

DATA SCIENCE

CLASS 6: LINEAR REGRESSION

- 0. BASIC FORM**
- I. COEFFICIENTS**
- II. INTERPRETATION**
- III. COMMON PROBLEMS**
- IV. CATEGORICAL VARIABLES**

LINEAR REGRESSION

0. BASIC FORM

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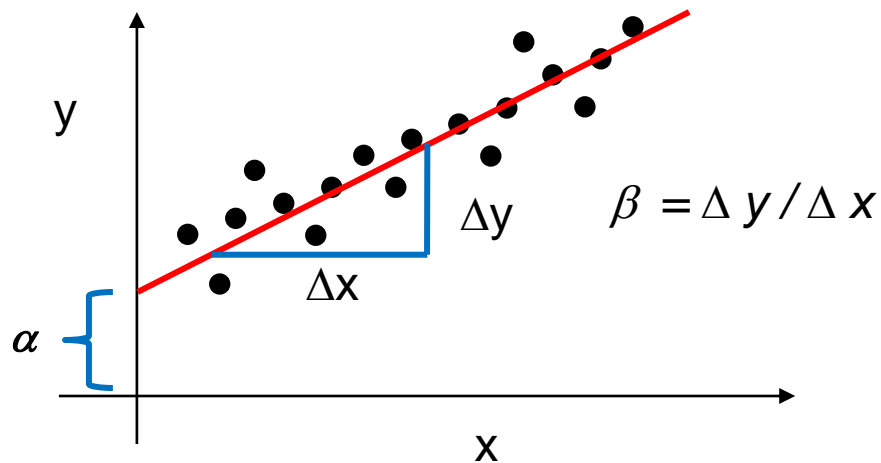
*α = **intercept** (where the line crosses the y-axis)*

*β = **regression coefficient** (the model parameter)*

*ε = **residual** (the error)*

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

LINEAR REGRESSION

I. ESTIMATING COEFFICIENTS

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

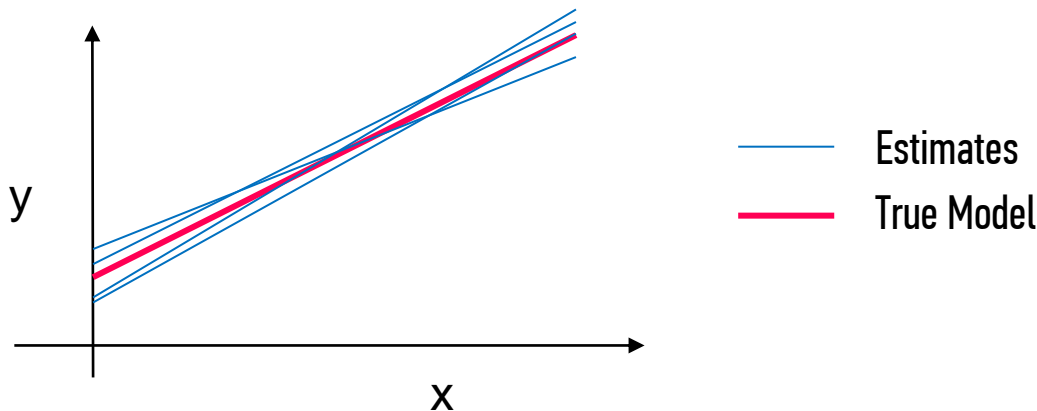
A: The coefficient estimates ($\hat{\beta}$)

Q: What is meant by estimates?

A: We are making an inference based off of a sample.

