Wine: Chemical Analysis
Full-Out Linear Regression
- Model
- Diagnostics
- Transformation
- Random Effect Model

I

I fit a linear model with quality as a response and the rest of variables as predictors, but I noticed that response is a discrete variable which can be thought of as being treated a continuous variable in this regression, and the problem naturally arises later in residual vs fit plot.

```
> summary(lmod)

Call:
lm(formula = quality ~ facidity + vacidity + citric + rsugar +
    chlorides + fso2 + tso2 + density + pH + so4 + alcohol)

Residuals:
     Min       1Q   Median       3Q      Max
-2.68911 -0.36652 -0.04699  0.45202  2.02498

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  2.197e+01  2.119e+01   1.036   0.3002
facidity     2.499e-02  2.595e-02   0.963   0.3357
vacidity    -1.084e+00  1.211e-01  -8.948  < 2e-16 ***
citric      -1.826e-01  1.472e-01  -1.240   0.2150
rsugar       1.633e-02  1.500e-02   1.089   0.2765
chlorides   -1.874e+00  4.193e-01  -4.470 8.37e-06 ***
fso2         4.361e-03  2.171e-03   2.009   0.0447 *
tso2        -3.265e-03  7.287e-04  -4.480 8.00e-06 ***
density     -1.788e+01  2.163e+01  -0.827   0.4086
pH          -4.137e-01  1.916e-01  -2.159   0.0310 *
so4          9.163e-01  1.143e-01   8.014 2.13e-15 ***
alcohol      2.762e-01  2.648e-02  10.429  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.648 on 1587 degrees of freedom
Multiple R-squared:  0.3606,     Adjusted R-squared:  0.3561
F-statistic: 81.35 on 11 and 1587 DF,  p-value: < 2.2e-16
```

I perform model selection by backward selection based on elimination of variable with the largest p-value.

The largest p-value is with the variate density

```
> lmod1 = update(lmod, .~., -density)
> summary(lmod1)

Call:
lm(formula = quality ~ facidity + vacidity + citric + rsugar +
    chlorides + fso2 + tso2 + pH + so4 + alcohol)

Residuals:
     Min       1Q   Median       3Q      Max
-2.67204 -0.36527 -0.04523  0.45628  2.03894

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  4.4538341  0.6125783   7.271 5.59e-13 ***
facidity     0.0081441  0.0160586   0.507  0.61212
vacidity    -1.0964449  0.1200866  -9.130  < 2e-16 ***
citric      -0.1836098  0.1471561  -1.248  0.21232
rsugar       0.0089507  0.0120542   0.743  0.45787
chlorides   -1.9067341  0.4173928  -4.568 5.30e-06 ***
fso2         0.0045147  0.0021631   2.087  0.03704 *
tso2        -0.0033120  0.0007264  -4.560 5.52e-06 ***
pH          -0.5042762  0.1571117  -3.210  0.00136 **
so4          0.8928974  0.1107548   8.062 1.46e-15 ***
alcohol      0.2927427  0.0173394  16.883  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.6479 on 1588 degrees of freedom
Multiple R-squared:  0.3603,     Adjusted R-squared:  0.3562
F-statistic: 89.43 on 10 and 1588 DF,  p-value: < 2.2e-16
```

The largest p-value is now with the variate rsugar

```
> lmod2 <- lm(quality ~ facidity + vacidity + citric + chlorides +
fso2 + tso2 + pH + so4 + alcohol)
> summary(lmod2)

Call:
lm(formula = quality ~ facidity + vacidity + citric + chlorides +
    fso2 + tso2 + pH + so4 + alcohol)
```

```
Residuals:
     Min       1Q   Median       3Q      Max 
-2.68601 -0.36723 -0.04516  0.45629  2.02723 

Coefficients:
              Estimate Std. Error t value Pr(>|t|)    
(Intercept)  4.4410923  0.6122514   7.254 6.31e-13 ***
facidity     0.0090201  0.0160129   0.563  0.57331    
vacidity    -1.0905804  0.1198096  -9.103  < 2e-16 ***
citric      -0.1756500  0.1467444  -1.197  0.23149    
chlorides   -1.8893071  0.4166737  -4.534 6.21e-06 ***
fso2         0.0046664  0.0021532   2.167  0.03036 *  
tso2        -0.0032560  0.0007224  -4.507 7.04e-06 ***
pH          -0.5022333  0.1570654  -3.198  0.00141 ** 
so4          0.8872849  0.1104810   8.031 1.86e-15 ***
alcohol      0.2940206  0.0172514  17.043  < 2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.6479 on 1589 degrees of freedom
Multiple R-squared:  0.3601,	Adjusted R-squared:  0.3564 
F-statistic: 99.34 on 9 and 1589 DF,  p-value: < 2.2e-16

> lmod3 <- lm(quality ~ vacidity + citric + chlorides + fso2 + tso2 + 
pH + so4 + alcohol)
> summary(lmod3)

Call:
lm(formula = quality ~ vacidity + citric + chlorides + fso2 + 
    tso2 + pH + so4 + alcohol)

Residuals:
     Min       1Q   Median       3Q      Max 
-2.66890 -0.37044 -0.04474  0.45697  2.02363 

Coefficients:
              Estimate Std. Error t value Pr(>|t|)    
(Intercept)  4.6680876  0.4608410  10.129  < 2e-16 ***
vacidity    -1.0736123  0.1159362  -9.260  < 2e-16 ***
citric      -0.1295444  0.1217717  -1.064   0.2876    
chlorides   -1.9494185  0.4026906  -4.841 1.42e-06 ***
fso2         0.0047601  0.0021463   2.218   0.0267 *  
tso2        -0.0033658  0.0006954  -4.840 1.42e-06 ***
pH          -0.5491501  0.1331350  -4.125 3.90e-05 ***
```

```
so4           0.8914283  0.1102122   8.088 1.19e-15 ***
alcohol       0.2928780  0.0171280  17.099  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.6477 on 1590 degrees of freedom
Multiple R-squared:  0.3599,     Adjusted R-squared:  0.3567
F-statistic: 111.8 on 8 and 1590 DF,  p-value: < 2.2e-16

> lmod4 <- lm(quality ~ vacidity + chlorides + fso2 + tso2 + pH + so4
+ alcohol)
> summary(lmod4)

Call:
lm(formula = quality ~ vacidity + chlorides + fso2 + tso2 + pH + 
    so4 + alcohol)

Residuals:
     Min       1Q   Median       3Q      Max 
-2.68918 -0.36757 -0.04653  0.46081  2.02954 

Coefficients:
              Estimate Std. Error t value Pr(>|t|)    
(Intercept)  4.4300987  0.4029168  10.995  < 2e-16 ***
vacidity    -1.0127527  0.1008429 -10.043  < 2e-16 ***
chlorides   -2.0178138  0.3975417  -5.076 4.31e-07 ***
fso2         0.0050774  0.0021255   2.389    0.017 *  
tso2        -0.0034822  0.0006868  -5.070 4.43e-07 ***
pH          -0.4826614  0.1175581  -4.106 4.23e-05 ***
so4          0.8826651  0.1099084   8.031 1.86e-15 ***
alcohol      0.2893028  0.0167958  17.225  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.6477 on 1591 degrees of freedom
Multiple R-squared:  0.3595,     Adjusted R-squared:  0.3567
F-statistic: 127.6 on 7 and 1591 DF,  p-value: < 2.2e-16
```

