

## STAT 571A — Advanced Statistical Regression Analysis

## <u>Chapter 3 NOTES</u> Diagnostics and Remedial Measures

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## **Predictor Diagnostics**

It's always a good idea to study the nature of the predictor variable, X<sub>i</sub>, and ensure it's not harboring any surprises.

#### Useful tools:

- Dot plots
- Sequence plots (scatterplot of X<sub>i</sub> vs. *i* with dots connected — useful if *i* is a surrogate for time)
- Stemplots
- Boxplots

### **Residual Diagnostics**

The residuals from the LS fit for a Simple Linear Regression (SLR) model are the differences between the observed response and the predicted response:

$$\mathbf{e}_{i} = \mathbf{Y}_{i} - \mathbf{\hat{Y}}_{i}$$
.

The e<sub>i</sub>'s contain useful info. Recall that  $\sum e_i = \sum e_i X_i = \sum e_i \hat{Y}_i = 0$ . Thus  $\overline{e} = \sum e_i/n = 0$ while

$$\mathbf{s_e}^2 = \frac{1}{n-2} \Sigma (\mathbf{e_i} - \overline{\mathbf{e}})^2 = \frac{1}{n-2} \Sigma \mathbf{e_i}^2 = \frac{SSE}{n-2} = MSE$$

#### **Residual Plots**

- A powerful diagnostic tool for assessing model fit is the Residual Plot, i.e., a plot of e<sub>i</sub> = Y<sub>i</sub> - Ŷ<sub>i</sub> vs. Ŷ<sub>i</sub>.
- If the SLR model fit is adequate, the residuals, e<sub>i</sub>, should cluster around the horizontal line e = 0, with no apparent pattern. See, e.g., next slide →

## Prototypical Residual Plot with Random Scatter



Fitted value

#### **Residual Plots (cont'd)**

Can also use residual plots to study:

- departure from linearity in E{Y}
- departure from constant  $\sigma^2$  in  $\sigma^2$ {Y}
- departure from indep. assumption
- outlying values of Y<sub>i</sub>
- departure from normality in  $\epsilon_i \sim N(0,\sigma^2)$
- other values of X that could be useful (see Ch. 6)

#### **Residual Plots (cont'd)**

Alternate versions of the residual plot include:

- plot  $e_i$  vs.  $\hat{Y}_i$  (std. version)
- plot e<sub>i</sub> vs. X<sub>i</sub>
- plot |e<sub>i</sub>| or e<sub>i</sub><sup>2</sup> vs. X<sub>i</sub>
- plot  $e_i$  vs. *i* (if sequence is surrogate for time)  $\rightarrow$  see Fig. 3.2b
- boxplot and/or histogram of e<sub>i</sub>'s → see Fig.
   3.2c
- normal probab. plot of of  $e_i$ 's  $\rightarrow$  see Fig. 3.2d

#### **Residual Plots in R**

- In R, the plot() function can extract the raw residual plot from the lm() object.
- Or, use plot() directly with the functions resid() and fitted().

#### **Toluca Example** (cont'd)

In the Toluca Data example (CH01TA01), we produce a residual plot via:

- > CH01TA01.lm = lm(  $Y \sim X$  )
- > plot( resid(CH01TA01.lm) ~ X )
- > abline( h=0 ) #add horiz. e=0 line

## **Toluca Example Residual Plot**



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#### Toluca Resid. Plot (cont'd)

As mentioned, residual plots are usually drawn against the fitted values:

- > CH01TA01.lm = lm(  $Y \sim X$  )
- > abline( h=0 ) #add horiz. e=0 line

Residual pattern will be identical under an SLR model (reversed if  $b_1 < 0$ ).

#### **Example TA01 Residual Plot**



#### **Quadratic Curvature**

Curvature in the scatterplot and the resid. plot may indicate a parabolic (quadratic) pattern:



#### Variance heterogeneity

# Departure from constant $\sigma^2$ in $\sigma^2$ {Y} will be evident in a widening residual pattern, e.g.



#### **Possible Outliers**

# Unusual observations (possible 'outliers') can be recognized quickly in resid. plots:



## **Possible** Outliers

- Keep in mind that detection of an unusual observation does not immediately condemn the data point or call for its deletion.
- Always examine <u>why</u> the point is flagged: it may involve a simple data entry error or some other explanation.

