FINAL PROJECT REPORT

Audrey Anggitawijaya (20824582, aanggita) Aurelya Wibowo (20853893, arwibowo)
Callista Chong (20838195, c23chong) Clara Putri Ong (20846106, cp2ong)

SUMMARY

In this report, we analyze the pollutant.csv data which contains a sample of n = 864 adults included in a study investigating the relationship between exposure to persistent organic pollutants and leukocyte telomere length—a marker of cellular aging that may be related to certain cancers. Our goal is to determine whether/which pollutants improve prediction of the outcome (i.e. length).

Our methods for achieving this goal is by making a model for prediction where we consider various types of model selection: forward, backward, stepwise where we use both criteria AIC and BIC, and LASSO. Next, we will verify that the LINE assumption is met for the chosen model and answer the question to our objective. In the end, we understood that 1 particular pollutant type assisted in the improvement of prediction of the outcome with respect to our model.

Finally, we will discuss what we did differently in our methods which could be improved on, and some limitations to our analysis.

OBJECTIVE

The main objective of this project is to determine whether/which pollutants improve prediction of the outcome (i.e. length) by finding the best predictive model.

DATA PREPROCESSING

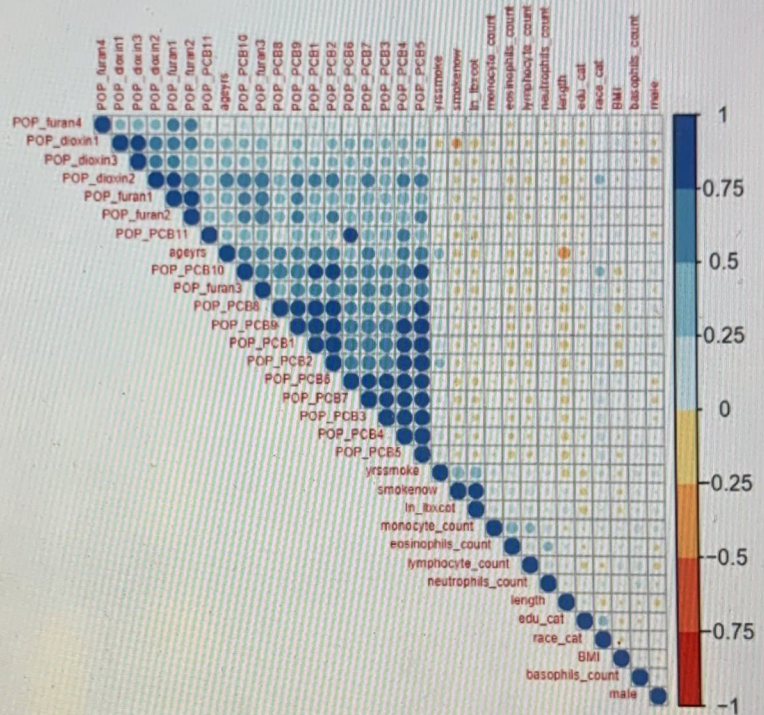
Our group did the regular data-preprocessing step: change categorical data to the factor data type. Also, we removed the whitecell_count (= number of white blood cells) covariate since we muliplied the covariates which represent the percentage of these cells with this value. The main reason we did this was for the model matrix to have independent columns (i.e. percentage of white blood cell does not rely on the number of white blood cell). Lastly, we acknowledge how the 'pollutant' dataset is a complete dataset without missing values.

EDA

In this section, we made plots of different kinds for all the covariates of the dataset in hopes of finding some interesting results.

