Regression 3

Diagnostic Procedures for aptness of model

Consider the simple linear regression model

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i.$$

This model is based on a series of assumptions which may not be met in practice. Departures from the simple linear regression model with normal errors happen when:

1. The regression function is not linear,

$$(\Rightarrow \hat{\epsilon}_i \text{ vs. } \hat{Y}_i \text{ plot})$$

2. The $Var(\epsilon_i)$ is not constant,

$$(\Rightarrow \hat{\epsilon}_i^2 \text{ vs. } \hat{Y}_i \text{ plot})$$

3. The errors ϵ_i are not independent,

$$(\Rightarrow \hat{\epsilon}_i \text{ vs. time-order plot})$$

- 4. The errors ϵ_i are not normally distributed,
 - $(\Rightarrow \text{histogram}, \, \text{normal probability plot or Q-Q plot})$
- 5. Other important predictor variables have been omitted,

$$(\Rightarrow \hat{\epsilon}_i \text{ vs. other predictors})$$

6. The model fits all but one or a few outliers.

$$(\Rightarrow \hat{\epsilon}_i/\sqrt{\text{MSE}} \text{ vs. } \hat{Y}_i \text{ plot})$$

1 Residuals

Direct diagnostic plots for the response Y are ordinarily not so useful in regression analysis because the values of the observations on the response are a function of the predictor X. Instead, diagnostics for the response Y are usually carried out indirectly through an examination of the residuals, $\hat{\epsilon}_i$. The residuals $\hat{\epsilon}_i$ is defined as

$$\hat{\epsilon}_i = Y_i - \hat{Y}_i = Y_i - (\hat{\beta}_0 + \hat{\beta}_1 X_i).$$

They have the following properties:

- 1. Sample mean: $\bar{\hat{\epsilon}} = \frac{1}{n} \sum \hat{\epsilon}_i = 0$.
- 2. Sample variance: $MSE = \frac{1}{n-2} \sum (\hat{\epsilon}_i \overline{\hat{\epsilon}})^2 = \frac{1}{n-2} \sum (\hat{\epsilon}_i)^2 = \frac{1}{n-2} SSE$. $E(MSE) = \sigma^2$ (unbiased).
- 3. The error terms ϵ_i are *iid* $N(0, \sigma^2)$. But the residuals $\hat{\epsilon}_i$ are *not* fully independent because there are two constraints from the normal equation:

(i)
$$\sum \hat{\epsilon}_i = 0$$
 and (ii) $\sum X_i \hat{\epsilon}_i = 0$.

Let n= sample size and p= the # of parameters in the regression model, for example p=2 for the simple linear regression. If $n\gg p$, then we can usually ignore the dependencies of $\hat{\epsilon}_i$.

2 Diagnostic for residuals

Minitab and R offer a convenient informal graphic analysis of residuals. The plot() command in R gives four graphics, which are a scatter plot of $\hat{\epsilon}_i$ vs. \hat{Y}_i , a norm Q-Q plot, absolute value of standardized $\hat{\epsilon}_i$ vs. \hat{Y}_i , and standardized $\hat{\epsilon}_i$ vs. leverages.

The Minitab macro command %resplots (old version) also gives four graphics, which are a normal probability plot, a time-series plot, a histogram, and a scatter plot of $\hat{\epsilon}_i$ vs. \hat{Y}_i .

Example 3.1. Graphic analysis of residuals.

Minitab

```
Read Data
```

```
SUBC> file "S:\LM\CH01TA01.txt" .

Entering data from file: S:\LM\CH01TA01.TXT

zero constant to the state of the state of
```

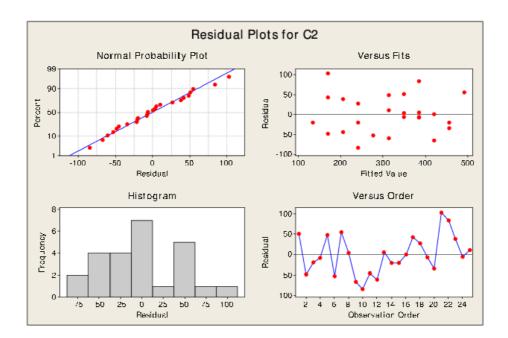
The Minitab macro command %resplots (old version) also gives four graphics, which are a normal probability plot, a time-series plot, a histogram, and a scatter plot of $\hat{\epsilon}_i$ vs. \hat{Y}_i .

Residual Plots

```
## store residuals into c3 and fitted Y into c21
regr c2 1 c1;
fits c21;
resid c3.

## Call resplots.mac (older version)
%resplots c3 c21.

## New version
## Stat -> Regression -> Graphs... -> (click four in one) -> OK
```



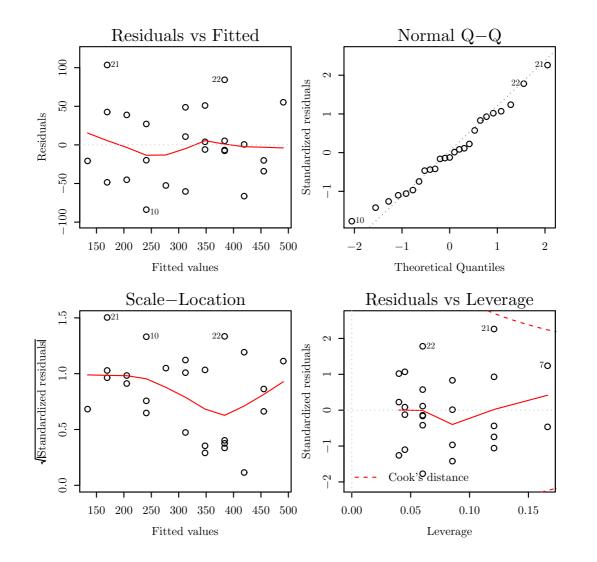


Read the data set

Residuals Plot

```
x = mydata[,1]
y = mydata[,2]
LM = lm(y ~ x )

par ( mfrow=c(2,2) ) ## Put four plots into one sheet
plot(LM)
```



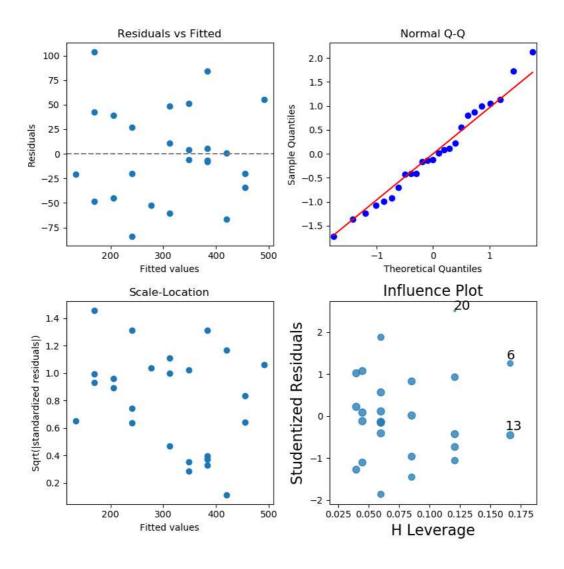
Python

Read the data set

```
#!/usr/bin/python3
  # If you have " CHO1TA01.txt " in your current computer .
   # mydata = open("S:/LM/CHO1TA01.txt", "r")
4
   # file = mydata.read().splitlines()
   # If PC is connected to Internet, then the following works.
   from urllib.request import urlopen
  link = "https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt"
url = urlopen(link)
11
   file = url.read().splitlines()
url.close()
13
  x = []
14
15 y = []
16 for line in file:
       p = line.split()
17
       x.append(float(p[0]))
18
       y.append(float(p[1]))
```

