Linear Regression Models

Dinesh K. Vishwakarma, Ph.D.

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**: $BMI = \dfrac{Weight\ in\ Kilograms}{(Height\ in\ Meters)2}$

- **Non-metric Formula**: $BMI = \dfrac{Weight\ (pounds) \times 703}{(Height\ in\ inches)2}$

Probabilistic Models

1. **Hypothesize 2 Components**
   - Deterministic
   - Random Error
2. **Example:** Systolic blood pressure of newborns is **6 Times** 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)

Bivariate & multivariate models

(Education) $x \longrightarrow y$ (Income) Bivariate

(Education) x_1

(Sex) x_2

(Experience) x_3

(Age) x_4

y (Income)

Multivariate

Model with simultaneous relationship

Price of wheat $\longleftrightarrow$ Quantity of wheat produced

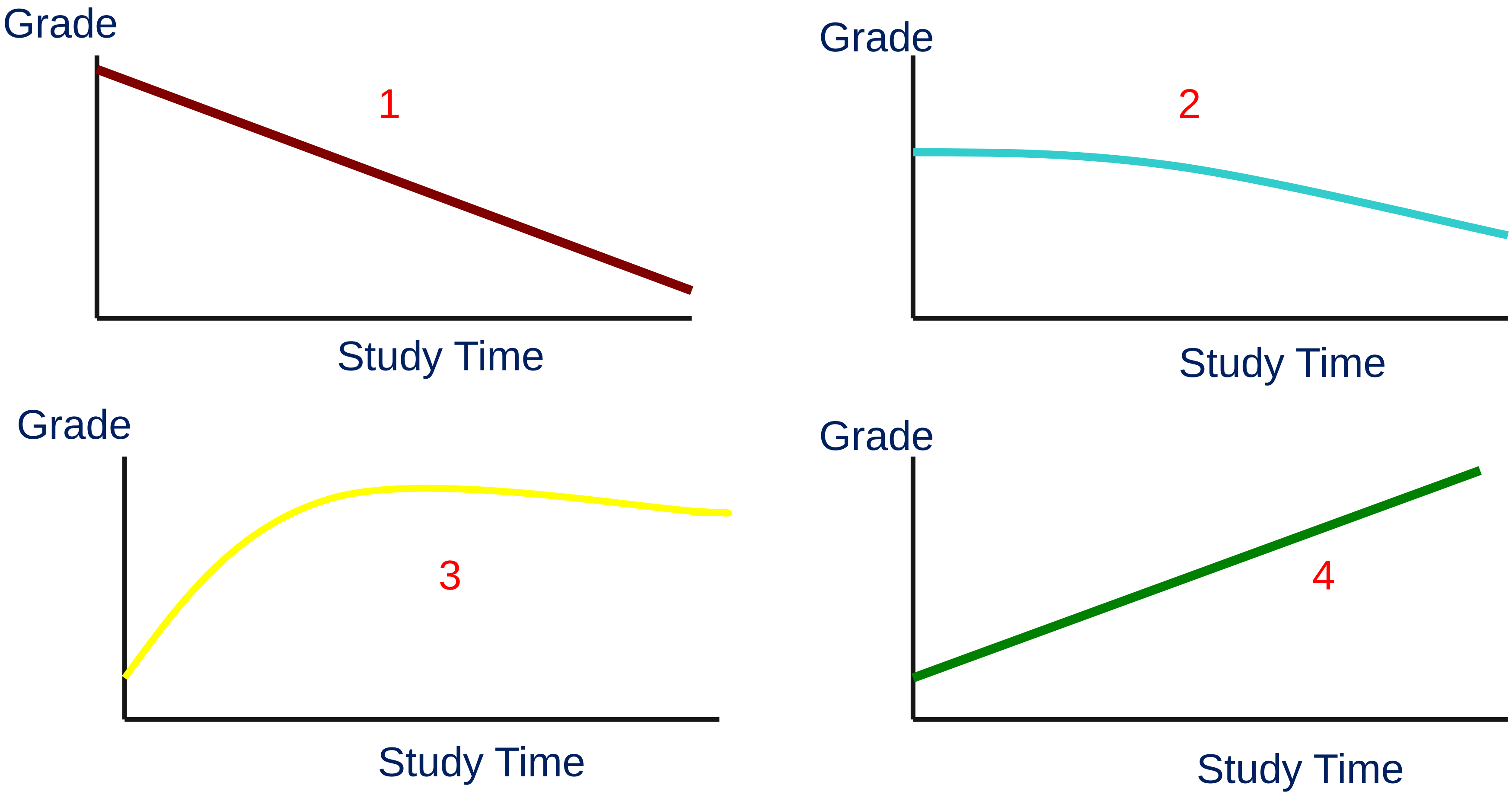
Regression Modeling Steps

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

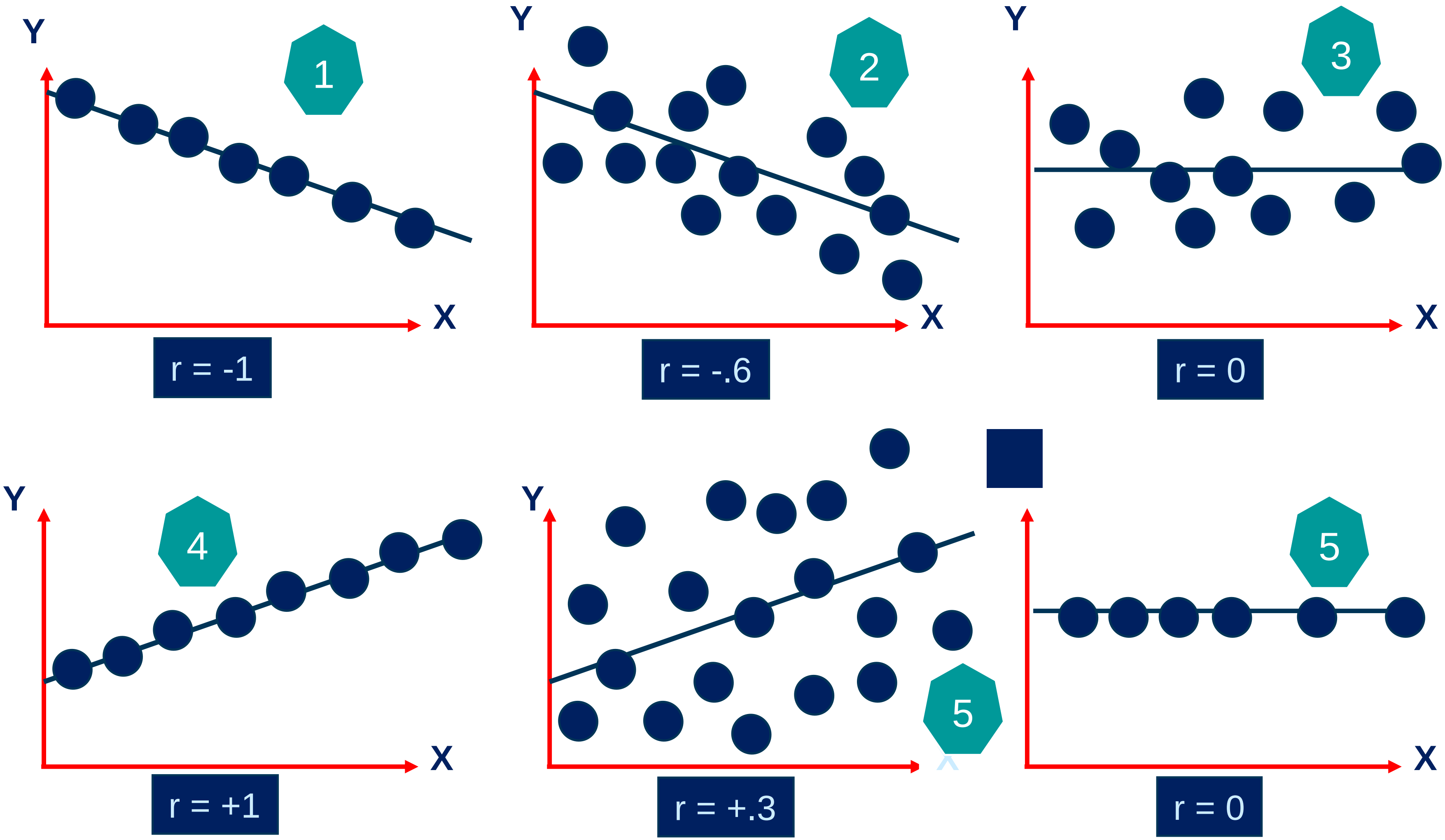
Models Facts

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

Thinking Challenge: Which is more logical?



