg.)] <- median(
  data_cleaned$Caffeine..mg., na.rm = TRUE)
# Summary of the Caffeine column after cleaning
summary(data_cleaned$Caffeine..mg.)
##
      Min. 1st Qu.
                    Median
                              Mean 3rd Qu.
                                               Max.
##
             70.00
                     75.00
                             88.14 130.00
                                            410.00
```

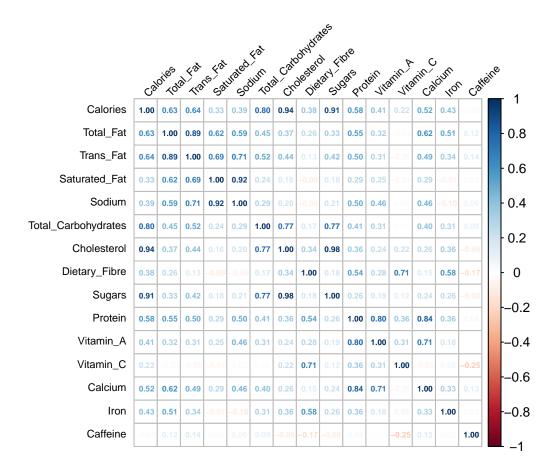
2.3 Rename Columns

Lastly, taking in consideration our cleaned data, we rename the columns by removing dots and units of measure, in order to obtain a more readable dataset.

3 Correlation Analysis

After completing these preliminary preprocessing steps, we calculate the correlation matrix for our dataset. This computation helps us in comprehending the interrelationships among the dataset's variables. In the correlation matrix, a value near to 1 at the ij position indicates a strong positive correlation between the i-th and j-th variables. Conversely, a value close to -1 signifies a strong negative correlation. A value near 0 suggests that the two variables do not significantly influence each other.

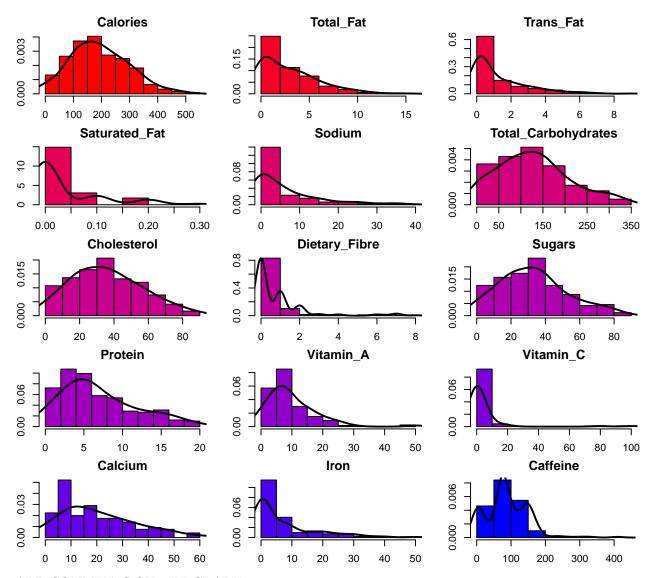
Observe that the first three columns of our data are categorical features, thus for these we cannot compute Pearson's correlation coefficient. In the following code lines we remove them to compute and plot such matrix.



4 Data Visualization

4.1 Histograms

We will plot some histograms to visualize the data.



ADD COMMENTS ON THE GRAPH

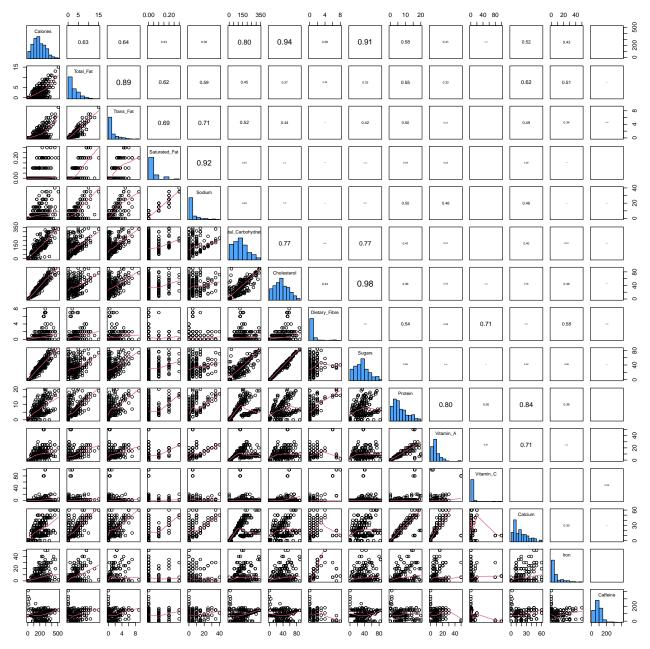
4.2 Pairplot