First, here is a correlation plot showing the correlation of all the covariates and outcome in the dataset.

```
## corrplot 0.84 loaded
```



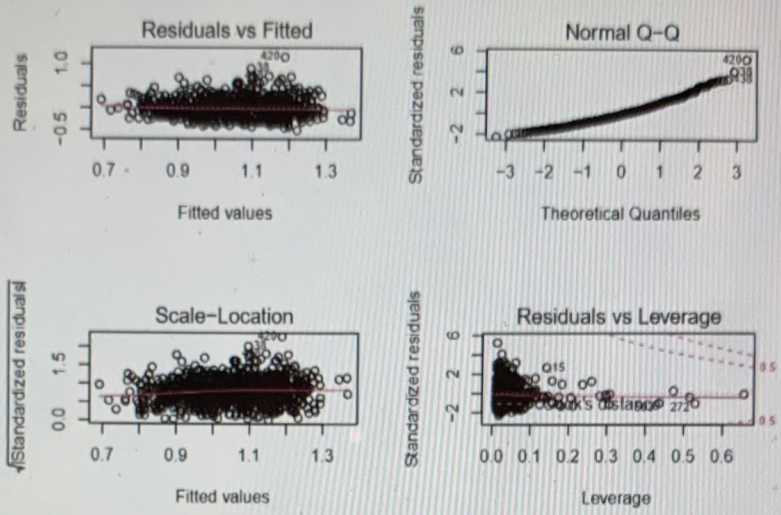
From this correlation plot, interesting findings include age and the outcome(telomere length) being fairly negatively-correlated, and the pollutant dioxin1 also being quite negatively-correlated to the covariate smoke_now.

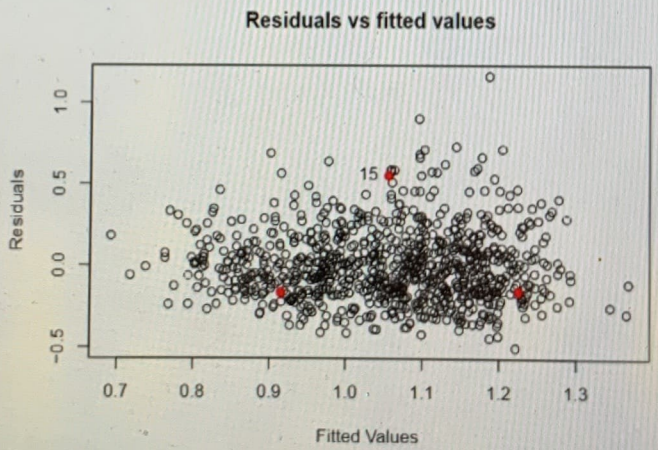
Also, looking at the vertical column (length), we can deduce that there is almost no correlation between length and the covariates POP_furan4 (first row), and all the white blood cell components. So, from this, in our work of finding a prediction model, we will consider removing the insignificant covariates which almost have no correlation with length. We will do this using hypothesis testing (Appendix: Section Applying LASSO as well as stepwise selection using AIC and BIC to select models. Data used here only contain significant covariates).

Now, we summarize the prominent findings of the code in the Appendix: Section Explanatory Data Analysis.

Focusing on the adults taking part in this study, from the box-plots generated in the EDA section of the appendix, we can summarize the majority of them are non-smokers of the non-Hispanic White race. Also, there are more females taking part in this study than males. The average BMI indicates that the participants taking part in this study are on average overweight. Next, they are between the age-group of around 34-63.

Next, we fit the full model M <- lm(length~., data = dat), to see how all covariates affect each other.





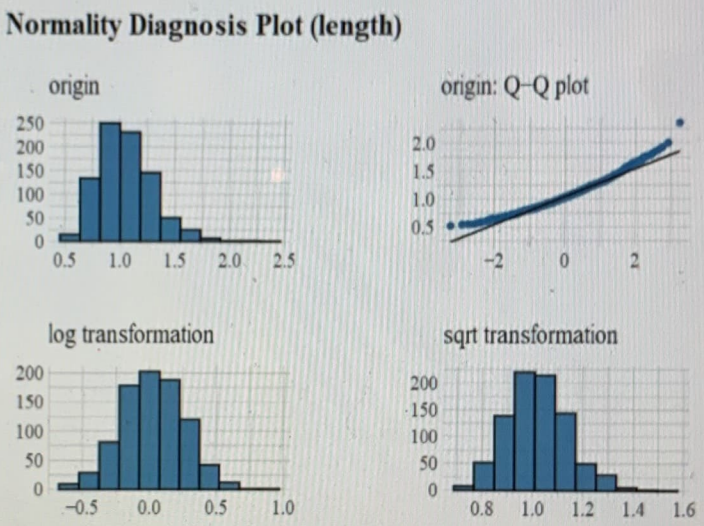
From the Residuals vs fitted plot and the scale-location plot, notice that the overall red line is pretty straight. This suggests an overall constant variance throughout the full model (heteroskedasticity). However, here we also point out the three most extreme points (high leverage) observations 38, 420, and 438, which can be seen more clearly from the same enlarged scatterplot in the Appendix: Section EDA.