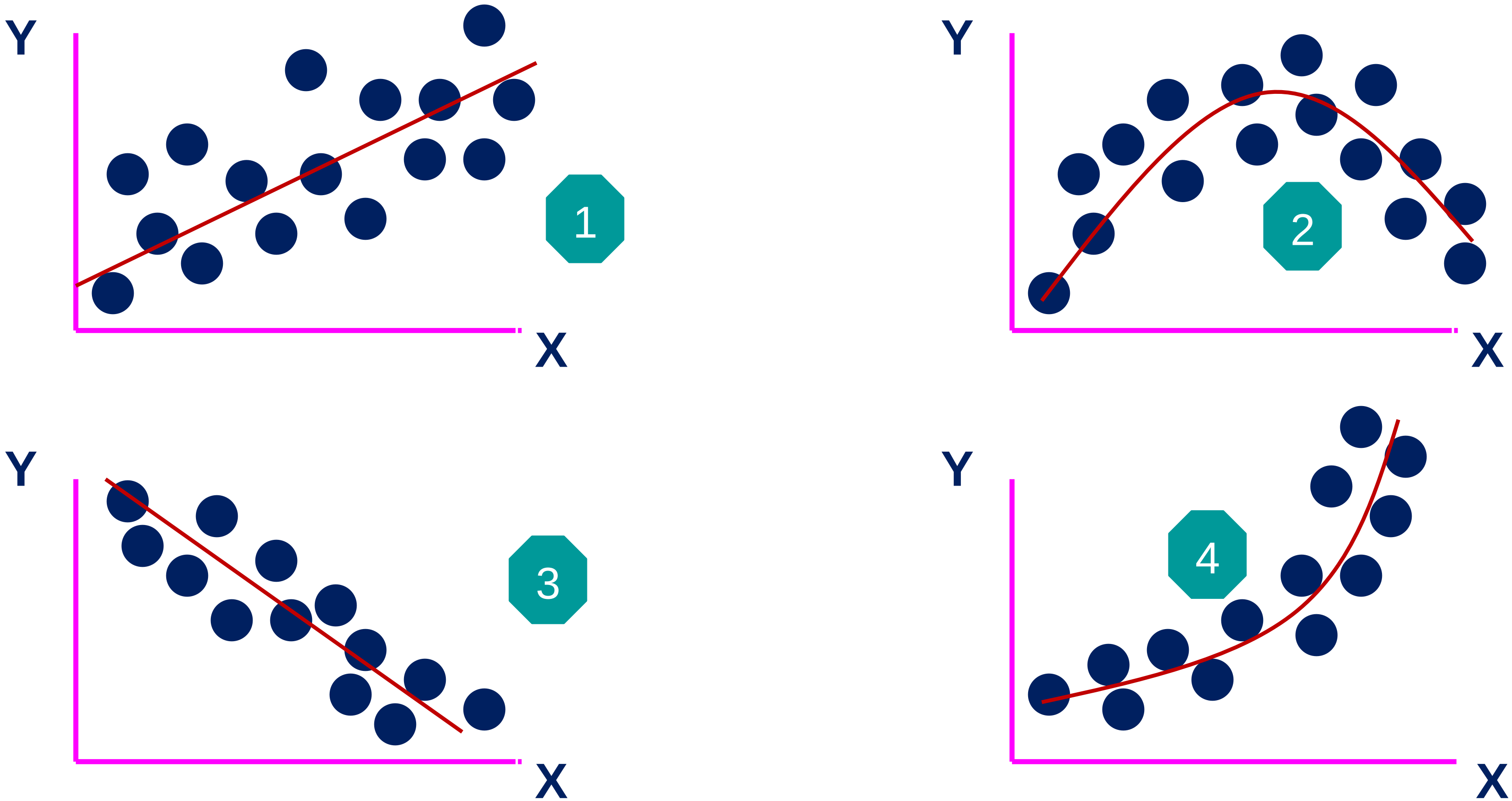
Scatter Plot of Data



Types of Relationship

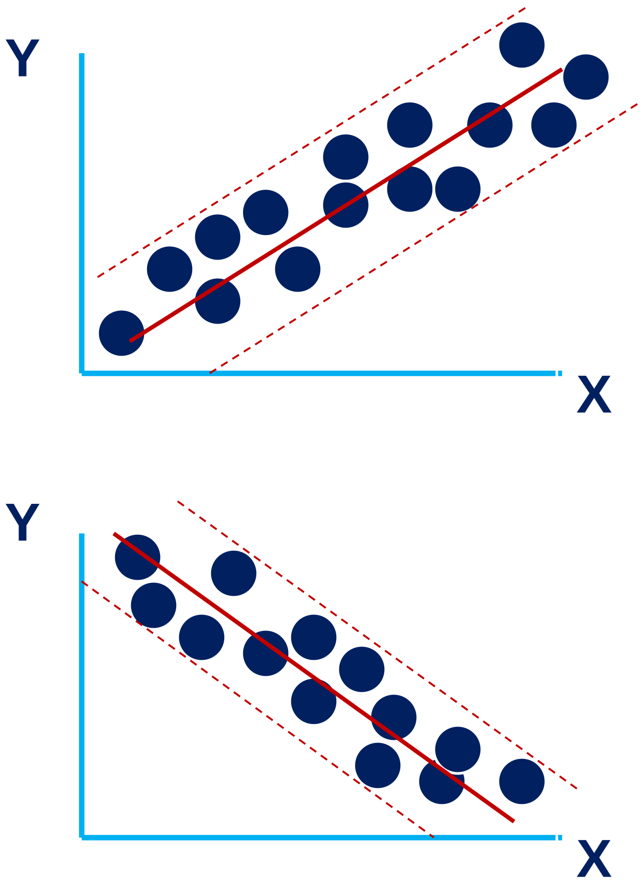
Linear relationships

Curvilinear relationships

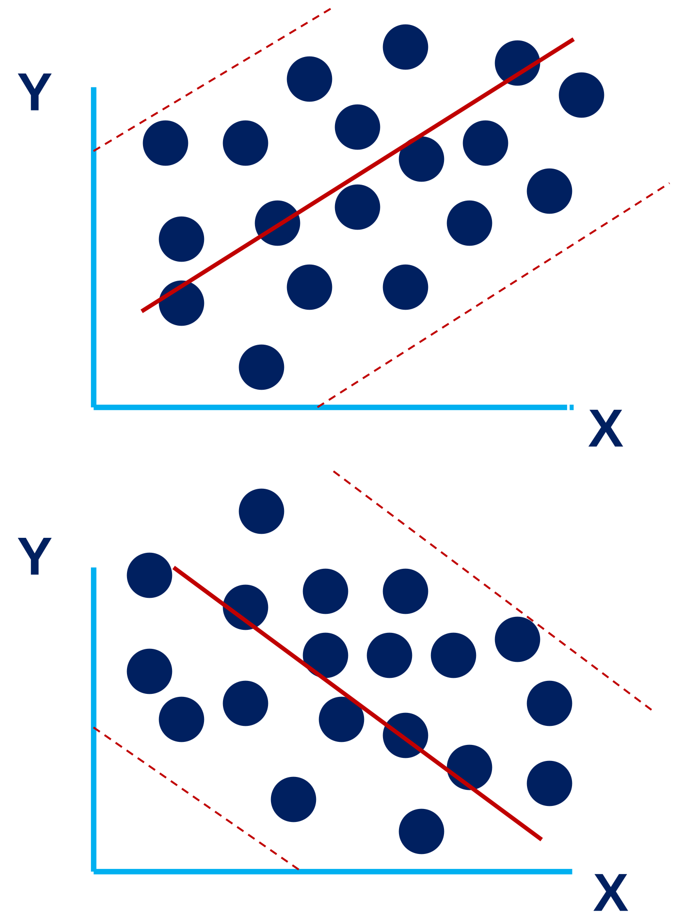


Types of Relationship…

Strong relationships

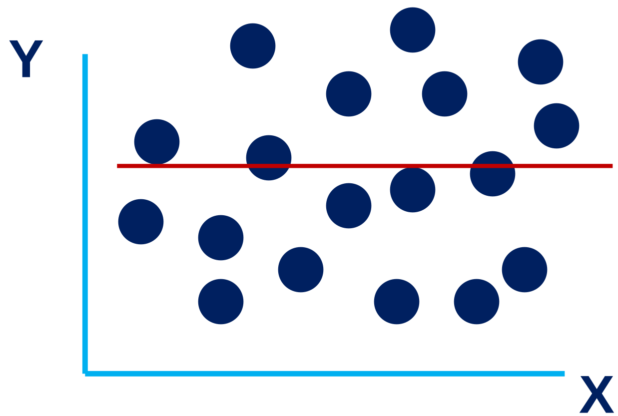


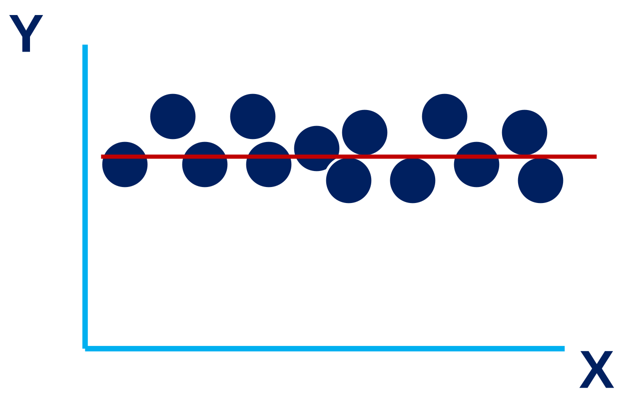
Weak relationships



Types of Relationship…

No relationship





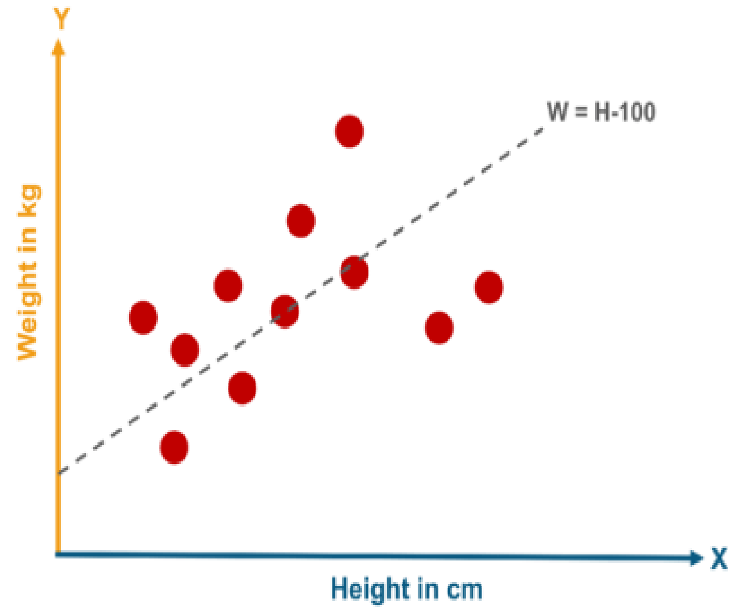