Residuals Plot

```
import statsmodels.formula.api as smf
2 import pandas as pd
  data1 = pd.DataFrame({"x":x, "y":y})
lm = smf.ols(formula = 'y ~ x', data = data1).fit()
   import matplotlib.pyplot as plt
8 import statsmodels.api as sm
fitted = lm.predict()
11 resids = lm.resid
std_resids = lm.resid_pearson
13
14 # 4 plots in one window
fig = plt.figure(figsize = (8, 8), dpi = 100)
16
17 ## raw residuals vs. fitted
ax1 = fig.add_subplot(2, 2, 1)
   ax1.plot(fitted, resids, 'o')
20 l = plt.axhline(y = 0, color = 'grey', linestyle = 'dashed')
21 ax1.set_xlabel('Fitted values')
  ax1.set_ylabel('Residuals')
22
23 ax1.set_title('Residuals vs Fitted')
24
25 ## q-q plot
26 ax2 = fig.add_subplot(2, 2, 2)
sm.qqplot(std_resids, line='s', ax = ax2)
ax2.set_title('Normal Q-Q')
29
30 ## scale-location
31 ax3 = fig.add_subplot(2, 2, 3)
ax3.plot(fitted, abs(std_resids)**.5, 'o')
33 ax3.set_xlabel('Fitted values')
34 ax3.set_ylabel('Sqrt(|standardized residuals|)')
35
   ax3.set_title('Scale-Location')
37 ## residuals vs. leverage
   ax4 = fig.add_subplot(2, 2, 4)
39 sm.graphics.influence_plot(lm, criterion = 'Cooks', size = 2, ax = ax4)
40
41 plt.tight_layout()
42 fig.savefig('regplots.png')
```



We will study some informal diagnostic plots of residuals to provide information on whether any of the six types of departures from the simple linear regression model are present. Graphic analysis of residuals provides very useful and attractive information. One has to be careful with looking at these plots, however, as sometimes they are difficult to interpret. Unless the effect is very strong, one usually needs a lot of points, say 100 or more, to really notice the effect. Graphic analysis of residuals is inherently subjective. We introduce some informal diagnostic plots of residuals and some objective tests to check departures from the simple linear regression model.

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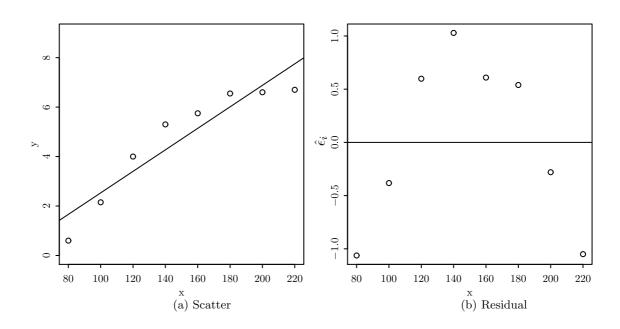
2.1 Non-linearity of regression function

Plot

Nonlinearity of the regression function can be investigated from:

- (a) $\hat{\epsilon}_i$ vs. $\hat{Y}_i \Rightarrow$ recommended.
- (b) $\hat{\epsilon}_i$ vs. $X_i \Rightarrow$ essentially equivalent to (a).
- (c) (X_i, Y_i) scatter plot \Rightarrow not always effective.

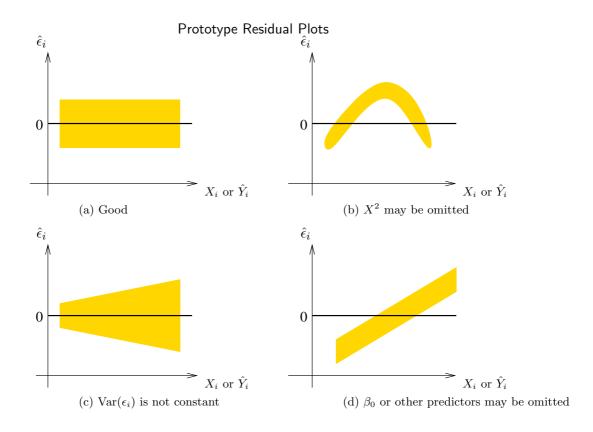
Scatter plot and residual plot



The above plots were made by R using the data in Table 3.1 on Page 105 of the text.

R

```
1  x = c(80, 220, 140, 120, 180, 100, 200, 160)
2  y = c(0.60,6.70,5.30,4.00,6.55,2.15,6.60,5.75)
3
4  LM = lm(y~x)
5  y1 = fitted(LM)
6  r = y - y1
7
8  par(mfrow=c(1,2))  ## two plots into one sheet
9  plot(x,y, ylim=c(0,9), sub="(a)")
10  abline(coef(LM))
11
12  plot(x,r, sub="(b)")
13  abline(h=0)
```



Test

Regress $\hat{\epsilon}_i$ on \hat{Y}_i and \hat{Y}_i^2 :

$$\hat{\epsilon}_i = \gamma_0 + \gamma_1 \hat{Y}_i + \gamma_2 \hat{Y}_i^2.$$

If the coefficient of \hat{Y}_i^2 (i.e., γ_2) is significant (usually when p-value is less than $\alpha = 0.05$), then this suggests that the model should include a quadratic term.

Example 3.2.

Minitab

```
## Data set from Table 3.1 pg. 105
   MTB > set c1
   DATA > 80 220 140 120 180 100 200 160
   DATA > end
   MTB > set c2
   DATA> .60 6.70 5.30 4.0 6.55 2.15 6.6 5.75
   DATA > end
   MTB > regr c2 1 c1;
   SUBC> fits c3;
   SUBC > resid c5.
10
11
   Regression Analysis: C2 versus C1
12
   The regression equation is
14
   C2 = -1.82 + 0.0435 C1
15
   Predictor
                   Coef
                          SE Coef
```

```
-1.816 1.052 -1.73 0.135
0.043482 0.006706 6.48 0.001
18 Constant
19 C1
20
S = 0.869241 R-Sq = 87.5% R-Sq(adj) = 85.4%
23 Analysis of Variance
               DF
24 Source
                           SS
                                   MS
                    1 31.764 31.764 42.04 0.001
   Regression
25
26 Residual Error 6 4.533
27 Total 7 36.297
                                0.756
28
29 MTB > let c4 = c3**2.
30 MTB > regr c5 2 c3 c4.
31
32 Regression Analysis: C5 versus C3, C4
33
34 The regression equation is
   C5 = -3.87 + 2.00 C3 - 0.213 C4
35
36
                  Coef SE Coef
                                       Т
37 Predictor
                                  -9.93 0.000
10.87 0.000
               -3.8702 0.3896
2.0039 0.1843
   Constant
39 C3
40 C4
              -0.21290 0.01925 -11.06 0.000
42 S = 0.188738 R-Sq = 96.1\% R-Sq(adj) = 94.5\%
43
44 Analysis of Variance
                DF
                           SS
                                    MS
45 Source
46 Regression
                    2 4.3554 2.1777 61.13 0.000
47 Residual Error 5 0.1781
48 Total 7 4.5335
                                0.0356
   Total
50 Source DF Seq SS
51 C3 1 0.0000
       1 4.3554
52 C4
```

