

# ST5202: Applied Regression Analysis

Department of Statistics and Applied Probability  
National University of Singapore

05-Feb-2018  
Week 4

## Announcement

- Assignment #2 available online
  - Due on 12 Feb by 9 pm
  - Submit either in-class or via email (in-class submission preferred)
  - Please write BOTH your name and metric number
- Make-up midterm request due on 26 Feb
  - Better to make request as soon as possible
  - Official supporting document required
  - Request after the due date would not be considered

# Week 4

## Reviews & Diagnostics and Remedial Measures (Chapter 3)

### Some Reviews & Construction of Confidence Band

- Inference about the mean response  $E\{Y_h\}$
- Predicting new observations  $Y_{h(new)}$
- Confidence bound for a regression line (new stuff!)
- General linear test approach

### Review:

Inference about the mean response  $E\{Y_h\}$  at  $X = X_h$

- $E\{Y_h\}$  is the expected/mean outcome with the given level of  $X$  is  $X_h$ 
  - Estimator for  $E\{Y_h\}$  given by:  $\hat{Y}_h = b_0 + b_1 X_h$ , with sampling distribution:

$$\hat{Y}_h \sim N(\beta_0 + \beta_1 X_h, \sigma^2 \{ \hat{Y}_h \})$$

$$\text{with } \sigma^2 \{ \hat{Y}_h \} = \sigma^2 \left( \frac{1}{n} + \frac{(X_h - \bar{X})^2}{\sum (X_i - \bar{X})^2} \right)$$

- As with the sampling distribution of the  $b_i$ 's,  $\sigma^2$  is unknown and estimated by  $s^2$ , which then gives a t-distribution for studentized  $\hat{Y}_h$ :  
$$\frac{\hat{Y}_h - E\{Y_h\}}{s\{\hat{Y}_h\}} \sim t_{n-2} \text{ with } s^2 \{ \hat{Y}_h \} = s^2 \left( \frac{1}{n} + \frac{(X_h - \bar{X})^2}{\sum (X_i - \bar{X})^2} \right)$$

### Review:

Inference about the mean response  $E\{Y_h\}$  at  $X = X_h$

- Using this sampling distribution, we can construct  $(1 - \alpha)100\%$  confidence interval for  $E\{Y_h\}$ :

$$\hat{Y}_h \pm t(1 - \alpha/2; n - 2)s\{\hat{Y}_h\}$$

## Review:

Prediction of a new observation given  $X = X_h$

- We have

$$\begin{aligned}Y_{h(new)} &\sim N(\beta_0 + \beta_1 X_h, \sigma^2) \\ \hat{Y}_h &\sim N(\beta_0 + \beta_1 X_h, \sigma^2 \{\hat{Y}_h\})\end{aligned}$$

- We utilize the distribution of  $(Y_{h(new)} - \hat{Y}_h)$  :

$$\begin{aligned}(Y_{h(new)} - \hat{Y}_h) &\sim N(0, \sigma^2 \{\text{pred}\}) \text{ where} \\ \sigma^2 \{\text{pred}\} &= \text{Var}(Y_{h(new)} - \hat{Y}_h) \\ &= \text{Var}(Y_{h(new)}) + \text{Var}(\hat{Y}_h) \\ &= \sigma^2 + \sigma^2 \{\hat{Y}_h\} \\ &= \sigma^2 \left( 1 + \frac{1}{n} + \frac{(X_h - \bar{X})^2}{\sum (X_i - \bar{X})^2} \right)\end{aligned}$$

## Review:

### Prediction of a new observation given $X = X_h$

- ▶ We have

$$\frac{(Y_{h(new)} - \hat{Y}_h)}{\sigma\{pred\}} \sim N(0, 1)$$

- ▶ To construct prediction intervals for  $Y_{h(new)}$  based on its distribution, we need to estimate  $\sigma\{pred\}$  by  $s\{pred\}$ , which gives:

$$\frac{Y_{h(new)} - \hat{Y}_h}{s\{pred\}} \sim t_{n-2}$$

and the  $(1 - \alpha)100\%$  prediction interval (PI) is given by  $\hat{Y}_h \pm t(1 - \alpha/2; n - 2)s\{pred\}$ .

- ▶ Interpretation: We are  $(1 - \alpha)\%$  confident that the PI will contain the new observation
- ▶ Note: we can NOT state  $Pr(Y_{h(new)} \in (1 - \alpha)100\%PI) = 1 - \alpha$ , because the bounds of the PI have been constructed based on one sample (e.g. based on the estimate  $\hat{Y}_h$ )



## New Stuff

### Confidence band for a regression line

- Note: we **CANNOT** state  $Pr(Y_{h(new)} \in (1 - \alpha)100\%PI) = 1 - \alpha$  because the bounds of the PI have been constructed based on one batch of sample (i.e., based on the estimate  $\hat{Y}_h$ )
- GPA example:
  - for  $\hat{X}_h = 27$ , we have  $\hat{Y}_h = 3.16238$  and  $s\{pred\} = 0.6263652$ .  
Is  $\frac{Y_{h(new)} - 3.16238}{\sigma\{pred\}} \sim N(0, 1)$ ?  
Is  $\frac{Y_{h(new)} - 3.16238}{0.6263652} \sim t_{n-2}$ ?

