Regression Assumptions & Diagnostics

Fundamental Techniques in Data Science with R

Kyle M. Lang

Department of Methodology & Statistics
Utrecht University

Utrecht University

Outline

Motivation

Assumptions of MLR
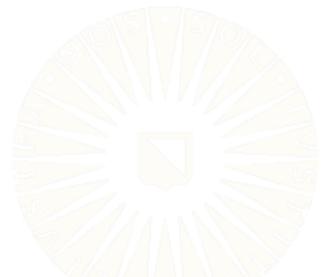
Regression Diagnostics
  Heteroscedasticity
  Correlated Errors
  Linearity
  Omitted Variables
  Normality

Why Assume?

Consider the following equation:

$$5 = x + y$$
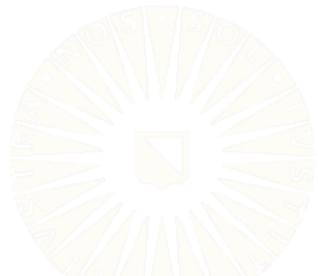
What are the values of x and y?

Why Assume?

Consider the following equation:

$$5 = x + y$$

What are the values of x and y?

$$y = 5 - x$$

Why Assume?

Consider the following equation:

$$5 = x + y$$

What are the values of x and y?

$$y = 5 - x$$

What if we assume that $y = x$?

Why Assume?

Consider the following equation:

$$5 = x + y$$

What are the values of x and y?

$$y = 5 - x$$
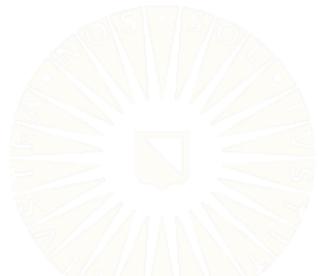
What if we assume that $y = x$?

$$5 = x + y$$
$$0 = x - y$$

Why Assume?

Consider the following equation:

$$5 = x + y$$

What are the values of x and y?

$$y = 5 - x$$
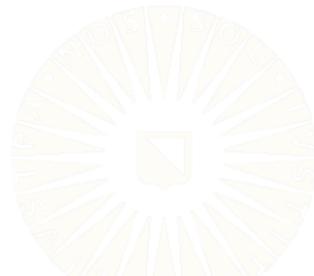
What if we assume that $y = x$?

$$5 = x + y$$
$$0 = x - y$$

Now we have enough information:

$$5 = x + x = 2x \implies x = y = 2.5$$

Why Assume?
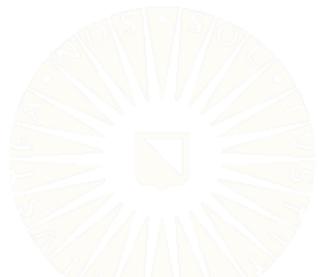
Given Foo, Bar → Baz

Assumptions of MLR

The assumptions of the linear model can be stated as follows:

1. The model is linear in the parameters.

   - This is OK: $Y = \beta_0 + \beta_1 X + \beta_2 Z + \beta_3 XZ + \beta_4 X^2 + \beta_5 X^3 + \varepsilon$
   - This is not: $Y = \beta_0 X^{\beta_1} + \varepsilon$

2. The predictor matrix is *full rank*.

   - $N > P$
   - No X_p can be a linear combination of other predictors.

Assumptions of MLR

3. The predictors are strictly exogenous.
   - The predictors do not correlated with the errors.
   - $\text{Cov}(\hat{Y}, \varepsilon) = 0$
   - $\text{E}[\varepsilon_n] = 0$

4. The errors have constant, finite variance.
   - $\text{Var}(\varepsilon_n) = \sigma^2 < \infty$
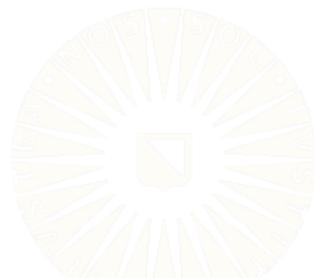
5. The errors are uncorrelated.
   - $\text{Cov}(\varepsilon_i, \varepsilon_j) = 0, \ i \neq j$

6. The errors are normally distributed.
   - $\varepsilon \sim \text{N}(0, \sigma^2)$
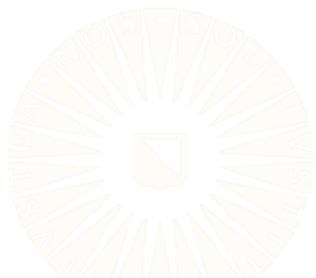
Assumptions of MLR