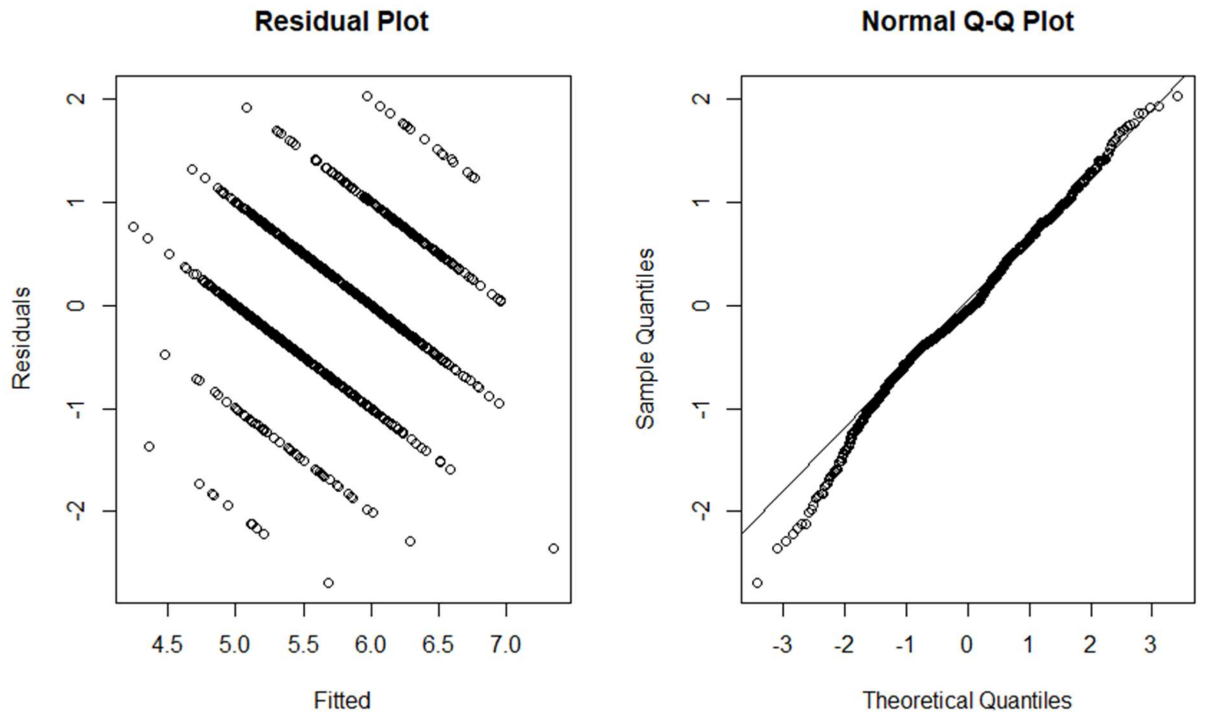
We have eliminated the following variables in order: density, residual sugar, fixed acidity, and citric acid.

No other variables have high enough p-value to be eliminated anymore.

Using backward elimination based on AIC value also reaches the same model.

```
> step(lmod)
Start:  AIC=-1375.49
quality ~ facidity + vacidity + citric + rsugar + chlorides + 
    fso2 + tso2 + density + pH + so4 + alcohol

            Df Sum of Sq    RSS     AIC
- density    1     0.287 666.70 -1376.8
- facidity   1     0.389 666.80 -1376.5
- rsugar     1     0.498 666.91 -1376.3
- citric     1     0.646 667.06 -1375.9
<none>                   666.41 -1375.5
- fso2       1     1.694 668.10 -1373.4
- pH         1     1.957 668.37 -1372.8
- chlorides  1     8.391 674.80 -1357.5
- tso2       1     8.427 674.84 -1357.4
- so4        1    26.971 693.38 -1314.0
- vacidity   1    33.620 700.03 -1298.8
- alcohol    1    45.672 712.08 -1271.5

Step:  AIC=-1376.8
quality ~ facidity + vacidity + citric + rsugar + chlorides + 
    fso2 + tso2 + pH + so4 + alcohol

            Df Sum of Sq    RSS     AIC
- facidity   1     0.108 666.81 -1378.5
- rsugar     1     0.231 666.93 -1378.2
- citric     1     0.654 667.35 -1377.2
<none>                   666.70 -1376.8
- fso2       1     1.829 668.53 -1374.4
- pH         1     4.325 671.02 -1368.5
- tso2       1     8.728 675.43 -1358.0
- chlorides  1     8.761 675.46 -1357.9
- so4        1    27.287 693.98 -1314.7
- vacidity   1    35.000 701.70 -1297.0
- alcohol    1   119.669 786.37 -1114.8

Step:  AIC=-1378.54
quality ~ vacidity + citric + rsugar + chlorides + fso2 + tso2 + 
    pH + so4 + alcohol

            Df Sum of Sq    RSS     AIC
- rsugar     1     0.257 667.06 -1379.9
- citric     1     0.565 667.37 -1379.2
<none>                   666.81 -1378.5
- fso2       1     1.901 668.71 -1376.0
- pH          1     7.065 673.87 -1363.7
- chlorides   1     9.940 676.75 -1356.9
- tso2        1    10.031 676.84 -1356.7
- so4         1    27.673 694.48 -1315.5
- vacidity    1    36.234 703.04 -1295.9
- alcohol     1   120.633 787.44 -1114.7

Step:  AIC=-1379.93
quality ~ vacidity + citric + chlorides + fso2 + tso2 + pH +
    so4 + alcohol

            Df Sum of Sq    RSS     AIC
- citric     1     0.475 667.54 -1380.8
<none>                   667.06 -1379.9
- fso2       1     2.064 669.13 -1377.0
- pH         1     7.138 674.20 -1364.9
- tso2       1     9.828 676.89 -1358.5
- chlorides  1     9.832 676.89 -1358.5
- so4        1    27.446 694.51 -1317.5
- vacidity   1    35.977 703.04 -1297.9
- alcohol    1   122.667 789.73 -1112.0

Step:  AIC=-1380.79
quality ~ vacidity + chlorides + fso2 + tso2 + pH + so4 + alcohol

            Df Sum of Sq    RSS     AIC
<none>                   667.54 -1380.8
- fso2       1     2.394 669.93 -1377.1
- pH         1     7.073 674.61 -1365.9
- tso2       1    10.787 678.32 -1357.2
- chlorides  1    10.809 678.35 -1357.1
- so4        1    27.060 694.60 -1319.2
- vacidity   1    42.318 709.85 -1284.5
- alcohol    1   124.483 792.02 -1109.4

Call:
lm(formula = quality ~ vacidity + chlorides + fso2 + tso2 + pH +
    so4 + alcohol)

Coefficients:
(Intercept)     vacidity    chlorides         fso2         tso2
pH          so4      alcohol
   4.430099    -1.012753    -2.017814     0.005077    -0.003482    -
0.482661     0.882665     0.289303
```

I check the model assumptions. The two diagnostic plots are presented:



It is difficult to interpret this residual plot. The diagonal streaks arise from discrete values of wine quality. The qqplot suggests that the distribution of residuals is slightly light-tailed on the left tail of distribution.

```
> shapiro.test(residuals(lmod))

        Shapiro-Wilk normality test

data:  residuals(lmod)
W = 0.99137, p-value = 4.321e-08
```