We will plot a pairplot to visualize the relationship between the variables. The pairplot is a grid of scatterplots that shows the relationship between each pair of variables in the dataset. This visualization helps us to identify patterns and correlations between the variables.

First of all we have to define the function for the pairplot. We will define a function for the histogram, the correlation and the smooth line.

Then we create the pairplot using the defined functions.

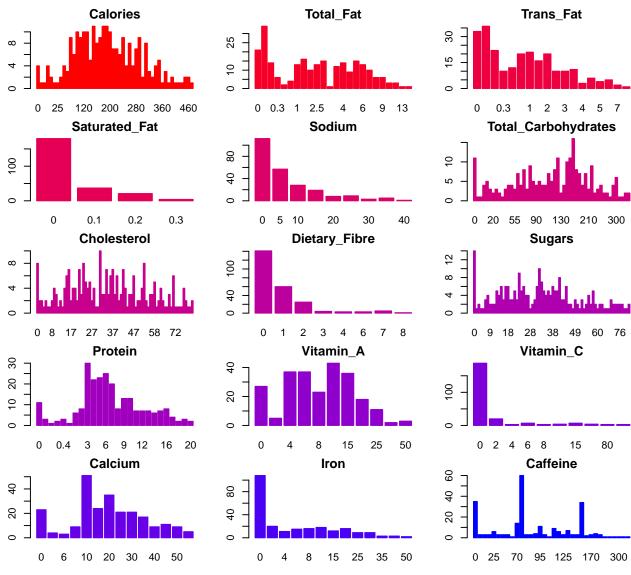
```
pairs(data_num,
    diag.panel = panel.hist,
    upper.panel = panel.cor,
    lower.panel = panel.smooth,
    colour = "#4ea5ff")
```



ADD COMMENTS ON THE GRAPH

4.3 Barplot

We will plot a barplot of the data. The barplot is a graphical representation of the data that displays the frequency of each category in a categorical variable. This visualization helps us to understand the distribution of the data and identify the most common categories in the dataset.

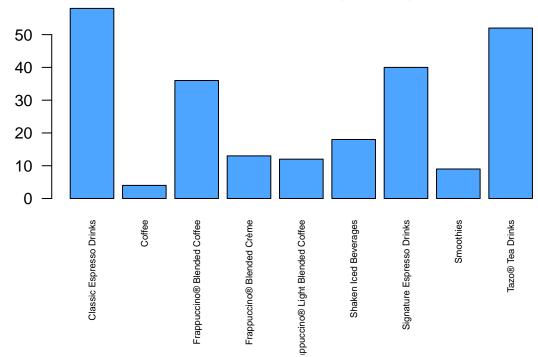


ADD COMMENTS ON THE GRAPH

4.3.1 Beverages Barplot

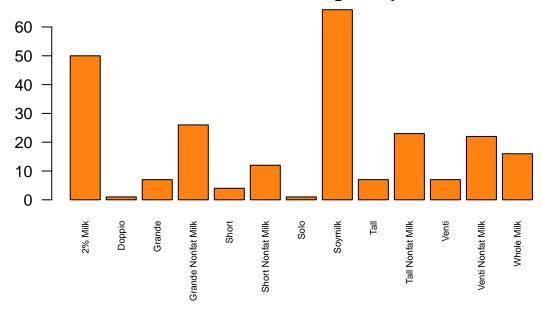
We create a barplot to visualize the distribution of the 'Beverage_category' variable and the 'Beverage_prep' variable in order to understand the most common beverages and preparation methods.

Distribution of Beverage Categories



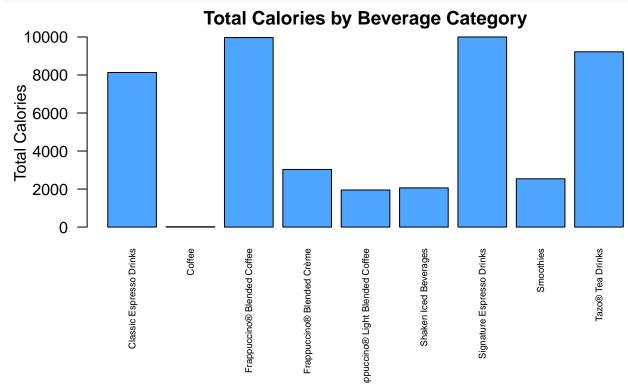
```
barplot(table(data$Beverage_prep),
    main = "Distribution of Beverage Preparation",
    ylab = "Count", col = "#ff810f", las = 2, cex.names = 0.6)
```

Distribution of Beverage Preparation



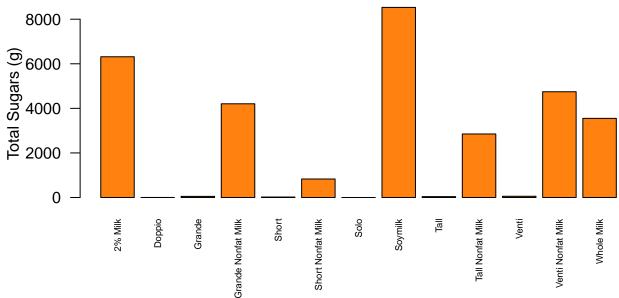
Now we want to compare the total calories for each categories of bevarage. First we aggreate the data to obtain the total calories for each categories of bevarage and then we create a barplot to visualize the results.