R

```
x = c(80, 220, 140, 120, 180, 100, 200, 160)
x = c(0.60, 6.70, 5.30, 4.00, 6.55, 2.15, 6.60, 5.75)
   > LM = lm(y^x)
   > c3 = fitted(LM)
   > c4 = c3^2
   > c5 = resid(LM)
  > LM2 = lm(c5 ~c3 + c4)
10 > summary(LM2)
11
12 Call:
lm(formula = c5 ~c3 + c4)
14
15 Residuals:
    1 2 3 4 5 6 7 8
0.06458 0.07708 0.22351 0.11518 0.05625 -0.22113 -0.11935 -0.19613
17
18
19 Coefficients:
20 Estimate Std. Error t value Pr(>|t|)
21 (Intercept) -3.87017 0.38961 -9.933 0.000177 ***
22 c3
                 2.00392
                              0.18430 10.873 0.000114 ***
23 c4
                 -0.21290
                              0.01925 -11.057 0.000105 ***
25 Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
27 Residual standard error: 0.1887 on 5 degrees of freedom
28 Multiple R-Squared: 0.9607, Adjusted R-squared: 0.945
_{29} F-statistic: 61.13 on 2 and 5 DF, \, p-value: 0.0003059
```

Python

```
#!/usr/bin/python3
   import pandas as pd
   import statsmodels.formula.api as smf
   x = [80, 220, 140, 120, 180, 100, 200, 160]
   y = [0.60, 6.70, 5.30, 4.00, 6.55, 2.15, 6.60, 5.75]
   data1 = pd.DataFrame({"x":x, "y":y})
   LM = smf.ols(formula = 'y ~ x', data = data1).fit()
10
11
   c3 = LM.fittedvalues
   c4 = c3 ** 2
12
   c5 = LM.resid #Residuals
13
14
   data2 = pd.DataFrame({"c3":c3, "c4":c4, "c5":c5})
15
  LM2 = smf.ols(formula = 'c5 ~ c3 + c4', data = data2).fit()
16
   print(LM2.summary())
```

Remark 3.1. Note: From the Minitab result, the coefficient of \hat{Y}^2 (C4) is significant, *i.e.*, *p*-value for two-sided hypothesis test $(H_0: \gamma_2 = 0 \text{ vs. } H_1: \gamma_2 \neq 0)$ is 0 from the Minitab result and $0.000105 \approx 0$ from the R result both of which are less than $\alpha = 0.05$. This result suggests that $\hat{\epsilon}_i$ have a quadratic term and so the model should include a quadratic term.

2.2 Non-constancy of variance of error

Plot

- (i) $\hat{\epsilon}_i^2$ or $|\hat{\epsilon}_i|$ vs. $\hat{Y}_i \Rightarrow$ recommended.
- (ii) $\hat{\epsilon}_i^2$ or $|\hat{\epsilon}_i|$ vs. $X_i \Rightarrow$ essentially equivalent to (a).

Test

- (a) Regress $\hat{\epsilon}_i^2$ on \hat{Y}_i . If the coefficient of \hat{Y}_i is significant, *i.e.*, *p*-value is less than $\alpha = 0.05$, then this suggests that variance of error is not constant.
- (b) Brown-Forsythe (Modified Levene) Test.

The modified Levene test is the test of the equality of variances of two groups. This test can be used to test the constant error variance. To conduct this test, we divide the data set into two groups, according to the level of X, so that one group consists of cases where the X level is low and the other group consists of cases where the X level is high. We shall use $\hat{\epsilon}_{i1}$ to denote the ith residual for group I and $\hat{\epsilon}_{i2}$ to denote the ith residual for group II. Also we denote n_1 and n_2 to be the sample sizes of the

⑥ 亞△士 CHANSEOK PARK

two groups. Denote

$$d_{i1} = |\hat{\epsilon}_{i1} - \tilde{\epsilon}_1|$$
 and $d_{i2} = |\hat{\epsilon}_{i2} - \tilde{\epsilon}_2|$,

where $\tilde{\epsilon}_1 = \text{median}_i(\hat{\epsilon}_{i1})$ and $\tilde{\epsilon}_2 = \text{median}_i(\hat{\epsilon}_{i2})$. Note that the original Levene test uses the mean instead of the median.

The two-sample t test statistic is given as

$$t_L^* = \frac{\bar{d}_1 - \bar{d}_2}{s\sqrt{1/n_1 + 1/n_2}},$$

where \bar{d}_1 and \bar{d}_2 are the sample means of d_{i1} and d_{i2} , respectively and the pooled variance s^2 is

$$s^{2} = \frac{\sum (d_{i1} - \bar{d}_{1})^{2} + \sum (d_{i2} - \bar{d}_{2})^{2}}{n_{1} + n_{2} - 2}.$$

The decision rule is:

- If $|t_L^*| \le t(1 \frac{\alpha}{2}; n_1 + n_2 2)$, conclude the error variance is constant.
- If $|t_L^*| > t(1 \frac{\alpha}{2}; n_1 + n_2 2)$, conclude the error variance is not constant.

It should be noted that if the usual ANOVA F statistic for testing equality of means applied to the absolute deviations of k samples $(d_{i_11}, d_{i_22}, \ldots, d_{i_kk})$, we can perform the homogeneity of variances of k populations.

(c) Breusch-Pagan Test.

This test assumes that the error terms are independent and normally distributed and the variance of the error term ϵ_i , denoted by σ_i^2 is related to the levels of X in the following way:

$$\ln \sigma_i^2 = \gamma_0 + \gamma_1 X_i.$$

The test of H_0 : $\gamma_1 = 0$ is carried out by means of regressing the squared residuals $\hat{\epsilon}_i^2$ on X_i in the usual manner and obtaining the regression sum of squares SSR*. The test statistic X_{BP}^2 is as follows:

$$X_{BP}^2 = \frac{SSR^*}{2} \div \left(\frac{SSE}{n}\right)^2 \dot{\sim} \chi_{df=p-1}^2,$$

where

SSR* is the regression sum of squares when regressing $\hat{\epsilon}_i^2$ on X_i and

SSE is the error sum of squares when regressing Y_i on X_i .

The test statistic X_{BP}^2 follows approximately the χ^2 distribution with p-1 degree of freedom (p is the number of parameters. So p=2.) Large values of X_{BP}^2 lead to H_1 : non-constancy of error variance.

(d) Other tests of homogeneity of variances.