Linear Regression Models

- 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

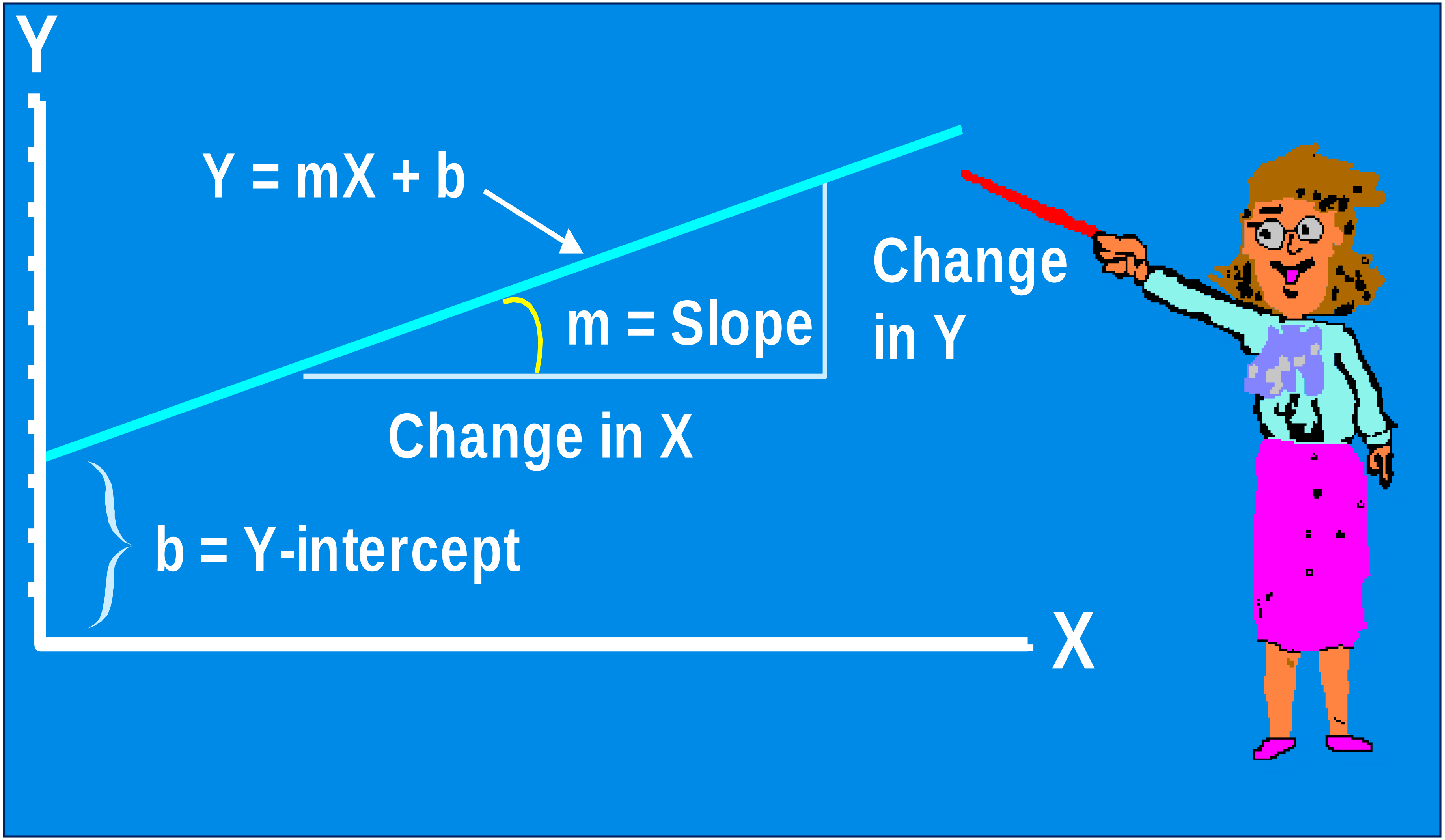
- **Types of Regression**
- Linear Regression
- Logistic Regression
- Polynomial Regression
- Stepwise Regression

Basis	Linear Regression	Logistic Regression
Core Concept	The data is modelled using a straight line	The data is modelled using a sigmoid
Used with	Continuous Variable	Categorical Variable
Output/Prediction	Value of the variable	Probability of occurrence of an event
Accuracy and Goodness of Fit	Measured by loss, R squared, Adjusted R squared etc.	Measured by 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

Linear Equations



Linear Regression Model

- **Relationship Between Variables is a Linear Function**

Population Y-Intercept

Population Slope

Random Error

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$

Dependent (Response Variable)