The assumption of *spherical errors* combines Assumptions 4 and 5.

$$\text{Var}(\varepsilon) = \begin{bmatrix} \sigma^2 & 0 & \cdots & 0 \\ 0 & \sigma^2 & \cdots & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & \cdots & \sigma^2 \end{bmatrix} = \sigma^2 \mathbf{I}_N$$

We can combine Assumptions 3, 4, 5, and 6 by assuming independent and identically distributed normal errors:

- $\varepsilon \overset{iid}{\sim} \text{N}(0, \sigma^2)$
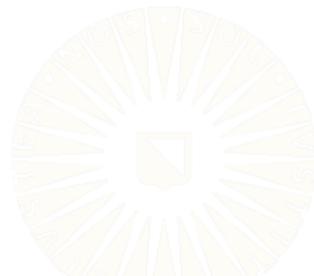
Consequences of Violating Assumptions

1. If the model is not linear in the parameters, then we're not even working with linear regression.
   - We need to move to entirely different modeling paradigm.
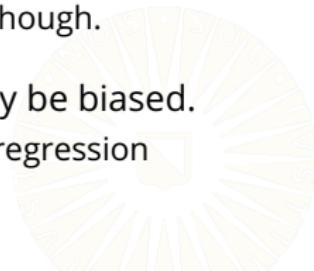
Consequences of Violating Assumptions

1. If the model is not linear in the parameters, then we're not even working with linear regression.
   - We need to move to entirely different modeling paradigm.

2. If the predictor matrix is not full rank, the model is not estimable.
   - The parameter estimates cannot be uniquely determined from the data.

Consequences of Violating Assumptions

1. If the model is not linear in the parameters, then we're not even working with linear regression.
   - We need to move to entirely different modeling paradigm.

2. If the predictor matrix is not full rank, the model is not estimable.
   - The parameter estimates cannot be uniquely determined from the data.

3. If the predictors are not exogenous, the estimated regression coefficients will be biased.

4. If the errors are not spherical, the standard errors will be biased.
   - The estimated regression coefficients will be unbiased, though.

5. If errors are non-normal, small-sample inferences may be biased.
   - The justification for some tests and procedures used in regression analysis may not hold.
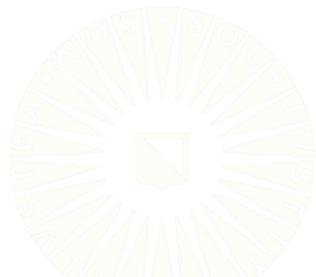
Regression Diagnostics

If some of the assumptions are (grossly) violated, the inferences we make using the model may be wrong.

- We need to check the tenability of our assumptions before leaning too heavily on the model estimates.
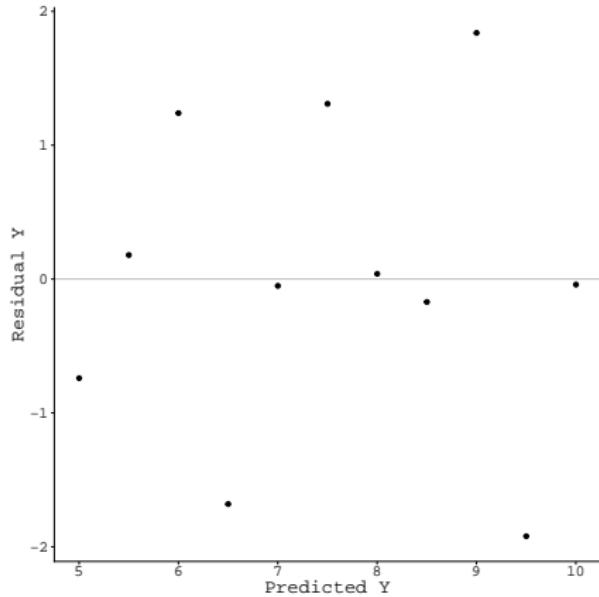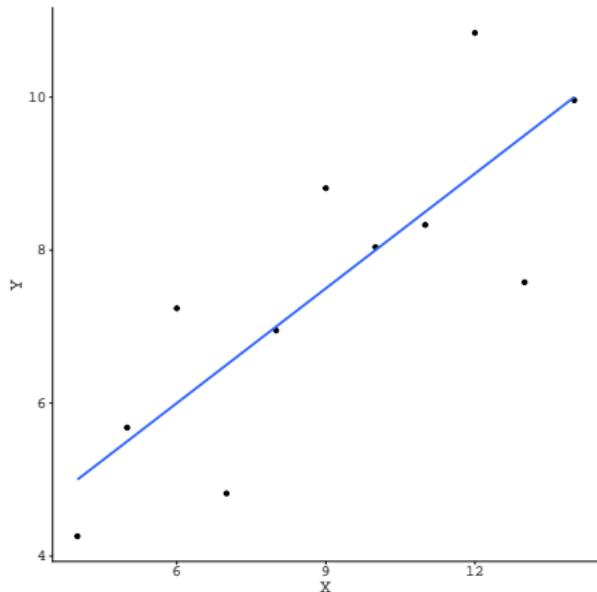
These checks are called *regression diagnostics*.

