Data Analysis Notebook - MP2

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Contents

Our Team

Our team members and their roles were the following:

- **Bella Cruz:** Data Cleaning; Data Exploration; Model Fitting
- **Abhi Thanvi:** Formatting; Model Fitting; Predictive Selection and Power
- **Maria Larmon:** Classification tables; Predictive power; Cross-Validation

Data Exploration

```
water_pot <- read.csv("data/water_potability.csv", header = TRUE)
head(water_pot)
```

```
##         ph Hardness   Solids Chloramines  Sulfate Conductivity Organic_carbon
## 1       NA 204.8905 20791.32    7.300212 368.5164     564.3087      10.379783
## 2 3.716080 129.4229 18630.06    6.635246       NA     592.8854      15.180013
## 3 8.099124 224.2363 19909.54    9.275884       NA     418.6062      16.868637
## 4 8.316766 214.3734 22018.42    8.059332 356.8861     363.2665      18.436524
## 5 9.092223 181.1015 17978.99    6.546600 310.1357     398.4108      11.558279
## 6 5.584087 188.3133 28748.69    7.544869 326.6784     280.4679       8.399735
##   Trihalomethanes Turbidity Potability
## 1        86.99097  2.963135          0
## 2        56.32908  4.500656          0
## 3        66.42009  3.055934          0
## 4       100.34167  4.628771          0
## 5        31.99799  4.075075          0
## 6        54.91786  2.559708          0
```

The dataset initially has 3276 rows and 10 columns.

Columns:

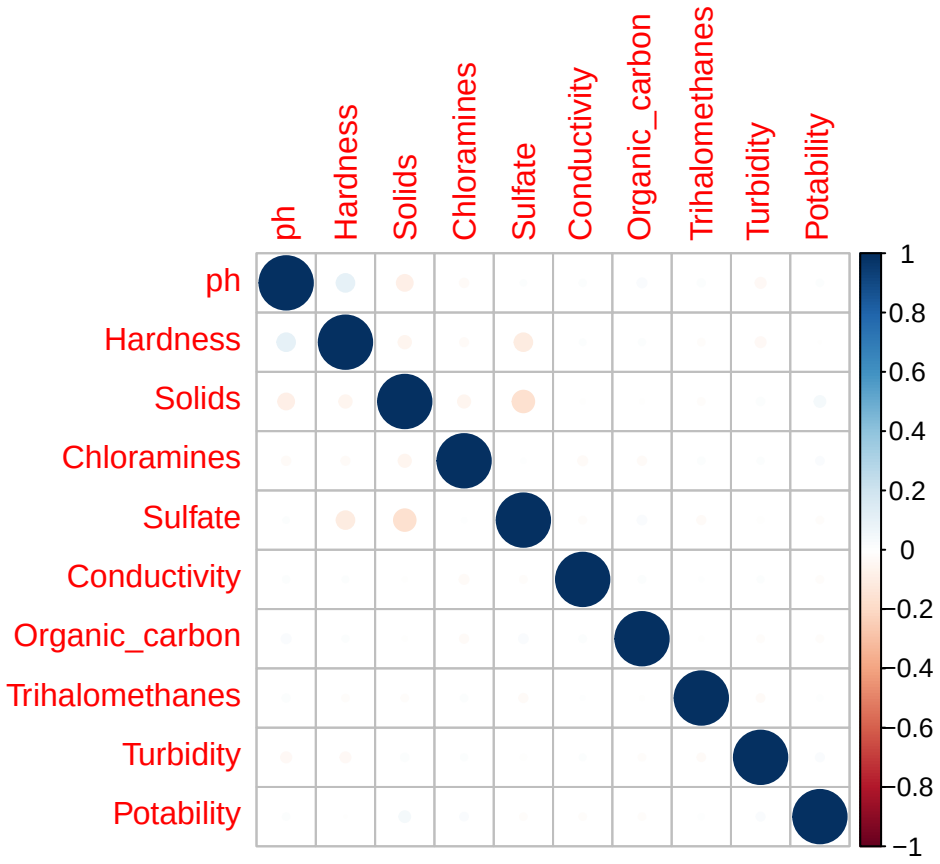
- **ph:** Represents the pH levels.
- **Hardness:** Indicates water hardness.
- **Solids:** Denotes the concentration of dissolved solids.
- **Chloramines:** Reflects the presence of chloramines in the water.
- **Sulfate:** Indicates sulfate levels.
- **Conductivity:** Represents the electrical conductivity of the water.
- **Organic_carbon:** Denotes the concentration of organic carbon.
- **Trihalomethanes:** Reflects the presence of trihalomethanes.
- **Turbidity:** Indicates water turbidity.
- **Potability:** Binary variable (0 or 1) indicating water potability, where 1 represents potable water.