Next, from the Normal Q-Q plot, notice how towards the middle, there are many observations on the line so we can assume normality. However, towards the ends, the observations lie above the line. Because of this, we can infer that the data is skewed right (i.e. more datapoints lie on the lower side). We can also take note on the high leverage points, which are quite far from the straight line.

Lastly, from the Cook's Distance plot (bottom right of 4 block plots), we note that the 3 most highly influential observations are 15, 272, and 503, which can be seen more clearly from the same enlarged scatterplot

in the Appendix: Section EDA.
Plotting these points into a scatterplot of residual vs. fitted values shows that these points fit the overall model, and will not have much effect on the model with or without them. This will be further explained in the limitations section of the discussions section.

Besides this, another interesting observation we noticed from the appendix code was that all the variables except ageyrs, yrssmoke and ln_lbxcot in the dataset were right-skewed. This is seen from all the normality diagnosis plots in the Appendix: Section EDA, plot origin. However, in all the normality diagnosis plots, the log transformation fixes this skew, since the histogram of the log transformed data is bell-shaped. Here is an example with the variable length:

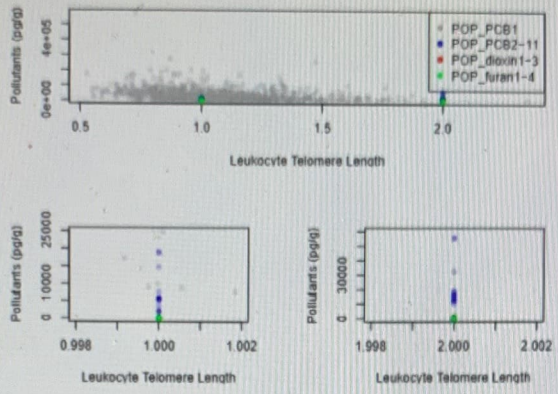


Next, after modelling the outcome with all the covariates, we modelled the outcome with each covariate individually.

From fitting individually, we get the following results:

1. The covariate with the largest change every 1 unit increase in length (i.e. largest abs(beta)) is basophils_pct with beta 0.1064593.
2. The covariate with the smallest change every 1 unit increase in length (i.e. smallest abs(beta)) is POP_PCB4 with beta 9.759999e-07.
3. The covariate with the smallest p-value (most statistically significant) is BMI with p-value 2.445749e-43.
4. The covariate with the largest p-value (least statistically significant) is POP_furan3 with p-value 0.6411889.

Finally, since the dataset is provided by conducting a study aimed to investigate the relationship between length and the pollutants, a scatterplot of pollutants(pg/g) vs. telomere length has been plotted.



The first plot considers all the telomere length, whereas the bottom two plots are enlarged versions of the plot focusing on length 1 and 2.

From here, we can see that pollutants of type PCB1 seem to have occurences over all the telomere lengths, whereas pollutants of type PCB2-11, dioxin1-3, and furan1-4 only have occurences for leukocyte telomere length of length 1 and 2.

METHODS

We divide our observations into two separate datasets, training set (traindat) and a test set (testdat). Traindat contains 664 of the observations in pollutant.csv and testdat contains the other 200 observations. We let testdat be the holdout set that we will later use to evaluate the MSPE of our selected models on different data with the goal of providing unbiased results.

We decided to use three different model selection methods to select three different best models according to the criteria of each respective model selection method. We start with the full model which contains all the potential covariates and the intercept. Next, we will get our candidate models using some selection algorithm. The criteria for our candidates are based on AIC, BIC, and LASSO.