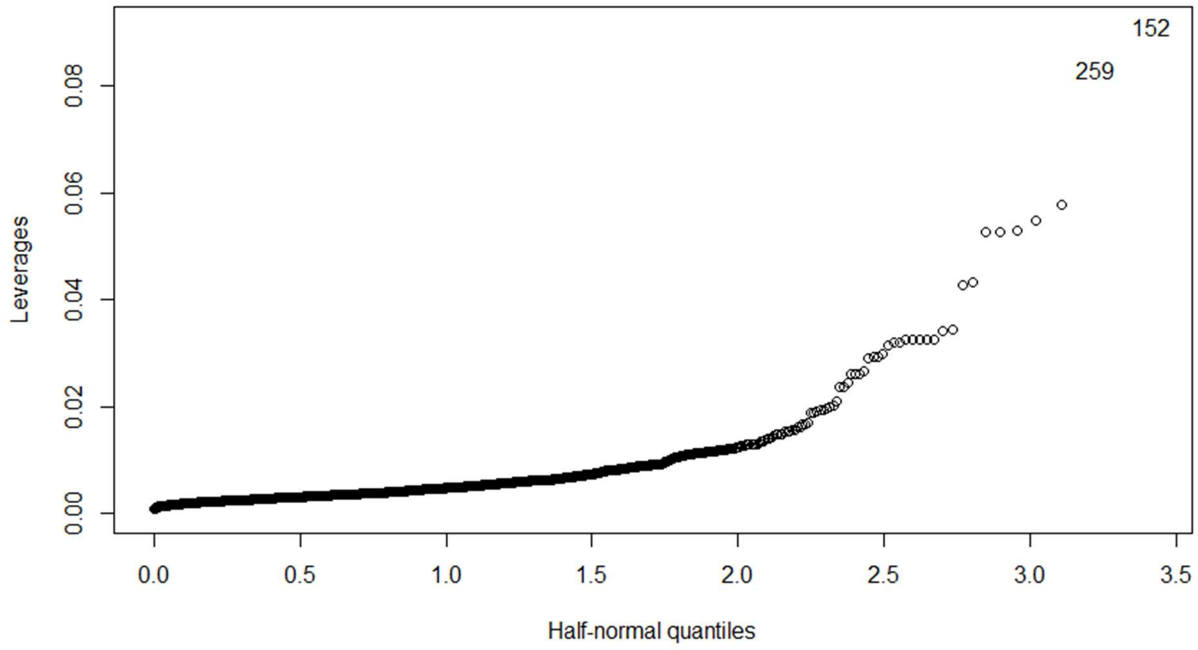
Shapiro test punishes hard for mild deviation from normality and as such gives a verdict that the distribution is clearly not normal.
Recall that for short-tailed distribution the large sample size allows us to make estimation of coefficients, so we have little reason to abandon linear regression. However, it does not allow inference such as confidence intervals.
The model also fails Durbin Watson test implying errors are heavily correlated.

```
> dwtest(quality ~ vacidity + chlorides + fso2 + tso2 + pH + so4 +
alcohol)

        Durbin-Watson test
```

```
data:  quality ~ vacidity + chlorides + fso2 + tso2 + pH + so4 +
alcohol
DW = 1.75, p-value = 2.345e-07
alternative hypothesis: true autocorrelation is greater than 0
As such I use bootstrap confidence intervals for coefficients.
```

One solution is to build covariance structure into the model via GLS, but it is not done here.

Now checking to see if we need to remove any data points, I first make a half-normal plot of leverage. There are two data points (152 and 259) that have high leverages and diverge substantially from the rest of the data.

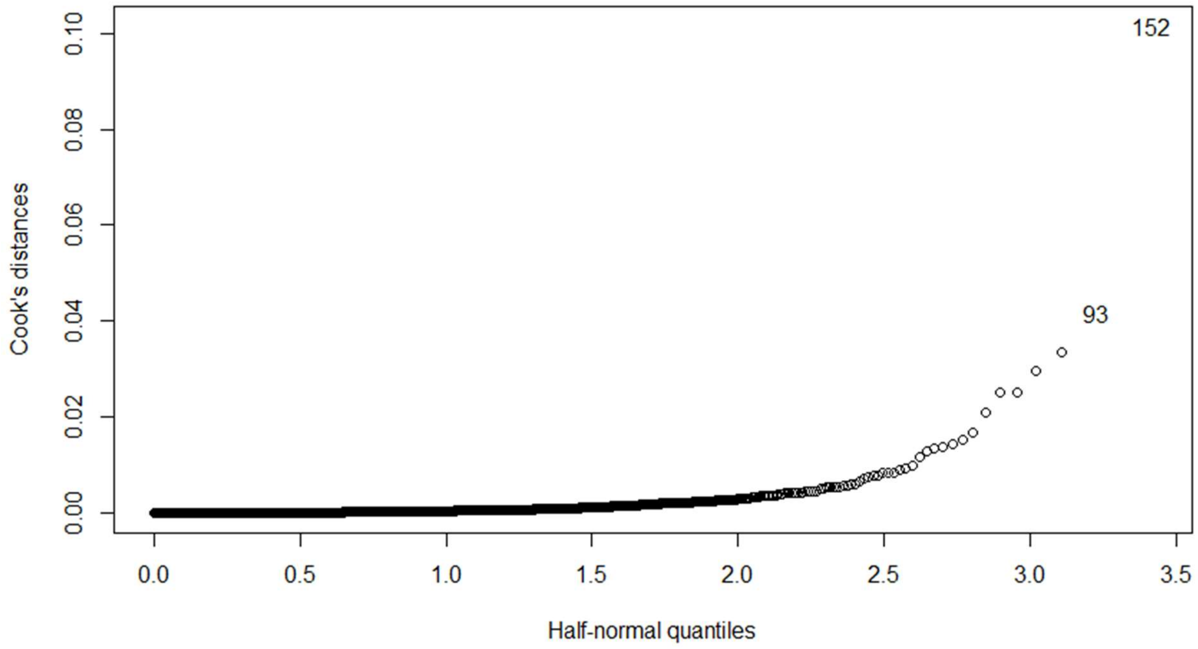


Next, I compute leave-one-out residuals

```
> tail(jack[order(abs(jack))])
      460       900      1506      1277       653       833
-3.284724 -3.349168 -3.434795 -3.550248 -3.678457 -4.185391
> qt(.05/(1599*2),1599-8)
[1] -4.176048
> jack[152]
      152
-2.851774
```

Considering I used Bonferronni correction which is conservative in finding fewer outliers than the nominal level of confidence would dictate, the data point 833 is way beyond the confidence level.

Next we find the most influential points:



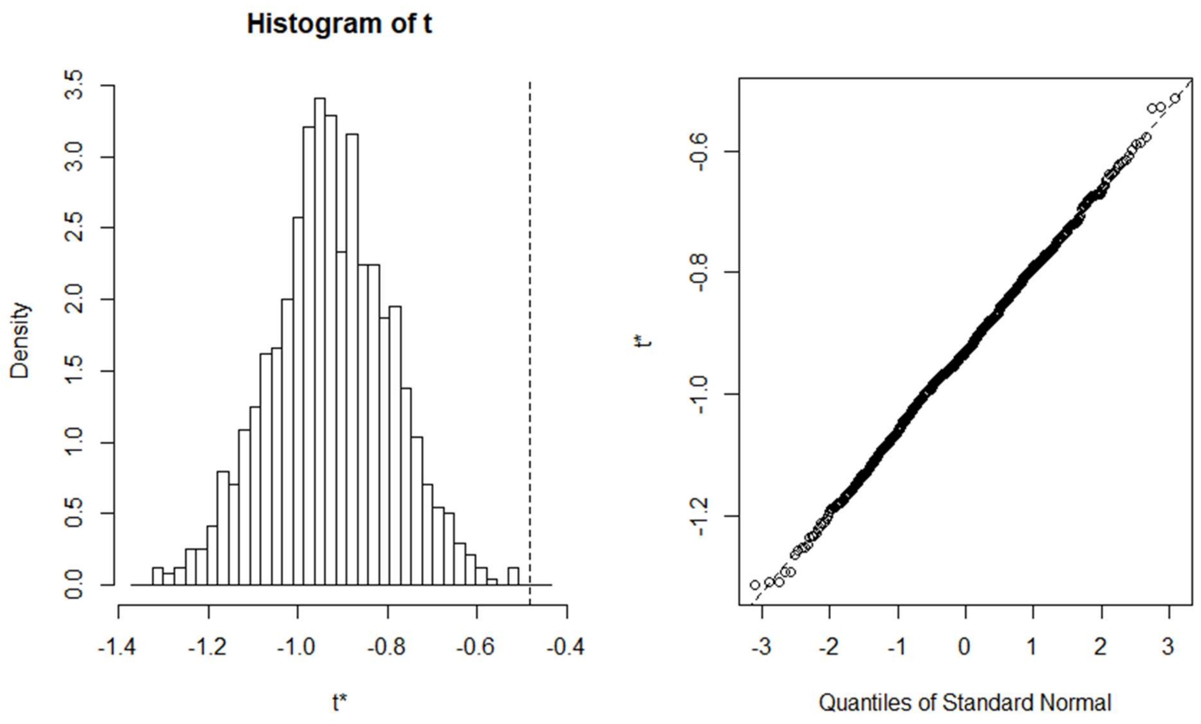
We try excluding this particular point 152, which also had the highest leverage. Recall that 152 had t-score of -2.85 which is quite high.

```
> summary(lm(quality ~ vacidity + chlorides + fso2 + tso2 + pH + so4 +
alcohol, subset=(cook<max(cook))))

Call:
lm(formula = quality ~ vacidity + chlorides + fso2 + tso2 + pH +
    so4 + alcohol, subset = (cook < max(cook)))

Residuals:
     Min       1Q   Median       3Q      Max
-2.71375 -0.36843 -0.04987  0.46154  2.03385

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  4.4002381  0.4021530  10.942  < 2e-16 ***
vacidity    -1.0051906  0.1006526  -9.987  < 2e-16 ***
chlorides   -1.7757498  0.4056341  -4.378 1.28e-05 ***
fso2         0.0053602  0.0021231   2.525   0.0117 *
tso2        -0.0035385  0.0006855  -5.162 2.76e-07 ***
pH          -0.4912605  0.1173342  -4.187 2.98e-05 ***
so4          0.9136403  0.1101995   8.291 2.37e-16 ***
```

```
alcohol      0.2904650  0.0167632  17.328  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.6463 on 1590 degrees of freedom
Multiple R-squared:  0.3611,    Adjusted R-squared:  0.3583
F-statistic: 128.4 on 7 and 1590 DF,  p-value: < 2.2e-16
```