#### **Standardizing the Residuals**

- A problem with raw residuals is that they are scale/measurement-dependent: in one data set an absolute residual of |e<sub>i</sub>| = 8.2 may be *less* egregious than a residual of |e<sub>i</sub>| = 0.7 in another data set.
- We can stabilize residuals across data sets/model fits by standardizing them to similar scales (sort of like a z-score).

#### **Semistudentized Residuals**

A *Semistudentized Residual* is a raw residual, e<sub>i</sub>, divided by its sample std. deviation:

$$e_i^* = \frac{e_i}{s_e} = \frac{e_i}{\sqrt{MSE}}$$

(Some authors call this a *Studentized Residual*. Others don't! Be careful of terminology.)

There are more effective ways to adjust resid's; we expand on this in Ch. 10.

## Semistudentized Residuals in R

- In R, we can plot the e<sub>i</sub>\*s.
- E.g., with the Toluca data (CH01TA01), use
  - > CH01TA01.lm = lm(  $Y \sim X$  )
  - > eistar = resid( CH01TA01.lm )/

sqrt( anova(CH01TA01.lm)\$"Mean Sq"[2] )

- > plot( eistar ~ fitted(CH01TA01.lm) )
- > abline( h=0 )

#### Toluca Example: Semistudentized Residual Plot

Pattern is similar to raw residual plot, but now on a standardized scale.



## **Normal Probability Plots**

- To assess departure from normality in ε<sub>i</sub> ~ N(0,σ<sup>2</sup>), display the e<sub>i</sub>'s via a boxplot, histogram, or normal probab. plot (NPP).
- E.g., with NPP's, if normality holds, the NPP will show a 45° line.
- Departure from normality will be evident as deviations from the 45° line.

(See Fig. 3.9)

#### **Right Skew in NP Plot**

#### Right-skewed residuals display convex shape in NPP



Normal Q-Q Plot



#### **Thick Tails in NP Plot**

Thick-tailed (but still symmetric) residuals display as flattened shape in NPP



Normal Q-Q Plot

## **Test of Normality**

- Besides visualizations, we can apply a univariate test of Normality to the  $e_i$ 's, and assess whether the  $\epsilon_i$ 's appear to deviate from the N(0, $\sigma^2$ ) assumption.
- The basic test is due to Shapiro and Wilk.
   Applied to the residuals, it gives a test statistic (W\*) and an associated P-value.
- If *P* is too small (below a pre-set α-level), reject the null hypothesis of normality.

#### **Toluca Example (cont'd)**

In the Toluca example (CH01TA01), we test the residuals for normality:

> CH01TA01.lm = lm(Y ~ X)

> shapiro.test( resid(CH01TA01.lm) )

Shapiro-Wilk normality test data: resid(CH01TA01.lm) W = 0.9789, p-value = 0.8626

P-value is large, so no departure from normality is evidenced.

#### **Test of Variance Homogeneity**

- From an SLR model, we test the residuals for variance homogeneity (i.e., constant σ<sup>2</sup>) via the 'robust' Brown-Forsythe test, a special case of the more-general Levene test.
- The test breaks the e<sub>i</sub>'s into 2 groups: (1) e<sub>i</sub>'s from small X<sub>i</sub>'s vs. (2) e<sub>i</sub>'s from large X<sub>i</sub>'s. Then, it compares deviations from median between the 2 groups.

#### **Brown-Forsythe Test**

- For (small-X) group 1, let n₁ = # resid's from small X<sub>i</sub>'s, and denote the median resid. in that group as e₁. Compute d<sub>i1</sub> = |e<sub>i1</sub> – e₁|.
- For (large-X) group 2, let n<sub>2</sub> = # resid's from large X<sub>i</sub>'s, and denote the median resid. in that group as e<sub>2</sub>. Compute d<sub>i2</sub> = |e<sub>i2</sub> - e<sub>2</sub>|.