Recall that to do a selection algorithm, we need a starting model. The starting model we decided to go with contains all the potential covariates and intercept (i.e., full model). Here, we chose the stepwise selection because it is the most efficient compared to forward and backward selection. In addition to that, using forward or backward selection may cause the wrong removal of some covariates. Next, we also consider the more modern approach, LASSO, to also be a candidate for the best fitting model.

After obtaining the three candidate models, we wanted to take interactions between the covariates and itself into consideration. Therefore, we also applied the stepwise selection with AIC and BIC, as well as LASSO, taking into account all possible one-to-one interactions. Our starting model contains all the potential covariates squared and the intercept. Looking at the covariates present in each model, we realized that the model with interactions obtained from stepwise selection using BIC, is the same with the model obtained using the same method but without interactions. Thus, we have 5 models to consider.

From EDA, based on the correlation plot, we also notice that POP_furan4, and all the white blood cell components seems to be uncorrelated to length. Also, in the Appendix: Section Applying LASSO as well as stepwise selection using AIC and BIC to select models. Data used here only contain significant covariates, we observed that the p-values of lymphocyte, eosinophils, basophils, neutrophils, BMI, edu_cat (1= less than 9th grade of 9-11th grade), edu_cat (2= highschool grad/ GED or equivalent) and all the race_cat assessed individually are not significant at the $\alpha = 0.05$ level. Hence, we removed those covariates from our

data and repeated our above procedure. We split the data into training and testing datasets, and conducted stepwise selection based on AIC and BIC as well as LASSO on the training set, considering both all possible one-to-one interactions and no interactions at all.

Thereafter, we realized that the models (with and without interactions) we obtained applying stepwise selection based on BIC are identical to the stepwise selection based on BIC that we did on the data that we did not manipulate. For that reason, we only take the model (no data manipulations and no interactions) obtained by stepwise using BIC into account.

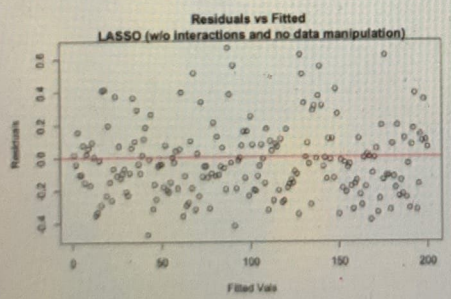
Onward, we checked all nine models for the assumptions of linear regression: linearity, independence, normality and heteroskedasticity. We also calculated their respective mean squared prediction error and its square root to measure the prediction accuracy of each model. Below is the summary of the RMSPE of each models:

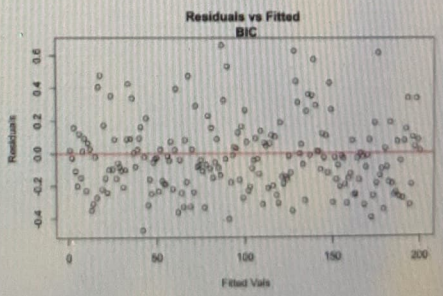
	From model with all covariates		From model with only significant covariates	
Without Interactions i.e. .	**AIC**	0.228444*	**AIC**	0.227353*
	BIC	0.221453	**LASSO**	0.223235
	LASSO	0.222867		
With Interactions i.e. .^2	**AIC**	0.242596*	**AIC**	0.243453*
	LASSO	0.228189*	**LASSO**	0.227725*

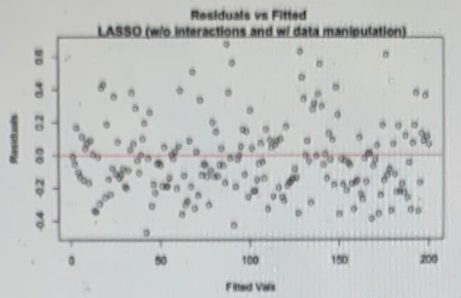
Top 3 models based on RMSPE:

1. Model selected based on stepwise selection (criteria: BIC).
2. Model selected based on LASSO with no interactions and no data manipulation.
3. Model selected based on LASSO with no interactions, done on the data containing only significant covariates.

