Regression Model to Predict Viscosity of a Blend from its Composition

Mohammed Quazi

PhD Candidate – Statistics
Department of Mathematics & Statistics
University of New Mexico
mquazi@unm.edu
https://math.unm.edu/~mquazi/
https://github.com/mquazi

Overview

Viscosity Data Exercise

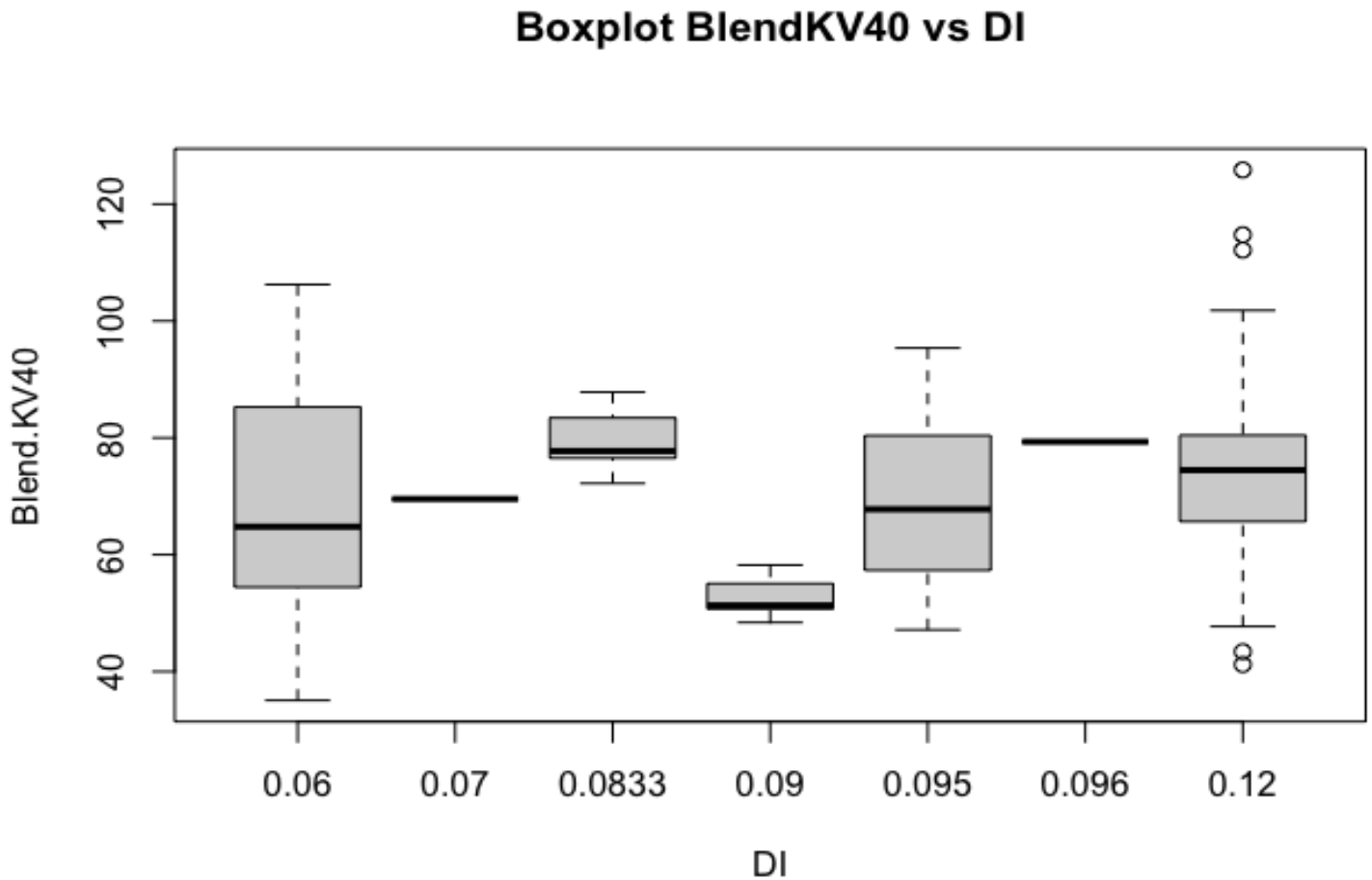
- Files to execute this study are here: github.com/mquazi/Intro_OW_ANOVA
- Main question: Build a predictive model to predict Blend KV40
- Viscosity of a blend is the response variable – Blend KV40
- Predictor variables considered are 6 – performance package (DI), viscosity modifier (VM), base stock density (BS Density), base stock KV40 (BS KV40), base stock KV100 (BS KV100), base stock total (BS total)
- If the prediction model is not accurate enough, need to include the individual base stocks

Preliminary Data Analysis

- No NAs or missing data points
- 86 rows and 20 columns
- Correlation between Blend KV40 and BS KV100 is 0.708 (good)
- Correlation between Blend KV40 and BS KV40 is 0.718 (good)
- Correlation between BS KV40 and BS KV100 is 0.9888 (bad)