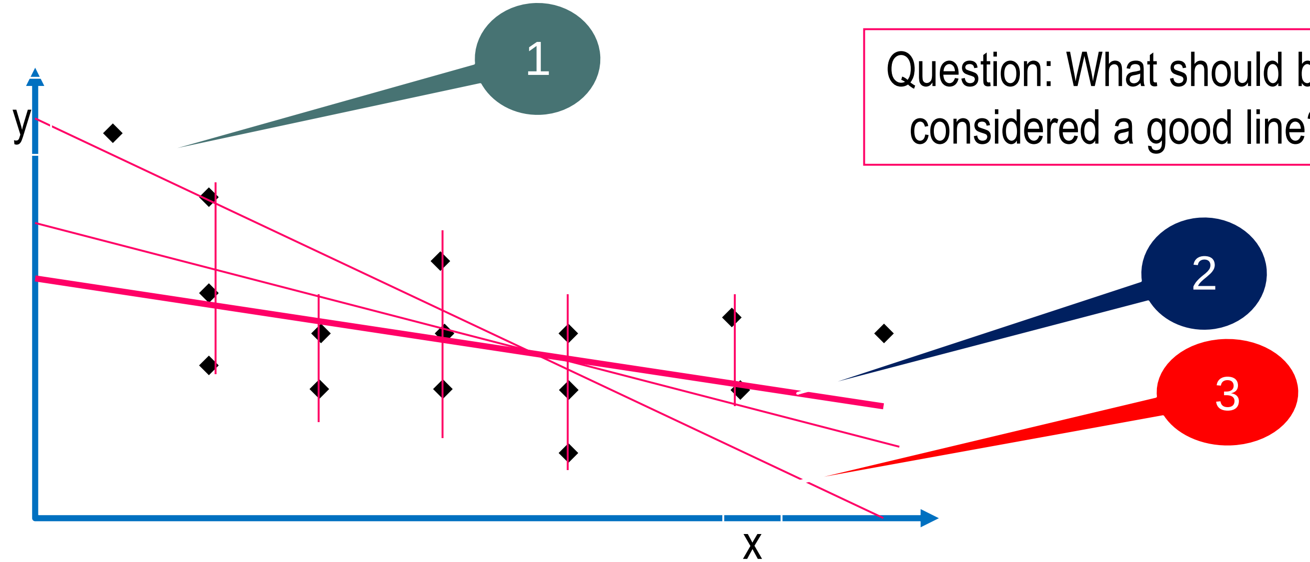
E.g. Grade

Independent (Explanatory) Variable

E.g. Study Time

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.

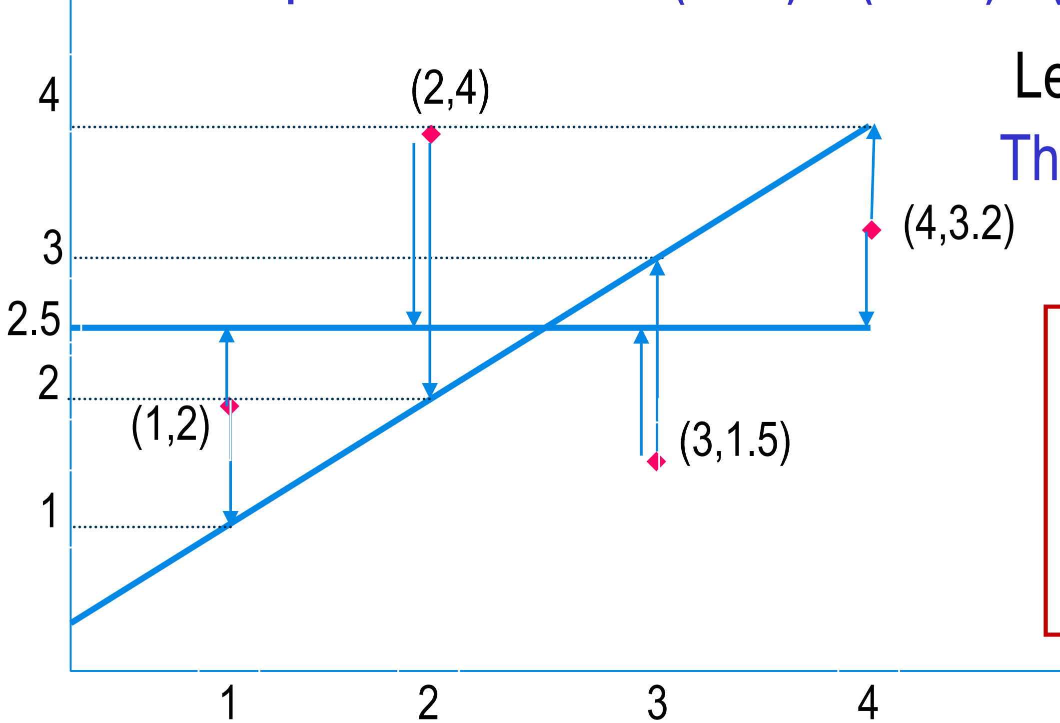


Question: What should be considered a good line?

Sum Squared Difference

Sum of squared differences = $(2 - 1)^2 + (4 - 2)^2 + (1.5 - 3)^2 + (3.2 - 4)^2 = 6.89$

Sum of squared differences = $(2 - 2.5)^2 + (4 - 2.5)^2 + (1.5 - 2.5)^2 + (3.2 - 2.5)^2 = 3.99$