## New Stuff

### Confidence band for a regression line

- ▶ Regression line  $\beta_0 + \beta_1 X$  is estimated by  $\hat{Y} = b_0 + b_1 X$
- ▶ Construct a confidence band for  $\beta_0 + \beta_1 X$ :  
The band (area) is expected to contain the true regression line 95/100 repeated samples
- ▶ The bounds of the band will be (slightly) wider than the individual CIs at each level of  $X_h$ , because the band has to include the entire regression line 95/100 times, instead of just one expected value
- ▶ The “Working-Hotelling” confidence band for the regression line is given by:

$$\hat{Y}_h \pm W \cdot s\{\hat{Y}_h\},$$

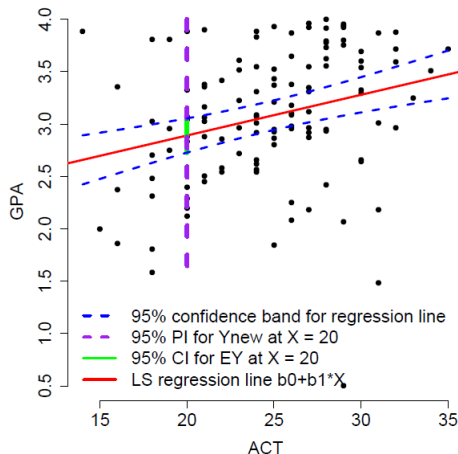
with

$$W = \sqrt{2F(1 - \alpha; 2, n - 2)}$$

- ▶  $F(1 - \alpha; 2, n - 2)$  is the  $(1 - \alpha)$  percentile of the F-distribution with 2 and  $(n - 2)$  degrees of freedom

## Week 4: Diagnostics and Remedial Measures

### Confidence band for a regression line GPA example



### Review: General Linear Test Approach

- Three steps: 1) full Model, 2) reduced model, and 3) test statistic
- Error sum of squares of the full model ( $SSE(F)$ ) measures the variability of the  $Y_i$  observations around the fitted regression line from the full model
- Error sum of squares of the reduced model ( $SSE(R)$ ) is the variability of the observation  $Y_i$  around the fitted regression line from the reduced model
- IDEA: if  $SSE(F)$  is not much less than  $SSE(R)$ , then it implies that full model does not explain the data much better than the reduced model

## General Linear Test Approach

- The test statistic

$$F^* = \frac{SSE(R) - SSE(F)}{df_R - df_F} \div \frac{SSE(F)}{df_F} \sim F(df_R - df_F, df_F) \text{ when } H_0 \text{ holds}$$

where  $df_R$  and  $df_F$  are the degrees of freedom associated with the reduced model and the full model respectively

- The decision rule:

If  $F^* \leq F(1 - \alpha; df_R - df_F, df_F)$ , conclude  $H_0$

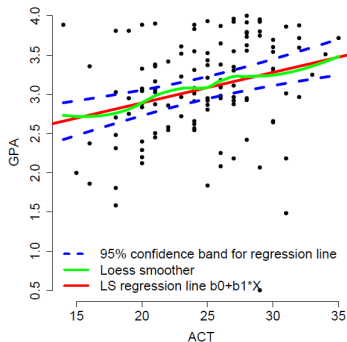
If  $F^* > F(1 - \alpha; df_R - df_F, df_F)$ , conclude  $H_a$

### Diagnostics and Remedial Measures

### Exploration of Shape of Regression Function: Smoothing (Nonparametric Regression Curves)

- Fit a smooth curve without any constraints on the regression function to the data  
→ Helpful to explore the nature of the regression relationship, if any, by fitting a smoothed curve
- Nice method to find such a smoothed curve:  
Lowess method (or simply loess)
  - Stands for “Locally Weighted Regression Scatter Plot Smoothing”
  - Fits a regression function locally;  
Span parameter determines size of the neighborhood that is used to fit the curve (thus how smooth the curve is)
  - Sometimes an iterative procedure is used, to down-weight outliers
- R command: “loess”

### Exploration of Shape of Regression Function: Smoothing (GPA example)



Linear relation seems appropriate



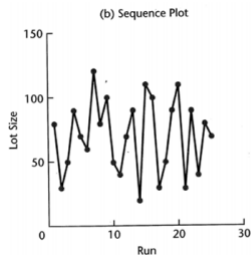
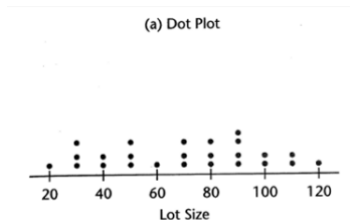
## Week 4: Diagnostics and Remedial Measures

- How can we tell that our regression model is appropriate?
  - Graphic diagnostics
  - Tests
- What do we do if not?
  - Depends on our data  
(transformation of variables, perform weighted least squares, etc)

### Graphical Diagnostics for Predictor Variable

- Dot plot
  - Useful for visualizing distributions of inputs when the data points are not too many
- Sequence plot
  - Useful for visualizing pattern (if there exists any)
- Stem-and-leaf-plot
  - Similar to histogram
- Box plot
  - Useful for visualizing distribution of inputs