I observed that there is no significant change in the model. P-values are roughly the same for predictors and the estimates do not change. As a final model I decided not to exclude any data point for the reason that they do not change the model substantially and removing outlier automatically without understanding physical context of data can be dangerous.

In order to estimate confidence interval, I use bootstrap method because it does not require any distributional assumptions and provide more accurate inferences when the data are not well behaved.



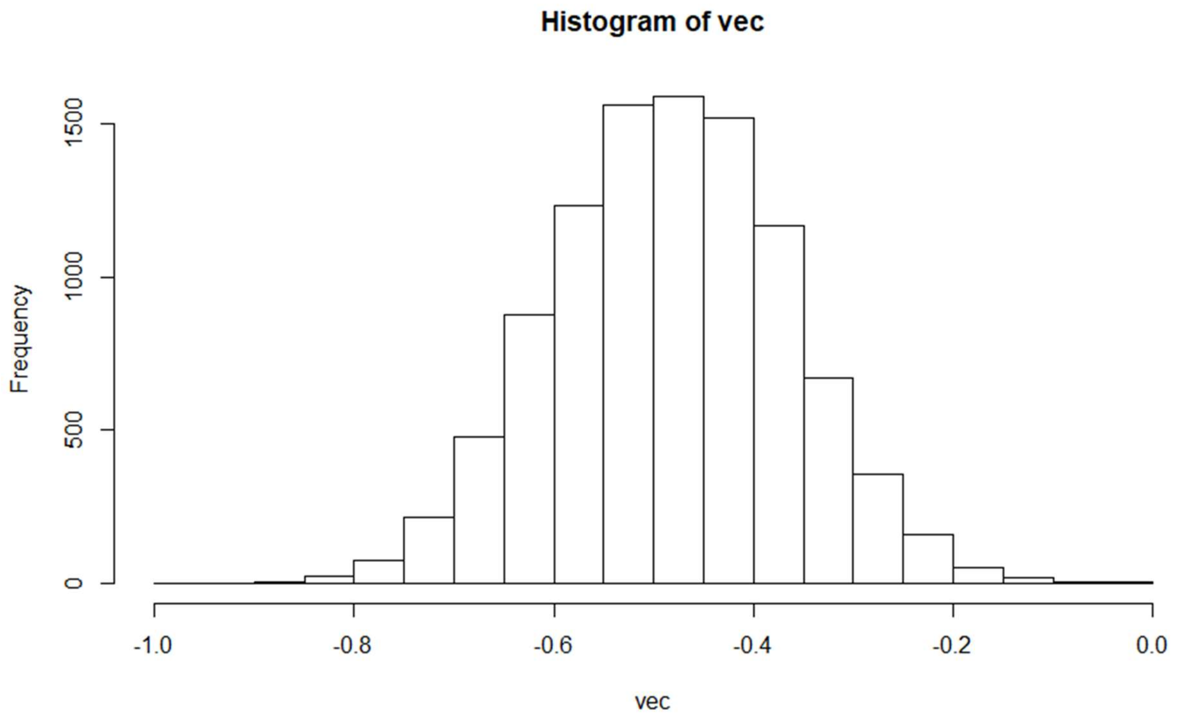
```
ORDINARY NONPARAMETRIC BOOTSTRAP


Call:
boot(data = wine, statistic = bs, R = 1000, formula = quality ~
    vacidity + chlorides + fso2 + tso2 + pH + so4 + alcohol)


Bootstrap Statistics :
        original       bias     std. error
t1*  4.430098698  0.433583029 0.4640263454
t2* -1.012752700  1.005001221 0.1023640512
t3* -2.017813817  0.912322429 0.4125870793
t4*  0.005077370 -0.004975567 0.0022538235
t5* -0.003482245  0.003449912 0.0007027508
t6* -0.482661444 -0.444583503 0.1329182029
t7*  0.882665133 -0.877056724 0.1056710125
t8*  0.289302753  0.088698475 0.0192353832
```

`t6` represents the coefficient for pH.

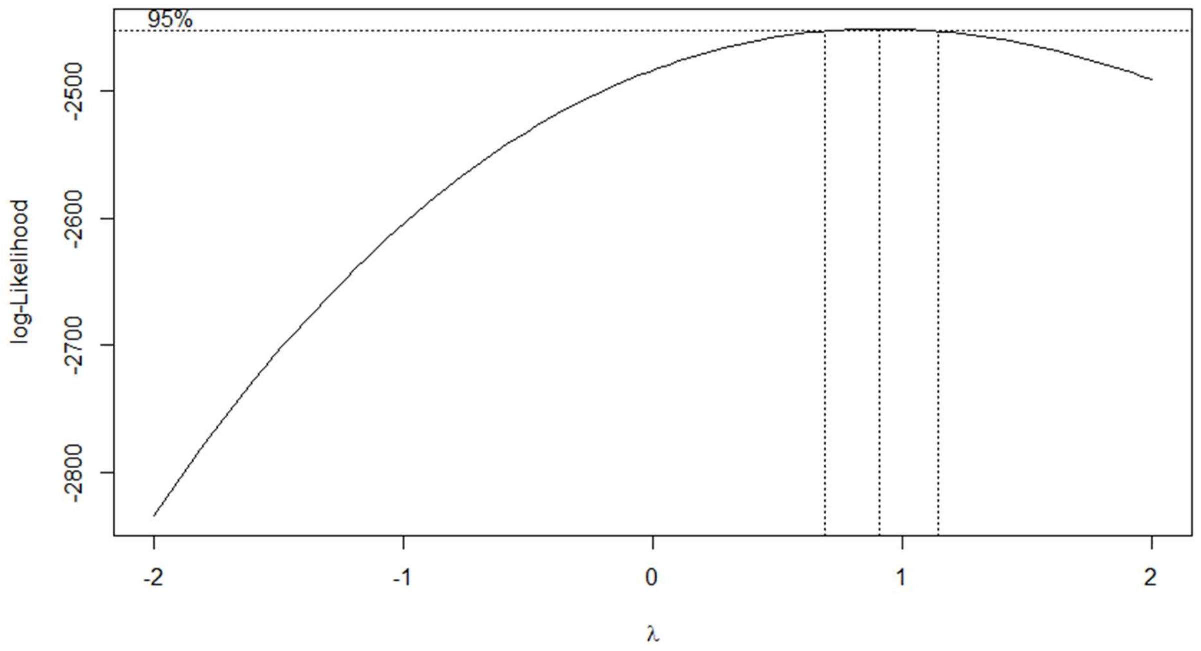
The confidence interval is obtained via:

```
> lmod = lm(quality ~ vacidity + chlorides + fso2 + tso2 + pH + so4 +
alcohol)
> preds = fitted(lmod)
> resids = residuals(lmod)
> vec=numeric(10000)
> for(i in 1:10000) {
+   ynew = preds + sample(resids, rep=TRUE)
+   vec[i]=summary(lm(ynew ~ vacidity + chlorides + fso2 + tso2 + pH +
so4 + alcohol))$coef[6]
+ }
> par(mfrow=c(1,1))

> a = -0.48266
> length(vec[vec>a])/10000
[1] 0.4976
> sort(vec)[250]
[1] -0.7126148
> sort(vec)[9750]
[1] -0.2534445
```