In general, F-test is used for comparing two variances, where the test statistic given by the ratio of two sample variances. For the modified Levene test, we divided the data set into two groups, according to the level of X, so that one group consists of cases where the X level is low and the other group consists of cases where the X level is high. We denoted the residuals for group I by $\hat{\epsilon}_{i1}$ and the residuals for group II by $\hat{\epsilon}_{j2}$, where $i = 1, 2, ..., n_1$ and $j = 1, 2, ..., n_2$. Thus, using two samples for groups I and II, we can easily perform the F-test and its test statistic is given by

$$F = \frac{S_1^2}{S_2^2} \sim F(n_1 - 1, n_2 - 1),$$

where S_1^2 is the sample variance of the first sample and S_1^2 is the sample variance of the second. This is easily performed by using the R function, var.test. It should be noted that this test is very sensitive to the departure from the normality assumption. For robust alternative to this test, one can refer to the Ansari-Bradley Test (Hollander and Wolfe, 2013) and the R has the function ansari.test for this test.

If there are more than k populations, the above tests can not be applied. For homoscedasticity or homogeneity of variances of k populations, one can refer to Brown-Forsythe test, Bartlett, Fligner-Killeen, Hartley's F-max test, and Cochran's C test. The R program provides bartlett.test and fligner.test. Note that Bartlett, Hartley's F-max and Cochran's C tests are sensitive to departure from normality.

Example 3.3. (a) Regress $\hat{\epsilon}_i^2$ on \hat{Y}_i .

Minitab

```
MTB > READ C1 C2;
SUBC> file "S:\LM\CH01TA01.txt" .
Entering data from file: S:\LM\CH01TA01.TXT

25 rows read.
MTB > regr c2 1 c1;
SUBC> resid c3;
SUBC> fits c4.

MTB > let c5 = c3**2
MTB > regr c5 1 c4.
```

```
12 Regression Analysis: C5 versus C4
13
14 The regression equation is
15 C5 = 3940 - 5.59 C4
                                   Т
              Coef SE Coef
17 Predictor
                        1756 2.24 0.035
5.354 -1.04 0.307
18 Constant
                3940
19 C4
               -5.593
20
S = 2689.72  R-Sq = 4.5\%  R-Sq(adj) = 0.4\%
22
23 Analysis of Variance
                DF
                                              F
24 Source
                              SS
                                     MS
   Regression 1 7896142 7896142 1.09 0.307
Residual Error 23 166395896 7234604
Total 24 174292038
25 Regression
28
29 Unusual Observations
30 Obs C4 C5 Fit SE Fit Residual St Resid
   21 169 10718 2992
22 384 7109 1794
                           935
                                              3.06R
                                    7726
31
32
                              660
                                        5316
                                                  2.04R
33
34 R denotes an observation with a large standardized residual.
```

R

Read the data set

Regression analysis

```
1 > c1 = mydata[,1]
2 > c2 = mydata[,2]
   > LM = lm(c2 ~c1)
   > c3 = resid(LM)
   > c4 = fitted(LM)
   > c5 = c3^2
   > LM2 = lm(c5 ~c4)
10 > summary(LM2)
11
   Call:
12
13 lm(formula = c5 ~ c4)
15 Residuals:
  Min 1Q Median -2760.1 -1765.4 -990.7
16
                                 3 Q
                             609.5 7726.3
17
18
19
   Coefficients:
               Estimate Std. Error t value Pr(>|t|)
20
21 (Intercept) 3939.750 1756.371 2.243 0.0348 *
22 c4 -5.593 5.354 -1.045 0.3070
23
24 Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
\, Residual standard error: 2690 on 23 degrees of freedom
                                    Adjusted R-squared: 0.003796
Multiple R-Squared: 0.0453,
28 F-statistic: 1.091 on 1 and 23 DF, p-value: 0.307
```

Python

Read the data set

```
#!/usr/bin/python3
   # If you have " CH01TA01.txt " in your current computer .
   # mydata = open("S:/LM/CH01TA01.txt", "r")
4
   # file = mydata.read().splitlines()
   \mbox{\tt\#} If PC is connected to Internet, then the following works.
   from urllib.request import urlopen
  link = "https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt"
url = urlopen(link)
   file = url.read().splitlines()
url.close()
13
   c1 = []
14
c2 = []
16 for line in file:
17
       p = line.split()
       c1.append(float(p[0]))
18
       c2.append(float(p[1]))
```

Regression analysis

```
import pandas as pd
import statsmodels.formula.api as smf

data1 = pd.DataFrame({"c1":c1, "c2":c2})
LM = smf.ols(formula = 'c2 ~ c1', data = data1).fit()

c3 = LM.resid
c4 = LM.fittedvalues
c5 = c3 ** 2

data2 = pd.DataFrame({"c4":c4, "c5":c5})
LM2 = smf.ols(formula = 'c5 ~ c4', data = data2).fit()
print(LM2.summary())
```

Example 3.4. (b) Modified Levene Test.

Minitab The Minitab macro for the Levene test (file: levene.MAC) is available at

https://github.com/AppliedStat/LM

```
1 MTB > READ C1 C2;
  SUBC> file "S:\LM\CHO1TAO1.txt"
   Entering data from file: S:\LM\CH01TA01.TXT
   25 rows read.
   MTB > regr c2 1 c1;
   SUBC> resid c3.
   MTB > sort c1 c3 c4 c5;
  SUBC > by c1.
10
  MTB > print c1 c3 c4 c5
12
13
   Data Display
  Row C1
                  C3
                     C4
                               C5
         80
              51.018
                      20 -20.770
   1
15
```

```
30 -48.472
50 -19.876
                       30
30
                        30 -48.472
16
     2
17
                            42.528
18
19
   MTB > copy c5 c11
  MTB > copy c5 c12
21
22 MTB > delete 14:25 c11
   MTB > delete 1:13 c12
23
24
   MTB > %S:\LM\levene c11 c12 k1
   Executing from file: S:\LM\levene.MAC
26
27
   Data Display
29
30
   K1
         1.31648
31
   MTB > invcdf 0.975;
32
33
   SUBC> t 23.
34
  Inverse Cumulative Distribution Function
35
   Student's t distribution with 23 DF
37
38
   P(X \le x)
39
         0.975 2.06866
40
```

Remark 3.2. From the Minitab result above, we have $|t_L^*| = 1.31648 < 2.06866$. Hence we conclude that the error variance is constant.