```
barplot(height = total_calories_by_category$Calories,
    names.arg = total_calories_by_category$Beverage_category,
    main = "Total Calories by Beverage Category",
    ylab = "Total Calories", col = "#4ea5ff", las = 2, cex.names = 0.6)
```



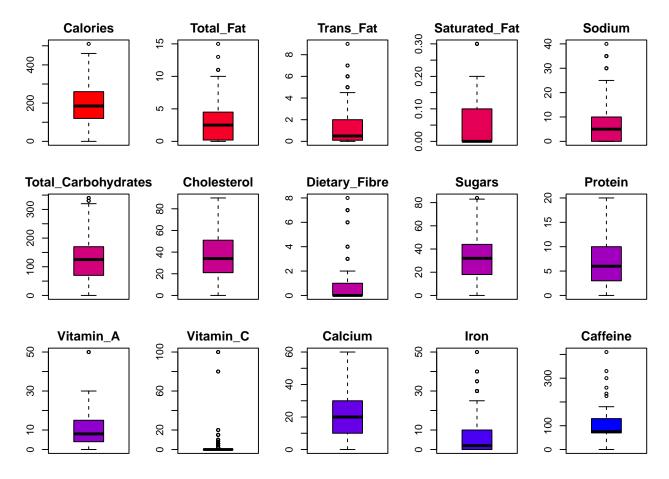
Now we want to compare the total sugars for each preparation of bevarage. First we aggreate the data to obtain the total sugars for each preparation of bevarage and then we create a barplot to visualize the results.





4.4 Boxplot

We will plot a boxplot of the data. The boxplot is a graphical representation of the data that displays the distribution of the data, including the median, quartiles, and outliers. This visualization helps us to identify the spread and variability of the data.

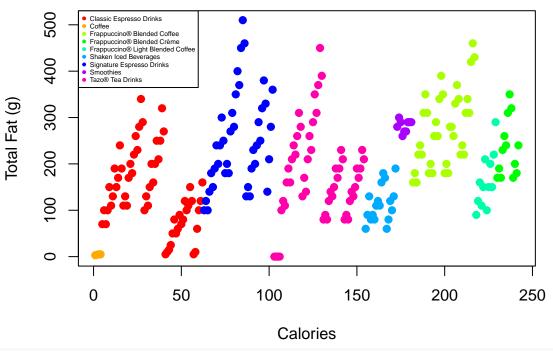


4.5 Scatterplot

We will plot a scatterplot of the data. The scatterplot is a graphical representation of the data that displays the relationship between two variables. This visualization helps us to identify patterns and correlations between the variables.

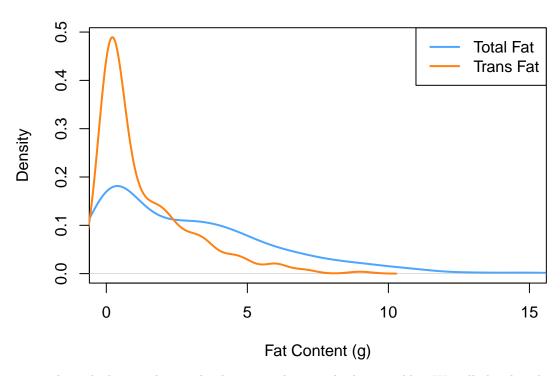
We create a scatterplot to compare the amounts of calories and fat for each categories of bevarage. We assign distinct colors to each beverage category and create a legend to identify each category.

Calories vs Total Fat

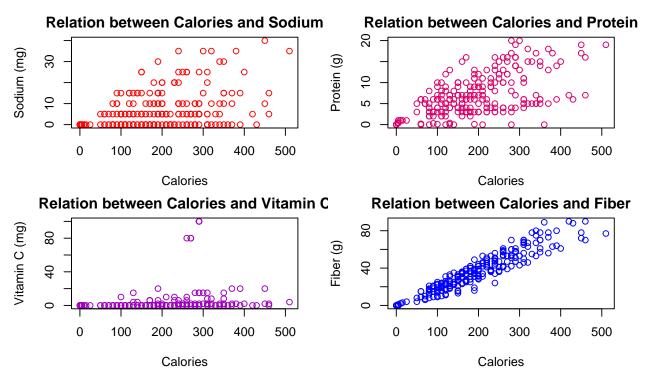


