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
```

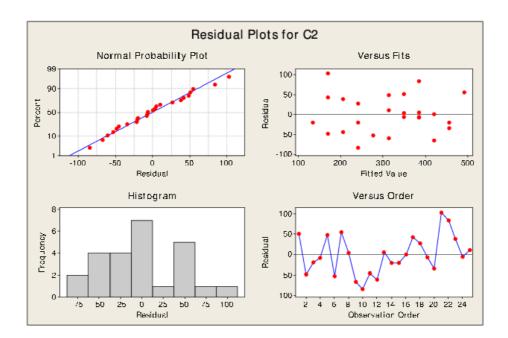
The Minitab macro command %resplots (old version) also gives four graphics, which are a normal probability plot, a time-series plot, a histogram, and a scatter plot of $\hat{\epsilon}_i$ vs. \hat{Y}_i .

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
```



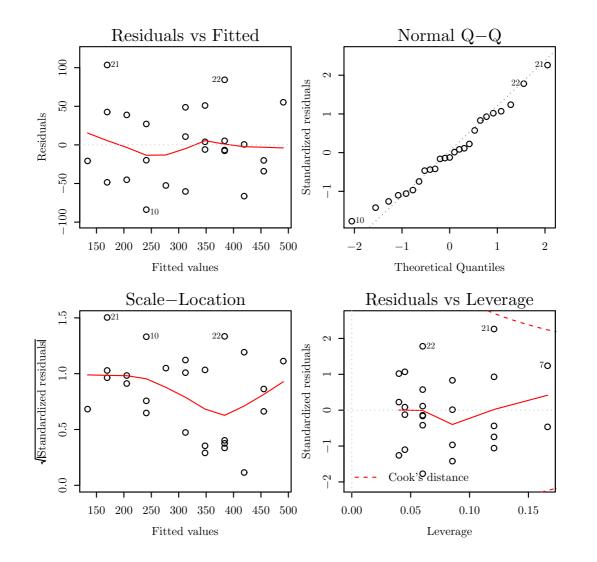


Read the data set

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)
```



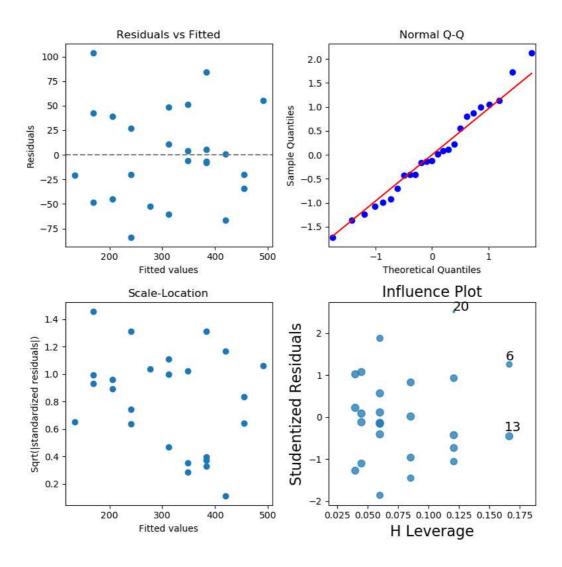
Python

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.

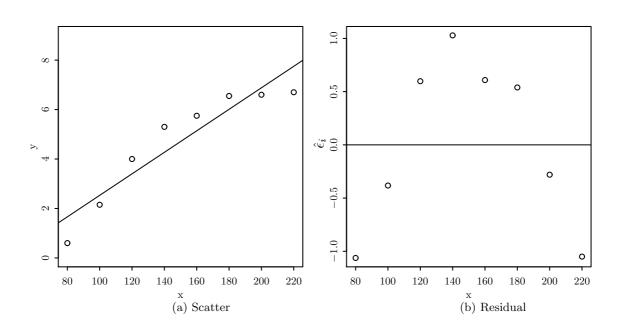
2.1 Non-linearity of regression function

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.

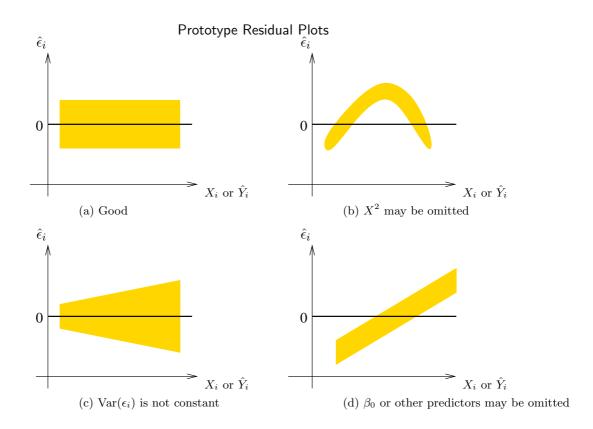
Scatter plot and residual plot



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

R

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



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