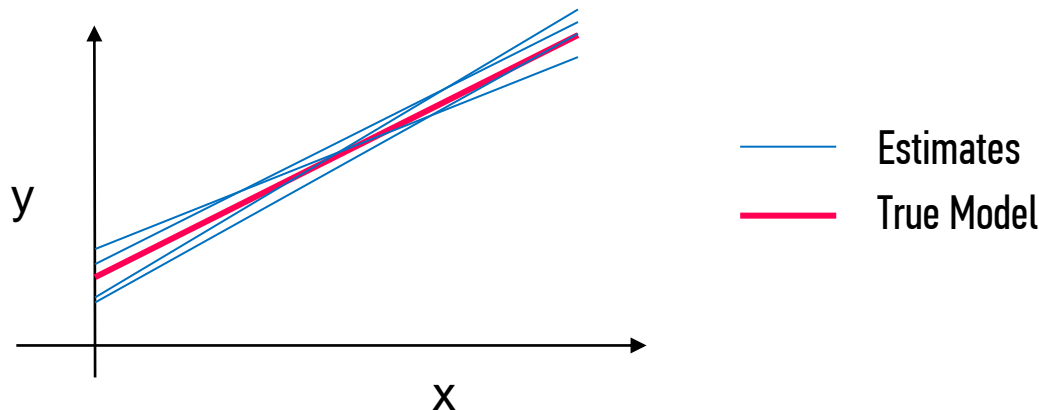
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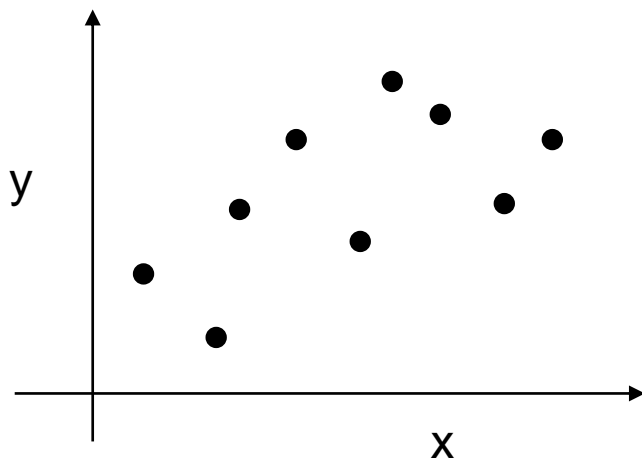
A: We are making an inference based off of a sample.



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

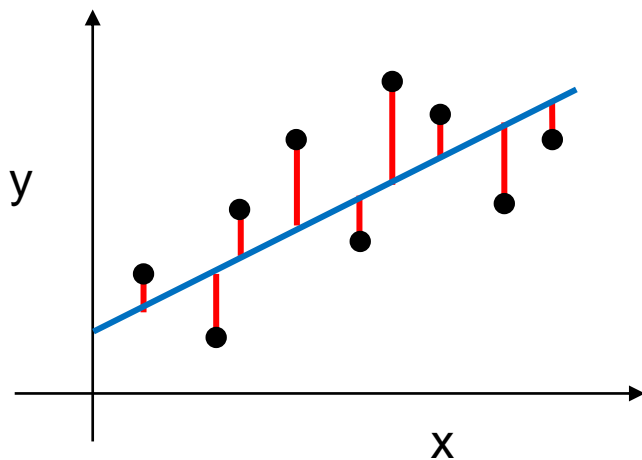
*Q: How to **estimate** coefficients for a linear model?*

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



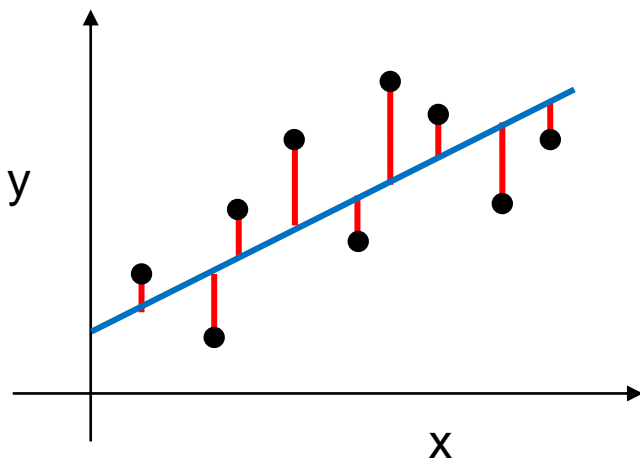
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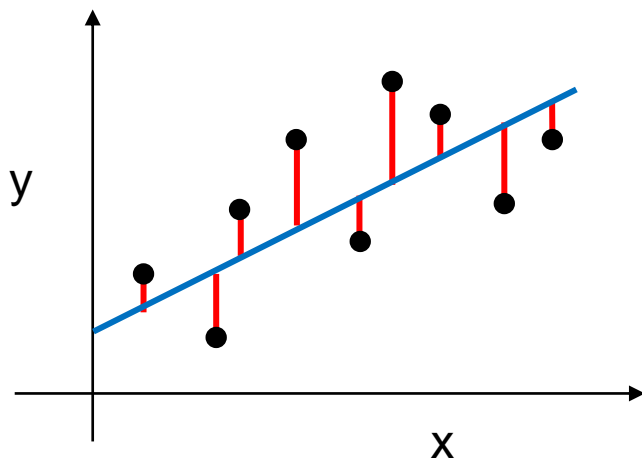
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Model Prediction

Observed Result

The diagram shows the formula for the sum of squared residuals. A red arrow points from the text 'Model Prediction' to the predicted value \hat{y}_i in the formula. Another red arrow points from the text 'Observed Result' to the observed value y_i in the formula.

