$_{\text{Chapter}}$ 

# 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  $\epsilon_i$  are not independent,

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

4. The errors  $\epsilon_i$  are not normally distributed,

 $(\Rightarrow$  histogram, normal probability plot or Q–Q plot)

3.1. RESIDUALS IE-34243

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.

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

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

# 3.2 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

```
MTB > READ C1 C2;

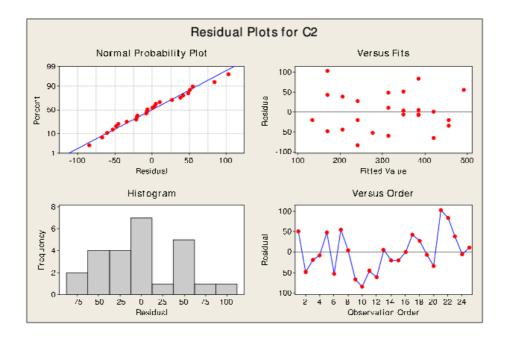
SUBC> file "U:\math8050\data\CH01TA01.txt" .

Entering data from file: U:\MATH8050\DATA\CH01TA01.TXT 25 rows read.

## 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
```

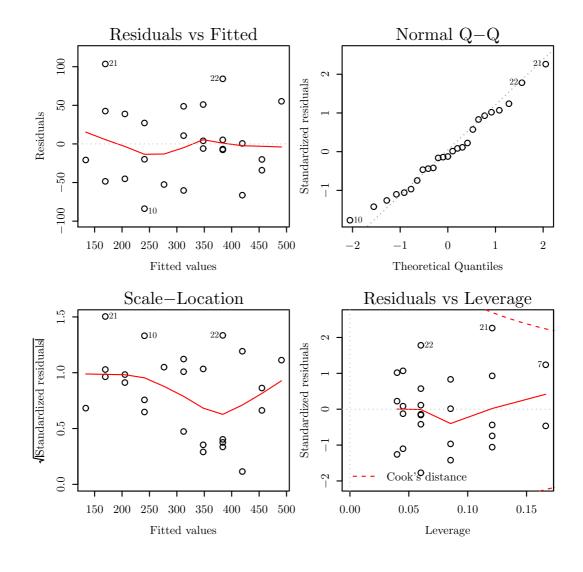


R

```
# Read the data set
mydata = read.table("U:\\math8050\\data\\CH01TA01.txt")
```

# If PC is connected to Internet, then the following works.
mydata = read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt")

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



 $\triangle$ 

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.

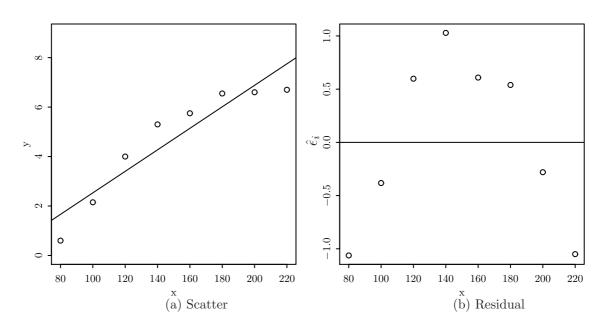
# 3.2.1 Non-linearity of regression function

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.

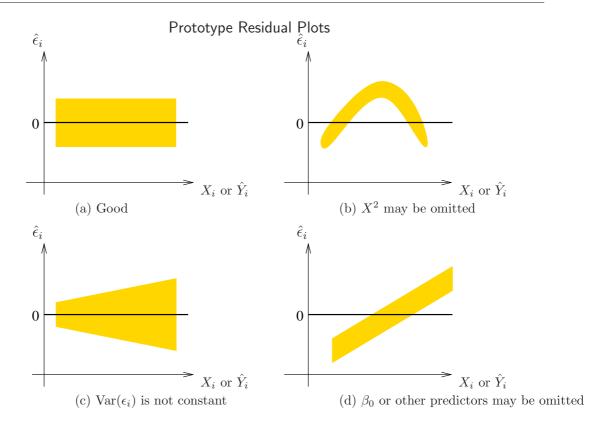
```
R
x = c(80, 220, 140, 120, 180, 100, 200, 160)
y = c(0.60,6.70,5.30,4.00,6.55,2.15,6.60,5.75)

LM = lm(y~x)
y1 = fitted(LM)
r = y - y1

par(mfrow=c(1,2))  ## two plots into one sheet plot(x,y, ylim=c(0,9), sub="(a)")
abline(coef(LM))

plot(x,r, sub="(b)")
abline(h=0)
```