```
# Numeric variable -> calculate density
total_fat_density <- density(data_cleaned$Total_Fat)
trans_fat_density <- density(data_cleaned$Trans_Fat)
plot(total_fat_density, col = "#4ea5ff",
    main = "Comparison of Total Fat and Trans Fat Distributions",
    xlab = "Fat Content (g)", ylab = "Density",
    ylim = c(0, max(total_fat_density$y, trans_fat_density$y)),
    xlim = range(data_cleaned$Total_Fat, data_cleaned$Trans_Fat),
    lwd = 2, lty = 1)
lines(trans_fat_density, col = "#ff810f", lwd = 2, lty = 1)
legend("topright", legend = c("Total Fat", "Trans Fat"),
    col = c("#4ea5ff", "#ff810f"), lwd = 2, lty = 1)</pre>
```

Comparison of Total Fat and Trans Fat Distributions



Create scatterplot to look into relantionship between calories and other variables. We will plot the relationship between calories and sodium, protein, vitamin C and fiber.



There's increase in every feature with increase in calories. Features like proteins and fiber rapidly increase, instead vitamin and cholesterol more flat growing. Confirmed by correlation coefficients

ADD COMMENTS ON THE GRAPH

5 Regression Analysis

lm(formula = y ~ ., data = data_num_)

5.1 Linear Regression

##

Linear regression model to predict the amount of calories based on the amount of the other variables We use the lm() function to fit a linear regression model