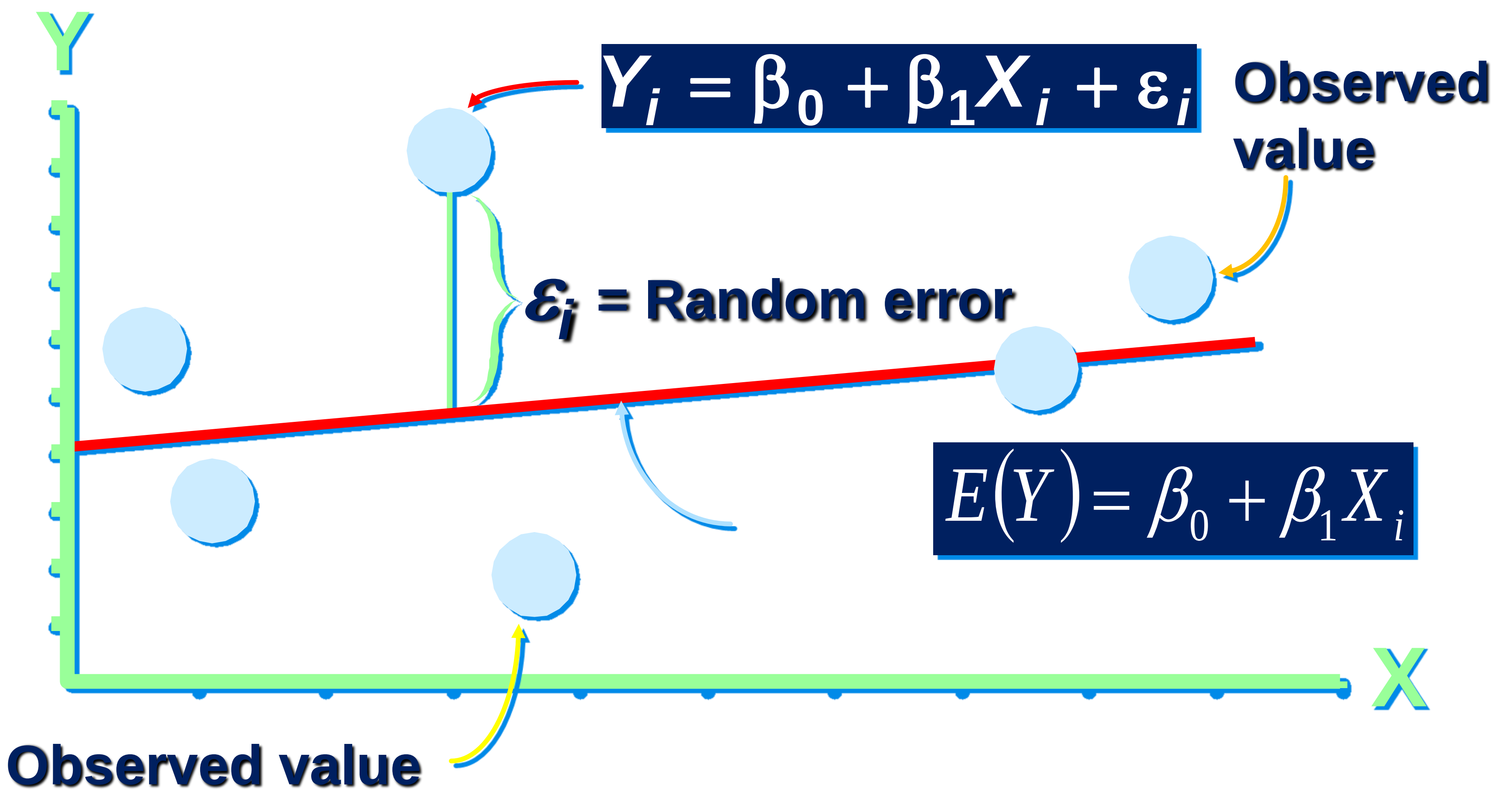
Let us compare two lines

The second line is horizontal

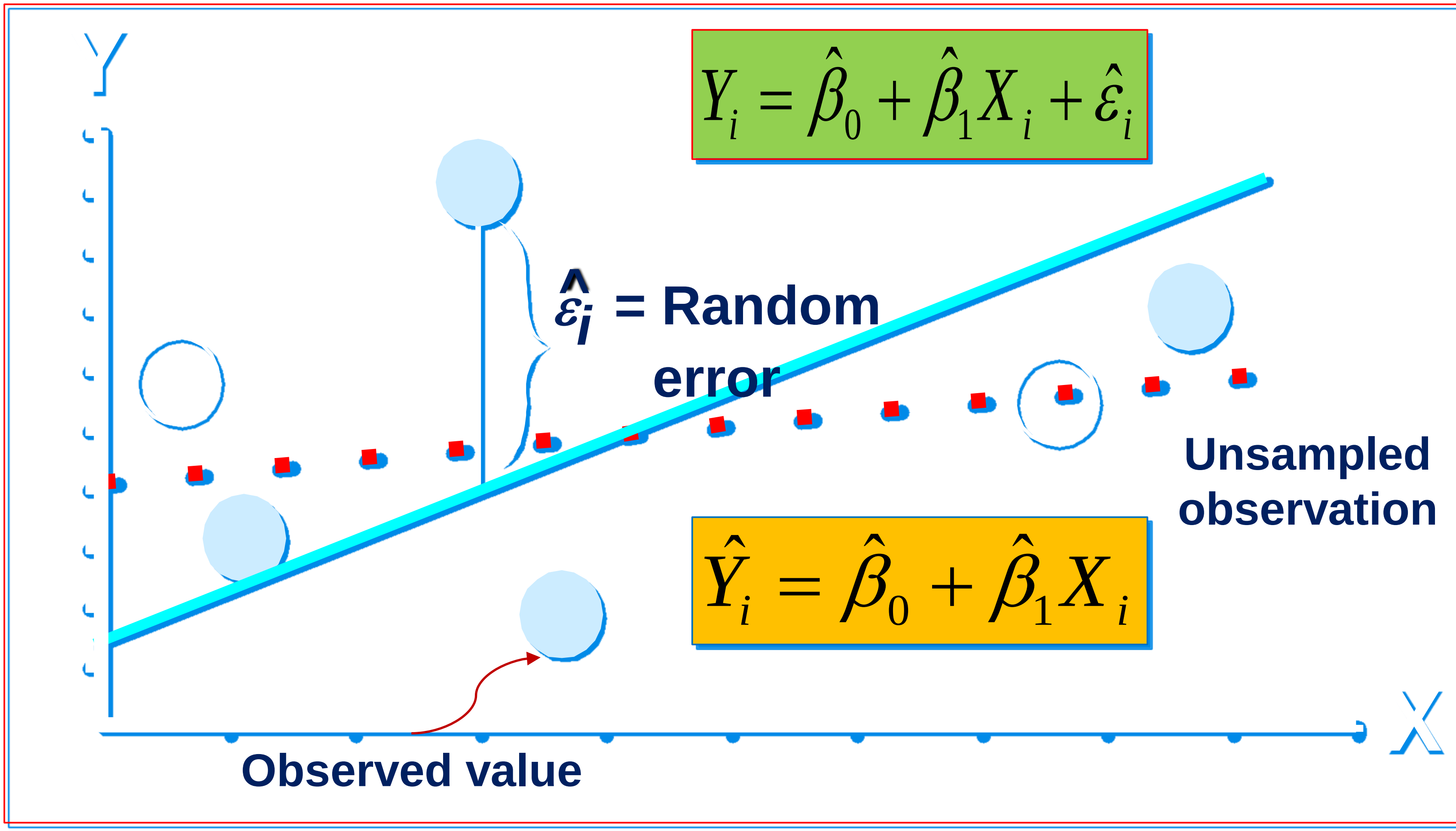
The smaller the sum of squared differences the better the fit of the line to the data.

