GENERAL ASSEMBLY

DATA SCIENCE
CLASS 6: LINEAR REGRESSION

0. BASIC FORM

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ε = **residual** *(the error)*

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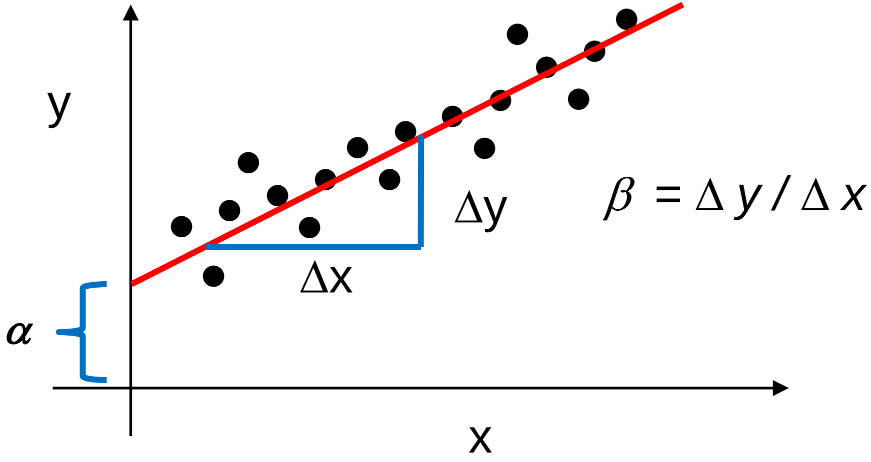

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$$y = \alpha + \beta_1 x_1 + \ldots + \beta_n x_n + \varepsilon$$

I. ESTIMATING COEFFICIENTS

*Q: How to determine the **impact** of a particular input variable on the response variable?*

A: The coefficient estimates $(\hat{\beta})$

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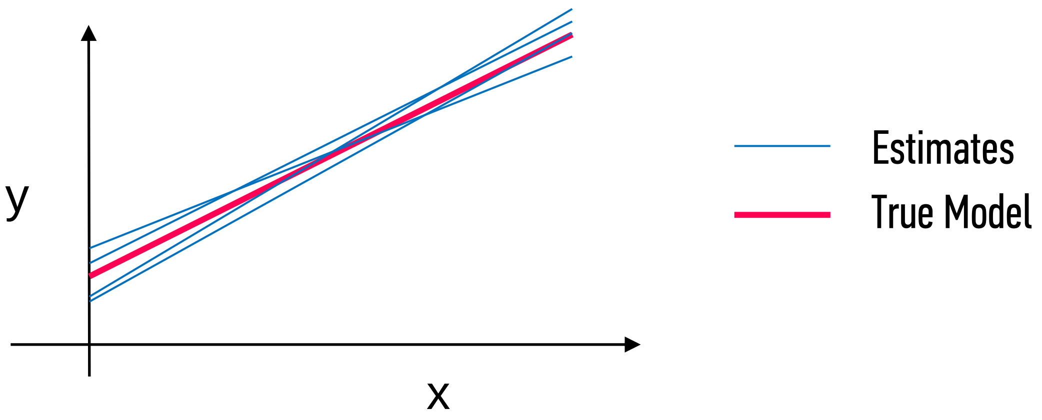