The confidence interval (95%) for the parameter is (-0.7126,-0.2534)



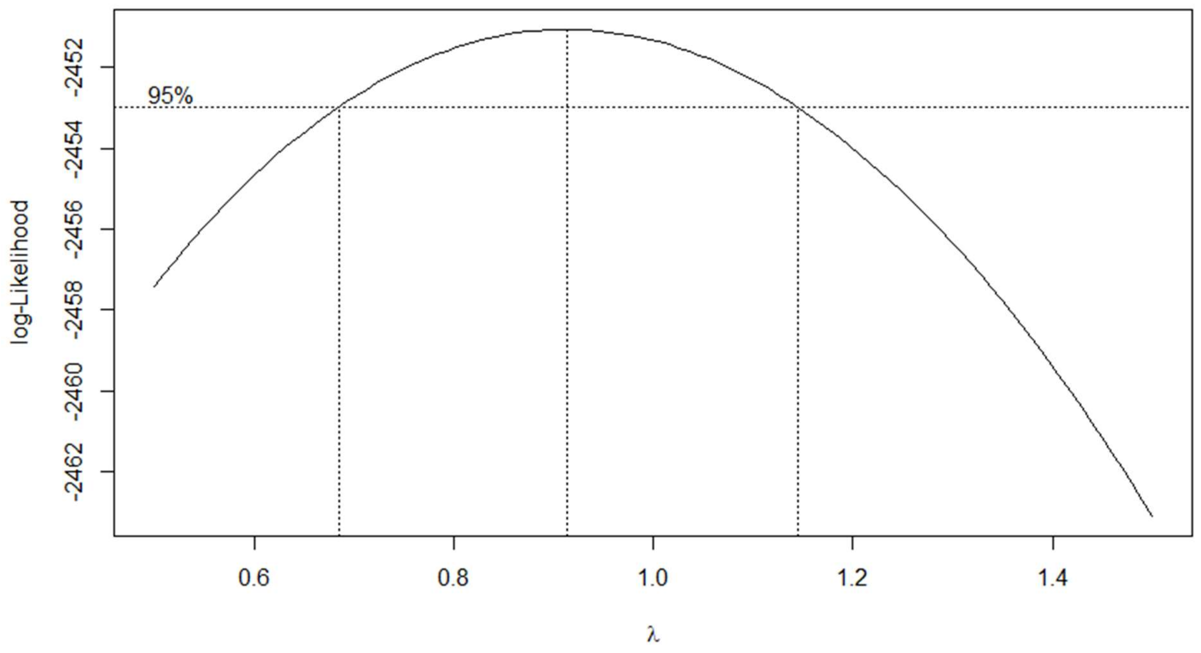
I look to find a suitable box-cox transformation that can change the model. Following is the log-likelihood of the box-coefficient parameter lambda.



The plot suggests that the box-cox parameter is nearly 1. To be more precise,

```
> head(cbind(boxcox(lmod)$x, boxcox(lmod)$y)[order(-boxcox(lmod)$y),])
          [,1]      [,2]
[1,] 0.9090909 -2451.054
[2,] 0.9494949 -2451.103
[3,] 0.8686869 -2451.125
[4,] 0.9898990 -2451.269
[5,] 0.8282828 -2451.315
[6,] 1.0303030 -2451.552
```

The parameter is approximately 0.91.



The 95% confidence interval runs from 0.7 to 1.15. There is no good reason to transform.

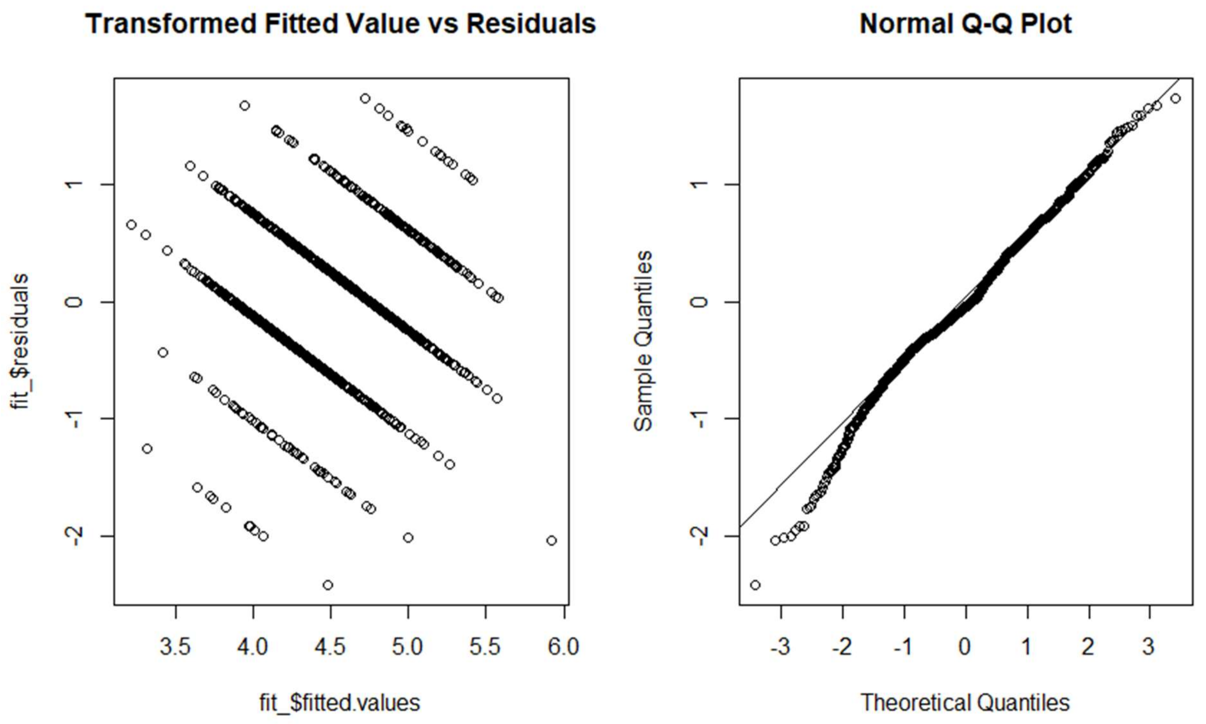
However, it might be a good idea to compare the transformed model with the original. With the techniques I learned in class, R-squared and AIC/BIC cannot be used to compare the models that are not nested or use the same set of data. Once the model is transformed by power transform or logarithm, response or predictor variable has different values, and R-squared cannot be compared between a model with untransformed Y and one with transformed Y. Not only that, we know the original model is flawed in that residuals are correlated and slightly non-normal, sowe cannot quite compute R-squared.