• Calculate 
$$t_{BF}^* = \frac{\overline{d}_1 - \overline{d}_2}{S_D \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}}$$
 with  
 $S_D^2 = \frac{\sum_{i=1}^{n_1} (d_{i1} - \overline{d}_1)^2 + \sum_{i=1}^{n_2} (d_{i2} - \overline{d}_2)^2}{n - 2}$ 

## **Brown-Forsythe Test (cont'd)**

- Then, conclude significant departure from homogeneous variance if
   |t<sup>\*</sup><sub>BF</sub>| > t(1-<sup>α</sup>/<sub>2</sub>; n-2).
- P-value is 2P[ t(n-2) > |t<sup>\*</sup><sub>BF</sub>| ]
- Can do this in R, but must first download and install the *lawstat* package, then load it into the current workspace:
  - > require( lawstat )

### **Toluca Example** (cont'd)

In the Toluca Data example (CH01TA01), test the residuals for variance homogeneity:

```
> ei = resid( CH01TA01.lm )
```

> BF.htest = levene.test( ei[order(X)],
 group=c(rep(1,13),rep(2,12)),
 location="median" )

Note use of  $ei[order(\hat{x})]$  to <u>sort</u> residuals by order of X. (Could also sort by  $\hat{Y}$ .)

The group= specifier factors into 2 groups for constructing the t\*statistic. (Actually, it gives  $F^* = t^{*2}$ .)

## **Toluca Example (cont'd)**

#### **Browth-Forsythe output:**

modified robust Brown-Forsythe Levene-type test based on the absolute deviations from the median data: ei[order(X)] Test Statistic = 1.7331, p-value = 0.201 > sqrt( BF.htest\$statistic ) #for t\*/statistic Test Statistic 1.316482  $P = 0.201 > 0.05 = \alpha$ . No significant departure from constant  $\sigma^2$  is evidenced.

### **Brown-Forsythe Test: Caveats**

- The Brown-Forsythe test works if variance heterogeneity is of the "megaphone" style (in the textbook's terminology).
- But (!), it may fail with stranger patterns, such as two megaphones back-to-back:



## Replication

- When there are multiple Y<sub>i</sub>'s observed at the <u>same</u> X<sub>i</sub>, we say the data/design exhibits Replication.
- The multiple Y<sub>i</sub>'s are called Replicates.
- In this case, it is possible to cleanly test the 'fit' of an assumed model for E{Y<sub>i</sub>}.

## Lack Of Fit (LOF) Testing

## Need to expand our notation: the observations are now indexed as Y<sub>ij</sub>, where i = 1,...,n<sub>j</sub> (replicates) and j = 1,...,c (unique X values)

Sample size is  $n = \sum_{j=1}^{c} n_j$ .

We approach the lack-of-Fit (LOF) test using the FM vs. RM discrepancy measure from §2.7.

## LOF Testing (cont'd)

- The Full Model (FM) here is  $Y_{ij} = \mu_j + \varepsilon_{ij}$ with  $\varepsilon_{ij} \sim i.i.d. N(0,\sigma^2)$ .
- The model allows for c > 1 different, unspecified means, μ<sub>j</sub>, at each j.
- The Reduced Model (RM) is the SLR: Y<sub>ij</sub> = β<sub>0</sub> + β<sub>1</sub>X<sub>j</sub> + ε<sub>ij</sub>
   with ε<sub>ij</sub> ~ i.i.d. N(0,σ<sup>2</sup>)
   (or whatever posited model is under
   study).