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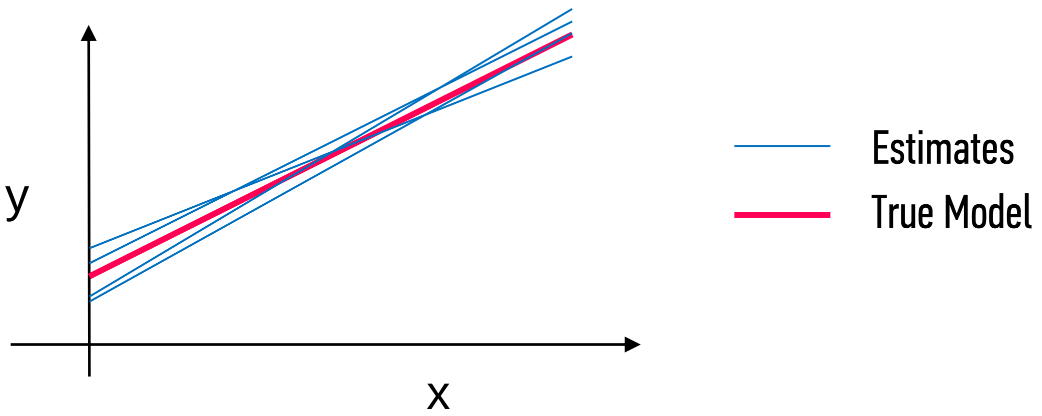
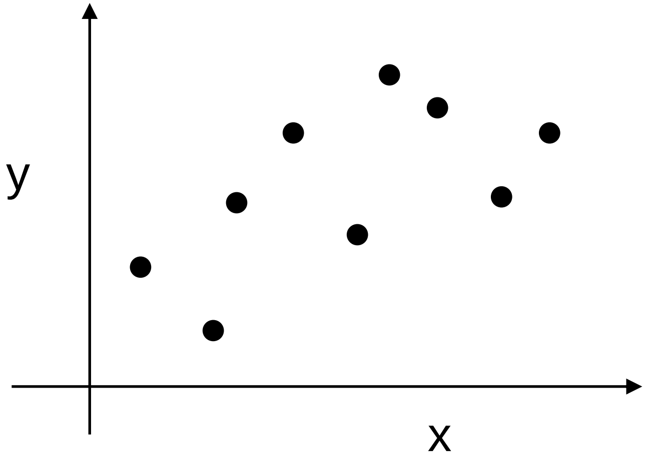


A fundamental part of statistics is quantifying our confidence that our estimates are reflective of truth.

*Q: How to **estimate** coefficients for a linear model?*

A: By finding the line that minimizes the sum of squared residuals.



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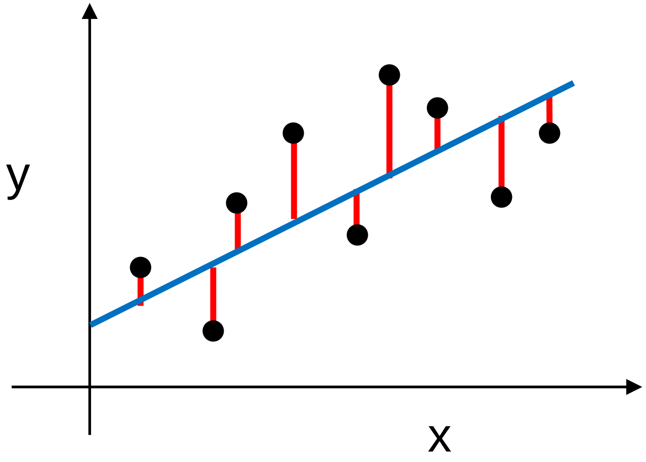

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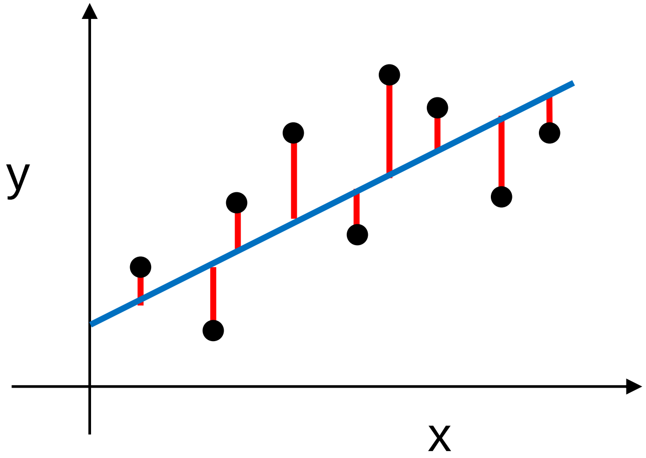