- Graphical visualizations
- Quantitative indices/measures
- Formal statistical tests

Residual Plots
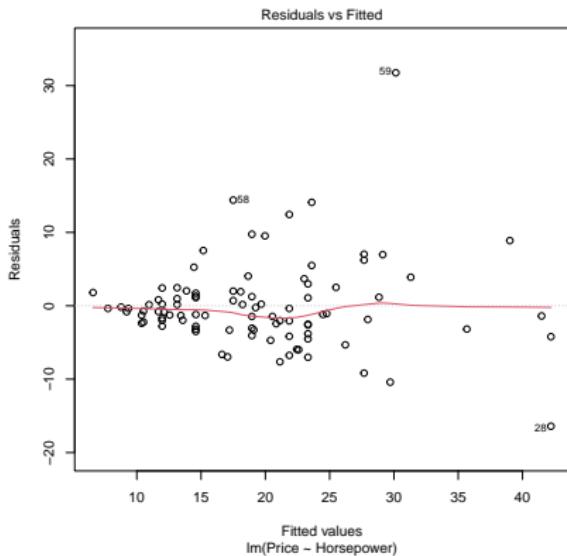
One of the most useful diagnostic graphics is the plot of residuals vs. predicted values.

Residual Plots

We can easily generate a simple plot of residuals vs. fitted values by plotting the fitted lm object in R.
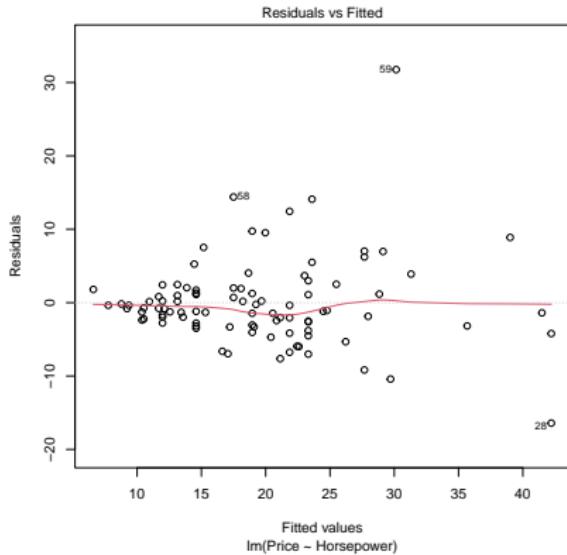
```
out1 <- lm(Price ~ Horsepower,
           data = Cars93)

plot(out1, 1)
```


Residuals vs Fitted
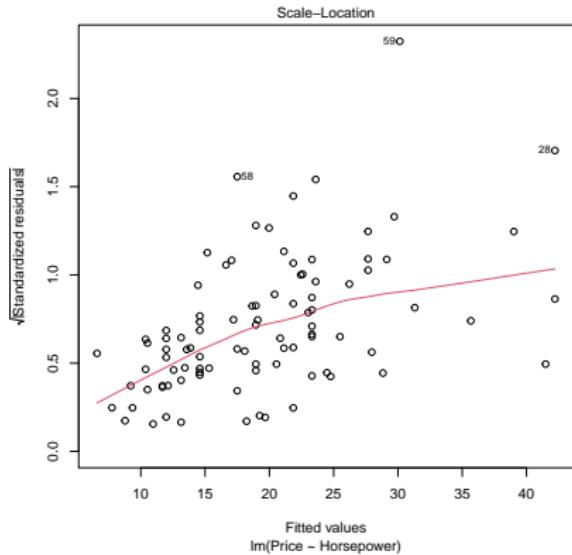
Heteroscedasticity

Non-constant error variance (*heteroscedasticity*) violates Assumption 4.