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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.,  $\gamma_2$ ) 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.

Regression Analysis: C2 versus C1

The regression equation is C2 = -1.82 + 0.0435 C1

 Predictor
 Coef
 SE Coef
 T
 P

 Constant
 -1.816
 1.052
 -1.73
 0.135

 C1
 0.043482
 0.006706
 6.48
 0.001

S = 0.869241 R-Sq = 87.5% R-Sq(adj) = 85.4%

Analysis of Variance

 Source
 DF
 SS
 MS
 F
 P

 Regression
 1
 31.764
 31.764
 42.04
 0.001

 Residual Error
 6
 4.533
 0.756

 Total
 7
 36.297

MTB > let c4 = c3\*\*2. MTB > regr  $c5 \ 2 \ c3 \ c4$ .

Regression Analysis: C5 versus C3, C4

The regression equation is C5 = -3.87 + 2.00 C3 - 0.213 C4

 Predictor
 Coef
 SE Coef
 T
 P

 Constant
 -3.8702
 0.3896
 -9.93
 0.000

 C3
 2.0039
 0.1843
 10.87
 0.000

 C4
 -0.21290
 0.01925
 -11.06
 0.000

S = 0.188738 R-Sq = 96.1% R-Sq(adj) = 94.5%

Analysis of Variance

 Source
 DF
 SS
 MS
 F
 P

 Regression
 2
 4.3554
 2.1777
 61.13
 0.000

 Residual Error
 5
 0.1781
 0.0356
 0.000

Total 7 4.5335

Source DF Seq SS C3 1 0.0000 C4 1 4.3554

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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
> c5 = resid(LM)
> LM2 = lm(c5 ~c3 + c4)
> summary(LM2)
Call:
lm(formula = c5 ~c3 + c4)
Residuals:
             2
                  3
                         4 5
                                        6
     1
Coefficients:
         Estimate Std. Error t value Pr(>|t|)
0.18430 10.873 0.000114 ***
0.01925 -11.057 0.000105 ***
сЗ
         2.00392
c4
         -0.21290
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
Residual standard error: 0.1887 on 5 degrees of freedom
Multiple R-Squared: 0.9607, Adjusted R-squared: 0.945
F-statistic: 61.13 on 2 and 5 DF, p-value: 0.0003059
```

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.

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### 3.2.2 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  $|t_L^*| \leq t(1-\frac{\alpha}{2}; n_1+n_2-2)$ , 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  $(d_{i_1}, d_{i_2}, \ldots, d_{i_k})$ , 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  $\epsilon_i$ , denoted by  $\sigma_i^2$  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:

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

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  $\chi^2$  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  $i=1,2,\ldots,n_1$  and  $j=1,2,\ldots,n_2$ . 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<sup>1</sup> 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

<sup>&</sup>lt;sup>1</sup>Hollander, M./Wolfe, D. A. Nonparametric Statistical Methods. 3rd edition. New York: Wiley, 2013.

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 "U:\math8050\data\CH01TA01.txt" .
Entering data from file: U:\MATH8050\DATA\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.
Regression Analysis: C5 versus C4
The regression equation is
C5 = 3940 - 5.59 C4
Predictor Coef SE Coef
                             Т
           3940 1756 2.24 0.035
                  5.354 -1.04 0.307
          -5.593
S = 2689.72  R-Sq = 4.5\%  R-Sq(adj) = 0.4\%
```