R The R function for the Levene test (file: levene.R) is available at

https://github.com/AppliedStat/LM

```
> # First, save the levene.R file at your current directory.
   > # source("S:/LM/levene.R")
   > # If your PC is connected to Internet, the following will work:
   > source("https://raw.githubusercontent.com/AppliedStat/LM/master/levene.R")
       read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt")
8
   > c1 = mydata[,1]
10
   > c2 = mydata[,2]
11
   > LM = lm(c2 ~c1)
12
13
14
   > c3 = resid(LM)
15
16
   > c1.order = order(c1)
17
   > c4 = c1 [ c1.order ]
   > c5 = c3 [ c1.order ]
18
19
   > print( cbind(c1,c3,c4,c5) )
20
                   c3 c4
21
       c1
22
  1
       80 51.0179798 20 -20.7698990
       30 -48.4719192 30 -48.4719192
50 -19.8759596 30 42.5280808
23
24
   3
       90 -7.6840404 30 103.5280808
26
```

Python

```
1 #!/usr/bin/python3
  # If you have " CHO1TA01.txt " in your current computer .
4 # mydata = open("S:/LM/CH01TA01.txt", "r")
  # file = mydata.read().splitlines()
  # If PC is connected to Internet, then the following works.
8 from urllib.request import urlopen
  link = "https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt"
url = urlopen(link)
file = url.read().splitlines()
url.close()
13
14 c1 = []
15 c2 = []
   for line in file:
16
       p = line.split()
17
       c1.append(int(p[0]))
18
19
       c2.append(int(p[1]))
20
21 import numpy as np
   import pandas as pd
22
23 import scipy.stats as stats
^{24} import statsmodels.formula.api as smf
25 data1 = pd.DataFrame({"c1":c1, "c2":c2})
26 LM = smf.ols(formula = 'c2 ~ c1', data = data1).fit()
28 c3 = LM.resid
30 c1 = np.asarray(c1)
c3 = np.asarray(c3)
32
   c1_order = np.argsort(c1, kind = 'stable')
c4 = c1[c1\_order]
c5 = c3[c1\_order]
36 # cbind = np.vstack((c1, c3, c4, c5))
37 cbind = pd.DataFrame({"c1":c1, "c2":c2, "c3":c3, "c4":c4})
38 print(cbind)
39
40 gr1 = c5[0:13]
gr2 = c5[13:25]
w, p = stats.levene(gr1, gr2)
44 print(p)
```

 Remark 3.3. Note that the t-distribution critical value for the modified Levene's test at the significance level α with df can be found in R as follows:

$$>$$
 qt(1 - α /2, df).

To test with $\alpha = 0.05$ and 23 degrees of freedom, we use qt(1-0.05/2, df=23) which results in 2.068658.

Example 3.5. (c) Breusch-Pagan Test.

Minitab The Minitab macro for the Breusch-Pagan test (file: BPtest.MAC) is available

https://github.com/AppliedStat/LM

```
MTB ># 1. Read the data
   MTB > READ C1 C2;
               file "S:\LM\CHO1TAO1.TXT"
   SUBC >
   Entering data from file: S:\LM\CH01TA01.TXT
   25 rows read.
5
   MTB > # 2. RUN BPtest Macro
   MTB > %S:\LM\BPtest C2 C1 .
8
   Executing from file: S:\LM\BPtest.MAC
10
11
  Data Display
12
  Breusch-Pagan Test Statistic:
                                       0.82092
13
14 Degrees of Freedom:
                                       1
   p-value:
                                       0.36491
15
```

R

```
> mydata =
       read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt")
   > c1 = mydata[,1]
   > c2 = mydata[,2]
   > LM = lm(c2 ~c1)
8
   > e = resid(LM)
   > sigma2 = e^2
10
11
   > LM2 = lm ( sigma2 ~ c1 )
12
13
   > SSR.star = sum( (fitted(LM2)-mean(sigma2))^2)
15
   > SSE = sum( (fitted(LM)-c2)^2 )
16
  > n = length(c2)
```

Python

```
#!/usr/bin/python3
   # If you have " CHO1TA01.txt " in your current computer .
   # mydata = open("S:/LM/CH01TA01.txt", "r")
   # file = mydata.read().splitlines()
   \mbox{\tt\#} If PC is connected to Internet, then the following works.
8 from urllib.request import urlopen
  link = "https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt"
url = urlopen(link)
file = url.read().splitlines()
url.close()
13
14 c1 = []
c2 = []
16 for line in file:
     p = line.split()
17
       c1.append(int(p[0]))
18
       c2.append(int(p[1]))
19
20
21 import numpy as np
22 import pandas as pd
   import scipy.stats as stats
23
24 import statsmodels.formula.api as smf
26 data1 = pd.DataFrame({"c1":c1, "c2":c2})
27 LM = smf.ols(formula = 'c2 ~ c1', data = data1).fit()
28
29 e = LM.resid
   sigma2 = e**2
31  data2 = pd.DataFrame({"c1":c1, "sigma2":sigma2})
32 LM2 = smf.ols(formula = 'sigma2 ~ c1', data = data2).fit()
   SSR_star = sum((LM2.fittedvalues-np.mean(sigma2))**2)
34 SSE = sum((LM.fittedvalues-c2)**2)
n = len(c2)
37 cbind = pd.DataFrame({"SSR_star":SSR_star, "SSE":SSE, "n":n}, index = [0])
38 print('\nData Display of SSR_star,SSE and n:')
39 print(cbind)
40
X_BP = SSR_star/2/((SSE/n)**2)
42 print('\nX_BP:')
43
   print(X_BP)
45 qchisq = stats.chi2.ppf(0.95, df=1)
46 print('\n qchisq:')
47 print(qchisq)
```

Remark 3.4. Note that the χ^2 critical value for the Breusch-Pagan test at the significance level

 α with df can be found in R as follows:

```
> qchisq(1 - \alpha, df).
```

Since $X_{\rm BP}^2=0.8209192$ is less than $\chi^2(0.95;1)=3.841459$, we conclude H_0 : constant error variance.

Δ

The R function for the Breusch-Pagan test (file: Breusch-Pagan.R) is also available at

https://github.com/AppliedStat/LM

2.3 Presence of outliers

Outliers are extreme observations.

Plot

It is convenient to use semi-Studentized residuals which are defined as

$$\hat{\epsilon}_i^* = \frac{\hat{\epsilon}_i - \overline{\hat{\epsilon}}}{\sqrt{\text{MSE}}} = \frac{\hat{\epsilon}_i}{\sqrt{\text{MSE}}},$$

since they do not depend on the unit of Y.

- (a) $\hat{\epsilon}_i^*$ vs. \hat{Y}_i . A rule of thumb is to identify Y_i as outliers if $|\hat{\epsilon}_i^*| > 4$
- (b) Use the Studentized deleted residuals defined as

$$t_i = \frac{\hat{\epsilon}_i}{\sqrt{\text{MSE}_{(i)}(1 - h_{ii})}}.$$

It is better than (a). We will study this later.

(c) Residuals can also be identified from box plot, stem-and-leaf plot, and histogram or dot plot.

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- Minitab: Use BOXPLOT, STEM-AND-LEAF, HISTOGRAM.
- R: Use boxplot(), stem(), hist().

Test

We will discuss this later (textbook: chapter 9).

2.4 Non-independence of error terms

Plot

 $\hat{\epsilon}_i$ vs. time-order (sequence) plot.

Test

Runs test and Durbin-Watson test are frequently used to test for lack of randomness in the residuals arranged in time or sequence order. We will discuss this later (textbook: chapter 12).