# Week 4: Diagnostics and Remedial Measures

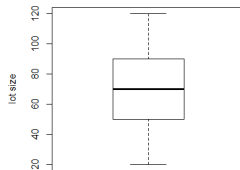


(c) Stem-and-Leaf Plot

The decimal point is 1 digit(s) to the right of the |

```
2 | 0
3 | 000
4 | 00
5 | 000
6 | 0
7 | 000
8 | 000
9 | 0000
10 | 00
11 | 00
12 | 0
```

(d) Box Plot



### Diagnostics of Residuals: Residuals

- The residual  $e_i$  can be regarded as the observed error:

$$e_i = Y_i - \hat{Y}_i$$

- The true error  $\epsilon_i$  is

$$\epsilon_i = Y_i - E\{Y_i\}$$

- Semistudentized residual

$$e_i^* = \frac{e_i - \bar{e}}{\sqrt{MSE}} = \frac{e_i}{\sqrt{MSE}}$$

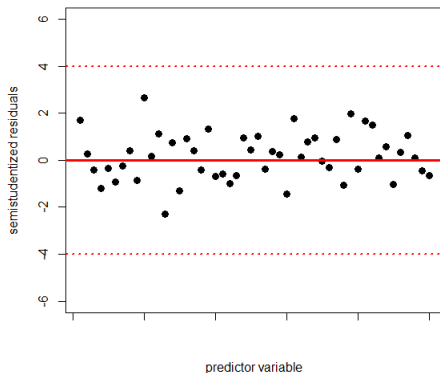
### Diagnostics of Residuals: Departures from Model to be Studied by Residuals

- The regression function is not linear
- The error term do not have constant variance
- The error terms are not independent
- The model fits all but one or a few outlier observations
- The error terms are not normally distributed
- One or several important predictor variables have been omitted from the model

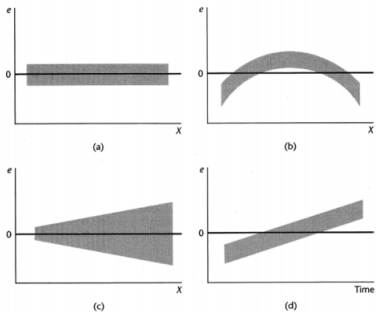
### Diagnostics plots of residuals

- Informal diagnostic plots
- Provides information on whether departure from the simple linear regression model exists

## Diagnostics plots of residuals: Prototypes



## Diagnostics plots of residuals: Prototypes

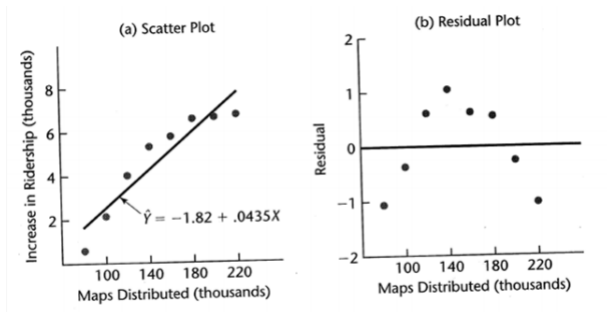




# Week 4: Diagnostics and Remedial Measures

## Diagnostics plots of residuals: Nonlinearity of Regression Function

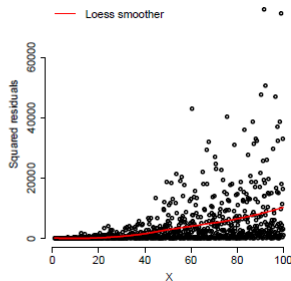
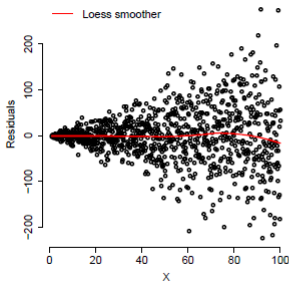
- Can be studied from a residual plot against the predictor variable or, equivalently, a residual plot against the fitted values
- Systematic patterns suggests points out the lack of linearity in true regression function



# Week 4: Diagnostics and Remedial Measures

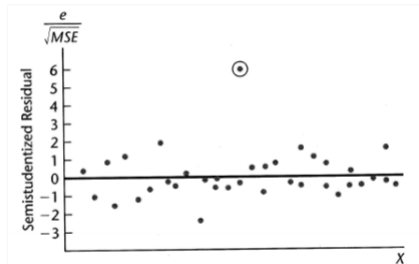
## Diagnostics plots of residuals: Nonconstancy of Error Variance

- Can be studied from " $e_i$  vs.  $X$ "
- Can be studied from " $|e_i|$  vs  $X$ " or " $e_i^2$  vs.  $X$ "
- "Megaphone" type as below suggests the variance increases as the values of the predictor variable increases

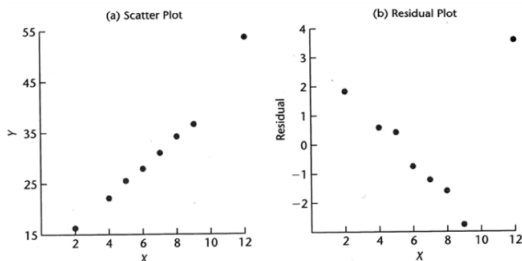


## Diagnostics plots of residuals: Presence of Outliers

- We can use box plots, stem-and-leaf plots, dot plots, and residual plots against  $X$  or  $\hat{Y}$
- Using a rule of thumb, semistudentized residuals with absolute value of four or more can be considered as outliers ( $\frac{|e_i|}{\sqrt{MSE}} > 4$ )