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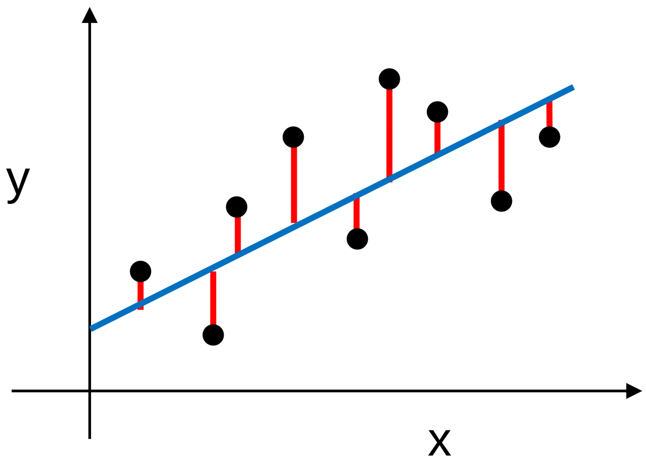

Model Prediction

$$SS_{residuals} = \sum_{i=1}^{N} (\hat{y}_i - y_i)^2$$

Observed Result

Q: How to calculate estimates that minimize the sum of squared errors?

A: Through calculus, it can be shown that the following equation minimizes the sum of squared errors.

$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

Let's walk through an trivial calculation to see how this works.

$$X = \begin{pmatrix} 1, & 3.385 \\ 1, & 0.48 \\ 1, & 1.35 \\ 1, & 465 \\ 1, & 36.33 \end{pmatrix} \qquad Y = \begin{pmatrix} 44.5 \\ 15.5 \\ 8.1 \\ 423 \\ 119.5 \end{pmatrix}$$

Along the way, we'll review some matrix math.

$$\hat{\beta} = \boxed{(X^T X)}^{-1} X^T Y$$

Transposing simply means flipping the columns and rows

$$X^T X = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 3.385 & 0.48 & 1.35 & 465 & 36.33 \end{pmatrix} \begin{pmatrix} 1, & 3.385 \\ 1, & 0.48 \\ 1, & 1.35 \\ 1, & 465 \\ 1, & 36.33 \end{pmatrix} = \begin{pmatrix} 5 & 506.54 \\ 506.54 & 217558.38 \end{pmatrix}$$

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$$\hat{\beta} = \boxed{(X^T X)^{-1}} X^T Y$$

Only square matrices can be inverted

$$(XX^T)^{-1} = \begin{pmatrix} 5 & 506.54 \\ 506.54 & 217558.38 \end{pmatrix}^{-1} = \begin{pmatrix} \boxed{0.26} & -6.1 \cdot 10^{-4} \\ -6.1 \cdot 10^{-4} & 6.0 \cdot 10^{-6} \end{pmatrix}$$

Taking the inverse of a 2x2 matrix simply means swapping across diagonals, and dividing each value by the determinant.

$$\frac{217558.38}{5 \times 217558.38 - 506.54 \times 506.54}$$

$$\hat{\beta} = (X^T X)^{-1} \boxed{X^T Y}$$

$$X^T Y = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 3.385 & 0.48 & 1.35 & 465 & 36.33 \end{pmatrix} \begin{pmatrix} 44.5 \\ 15.5 \\ 8.1 \\ 423 \\ 119.5 \end{pmatrix} = \begin{pmatrix} 610.6 \\ 201205.4 \end{pmatrix}$$

$$\hat{\beta} = \boxed{(X^T X)^{-1} X^T Y}$$

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II. INTERPRETING THE OUTPUT

There are many important features to understand of a linear regression output. For our purposes, we will discuss the following:

1) *Coefficient estimate significance using p-value*
2) *Confidence Intervals*
3) *Fit assessment using R^2*

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Q: What is a p-value?