Now, looking at the residual plots to assist in choosing the model from these 3,







	BIC	LASSO with no interactions and no data manipulation	LASSO with no interactions, done on the data containing only significant covariates
Proportion of residuals inside [-0.25, 0.25]	146/200	146/200	147/200

Interestingly, we can see that the proportions are almost the same for all 3 models.

However, we choose the BIC, since:

1. It has the lowest RMSPE,
2. Parsimony -> model with the least covariate
3. It is very interpretable: Since it has no interactions and has the least covariate it is very easy to interpret the data.

RESULTS

We have

$$\text{Length} \sim 1.4351718 + 0.0070121\text{POP\_furan3} - 0.1453943\text{monocyte\_count} - 0.0070514\text{ageyrs}$$

as our chosen model.

	Estimate	Standard Error	P-values
Intercept	1.4351718	0.0363128	< 2e-16
POP_furan3	0.0070121	0.0018724	0.000196
monocyte_count	-0.1453943	0.0494699	0.003407
ageyrs	- 0.0070514	0.0005721	< 2e-16

We ended up having 3 variables in the final model. The table above can be interpreted as follows:

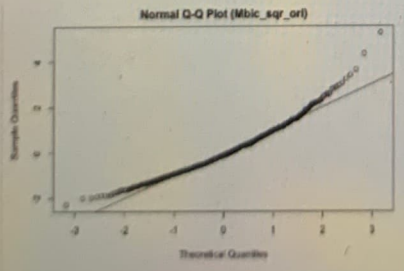
1. The mean outcome when the covariates POP_furan3, monocyte_count, and ageyrs are zero is 1.4351718.
2. The mean difference in the outcome for every 1 unit increase in POP_furan3, holding other covariates fixed is 0.0070121.
3. The mean difference in the outcome for every 1 unit increase in monocyte_count, holding other covariates fixed is -0.1453943.
4. The mean difference in the outcome for every 1 unit increase in ageyrs, holding other covariates fixed is -0.0070514. Out of all three covariates, the largest mean change in the outcome for some 1 unit increase is the monocyte_count.

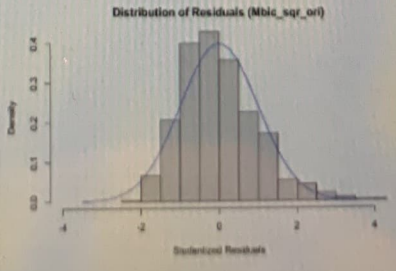
All the p-values for our covariates are very small, and hence, they are all very statistically significant, with the most statistically significant being ageyrs.

Overall, based on the residual plot and RMSPE, our final prediction model predicts the test data the best. We have assumed independence for our data. Then, here is how we prove the assumptions linearity, normality, and homoskedasticity.

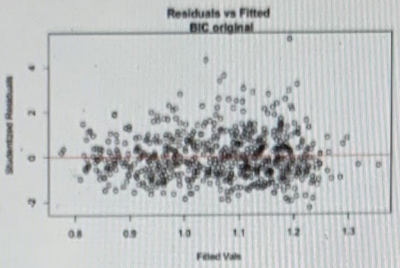
Assumptions

Normality: From the QQPlot and plot distribution of studentized residuals we can see that the data is slightly skewed to the right. Besides the slight skew, we can say that the normality assumption is fairly reasonable.



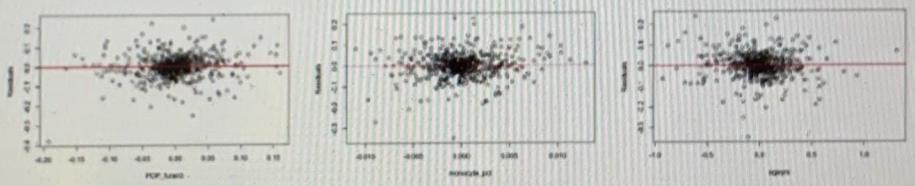


Heteroskedasticity: From the studentized residuals vs fitted values scatterplot, we can see that the points lie more or less horizontally within a constant band around the horizontal line where residual is zero. Therefore, we may conclude that our data has constant variability.



