

Regression Analysis

Multiple Linear Regression

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Assumptions and Diagnostics



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About This Lesson



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Multiple Linear Regression: Model

Data: $\{(x_{1,1}, \dots, x_{1,p}), y_1\}, \dots, \{(x_{n,1}, \dots, x_{n,p}), y_n\}$

Model: $y_i = \beta_0 + \beta_1 x_{i,1} + \dots + \beta_p x_{i,p} + \varepsilon_i, i = 1, \dots, n$

Assumptions:

- **Linearity/Mean Zero Assumption:** The relationship between the response variable and each predicting variable is linear. (For each $j, j = 1, \dots, p, y_i$ and x_{ij} are linearly related, $i = 1, \dots, n$.) $E(\varepsilon_i) = 0$
- **Constant Variance Assumption:** $\text{Var}(\varepsilon_i) = \sigma^2$
- **Independence Assumption:** $\{\varepsilon_1, \dots, \varepsilon_n\}$ are independent random variables
- Assumption that $\varepsilon_i \sim \text{Normal}$ for confidence/prediction intervals, hypothesis testing



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Properties of the Errors & Residuals

Properties of (true) errors:

- $E(\varepsilon_i) = 0$
- $\text{Var}(\varepsilon_i) = \sigma^2$
- $E(\boldsymbol{\varepsilon}) = \mathbf{0}$
- $\text{Var}(\boldsymbol{\varepsilon}) = \sigma^2 \mathbf{I}$

Properties of the (estimated) residuals:

- $\hat{\boldsymbol{\varepsilon}} = \mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}$
- $E(\hat{\boldsymbol{\varepsilon}}) = \mathbf{0}$ (or $E(\hat{\varepsilon}_i) = 0$)
- $\mathbf{V}(\hat{\boldsymbol{\varepsilon}}) = \sigma^2(\mathbf{I} - \mathbf{H})$ (or $\text{Var}(\hat{\varepsilon}_i) = \sigma^2(1 - h_{i,i})$)
 - Where \mathbf{H} is the hat matrix, and $h_{i,i}$ is the i -th element on its diagonal



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- While the true errors have constant variance, the estimated residuals do not.

- To use the estimated residuals for assessing the model assumptions, we need to standardize:

$$r_i = \hat{\varepsilon}_i / (\hat{\sigma} \sqrt{1 - h_{i,i}})$$

Residuals Analysis

Standardized Residual Values: $r_i = \hat{\varepsilon}_i / (\hat{\sigma} \sqrt{1 - h_{i,i}})$

Graphical assessment of MLR assumptions:

- Plot standardized residuals r_i against each predictor
 - *Linearity*
- Plot standardized residuals r_i against fitted values
 - *Constant Variance & Independence*
- QQ normal plot & histogram
 - *Normality*

Residuals Analysis

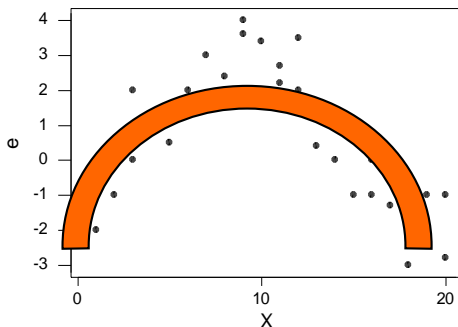
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Graphical assessment of MLR assumptions:

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 - Plot standardized residuals r_i against fitted values
 - *Constant Variance & Independence*
 - QQ normal plot & histogram
 - *Normality*
- We evaluate the normality assumption using the residuals, not the response variable.
 - We do not check the predicting variables for normality.
 - However, if the distribution of a predicting variable is strongly skewed, it is possible that the linearity assumption with respect to that variable will not hold.

Residual Analysis: Linearity Assumption

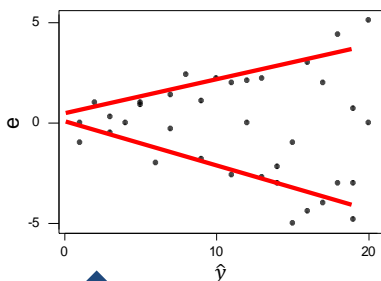
Linearity: Plot the residuals against each predicting variable.



This shows that there may be a non-linear relationship between X and Y .

Residual Analysis: Constant Variance Assumption

Constant Variance: Plot the residuals against fitted values.



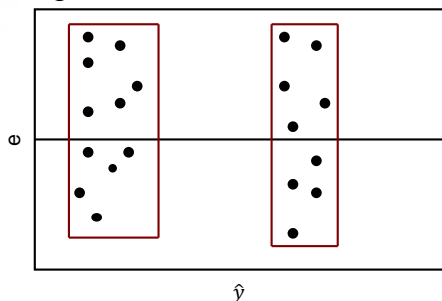
The residuals show larger variance as the predicting variable increases.



Here, it is an example for which σ^2 is not constant.

Residual Analysis: Independence Assumption

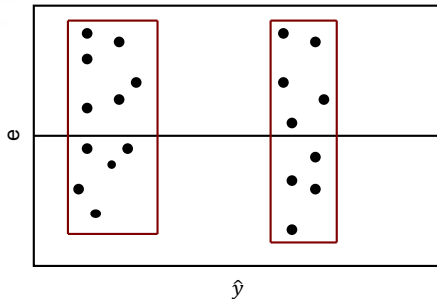
Independence (*uncorrelated errors*): Plot the residuals against fitted values.