## LOF Testing (cont'd)

- To construct the F-statistic use (2.70): compare SSE(R) under the SLR with SSE(F) under the full, unspecified model.
- If the SSE's differ too much, this implies that significant, explainable variation is still present, even after fitting the SLR model.
- Use the F-statistic to quantify this departure.
# LOF Testing (cont'd)

- Recall: the general form of the discrepancy F-statistic is  $F^* = \frac{SSE(R) SSE(F)}{df_{ER} df_{EF}} / \frac{SSE(F)}{df_{EF}}$
- For LOF, the numerator is the mean square for lack-of-fit: MSLF. The denominator is MSE(F).
- Reject the null hypoth. of acceptable fit if F\* > F(1-α; df<sub>ER</sub>-df<sub>EF</sub>, df<sub>EF</sub>).

### LOF Testing (cont'd)

# Notice: The RM SSE is based on the SLR, $SSE(R) = \sum_{j=1}^{c} \sum_{i=1}^{n_j} (Y_{ij} - \hat{Y}_{ij}(R))^2$ $= \sum_{j=1}^{c} \sum_{i=1}^{n_j} (Y_{ij} - b_0 - b_1 X_j)^2$

The FM SSE has similar form: SSE(F) =  $\sum_{j=1}^{c} \sum_{i=1}^{n_j} (Y_{ij} - \hat{Y}_{ij}(F))^2$ , but what is  $\hat{Y}_{ij}(F)$ ?

Answer: The FM makes no specification on  $E[Y_{ij}]$ , so the LS estimators are simply the replicate means  $\hat{Y}_{ij}(F) = \overline{Y}_j$ .

#### **Pure Error**

With this, find SSE(F) =  $\sum_{j=1}^{c} \sum_{i=1}^{n_j} (Y_{ij} - \overline{Y}_j)^2$ . This is called the **Pure Error**, and denoted as SSPE. Then,

$$MSE(F) = MSPE = \sum_{j=1}^{c} \sum_{i=1}^{n_j} (Y_{ij} - \overline{Y}_j)^2 / (n-c).$$

# The F-statistic becomes $F_{LOF}^{*} = \frac{SSE(R) - SSPE}{(n-2) - (n-c)} / MSPE.$

Reject the null hypoth. of acceptable fit if  $F^* > F(1-\alpha; c-2, n-c)$ .

# LOF ANOVA Table

We collect all these terms together into a special LOF ANOVA table:

Source	d.f.	SS	MS
Regr.	1	$SSR=\sum (\hat{Y}_{ij}-\overline{Y})^2$	MSR
Error	n–2	$SSE(R) = \sum (Y_{ij} - \hat{Y}_{ij})$	) <sup>2</sup> MSE(R)
LOF	c–2	SSLF= $\sum (\overline{\mathbf{Y}}_{j} - \hat{\mathbf{Y}}_{ij})^{2}$	<sup>2</sup> MSLF
Pure E	rror n–c	$SSPE=\sum (Y_{ij} - \vec{Y}_j)$	<sup>2</sup> MSPE
Total	n–1	SSTO= $\sum (Y_{ij} - \overline{Y})^2$	

The F-test employs the LOF statistic  $F_{LOF}^* = MSLF/MSPE$ .

#### Example: Lack of Fit (LOF) test



#### Example CH03TA04 (cont'd)

To test for LOF with the Bank Data (CH03TA04), can use:

> # fit reduced model

>

- > rmCH03TA04.lm = lm(Y ~ X)
- > # fit full model via factor() command
- > fmCH03TA04.lm = lm(  $Y \sim factor(X)$  )

#### Example CH03TA04 (cont'd)

- > #SLR anova component
- > anova( rmCH03TA04.lm )

Analysis of Variance Table
Response: Y
 Df Sum Sq Mean Sq F value Pr(>F)
X 1 5141.3 5141.3 3.1389 0.1102
Resid 9 14741.6 1638.0

#### Example CH03TA04 (cont'd)

> #SSPE with F\* for LOF

> anova( rmCH03TA04.lm, fmCH03TA04.lm )



#### **Comments on LOF Approach**

- We don't need replication at every X<sub>j</sub>. As long as at least 1 X<sub>j</sub> has replicated Y's, the test can proceed, if poorly (& assuming the replicated Y's are different).
- Can show that E{MSPE} =  $\sigma^2$  (always). For that matter, E{MSLF} =  $\sigma^2 + \sum n_i \{\mu_i - (\beta_0 + \beta_1 X_j)\}^2/(c-2)$ .
- Any p-parameter model can be tested in this manner, as long as some replication is present and c > p.
- (Also see pp. 126-127)

#### Remediation

- What if our diagnostics uncover failure in the SLR model?
- If it's just heterogeneous variance, we can move to Weighted Least Squares (WLS) → discussed in Ch. 11.
- If the linearity is in question, we might be able to transform Y (or X) to "linearize" the regression. (This can also stabilize non-constant variance.)