Independence: Looking at our data, none of their observations seem to depend on each other. Moreover, we removed the covariate whiteblood cell and changed all its components into their own amounts. Therefore, it seems reasonable to assume that our data is independent.

Linearity: By plotting the residuals of y to residuals of each of the covariates, notice that the points on the normal qqplot lie more or less along a straight line. Thus, linearity assumption may be assumed.



Hence, all of our regression assumptions have been reasonably satisfied by the final model. There are a couple of outliers, but not too much that it affects the assumptions.

One interesting finding is that we thought we would end up with the LASSO model, because it is the newest and more complicated algorithm out of them all. However, we ended up with the BIC model, which was quite unexpected.

DISCUSSIONS

The covariates chosen in our best model are POP_furan3, monocyte_count, and ageyrs. Recall that from the EDA section, ageyrs was strongly negatively-correlated with length which helps shed some light to why it is in our chosen model.

Using the model found in results, we can answer the objective question: Determine whether/which pollutants improve prediction of the outcome (i.e., length) to an extent. Since the model only includes pollutant POP_furan3, this is the pollutant which improves prediction of the outcome, which is quite interesting given how this type of pollutant was only a component of telomere lengths 1 and 2. Other telomere lengths didn't have any of the furan3 pollutants recorded for it. Note that we can only answer the objective question limited to the model we chose as the best predictive model. Other predictive models chosen with other methods might have different pollutants. So, according to our model chosen by stepwise selection(criteria: BIC) states that the pollutant is POP_furan3. However, this result is true due to some decisions we made in the methods which could be improved on:

Improvements

First, recall that in the EDA section, we observed that most of the variables in the data are right-skewed, and that using a log-transformation on the data fixes this skew and makes the variable normally-distributed. So, from here, it would have been a good decision to use log-transformed variables instead to find the best predictive model. However, we chose to not do that as it would be difficult to interpret the meaning behind the log-transformed data, although using the transformed data might yield a more accurate model and possibly a different answer to our objective.

Next, we did not remove the outliers(influential units) we found in the EDA section before dividing the data into a test and training set as we assumed that all the outliers(influential units) we found in the EDA sections are correct (i.e. no wrong inputs, data are from the same population, etc.) and decided to not remove it. However, this assumption could affect our model and it would be useful to examine its impact on our model further.

Finally, there are many more methods beyond our scope such as the log accuracy ratio(Tofallis, 2014) that could help us decide our final model. More comparisons could be made using these methods, which could give us different results on what model is chosen.

Limitations

First, in the EDA section, we mentioned that there were outliers in the data. However, earlier, we said that we did not removed it due to our assumptions that they are "correct". In the case that we are wrong, our model might not be correct as removing the outliers would affect our model entirely.

Second, one of our model-selection methods was LASSO. Recall that LASSO shrinks coefficients. However, in our case, we actually prefer that the coefficients are not shrunk since our objective is about fitting the best fitting model. So, a suggestion to this limitation would be to use relaxed LASSO instead. Also, we found it difficult to prove the regression diagnostics (assumptions) using LASSO.

Lastly, there is a limitation to our LINE assumptions for all the models we considered. All the residuals histograms and qqplots show that the model is not perfectly normal,but a little right skewed. So, the normality assumption is actually violated. Also, the independence assumption is only fulfilled since we assumed that was the case.

Now, we address the sampling error in the dataset. As mentioned in EDA, the dataset has the following biases: The majority of the adults in the study are non-smokers of the non-Hispanic White race. Also, there are more females taking part in this study than males. Next, the average BMI indicates that the participants taking part in this study are on average overweight. Finally, they are between the age-group of around 34-63. More variation might increase the credibility of the results found.

References

Tofallis, C. (2014, November 12). A better measure of relative prediction accuracy for model selection and model estimation. Retrieved April 14, 2021, from https://link.springer.com/article/10.1057/jors.2014.103