```
1 ## Data set from Table 3.1 pg. 105
2 MTB > set c1
   DATA > 80 220 140 120 180 100 200 160
   DATA > end
 5 MTB > set c2
6 DATA> .60 6.70 5.30 4.0 6.55 2.15 6.6 5.75
   DATA > end
8 MTB > regr c2 1 c1;
9 SUBC> fits c3;
10 SUBC > resid c5.
11
12 Regression Analysis: C2 versus C1
13
14 The regression equation is
15 C2 = - 1.82 + 0.0435 C1
16
                            SE Coef
17 Predictor
                     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%
22
23 Analysis of Variance
                   DF
                               SS
                                        MS
24 Source
                       1 31.764 31.764 42.04 0.001
25 Regression
26 Residual Error
                        6
                            4.533
                                      0.756
                       7 36.297
27 Total
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
35 C5 = -3.87 + 2.00 C3 - 0.213 C4
36
37 Predictor

        Coef
        SE Coef
        T
        P

        -3.8702
        0.3896
        -9.93
        0.000

        2.0039
        0.1843
        10.87
        0.000

        -0.21290
        0.01925
        -11.06
        0.000

                     Coef SE Coef
                                            T
38 Constant
39 C3
41
42 S = 0.188738 R-Sq = 96.1% R-Sq(adj) = 94.5%
43
44 Analysis of Variance
                  DF
                               SS
45
                                        MS
                      2 4.3554 2.1777 61.13 0.000
46 Regression
47 Residual Error 5 0.1781 0.0356
48 Total 7 4.5335
49
50 Source DF Seq SS
51 C3 1 0.0000
52 C4 1 4.3554
```

R

```
> x = c(80, 220, 140, 120, 180, 100, 200, 160)
  y = 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
6
   > c5 = resid(LM)
  > LM2 = lm(c5 ~c3 + c4)
9
10
   > summary(LM2)
11
12
  Call:
  lm(formula = c5 ~c3 + c4)
13
14
15
  Residuals:
16
                         3
   17
   Coefficients:
19
              Estimate Std. Error t value Pr(>|t|)
20
  (Intercept) -3.87017
                       0.38961 -9.933 0.000177 ***
21
                         0.18430 10.873 0.000114 ***
0.01925 -11.057 0.000105 ***
               2.00392
22 c3
23
  c4
              -0.21290
25 Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
27 Residual standard error: 0.1887 on 5 degrees of freedom
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
4
6 	 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\})
10 LM = smf.ols(formula = 'y ~ x', data = data1).fit()
   c3 = LM.fittedvalues
11
c4 = c3 ** 2
13 c5 = LM.resid #Residuals
14
data2 = pd.DataFrame({"c3":c3, "c4":c4, "c5":c5})
16 LM2 = smf.ols(formula = 'c5 ~ c3 + c4', data = data2).fit()
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 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:

$$\mathbf{X}^2_{\mathrm{BP}} = \frac{\mathrm{SSR}^*}{2} \div \left(\frac{\mathrm{SSE}}{n}\right)^2 \dot{\sim} \chi^2_{\mathrm{df}=p-1},$$

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\CHO1TAO1.TXT
   25 rows read.
  MTB > regr c2 1 c1;
   SUBC> resid c3;
   SUBC > fits c4.
  MTB > let c5 = c3**2
10
   MTB > regr c5 1 c4.
11
12 Regression Analysis: C5 versus C4
13
14
   The regression equation is
15 C5 = 3940 - 5.59 C4
16
               Coef SE Coef
17
   Predictor
                                  Т
               3940
                      1756
                              2.24 0.035
18
  Constant
              -5.593
                        5.354 -1.04 0.307
19 C4
20
S = 2689.72  R-Sq = 4.5\%  R-Sq(adj) = 0.4\%
22
23
   Analysis of Variance
               DF
                             SS
   Source
24
25
  Regression
                   1
                        7896142
                                 7896142 1.09 0.307
   Residual Error 23
                      166395896
                                 7234604
                  24 174292038
27
   Total
28
   Unusual Observations
29
                         SE Fit
30
   Obs C4 C5 Fit
                                 Residual
                                           St Resid
    21
        169 10718 2992
                            935
                                     7726
                                               3.06R
31
       384
            7109 1794
                            660
                                     5316
32
33
  R denotes an observation with a large standardized residual.
```

R

Read the data set

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

property mydata = read.table("S:\\LM\\CH01TA01.txt")

# If your computer is connected to Internet
```