2.5 Non-normality of error terms

Plot

(a) Normal probability plot $(\hat{\epsilon}_{[k]} \text{ vs. } E(\hat{\epsilon}_{[k]}))$ or Q-Q plot \Rightarrow recommended. Normal probability plot of the residuals is a plot of $\hat{\epsilon}_{[k]}$ vs. $E(\hat{\epsilon}_{[k]})$, where $\hat{\epsilon}_{[k]}$ is the k-th smallest among the n residuals. A good approximation of $E(\hat{\epsilon}_{[k]})$ is

$$E(\hat{\epsilon}_{[k]}) \approx \sqrt{\text{MSE}} \Phi^{-1} \left(\frac{k - 0.375}{n + 0.25} \right),$$

where $\Phi^{-1}(\cdot)$ is the inverse cdf of N(0,1).

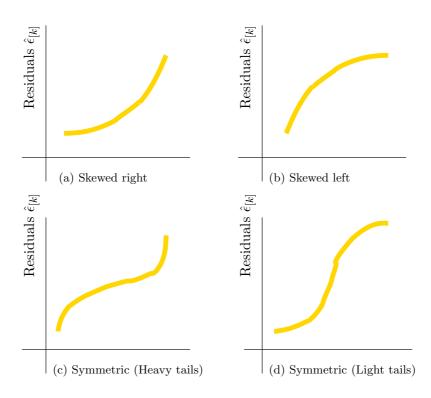
Note: the R function qqnorm() gives the Q-Q plot.

- (b) Distribution plots such as box plot, histogram, dot plot, stem-and-leaf.
- (c) Comparison of frequencies: $100(1-\alpha)\%$ of the residuals $\hat{\epsilon}_i$ fall between $\pm\sqrt{\text{MSE}}\cdot t(1-\frac{\alpha}{2};\text{df}=n-p)$, where p is the number of parameters.

Test

Calculate the sample correlation coefficient between $\hat{\epsilon}_{[k]}$ and $E(\hat{\epsilon}_{[k]}) \approx \sqrt{\text{MSE}} \Phi^{-1}\left(\frac{k-0.375}{n+0.25}\right)$. Find the critical value for n with α from Table B.6 of Kutner et al. (2005) or Table 2 of Looney and Gulledge, Jr. (1985). If the sample correlation coefficient is at least as large as

Q-Q Plots when error term is not Normal



the critical value from Table B.6 (Kutner et al., 2005) or Table 2 (Looney and Gulledge, Jr., 1985), then one can conclude that the error terms are reasonably normally distributed.

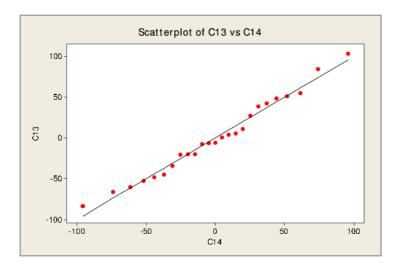
Remark 3.5. Personally, I am more concerned with getting the variance constant. And residuals may appear to be not normal because an inappropriate regression function is used or because the variance of error terms is not constant. \triangle

Example 3.6. Normal Probability Plot, which is based on the Table B.6 of Kutner et al. (2005) (textbook). Note that the normal probability plot using the Minitab built-in function, %resplot, uses the horizontal axis for the residuals.

Minitab

```
MTB > READ C1 C2;
SUBC> file "S:\LM\CHO1TAO1.txt" .
Entering data from file: S:\LM\CHO1TAO1.TXT
25 rows read.

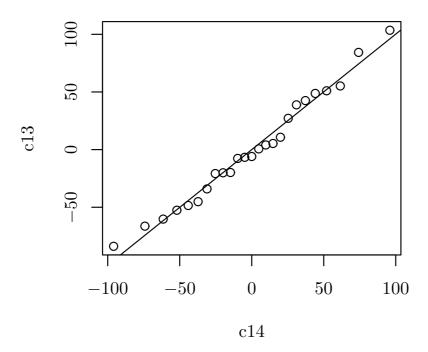
MTB > regr c2 1 c1;
SUBC> resid c3;
SUBC> mse k2.
```



```
10  MTB >let k1 = count(c3)
11
12  MTB > set c10
13  DATA >   1:k1
14  DATA > end .
15
16  MTB >sort c3 c13
17  MTB > let c11 = (c10 - .375) / (k1+.25)
18
19  MTB >invcdf c11 c12;
20  SUBC > normal 0 1.
21  MTB >let c14 = sqrt(k2)*c12
22  MTB >plot c13*c14;
23  SUBC > line c14 c14 .
```

R

```
\vspace{-0.5\baselineskip}
2
  > mydata =
       read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt")
   > c1 = mydata[,1]
> c2 = mydata[,2]
4
   > LM = lm(c2 ~c1)
8
   > c3 = resid(LM)
9
10
11
   > LM.sum = summary(LM)
12
  > attributes(LM.sum)
13
   $names
14
    [1] "call"
                         "terms"
                                          "residuals"
                                                           "coefficients"
15
                         "sigma"
                                         "df"
   [5] "aliased"
                                                          "r.squared"
   [9] "adj.r.squared" "fstatistic"
                                          "cov.unscaled"
17
18
19 $class
20 [1] "summary.lm"
```



```
21
   > s = LM.sum[[ "sigma" ]]
22
23
24
   > c13 = sort(c3)
25
26
   > n = length(c3)
27
   > k = 1:n
28
   > c11 = (k - 0.375) / (n+0.25)
30
31
32
   > c12 = qnorm( c11 )
33
   > c14 = s * c12
35
   > postscript( "ex4a.ps", width=4, height=4)
36
37
   > plot ( c14, c13)
38
   > abline(lm(c13~c14))
```

Python

```
#!/usr/bin/python3

# !!/usr/bin/python3

# If you have " CH01TA01.txt " in your current computer .

# mydata = open("S:/LM/CH01TA01.txt", "r")

# file = mydata.read().splitlines()

# If PC is connected to Internet, then the following works.

# from urllib.request import urlopen

| link = "https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt"

| url = urlopen(link)
```

```
file = url.read().splitlines()
url.close()
13
14 c1 = []
c2 = []
16 for line in file:
        p = line.split()
17
18
        c1.append(int(p[0]))
19
       c2.append(int(p[1]))
20
21
   import seaborn as sns
22 # The below may be needed for install seaborn and pandas (numexpr), etc
23 # sudo apt-get update -y
24 # sudo apt-get install -y python3-seaborn
25 # sudo apt-get install -y python3-pandas
26 # sudo apt-get install -y python3-numexpr
                                                   # latest numexpr is needed for pandas
import numpy as npimport scipy.stats as stats
29 import pandas as pd
30
31 import statsmodels.formula.api as smf
32 import matplotlib.pyplot as plt
   data1 = pd.DataFrame({"c1":c1, "c2":c2})
34
35 LM = smf.ols(formula = 'c2 ~ c1', data = data1).fit()
36
   c3 = LM.resid
37
38 LM_sum = LM.summary()
40
41 # get the residual standard error
42 squared_sigma = LM.mse_resid
43 s = squared_sigma ** 0.5
44
45 c13 = np.sort(c3)
46 n = len(c3)
48 c14 = []
49 for k in range(1,n+1):
       c11 = (k - 0.375)/(n + 0.25)
        c12 = stats.norm.ppf(c11)
51
52
       c14.append(s * c12)
53
c14 = np.asarray(c14)
56 fig = plt.figure(figsize = (4,4), dpi = 100)
57 data2 = pd.DataFrame({"c13":c13, "c14":c14})
sns.regplot(x="c14",y="c13",data=data2)
59 #sns.lmplot(x="c14",y="c13",data=data2)
60 plt.savefig('ex4a.png')
```

Example 3.7. Correlation test for normality.

