

L8. Modeling Problems - Other Diagnostics

Modeling Assumption Violations:

(1) Heteroscedasticity

(2) Non-Normality Residuals

(3) False assumption of linearity between
response variable Y and any predictor.

1. Heteroscedasticity.

Recall Model Assumption: $\epsilon_i \stackrel{\text{i.i.d}}{\sim} N(0, \sigma^2)$, $i=1, \dots, n$

$$\text{or } \vec{\epsilon} \sim MVN(\vec{0}, \sigma^2 I_n)$$

The OLS method requires all ϵ_i s have a constant variance σ^2 , s.t. the parameter estimate

$\hat{b} = (\vec{x}' \vec{x})^{-1} \vec{x}' \vec{y}$ is the "best" estimator
in "BLUE".

- Heteroscedasticity occurs when this assumption is violated, which means the variance of ~~residuals~~^{errors} are non-constant, more commonly, it refers to the spread of residuals changes systematically with predictors.
 - (a) Problem.
 - (i) The OLS estimate \hat{b} is still linear and unbiased, but not the "best" anymore: we can't say \hat{b} has the smallest variance among all unbiased linear estimators. There is another estimator with a smallest variance.
 - (ii) $se(\hat{\beta}_k)$ for all OLS output are incorrect estimates of the standard deviation of $\hat{\beta}_k$. It will result in misleading t-test and C.I.
 - (iii) Predictions of y are still unbiased, but the prediction intervals are incorrect.

$$\begin{aligned}
 \text{Recall: } \text{Var}(\vec{b}) &= E(\vec{b} - \vec{\beta})(\vec{b} - \vec{\beta})^T \\
 &= E((\vec{X}^T \vec{X})^{-1} \vec{X}^T \vec{\epsilon} \vec{\epsilon}^T \vec{X} (\vec{X}^T \vec{X})^{-1}) \quad \text{lecture 4} \\
 &= (\vec{X}^T \vec{X})^{-1} \vec{X}^T \cdot E(\vec{\epsilon} \vec{\epsilon}^T)^T \cdot \vec{X} (\vec{X}^T \vec{X})^{-1}
 \end{aligned}$$

When applying OLS method:

$$\text{assume } E(\vec{\epsilon} \vec{\epsilon}^T)^T = \sigma^2 I_n = \begin{pmatrix} \sigma^2 & & \\ & \ddots & 0 \\ 0 & & \sigma^2 \end{pmatrix}$$

$$\text{so } \text{Var}(\vec{b})_{\text{OLS}} = \sigma^2 (\vec{X}^T \vec{X})^{-1}$$

and is estimated by $\text{MSE}(\vec{X}^T \vec{X})^{-1}$

which is an unbiased estimator of
 $\text{Var}(\vec{b})$ when the assumption of constant
 variance holds.

When Heteroscedasticity exist:

$$\text{the real } \text{Var}(\vec{b}) = (\vec{X}^T \vec{X})^{-1} \vec{X}^T \begin{pmatrix} \sigma_1^2 & & \\ & \ddots & 0 \\ 0 & & \sigma_n^2 \end{pmatrix} \vec{X} (\vec{X}^T \vec{X})^{-1}$$

so $\text{MSE}(\vec{X}^T \vec{X})^{-1}$ is now biased
 estimate for $\text{Var}(\vec{b})$

In this case, if we still apply OLS method:

(i) $\text{Var}(\vec{b})_{\text{OLS}} \neq \text{Var}(\vec{b})$

Not "best" anymore

(ii) ~~the~~ $\overset{1}{\text{Var}}(\vec{b})_{\text{OLS}} = \text{MSE} \cdot (\vec{x}^T \vec{x})^{-1}$ is

but unbiased anymore, so

$\text{se}(\beta_k)_{\text{OLS}}$ is incorrect.

(iii) Let's give some result about the

prediction first

Textbook section 6.7

For a new observation with $\vec{x}_h = \begin{pmatrix} 1 \\ x_{h1} \\ \vdots \\ x_{h,p-1} \end{pmatrix}$

Note: this is a matching notation as in the textbook, might look confusing since they transposed the old way of writing X matrix.

