

# Linear Regression Models

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#### **Learning Objectives**

- 1. Describe the Linear Regression Model
- 2. State the Regression Modeling Steps
- 3. Explain Ordinary Least Squares
- 4. Compute Regression Coefficients
- 5. Understand and check model assumptions
- 6. Predict Response Variable

#### Learning Objectives...

- 7. Correlation Models
- 8. Link between a correlation model and a regression model
- 9. Test of coefficient of Correlation

#### What is a Model?

- 1. Representation of Some Phenomenon
- 2. Non-Maths/Stats Model





#### What is a Maths/Stats Model?

- 1. Often Describe Relationship between Variables
- 2. Types
  - Deterministic Models (no randomness)
  - Probabilistic Models (with randomness)

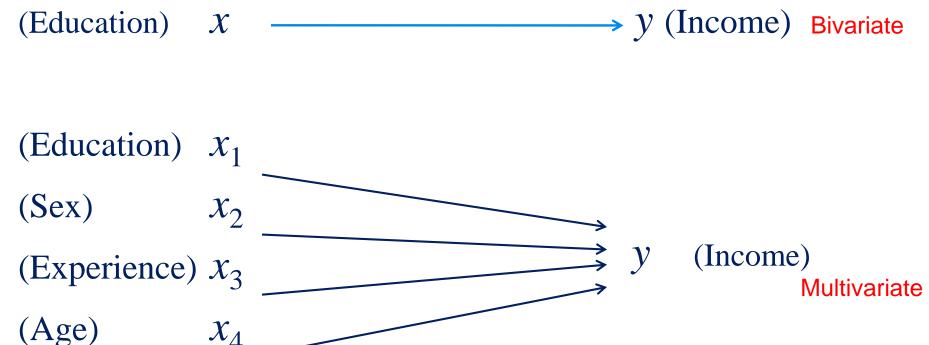
#### **Deterministic Models**

- 1. Hypothesize Exact Relationships
- 2. Suitable When Prediction Error is Negligible
- 3. Example: Body mass index (BMI) is measure of body fat based.
  - Metric Formula:  $BMI = \frac{Weight \ in \ Kilograms}{(Height \ in \ Meters)2}$
  - Non-metric Formula:  $BMI = \frac{Weight (pounds) \times 703}{(Height in inches)2}$

#### **Probabilistic Models**

#### 1. Hypothesize 2 Components

- Deterministic
- Random Error
- Example: Systolic blood pressure of newborns is 6Times the Age in days + Random Error
  - $SBP = 6 \times age(d) + \varepsilon$
  - Random Error may be due to factors other than age in days (e.g. Birth weight)



Model with simultaneous relationship

Price of wheat Quantity of wheat produced

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#### Regression Modeling Steps

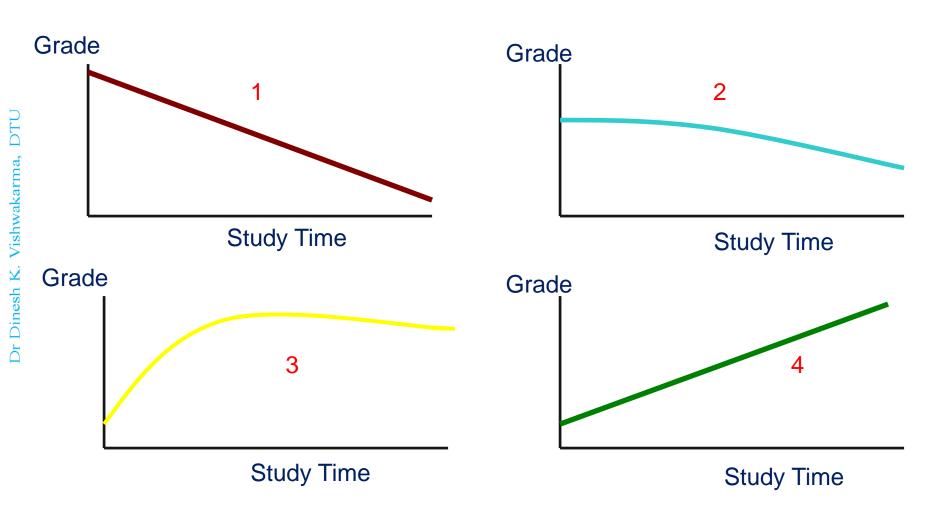
- > 1. Hypothesize Deterministic Component
  - Estimate Unknown Parameters
- Specify Probability Distribution of Random Error Term
  - Estimate Standard Deviation of Error
- > 3. Evaluate the fitted Model
- > 4. Use Model for Prediction & Estimation

#### **Models Facts**

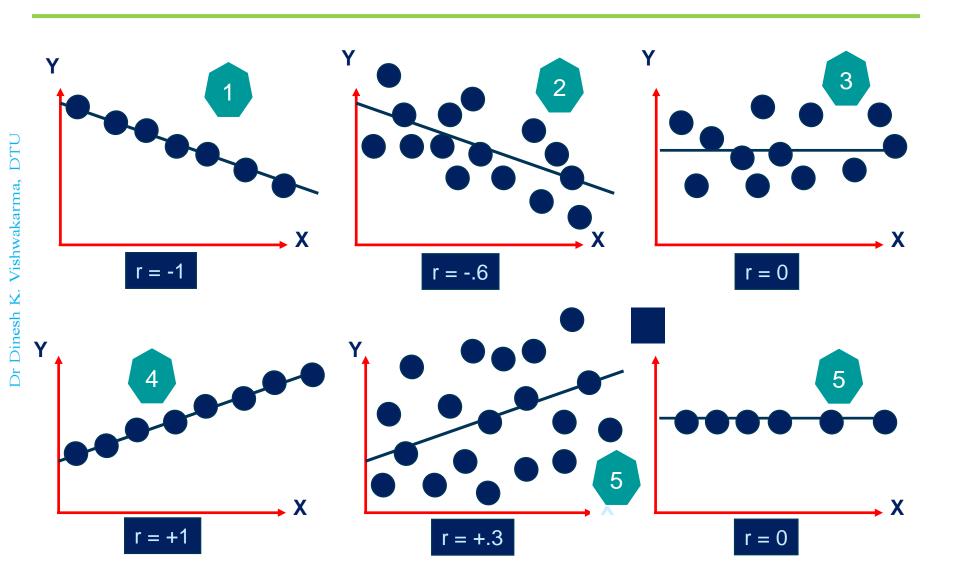
- ➤ 1. Theory of Field (e.g., Epidemiology)
- ➤ 2. Mathematical Theory
- > 3. Previous Research
- > 4. 'Common Sense'