A: The probability of getting the observed outcome (e.g., the coefficient estimate) if the null hypothesis were true ($p < 0.05$ is typically considered significant).

Q: What is the null hypothesis for linear regression coefficients?

A: There is no relationship between X and Y.

$$H_0: \beta_j = 0$$

$$H_a: \beta_j \neq 0$$

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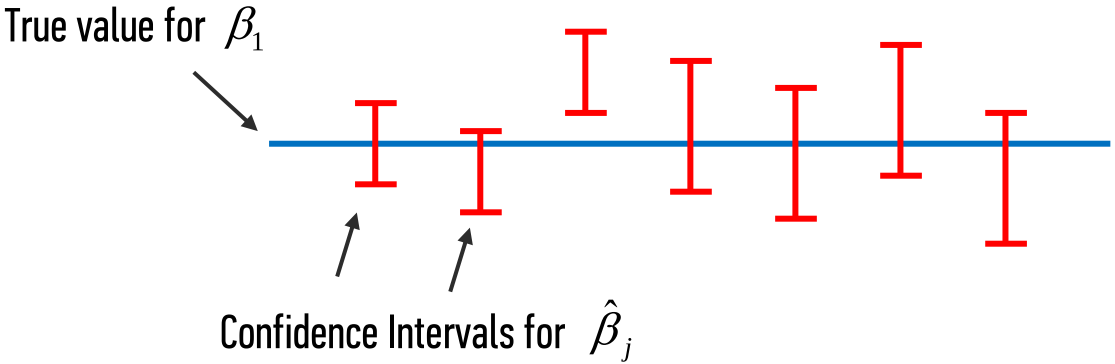
Q: What does the confidence interval mean?

A: 95% of the time, the true coefficients will be in this range.



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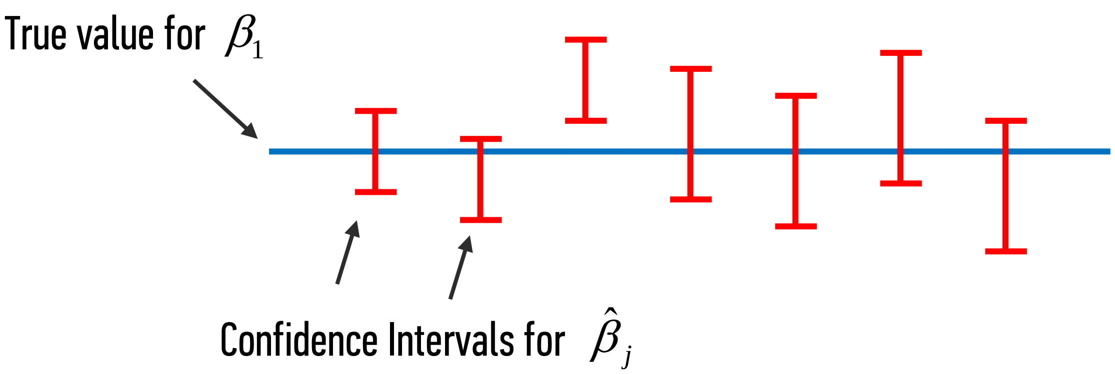

Confidence intervals are calculated based off of the error variance

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Q: How to determine model fit?

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Q: What is the R^2 value?

A: The proportion of explained variance, ranges from 0 to 1.