Minitab

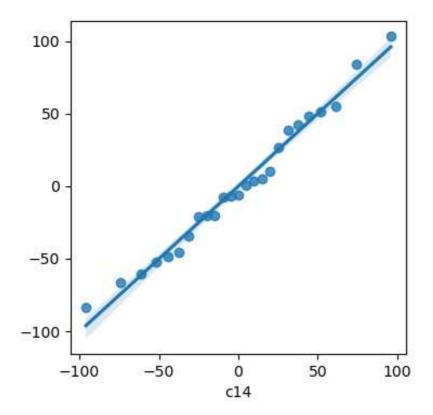
```
MTB > READ C1 C2;
SUBC> file "S:\LM\CH01TA01.txt" .
Entering data from file: S:\LM\CH01TA01.TXT

25 rows read.

6 MTB > regr c2 1 c1;
7 SUBC> resid c3;
8 SUBC> mse k2.

9

10 MTB > let k1 = count(c3)
```



```
11
   MTB > set c10
12
   DATA >
13
             1:k1
14
   DATA > end.
15
16
   MTB > sort c3 c13
17
   MTB > let c11 = (c10 - .375) / (k1+.25)
18
19
   MTB >invcdf c11 c12;
20
   SUBC > normal 0 1.
21
22
   MTB >let c14 = sqrt(k2)*c12
23
   MTB > correlation c13 c14 .
25
26
27
   Correlations: C13, C14
28
29
   Pearson correlation of C13 and C14 = 0.992
   P-Value = 0.000
```

Do not use the above p-value for the normality test.

R

```
1 > # Using Normal Probability Plot
2 > mydata =
       read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt")
  > c1 = mydata[,1]
4 > c2 = mydata[,2]
5 > LM = lm(c2 ~ c1)
   > c3 = resid(LM)
   > LM.sum = summary(LM)
   > s = LM.sum[[ "sigma" ]]
   > c13 = sort(c3)
n > n = length(c3)
   > k = 1:n
11
12 > c11 = (k - 0.375) / (n+0.25)
13 > c12 = qnorm( c11 )
   > c14 = s * c12
14
15 >
16 > cor(c13, c14)
17 [1] 0.9915055
19 >
20 > ## Using Q-Q plot
_{21} > pp = ppoints(c13, a=3/8)  # option "a=3/8=0.375" gives (k-0.375)/(n+0.25)
22 > qq = qnorm(pp)
23 > cor(c13, qq)
24 [1] 0.9915055
```

Python

```
#!/usr/bin/python3
  # If you have " CH01TA01.txt " in your current computer .
# mydata = open("S:/LM/CH01TA01.txt", "r")
3
   # file = mydata.read().splitlines()
8 # If PC is connected to Internet, then the following works.
9 from urllib.request import urlopen
10 link = "https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt"
url = urlopen(link)
file = url.read().splitlines()
13
   url.close()
14
15 c1 = []
16 c2 = []
17 for line in file:
       p = line.split()
       c1.append(int(p[0]))
19
20
       c2.append(int(p[1]))
21
import numpy as npimport scipy.stats as stats
24 import pandas as pd
25 import statsmodels.formula.api as smf
27  data1 = pd.DataFrame({"c1":c1, "c2":c2})
28 LM = smf.ols(formula = 'c2 ~ c1', data = data1).fit()
30 c3 = LM.resid
31 LM_sum = LM.summary()
32
squared_sigma = LM.mse_resid
s = squared_sigma ** 0.5
35
36 c13 = np.sort(c3)
n = len(c3)
38
```

```
c11 = [(k - 0.375)/(n + 0.25) for k in range(1,n+1)]
39
41 c12 = stats.norm.ppf(c11)
42
  c14 = s * c12
  cor1 = np.corrcoef(c13, c14)
44
45
  print(cor1)
46
   a = 3/8
47
48 m = len(c13)
49
50
51 # pp is written by ourselves, equivalent to ppints in R
52 pp = [(i-a)/(m+1/4) for i in range(1, m+1)]
54 qq = stats.norm.ppf(pp)
55 cor2 = np.corrcoef(c13, qq)
   print(cor2)
```

From Table B.6 of Kutner et al. (2005) (textbook) or Table 2 of Looney and Gulledge, Jr. (1985), the critical value for n = 25 and $\alpha = 0.05$ is 0.959. Since the sample correlation coefficient exceeds this critical value, we can conclude that the distribution the error terms does not depart from a normal distribution.

3 Transformations

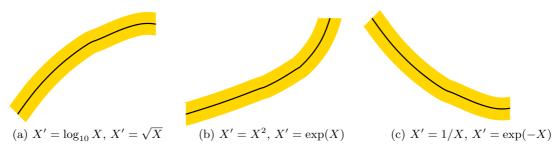
We consider transformations of the predictor X and the response Y.

3.1 Transformations of the predictor X

If the distribution of the error terms is reasonably close to normal distribution and the error terms have approximately constant variance, the transformations on X should be attempted. The transformations on Y is not desirable because the transformations on Y may change the shape of the distribution of the error terms from the normal distribution and may also leads to substantially differing error term variances.

Applied Statistics Lab, PNU 27 © $\oplus \wedge \pm$ Chanseok Park

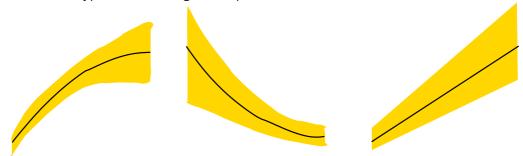
Prototype Nonlinear regression pattern with constant error variance.



3.2 Transformations of the response Y

Non-constant error variances and non-normality of the error terms frequently appear together. To remedy these departures from the simple linear regression model, we need a transformation of Y. We recommend the following transformations.





Possible transformations: $Y' = \sqrt{Y}, \ Y' = \log_{10} Y, \ \text{or} \ Y' = 1/Y.$

3.3 Box-Cox transformations

It is often difficult to determine from diagnostic plots which transformation of Y is most appropriate for correcting unequal error variances and nonlinearity of the regression function. The Box-Cox procedure automatically identifies a transformation from the family of power transformations on Y. The family of power transformations is of the form

$$Y' = \frac{Y^{\lambda} - 1}{\lambda} \approx Y^{\lambda},$$

for some λ and if $\lambda = 0$, use $Y' = \ln Y$. The normal error regression model of the above power transformations become

$$Y_i^{\lambda} = \beta_0 + \beta_1 X_i + \epsilon_i.$$

The Box-Cox procedure shows how to estimate $\hat{\lambda}$, the maximum likelihood estimate of λ to use in the power transformation. Note that the textbook use λ which has the smallest SSE.