Please note that some values are missing (NA) in the dataset so we drop them before furthering our analysis. Now our row count is 2011 and we call our data as `df` for simplicity.

Part A: Data Exploration

This section is a exploratory analysis of this data set in order to evaluate the water quality attributes and their relationship with the drinking water status. We aim to better understand what patterns we are dealing with in our data to make a better decision during modelling process.

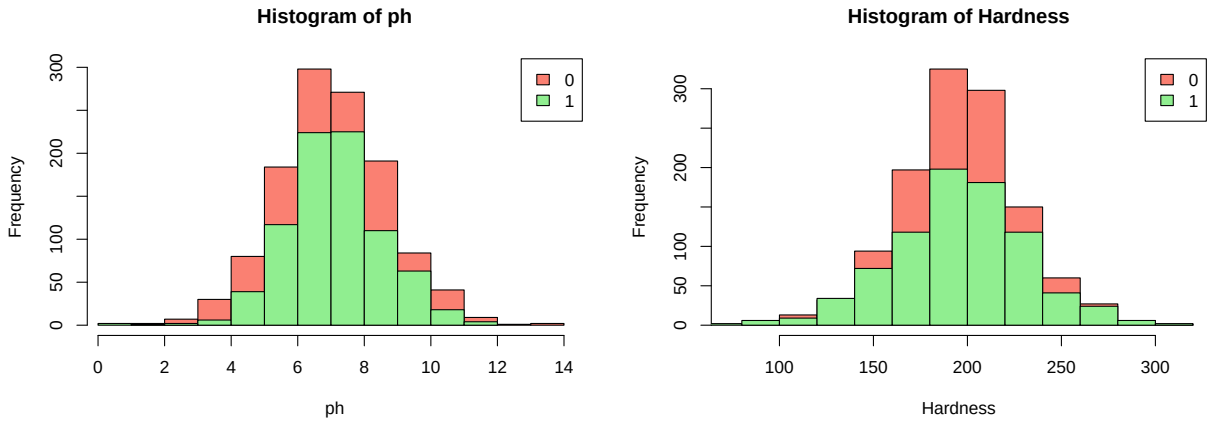
```
corrplot(cor(df))
```



Based on the correlation matrix plot, it seems like the dataset is forgiving in that no two variables are strongly correlated with one another. So, we should be good and not see any multicollinearity issue when fitting model.

BUT when we initially fit a full linear logit model (can be seen in our Analysis.Rmd) on the data, we saw an issue that none of our predictors were significant. So we decided to look more closely at how our data is dispersed.

Dispersion of Data



The `pH vs. Potability` graph and `Hardness vs. Potability` histogram graphs both imply that the dispersion of points for when the water is not potable (Potability=0) tends to cluster around the center range of their respective levels compared to the dispersion of points when the water is deemed potable (Potability=1). This could have been the reason for our main effects model to not suffice and suggest that we consider adding quadratic terms into the fitted model as well.