## Thinking Challenge: Which is more logical?

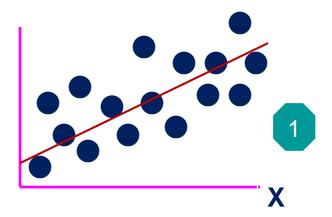


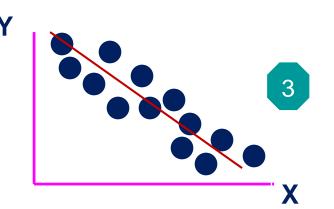
#### **Scatter Plot of Data**



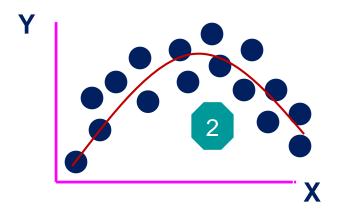
#### **Types of Relationship**

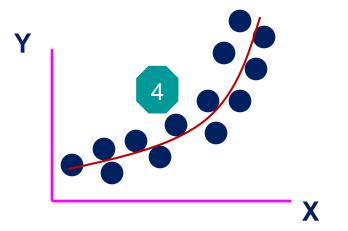
#### **Linear relationships**



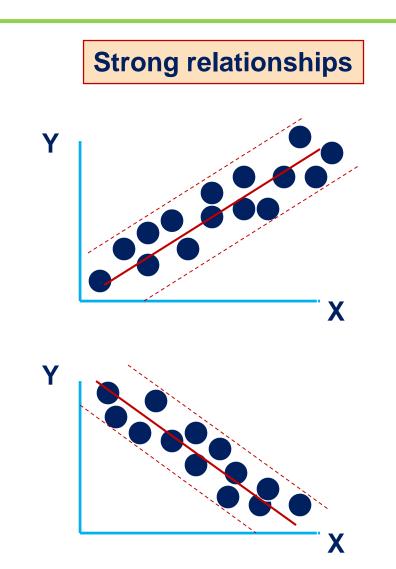


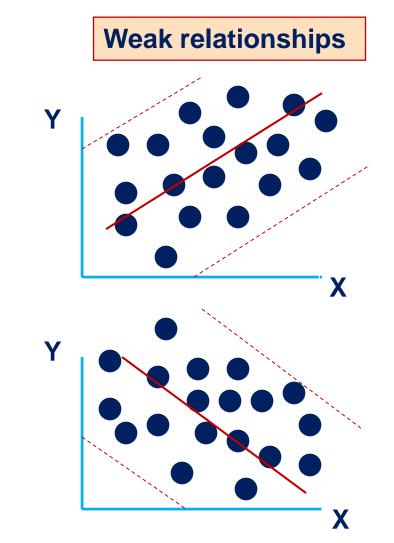
#### **Curvilinear relationships**



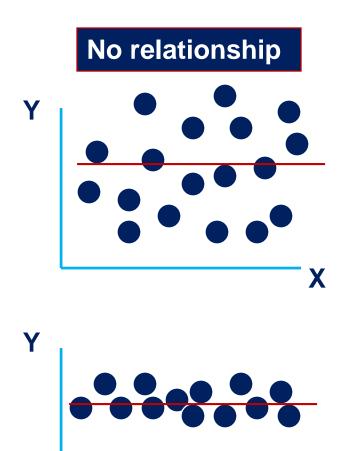


## Types of Relationship...





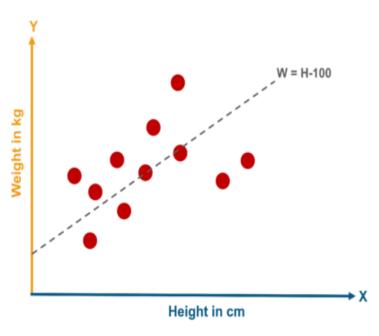
#### Types of Relationship...



X

#### **Linear Regression Models**

- A linear regression is one of the easiest statistical models in machine learning.
- It is used to show the linear relationship between a dependent variable and one or more independent variables.
- Relationship between one dependent variable(y) and explanatory variable (s).
- Regression analysis is a form of predictive modelling technique which investigates the relationship between a dependent and independent variable



## **Types of Regression**

> Types of	Basis	Linear Regression	Logistic Regression
<ul><li>Regression</li><li>Linear Regression</li></ul>	Core Concept	The data is modelled using a straight line	The data is modelled using a sigmoid
Logistic Regression	Used with	Continuous Variable	Categorical Variable
Polynomial	Output/Prediction	Value of the variable	Probability of occurrence of an event
Regression			Measured by
> Stepwise Regression	Accuracy and Goodness of Fit	Measured by loss, R squared, Adjusted R squared etc.	Accuracy, Precision, Recall, F1 score, ROC curve, Confusion

Matrix, etc

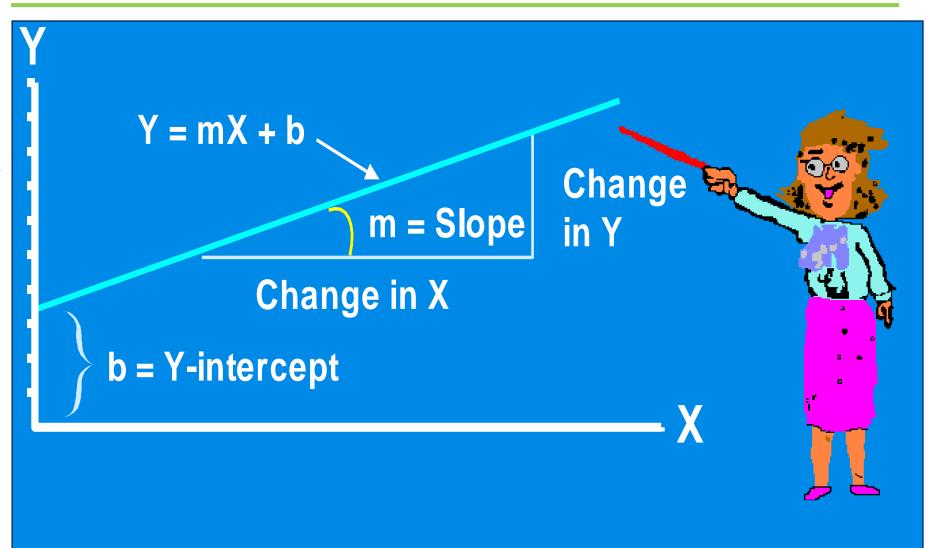
#### **Applications of LR**

- > Evaluating Trends and Sales Estimates
  - A company sales analysis (monthly sales vs time)
- > Analyzing the Impact of Price Changes
  - If company changes the price of a product several times
- > Assessing Risk E.g. health care
  - Number claims vs age

#### **Benefits of LR Model**

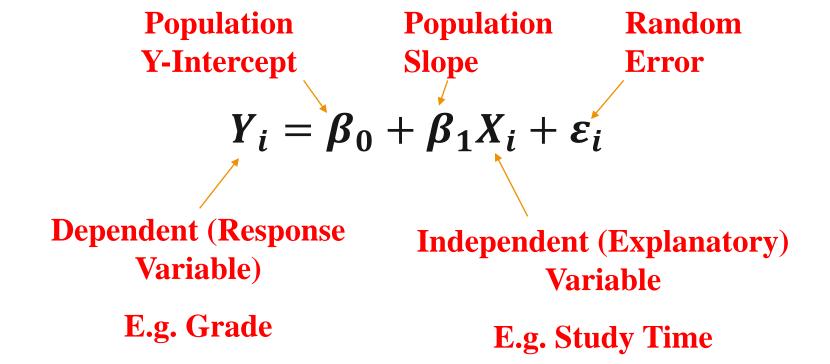
- > Ease
- > Interpretability
- > Scalability
- > Deploys and Performs well on Online Settings