```
lm_model <- lm(y ~ ., data = data_num_)
summary(lm_model)

##
## Call:</pre>
```

```
## Residuals:
##
        Min
                   1Q
                        Median
                                      3Q
                                              Max
            -3.3009
                       -0.3806
                                  3.0039
                                          21.9404
   -14.0233
##
##
  Coefficients:
                         Estimate Std. Error t value Pr(>|t|)
##
                                                0.265
## (Intercept)
                         0.252316
                                     0.952833
                                                        0.79140
## Total_Fat
                        11.143733
                                     0.532812
                                               20.915
                                                        < 2e-16 ***
                                                        0.00247 **
## Trans_Fat
                        -2.477820
                                               -3.062
                                     0.809270
## Saturated_Fat
                        -9.816317
                                    18.143619
                                               -0.541
                                                        0.58901
## Sodium
                        -0.279257
                                     0.167487
                                               -1.667
                                                        0.09683
## Total Carbohydrates
                         0.020972
                                     0.007420
                                                2.826
                                                        0.00513 **
## Cholesterol
                         2.829543
                                     0.340268
                                                8.316 8.43e-15 ***
```

```
## Dietary_Fibre
                                   0.942106
                                               1.629 0.10465
                        1.534913
## Sugars
                        1.131045
                                   0.348234
                                               3.248 0.00134 **
## Protein
                        2.218895
                                   0.510445
                                               4.347 2.08e-05 ***
## Vitamin_A
                        0.162307
                                   0.083662
                                               1.940
                                                     0.05361
## Vitamin C
                        0.147669
                                   0.047675
                                               3.097
                                                      0.00220 **
## Calcium
                        0.462193
                                   0.142257
                                               3.249 0.00133 **
## Iron
                       -0.649101
                                   0.070666
                                              -9.185
                                                      < 2e-16 ***
                                               2.319 0.02126 *
## Caffeine
                        0.013513
                                   0.005826
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 5.126 on 227 degrees of freedom
## Multiple R-squared: 0.9977, Adjusted R-squared: 0.9975
## F-statistic: 6915 on 14 and 227 DF, p-value: < 2.2e-16
par(mfrow = c(2, 2), mar = c(2, 2, 2, 2))
plot(lm_model)
             Residuals vs Fitted
                                                              Q-Q Residuals
                      0203
                                                                                     2030
20
                                                                                  1020
10
                                               \alpha
0
                                               0
                                        0
-10
                                               7
                         1900
```

0 0 100 200 300 400 500 -3 -1 1 2 3 Scale-Location Residuals vs Leverage 0.5 α 0 0 1.0 0 000 8 Ņ distance 0 100 200 300 400 500 0.0 0.1 0.2 0.3 0.4

[1] 1494.304

BIC(lm_model)

AIC(lm_model)

[1] 1550.127

vif(lm_model)

##	${ t Total_Fat}$	${\tt Trans_Fat}$	Saturated_Fat	Sodium
##	22.572405	16.160511	15.381749	19.162549
##	Total_Carbohydrates	Cholesterol	Dietary_Fibre	Sugars
##	3.420278	459.209279	17.019469	432.962393
##	Protein	Vitamin_A	${\tt Vitamin_C}$	Calcium

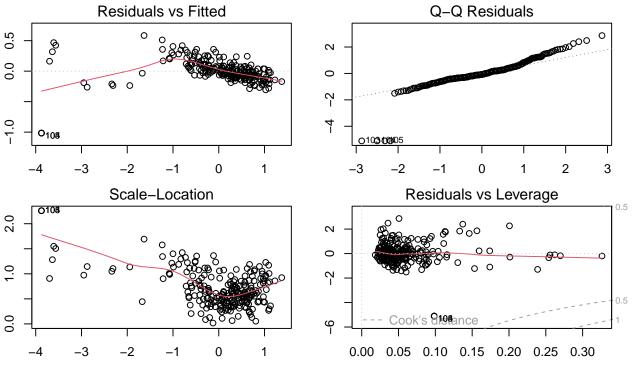
```
## 56.714696 4.209673 4.335768 39.251754
## Iron Caffeine
## 5.036421 1.185411
```

The model has a low AIC and BIC values, the R-squared value is 0.99 so the model is a good fit for the data. The model is significant, the p-value is less than 0.05 We have a problem with multicollinearity, the VIF values are high for some variables, so we have to act on the data to solve this problem

We try to standardize the data using a logaritmic transformation