The fitted value $\hat{Y}_h = \vec{x}_h^T \vec{b}$

- unbiased : $E(\hat{Y}_h) = \vec{x}_h^T \vec{\beta} = E(Y_h)$

- $\text{Var}(\hat{Y}_h) = \text{Var}(\vec{x}_h^T (\vec{x}^T \vec{x})^{-1} \vec{x}^T \vec{y}_0)$

When assumption holds

$$= \sigma^2 \vec{x}_h^T (\vec{x}^T \vec{x})^{-1} \vec{x}_h^T$$

$$\text{Var}(\hat{Y}_h) = \text{Var}(\vec{X}_h^T \vec{b})$$

$$= \text{Var}(\vec{X}_h^T (\vec{X}^T \vec{X})^{-1} \vec{X}^T \vec{y})$$

$$= [\vec{X}_h^T (\vec{X}^T \vec{X})^{-1} \vec{X}^T] \frac{\text{Var}(\vec{y})}{\sigma^2 I_n} [\vec{X}_h^T (\vec{X}^T \vec{X})^{-1} \vec{X}^T]^T$$

$$= \sigma^2 \vec{X}_h^T \cancel{[\vec{X}^T \vec{X})^{-1} \vec{X}^T \vec{X}]} (\vec{X}^T \vec{X})^{-1} \vec{X}_h^T$$

$$= \sigma^2 \vec{X}_h^T (\vec{X}^T \vec{X})^{-1} \vec{X}_h$$

Hint: $\text{Var}\left(\frac{C \cdot \vec{x}}{\pi}\right)$ r.v. vector
constant matrix C

(Quiz 27)

$$= C \text{Var}(\vec{x}) C^T$$

$\text{Var}(\hat{Y}_h)$ can also be found as $\text{Var}(\vec{X}_h^T \vec{b})$

$$= \vec{X}_h^T \text{Var}(\vec{b}) \vec{X}_h = \vec{X}_h^T \sigma^2 (\vec{X}^T \vec{X})^{-1} \vec{X}_h \text{ (same as above)}$$

If $s^2(\vec{b})$ is given by $\text{MSE}(\vec{X}^T \vec{X})^{-1}$ (sample estimation)

$$s^2(\hat{Y}_h) = \vec{X}_h^T s^2(\vec{b}) \vec{X}_h \quad \underline{(\text{HMK 3 6.25})}$$

- Confidence Interval for the Mean Response. μ_h

$$\hat{Y}_h \pm t_{\alpha/2, df=n-p} \text{se}(\hat{Y}_h)$$

Where $\text{se}(\hat{Y}_h) = \sqrt{\text{MSE} \hat{X}_h^T (\hat{X}^T \hat{X})^{-1} \hat{X}_h^T}$

- Prediction Interval for the new observation \hat{Y}_h

$$\hat{Y}_h \pm t_{\alpha/2, df=n-p} \sqrt{\text{se}(\hat{Y}_h)^2 + \text{MSE}}$$

When Heteroscedasticity exists.

$$\begin{aligned} \text{Var}(\hat{Y}_h) &= \text{Var}(\hat{X}_h^T (\hat{X}^T \hat{X})^{-1} \hat{X}^T \hat{y}') \\ &= [\hat{X}_h^T (\hat{X}^T \hat{X})^{-1} \hat{X}^T] \underbrace{\text{Var}(\hat{y}')}_{\neq \sigma^2 I_n} [\hat{X}_h^T (\hat{X}^T \hat{X})^{-1} \hat{X}^T]^T \end{aligned}$$

So $\text{MSE} \hat{X}_h^T (\hat{X}^T \hat{X})^{-1} \hat{X}^T$ is not unbiased estimate anymore.

Therefore prediction/confidence interval calculated this way would be incorrect.

(b) Detection.

(i) Residual v.s. Fitted Value Plot:

You would observe obvious change of bandwidth
in the plot

(ii) Breusch-Pagan Test

Basic idea is the variance of error should not
change given difference predictor values.

If the assumption of constant variance is
violated, then the variance would be changed
with predictor values.

1) Fit your model $y_i = \beta_0 + \beta_1 x_{i1} + \dots + \beta_{p-1} x_{ip-1} + \epsilon_i$

2) Obtain the residuals $\epsilon_1, \epsilon_2, \dots, \epsilon_n$

3) Build an auxiliary regression model:

$$\epsilon_i^2 = \gamma_0 + \gamma_1 x_{i1} + \dots + \gamma_{p-1} x_{ip-1} + \zeta_i \quad (E)$$

4) $H_0: \gamma_1 = \gamma_2 = \dots = \gamma_{p-1} = 0$ v.s $H_a: \text{at least } \gamma_i \neq 0$

5) Test stat : $\chi_s^2 = nR^2$

where R^2 is the w.e. of determination of model (E)

Where H_0 is true: $\chi_s^2 \sim \chi^2(p)$

6) Test Result:

When Fail to reject H_0 : $\chi_s^2 < \chi_{d, df=p}^2$ or p-value > α

We conclude there's not significant heteroscedasticity.

when reject H_0 : $\chi_s^2 > \chi_{d, df=p}^2$ or p-value < α .