## **Linear Equations**



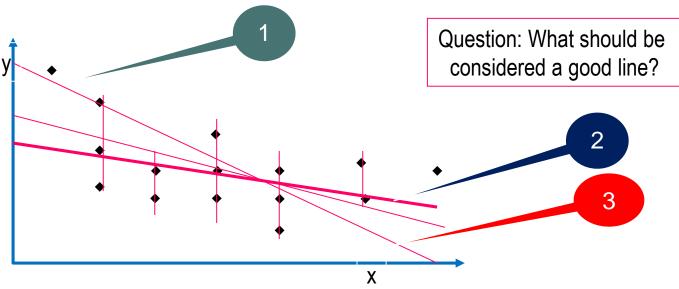
## **Linear Regression Model**

Relationship Between Variables is a Linear Function

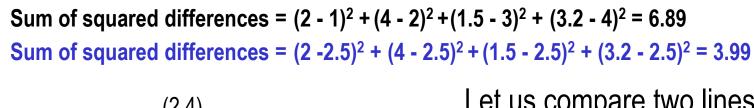


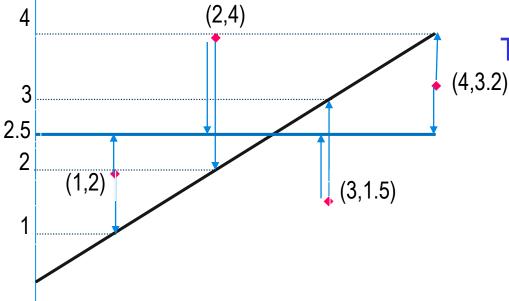
#### **Estimating the Coefficients**

- > The estimates are determined by
  - drawing a sample from the population of interest,
  - calculating sample statistics.
  - producing a straight line that cuts into the data.



#### **Sum Squared Difference**





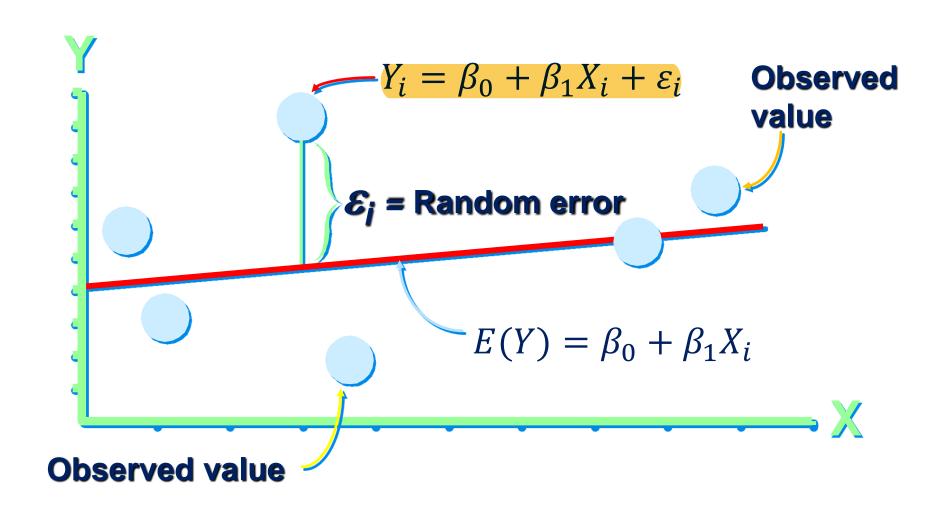
Let us compare two lines
The second line is horizontal

The smaller the sum of squared differences the better the fit of the line to the data.

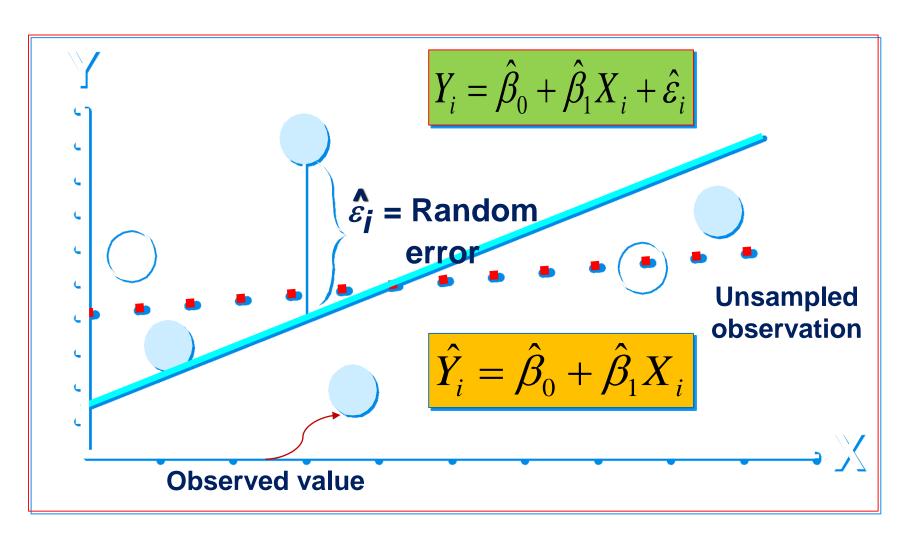
A good line is one that minimizes the sum of squared differences between the points and the line.