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.

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

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

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

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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Only square
matrices can be
inverted

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

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

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

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

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

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

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LINEAR REGRESSION

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 .

$$H_0: \beta_j = 0$$

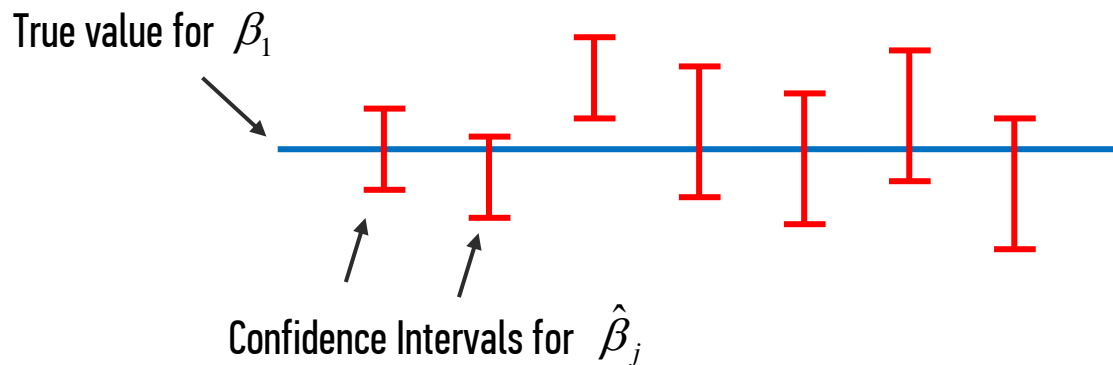
$$H_a: \beta_j \neq 0$$

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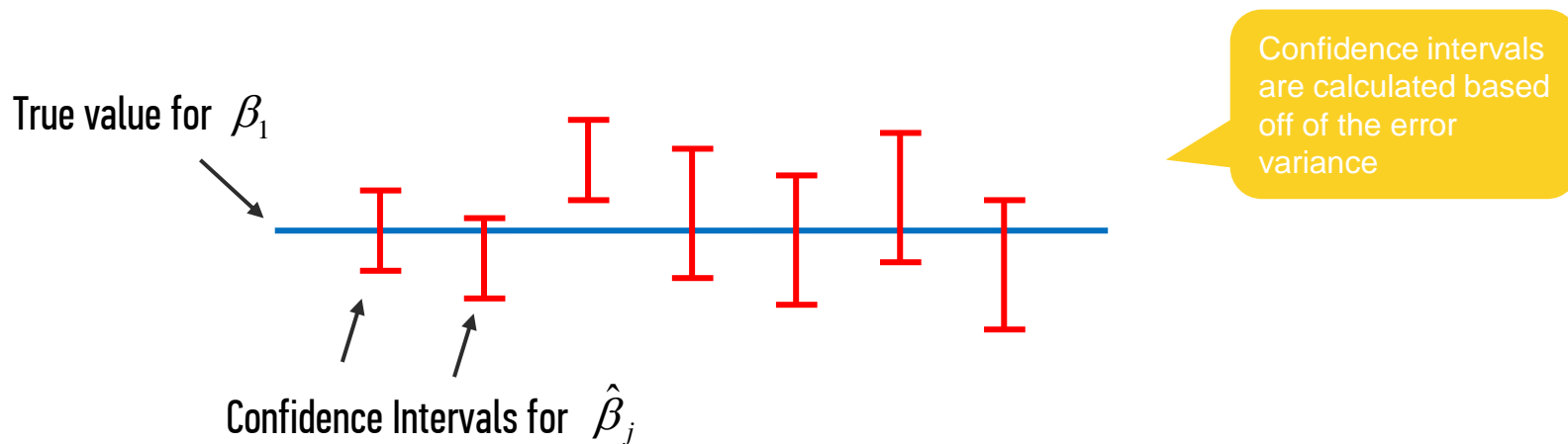
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Q: How to determine model fit?

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Q: What is the R^2 value?