`plot(out1, 1)`   `plot(out1, 3)`

Consequences of Heteroscedasticity

Non-constant error variance will not bias the parameter estimates.

- The best fit line is still correct.
- Our measure of uncertainty around that best fit line is wrong.

Heteroscedasticity will bias standard errors (usually downward).

- Test statistics will be too large.
- CIs will be too narrow.
- We will have inflated Type I error rates.

To get valid inference, we need to address (severe) heteroscedasticity.

Treating Heteroscedasticity

1. Transform your outcome using a concave function (e.g., $\ln(Y)$, $\sqrt{Y}$).
   - These transformations will shrink extreme values more than small/moderate ones.
   - It's usually a good idea to first shift the variable's scale by setting the minimum value to 1.

2. Refit the model using *weighted least squares*.
   - Create inverse weights using functions of the residual variances or quantities highly correlated therewith.

3. Use a *Heteroscedasticity Consistent* (HC) estimate of the asymptotic covariance matrix.
   - Robust standard errors, Huber-White standard errors, Sandwich estimators
   - HC estimators correct the standard errors for non-constant error variance.

Example

```r
## The 'sandwich' package provides several HC estimators:
library(sandwich)

## the 'lmtest' package provides fancy testing tools for linear models:
library(lmtest)

## Use sandwich estimator to compute ACOV matrix:
hcCov <- vcovHC(out1)

## Test coefficients with robust SEs:
robTest <- coeftest(out1, vcov = hcCov)

## Test coefficients with default SEs:
defTest <- summary(out1)$coefficients
```

Example

```
## Compare robust and default approaches:
robTest


t test of coefficients:

             Estimate Std. Error t value  Pr(>|t|)
(Intercept) -1.398769   2.078200 -0.6731    0.5026
Horsepower   0.145371   0.017164  8.4696 4.051e-13 ***
---
Signif. codes:
0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

defTest

              Estimate Std. Error     t value     Pr(>|t|)
(Intercept) -1.3987691  1.8200164  -0.7685475 4.441519e-01
Horsepower   0.1453712  0.0118978  12.2183251 6.837464e-21
```

Correlated Errors

Errors can become correlated in two basic ways:

1. Serial dependence
   - When modeling longitudinal data, the errors for a given observational unit are correlated over time.
   - We can detect temporal dependence by examining the *autocorrelation* of the residuals.
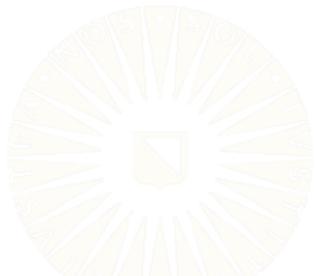
2. Clustering
   - Your data have some important, unmodeled, grouping structure.
     - Children nested within classrooms
     - Romantic couples
     - Departments within a company
   - We can detect problematic levels of clustering with the *intraclass correlation coefficient* (ICC).
     - We need to know the clustering variable to apply the ICC.

Treating Correlated Errors

Serially dependent errors in a longitudinal model usually indicate an inadequate model.

- Your model is ignoring some important aspect of the temporal variation that is being absorbed by the error terms.

- Hopefully, you can add the missing component to your model.

Treating Correlated Errors

Clustering can be viewed as theoretically meaningful or as a nuisance factor that just needs to be controlled.

- If the clustering is meaningful, you should model the data using *multilevel modeling*.
  - Hierarchical linear regression
  - Mixed models
  - Random effects models

- If the clustering is an uninteresting nuisance, you can use specialized HC variance estimators that deal with clustering.