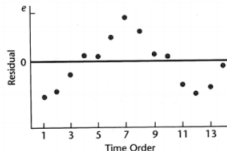
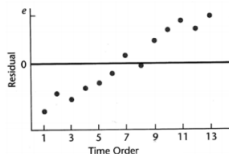
## Diagnostics plots of residuals: Presence of Outliers



- Distorting effect on residuals caused by an outlier when remaining data follow linear regression

## Diagnostics plots of residuals: Nonindependence of Error Terms

- Investigate the residuals against some type of sequence regarding  $X$  if there is any (e.g., time, geographical location, etc)
- Any systematic trends implies correlation between error terms that are near each other in the sequence
- (Note:  $e_i$ 's are not independent unlike  $\epsilon_i$ 's, but for large sample size, the dependency effect among  $e_i$  can be ignored)



### Diagnostics plots of residuals: Nonnormality of Error Terms

- Boxplot: graphical summary of important numbers (median, quartiles and outliers), good to check symmetry
- Histogram
- Quantile-quantile plot (QQ-plot)
- (Note: the number of samples must be reasonably large)

### Diagnostics plots of residuals: Quantile-quantile plot

- Graphical tool to determine whether a sample is consistent with a certain theoretical distribution  
(in this case, it is a standard normal distribution  $N(0, 1)$ )
- Each point in a QQ-plot corresponds to a probability  $p$ :
  - x-coordinate:  $p^{th}$  quantile of theoretical distribution
  - y-coordinate:  $p^{th}$  quantile of sample
- $p^{th}$  quantile (=percentile) of a distribution:  
point  $x$  such that  $P(X \leq x) = p$
- $p^{th}$  quantile of sample:  
point  $x$  such that  $\frac{\#obs \leq x}{n} \approx p$

### Diagnostics plots of residuals: Quantile-quantile plot

- If the sample is drawn from the compared theoretical distribution, then
  - the sample quantiles and the theoretical quantiles are approximately equal → hence the  $x$  and  $y$  coordinates of points in QQ-plot are approximately equal
  - hence the QQ-plot lies close to the line  $y = x$



# Week 4: Diagnostics and Remedial Measures

## Diagnostics plots of residuals: Quantile-quantile plot

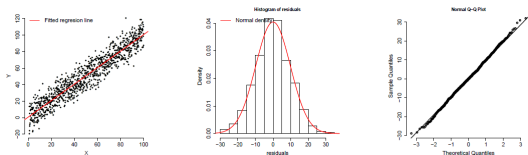


Figure: No visible violation of normality assumption

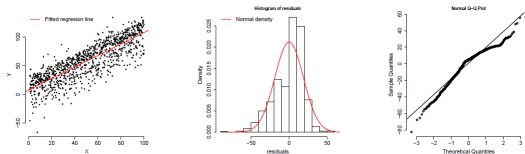


Figure: Residuals are left skewed

## Diagnostics plots of residuals: Quantile-quantile plot

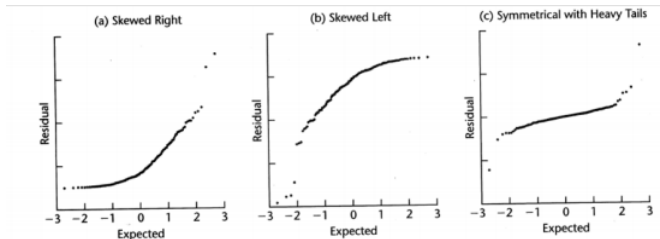


Figure: QQ-plots when normality does not hold

## Diagnostics plots of residuals: Omission of Important Predictor Variables

- Example—partitioned the data set with respect to type of machine
- Partitioning data can reveal dependence on omitted variable
- Can suggest that inclusion of other inputs is important



## Overview of Tests Involving Residuals

- Tests of randomness (run test, Durbin-Watson test, Chapter 12)
- Tests for constancy of variance (Brown-Forsythe test, Breusch-Pagan test, Section 3.6)
- Tests for Outliers (Chapter 10)
- Tests for normality (Correlation test, Section 3.5)

## Correlation Test for Normality

- Test statistic: correlation between sample quantiles and theoretical (normal) quantiles  
→ A high value of correlation is indicative of normality
- Table B.6 in the textbook provides critical values for a given level  $\alpha$  and various sample sizes
  - If, the observed coefficient of correlation is at least as large as the provided critical value, then conclude that the error terms are reasonably normally distributed

### Tests for Constancy of Error Variance

- Brown-Forsythe Test
- Breusch-Pagan Test

### Tests for Constancy of Error Variance: Brown-Forsythe Test

- Works well when the variance of the error terms either increase or decreases with  $X$
- Works well when the sample size should be large enough to ignore dependencies between the residuals