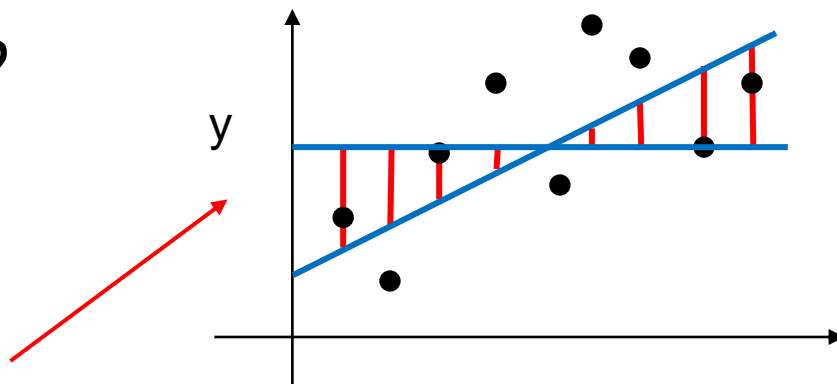
A: The proportion of explained variance, ranges from 0 to 1.

Q: How is the R^2 value calculated?

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

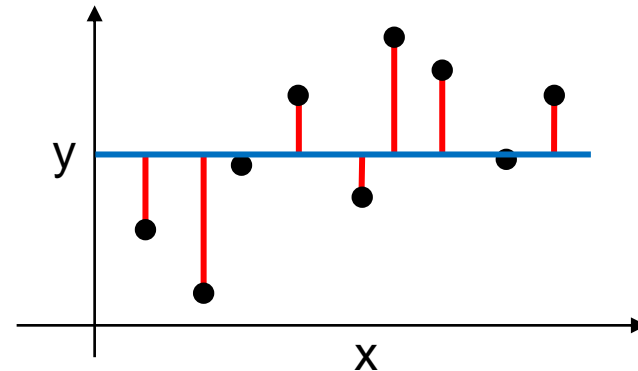
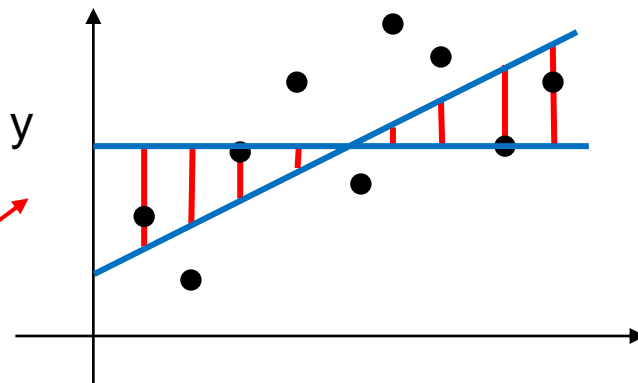
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However, it provides a benchmark to evaluate different models against one another. We will devote an entire class to model evaluation next week.

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.

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

$p = \text{Input Variables}$ $n = \text{Samples}$

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 underlying data:

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

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.*

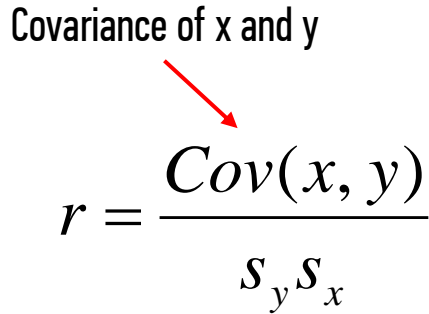
Q: How do I identify whether multicollinearity is present in my data?

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?

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

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

Observed x Average x



Q: How can I deal with multicollinearity?