Example

```
## Read in some data:
LeeBryk <- readRDS(here::here("data", "lee_bryk.rds"))

## Check the data:
str(LeeBryk, vec.len = 3)

'data.frame': 7185 obs. of  5 variables:
 $ schoolid: int  1 1 1 1 1 1 1 1 ...
 $ math    : num  5.88 19.71 20.35 8.78 ...
 $ ses     : num  -1.53 -0.59 -0.53 -0.67 -0.16 0.02 -0.62 -1 ...
 $ mses    : num  -0.43 -0.43 -0.43 -0.43 -0.43 -0.43 -0.43 -0.43 ...
 $ sector  : Factor w/ 2 levels "public","private": 1 1 1 1 1 1 1 1 ...

## Estimate a linear regression model:
fit <- lm(math ~ ses + sector, data = LeeBryk)

## Calculate the residual ICC:
ICC::ICCbare(x = LeeBryk$schoolid, y = resid(fit))

[1] 0.07487712
```
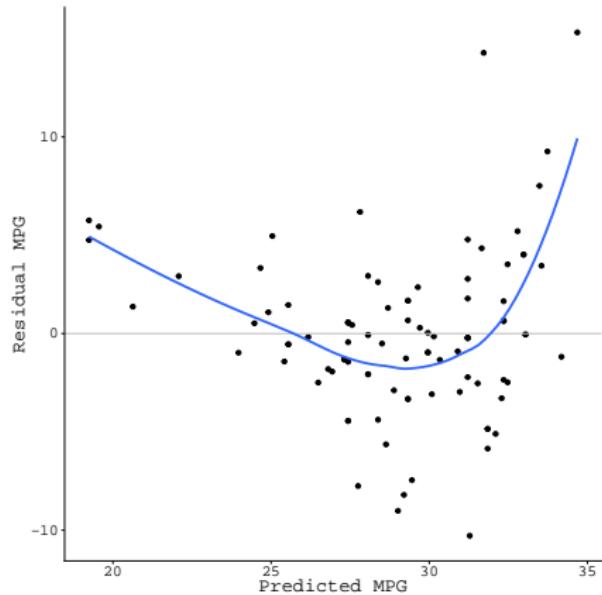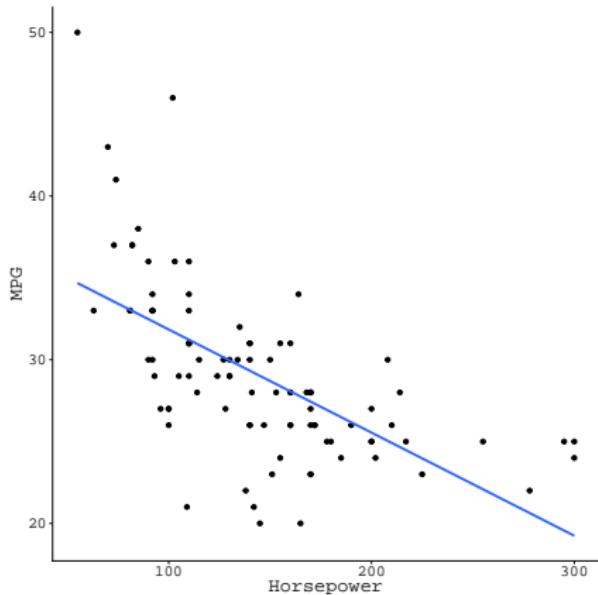
Example

```
## Robust tests:
coeftest(fit, vcov = vcovCL(fit, ~ schoolid))


t test of coefficients:

               Estimate Std. Error t value  Pr(>|t|)
(Intercept)    11.79965    0.20318 58.0746 < 2.2e-16 ***
ses             2.94860    0.12794 23.0475 < 2.2e-16 ***
sectorprivate   1.93495    0.31717  6.1006 1.111e-09 ***
---
Signif. codes:
0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

## Raw tests:
summary(fit)$coefficients

               Estimate Std. Error   t value      Pr(>|t|)
(Intercept)   11.799654 0.10612759 111.18366  0.000000e+00
ses            2.948605 0.09782968  30.14019 5.002687e-188
sectorprivate  1.934953 0.15249200  12.68888 1.676478e-36
```

Linearity

Each modeled X must exhibit a linear relation with Y.

- We can define X via nonlinear transformations of the original data.

Treating Residual Nonlinearity

Nonlinearity in the residual plots is usually a sign of either:

1. Model misspecification
2. Influential observations

This type of model misspecification usually implies omitted functions of modeled variables.