Q: How is the R^2 value calculated?

$$R^2 = \frac{SS_{regression}}{SS_{total}} = \frac{\sum_{i=1}^{N} (\hat{y}_i - \bar{y})^2}{\sum_{i=1}^{N} (y_i - \bar{y})^2}$$

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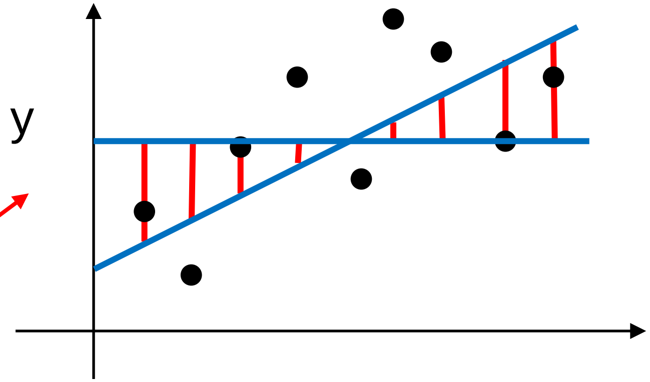

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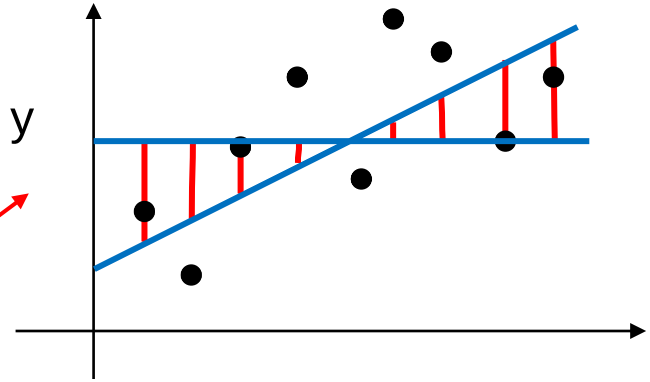

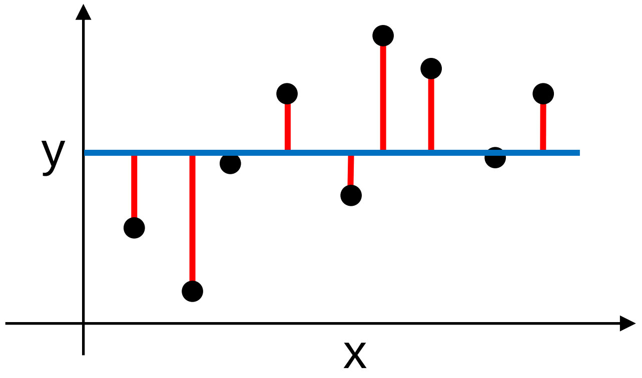

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However, it provides a benchmark to evaluate different models against one another. We will devote an entire class to model evaluation next week.

One additional caveat: *The R^2 should be taken with a grain of salt, since adding more variables will always increase the R^2, however, this does not mean we are necessarily improving our model.*

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In reality, the Adjusted R^2, which takes into account the model complexity, is a better measure of performance.

$$Adjusted\ \ R^2 = 1 - (1 - R^2)\frac{n-1}{n-p-1}$$

$p = Input\ Variables \quad n = Samples$

As p increases:

- Denominator decreases
- Fraction increases
- Adjusted R^2 decreases

III. COMMON PROBLEMS

Linear modeling is a parametric technique, meaning that it relies on specific assumptions about the underlying data:

1) *Linearity and additivity of the relationship between input and response variables*
2) *Homoscedasticity of the errors*
3) *Normality of the Error Distribution*
4) *Statistical independence of the errors*

Source: http://people.duke.edu/~rnau/testing.htm

This section defines two common problems that arise when these assumptions are not met, along with how to identify and remediate them.

1) *Multicollinearity*
2) *Heteroskedasticity*

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1) ***Multicollinearity***
2) *Heteroskedasticity*

Q: What is multicollinearity?

A: Multicollinearity (also called collinearity) exists whenever there is a correlation between 2 or more dependent variables.

Q: How does multicollinearity affect my model?

A: Generally, Linear Regression relies on the assumption that each input variable is independent of the other.