### Tests for Constancy of Error Variance: Brown-Forsythe Test

- Procedure:
  1. Select a cut-off value  $X_0$  for  $X$ 
    - Group 1 consists of  $n_1$  samples with  $X_i \leq X_0$ . Associated residuals are denoted by  $e_{i1}$
    - Group 2 consists of  $n_2$  samples with  $X_i > X_0$ . Associated residuals are denoted by  $e_{i2}$
  2. Calculate the absolute deviation of the residuals of medians in each group.
    - e.g., for group 1:  $d_{i1} = |e_{i1} - \tilde{e}_1|$ , with  $\tilde{e}_1 = \text{median}(e_{i1})$



### Tests for Constancy of Error Variance: Brown-Forsythe Test

- Procedure (continued):
  3. Run a two-sample t-test for the  $d_{i1}$ 's and  $d_{i2}$ 's to test whether their means are equal:

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

where  $\bar{d}_k$  denotes the group mean in group  $k$ , and

$$s = \sqrt{\frac{1}{n-2} \left( \sum_{i=1}^{n_1} (d_{i1} - \bar{d}_1)^2 + \sum_{i=1}^{n_2} (d_{i2} - \bar{d}_2)^2 \right)}$$

(note the different definition of  $s$ !)

### Tests for Constancy of Error Variance: Brown-Forsythe Test

- Procedure (continued):
  4. Approximately,  $t_{BF}^* \sim t(n - 2)$  holds under  $H_0$ . Therefore, with confidence level  $\alpha$ ,
    - If  $|t_{BF}^*| \leq t(1 - \alpha/2; n - 2)$ , conclude the error variance is constant
    - If  $|t_{BF}^*| > t(1 - \alpha/2; n - 2)$ , conclude the error variance is NOT constant

### Tests for Constancy of Error Variance: Breush-Pagan Test

- Assume error terms are independently and normally distributed and

$$\log \sigma_i^2 = \gamma_0 + \gamma_1 X_i$$

- Tests

$$H_0 : \gamma_1 = 0 \text{ vs. } H_a : \gamma_1 \neq 0$$

### Tests for Constancy of Error Variance: Breush-Pagan Test

- Procedure

1. Regress  $Y$  on  $X$ , and get  $SSE$
2. Regress  $e_i^2$  on  $X_i$ , and get the regression sum of squares  $SSR^*$
3. Get test statistic  $X_{BP}^2 = \frac{SSR^*}{2} \div \left(\frac{SSE}{n}\right)^2$
4. When  $n$  is reasonably large,  $X_{BP}^2 \sim \chi^2(1)$  under  $H_0$ . Therefore,

If  $X_{BP}^2 > \chi^2(1 - \alpha; 1)$ , conclude  $H_a$

If  $X_{BP}^2 \leq \chi^2(1 - \alpha; 1)$ , conclude  $H_0$

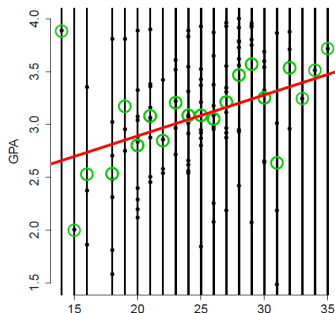
### F-Test for Lack of Fit

- Tests whether a linear function adequately fits the data
- Main idea: Assess if linear relation is appropriate by comparing the fits of a linear regression model to “just estimating the mean  $E\{Y\}$  at each  $X$  level”
- Assumes  $Y_i|X_i$  are 1) independent, 2) normally distributed, and 3) have the same variance  $\sigma^2$
- The tests requires replicates of  $Y$  at some  $X$  levels (or, if there are no replicates, group observations with similar values of  $X$ 's)

### F-Test for Lack of Fit

- Notation:  $Y_{ij}$ 's are then  $Y$ 's at level  $X_j$ ,  
with  $j = 1, \dots, c$  ( $c$ =number of  $X$  levels),  
and  $i = 1, \dots, n_j$  ( $n_j$ =number of outcomes at level  $X_j$ )
- The test is based on a general linear test approach
  - Full model:  $Y_{ij} = \mu_j + \epsilon_{ij}$
  - Reduced model:  $Y_{ij} = \beta_0 + \beta_1 X_j + \epsilon_{ij}$   
( $\epsilon_{ij}$  are independent  $N(0, \sigma^2)$ )

### GPA example: F-test for lack of fit



**Figure:** Fitted regression line (red,  $\hat{Y}$  under reduced model) and means at each  $X$  level (green,  $\hat{Y}$  under full model)

### F-test for Lack of Fit

- General linear test approach to compare the linear regression model (reduced model under  $H_0$ ) to “just estimation the mean  $E\{Y\}$  at each  $X$  level” (full model)
- Test

$$H_0 : E\{Y\} = \beta_0 + \beta_1 X$$

$$H_a : E\{Y\} \neq \beta_0 + \beta_1 X$$



### F-test for Lack of Fit

- Full model:  $E\{Y_{ij}\} = \mu_j$ 
  - Predicted values  $\hat{Y}_{ij} = \hat{\mu}_j = \bar{Y}_{.j}$
  - $SSE(F) = \sum_{j=1}^c \sum_{i=1}^{n_j} (Y_{ij} - \bar{Y}_{.j})^2$ , and  $df_R = n - c$
  - $SSE(F)$  is called the pure error sum of squares (SSPE)
  - Based on the best fit under all possible regression relations
- Reduced model under  $H_0 : E\{Y_{ij}\} = \beta_0 + \beta_1 X_j$ 
  - Predicted values  $\hat{Y}_{ij} = b_0 + b_1 X_j$
  - $SSE(R) = \sum_{j=1}^c \sum_{i=1}^{n_j} (Y_{ij} - \hat{Y}_{ij})^2$ , and  $df_R = n - 2$