- Polynomial terms
- Interactions

The solution is to include the omitted term into the model and refit.
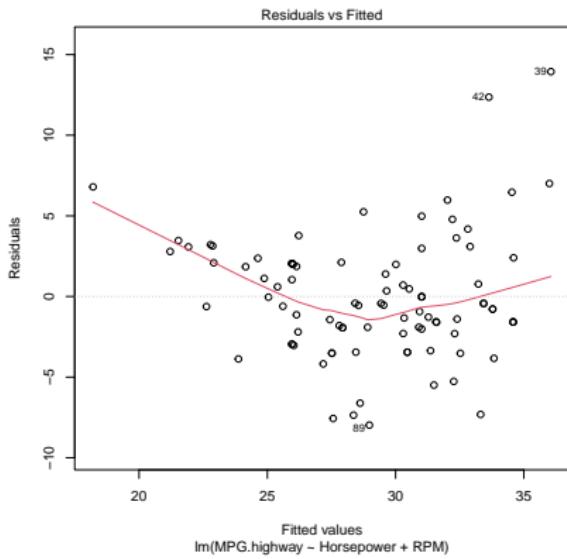
- This is very much easier said than done.

Limitations of Residual Plots

In multiple regression models, basic
residual plots won't tell us which
predictors exhibit nonlinear
associations.
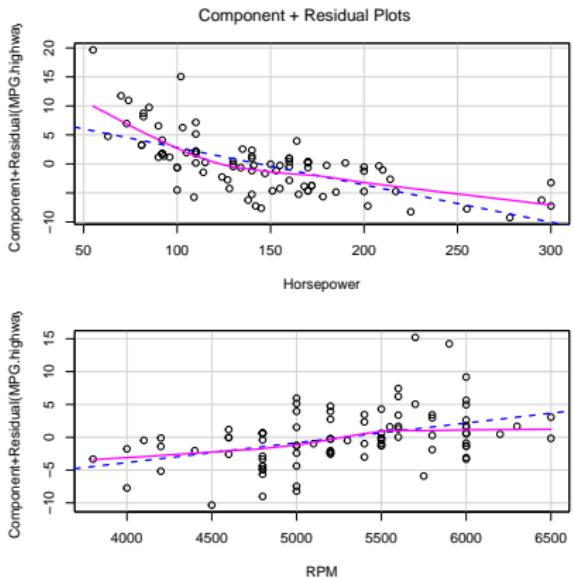
```
out3 <-
  lm(MPG.highway ~ Horsepower + RPM,
     data = Cars93)
```


Residuals vs Fitted

Fitted values
lm(MPG.highway ~ Horsepower + RPM)

Component + Residual Plots

We can use *Component + Residual Plots* (AKA, partial residual plots) to visualize the unique effects of each X variable.
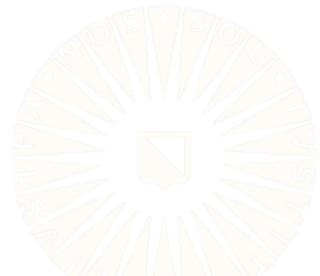
```
library(car)
crPlots(out3)
```


Component + Residual Plots

Omitted Variables

The most common cause of endogeneity (i.e., violating Assumption 3) is *omitted variable bias*.

- If we leave an important predictor variable out of our equation, some modeled predictors will become endogenous and their estimated regression slopes will be biased.

- The omitted variable must be correlated with Y and at least one of the modeled X_p, to be a problem.

Omitted Variables

Assume the following is the true regression model.

$$Y = \beta_0 + \beta_1 X + \beta_2 Z + \varepsilon$$

Now, suppose we omit Z from the model:

$$Y = \beta_0 + \beta_1 X + \omega$$
$$\omega = \varepsilon + \beta_2 Z$$

Our new error, ω, is a combination of the true error, ε, and the omitted term, $\beta_2 Z$.
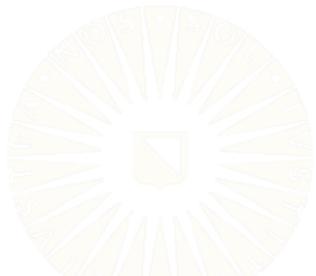
- Consequently, if X and Z are correlated, omitting Z induces a correlation between X and ω (i.e., endogeneity).

Treating Omitted Variable Bias

Omitted variable bias can have severe consequences, but you can't really test for it.

- The *errors* are correlated with the predictors, but our model is estimated under the assumption of exogeneity, so the *residuals* from our model will generally be uncorrelated with the predictors.