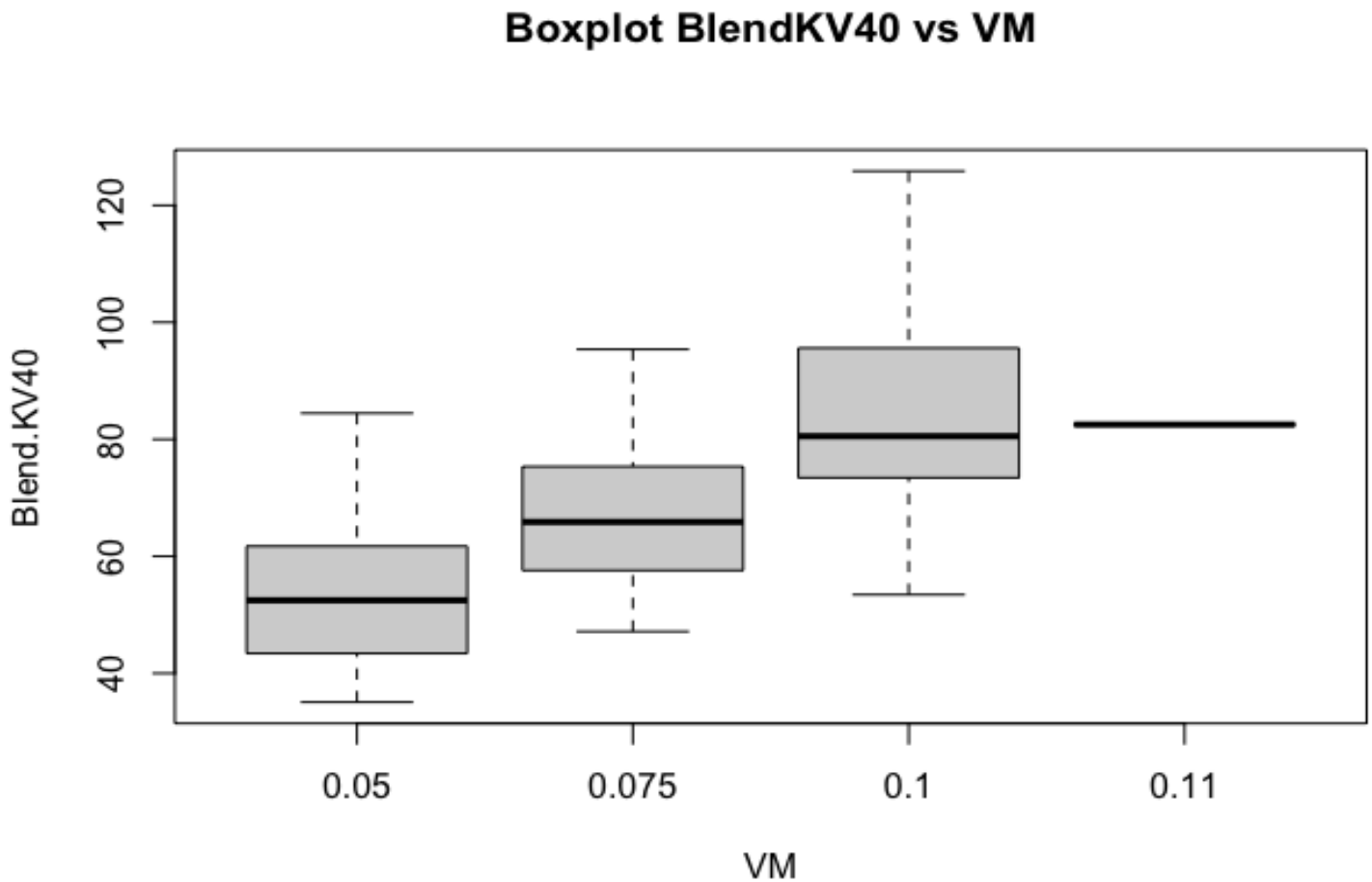
Boxplot DI

- No real takeaways, DI median Blend KV40 levels do not really differ

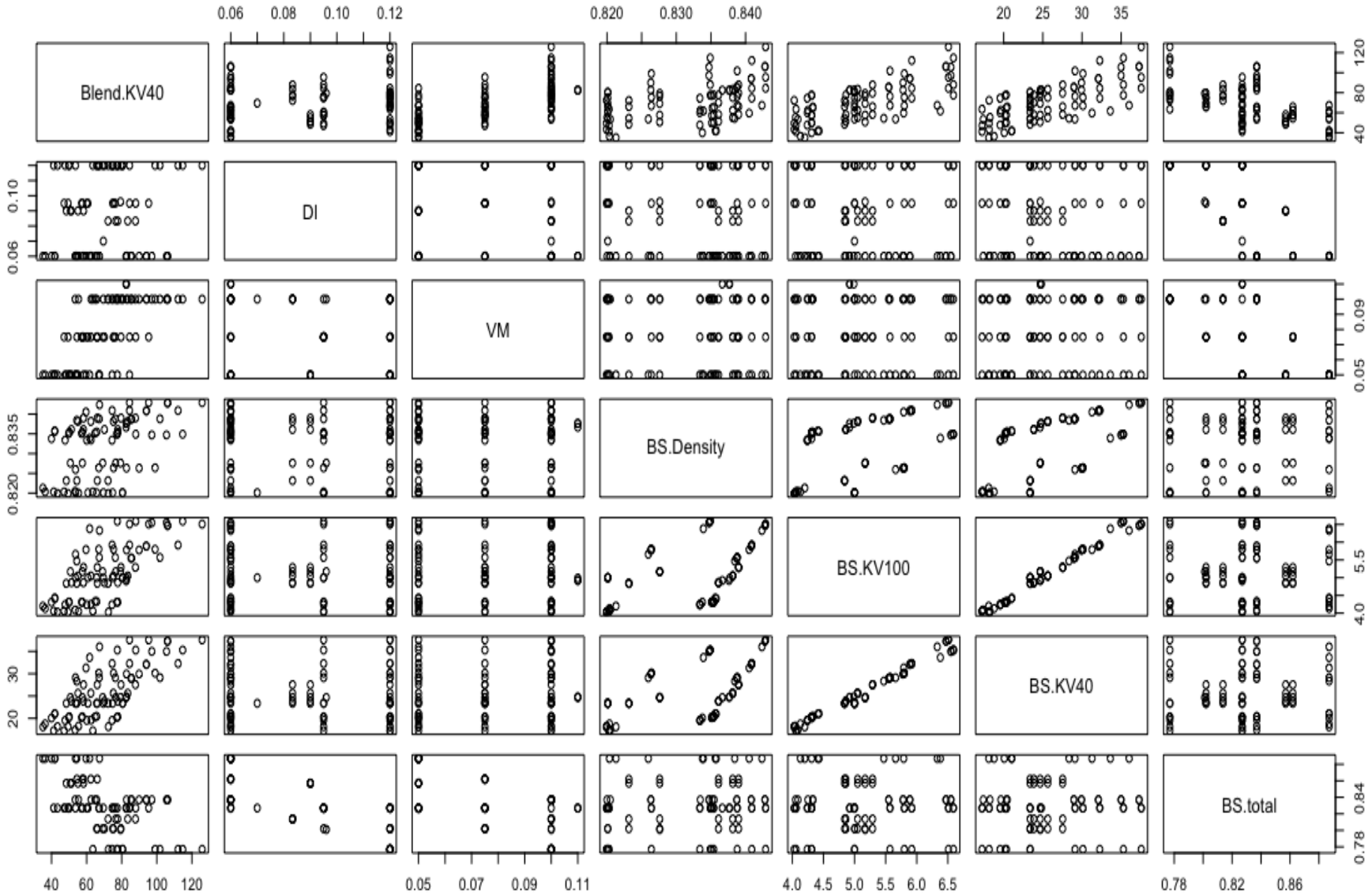


Boxplot VM

- Upward trend, 0.11's Blend KV40 median to lookout for



Pairplot



Multiple Linear Regression

- After constructing the required interactions
- Model form is:

$$Y = \beta_0 + \sum_{i=1}^{6} \beta_i X_i + \sum_{i=4}^{5} \delta_i X_2 X_i + \epsilon \quad (1)$$

β_0, β_i, & δ_i are constants

ϵ iid Normal$(0, \sigma^2)$

- But the interaction terms have correlations with other predictors

- I built another additive model and the dropped interactions are considered later using added variable plots
- Model form is:

$$Y = \beta_0 + \sum_{i=1}^{6} \beta_i X_i + \epsilon \quad (2)$$

β_0, β_i, & δ_i are constants

ϵ iid Normal$(0, \sigma^2)$

Model Selection

- Backward elimination and best subsets criteria based on adjusted R^2, R^2, C_p, BIC suggested models are

Procedure	**Variables included**	R^2	**Adj**R^2	$C_p(p+1)$	**BIC(lowest)**
Backward elimination	X_1, X_2, X_3, X_5	0.98	0.98	4.5	-320
Best subsets	X_1, X_2, X_3, X_4, X_5	0.98	0.98	5	-320
Best subsets	X_1, X_3, X_4, X_5, X_6	0.98	0.98	5	-320
Best subsets	X_1, X_2, X_3, X_5	0.98	0.98	4.5	-320