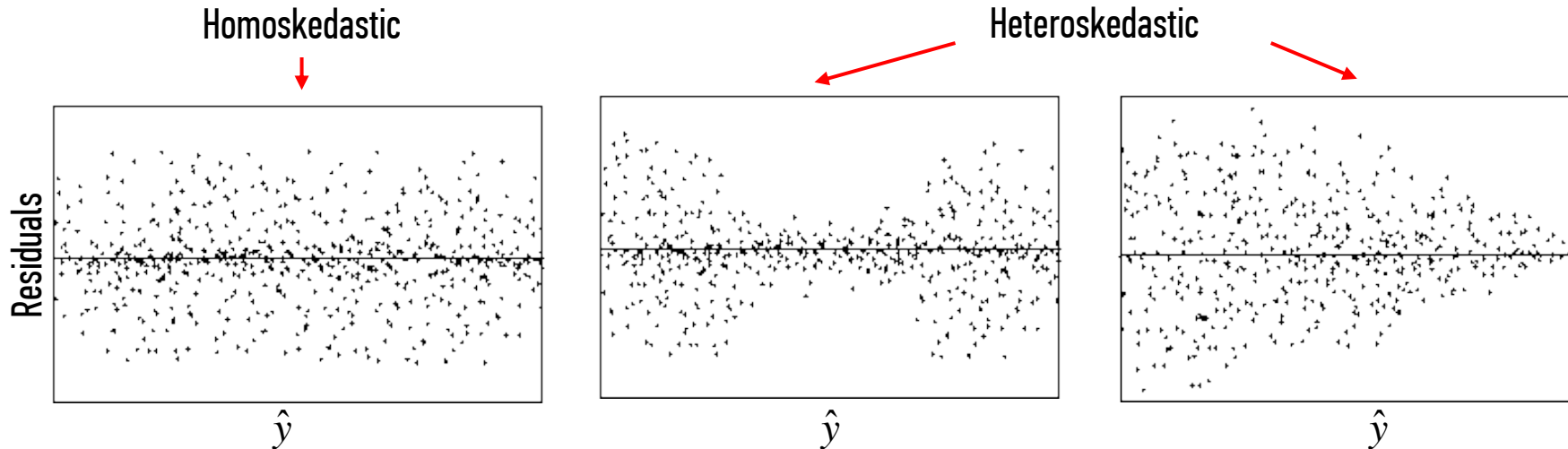
A: These variables can be removed, or included in the model as an interaction term.

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?

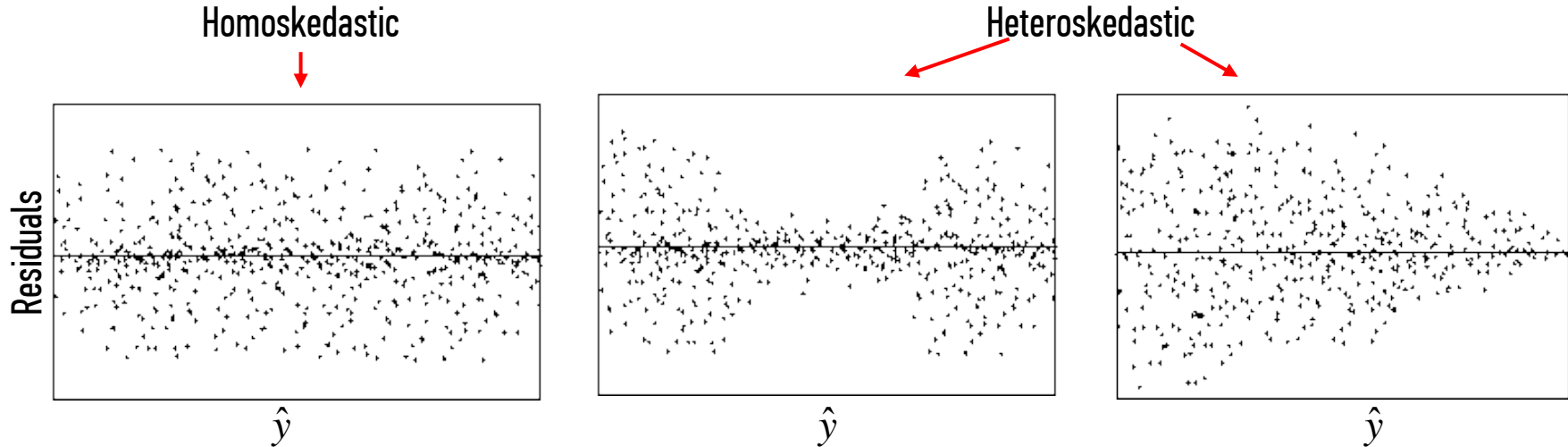
A: It will distort and therefore decrease confidence in coefficient and prediction estimates.

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)		Engineering	Business	Literature
Computer Science	→	0	0	0
Engineering		1	0	0
Business		0	1	0
Literature	→	0	0	1
Business		0	1	0
Engineering		1	0	0

Computer Science is the reference

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Q: Is this the only way to represent categorical data?

A: This is the conventional way to represent nominal data, however, ordinal data can be represented with integers.

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.

What we covered:

- *Basic Form*
- *Estimating Coefficients*
- *Interpreting Coefficient Significance*
- *Confidence Intervals*
- *R^2 and Adjusted R^2*
- *Heteroskedasticity*
- *Multicollinearity*
- *Categorical Variables*

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What did we not cover:

- *The F and t Distributions*
- *Deriving the line that minimizes the squared error*
- *Statistical independence of errors*
- *Normality of error distribution*
- *Log-Log / Lin-Log interpretation*
- *Polynomial Regression*
- *Stepwise Regression*
- *Regularization*