#### Analysis of Variance

SS MSF Regression 1 7896142 7896142 1.09 0.307 Residual Error 23 166395896 7234604 24 174292038

#### Unusual Observations

```
Obs C4
          C5
              Fit SE Fit Residual St Resid
21 169 10718 2992
                      935
                              7726
                                       3.06R
22 384 7109 1794
                      660
                                       2.04R
                              5316
```

R denotes an observation with a large standardized residual.

R

```
\mbox{\tt \#\#} if you have "CHO1TA01.txt" in your current computer.
> mydata = read.table("U:\\math8050\\data\\CH01TA01.txt")
## if your computer is connected to Internet
> mydata = read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt")
> c1 = mydata[,1]
> c2 = mydata[,2]
> LM = lm(c2 ~c1)
> c3 = resid(LM)
> c4 = fitted(LM)
> c5 = c3^2
> LM2 = lm(c5 ~c4)
> summary(LM2)
Call:
lm(formula = c5 ~ c4)
Residuals:
Min 1Q Median 3Q Max -2760.1 -1765.4 -990.7 609.5 7726.3
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 3939.750 1756.371 2.243 0.0348 * c4 -5.593 5.354 -1.045 0.3070
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
Residual standard error: 2690 on 23 degrees of freedom
Multiple R-Squared: 0.0453, Adjusted R-squared: 0.003796
F-statistic: 1.091 on 1 and 23 DF, p-value: 0.307
```

Δ

#### 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

```
MTB > READ C1 C2;
SUBC> file "U:\math8050\data\CH01TA01.txt" .
Entering data from file: U:\MATH8050\DATA\CH01TA01.TXT
25 rows read.
MTB > regr c2 1 c1;
SUBC> resid c3.
MTB > sort c1 c3 c4 c5;
SUBC> by c1.
MTB > print c1 c3 c4 c5
Data Display
 cow C1 C3 C4 C5
1 80 51.018 20 -20.770
2 30 -48.472 30 -48.472
3 50 -19.876 30 42.528
Row C1
MTB > copy c5 c11
MTB > copy c5 c12
MTB > delete 14:25 c11
MTB > delete 1:13 c12
MTB > U:\mathbb{50} minitab\levene c11 c12 k1
Executing from file: U:\math8050\minitab\levene.MAC
Data Display
     1.31648
MTB > invcdf 0.975;
SUBC> t 23.
Inverse Cumulative Distribution Function
Student's t distribution with 23 DF
P( X <= x )
      0.975 2.06866
```

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 file at your current directory.
> source("U:/math8050/R/levene.R")
> ## If your PC is connected to Internet, the following will work:
> source("https://raw.githubusercontent.com/AppliedStat/LM/master/levene.R")
> mydata = read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt")
> c1 = mydata[,1]
> c2 = mydata[,2]
> LM = lm(c2 ~c1)
> c3 = resid(LM)
> c1.order = order(c1)
> c4 = c1 [ c1.order ]
> c5 = c3 [ c1.order ]
> print( cbind(c1,c3,c4,c5) )
   c1
            c3 c4
   80 51.0179798 20 -20.7698990
   30 -48.4719192 30 -48.4719192
  50 -19.8759596 30 42.5280808
  90 -7.6840404 30 103.5280808
> gr1 = c5[1:13]
> gr2 = c5[14:25]
> levene.test(gr1, gr2)
$t.test.stat
[1] 1.316482
$df
[1] 23
$p.value
[1] 0.2009812
```

Note that the t-distribution critical value for the modified Levene's test at the significance level  $\alpha$  with df can be found in R as follows:

> qt(1 - 
$$\alpha$$
/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.

 $\triangle$ 

[1] 3.841459

#### 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