3

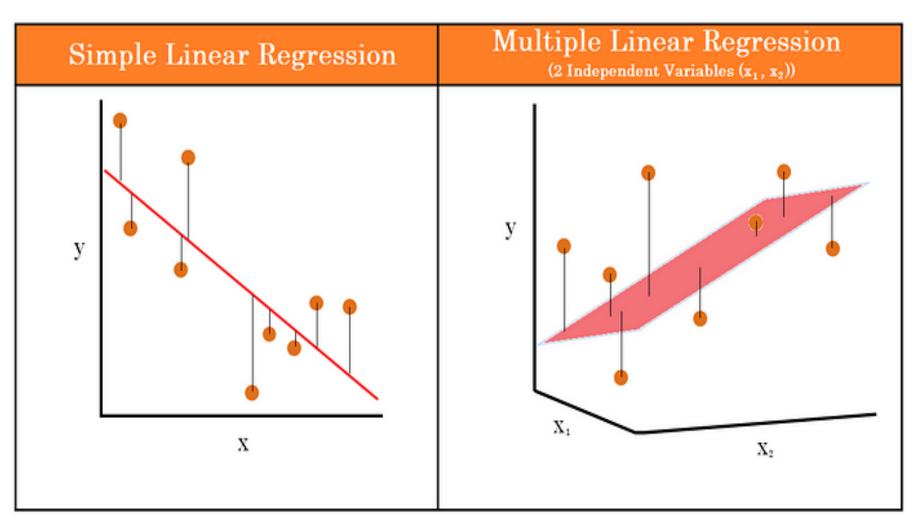
## Population Linear Regression Model



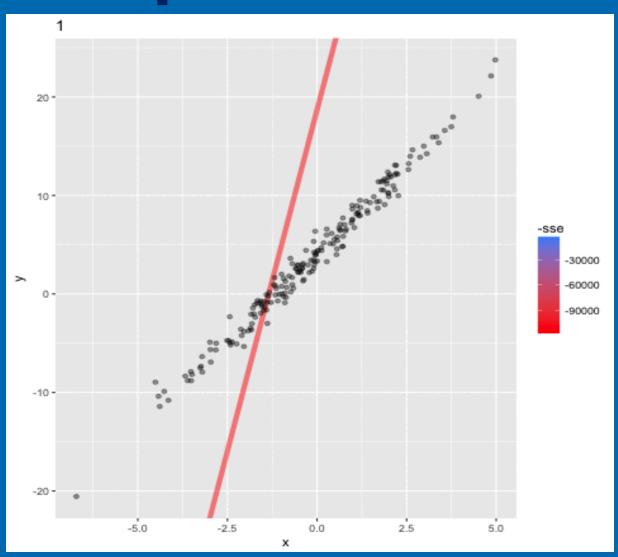
## Simple Linear Regression Model



## Simple LR Model vs Multiple LR

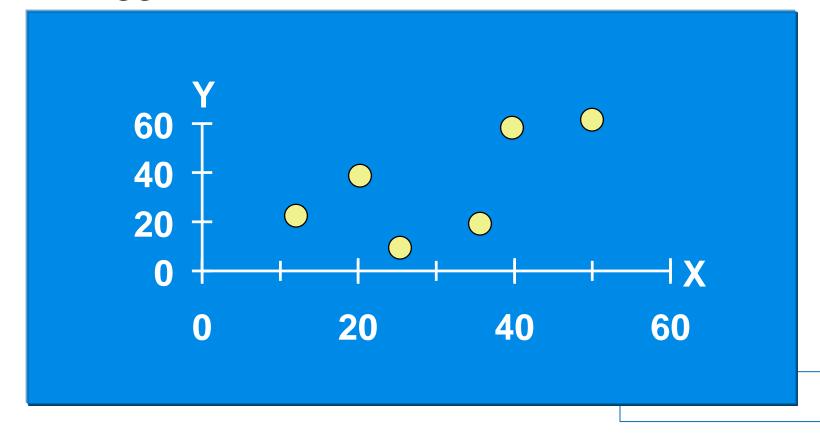


## Estimating Parameters: Least Squares Method



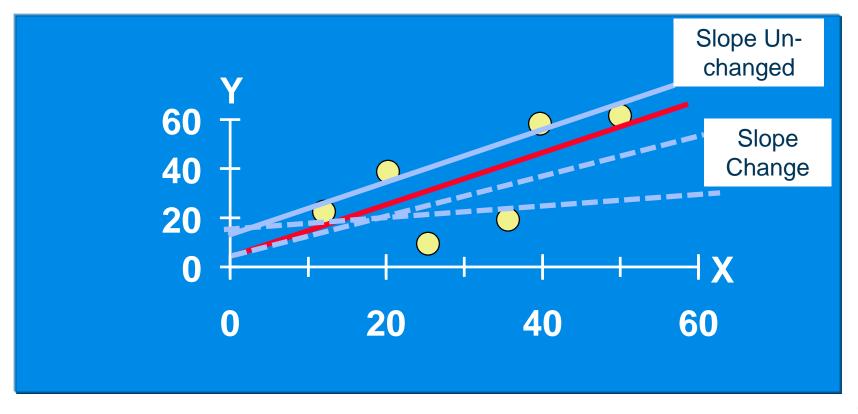
## Scatter plot

- $\triangleright$  1. Plot of All  $(X_i, Y_i)$  Pairs
- ➤ 2. Suggests How Well Model Will Fit



## **Thinking Challenge**

How would you draw a line through the points? How do you determine which line 'fits best'?



## Least Squares Error

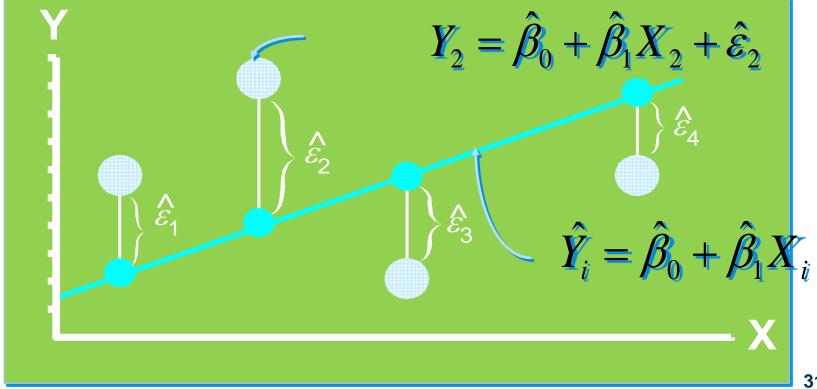
- Best Fit' Means Difference Between Actual Y Values & Predicted  $\widehat{Y}$  Values are a Minimum. But Positive Differences Off-Set Negative ones
- > So square errors!

$$\sum_{i=1}^{n} (Y_i - \widehat{Y}_i)^2 = \sum_{i=1}^{n} \widehat{\varepsilon}_i^2$$

LS Minimizes the Sum of the Squared Differences (errors) (SSE)

#### **Least Squares Graphically**

LS Minimizes 
$$\sum_{i=1}^{n} \hat{\varepsilon}_{i}^{2} = \hat{\varepsilon}_{1}^{2} + \hat{\varepsilon}_{2}^{2} + \hat{\varepsilon}_{3}^{2} \dots \dots + \hat{\varepsilon}_{n}^{2}$$



## **Coefficient Equations**

#### Prediction equation

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

Sample slope

$$\hat{\beta}_1 = \frac{SS_{xy}}{SS_{xx}} = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2}$$

Sample Y - intercept

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

## Finding $\beta_0$ MSE Method

$$\sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} (y_i - \beta_0 + \beta_1 \cdot x_i)^2$$

$$> 0 = \frac{\partial \sum_{i=1}^{n} (y_i - \beta_0 + \beta_1 \cdot x_i)^2}{\partial \beta_0}$$

$$\geq \frac{\partial \sum_{i=1}^{n} y_i^2 + \beta_0^2 + \beta_1^2 \cdot x_i^2 + 2\beta_0 \beta_1 \cdot x_i - 2y_i \cdot \beta_0 - 2y_i \beta_1 \cdot x_i}{\partial \beta_0} = 0$$

$$\frac{\partial \beta_0}{\partial x_i} > 0 = 2 \sum_{i=1}^n \beta_0 + 2\beta_1 \sum_{i=1}^n x_i - 2 \sum_{i=1}^n y_i$$

$$> 0 = 2(n\beta_0 + n\beta_1 \bar{x} - n\bar{y})$$

$$> \widehat{\boldsymbol{\beta}}_0 = \overline{\mathbf{y}} - \widehat{\boldsymbol{\beta}}_1 \overline{\mathbf{x}}$$