Part B. Model Fitting

This section fits an appropriate model to this data set in order to make predictions about the potability of water given a set of measurements on water quality attributes. We learnt that a Main Effects model will not suffice and therefore will attempt to fit a model with quadratic terms and see the results.

```
full_quad_mod <- glm(Potability ~
                       ph + I(ph^2) +
                       Hardness + I(Hardness^2) +
                       Solids + I(Solids^2) +
                       Chloramines + I(Chloramines^2) +
                       Sulfate + I(Sulfate^2) +
                       Conductivity + I(Conductivity^2) +
                       Organic_carbon + I(Organic_carbon^2) +
                       Trihalomethanes + I(Trihalomethanes^2) +
                       Turbidity + I(Turbidity^2), family=binomial, data=df)
summary(full_quad_mod)
```

```
##
## Call:
## glm(formula = Potability ~ ph + I(ph^2) + Hardness + I(Hardness^2) +
##     Solids + I(Solids^2) + Chloramines + I(Chloramines^2) + Sulfate +
##     I(Sulfate^2) + Conductivity + I(Conductivity^2) + Organic_carbon +
##     I(Organic_carbon^2) + Trihalomethanes + I(Trihalomethanes^2) +
##     Turbidity + I(Turbidity^2), family = binomial, data = df)
##
## Coefficients:
##                          Estimate Std. Error z value Pr(>|z|)
## (Intercept)           1.415e+01  2.894e+00   4.890 1.01e-06 ***
## ph                    9.563e-01  2.080e-01   4.599 4.25e-06 ***
## I(ph^2)              -6.544e-02  1.439e-02  -4.549 5.40e-06 ***
## Hardness             -3.656e-02  1.129e-02  -3.240  0.00120 **
## I(Hardness^2)         9.306e-05  2.868e-05   3.244  0.00118 **
## Solids                8.707e-06  2.347e-05   0.371  0.71060
## I(Solids^2)           1.479e-11  4.674e-10   0.032  0.97476
## Chloramines          -5.348e-01  1.782e-01  -3.000  0.00270 **
## I(Chloramines^2)      3.946e-02  1.237e-02   3.190  0.00142 **
## Sulfate              -7.494e-02  1.345e-02  -5.570 2.55e-08 ***
## I(Sulfate^2)          1.119e-04  2.001e-05   5.592 2.24e-08 ***
## Conductivity         -5.466e-03  4.823e-03  -1.133  0.25708
## I(Conductivity^2)     5.716e-06  5.473e-06   1.044  0.29627
## Organic_carbon        1.032e-01  8.751e-02   1.179  0.23844
## I(Organic_carbon^2)  -3.747e-03  3.016e-03  -1.242  0.21414
## Trihalomethanes      -1.212e-02  1.613e-02  -0.752  0.45227
## I(Trihalomethanes^2)  9.967e-05  1.201e-04   0.830  0.40653
## Turbidity             1.578e-01  4.408e-01   0.358  0.72027
## I(Turbidity^2)       -1.352e-02  5.508e-02  -0.245  0.80616
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 2712.1  on 2010  degrees of freedom
```

```
## Residual deviance: 2609.3  on 1992  degrees of freedom
## AIC: 2647.3
##
## Number of Fisher Scoring iterations: 4
```

Perfect! Now at least we can see some predictors being significant. This means this transformation/switch was good. We will later do predictor selection so we can move on from this section!

Part C. Predictor Selection

We just chose a full model with quadratic terms (`full_quad_model`) and saw better results. However, only few predictors were significant while others were not. In this section, we aim to select the best predictors determining the water potability.

We will consider all three `forward, backward, step-wise` selection methods and choose the one that produces model (i.e. smallest AIC)