We are interested in formulating a model that has predictive power. As such, we compare how much less error a model. We can root-mean-squared/ cross-validation approach, where we compare the predictive power of each model.

Here is the box-cox transformed model with the power =0.91.

```
Call:
lm(formula = quality_ ~ vacidity + chlorides + fso2 + tso2 + 
    pH + so4 + alcohol)

Residuals:
     Min       1Q   Median       3Q      Max 
-2.41485 -0.31422 -0.03772  0.40452  1.73805 

Coefficients:
             Estimate Std. Error t value Pr(>|t|)    
(Intercept)  3.395289   0.351431   9.661  < 2e-16 ***
vacidity    -0.888548   0.087957 -10.102  < 2e-16 ***
chlorides   -1.758634   0.346743  -5.072 4.40e-07 ***
fso2         0.004448   0.001854   2.399   0.0165 *  
tso2        -0.003014   0.000599  -5.032 5.40e-07 ***
pH          -0.418804   0.102536  -4.084 4.64e-05 ***
so4          0.766301   0.095864   7.994 2.50e-15 ***
alcohol      0.250546   0.014650  17.103  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.565 on 1591 degrees of freedom
Multiple R-squared:  0.3579,	Adjusted R-squared:  0.3551 
F-statistic: 126.7 on 7 and 1591 DF,  p-value: < 2.2e-16
```

Looking at the diagnostics, the transformation doesn't significantly improve the assumptions.



```
> trainwine <- wine[1:1400,]
> testwine <- wine[1401:1599,]
>
> mod1 <- lm(quality ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates +
alcohol, data=trainwine)
> mod2 <- lm(((quality -1)^0.91)/0.91 ~ volatile.acidity +
chlorides + free.sulfur.dioxide + total.sulfur.dioxide + pH +
sulphates + alcohol, data=trainwine)
>
> rmse(predict(mod1,testwine), testwine$quality)
[1] 0.6994192
> rmse(predict(mod2,testwine), testwine$quality)
[1] 1.304175
```

I noticed that the RMSE of the original model is smaller, which means it incurs smaller prediction error. I divided the data into 8 training/testing sets, computed rmse for each, and averaged them. Then I have 0.658for the first model and 1.367.

```
> (0.699 + 0.631+0.623 + 0.692 + 0.613 + 0.679 +0.666 + 0.662)/8
[1] 0.658125
> (1.304 + 1.269 + 1.495 + 1.412 + 1.296 + 1.425 + 1.53 + 1.207)/8
[1] 1.36725
```

There is a caution to this result however. The root mean squared contains error sigma-squared, and if they are substantially different, it becomes difficult to compare the root mean squared. Looking at the estimated residual standard error, we see that they are slightly different: 0.64 vs 0.56. However, the difference appears small enough that we can compare the root mean squared (data-driven comparison measure) to see which model is better in terms of prediction error given the data.

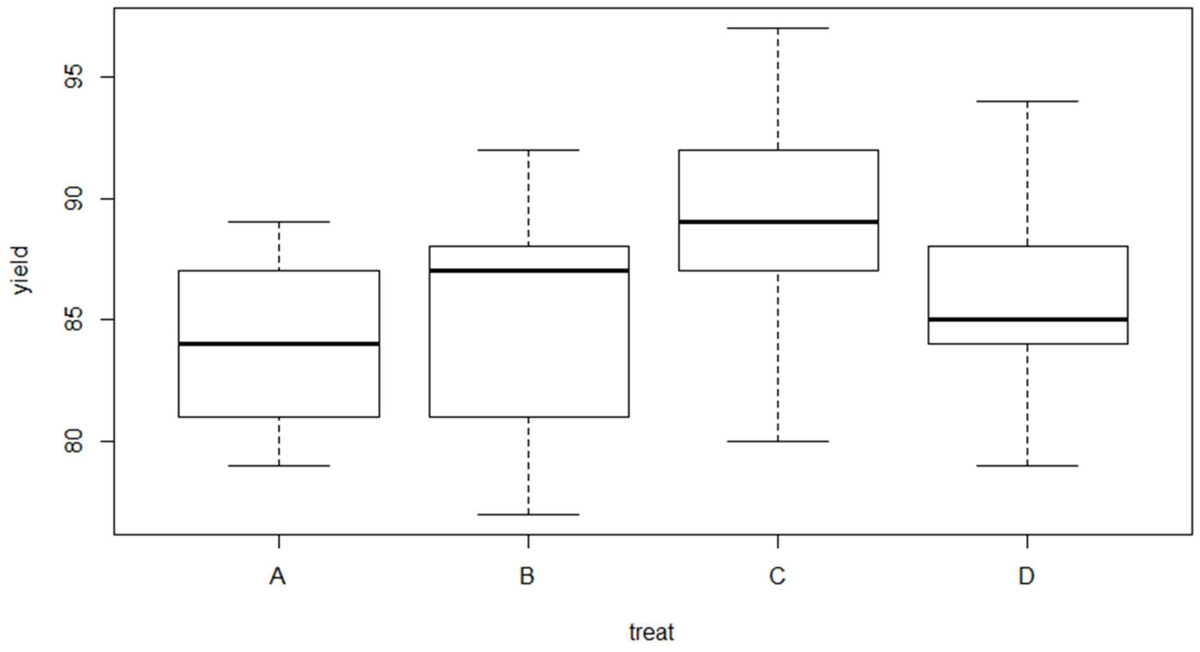
II.

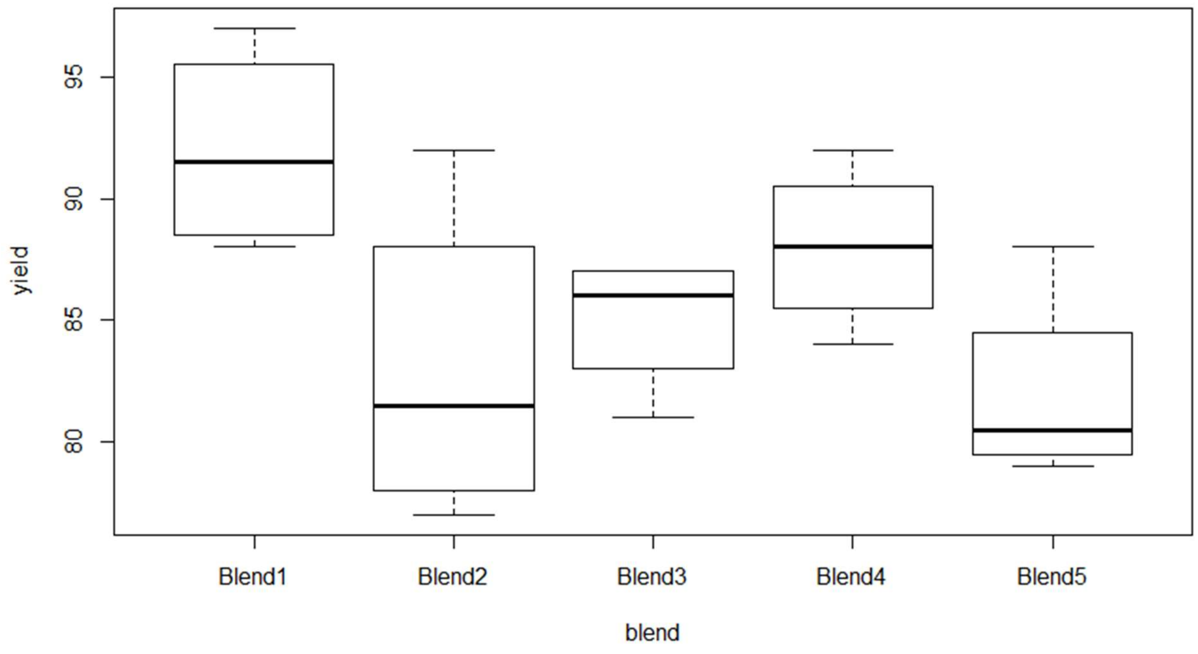
To reiterate the problem and identify its components, we have four processes of production from A to D - labeled as “treat”,and the five types of blend are the fixed effect (which will be changed to random effect later)