Minimum Sum Square Error Method

#### Finding $\beta_1$ MSE Method

- $\sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} (y_i \hat{y}_i)^2 = y_i^2 + \hat{y}_i^2 2y_i \cdot \hat{y}_i$  Where  $\hat{y}_i = \beta_0 + \beta_1 \cdot x_i$
- $\sum_{i=1}^{n} y_i^2 + (\beta_0 + \beta_1 \cdot x_i)^2 2y_i \cdot (\beta_0 + \beta_1 \cdot x_i)^2$ 
  - $\rightarrow$

$$\sum_{i=1}^{n} y_i^2 + \beta_0^2 + \beta_1^2 \cdot x_i^2 + 2\beta_0 \beta_1 \cdot x_i - 2y_i \cdot \beta_0 - 2y_i \beta_1 \cdot x_i$$

> Finding minimum error, the derivative must be zero:

#### **Optimization**

$$\frac{\partial (\sum_{i=1}^{n} \varepsilon_i^2)}{\partial \beta_1} = \frac{\partial \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 \cdot x_i)^2)}{\partial \beta_1} = 0$$

$$\triangleright 0 = -2\sum_{i=1}^{n} x_i (y_i - \beta_0 - \beta_1 x_i)$$

$$\rightarrow 0=-2\sum_{i=1}^n x_i(y_i-\bar{y}+\beta_1\bar{x}-\beta_1x_i)$$
 substituting the value of  $\beta_0$ 

#### Minimum Square Error Method...

$$> 0 = -2 \sum_{i=1}^{n} x_i (y_i - \bar{y} + \beta_1 \bar{x} - \beta_1 x_i)$$

• substituting the value of  $\beta_0$ 

$$\beta_1 \sum_{i=1}^n x_i (x_i - \bar{x}) = \sum_{i=1}^n x_i (y_i - \bar{y})$$

$$\beta_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})(x_i - \bar{x})}$$

$$\beta_1 = \frac{SS_{xy}}{SS_{xx}}$$

## **Computation Table**

Xi	Yi	$X_i^2$	$Y_i^2$	$X_iY_i$
<b>X</b> <sub>1</sub>	<b>Y</b> <sub>1</sub>	$X_1^2$	Y <sub>1</sub> <sup>2</sup>	$X_1 Y_1$
<b>X</b> <sub>2</sub>	Y <sub>2</sub>	$X_2^2$	Y <sub>2</sub> <sup>2</sup>	$X_2Y_2$
:	:	:	•	:
X <sub>n</sub>	Y <sub>n</sub>	$X_n^2$	Y <sub>n</sub> <sup>2</sup>	$X_nY_n$
$\Sigma X_i$	$\sum Y_i$	$\sum X_i^2$	$\sum Y_i^2$	$\Sigma X_i Y_i$

## Interpretation of Coefficients

ightharpoonup Slope  $(\widehat{\beta_1})$ 

- $\beta_1 > 0 \implies$  Positive Association
- $\beta_1 < 0 \Rightarrow$  Negative Association
- $\beta_1 = 0 \implies \text{No Association}$
- Estimated *Y* Changes by  $\widehat{\beta_1}$  for each 1 Unit Increase in *X* 
  - If  $\widehat{\beta_1} = 2$ , then *Y* Is Expected to Increase by 2 for each 1 Unit Increase in *X*

- $\triangleright$  Y-Intercept  $(\beta_0)$ 
  - Average Value of Y When X = 0
    - If  $\beta_0 = 4$ , then Average Y is expected to be 4 When X is 0

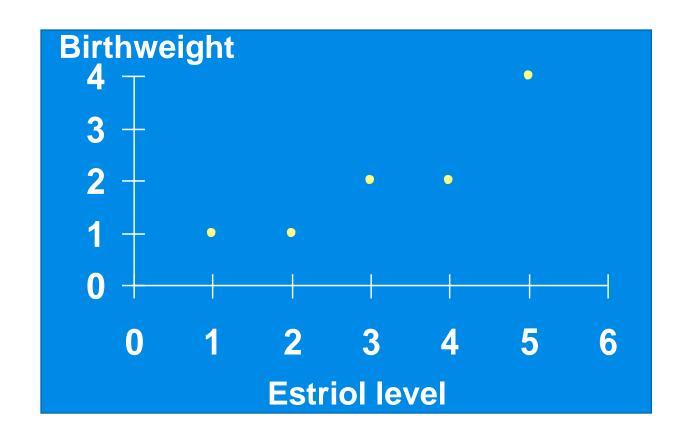
## E.g. Parameter Estimation

What is the relationship between Mother's Estriol level & Birthweight using the following data?

<b>Estriol</b>	<b>Birthweight</b>
(mg/24h)	(g/1000)
1	1
2	1
3	2
4	2
5	4



# Scatterplot Birthweight vs. Estriol level



# Parameter Estimation Solution Table

Xi	Yi	$X_i^2$	$Y_i^2$	$X_iY_i$
1	1	1	1	1
2	1	4	1	2
3	2	9	4	6
4	2	16	4	8
5	4	25	16	20
15	10	55	26	37

### Parameter Estimation Solution

$$\hat{\beta}_{1} \triangleq \frac{\sum_{i=1}^{n} X_{i} Y_{i}}{\sum_{i=1}^{n} X_{i}} = \frac{37 - \frac{(15)(10)}{5}}{5} = 0.70$$

$$\sum_{i=1}^{n} X_{i}^{2} = \frac{\sum_{i=1}^{n} X_{i}}{n}$$

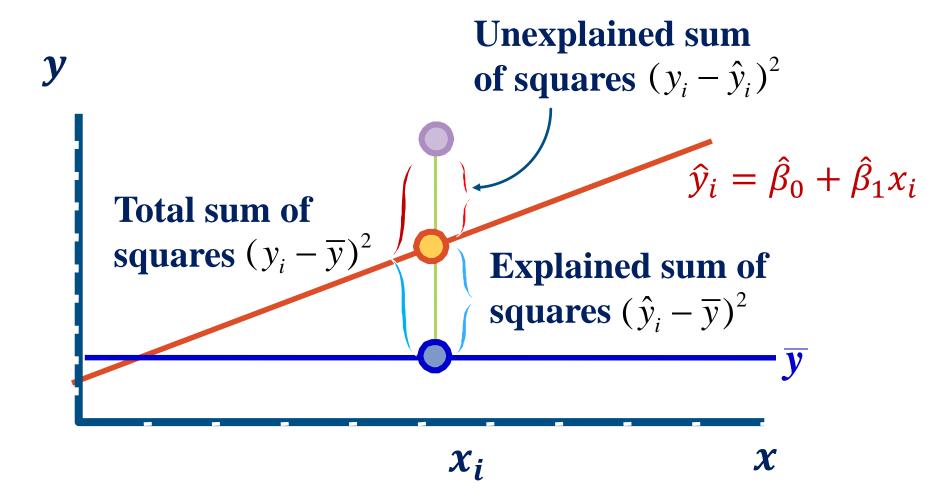
$$\hat{\beta}_0 = \overline{Y} - \hat{\beta}_1 \overline{X} = 2 - (0.7)(3) = -0.1$$
  $\hat{y} = -0.1 + 0.7x$ 