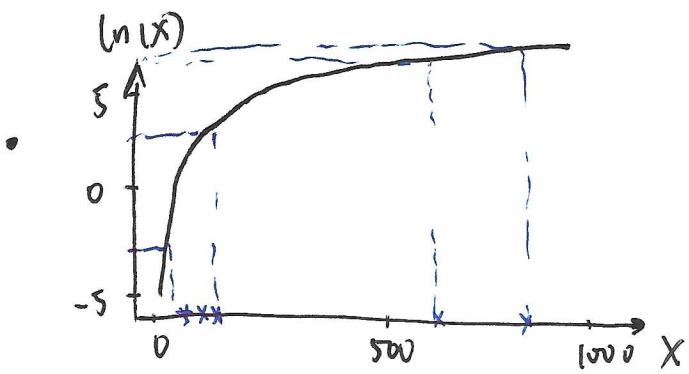
We conclude there's significant heteroscedasticity problem.

(iii) White Test * is another common one.

(c) Solution

(i) log-transformation on y

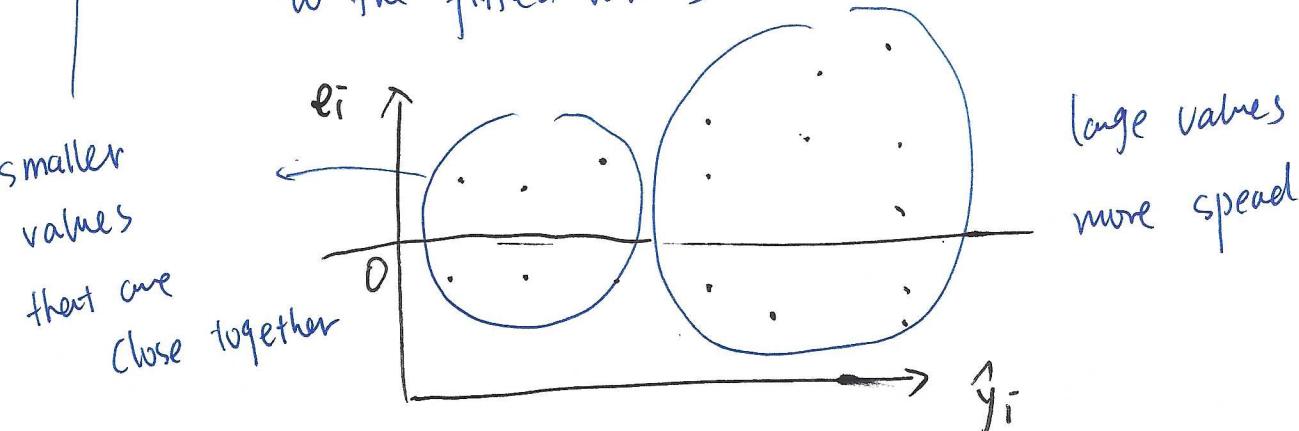
- Natural logarithm, \ln , transformation is the most common transformation in MLR



From the plot, the effects of taking natural log transformation are:

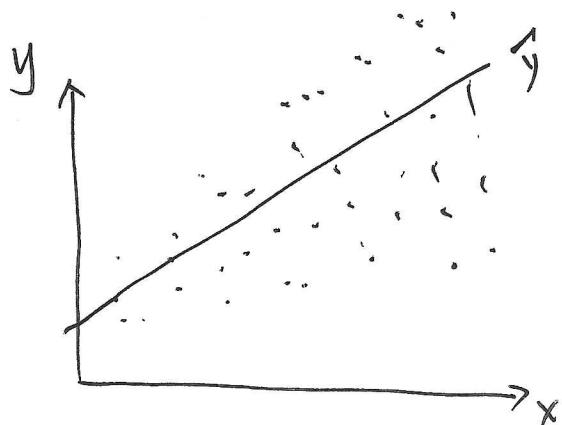
- small values that are close together are spread further out
- large values that are spread out are brought close together

Therefore, it works when the residuals changes proportionally to the fitted values



$$\text{since } e_i = y_i - \hat{y}_i$$

the heteroscedasticity problem lands on "y" in the data.



distribution of y around the fitted line
also changes from clusters of
smaller values to the spread
of large values.

- In this case, a natural-log transformation on y

could help "even-out" the points:

$$y_{\text{new}} = \ln(y)$$

smf.ols("y_{\text{new}} \sim x_1 + \dots + x_{p-1}")

$$\hat{y}_{\text{new}} = \ln(\hat{y}) \rightarrow \hat{y} = e^{\hat{y}_{\text{new}}}$$

Since $\ln y$ only works for the case of e_i is proportional with y_i .

or "Funnel" shape, other solutions can be

(iii) Weighted least-square regression. — count different variances in the estimation.