#### Transformations

When the Y-vs.-X relationship does not conform to a simple linear model, it may be possible to transform either the X<sub>i</sub>'s or the Y<sub>i</sub>'s (or both!) to at least approximately satisfy the SLR requirements.

We don't know this in advance, of course, so <u>always</u>

 (a) plot the data, and
 (b) plot/examine the residuals
 for guidance.

# Transforming X to $\sqrt{X}$

- When a curvilinear relationship is evidenced in the data, a transform of X to √X might be called for.
- That is, replace the SLR model with  $Y_i = \beta_0 + \beta_1 X_i^{1/2} + \varepsilon_i \quad (i = 1,...,n).$
- Sales Training example (CH03TA07):
  - > par( mfrow=c(1,2) )
  - > plot( Y ~ X )
  - > plot( Y ~ sqrt(X) )



#### Sales Train'g (CH03TA07) (cont'd)

Resid. plot and normal probability plots seem reasonable after  $\sqrt{X}$  transform:

- > sqrtX = sqrt(X)
- > trCH03TA07.lm = lm(  $Y \sim sqrtX$  )
- > par(mfrow=c(1,2))
- > plot( resid(trCH03TA07.lm) ~

sqrtX, xlab=expression(sqrt(X)) )

> abline( h=0 )

> qqnorm( resid(trCH03TA07.lm), main=""

#### Sales Train'g (CH03TA07) (cont'd)



#### Transforming X to *ln*(X)

- Sometimes, a few X<sub>i</sub>-values are very far away from the bulk of the data, or the X's are geometrically or exponentially spaced (e.g., X = 1, 3, 10, 30, 100, 300, ...)
- If so, and if all the X<sub>i</sub>'s are positive (X > 0), then a logarithmic transform may be called for; i.e., replace the SLR model with

 $Y_i = β_0 + β_1 ln(X_i) + ε_i$  (i = 1, ..., n).

#### Example

#### **Brain Weight/Body Weight**

In a study of mammalian body features, X = avg. body weight (kg) and Y = avg. brain weight (g) were determined for n = 62 terrestrial mammals.

On the original scale, a scatterplot shows little distinguishability, due to the extreme observations at high X (next slide  $\rightarrow$ )

#### **Brain Weight Scatterplot**





#### Brain Weight Scatterplot after *ln*(X)-*ln*(Y) transform



#### Brain Weight Scatterplot after *ln*(X)-*ln*(Y) transform



#### Brain Weight Scatterplot after *ln*(X)-*ln*(Y) transform



#### Brain Weight Example (cont'd)

- We see that the logarithmic transform applied to X (and here, also to Y) can increase distinguishability in the scatterplot.
- In this example, it also "reduced" the outlying effect of the extreme observations (elephants), while also enhancing our ability to identify other possible extreme observations (maybe humans?).

#### Other Useful Transformations

Some other useful transformations of the X variable include

- $X' = \log_{10}(X)$
- X' = 1/(X + k) (for some  $k \ge 0$ )
- X' = X (1/X)

# Transforming Y to log<sub>10</sub>Y

- When a curvilinear relationship is evidenced in the data, a transform of Y to log<sub>10</sub>Y might be called for.
- That is, replace the SLR model with  $\log_{10} Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$  (i = 1, ..., n).
- Blood plasma example (CH03TA08):
  - > par( mfrow=c(1,2) )
  - > plot( Y ~ X )
  - > plot( log10(Y) ~ X )