```
MTB ># 1. Read the data
MTB > READ C1 C2;
SUBC>
           file "U:\math8050\data\CH01TA01.TXT" .
Entering data from file: U:\MATH8050\DATA\CH01TA01.TXT
25 rows read.
MTB > # 2. RUN BPtest Macro
MTB > %U:\math8050\minitab\BPtest C2 C1 .
Executing from file: U:\math8050\minitab\BPtest.MAC
Data Display
Breusch-Pagan Test Statistic:
                                  0.82092
Degrees of Freedom:
                                  0.36491
p-value:
R
> mydata = read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt")
> c1 = mydata[,1]
> c2 = mydata[,2]
> LM = lm(c2 \sim c1)
> e = resid(LM)
> sigma2 = e^2
> LM2 = lm (sigma2 ~c1)
> SSR.star = sum( (fitted(LM2)-mean(sigma2))^2 )
> SSE = sum( (fitted(LM)-c2)^2 )
> n = length(c2)
> cbind(SSR.star, SSE, n)
                 SSE n
    SSR.star
[1,] 7896142 54825.46 25
> X.BP = SSR.star/2 / ( (SSE/n)^2 )
> X.BP
[1] 0.8209192
> qchisq(0.95, df = 1) ## chi-square critical value
```

Note that the  $\chi^2$  critical value for the Breusch-Pagan test at the significance level  $\alpha$  with df can be found in R as follows:

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$$>$$
 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.

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

#### https://github.com/AppliedStat/LM

```
> source("https://raw.githubusercontent.com/AppliedStat/LM/master/Breusch-Pagan.R")
>
> BP.test ( c2 ~ c1)
$test.stat
[1] 0.8209192
$df
[1] 1
$p.value
[1] 0.3649116
```

 $\triangle$ 

#### 3.2.3 Presence of outliers

Outliers are extreme observations.

Plot

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

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

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).

# 3.2.4 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).

# 3.2.5 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:  $100(1-\alpha)\% \text{ of the residuals } \hat{\epsilon}_i \text{ fall between } \pm \sqrt{\text{MSE}} \cdot t(1-\frac{\alpha}{2}; \text{df} = n-p), \text{ where } p \text{ is the number of parameters.}$

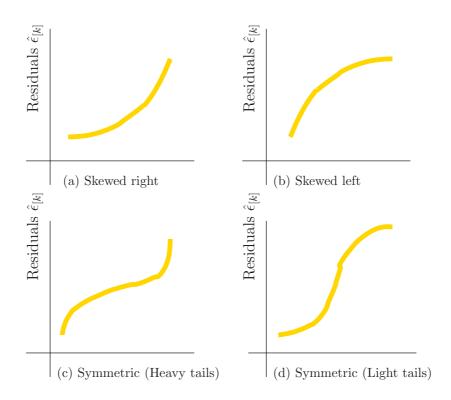
Test

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  $\alpha$  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 therms are reasonably normally distributed.

Personal Note: 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.

Example 3.6. Normal Probability Plot (based on the textbook). Note that the normal probability plot using the Minitab built-in function, %resplot,

### Q-Q Plots when error term is not Normal



uses the horizonal axis for the residuals.

#### Minitab

```
MTB > READ C1 C2;
       file "U:\math8050\data\CH01TA01.txt" .
Entering data from file: U:\MATH8050\DATA\CH01TA01.TXT
25 rows read.
MTB > regr c2 1 c1;
SUBC> resid c3;
SUBC> mse k2.
MTB >let k1 = count(c3)
MTB > set c10
DATA> 1:k1
DATA> end .
MTB >sort c3 c13
MTB > let c11 = (c10 - .375) / (k1+.25)
MTB >invcdf c11 c12;
SUBC> normal 0 1.
MTB >let c14 = sqrt(k2)*c12
MTB >plot c13*c14;
```

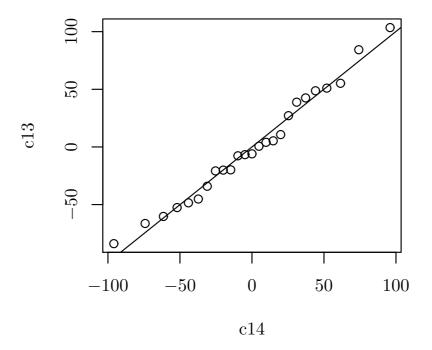
SUBC> line c14 c14 .

Scatterplot of C13 vs C14

# R