Selection Algorithms

```
intercept_model <- glm(Potability ~ 1, family=binomial, data=df)

# Forward Selection
forward_mod <- step(intercept_model, ~ ph + I(ph^2) + Hardness + I(Hardness^2)
                    + Solids + I(Solids^2) + Chloramines + I(Chloramines^2)
                    + Sulfate + I(Sulfate^2) + Conductivity + I(Conductivity^2)
                    + Organic_carbon + I(Organic_carbon^2)
                    + Trihalomethanes + I(Trihalomethanes^2)
                    + Turbidity + I(Turbidity^2), direction="forward", trace=0)
summary(forward_mod)
```

```
##
## Call:
## glm(formula = Potability ~ I(Solids^2) + I(Chloramines^2) + Chloramines,
##     family = binomial, data = df)
##
## Coefficients:
##                     Estimate Std. Error z value Pr(>|z|)
## (Intercept)       1.732e+00  6.057e-01   2.860  0.00424 **
## I(Solids^2)       1.930e-10  1.041e-10   1.854  0.06379 .
## I(Chloramines^2)  5.041e-02  1.169e-02   4.311 1.63e-05 ***
## Chloramines      -6.905e-01  1.689e-01  -4.088 4.35e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 2712.1  on 2010  degrees of freedom
## Residual deviance: 2687.8  on 2007  degrees of freedom
## AIC: 2695.8
##
## Number of Fisher Scoring iterations: 4
```

```
# Backward Selection
backward_mod <- step(full_quad_mod, direction="backward", trace=0)
summary(backward_mod)
```

```
##
## Call:
## glm(formula = Potability ~ ph + I(ph^2) + Hardness + I(Hardness^2) +
```

```
##     Solids + Chloramines + I(Chloramines^2) + Sulfate + I(Sulfate^2),
##     family = binomial, data = df)
##
## Coefficients:
##                     Estimate Std. Error z value Pr(>|z|)
## (Intercept)       1.353e+01  2.384e+00   5.676 1.38e-08 ***
## ph                9.712e-01  2.071e-01   4.690 2.73e-06 ***
## I(ph^2)          -6.648e-02  1.432e-02  -4.644 3.42e-06 ***
## Hardness         -3.623e-02  1.127e-02  -3.216  0.00130 **
## I(Hardness^2)     9.195e-05  2.862e-05   3.213  0.00132 **
## Solids            9.031e-06  5.542e-06   1.629  0.10322
## Chloramines      -5.172e-01  1.771e-01  -2.920  0.00350 **
## I(Chloramines^2)  3.822e-02  1.229e-02   3.109  0.00188 **
## Sulfate          -7.518e-02  1.336e-02  -5.627 1.84e-08 ***
## I(Sulfate^2)      1.123e-04  1.987e-05   5.653 1.58e-08 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 2712.1  on 2010  degrees of freedom
## Residual deviance: 2614.3  on 2001  degrees of freedom
## AIC: 2634.3
##
## Number of Fisher Scoring iterations: 4
```

```
# Step Selection
step_mod <- step(intercept_model, ~ ph + I(ph^2) + Hardness + I(Hardness^2)
                   + Solids + I(Solids^2) + Chloramines + I(Chloramines^2)
                   + Sulfate + I(Sulfate^2) + Conductivity + I(Conductivity^2)
                   + Organic_carbon + I(Organic_carbon^2)
                   + Trihalomethanes + I(Trihalomethanes^2)
                   + Turbidity + I(Turbidity^2), direction="both", trace=0)
summary(step_mod)
```

```
##
## Call:
## glm(formula = Potability ~ I(Solids^2) + I(Chloramines^2) + Chloramines,
##     family = binomial, data = df)
##
## Coefficients:
##                     Estimate Std. Error z value Pr(>|z|)
## (Intercept)       1.732e+00  6.057e-01   2.860  0.00424 **
## I(Solids^2)       1.930e-10  1.041e-10   1.854  0.06379 .
## I(Chloramines^2)  5.041e-02  1.169e-02   4.311 1.63e-05 ***
## Chloramines      -6.905e-01  1.689e-01  -4.088 4.35e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 2712.1  on 2010  degrees of freedom
## Residual deviance: 2687.8  on 2007  degrees of freedom
## AIC: 2695.8
```

```
##
## Number of Fisher Scoring iterations: 4
```

Observations:

- Seems like `Forward Selection` and `Step-Wise Selection` both converged to the same subset of predictors
  - `Intercept`, `Solids^2^` (not super signif.), `Chloramines^2^`, `Chloromines`
  - Both have **AIC = 2695.8**
- `Backward Selection` had a longer list of selected predictors and can be seen above
  - `Solids` is selected in the model but is not significant (we shall see what to with this later)
  - Has the smaller **AIC = 2634.3** Since the `Backward Selection` produced the smaller AIC among the three selection algorithms, we shall move forward with running diagnositcs on `backward_mod`.