Model Selection

- Final model selected by me by striking a balance between a simpler model and good model attributes for further analysis is

$$Y = \beta_0 + \sum_{i=1}^{3} \beta_i X_i + \beta_5 X_5 + \epsilon \tag{3}$$

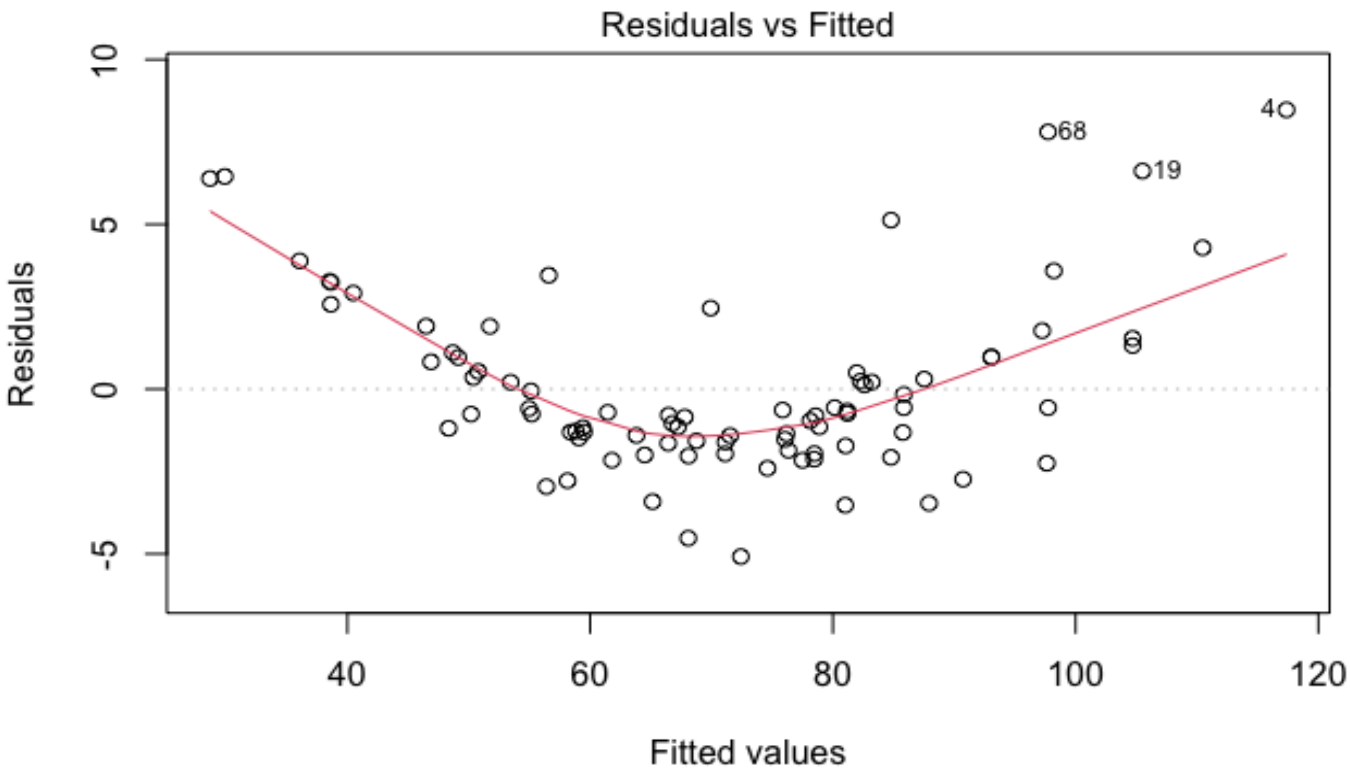
β_0, β_i, & β_5 are constants

ϵ iid Normal$(0, \sigma^2)$

- Retained variables are: DI, VM, BS Density and BS KV40

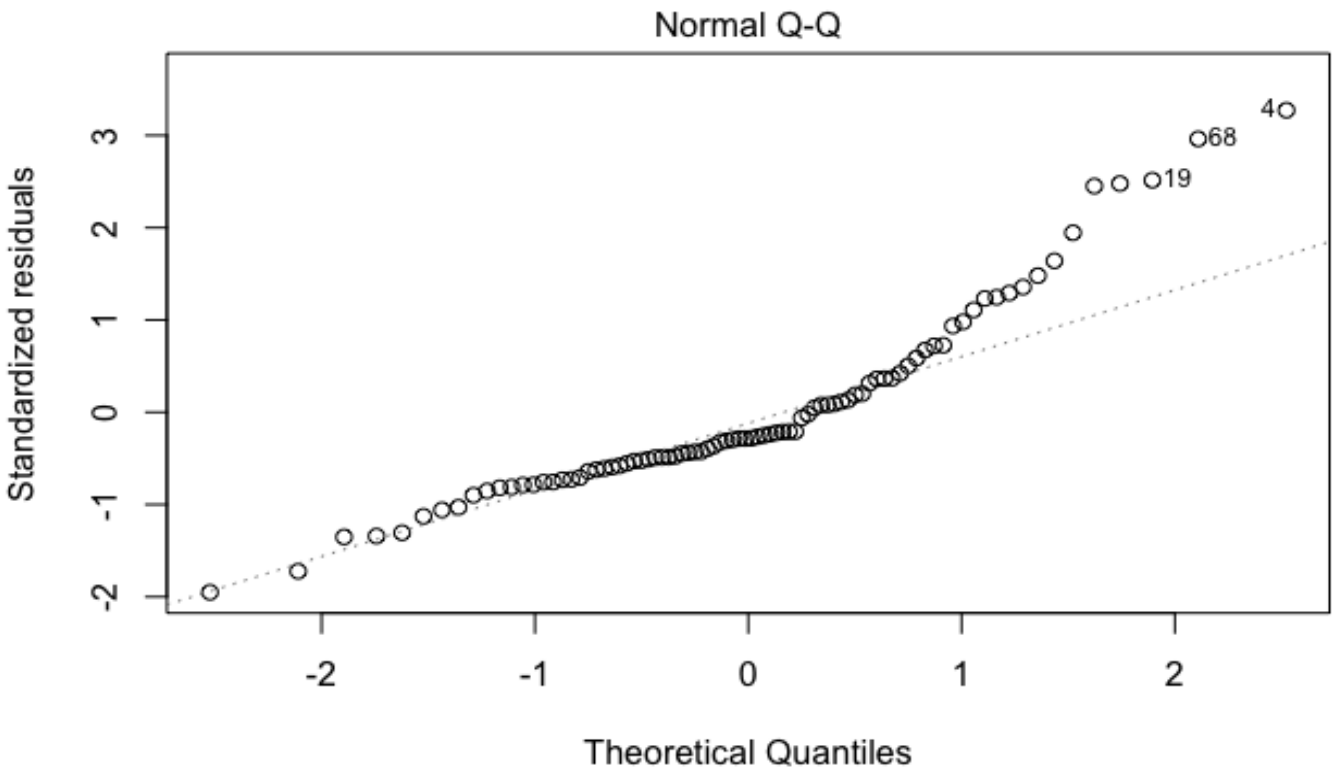
