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

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, $i = 1, \dots, n$.) $\mathrm{E}(\varepsilon_i) = 0$
- *Constant Variance Assumption*: $\mathrm{Var}(\varepsilon_i) = \sigma^2$
- *Independence Assumption*: $\{\varepsilon_1, \dots, \varepsilon_n\}$ are independent random variables
- Assumption that $\varepsilon_i \sim$ Normal *for confidence/prediction intervals, hypothesis testing*

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Properties of the Errors & Residuals

Properties of (true) errors:

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

Properties of the (estimated) residuals:

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

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  - Where $\mathbf{H}$ is the hat matrix, and $h_{i,i}$ is the *i*-th element on its diagonal

- **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:**

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

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Residuals Analysis

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

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*

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- 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.**

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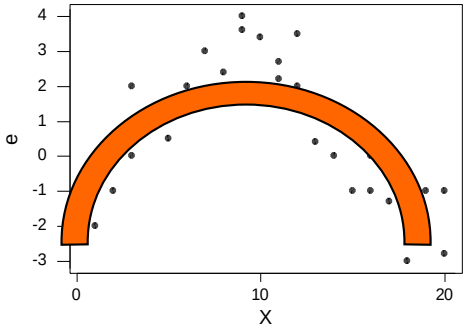
Residual Analysis: Linearity Assumption

Linearity: Plot the residuals against each predicting variable.



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

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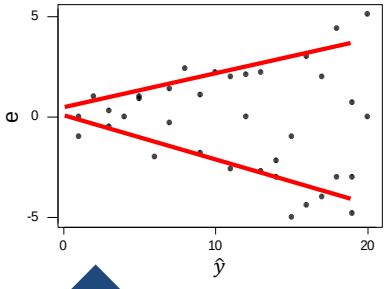
Residual Analysis: Constant Variance Assumption

Constant Variance: Plot the residuals against fitted values.

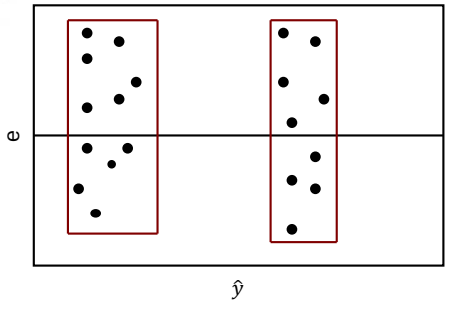


The residuals show larger variance as the predicting variable increases.

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

Residual Analysis: Independence Assumption

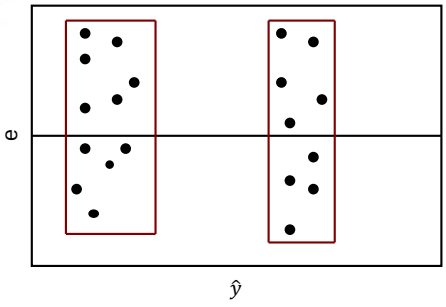
Independence *(uncorrelated errors)***:** Plot the residuals against fitted values.



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

Residual Analysis: Independence Assumption

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



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

- **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.**

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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
- **Curviture (especially at the ends)** shows non-normality

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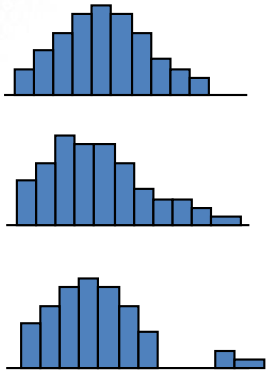
Residual Analysis: Normality Assumption

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.

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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

or

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

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

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Normality Transformation

Problem: Constant variance or/and normality assumption

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

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

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

$\sigma_y(x) \propto const$	$\lambda = 1$	(don't transform)
$\sigma_y(x) \propto \sqrt{\mu_x}$	$\lambda = 1/2$	$\boldsymbol{y}^* = \sqrt{\boldsymbol{y}}$
$\sigma_y(x) \propto \mu_x$	$\lambda = 0$	$\boldsymbol{y}^* = \ln(\boldsymbol{y})$
$\sigma_y(x) \propto \mu_x^2$	$\lambda = -1$	$\boldsymbol{y}^* = \frac{1}{\boldsymbol{y}}$

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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: $\mathrm{D}_i = \frac{(\hat{\boldsymbol{Y}}_{(i)} - \hat{\boldsymbol{Y}})^{\mathrm{T}}(\hat{\boldsymbol{Y}}_{(i)} - \hat{\boldsymbol{Y}})}{(k+1)\hat{\sigma}^2}$

where $\hat{\boldsymbol{Y}}_{(i)}$ are the fitted values from the model fitted without the *i*th observation (i.e., excluding the *i*th observation from the data) and $\hat{\boldsymbol{Y}}$ 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: $\mathrm{D}_i > 4/n$, $\mathrm{D}_i > 1$, OR any "large" D_i should be investigated.

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- 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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