Model Diagnostics - Backward Selected

Here we are deciding if we should drop the 'Solids' predictor as it is insignificant when looking at the summary of our selected model

```r
drop_results <- drop1(backward_mod, test = "Chisq")

# Create a data frame with variable names and their p-values
drop_terms <- data.frame(
  Variable = rownames(drop_results),
  P_Value = drop_results$Pr
)
#print(drop_terms)
# Remove 'Solids' if it's in the list of drop-able terms
if ('Solids' %in% drop_terms$Variable[drop_terms$P_Value > 0.05]) {
  tmp_model <- update(backward_mod, . ~ . - Solids)
} else {
  tmp_model <- backward_mod
}

summary(tmp_model)
```

```
##
## Call:
## glm(formula = Potability ~ ph + I(ph^2) + Hardness + I(Hardness^2) +
##     Chloramines + I(Chloramines^2) + Sulfate + I(Sulfate^2),
##     family = binomial, data = df)
##
## Coefficients:
##                    Estimate Std. Error z value Pr(>|z|)
## (Intercept)       1.404e+01  2.362e+00   5.946 2.75e-09 ***
## ph                9.569e-01  2.067e-01   4.630 3.65e-06 ***
## I(ph^2)          -6.573e-02  1.429e-02  -4.601 4.21e-06 ***
## Hardness         -3.646e-02  1.125e-02  -3.240  0.00120 **
## I(Hardness^2)     9.218e-05  2.859e-05   3.224  0.00126 **
## Chloramines      -5.175e-01  1.768e-01  -2.927  0.00342 **
## I(Chloramines^2)  3.808e-02  1.227e-02   3.103  0.00191 **
```

```
## Sulfate          -7.614e-02  1.335e-02  -5.704 1.17e-08 ***
## I(Sulfate^2)      1.133e-04  1.986e-05   5.706 1.16e-08 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 2712.1  on 2010  degrees of freedom
## Residual deviance: 2617.0  on 2002  degrees of freedom
## AIC: 2635
##
## Number of Fisher Scoring iterations: 4
```