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Regression analysis

```
> c1 = mydata[,1]
2 > c2 = mydata[,2]
3 > LM = lm(c2 ~c1)
  > c3 = resid(LM)
  > c4 = fitted(LM)
   > c5 = c3^2
   > LM2 = lm(c5 ~c4)
10 > summary(LM2)
11
12 Call:
13 lm(formula = c5 \sim c4)
15 Residuals:
16
      Min
               1Q Median
                              30
                                      Max
                           609.5 7726.3
17
   -2760.1 -1765.4 -990.7
18
19 Coefficients:
20
               Estimate Std. Error t value Pr(>|t|)
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
26 Residual standard error: 2690 on 23 degrees of freedom
27 Multiple R-Squared: 0.0453,
                                 Adjusted R-squared: 0.003796
28 F-statistic: 1.091 on 1 and 23 DF, p-value: 0.307
```

Python

Read the data set

```
1 #!/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.
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 = []
16
   for line in file:
       p = line.split()
17
       c1.append(float(p[0]))
18
       c2.append(float(p[1]))
19
```

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
```

```
8  c4 = LM.fittedvalues
9  c5 = c3 ** 2
10
11  data2 = pd.DataFrame({"c4":c4, "c5":c5})
12  LM2 = smf.ols(formula = 'c5 ~ c4', data = data2).fit()
13  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;
2 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.
9
   MTB > sort c1 c3 c4 c5;
   SUBC > by c1.
10
11 MTB > print c1 c3 c4 c5
13
   Data Display
                 СЗ
14 Row C1
                      C4
                               C5
         80
             51.018
                     20 -20.770
         30
            -48.472
                       30
                          -48.472
16
                     30 42.528
       50 -19.876
17
    3
19
20
  MTB > copy c5 c11
21 MTB > copy c5 c12
22 MTB > delete 14:25 c11
23
   MTB > delete 1:13 c12
_{25} MTB > %S:\LM\levene c11 c12 k1
   Executing from file: S:\LM\levene.MAC
27
28 Data Display
        1.31648
30 K1
   MTB > invcdf 0.975;
32
33 SUBC> t 23.
   Inverse Cumulative Distribution Function
35
  Student's t distribution with 23 DF
38
   P( X <= x )
39
         0.975 2.06866
```

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

```
_{\rm 1} > # 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")
6
   > mydata =
       read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt")
   >
8
9
   > c1 = mydata[,1]
   > c2 = mydata[,2]
10
11
   > LM = lm(c2 ~c1)
13
   > c3 = resid(LM)
14
15
   > c1.order = order(c1)
16
  > c4 = c1 [ c1.order ]
   > c5 = c3 [ c1.order ]
18
19
  > print( cbind(c1,c3,c4,c5) )
20
       c1 c3 c4 c5
80 51.0179798 20 -20.7698990
21
22 1
       30 -48.4719192 30 -48.4719192
23 2
       50 -19.8759596 30 42.5280808
90 -7.6840404 30 103.5280808
24 3
25
   4
26
        . . . . . . . . . . . . . . . . . . .
27 >
28
   > gr1 = c5[1:13]
29 > gr2 = c5[14:25]
30
   > levene.test(gr1, gr2)
31
32
   $t.test.stat
33 [1] 1.316482
34
35 $df
36 [1] 23
37
38
   $p.value
   [1] 0.2009812
```

Python

```
1 #!/usr/bin/python3
  # If you have " CHO1TA01.txt " in your current computer .
3
   # 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)
10
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]))
        c2.append(int(p[1]))
19
20
21 import numpy as np
22 import pandas as pd
23 import scipy.stats as stats
   import statsmodels.formula.api as smf
24
25 data1 = pd.DataFrame({"c1":c1, "c2":c2})
26 LM = smf.ols(formula = 'c2 ~ c1', data = data1).fit()
27
c3 = LM.resid
30   c1 = np.asarray(c1)
31
    c3 = np.asarray(c3)
32 c1_order = np.argsort(c1, kind = 'stable')
33 c4 = c1[c1_order]
34
   c5 = c3[c1\_order]
35
36  # cbind = np.vstack((c1, c3, c4, c5))
37  cbind = pd.DataFrame({"c1":c1, "c2":c2, "c3":c3, "c4":c4})
38 print(cbind)
    gr1 = c5[0:13]
40
    gr2 = c5[13:25]
41
w, p = stats.levene(gr1, gr2)
    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.