Example 3.8. Box-Cox Transforms

The Minitab macro for the Box-Cox Transform (bxcx.MAC) is available at

https://github.com/AppliedStat/LM

Minitab

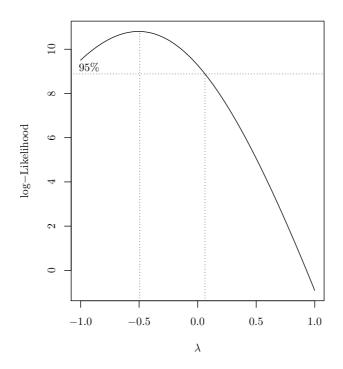
```
## See Table 3.9 (Section 3.9)
   MTB > READ c1 c2 c3;
  SUBC> file "S:\LM\CHO3TAO8.txt" .
   Entering data from file: S:\LM\CHO3TA08.TXT
   25 rows read.
   ## Generate 1.0, 0.9, ..., -1.0
  MTB >set c3
8
   DATA > 10:-10
10 DATA > end
11
12 MTB >let c3 = c3/10
13
14 MTB >%S:\LM\bxcx c2 c1 c3 c4
   Executing from file: S:\LM\bxcx.MAC
16
17 MTB >print c3 c4
18
   Data Display
        C3
19 Row
         1.0 77.9831
         0.9
              70.3505
21
         0.8 63.6693
22
     3
23
     4
         0.7 57.8369
     5
         0.6 52.7634
24
25
     6
         0.5 48.3707
         0.4 44.5905
    8
         0.3 41.3634
27
         0.2 38.6379
28
    9
   10
        0.1 36.3694
29
        0.0
30
    11
              34.5195
       -0.1
31
    12
              33.0552
       -0.2 31.9487
   13
32
33
    14
       -0.3 31.1763
34
    15
        -0.4
              30.7186
    16
       -0.5 30.5596
35
       -0.6 30.6868
36
    17
37
    18
        -0.7
              31.0907
        -0.8
    19
              31.7645
38
39
    20
       -0.9 32.7044
   21
        -1.0 33.9089
40
```

The R function for the Box-Cox Transform (bxcx.R) is available at

https://github.com/AppliedStat/LM

R

```
> ## Using web link:
1
   > source("https://raw.githubusercontent.com/AppliedStat/LM/master/bxcx.R")
4
       read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CH03TA08.txt")
   > c1 = mydata[,1]
6
   > c2 = mydata[,2]
  > lam = seq(1.0, -1.0, by=-0.1)
> sse = bxcx(c2, c1, lambda=lam)
10
11
12 > cbind(lam, sse)
13
          lam
         1.0 77.98306
   [1,]
14
   [2,] 0.9 70.35050
    [3,]
         0.8 63.66932
16
         0.7 57.83686
17
    [4,]
    [5,]
         0.6 52.76343
    [6,]
         0.5 48.37072
19
20
    [7,]
         0.4 44.59051
    [8,]
         0.3 41.36342
21
    [9,]
         0.2 38.63791
22
23
   [10,]
         0.1 36.36939
   [11,]
         0.0 34.51945
24
   [12,] -0.1 33.05520
25
   [13,] -0.2 31.94867
   [14,] -0.3 31.17631
27
   [15,] -0.4 30.71859
   [16,]
        -0.5 30.55961
   [17,] -0.6 30.68680
30
31
   [18,] -0.7 31.09066
   [19,] -0.8 31.76453
32
   [20,] -0.9 32.70442
33
  [21,] -1.0 33.90887
35
  36
  > # Using MASS library
  > # For help, use
38
  > # > library(help="MASS") or help("boxcox")
39
   > library("MASS")
41
  > # Note: 1. find the max. instead of the min.
43
             2. log-likelihood is used instead of SSE
44
  > lam = seq(1.0, -1.0, by=-0.1)
46
  > boxcox( c2 ~ c1 , lambda = lam )
```



Python

```
#!/usr/bin/python3
   # If you have " CHO1TA01.txt " in your current computer .
3
   # mydata = open("S:/LM/CH01TA01.txt", "r")
   # file = mydata.read().splitlines()
   \mbox{\tt\#} If PC is connected to Internet, then the following works.
   from urllib.request import urlopen
   link = "https://raw.githubusercontent.com/AppliedStat/LM/master/CHO3TAO8.txt"
9
   url = urlopen(link)
10
file = url.read().splitlines()
  url.close()
12
13
   c1 = []
14
15
   c2 = []
   for line in file:
       p = line.split()
17
        c1.append(float(p[0]))
18
        c2.append(float(p[1]))
19
20
21
   import numpy as np
22
   import pandas as pd
23
   {\tt import\ statsmodels.formula.api\ as\ smf}
   # Implement the boxcox function
def bxcx(y, x, lam):
25
26
27
       n = len(lam)
        sse = []
28
       k2 = np.exp(np.mean(np.log(y)))
29
        for i in range(0, n):
30
            if abs(lam[i]) > 0.0001:
31
32
                k1 = 1/(lam[i]* k2**(lam[i]-1))
                w = k1 * (y**lam[i]-1)
33
```

```
34
           else:
35
                w = k2 * np.log(y)
           data = pd.DataFrame({"x":x, "w":w})
36
           LM = smf.ols(formula = 'w
                                        x', data = data).fit()
37
           res = LM.resid
           sse.append(sum(res**2))
39
       return sse
41
   lam = np.arange(1.0, -1.1, -0.1)
42
43
   sse = bxcx(c2,c1,lam)
44
   #cbind = np.vstack((lam, sse))
45
   cbind = pd.DataFrame({"lam":lam, "sse":sse})
   print(cbind)
47
49
50
                 lam
                             sse
                      77.983064
51
   Ω
      1.000000e+00
   1
       9.000000e-01
                     70.350503
52
53
   2
       8.000000e-01
                      63.669322
54
   3
       7.000000e-01
                      57.836861
       6.000000e-01
                     52.763425
55
56
  5
       5.000000e-01
                      48.370723
       4.000000e-01
                      44.590514
57
       3.000000e-01
                      41.363420
58
59
   8
       2.000000e-01
                     38.637906
   9
       1.000000e-01
                      36.369386
60
   10 2.220446e-16
61
                      34.519452
  11 -1.000000e-01
                      33.055203
   12 -2.000000e-01
                      31.948669
63
64
   13 -3.000000e-01
                      31.176310
   14 -4.000000e-01
                      30.718590
65
   15 -5.000000e-01
                      30.559611
66
   16 -6.000000e-01
                      30.686803
  17 -7.000000e-01
                      31.090661
68
69
   18 -8.000000e-01
                      31.764528
70
   19 -9.000000e-01
                      32.704418
   20 -1.000000e+00
                      33.908874
```

Note:

- 1. Always check the plot of residuals after transformation.
- 2. Use the Box-Cox transformation only as a rough guide to selecting λ . It is better to use *nice* values like $\lambda = 0, 1/2, 1/3, -1$, etc. than *weird* values like $\lambda = 0.3645$.

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References

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