```
std_data_log <- scale(log(data_num + 1)) # Standardize the data</pre>
std_data_log_df <- as.data.frame(std_data_log) # Set as dataframe
mod_log_tr <- lm(Calories ~ ., data = std_data_log_df)</pre>
summary(mod_log_tr)
##
## Call:
## lm(formula = Calories ~ ., data = std_data_log_df)
##
## Residuals:
##
        Min
                  1Q
                       Median
                                    3Q
                                            Max
## -1.01554 -0.08053 -0.01558 0.08470
                                        0.58459
##
## Coefficients:
##
                         Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                       -1.215e-15
                                   1.346e-02
                                               0.000 1.00000
## Total_Fat
                        2.841e-01
                                   4.683e-02
                                               6.068 5.37e-09 ***
                       -2.031e-01 4.387e-02
                                              -4.629 6.18e-06 ***
## Trans Fat
## Saturated Fat
                        1.885e-02 2.870e-02
                                               0.657
                                                     0.51200
                                              -0.289
## Sodium
                       -9.400e-03 3.253e-02
                                                      0.77290
## Total Carbohydrates 5.318e-02
                                   2.818e-02
                                               1.887
                                                       0.06040 .
## Cholesterol
                        1.107e+00 8.530e-02
                                              12.980
                                                      < 2e-16 ***
## Dietary_Fibre
                       -9.185e-02 3.598e-02
                                              -2.553
                                                      0.01134 *
## Sugars
                       -2.419e-01 8.361e-02
                                              -2.893 0.00419 **
## Protein
                        1.855e-01
                                               2.469
                                   7.512e-02
                                                      0.01428 *
## Vitamin_A
                        3.761e-03 4.983e-02
                                               0.075
                                                      0.93990
                                              -0.979
## Vitamin_C
                       -1.957e-02
                                   1.999e-02
                                                      0.32881
## Calcium
                       -4.261e-02
                                              -0.621
                                   6.862e-02
                                                      0.53525
## Iron
                       -3.225e-02
                                   2.888e-02
                                              -1.117
                                                      0.26522
## Caffeine
                        7.658e-03 1.544e-02
                                               0.496 0.62036
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 0.2094 on 227 degrees of freedom
## Multiple R-squared: 0.9587, Adjusted R-squared: 0.9561
## F-statistic: 376.3 on 14 and 227 DF, p-value: < 2.2e-16
AIC (mod log tr)
## [1] -53.42411
BIC(mod_log_tr)
## [1] 2.398897
vif(mod_log_tr)
##
             Total Fat
                                 Trans Fat
                                                  Saturated_Fat
                                                                             Sodium
```