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Example 3.5. (c) Breusch-Pagan Test.

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

https://github.com/AppliedStat/LM

```
_{\rm 1} MTB ># 1. Read the data
   MTB > READ C1 C2;
   SUBC >
              file "S:\LM\CHO1TAO1.TXT" .
   Entering data from file: S:\LM\CH01TA01.TXT
   25 rows read.
  MTB > # 2. RUN BPtest Macro
   MTB > %S:\LM\BPtest C2 C1 .
8
  Executing from file: S:\LM\BPtest.MAC
9
11 Data Display
12
13 Breusch-Pagan Test Statistic:
                                       0.82092
14 Degrees of Freedom:
                                       1
   p-value:
                                       0.36491
```

R

```
read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt")
2
   > c1 = mydata[,1]
   > c2 = mydata[,2]
   > LM = lm(c2 ~c1)
   > e = resid(LM)
   > sigma2 = e^2
10
   > LM2 = lm ( sigma2 ~ c1 )
12
13
  > SSR.star = sum( (fitted(LM2)-mean(sigma2))^2)
15
   > SSE = sum( (fitted(LM)-c2)^2 )
16
17
  > n = length(c2)
18
19
20 > cbind(SSR.star, SSE, n)
21
        SSR.star
                      SSE n
   [1,] 7896142 54825.46 25
23
24 > X.BP = SSR.star/2 / ((SSE/n)^2)
25
   > X.BP
26
27 [1] 0.8209192
28
  > qchisq(0.95, df = 1) ## chi-square critical value
29
  [1] 3.841459
```

Python

```
#!/usr/bin/python3
   # If you have " CH01TA01.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/CH01TA01.txt"
   url = urlopen(link)
file = url.read().splitlines()
12
  url.close()
14 c1 = []
c2 = []
16
  for line in file:
       p = line.split()
17
       c1.append(int(p[0]))
       c2.append(int(p[1]))
19
20
21 import numpy as np
   import pandas as pd
22
   import scipy.stats as stats
  import statsmodels.formula.api as smf
25
   data1 = pd.DataFrame({"c1":c1, "c2":c2})
26
  LM = smf.ols(formula = 'c2 ~ c1', data = data1).fit()
27
28
   e = LM.resid
  sigma2 = e**2
30
data2 = pd.DataFrame({"c1":c1, "sigma2":sigma2})
   LM2 = smf.ols(formula = 'sigma2 ~ c1', data = data2).fit()
33 SSR_star = sum((LM2.fittedvalues-np.mean(sigma2))**2)
34 SSE = sum((LM.fittedvalues-c2)**2)
35
   n = len(c2)
36
  cbind = pd.DataFrame({"SSR_star":SSR_star, "SSE":SSE, "n":n}, index = [0])
  print('\nData Display of SSR_star, SSE and n:')
38
39
   print(cbind)
X_BP = SSR_star/2/((SSE/n)**2)
   print('\nX_BP:')
  print(X_BP)
44
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

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https://github.com/AppliedStat/LM