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- *This means that you can vary each input variable independently and still get accurate predictions.*
- ***When this assumption is not met, it reduces confidence in your coefficient estimates.***

Q: How do I identify whether multicollinearity is present in my data?

A: This can be difficult, however, a scatter matrix, or correlation coefficient matrix can help.

Q: How is the correlation coefficient matrix calculated?

A: Most popular method is the Pearson product-moment coefficient (a.k.a., correlation coefficient).

Covariance of x and y

$$r = \frac{Cov(x, y)}{s_y s_x}$$

Sample standard deviation

Q: How is the correlation coefficient matrix calculated?

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Observed x Average x

$$r = \frac{Cov(x, y)}{s_y s_x} = \frac{\sum_{i=1}^{N}(x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum_{i=1}^{N}(x_i - \overline{x})}\sqrt{\sum_{i=1}^{N}(y_i - \overline{y})}}$$

Q: How can I deal with multicollinearity?

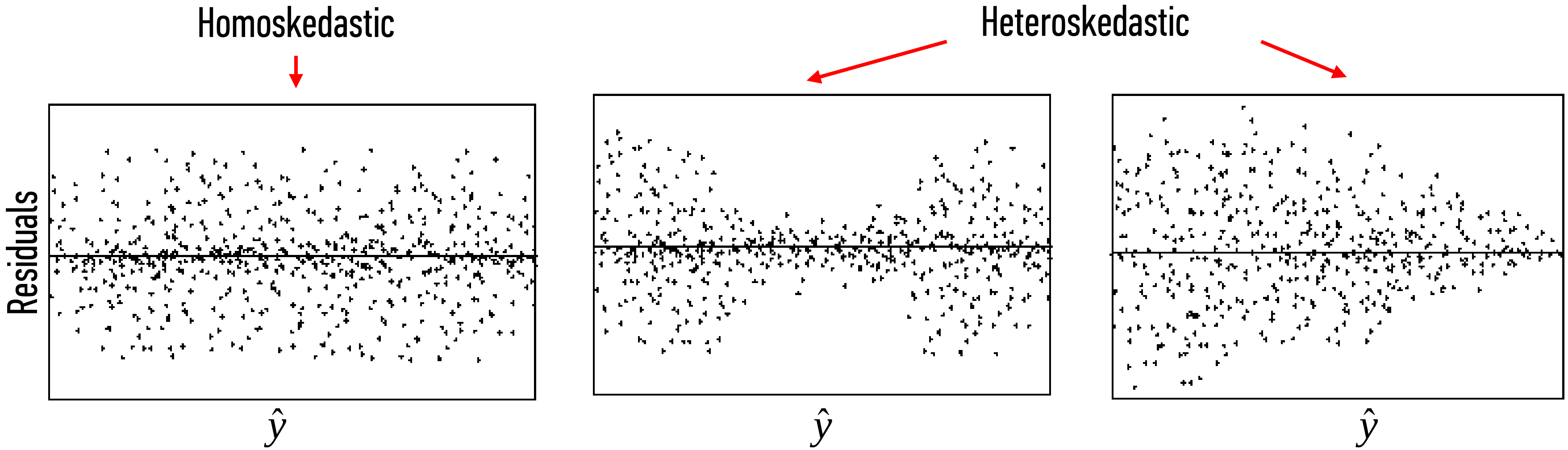
A: These variables can be removed, or included in the model as an interaction term.

This section defines two common problems that arise when these assumptions are not met, along with how to identify and remediate them.

1) *Multicollinearity*
2) ***Heteroskedasticity***

Q: What is heteroskedasticity?

A: Heteroskedasticity means non-constant variance in the residuals (literally: hetero=different, skedasis=dispersion).