### F-test for Lack of Fit

- Test statistic:

$$\begin{aligned} F^* &= \frac{SSE(R) - SSE(F)}{df_R - df_F} \div \frac{SSE(F)}{df_F} \\ &= \frac{SSE - SSPE}{c - 2} \div \frac{SSPE}{n - c} \\ &\sim F(c - 2, n - c) \text{ under } H_0 \end{aligned}$$

- Decision rule

If  $F^* > F(1 - \alpha; c - 2, n - c)$ , conclude  $H_a$

If  $F^* \leq F(1 - \alpha; c - 2, n - c)$ , conclude  $H_0$

### F-test for Lack of Fit: GPA example

```
Console C:/Users/Yunjin/Dropbox/teaching/ST5202/Week3/ ↗
> colnames(gpa.example) = c("Y", "X")
> full.model = lm(Y ~ factor(X), data = gpa.example)
> reduced.model = lm(Y ~ X, data=gpa.example)
> anova(reduced.model, full.model)
Analysis of Variance Table

Model 1: Y ~ X
Model 2: Y ~ factor(X)
  Res.Df    RSS Df Sum of Sq    F Pr(>F)
1     118 45.818
2      99 39.332 19     6.4857 0.8592 0.6324
> |
```

- We don't reject  $H_0$ , as there is no statistical evidence that the linear model is inappropriate.

### F-test for Lack of Fit: Interpretation and extended ANOVA table

- What's the difference between this test and the F-test for  $H_0 : \beta_1 = 0$  versus  $H_a : \beta_1 \neq 0$ ?
  - F-test for lack of fit is used to determine if a linear model is appropriate, rejecting  $H_0$  means that the linear model is not appropriate
  - F-test for slope is used to determine if the linear association between  $X$  and  $Y$  is significant, this F-test is not useful if a linear model is not appropriate!

### F-test for Lack of Fit: Interpretation and extended ANOVA table

- Extended ANOVA table:

- $SSE = \sum_{j=1}^c \sum_{i=1}^{n_j} (Y_{ij} - \hat{Y}_{ij})^2 = SSPE + SSLF$
- $SSPE$  = Pure error sum of squares =  $\sum_{j=1}^c \sum_{i=1}^{n_j} (Y_{ij} - \bar{Y}_j)^2$
- $SSLF$  = “Lack of fit” sum of squares of linear regression model

$$SSLF = \sum_{j=1}^c \sum_{i=1}^{n_j} (\hat{Y}_{ij} - \bar{Y}_j)^2$$

- Degrees of freedom:

$$\begin{aligned} df(SSE) &= df(SSPE) + df(SSLF) \\ n - 2 &= (n - c) + (c - 2) \end{aligned}$$

### Overview of Remedial Measures: What do we do if the linear regression model is inappropriate?

- If simple regression model is not appropriate, then we have two choices:
  - Abandon simple regression model, then develop and use a more appropriate model
  - Employ some transformation on the data so that linear regression model is appropriate for the transformed data

### Overview of Remedial Measures: What do we do if the linear regression model is inappropriate?


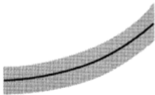
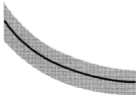
- Nonlinearity of regression function → Transformations (Section 3.9)
- nonconstancy of error variance → weighted least squares (Chapter 11) or transformations (Section 3.9)
- Nonindependence of Error terms → work with a model that calls for correlated error term (Chapter 12)
- Nonnormality of error terms → Transformations (Section 3.9)
- Omission of important predictor variables → modify the model (Multiple regression analysis in Chapter 6 and forward)
- Outlying Observations → robust regression (Chapter 11)

### Transformations: For nonlinearity relation only

- When the distribution of the error terms is reasonably close to a normal distribution and the error terms have approximately constant variance.
- Transformation of  $X$  should be attempted
- Transformation of  $Y$  should be refrained since it will affect the distribution of the error terms



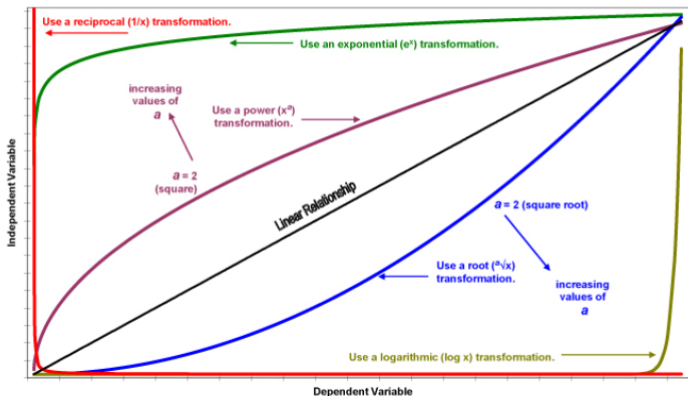
## Transformations: For nonlinearity relation only

	Prototype Regression Pattern	Transformations of $X$
(a)		$X' = \log_{10} X$ $X' = \sqrt{X}$
(b)		$X' = X^2$ $X' = \exp(X)$
(c)		$X' = 1/X$ $X' = \exp(-X)$