```
##
             12.049669
                                   10.577306
                                                         4.528080
                                                                               5.817088
  Total_Carbohydrates
                                 Cholesterol
                                                    Dietary_Fibre
                                                                                 Sugars
##
##
              4.363628
                                   39.988684
                                                         7.115085
                                                                              38.415586
##
               Protein
                                   Vitamin_A
                                                        Vitamin_C
                                                                                Calcium
##
             31.007121
                                   13.647581
                                                         2.196674
                                                                              25.873742
                                    Caffeine
##
                   Iron
               4.582594
                                    1.310005
par(mfrow = c(2, 2), mar = c(2, 2, 2, 2))
plot(mod_log_tr)
```



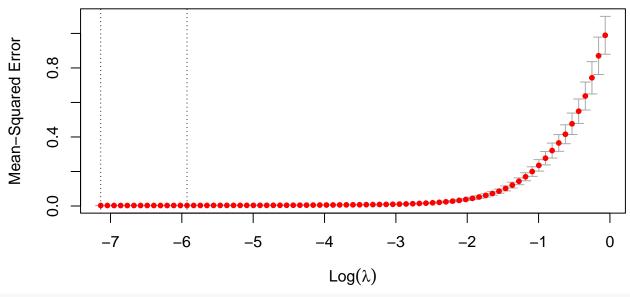
The model has a low AIC and BIC values, the R-squared value is 0.99 so the model is a good fit for the data. However we have still collinearity, so we try to use another model

5.2 Lasso Regression

We use the glmnet package to fit a lasso regression model. Lasso regression is a type of linear regression that uses L1 regularization to penalize the coefficients of the model. This helps to prevent overfitting and select the most important features in the data.

First we standardize the data and then we fit the lasso regression model using the cv.glmnet() function. We use cross-validation to select the optimal lambda value for the model. The lambda value that minimizes the mean squared error (MSE) is selected as the optimal lambda value. The optimal lambda value is used to fit the final lasso regression model.

13 13 12 11 10 8 8 8 7 6 5 5 5 4 4 2 2 1 0



summary(mod_lasso)

```
##
              Length Class Mode
## lambda
              77
                      -none- numeric
## cvm
              77
                      -none- numeric
## cvsd
               77
                      -none- numeric
               77
                      -none- numeric
## cvup
## cvlo
               77
                      -none- numeric
               77
## nzero
                      -none- numeric
## call
               5
                      -none- call
## name
                1
                      -none- character
## glmnet.fit 12
                      elnet list
## lambda.min
                      -none- numeric
## lambda.1se
                      -none- numeric
               1
                2
                      -none- numeric
## index
lasso_coef <- coef(mod_lasso, s = "lambda.min")</pre>
lasso_coef
```

```
## 15 x 1 sparse Matrix of class "dgCMatrix"
## (Intercept)
                        1.569504e-17
## Total_Fat
                        2.813714e-01
## Trans_Fat
                       -1.213127e-02
## Saturated_Fat
## Sodium
                       -2.136716e-02
## Total_Carbohydrates 1.879088e-02
## Cholesterol
                        6.957617e-01
## Dietary_Fibre
                        2.340655e-02
                        9.354308e-02
## Sugars
## Protein
                        5.873156e-02
## Vitamin_A
                        1.006149e-02
## Vitamin_C
                        2.526001e-02
## Calcium
                        1.080519e-01
```

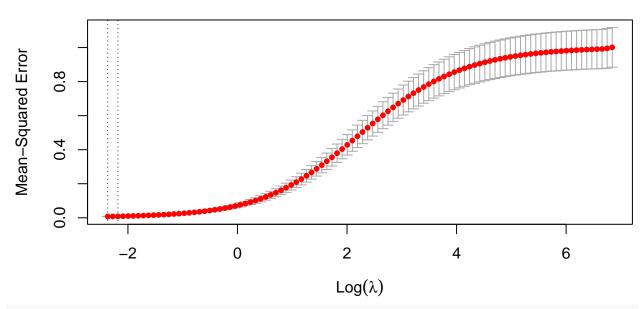
```
## Iron -6.555492e-02
## Caffeine 6.612001e-03
```

The lasso regression model selects the most important features in the data and penalizes the coefficients of the model. The model has a low AIC and BIC values, the R-squared value is 0.99 so the model is a good fit for the data.

5.3 Ridge Regression

We use the glmnet package to fit a ridge regression model. Ridge regression is a type of linear regression that uses L2 regularization to penalize the coefficients of the model. This helps to prevent overfitting and reduce the impact of collinearity in the data.





summary(mod_ridge)