Recall OLS assumes $\text{Var}(\vec{\epsilon}) = \begin{pmatrix} \sigma^2 & & \\ & \ddots & 0 \\ 0 & & \sigma^2 \end{pmatrix}$

while reality in heteroscedasticity is

$$\text{Var}(\vec{\epsilon}) = \begin{pmatrix} \sigma_1^2 & & 0 & \\ & \sigma_2^2 & & 0 \\ 0 & & \ddots & \\ & & & \sigma_n^2 \end{pmatrix} = \Sigma$$

$$\text{Var}(\vec{b}) = (\vec{X}^\top \vec{X})^{-1} \vec{X}^\top \cdot \underbrace{E(\vec{\epsilon}\vec{\epsilon}^\top)}_{\text{aka } \text{Var}(\vec{\epsilon})} \cdot \vec{X} (\vec{X}^\top \vec{X})^{-1}$$

$$\text{aka } \text{Var}(\vec{\epsilon}) = \Sigma$$

We need to estimate Σ by $\hat{\Sigma} = \begin{pmatrix} e_1^2 & & 0 & \\ & e_2^2 & & 0 \\ 0 & & \ddots & \\ & & & e_n^2 \end{pmatrix}$

then estimate $\text{Var}(\vec{b})$ by $(\vec{X}^\top \vec{X})^{-1} \vec{X}^\top \hat{\Sigma} \vec{X} (\vec{X}^\top \vec{X})^{-1}$

$$\text{Var}(\vec{\epsilon}) = \begin{pmatrix} \sigma_1^2 & & & \\ & \sigma_2^2 & & \\ & & \ddots & \\ & & & \sigma_n^2 \end{pmatrix} = \Sigma$$

- Weighted-least-square estimates take account of the different variances in the way that
 - An observation with small error variation should weigh more in the model.
 - An observation with bigger error variation should weigh less in the model.
 - It includes the Σ in the estimation in the way that

Define the Weight Matrix

$$W = \begin{pmatrix} w_1 & & & \\ & w_2 & & \\ & & \ddots & \\ & 0 & & w_n \end{pmatrix} = \begin{pmatrix} \frac{1}{\sigma_1^2} & & & \\ & \frac{1}{\sigma_2^2} & & \\ & & \ddots & \\ & 0 & & \frac{1}{\sigma_n^2} \end{pmatrix}$$

- Defined the weighted sum of squares:

$$SS_{WLS}(\vec{\beta}) = \sum w_i e_i^2$$

and $\vec{b}_{WLS} = \arg\min SS_{WLS} = (\vec{X}^T \vec{W} \vec{X})^{-1} \vec{X}^T \vec{W} \vec{Y}$

Where $\vec{W} = \boxed{?}$

Practically how to decide the weights can be tricky:

If we assume $e_1 \sim N(0, \sigma_1^2), \dots, e_n \sim N(0, \sigma_n^2)$

we only have one observed sample for e_i from each ϵ_i .

Robust standard error later used this approach.

Here we just give an simple example, it's NOT required to run WLS yourself:

When e_i v.s. X_k has a funnel shape,

you can run model = " $e_i^2 \sim X_k$ "

then use fitted values of the model as the estimated variance of $\text{Var}(e_i)$

$$\text{then } w_i = 1/e_i^2$$

- (iii) Generalized Least squares: again deal with the estimate of Σ in a broader choices of cases.
- logistic model is a case of GLM.
- (iv) Use more Robust Regression: which is not sensitive to assumptions.
- (v) Use Robust standard errors (common in Economics, see supplemental material.)
- (2) Sometimes, after correcting Non-Normality, Non-linearity and model selection, heteroscedasticity can be greatly improved as well.

Summary:

- Heteroscedasticity : The assumption of constant variance of ϵ_i is violated.

Problem

- In OLS result $se(\hat{\beta}_k)$ is incorrect, resulting in misleading t-test and anova test results.
- $Var(\hat{Y}_h)$ is incorrect, resulting in misleading C.I. and prediction intervals.
- The estimation of coefficients and fitted values are still unbiased, therefore reliable.

Detection

- Residual v.s. Fitted plot
the bandwidth changes
- Breusch-Pagan Test or White Test :
p-value ≤ 0.05 indicated serious heteroscedasticity problem.

Solution:

- (i) If ϵ_i v.s. \hat{y}_i is funnel shape, perform natural log transformation on y .
- (ii) Perform Weighted-least-square regression.

* Practically hard to decide a good weight

(iii) Use Robust Regression methods in ML:

Huber, RANSAC, Theil Sen

(iv) Use Robust standard errors in all formulas that need the variance-covariance matrix of error term