# Week 4: Diagnostics and Remedial Measures

## Transformations: For nonlinearity relation only

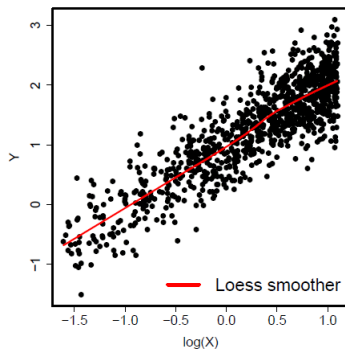
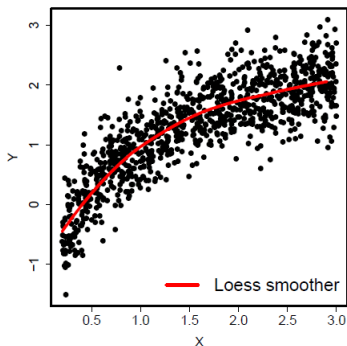
If a data relationship looks like one of these curves, try using a transformation of the independent variable to make the relationship linear.



## Week 4: Diagnostics and Remedial Measures

### Transformations: For nonlinearity relation only

- Transformations can help satisfy the assumption of a linear regression model
- Transform  $X$  to linearize a nonlinear regression function

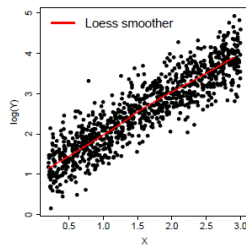
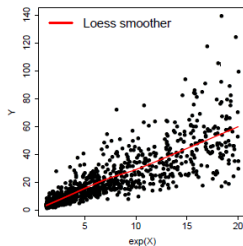
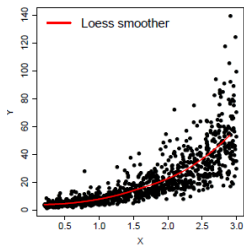


### Transformations: For Nonnormality and Unequal Error Variances

- Non-normality and unequal variances of error terms frequently appear together
- To remedy these in the normal regression model, we need to transform  $Y$ 
  - Shapes and spreads of distributions of  $Y$  need to be changed
  - May help linearize a curvilinear regression relation
  - Disadvantage: interpretations are on the transformed scale, so they can be more difficult
- Can be combined with transformation on  $X$

# Week 4: Diagnostics and Remedial Measures

## Transformations: For Nonnormality and Unequal Error Variances—example



### Transformations: Transforming $Y$ 's using Box-Cox Transformations

- Sometimes, it can be difficult to determine from diagnostic plots which transformation on  $Y$  is most appropriate
- The Box-Cox procedure automatically identifies a transformation from the family of power transformations on  $Y$ .

### Transformations: Transforming $Y$ 's using Box-Cox Transformations

- In Box-Cox transformations, a power transform  $Y' = Y^\lambda$  is used as the response variable:

$$Y' = \begin{cases} K_1(Y^\lambda - 1) & \lambda \neq 0 \\ K_2(\log_e Y) & \lambda = 0 \end{cases}$$

where  $K_1 = \frac{1}{\lambda K_2^{\lambda-1}}$  and  $K_2 = (\prod_{i=1}^n Y_i)^{1/n}$

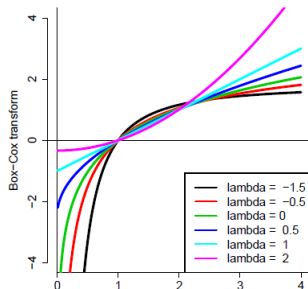
(standardized so that the magnitude of the error sum of squares does not depend on the value of  $\lambda$ )

- Or simply:

$$Y' \propto \begin{cases} Y^\lambda & \lambda \neq 0 \\ \log_e Y & \lambda = 0 \end{cases}$$

### Transformations: Transforming $Y$ 's using Box-Cox Transformations

$$Y' \propto \begin{cases} Y^\lambda & \lambda \neq 0 \\ \log_e Y & \lambda = 0 \end{cases}$$



- $\lambda > 1$  spreads out large values of  $Y$  and compress small values
- $\lambda < 1$  compress large values of  $Y$  and spreads out small values

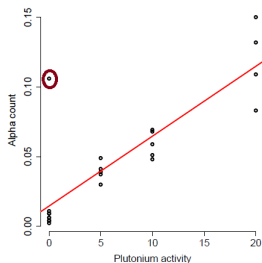


### Transformations: Transforming $Y$ 's using Box-Cox Transformations

- Select optimal  $\lambda$  with maximum likelihood estimation (plug in  $Y'$  as dependent variable instead of  $Y$ )
- Often likelihood is relatively flat around optimal  $\lambda$ , so choose a number that is easier to interpret, like 0.5, 2,  $-0.5$
- R command for finding  $\lambda$ : `"boxcox( $Y \sim X$ , plotit=T)"`

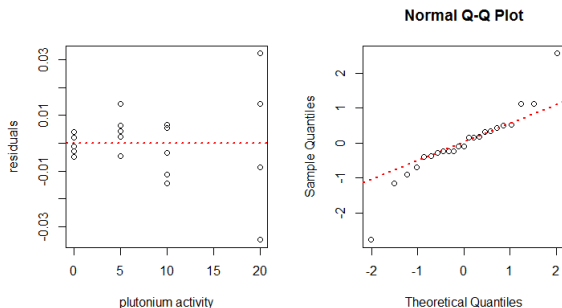
## Plutonium example (Section 3.11)

Examine the relation between plutonium activity and the number of alpha particles that it submits per second.