```
> mydata = read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt")
> c1 = mydata[,1]
> c2 = mydata[,2]
> LM = lm(c2 ~c1)
> c3 = resid(LM)
> LM.sum = summary(LM)
> attributes(LM.sum)
$names
[1] "call"
[5] "aliased"
                     "terms"
                                     "residuals"
                                                     "coefficients"
                    "sigma"
                                     "df"
                                                     "r.squared"
 [9] "adj.r.squared" "fstatistic"
                                   "cov.unscaled"
$class
[1] "summary.lm"
> s = LM.sum[[ "sigma" ]]
> c13 = sort(c3)
> n = length(c3)
> k = 1:n
```

```
> c11 = (k - 0.375) / (n+0.25)
> c12 = qnorm( c11 )
> c14 = s * c12
> postscript( "ex4a.ps", width=4, height=4)
> plot ( c14, c13)
> abline(lm(c13~c14))
```



 $\triangle$ 

Example 3.7. Correlation test for normality.

#### Minitab

```
MTB > READ C1 C2;
SUBC> file "U:\math8050\data\CH01TA01.txt" .
Entering data from file: U:\MATH8050\DATA\CH01TA01.TXT
25 rows read.
```

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```
MTB >regr c2 1 c1;
SUBC> resid c3;
SUBC> mse k2.
MTB > let k1 = count(c3)
MTB > set c10
DATA> 1:k1
DATA> end .
MTB > sort c3 c13
MTB > let c11 = (c10 - .375) / (k1+.25)
MTB >invcdf c11 c12;
SUBC> normal 0 1.
MTB >let c14 = sqrt(k2)*c12
MTB > correlation c13 c14 .
Correlations: C13, C14
Pearson correlation of C13 and C14 = 0.992
P-Value = 0.000
```

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

#### R

```
> ## Using Normal Probability Plot
> mydata = read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CH01TA01.txt")
> c1 = mydata[,1]
> c2 = mydata[,2]
> LM = lm(c2 ~c1)
> c3 = resid(LM)
> LM.sum = summary(LM)
> s = LM.sum[[ "sigma" ]]
> c13 = sort(c3)
> n = length(c3)
> k = 1:n
> c11 = (k - 0.375) / (n+0.25)
> c12 = qnorm( c11 )
> c14 = s * c12
> cor(c13, c14)
[1] 0.9915055
> ## Using Q-Q plot
> pp = ppoints(c13, a=3/8) # option "a=3/8=0.375" gives (k-0.375)/(n+0.25)
> qq = qnorm(pp)
> cor(c13, qq)
[1] 0.9915055
```

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

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correlation coefficient exceeds this critical value, we can conclude that the distribution the error terms does not depart from a normal distribution.

 $\triangle$ 

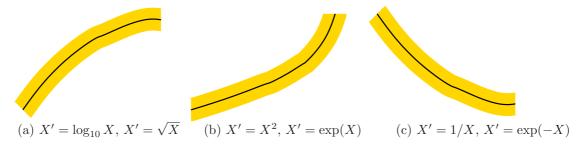
# 3.3 Transformations

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

### 3.3.1 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.

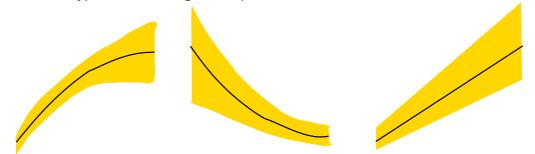
Prototype Nonlinear regression pattern with constant error variance.