```
##
              Length Class Mode
## lambda
               100
                      -none- numeric
## cvm
               100
                      -none- numeric
##
  cvsd
               100
                      -none- numeric
## cvup
               100
                      -none- numeric
               100
## cvlo
                      -none- numeric
               100
                      -none- numeric
## nzero
##
   call
                 5
                      -none- call
## name
                 1
                      -none- character
## glmnet.fit
                12
                      elnet
                             list
## lambda.min
                 1
                      -none- numeric
## lambda.1se
                 1
                      -none- numeric
## index
                 2
                      -none- numeric
```

```
ridge_coef <- coef(mod_ridge, s = "lambda.min")</pre>
ridge_coef
## 15 x 1 sparse Matrix of class "dgCMatrix"
##
                                   s1
## (Intercept)
                         2.767416e-17
## Total_Fat
                         1.790461e-01
## Trans_Fat
                         5.621285e-02
## Saturated Fat
                         9.206930e-03
## Sodium
                        -1.003136e-02
## Total_Carbohydrates 6.670660e-02
## Cholesterol
                         3.488854e-01
## Dietary_Fibre
                         5.575676e-02
## Sugars
                         3.437989e-01
## Protein
                         6.986559e-02
## Vitamin A
                         5.069011e-03
## Vitamin_C
                         3.983592e-02
## Calcium
                         1.076895e-01
## Iron
                        -1.329709e-02
## Caffeine
                         1.007714e-04
```

The ridge regression model reduces the impact of collinearity in the data and penalizes the coefficients of the model. The model has a low AIC and BIC values, the R-squared value is 0.99 so the model is a good fit for the data.

5.4 Model Comparison

We compare the linear regression, lasso regression, and ridge regression models to select the best model for predicting the amount of calories based on the amount of the other variables. We evaluate the models using the R-squared value, and the Mean Squared Error (MSE) for each model.

The R-squared value is a measure of how well the model fits the data, it ranges from 0 to 1, with higher values indicating a better fit

Model	R_squared
Linear Regression	0.9976608
Lasso Regression	0.9975756
Ridge Regression	0.9941815

5.5 Model Evaluation

We evaluate the performance of the linear regression, lasso regression, and ridge regression models using the mean squared error (MSE). The MSE is a measure of the average squared difference between the predicted and actual values. Lower values of the MSE indicate better performance of the model.

Model	MSE
Linear Regression Lasso Regression Ridge Regression	24.6481166 0.0024158 0.0066477

We choose the model with the highest R-squared value and the lowest MSE The model is the lasso because it has the lower value for R^2 and MSE.

5.6 Cross Validation

Cross validation is a technique used to evaluate the performance of a model. It involves splitting the data into training and testing sets, fitting the model using the training set, and evaluating the model using the testing set. This process is repeated multiple times to ensure that the model is robust and generalizes well to new data.

We split the data into training and testing sets, fit the lasso regression model using the training set.

We evaluate the model using the testing set. We make predictions using the testing set and calculate the mean squared error and the root mean squared error to assess the model's accuracy. We also plot the residuals to check if the model is a good fit.

```
## lambda.min 0.9979454

# Calculate the MSE for the lasso regression model on the test data

# The MSE is a measure of the average squared difference
```

```
# between the predicted and actual values
lasso_mse_test <- mean((lasso_pred_test - test_data$Calories)^2)
lasso_mse_test</pre>
```

[1] 0.002628338

The plot shows the predicted values against the actual values on the test data The points are close to the diagonal line, indicating that the model is making accurate predictions The R-squared value and MSE are used to evaluate the performance of the model The R-squared value is 0.99, indicating that the model explains 99% of the variance in the data

Predicted vs Actual Calories