Residual Analysis

- **Linearity** assumption is not in danger, the fit curve is not too erratic
- **Homoscedascity** is clearly violated with an obvious curvature. However, Breusch-Pagan test P-value is 0.2545



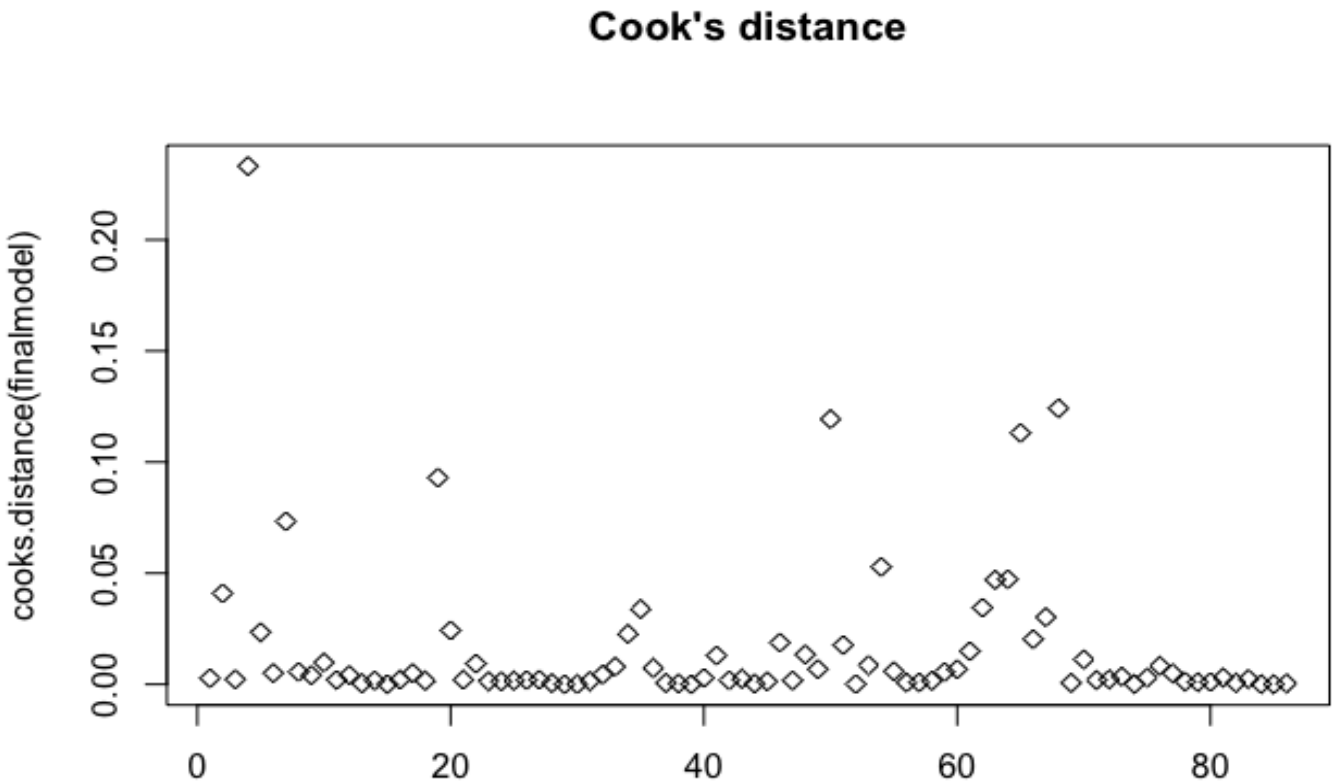
Residual Analysis

- **Normality** assumption regarding variances is violated. Plot shows points deviating too much from the straight line
- Shapiro-Wilks test yields the same result