# **3.3.2** 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.

Prototype Nonlinear regression pattern with nonconstant error variance.



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

#### 3.3.3 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  $\lambda$  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  $\lambda$  to use in the power transformation. Note that the textbook use  $\lambda$  which has the smallest SSE.

#### Example 3.8. Box-Cox Transforms

Minitab Th

The  ${\tt Minitab}$  macro for the Box-Cox Transform  $({\tt bxcx.MAC})$  is available

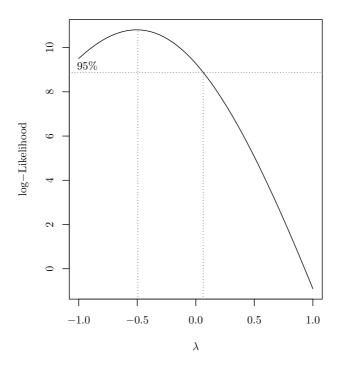
#### https://github.com/AppliedStat/LM

```
## See Table 3.9 (Section 3.9)
MTB > READ c1 c2 c3;
SUBC> file "U:\math8050\data\CH03TA08.txt" .
Entering data from file: U:\MATH8050\DATA\CH03TA08.TXT
25 rows read.
## Generate 1.0, 0.9, ..., -1.0
MTB >set c3
DATA> 10:-10
DATA> end
MTB >let c3 = c3/10
MTB >%U:\math8050\minitab\bxcx c2 c1 c3 c4
Executing from file: U:\mathbb{U}
MTB >print c3 c4
Data Display
    C3
     1.0 77.9831
 1
     0.9 70.3505
    0.8 63.6693
     0.7 57.8369
     0.6 52.7634
    0.5 48.3707
     0.4 44.5905
 8
     0.3 41.3634
    0.2 38.6379
 9
 10 0.1 36.3694
 11
    0.0 34.5195
 12 -0.1 33.0552
 13 -0.2 31.9487
 14 -0.3 31.1763
15 -0.4 30.7186
 16 -0.5 30.5596
17 -0.6 30.6868
18 -0.7 31.0907
 19 -0.8 31.7645
20 -0.9 32.7044
21 -1.0 33.9089
```

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

### https://github.com/AppliedStat/LM

```
> source("bxcx.R")
> ## Or, using web link:
> source("https://raw.githubusercontent.com/AppliedStat/LM/master/bxcx.R")
> mydata = read.table("https://raw.githubusercontent.com/AppliedStat/LM/master/CHO3TAO8.txt")
> c1 = mydata[,1]
> c2 = mydata[,2]
> lam = seq(1.0, -1.0, by=-0.1)
> sse = bxcx(c2, c1, lambda=lam)
> cbind(lam, sse)
      lam
 [1,] 1.0 77.98306
 [2,] 0.9 70.35050
[3,] 0.8 63.66932
 [4,] 0.7 57.83686
 [5,] 0.6 52.76343
[6,] 0.5 48.37072
 [7,] 0.4 44.59051
[8,] 0.3 41.36342
[9,] 0.2 38.63791
[10,] 0.1 36.36939
[11,] 0.0 34.51945
[12,] -0.1 33.05520
[13,] -0.2 31.94867
[14,] -0.3 31.17631
[15,] -0.4 30.71859
[16,] -0.5 30.55961
[17,] -0.6 30.68680
[18,] -0.7 31.09066
[19,] -0.8 31.76453
[20,] -0.9 32.70442
[21,] -1.0 33.90887
> # ========
> # Using MASS library
> # For help, use
> # > library(help="MASS") or help("boxcox")
> library("MASS")
> # Note: 1. find the max. instead of the min.
> #
        log-likelihood is used instead of SSE
> lam = seq(1.0, -1.0, by=-0.1)
> boxcox( c2 ~ c1 , lambda = lam )
```



Δ

#### Note:

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