$$\hat{y} = -.1 + .7x$$

# **Coefficient Interpretation Solution**

- $\triangleright$  1. Slope  $(\beta_1)^{\alpha}$ 
  - Birthweight (*Y*) is Expected to Increase by .7 Units for Each 1 unit Increase in Estriol (*X*).
- $\triangleright$  2. Intercept  $(\beta_0)$ 
  - Average Birthweight (Y) is -.10 Units When Estriol level (X) Is 0
    - Difficult to explain
    - The birthweight should always be positive

### **Goodness: Variation Measures**



### Estimation of $\sigma^2$

$$s^{2} = \frac{SSE}{n-2} \qquad \text{Where } SSE = \sum_{i=1}^{n} (y_{i} - \hat{y}_{i})^{2}$$

$$s = \sqrt{s^2} = \sqrt{\frac{SSE}{n-2}}$$

The subtraction of 2 can be thought of as the fact that we have estimated two parameters:  $\beta_0$  and  $\beta_1$ 

## E.g. Compute SSE, s<sup>2</sup>, s

You're a marketing analyst for any Toys. You gather the following data:

<b>Ad</b> (₹)	Sales (Qty)
1	1
2	1
3	2
4	2
5	4

Find SSE,  $s^2$ , and s.



## E.g. Solution: SSE, s<sup>2</sup>, s

$x_i$	$y_i$	$\hat{y} =1 + .7x$	$y - \hat{y}$	$(y-\hat{y})^2$
1	1	.6	.4	.16
2	1	1.3	3	.09
3	2	2	0	0
4	2	2.7	7	.49
5	4	3.4	.6	.36
				<b>SSE=1.1</b>

$$s^2 = \frac{SSE}{n-2} = \frac{1.1}{5-2} = .36667$$
  $s = \sqrt{.36667} = .6055$ 

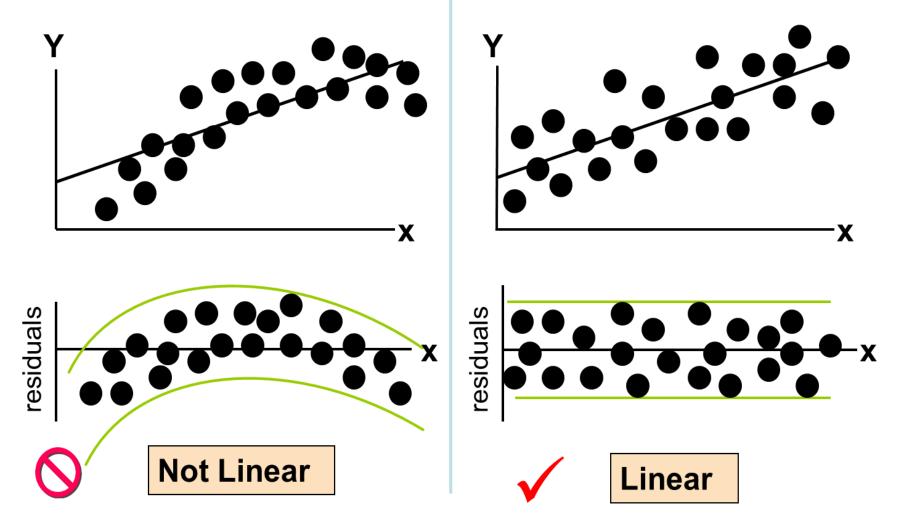
$$s = \sqrt{.36667} = .6055$$

## **Residual Analysis**

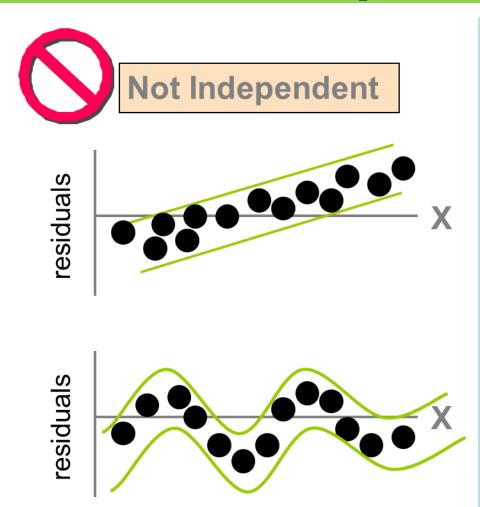
$$e_i = Y_i - \hat{Y}_i$$

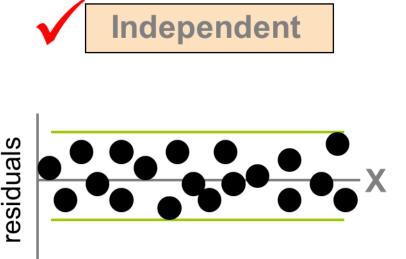
- The residual for observation i,  $e_i$ , is the difference between its observed and predicted value
- Check the assumptions of regression by examining the residuals
  - Examine for linearity assumption
  - Evaluate independence assumption
  - Evaluate normal distribution assumption
  - Examine for constant variance for all levels of X (homoscedasticity)