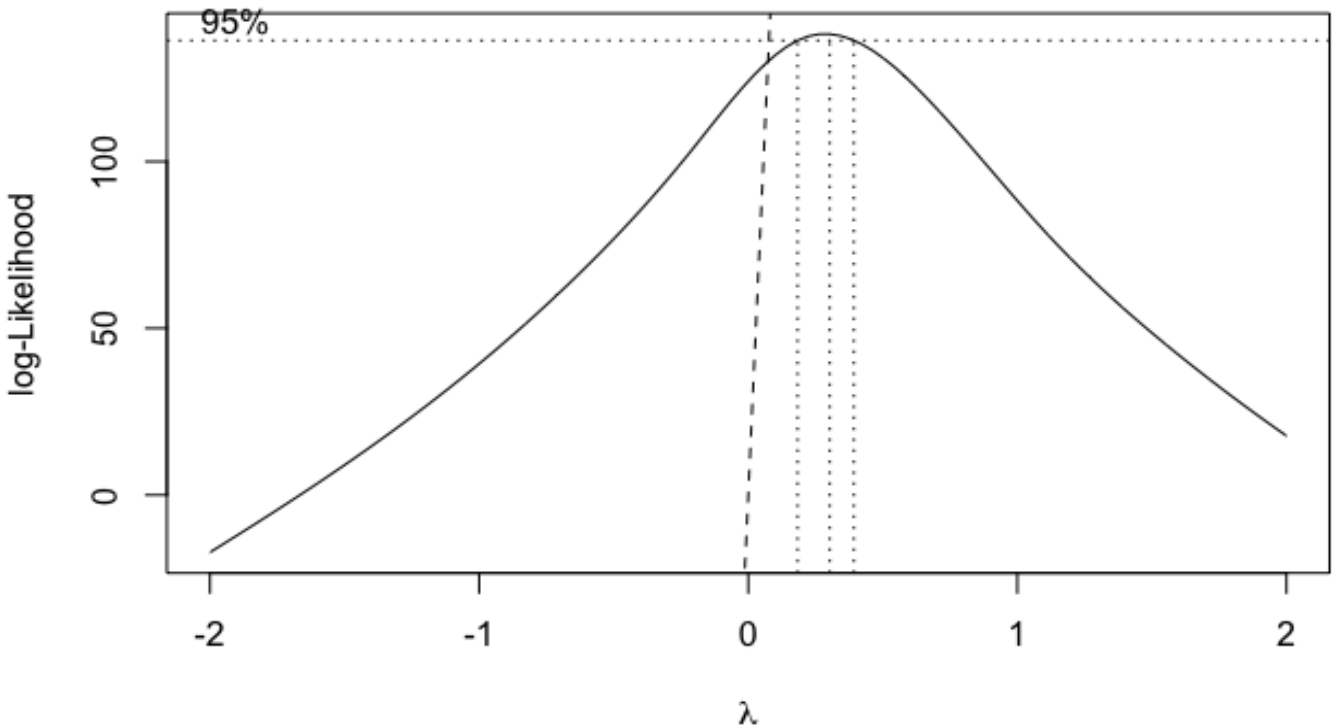
Residual Analysis

- **Multicollinearity** is not an issue at all, since all the VIFs are well within the critical value of 5
- After considering the Bonferroni limit, DFFITS and Cook's distances, leverage points, no case is particularly alarming as an **outlier**