- We mostly have to pro-actively work to include all relevant variables in our model.
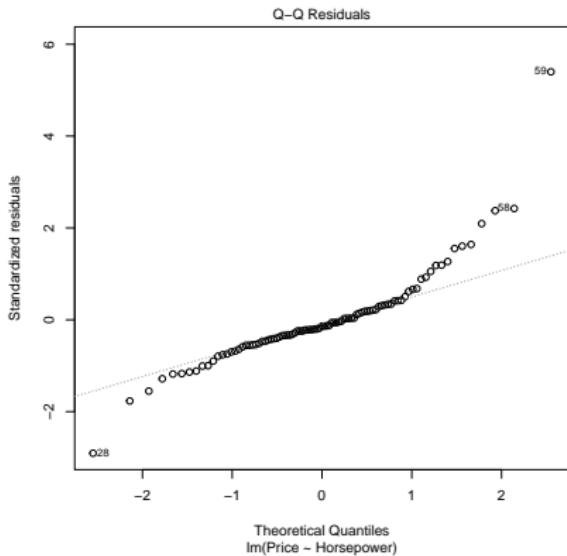
Normality Assumption

One of the best ways to evaluate
the normality of the error
distribution with a Q-Q Plot.
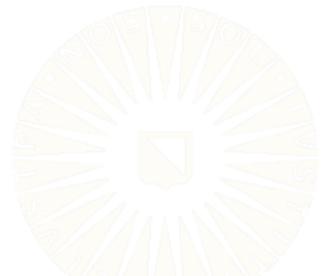
- Plot the quantiles of the residual
  distribution against the
  theoretically ideal quantiles.

- We can actually use a Q-Q Plot to
  compare any two distributions.

Consequences of Violating Normality

In small samples, with *fixed* predictors, normally distributed errors imply normal sampling distributions for the regression coefficients.

- In large samples, the central limit theorem implies normal sampling distributions for the coefficients, regardless of the error distribution.

Consequences of Violating Normality

In small samples, with *fixed* predictors, normally distributed errors imply normal sampling distributions for the regression coefficients.

- In large samples, the central limit theorem implies normal sampling distributions for the coefficients, regardless of the error distribution.

Prediction intervals require normally distributed errors.

- Confidence intervals for predictions share the same normality requirements as the coefficients' sampling distributions.

Consequences of Violating Normality

In small samples, with *fixed* predictors, normally distributed errors imply normal sampling distributions for the regression coefficients.
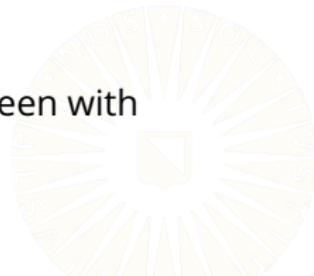
- In large samples, the central limit theorem implies normal sampling distributions for the coefficients, regardless of the error distribution.

Prediction intervals require normally distributed errors.

- Confidence intervals for predictions share the same normality requirements as the coefficients' sampling distributions.

Parameter estimates will not be fully efficient.
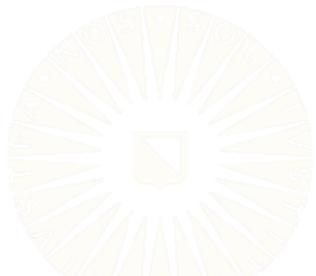
- Standard errors will be larger than they would have been with normally distributed errors.

Treating Violations of Normality

We usually don't need to do anything about non-normal errors.

- The CLT will protect our inferences.

Treating Violations of Normality

We usually don't need to do anything about non-normal errors.

- The CLT will protect our inferences.

We can use *bootstrapping* to get around the need for normality.

1. Treat your sample as a synthetic population from which you draw many new samples (with replacement).
2. Estimate your model in each new sample.
3. The replicates of your estimated parameters generate an empirical sampling distribution that you can use for inference.

Treating Violations of Normality

We usually don't need to do anything about non-normal errors.

- The CLT will protect our inferences.

We can use *bootstrapping* to get around the need for normality.

1. Treat your sample as a synthetic population from which you draw many new samples (with replacement).
2. Estimate your model in each new sample.
3. The replicates of your estimated parameters generate an empirical sampling distribution that you can use for inference.

Bootstrapping can be used for inference on pretty much any estimable parameter, but it won't work with small samples.

- Need to assume that your sample is representative of the population