- There are clusters of residuals.
- The independence assumption does not hold.

Residual Analysis: Independence Assumption

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- Using residual analysis, we are actually checking for uncorrelated errors, not independence.
- Independence is a more complicated matter. If the data are from a randomized experiment, then independence holds, but most data are from observational studies.
- We commonly correct for selection bias in observational studies using controlling variables.

Checking the Assumption of Normality

One way to check this assumption in a regression is using a **Normal Probability (Q-Q) Plot**

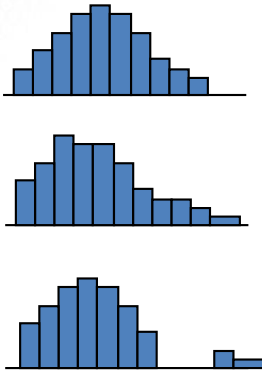
y-axis:	e_i
x-axis:	$\Phi^{-1}\left(\frac{r_i - 3/8}{n + 1/4}\right)$

r_i = rank of e_i (between 1, n)
 Φ = CDF of Normal Distribution

- Let the R statistical software do this for you!
- A straight line in a normal probability plot implies that the assumption is valid
- **Curvature (especially at the ends)** shows non-normality

Residual Analysis: Normality Assumption

A complementary approach for checking for the normality assumption is by plotting the histogram of the residuals.



Normality Assumption:

The residuals should have an approximately symmetric, unimodal distribution, with no gaps in the data.

Predicting Variable Transformation

- If the model fit is inadequate, it does not mean that a regression is not useful.
- One problem might be that one or more predicting variable X might not have a linear relationship with the response variable Y .
- To model the nonlinear relationship, we transform X by some nonlinear function such as

$$f(x) = x^a$$

or

$$f(x) = \log(x)$$

Normality Transformation

Problem: Constant variance or/and normality assumption

Solution: Transform the response variable from y to \hat{y}^* via

$$\hat{y}^* = y^\lambda$$

where the value of λ depends on how $\text{Var}(y)$ changes as x changes.

$$\sigma_y(x) \propto \text{const} \quad \lambda = 1 \quad (\text{don't transform})$$

$$\sigma_y(x) \propto \sqrt{\mu_x} \quad \lambda = 1/2 \quad \hat{y}^* = \sqrt{y}$$

$$\sigma_y(x) \propto \mu_x \quad \lambda = 0 \quad \hat{y}^* = \ln(y)$$

$$\sigma_y(x) \propto \mu_x^2 \quad \lambda = -1 \quad \hat{y}^* = \frac{1}{y}$$



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Outliers in Regression

A data point far from the majority of the data (in y and/or any x) may be called an *outlier*, especially if it does not follow the general trend of the rest of the data.

- Data points that are far from the means of the X s or near the edge of the observation space are called *leverage points*.
- A data point that is far from the means of y and/or an x is called an *influential point* if it influences the fit of the regression.
- Excluding a leverage point may or may not the regression fit significantly, thus a leverage point may or may not be an influential point.

The upshot: Sometimes there are good reasons to exclude subsets of data (e.g., errors in data entry or experimental errors). Sometimes an outlier belongs in the data. Outliers should always be examined.



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Checking for Outliers

Cook's Distance:
$$D_i = \frac{(\hat{Y}_{(i)} - \hat{Y})^T (\hat{Y}_{(i)} - \hat{Y})}{(k + 1) \hat{\sigma}^2}$$

where $\hat{Y}_{(i)}$ are the fitted values from the model fitted without the i^{th} observation (i.e., excluding the i^{th} observation from the data) and \hat{Y} are the fitted values from the model fitted with the i^{th} observation (i.e., including all observations).

Cook's Distance measures how much the estimated parameter values in the regression model change when the i^{th} observation is removed.

Rule of Thumb: $D_i > 4/n$, $D_i > 1$, OR any "large" D_i should be investigated.



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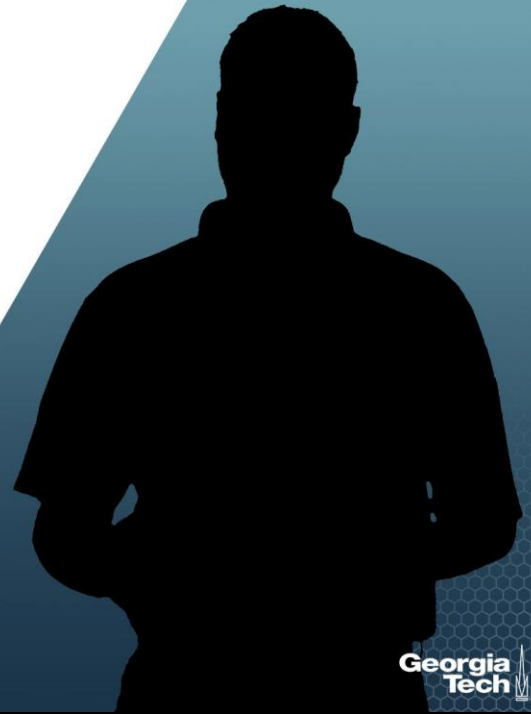
Rule of Thumb: $D_i > 4/n$, $D_i > 1$, OR any "large" D_i should be investigated.

- Outliers: are those few observations with much larger Cook's distance than the rest of observations;
- If a large number of outliers, then they probably point to a heavy tailed distribution rather than truly extreme values.



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Summary



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