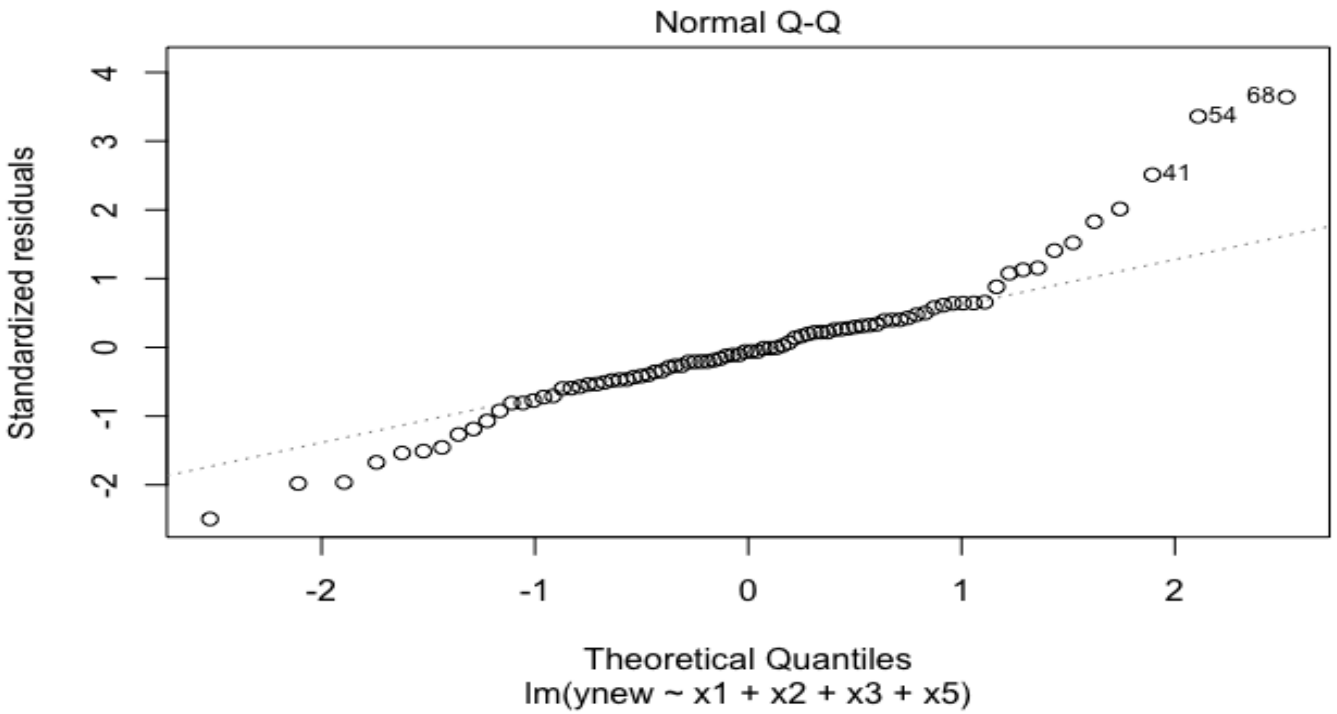
Residual Analysis

- To fix the issue of **non-constant variances**, from Box-Cox procedure, square root transformation of the Blend KV40 variable looks reasonable



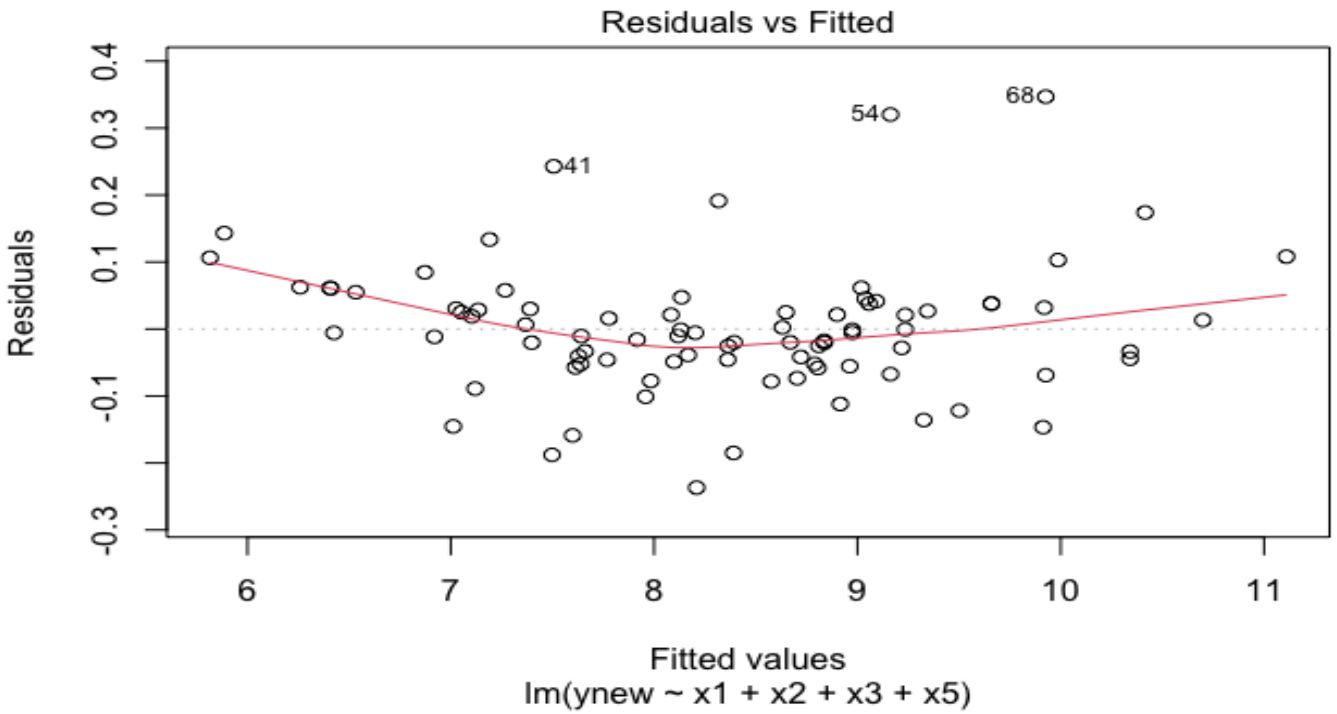
Residual Analysis

- After transformation, **linearity** and **independence** assumptions still hold **Multicollinearity** is not a serious issue, as all VIFs are well within the limit
- **Normality** of error terms is still not satisfied, but greatly improved