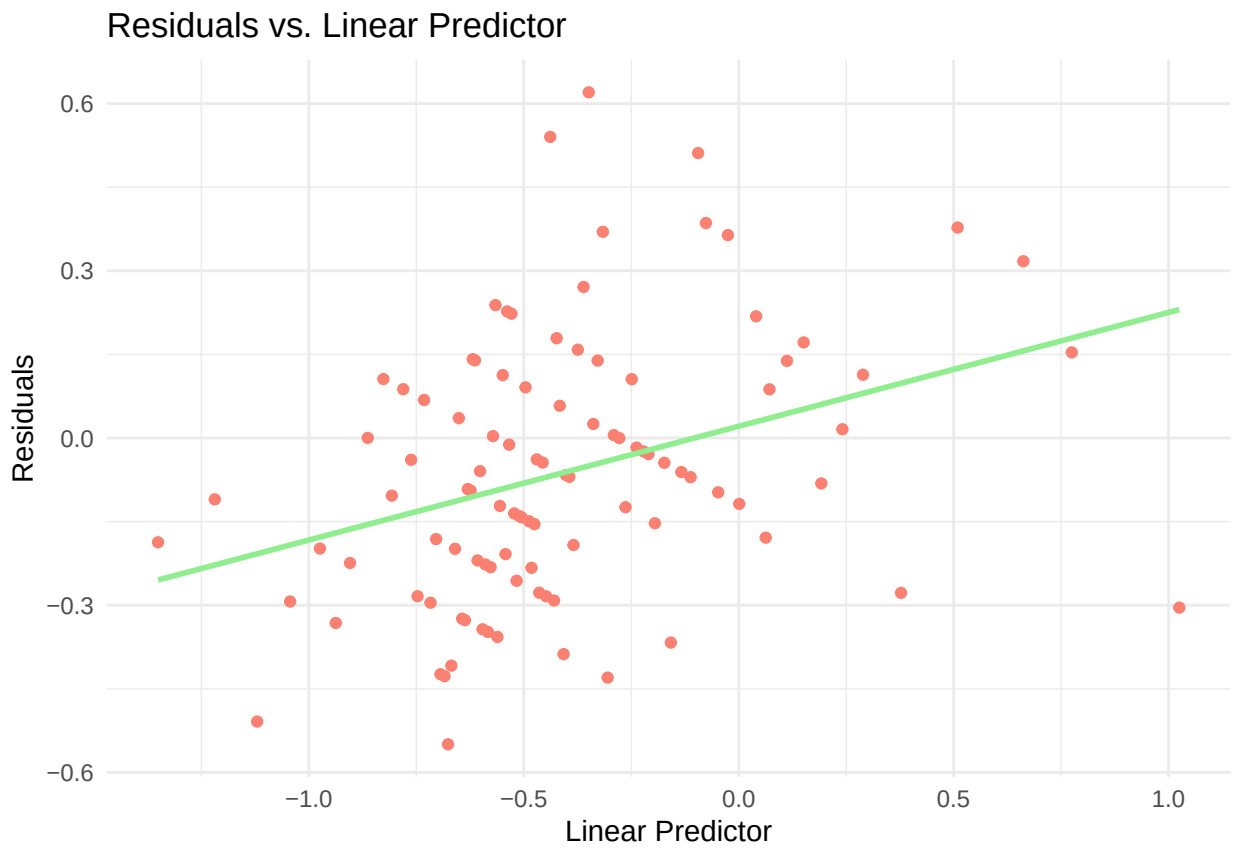
Dropping `Solids` Increased our AIC by 0.7. But we will use the Backward Selection model **with** the `Solids` predictor for 2 reasons:

- Most importantly, the AIC increased slightly by removing the predictor. Also, we are choosing model predictors based on AIC criterion. We are not doing hypothesis testing on the predictors significance, switching back-forth like that will be inconsistent and inaccurate in a way.
- Secondly, in real world intuition, it would make sense that solids dissolved in the water would be one of important factor to determine potability.

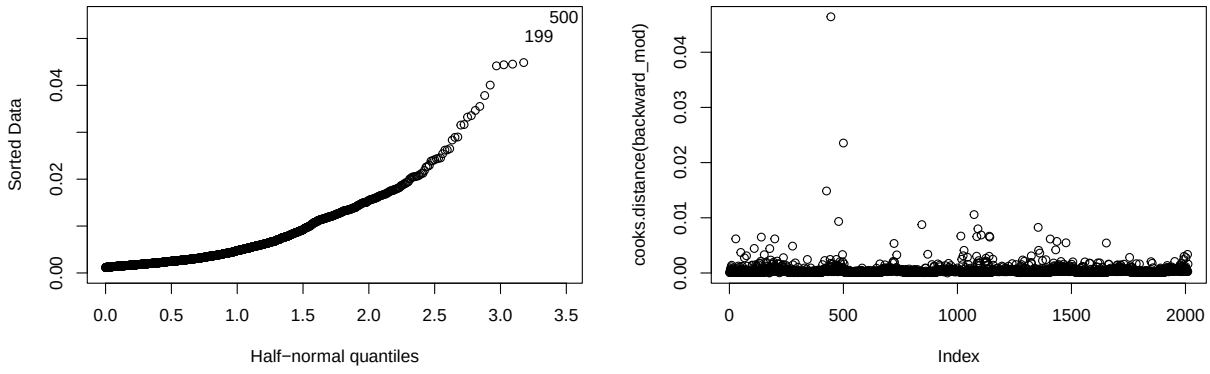
```r
library(dplyr)

tmp_df <- df %>%
  mutate(
    residuals = residuals(backward_mod),
    linpred = predict(backward_mod)
  ) %>%
  group_by(bin = cut(linpred, breaks = unique(quantile(linpred, (1:100)/101)))) %>%
  summarise(
    residuals = mean(residuals),
    linpred = mean(linpred)
  )

ggplot(tmp_df, aes(x = linpred, y = residuals, group = 1)) +
  geom_point(color = "salmon") +
  geom_smooth(method = "lm", se = FALSE, color = "lightgreen") +
  labs(
    title = "Residuals vs. Linear Predictor",
    x = "Linear Predictor",
    y = "Residuals"
  ) +
  theme_minimal()
```