# **Residual Analysis for Linearity**

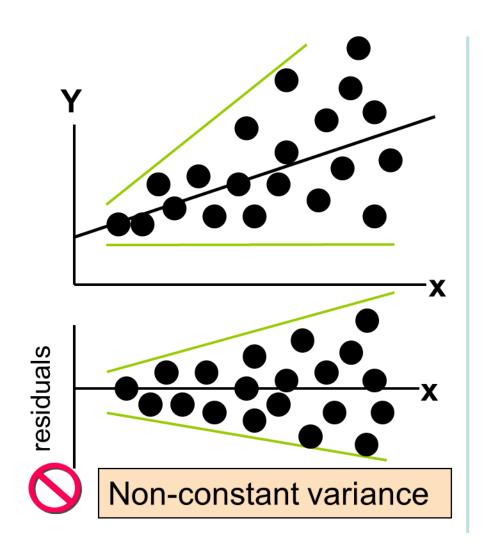


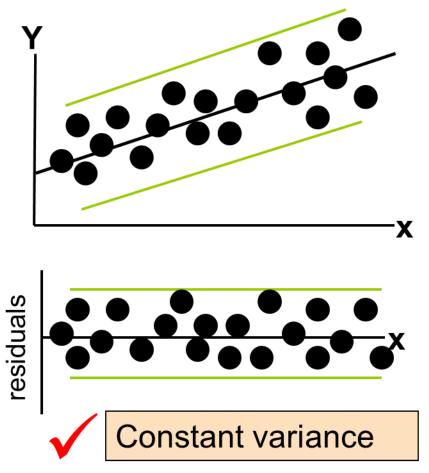
# Residual Analysis for Independence





## **RA for Equal Variance**





# **Evaluating the Model**

Testing for Significance

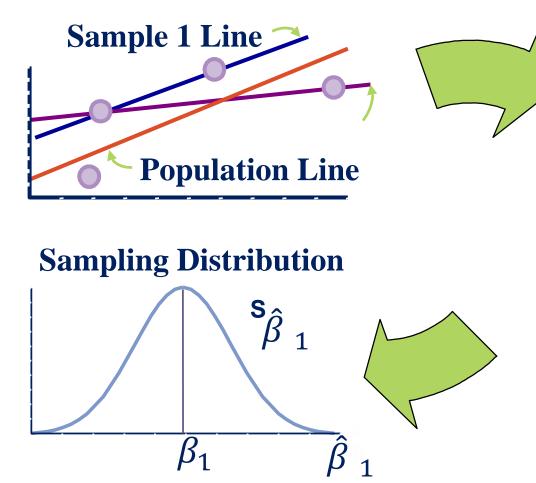
## Regression Modeling Steps

- 1. Hypothesize deterministic component
- 2. Estimate unknown model parameters
- 3. Specify probability distribution of random error term
  - Estimate standard deviation of error
- 4. Evaluate model
- 5. Use model for prediction and estimation

## **Test of Slope Coefficient**

- Shows if there is a linear relationship between x and y
- $\triangleright$  Involves population slope  $\beta_1$
- Hypotheses
  - $H_0$ :  $\beta_1 = 0$  (No Linear Relationship)
  - $H_a$ :  $\beta_1 \neq 0$  (Linear Relationship)
- Theoretical basis is sampling distribution of slope

## Distribution of Sample Slopes



# All Possible Sample Slopes

Sample 1: 2.5
Sample 2: 1.6
Sample 3: 1.8
Sample 4: 2.1

Very large number of sample slopes

## Slope Coefficient Test Statistic

$$t = \frac{\widehat{\beta_1}}{S_{\widehat{\beta_1}}} = \frac{\widehat{\beta_1}}{S}, \qquad df = 2$$

$$SS_{xx} = \sum_{i=1}^{n} x_i - \frac{(\sum_{i=1}^{n} x_i)^2}{n}$$

## E.g. Test of Slope Coefficient

You're a marketing analyst for any Toys.

You find  $\hat{\beta_0} = -.1$ ,  $\hat{\beta_1} = .7$  and s = .6055.

<u>Ad (₹)</u>	Sales (Qty)
1	1
2	1
3	2
4	2
5	4

Is the relationship **significant** at the **.05** level of significance?



## **Solution Table**

$x_i$	$y_i$	$x_i^2$	$y_i^2$	$x_i y_i$
1	1	1	1	1
2	1	4	1	2
3	2	9	4	6
4	2	<b>16</b>	4	8
5	4	25	16	20
15	10	55	26	37

# Slope Coefficient Test Statistic

$$t = \frac{\widehat{\beta}_1}{S_{\widehat{\beta}_1}} = \frac{\widehat{\beta}_1}{\frac{S}{\sqrt{SS_{xx}}}},$$

$$t = \frac{\widehat{\beta_1}}{S_{\widehat{\beta_1}}} = \frac{\widehat{\beta_1}}{\frac{S}{\sqrt{SS_{min}}}}, \qquad df = 2 \qquad \Longrightarrow \qquad Where \\ SS_{xx} = \sum_{i=1}^n x_i - \frac{(\sum_{i=1}^n x_i)^2}{n}$$

$$S_{\widehat{\beta}_1} = \frac{s}{\sqrt{SS_{XX}}} = \frac{0.6055}{\sqrt{55 - \frac{15^2}{5}}} = .1914$$

$$t = \frac{0.70}{1914} = 3.657$$

# Test of Slope Coefficient Solution

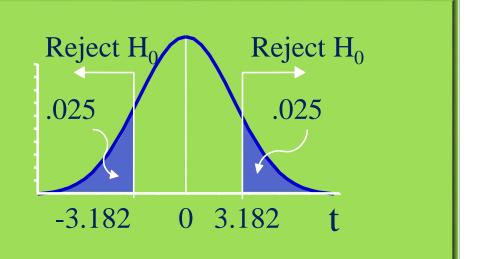
$$\rightarrow$$
 H<sub>0</sub>:  $\beta_1 = 0$ 

$$\triangleright$$
 Ha:  $β_1 ≠ 0$ 

$$\rightarrow \alpha = .05$$

$$\rightarrow$$
 df = 5 - 2 = 3

Critical Value(s):



Test Statistic: 
$$t = \frac{\widehat{\beta_1}}{S_{\widehat{\beta}_1}} = \frac{0.70}{.1914} = 3.657$$

**Decision:** Reject  $(H_0)$  at  $\alpha = .05$ ,

**Conclusion:** There is evidence of a relationship

## **Correlation Coefficient**

### **Correlation Models**

- Answers 'How strong is the **linear** relationship between two variables?'
- Coefficient of correlation
  - Sample correlation coefficient denoted *r*
  - Values range from −1 to +1
  - Measures degree of association
  - Does not indicate cause—effect relationship

### Coefficient of Correlation

$$r = \frac{SS_{xy}}{\sqrt{SS_{xx}SS_{yy}}}$$

$$SS_{xx} = \sum x^2 - \frac{\left(\sum x\right)^2}{n}$$

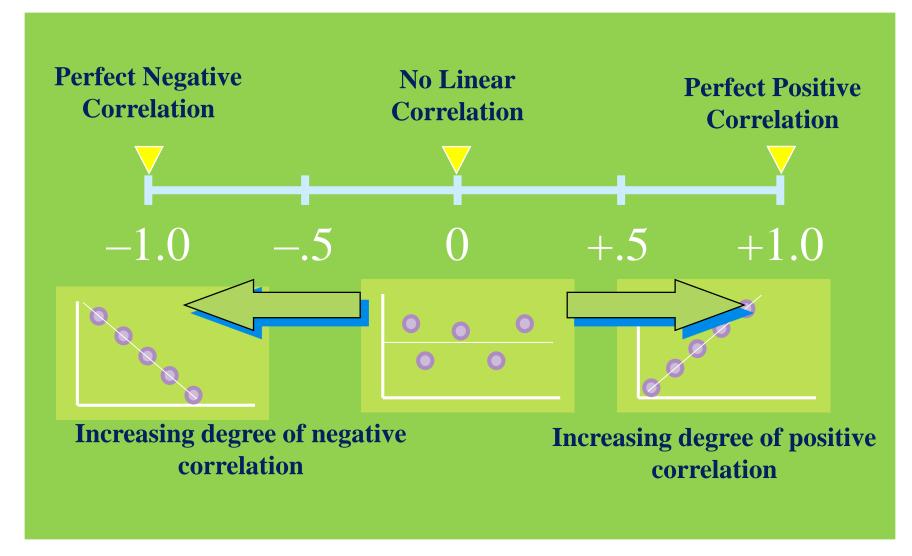
$$SS_{yy} = \sum y^2 - \frac{\left(\sum y\right)^2}{n}$$

$$SS_{xx} = \sum x^2 - \frac{\left(\sum x\right)^2}{n}$$

$$SS_{yy} = \sum y^2 - \frac{\left(\sum y\right)^2}{n}$$

$$SS_{xy} = \sum xy - \frac{\left(\sum x\right)\left(\sum y\right)}{n}$$

### **Correlation Coefficient Values**



## E.g. Coefficient of Correlation

You're a marketing analyst for any Toys.