```
1  > source("https://raw.githubusercontent.com/AppliedStat/LM/master/Breusch-Pagan.R")
2
3  > BP.test ( c2 ~ c1)
4  $test.stat
5  [1]  0.8209192
6
7  $df
8  [1]  1
9
10  $p.value
11  [1]  0.3649116
```

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.
 - 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.

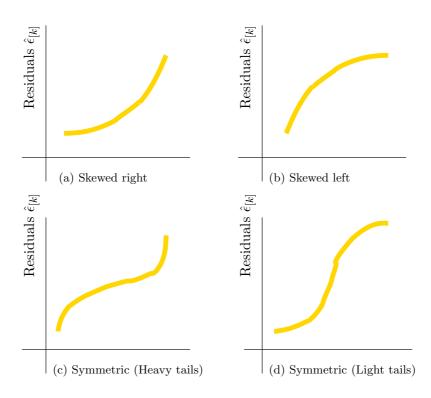
- (b) Distribution plots such as box plot, histogram, dot plot, stem-and-leaf.
- (c) Comparison of frequencies: $100(1-\alpha)\%$ of the residuals $\hat{\epsilon}_i$ fall between $\pm\sqrt{\text{MSE}}\cdot t(1-\frac{\alpha}{2};\text{df}=n-p)$, where p is the number of parameters.

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 the textbook or Table 2 of Looney and Gulledge (1985) in *The American Statistician* 39, pp. 75–79. If the sample correlation coefficient is at least as large as the critical value from Table B.6 (textbook) or Table 2 (Looney and Gulledge), 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

Q-Q Plots when error term is not Normal

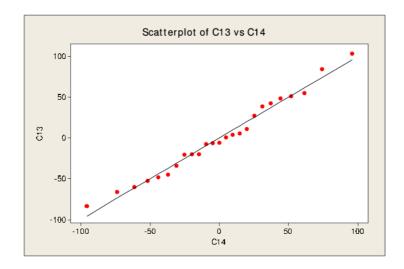


Example 3.6. Normal Probability Plot (based on the textbook).

Note that the normal probability plot using the Minitab built-in function, %resplot, uses the horizontal axis for the residuals.

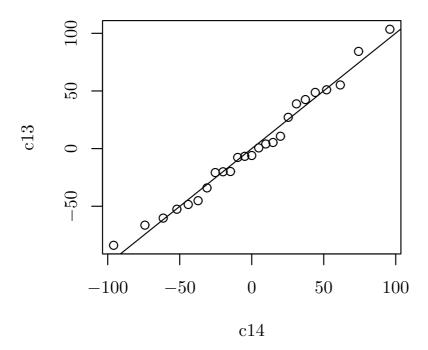
Minitab

```
MTB > READ C1 C2;
   SUBC >
             file "S:\LM\CH01TA01.txt" .
   Entering data from file: S:\LM\CHO1TA01.TXT
   25 rows read.
   MTB > regr c2 1 c1;
   SUBC > resid c3;
   SUBC > mse
                k2.
   MTB >let k1 = count(c3)
10
   MTB > set c10
12
   DATA >
13
              1:k1
   DATA > end.
14
15
   MTB >sort c3 c13
16
17
   MTB > let c11 = (c10 - .375) / (k1+.25)
18
19
   MTB >invcdf c11 c12;
   SUBC > normal 0 1.
20
   MTB >let c14 = sqrt(k2)*c12
21
   MTB >plot c13*c14;
   SUBC > line c14 c14.
```



R

```
> mydata =
1
       read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt")
   > c1 = mydata[,1]
3
   > c2 = mydata[,2]
4
   > LM = lm(c2 ~c1)
6
   > c3 = resid(LM)
8
9
10
   > LM.sum = summary(LM)
11
12
  > attributes(LM.sum)
   $names
13
   [1] "call"
                        "terms"
                                         "residuals"
                                                         "coefficients"
14
   [5] "aliased"
                                         "df"
                        "sigma"
                                                         "r.squared"
   [9] "adj.r.squared" "fstatistic"
                                         "cov.unscaled"
16
17
18 $class
  [1] "summary.lm"
19
20
21 > s = LM.sum[[ "sigma" ]]
22
   > c13 = sort(c3)
23
24 >
  > n = length(c3)
25
26
  > k = 1:n
27
28
   > c11 = (k - 0.375) / (n+0.25)
29
30 >
31 > c12 = qnorm( c11 )
32
  > c14 = s * c12
33
34
   > postscript( "ex4a.ps", width=4, height=4)
35
36 >
37 > plot ( c14, c13)
```



38 > abline(lm(c13~c14))

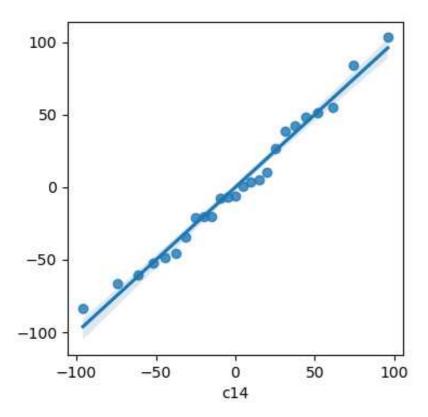
Python