The residual plots looks okay because the residuals are following the general trend of the linear predictor and seems like are equally below and above the prediction line. However, we need to run more diagnostics since our data is not grouped which makes us unconfident in our diagnostic-analysis. But as of now nothing seems to concerning



Based on the plots (code muted to save space :D)for leverages and cook's distance, it seems like there are some points that have higher influence than other points. A specific point would be Index 500 which seems to have a high leverage and high cook's distance. However, the cook's distance is less than 1, so we can consider this point to be okay and not really a problem for us! Let's move on to see our model's predictive power.

Model Evaluation - Predictive Power

This section summarizes the predictive power of the final model selected, using correlation based measures and likelihood based measures.

```
# correlation measure final model
cor(df$Potability, fitted(backward_mod))
```

```
## [1] 0.2195577
```

A correlation coefficient of 0.22 suggests a positive but weak linear relationship between the observed `Potability` values and the fitted values from the logistic regression model we got from backward selection.

```
# likelihood measure final model
lik <- (logLik(backward_mod) - logLik(intercept_model))/(0-logLik(intercept_model))
as.numeric(lik)
```

```
## [1] 0.0360592
```

Although, `Backward Model` gave us the lowest AIC, the Likelihood Test Statistic is 0.036 which is relatively small. Indicating that our `Backward Model` is not significantly better at prediction compared to the `Intercept Model`.

Model Evaluation - Classification Tables

This section uses classification tables to measure the predictive power of the best final model selected based on the results obtained in (c). Implement the leave-one-out cross-validation method for this step.

```
# CV
pi.0 <- 0.5
num = nrow(df)
pihat.cv <- numeric(num)

for (i in 1:num) {
  pihat.cv[i] <- predict(update(backward_mod, subset=-i), newdata=df[i, ],
                         type="response")
}
tab1 <- table(y=df$Potability, yhat=as.numeric(pihat.cv > pi.0))
tab1
```

```
##    yhat
## y      0    1
##   0 1087  113
##   1  654  157
```

```
sensitivity <- tab1[2,2] / (tab1[2,2] + tab1[2,1])
specificity <- tab1[1,1] / (tab1[1,1] + tab1[1,2])

cat("Sensitivity: ", sensitivity, "\n", "Specificity: ",
    specificity)
```

```
## Sensitivity:  0.1935882
##  Specificity:  0.9058333
```

In other words, our model can correctly identify potable water approximately 19% of the time (low sensitivity). However, our model excels at correctly identifying non-potable water with an accuracy of 90% (high specificity). Additionally, the higher specificity indicates that the risk of falsely categorizing non-potable water as potable is relatively low when using the backward_mod model.

The overall accuracy of our model is about 62.4% and the positive predictive value of our model is about 0.91

```
table(df$Potability)
```

```
##
##    0    1
## 1200  811
```

One reason we suspect could be that we more data for non-potable water compared to potable water. Later, we might considering sampling equal counts for each category. This isn't a conclusion, but rather just an exercise for future to maybe see if the distribution of our target variable in our dataset impacts the sensitivity and specificity. [This bit is not part of our analysis, but something we are curious about.]

```r
# Overall proportion correct
(tab1[1,1] + tab1[2,2]) / (tab1[1,1] + tab1[2,2] + tab1[1,2] + tab1[2,1])
```

```
## [1] 0.6185977
```

The estimated probability of the `backward_mod` overall correctly classifying the water as potable or not is 61.8% which is not terrible. But considering, that this is related to health of the people, we still suggest to be safe and use the specificity to detect non-potable water as it seems to be more accurate (and safer response for the people who will be drinking the water).