We run regression of yield on the sum of dummy variables for treatment and blend, which R sets up automatically. Intercept is the reference level (or treat A), and the others are its relative magnitude.

```
> lmod <- lm(yield ~ treat + blend, penicillin)
> summary(lmod)

Call:
lm(formula = yield ~ treat + blend, data = penicillin)

Residuals:
   Min     1Q Median     3Q    Max 
 -5.00  -2.25  -0.50   2.25   6.00 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)   90.000      2.745  32.791  4.1e-13 ***
treatB         1.000      2.745   0.364  0.72194    
treatC         5.000      2.745   1.822  0.09351 .  
treatD         2.000      2.745   0.729  0.48018    
blendBlend2   -9.000      3.069  -2.933  0.01254 *  
blendBlend3   -7.000      3.069  -2.281  0.04159 *  
blendBlend4   -4.000      3.069  -1.304  0.21686    
blendBlend5  -10.000      3.069  -3.259  0.00684 ** 
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 4.34 on 12 degrees of freedom
Multiple R-squared:  0.5964,     Adjusted R-squared:  0.361 
F-statistic: 2.534 on 7 and 12 DF,  p-value: 0.07535

> lmod_ <- lm(yield ~ blend, penicillin)
> anova(lmod,lmod_)
Analysis of Variance Table

Model 1: yield ~ treat + blend
Model 2: yield ~ blend
  Res.Df RSS Df Sum of Sq      F Pr(>F)
1     12 226
2     15 296 -3       -70 1.2389 0.3387
```

According to the summary of regression, none of the treatments is significant, which means none of the treatments is significantly different from A. When we look at the boxplots of each process with yield, the means are not very different from one another except C, whose p-value is low. On the other hand, there seems to be no block effect except blend 2, 3, and 5, which are significant. As seen in the boxplot, there seem to be significant difference in means among each blend. If we look at the anova test comparing the model without treatment and with treatment, the F-statistic p-value is high, so we can conclude the treatments are not significant.





Using blends increases efficiency as it reduces the variance of the model, where `lmod` is the blocked model whereas the unblocked model is `lmod2` whose variance is underlined. The efficiency is 30.625/18.833 = 1.62 > 1,which implies it is easier to detect treatment effect under RCBD.

```
> anova(lmod)
Analysis of Variance Table

Response: yield
          Df Sum Sq Mean Sq F value  Pr(>F)  
treat      3     70  23.333  1.2389 0.33866  
blend      4    264  66.000  3.5044 0.04075 *
Residuals 12    226  18.833                  
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1


> anova(lmod2)
Analysis of Variance Table

Response: yield
          Df Sum Sq Mean Sq F value Pr(>F)
treat      3     70  23.333  0.7619 0.5318
```

```
Residuals 16    490  30.625
```

Now I consider blend as the random effect whose noise is correlated with each block, so I am interested in the variance of this random effect.Using `gls` function simply as follows means we are considering both treatment and block as random variables, and is wrong.

```
> gls(yield ~ treat + blend, penicillin)
Generalized least squares fit by REML
  Model: yield ~ treat + blend
  Data: penicillin
  Log-restricted-likelihood: -39.82778

Coefficients:
(Intercept)      treatB      treatC      treatD blendBlend2
blendBlend3 blendBlend4 blendBlend5
         90           1           5           2          -9           -
7          -4         -10

Degrees of freedom: 20 total; 12 residual
Residual standard error: 4.339739
```

If we consider RCBD with one random effect and the variance of random effect, we can regress yield on treat with `gls` and treat its residual error as the sum of sigma-squared(variance of OLS) and v-squared (variance of random effect). Thus, we compute the residual variance of GLS and subtract by sigma-squared (variance of OLS), which is v-squared (variance of random effect). We have v^2 = 5.53^2 - 4.34^2 = 12.

```
> glmod <- gls(yield ~ treat, penicillin)
> summary(glmod) #5.533 = 30.61
Generalized least squares fit by REML
  Model: yield ~ treat
  Data: penicillin
       AIC      BIC    logLik
  116.5929 120.4558 -53.29643

Coefficients:
            Value Std.Error  t-value p-value
(Intercept)    84  2.474874 33.94113  0.0000
treatB          1  3.500000  0.28571  0.7788
treatC          5  3.500000  1.42857  0.1724
treatD          2  3.500000  0.57143  0.5756

 Correlation:
       (Intr) treatB treatC
treatB -0.707
```

```
treatC -0.707  0.500
treatD -0.707  0.500  0.500

Standardized residuals:
       Min         Q1        Med         Q3        Max
-1.6263142 -0.5872801  0.0000000  0.5421047  1.4456126

Residual standard error: 5.533986
Degrees of freedom: 20 total; 16 residual

> lmod <- lm(yield ~ treat + blend, penicillin)
> summary(lmod) #4.34 = 18.83

Call:
lm(formula = yield ~ treat + blend, data = penicillin)

Residuals:
   Min     1Q Median     3Q    Max
 -5.00  -2.25  -0.50   2.25   6.00

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   90.000      2.745  32.791  4.1e-13 ***
treatB         1.000      2.745   0.364  0.72194
treatC         5.000      2.745   1.822  0.09351 .
treatD         2.000      2.745   0.729  0.48018
blendBlend2   -9.000      3.069  -2.933  0.01254 *
blendBlend3   -7.000      3.069  -2.281  0.04159 *
blendBlend4   -4.000      3.069  -1.304  0.21686
blendBlend5  -10.000      3.069  -3.259  0.00684 **
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 4.34 on 12 degrees of freedom
Multiple R-squared:  0.5964,     Adjusted R-squared:  0.361
F-statistic: 2.534 on 7 and 12 DF,  p-value: 0.07535
```

III.

The idea of transformation is attached. I implement the idea where I re-defined y_ as y-x2 and x_ as x1-x2, and obtain the coefficients as follows:

```
Call:
lm(formula = y_ ~ x_)
```

```
Coefficients:
(Intercept)           x_
     3.1956       0.3668
```

```
Call:
lm(formula = y_ ~ x_)

Residuals:
     Min       1Q   Median       3Q      Max 
-2.93143 -0.78183  0.01373  0.86331  2.49095 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)  3.19563    0.14641  21.827  < 2e-16 ***
x_           0.36676    0.09119   4.022 0.000114 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 1.1 on 98 degrees of freedom
Multiple R-squared:  0.1417,	Adjusted R-squared:  0.1329 
F-statistic: 16.18 on 1 and 98 DF,  p-value: 0.0001136
```