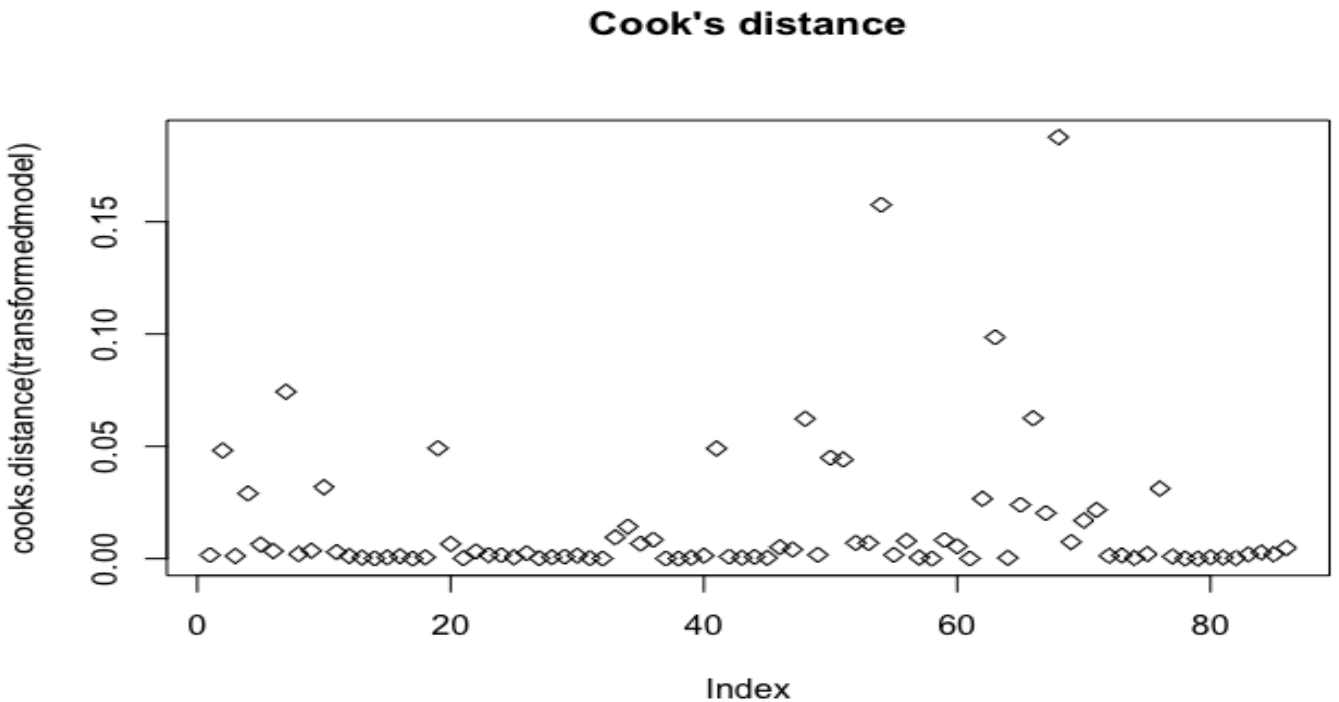
Residual Analysis

- **Homoscedasticity** is still not satisfied but greatly improved from previous plot. Curvature has weakened



Residual Analysis

- From Bonferroni limit, DFFITS and Cook's distances, and leverage points, no case is particularly alarming as an **outlier**



Final Model for future predictions of Blend KV40

- The interaction terms dropped just before variable selection were checked again using added variable plots, but none could have improved the model. Final transformed model is

$$Y' = \beta_0 + \sum_{i=1}^{3} \beta_i X_i + \beta_5 X_5 + \epsilon \tag{4}$$

$Y'$is the square root transformation of the Blend KV40 (response)

β_0, β_i, & β_5 are constants

ϵ iid Normal$(0, \sigma^2)$

- Retained variables are: DI, VM, BS Density and BS KV40

Final Model for future predictions of Blend KV40

Table: ANOVA Table for the Final Model

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
x1(DI)	1	1.334	1.334	137.238	0
x2(VM)	1	54.382	54.382	5,595.461	0
x3(BS Density)	1	24.667	24.667	2,538.046	0
x5(BS KV40)	1	30.015	30.015	3,088.242	0
Residuals	81	0.787	0.010		

Final Model for future predictions of Blend KV40

Table: Coefficients and SEs – All predictors are significant at $\alpha = 0.05$

	Dependent variable:
	ynew
x1(DI)	12.212^{***}
	(0.423)
x2(VM)	35.681^{***}
	(0.496)
x3(BS Density)	15.657^{***}
	(1.712)
x5(BS KV40)	0.125^{***}
	(0.002)
Constant	-11.825^{***}
	(1.399)
Observations	86
R^2	0.993
Adjusted R^2	0.993
Residual Std. Error	0.099 (df = 81)
F Statistic	$2{,}839.747^{***}$ (df = 4; 81)
Note:	*p<0.1; **p<0.05; ***p<0.01

Thank You!