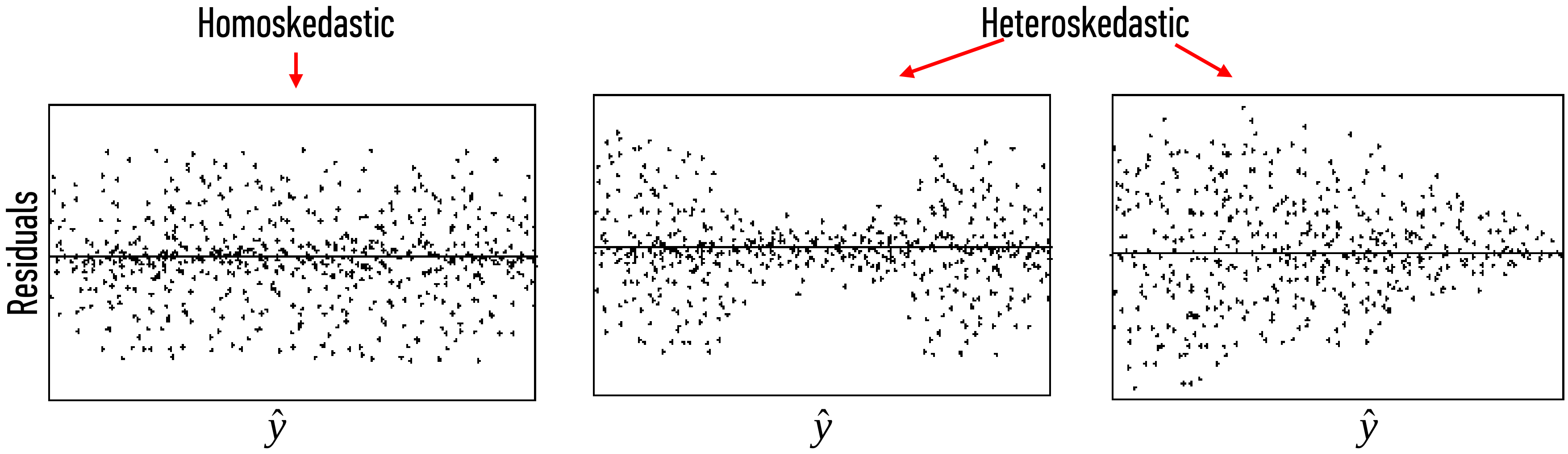


Q: How does heteroskedasticity affect my model?
A: It will distort and therefore decrease confidence in coefficient and prediction estimates.

Q: Why does heteroskedasticity reduce confidence in the model?
A: Because standard errors, confidence intervals, and hypothesis tests all rely on constant error variance.

Q: How to identify heteroskedasticity?

A: Plot the residuals against the predicted response variable (also input variables and time).



Q: How to deal with heteroskedasticity?

Option #1: Conduct log transformation of the response variable.

Coefficients now correspond to percentage change in response variable, rather than unit change.

Q: How to deal with heteroskedasticity?

Option #2: Use Weighted Least Squares.

The weights themselves are an input to the model. This typically means observations with greater deviation contribute less to estimates associated with the coefficients.

IV. CATEGORICAL VARIABLES

Q: How do we deal with categorical variables? (i.e., with k levels)

Major (k=4)
Computer Science
Engineering
Business
Literature
Business
Engineering

Q: How do we deal with categorical variables? (i.e., with k levels)

A: Create a k-1 binary ("dummy") variables.

Major (k=4)
Computer Science
Engineering
Business
Literature
Business
Engineering

Engineering	Business	Literature
0	0	0
1	0	0
0	1	0
0	0	1
0	1	0
1	0	0

Computer Science is the reference

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Q: Does it matter which factor level I leave out?
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Q: Is this a limitation?
A: Not really, a comparison must have a baseline.

Q: Is this the only way to represent categorical data?
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Q: What does this mean?
A: Categories that can be ranked (i.e., strongly disagree, disagree, neutral, agree, strongly agree) can be represented as 1, 2, 3, 4, 5.