Anything wrong?

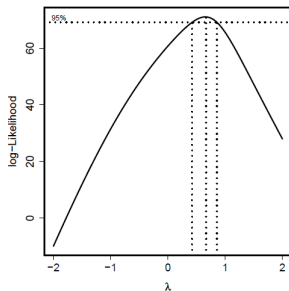
## Plutonium example (Section 3.11)



Anything wrong?

## Plutonium example (Section 3.11)

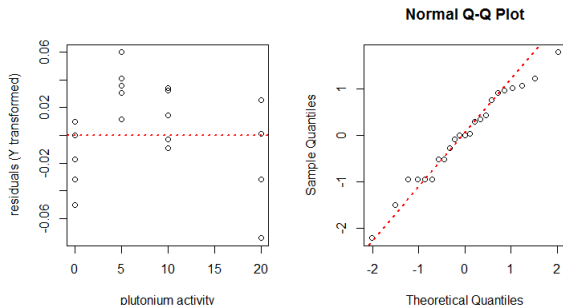
Box-Cox transformation to find  $\lambda$



## Week 4: Diagnostics and Remedial Measures

### Plutonium example (Section 3.11)

Transform  $Y$  so that  $Y' = \sqrt{Y}$  ( $\lambda = .5$ )



Anything wrong?

### Plutonium example (Section 3.11)

Transform  $Y$  so that  $Y' = \sqrt{Y}$  ( $\lambda = .5$ );  
Lack of fit F-test

Analysis of Variance Table

Model 1:  $\text{sqrt}(Y) \sim X$

Model 2:  $\text{sqrt}(Y) \sim \text{factor}(X)$

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	21	0.023453				
2	19	0.011346	2	0.012106	10.136	0.00101 **

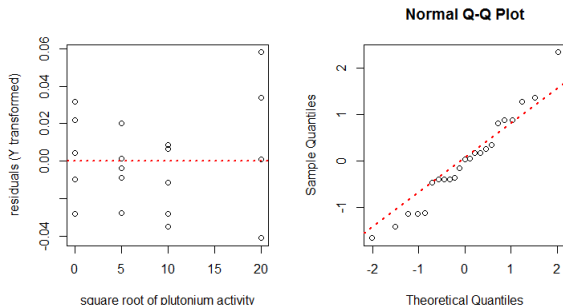
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## Week 4: Diagnostics and Remedial Measures

### Plutonium example (Section 3.11)

Transform both  $X$  and  $Y$  so that  $X' = \sqrt{X}$  and  $Y' = \sqrt{Y}$  ( $\lambda = .5$ )



Anything wrong?

### Plutonium example (Section 3.11)

Transform both  $X$  and  $Y$  so that  $X' = \sqrt{X}$  and  $Y' = \sqrt{Y}$  ( $\lambda = .5$ );  
Lack of fit F-test

Analysis of Variance Table

Model 1:  $\text{sqrt}(Y) \sim \text{sqrt}(X)$

Model 2:  $\text{sqrt}(Y) \sim \text{factor}(\text{sqrt}(X))$

	Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
1	21	0.012883				
2	19	0.011346	2	0.0015368	1.2868	0.2992

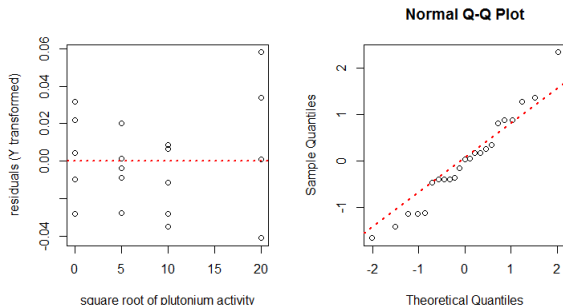
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## Week 4: Diagnostics and Remedial Measures

### Plutonium example (Section 3.11)

Transform both  $X$  and  $Y$  so that  $X' = \sqrt{X}$  and  $Y' = \sqrt{Y}$  ( $\lambda = .5$ )



Anything wrong?

## Diagnostics and Remedial Measures Summary

- ▶ Non-linear regression function:
  - ▶ Diagnose with residual plots ( $e_i$  versus  $X_i$ ) and F-test for lack of fit
  - ▶ Solve it with:
    - ▶ Transformations of  $X$  (not  $Y$ , why?)
    - ▶ Polynomial regression (chapter 8)
    - ▶ Non-linear regression (part III)
- ▶ Non-constancy of error variance
  - ▶ Diagnose with residual plots ( $|e_i|$  versus  $X_i$ ) and Brown-Forsythe/Breusch-Pagan test
  - ▶ Solve it with:
    - ▶ Transformations of  $Y$
    - ▶ Weighted least-squares (chapter 11)
- ▶ Outliers and influential points (chapter 11)
- ▶ Non-independence of errors (chapter 12)

Reading: Section 2.6 & whole Chapter 3