IV

R Code

```
# 1
load("C:/Users/jihun/Downloads/winequality.RData")
quality <- wine$quality
facidity <- wine$fixed.acidity
vacidity <- wine$volatile.acidity
citric <- wine$citric.acid
rsugar <- wine$residual.sugar
chlorides <- wine$chlorides
fso2 <- wine$free.sulfur.dioxide
tso2 <- wine$total.sulfur.dioxide
density <- wine$density
pH <- wine$pH
so4 <- wine$sulphates
alcohol <- wine$alcohol
# linear model
```

```
lmod <- lm(quality ~ facidity + vacidity + citric + rsugar + chlorides
+ fso2 + tso2 + density + pH + so4 + alcohol)
summary(lmod)
# model selection
step(lmod)
lmod4 <- lm(quality ~ vacidity + chlorides + fso2 + tso2 + pH + so4 +
alcohol)
summary(lmod4)
lmod=lmod4
# diagnostics
# homoscedasticity
par(mfrow=c(1,2))
plot(fitted(lmod),residuals(lmod),xlab="Fitted",ylab="Residuals",main=
"Residual Plot")
qqnorm(residuals(lmod))
qqline(residuals(lmod))
# normality
shapiro.test(residuals(lmod))
# independence
library(lmtest)
dwtest(quality ~ vacidity + chlorides + fso2 + tso2 + pH + so4 +
alcohol)

# outliers
# check leverages
halfnorm(lm.influence(lmod)$hat,ylab="Leverages")
# outlier
jack <- rstudent(lmod)
jack[which.max(abs(jack))]
tail(jack[order(abs(jack))])
qt(.05/(1599*2),1599-8)
jack[152]
# influence
cook <- cooks.distance(lmod)
halfnorm(cook, ylab="Cook's distances")
summary(lm(quality ~ vacidity + chlorides + fso2 + tso2 + pH + so4 +
alcohol, subset=(cook<max(cook))))



# bootstrap
library(boot)
# function to obtain regression weights
bs <- function(formula, data, indices) {
  d <- data[indices,] # allows boot to select sample
  fit <- lm(formula, data=d)
  return(coef(fit))
}
# bootstrapping with 1000 replications
results <- boot(data=wine, statistic=bs,
                R=1000, formula=quality ~ vacidity + chlorides + fso2
+ tso2 + pH + so4 + alcohol)

# view results
results
plot(results, index=6) # pH



lmod = lm(quality ~ vacidity + chlorides + fso2 + tso2 + pH + so4 +
alcohol)
preds = fitted(lmod)
resids = residuals(lmod)
vec=numeric(10000)
for(i in 1:10000) {
  ynew = preds + sample(resids, rep=TRUE)
  vec[i]=summary(lm(ynew ~ vacidity + chlorides + fso2 + tso2 + pH +
so4 + alcohol))$coef[6]
}
par(mfrow=c(1,1))
hist(vec)
a = -0.48266
length(vec[vec>a])/10000
sort(vec)[250]
sort(vec)[9750]
# Box-cox transformation
library(MASS)
boxcox(lmod, plotit=T)
head(cbind(boxcox(lmod)$x, boxcox(lmod)$y)[order(-boxcox(lmod)$y),])
boxcox(lmod,plotit=T,lambda=seq(0.5,1.5,by=0.1))

# data-driven approach

quality_ = ((quality -1)^0.91)/0.91
fit_ = lm(quality_ ~ vacidity + chlorides + fso2 + tso2 + pH + so4 +
alcohol)
summary(fit_)
par(mfrow=c(1,2))
plot(fit_$fitted.values,fit_$residuals,main="Transformed Fitted Value
vs Residuals")
```

```
qqnorm(fit_$residuals)
qqline(residuals(fit_))

library(Metrics)

trainwine <- wine[1:1400,]
testwine <- wine[1401:1599,]

mod1 <- lm(quality ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates + alcohol,
data=trainwine)
mod2 <- lm(((quality -1)^0.91)/0.91 ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates + alcohol,
data=trainwine)

rmse(predict(mod1,testwine), testwine$quality) # 0.6524137
rmse(predict(mod2,testwine), testwine$quality) # 1.283869

trainwine2 <- wine[-c(1201:1400),]
testwine2 <- wine[c(1201:1400),]
mod21 <- lm(quality ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates + alcohol,
data=trainwine2)
mod22 <- lm(((quality -1)^0.91)/0.91 ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates + alcohol,
data=trainwine2)

rmse(predict(mod21,testwine2), testwine2$quality) # 0.631
rmse(predict(mod22,testwine2), testwine2$quality) # 1.269

trainwine3 <- wine[-c(1001:1200),]
testwine3 <- wine[c(1001:1200),]
mod31 <- lm(quality ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates + alcohol,
data=trainwine3)
mod32 <- lm(((quality -1)^0.91)/0.91 ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates + alcohol,
data=trainwine3)

rmse(predict(mod31,testwine3), testwine3$quality) # 0.623
rmse(predict(mod32,testwine3), testwine3$quality) # 1.495

trainwine4 <- wine[-c(801:1000),]
testwine4 <- wine[c(801:1000),]
```

```
mod41 <- lm(quality ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates + alcohol,
data=trainwine4)
mod42 <- lm(((quality -1)^0.91)/0.91 ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates + alcohol,
data=trainwine4)

rmse(predict(mod41,testwine4), testwine4$quality) # 0.692
rmse(predict(mod42,testwine4), testwine4$quality) # 1.412

trainwine5 <- wine[-c(601:800),]
testwine5 <- wine[c(601:800),]
mod51 <- lm(quality ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates + alcohol,
data=trainwine5)
mod52 <- lm(((quality -1)^0.91)/0.91 ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates + alcohol,
data=trainwine5)

rmse(predict(mod51,testwine5), testwine5$quality) # 0.613
rmse(predict(mod52,testwine5), testwine5$quality) #1.296

trainwine6 <- wine[-c(401:600),]
testwine6 <- wine[c(401:600),]
mod61 <- lm(quality ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates + alcohol,
data=trainwine6)
mod62 <- lm(((quality -1)^0.91)/0.91 ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates + alcohol,
data=trainwine6)

rmse(predict(mod61,testwine6), testwine6$quality) # 0.679
rmse(predict(mod62,testwine6), testwine6$quality) # 1.425

trainwine7 <- wine[-c(201:400),]
testwine7 <- wine[c(201:400),]
mod71 <- lm(quality ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates + alcohol,
data=trainwine7)
mod72 <- lm(((quality -1)^0.91)/0.91 ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates + alcohol,
data=trainwine7)

rmse(predict(mod71,testwine7), testwine7$quality) # 0.666
rmse(predict(mod72,testwine7), testwine7$quality) # 1.53
```

```
trainwine8 <- wine[-c(1:200),]
testwine8 <- wine[c(1:200),]
mod81 <- lm(quality ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates + alcohol,
data=trainwine8)
mod82 <- lm(((quality -1)^0.91)/0.91 ~ volatile.acidity + chlorides +
free.sulfur.dioxide + total.sulfur.dioxide + pH + sulphates + alcohol,
data=trainwine8)

rmse(predict(mod81,testwine8), testwine8$quality) # 0.662
rmse(predict(mod82,testwine8), testwine8$quality) # 1.207

library(analogue)

pcrmod <- pcr(quality ~ volatile.acidity + chlorides +
                free.sulfur.dioxide + total.sulfur.dioxide +
                pH + sulphates + alcohol, data=trainwine,
              validation="CV",ncomp=50)

rmse(predict(pcrmod, testwine$quality))



# 2
library(faraway)
data(penicillin)
penicillin
plot(yield ~ treat, penicillin,pch=unclass(blend))
plot(yield ~ blend, penicillin,pch=unclass(treat))
# RCBD
lmod <- lm(yield ~ treat + blend, penicillin)
summary(lmod)
lmod_ <- lm(yield ~ blend, penicillin)
anova(lmod,lmod_)

# CRD
lmod2 <- lm(yield ~ treat, penicillin)
summary(lmod2)
anova(lmod2)

# random effect


library(nlme)
```

```
gls(yield ~ treat + blend, penicillin)

glmod <- gls(yield ~ treat, penicillin)
summary(glmod) #5.533 = 30.61

lmod <- lm(yield ~ treat + blend, penicillin)
summary(lmod) #4.34 = 18.83


# 3
load("C:/Users/jihun/Downloads/Constrained.RData")
y_ = y - x2
x_ = x1 - x2
summary(lm(y_ ~ x_))
```