Residual plot and normal probability plot under 'usual' SLR model:

- > CH03TA08.lm = lm( Y ~ X )
- > par( mfrow=c(1,2) )
- > plot( resid(CH03TA08.lm) ~ X )
- > abline( h=0 )
- > qqnorm( resid(CH03TA08.lm), main='')



Residual plot and normal probability plot under log<sub>10</sub>(Y) transform:

- > trCH03TA08.lm = lm( log10(Y) ~ X )
- > par( mfrow=c(1,2) )
- > plot( resid(trCH03TA08.lm) ~ X )
- > abline( h=0 )
- > qqnorm( resid(trCH03TA08.lm),
  - main=""



#### **Box-Cox Power Transform**

A general class of transformations that includes the square root and the log is the Box-Cox Power Transformation:

$$W_{i} = \frac{Y_{i}^{\lambda} - 1}{\lambda K_{2}^{\lambda - 1}}$$

where λ is a transform parameter and K<sub>2</sub> is the geometric mean of the Y<sub>i</sub>s:

$$\mathbf{K}_{2} = \left( \prod_{i=1}^{n} \mathbf{Y}_{i} \right)^{1/n}$$

#### **Box-Cox Transform** (cont'd)

If λ = 0, use the continuity-preserving logarithm for the Box-Cox transform:

$$W_i = K_2 ln(Y_i)$$
 at  $\lambda = 0$ .

- We can apply maximum likelihood (ML) to estimate λ from the data. (Alternatively, can minimize the regression SSE over a series λ values; see p. 135.)
- In R, this is performed via the boxcox() function in the MASS package.

Box-Cox transform analysis (mimics presentation in Neter *et al.*, p.136):

> require( MASS )

- > CH03TA08.lm = lm(  $Y \sim X$  )
- > CH03TA08.bc = boxcox( CH03TA08.lm, lambda=seq(-1, 1, 0.1), interp=F )

> cbind( CH03TA08.bc\$x, CH03TA08.bc\$y )

boxcox() function produces plot of loglikelihood (cf. to Fig. 3.17 in Neter *et al*.)



Call to cbind() prints out  $\lambda$  ('x' col.) and calculated values of log-likelihood ('y' col.):

[1,]	-1.0	9.5036602	[12,]	0.1	8.6280273
[2,]	-0.9	9.9557422	[13,]	0.2	7.8716970
[3,]	-0.8	10.3202421	[14,]	0.3	7.0196583
[4,]	-0.7	10.5882760	[15,]	0.4	6.0806054
[5,]	-0.6	10.7517109	[16,]	0.5	5.0634353
[6,]	-0.5	10.8036292	[17,]	0.6	3.9768915
[7,]	-0.4	10.7387696	[18,]	0.7	2.8292907
[8,]	-0.3	10.5538884	[19,]	0.8	1.6283340
[9,]	-0.2	10.2479881	[20,]	0.9	0.3809955
[10,]	-0.1	9.8223822	[21,]	1.0	-0.9065263
[11,]	0.0	9.2805821			

# **Transforming Y: Caveats**

We need to be careful when transforming the response, Y.

Say you use W = ln(Y), so that  $Y = exp{W}$ .

- The model becomes  $E[W] = \beta_0 + \beta_1 X$ .
- The fitted values have the form  $\hat{W}_h = b_0 + b_1 X_h$ . But don't stop there!
- Should reverse the transform to end with  $\hat{Y}_h = \exp\{b_0 + b_1 X_h\}$ .
- Use similar reverse-transforms for other transforming functions.
## **Transforming X: Caveats**

- By contrast, if you transform just the Xvariable/predictor, you only change the input scale.
- At that point, stay on the chosen, transformed, input scale throughout all the calculations.

<u>Example</u>: if you transform  $X_i$  to  $\sqrt{X_i}$  the model becomes  $E[Y_i] = \beta_0 + \beta_1 \sqrt{X_i}$ . Then stay on the  $\sqrt{X_i}$  scale for estimates, inferences, predictions, etc.