<u>Ad (₹)</u>	Sales (Qty)
1	1
2	1
3	2
4	2
5	4

Calculate the **coefficient of correlation**.



## **Solution Table**

$\boldsymbol{x}_{i}$	$y_i$	$x_i^2$	$y_i^2$	$x_i y_i$
1	1	1	1	1
2	1	4	1	2
3	2	9	4	6
4	2	16	4	8
5	4	25	16	20
15	10	55	26	37

#### **Coefficient of Correlation Solution**

$$SS_{xx} = \sum x^{2} - \frac{\left(\sum x\right)^{2}}{n} = 55 - \frac{(15)^{2}}{5} = 10$$

$$SS_{yy} = \sum y^{2} - \frac{\left(\sum y\right)^{2}}{n} = 26 - \frac{(10)^{2}}{5} = 6$$

$$SS_{xy} = \sum xy - \frac{\left(\sum x\right)\left(\sum y\right)}{n} = 37 - \frac{(15)(10)}{5} = 7$$

$$r = \frac{SS_{xy}}{\sqrt{SS_{xx}SS_{yy}}} = \frac{7}{\sqrt{10 \cdot 6}} = .904$$

It can be predicted using LR due High value of Correlation Coefficient

## **Coefficient of Correlation Challenge**

You're an economist for the county cooperative.

You gather the following data:

Fertilizer (lb.)	Yield (lb.)	
4	3.0	
6	5.5	
10	6.5	
<b>12</b>	9.0	

Find the coefficient of correlation.

## **Solution Table\***

$\boldsymbol{x}_i$	$y_i$	$x_i^2$	$y_i^2$	$x_i y_i$
4	3.0	16	9.00	12
6	5.5	36	30.25	33
10	6.5	100	42.25	65
12	9.0	144	81.00	108
32	24.0	296	162.50	218

# Coefficient of Correlation Solution\*

$$SS_{xx} = \sum x^2 - \frac{\left(\sum x\right)^2}{n} = 296 - \frac{(32)^2}{4} = 40$$

$$SS_{yy} = \sum y^2 - \frac{\left(\sum y\right)^2}{n} = 162.5 - \frac{(24)^2}{4} = 18.5$$

$$SS_{xy} = \sum xy - \frac{\left(\sum x\right)\left(\sum y\right)}{n} = 218 - \frac{(32)(24)}{4} = 26$$

$$r = \frac{SS_{xy}}{\sqrt{SS_{xx}SS_{yy}}} = \frac{26}{\sqrt{40.18.5}} = .956$$

### **Coefficient of Determination**

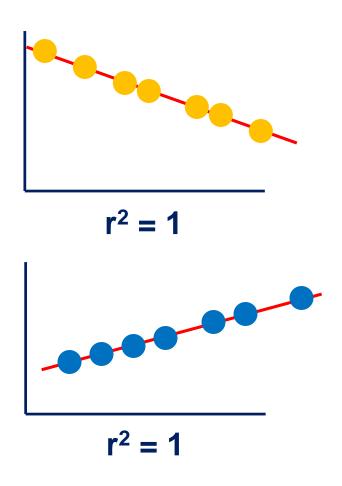
**Proportion** of variation 'explained' by relationship between *x* and *y* 

$$r^2 = \frac{\text{Explained Variation}}{\text{Total Variation}} = \frac{SS_{yy} - SSE}{SS_{yy}}$$

 $0 \le r^2 \le 1$ 

$$r^2$$
 = (coefficient of correlation)<sup>2</sup>

## E.g. Approximate r<sup>2</sup> Values

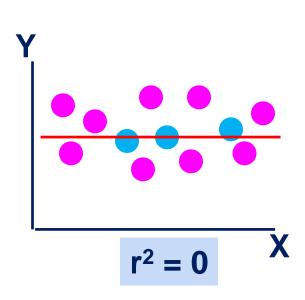


$$r^2 = 1$$

Perfect linear relationship between X and Y:

100% of the variation in Y is explained by variation in X

## E.g. Approximate r<sup>2</sup> Values...



$$r^2 = 0$$

- No linear relationship between X and Y:
- The value of Y does not depend on X. (None of the variation in Y is explained by variation in X)

## E.g. Determination Coefficient

You're a marketing analyst for any Toys. You

know r = .904.

<u>Ad (₹)</u>	Sales (Qty)
1	1
2	1
3	2
4	2
5	4

Calculate and interpret the coefficient of determination.



## E.g. Determination Coefficient

$$r^2$$
 = (coefficient of correlation)<sup>2</sup>  
 $r^2$  = (.904)<sup>2</sup>  
 $r^2$  = .817

**Interpretation:** About 81.7% of the sample variation in Sales (y) can be explained by using Ad  $\not\in$  (x) to predict Sales (y) in the linear model.

### Other Evaluation Metrics

- Mean Squared Error (MSE)
  - Most commonly used Metric
  - Differentiable due to convex shape
  - Easier to optimize.
  - Penalizes large errors
- Mean Absolute Error (MAE)

$$MAE = \frac{1}{m} \sum_{i=1}^{m} |y_i - \hat{y}_i|$$

 $MSE = \frac{1}{m} \sum_{i=1}^{m} (y_i - \widehat{y}_i)^2$ 

- Not preferred in cases where outliers are prominent = 1
- MAE does not penalize large errors.
- Small MAE suggests the model is great at prediction, while a large MAE suggests that model may have trouble in certain areas.

#### Other Evaluation Metrics...

- > Root Mean Squared Error (RMSE)
  - RMSE measures the scatter of these residuals
  - RMSE penalizes large errors.
  - Lower RMSE indicates model is better for predictions.
  - Higher RMSE indicates, large deviations between the predicted and actual value.

$$RMSE = \sqrt{\frac{1}{m} \sum_{i=1}^{m} (y_i - \widehat{y}_i)^2}$$

#### Conclusion

- 1. Described the Linear Regression Model
- 2. Stated the Regression Modeling Steps
- 3. Explained Least Squares
- 4. Computed Regression Coefficients
- 5. Explained Correlation
- 6. Predicted Response Variable