```
#!/usr/bin/python3
    \mbox{\tt\#} If you have \mbox{\tt "CH01TA01.txt} \mbox{\tt "in your current computer} .
3
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
    {\tt link = "https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt"}
   url = urlopen(link)
   file = url.read().splitlines()
11
12
    url.close()
13
14 c1 = []
    c2 = []
15
    for line in file:
16
         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
# sudo apt-get install -y python3-seaborn

# sudo apt-get install -y python3-pandas

# sudo apt-get install -y python3-pandas

# sudo apt-get install -y python3-numexpr # latest numexpr is needed for pandas
27 import numpy as np
```



```
import scipy.stats as stats
  import pandas as pd
29
30
31 import statsmodels.formula.api as smf
32 import matplotlib.pyplot as plt
  data1 = pd.DataFrame({"c1":c1, "c2":c2})
34
  LM = smf.ols(formula = 'c2 ~ c1', data = data1).fit()
35
36
   c3 = LM.resid
37
38
  LM_sum = LM.summary()
39
40
41
   # get the residual standard error
   squared_sigma = LM.mse_resid
42
43 s = squared_sigma ** 0.5
   c13 = np.sort(c3)
45
46
   n = len(c3)
47
   c14 = []
48
49
    for k in range(1,n+1):
        c11 = (k - 0.375)/(n + 0.25)
50
        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})
58 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

```
1 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;
8
   SUBC > mse
10 MTB > let k1 = count(c3)
11
12 MTB > set c10
13 DATA > 1:k1
14 DATA > end .
16 MTB > sort c3 c13
17
18 MTB > let c11 = (c10 - .375) / (k1+.25)
19
20 MTB >invcdf c11 c12;
21 SUBC > normal 0 1.
22
23 MTB >let c14 = sqrt(k2)*c12
24
_{25} MTB > correlation c13 c14 .
26
  Correlations: C13, C14
27
29 Pearson correlation of C13 and C14 = 0.992
30 P-Value = 0.000
```

Don't use the above p-value for the normality test.

R

```
> # Using Normal Probability Plot
2 > mydata =
       read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt")
  > c1 = mydata[,1]
  > c2 = mydata[,2]
   > LM = lm(c2)
   > c3 = resid(LM)
   > LM.sum = summary(LM)
  > s = LM.sum[[ "sigma" ]]
   > c13 = sort(c3)
10 > n = length(c3)
11 > k = 1:n
   > c11 = (k - 0.375) / (n+0.25)
^{13} > c12 = qnorm( c11 )
14 > c14 = s * c12
15
  > cor(c13, c14)
16
17 [1] 0.9915055
18
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

```
1 #!/usr/bin/python3
3 # If you have " CHO1TA01.txt " in your current computer .
  # mydata = open("S:/LM/CH01TA01.txt", "r")
5 # file = mydata.read().splitlines()
8 # If PC is connected to Internet, then the following works.
   from urllib.request import urlopen
10 link = "https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt"
url = urlopen(link)

file = url.read().splitlines()
url.close()
14
15 c1 = []
16 c2 = []
17 for line in file:
        p = line.split()
18
        c1.append(int(p[0]))
19
20
       c2.append(int(p[1]))
21
22 import numpy as np
23 import scipy.stats as stats
24 import pandas as pd
25 import statsmodels
   import statsmodels.formula.api as smf
27  data1 = pd.DataFrame({"c1":c1, "c2":c2})
28  LM = smf.ols(formula = 'c2 ~ c1', data = data1).fit()
29
30 c3 = LM.resid
31 LM_sum = LM.summary()
32
33 squared_sigma = LM.mse_resid
34 s = squared_sigma ** 0.5
35
36 c13 = np.sort(c3)
n = len(c3)
39 c11 = [(k - 0.375)/(n + 0.25) for k in range(1,n+1)]
40
41 c12 = stats.norm.ppf(c11)
c14 = s * c12
43
44 cor1 = np.corrcoef(c13, c14)
45 print(cor1)
46
47
   a = 3/8
48 m = len(c13)
49
_{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)]
53
54  qq = stats.norm.ppf(pp)
55 cor2 = np.corrcoef(c13, qq)
56 print(cor2)
```

From Table B.6 of the textbook or Table 2 of Looney and Gulledge (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.

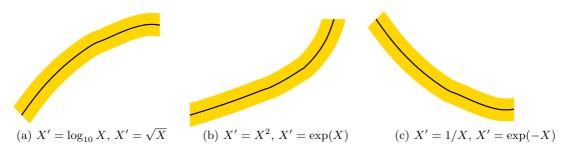
3 Transformations

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.

Prototype Nonlinear regression pattern with constant error variance.

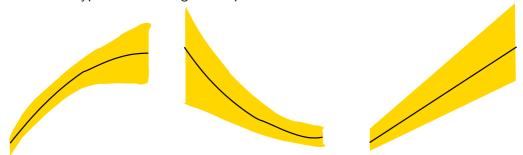


3.2 Transformations of the response Y

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.

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Prototype Nonlinear regression pattern with non-constant error variance.



Possible transformations: $Y' = \sqrt{Y}$, $Y' = \log_{10} Y$, 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

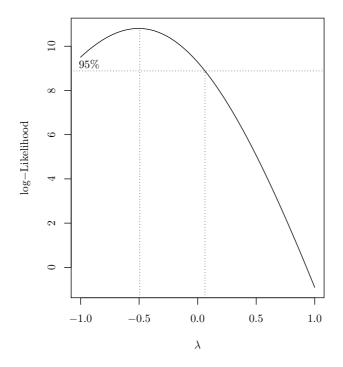
```
## See Table 3.9 (Section 3.9)
  MTB > READ c1 c2 c3;
   SUBC> file "S:\LM\CHO3TA08.txt" .
  Entering data from file: S:\LM\CHO3TAO8.TXT
   25 rows read.
   ## Generate 1.0, 0.9, ..., -1.0
  MTB >set c3
8
   DATA > 10:-10
10 DATA > end
11
12 MTB >let c3 = c3/10
13
14 MTB >%S:\LM\bxcx c2 c1 c3 c4
15 Executing from file: S:\LM\bxcx.MAC
16
17 MTB >print c3 c4
   Data Display
18
19
   Row
         C3
         1.0 77.9831
     2
         0.9
              70.3505
21
22
     3
         0.8 63.6693
         0.7 57.8369
23
         0.6 52.7634
     5
24
25
     6
         0.5
              48.3707
         0.4 44.5905
26
27
    8
         0.3 41.3634
         0.2 38.6379
28
    9
    10
        0.1 36.3694
29
30
    11
        0.0 34.5195
31
    12
        -0.1
              33.0552
        -0.2
              31.9487
    13
32
33
    14
        -0.3 31.1763
    15
        -0.4
34
              30.7186
        -0.5
              30.5596
35
    16
    17
        -0.6 30.6868
    18
        -0.7
              31.0907
37
38
    19
        -0.8
              31.7645
    20
        -0.9 32.7044
39
   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:
   > source("https://raw.githubusercontent.com/AppliedStat/LM/master/bxcx.R")
4
  > mydata =
       read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CH03TA08.txt")
  > c1 = mydata[,1]
   > 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
                   sse
         1.0 77.98306
14
   [1,]
   [2,]
         0.9 70.35050
15
    [3,]
         0.8 63.66932
16
         0.7 57.83686
17
    [4,]
         0.6 52.76343
    [5,]
18
19
    [6,]
         0.5 48.37072
20
    [7,]
         0.4 44.59051
         0.3 41.36342
21
    [8,]
22
    [9,]
         0.2 38.63791
23
   [10,]
         0.1 36.36939
         0.0 34.51945
   [11,]
24
   [12,] -0.1 33.05520
   [13,] -0.2 31.94867
26
   [14,] -0.3 31.17631
27
   [15,] -0.4 30.71859
   [16,] -0.5 30.55961
29
   [17,] -0.6 30.68680
30
   [18,] -0.7 31.09066
   [19,] -0.8 31.76453
[20,] -0.9 32.70442
32
33
  [21,] -1.0 33.90887
   > # Using MASS library
37
38 > # For help, use
   > # > library(help="MASS") or help("boxcox")
   > library("MASS")
41
   \gt # Note: 1. find the max. instead of the min.
            2. log-likelihood is used instead of SSE
45
46 > lam = seq(1.0, -1.0, by=-0.1)
47 > boxcox( c2 ~ c1 , lambda = lam )
```



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 $\lambda = 0.3645$.

References

Hollander, M. and Wolfe, D. A. (2013). *Nonparametric Statistical Methods*. Wiley, New York, 3rd edition.

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