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

Population Linear Regression Model



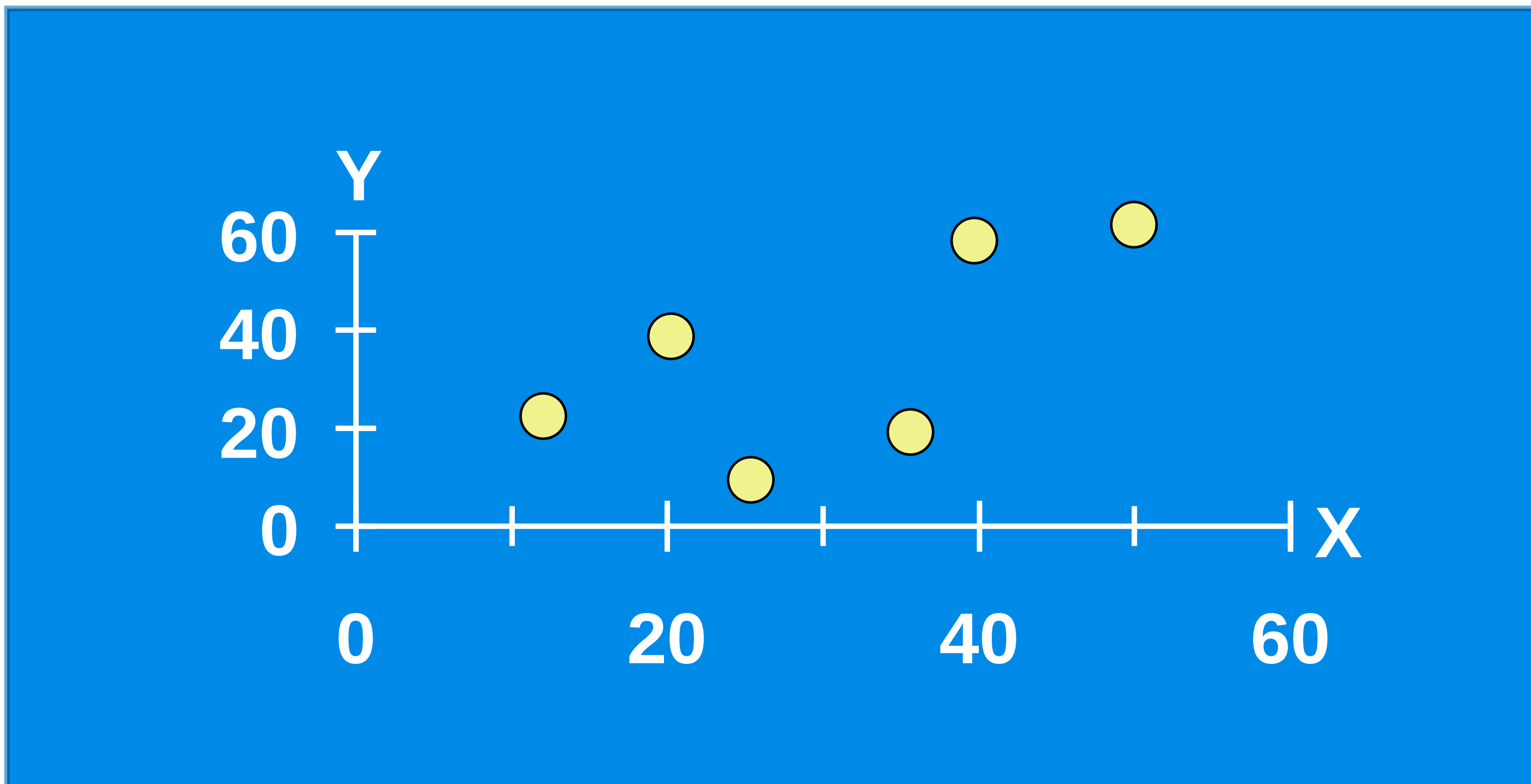
Simple Linear Regression Model



Estimating Parameters: Least Squares Method

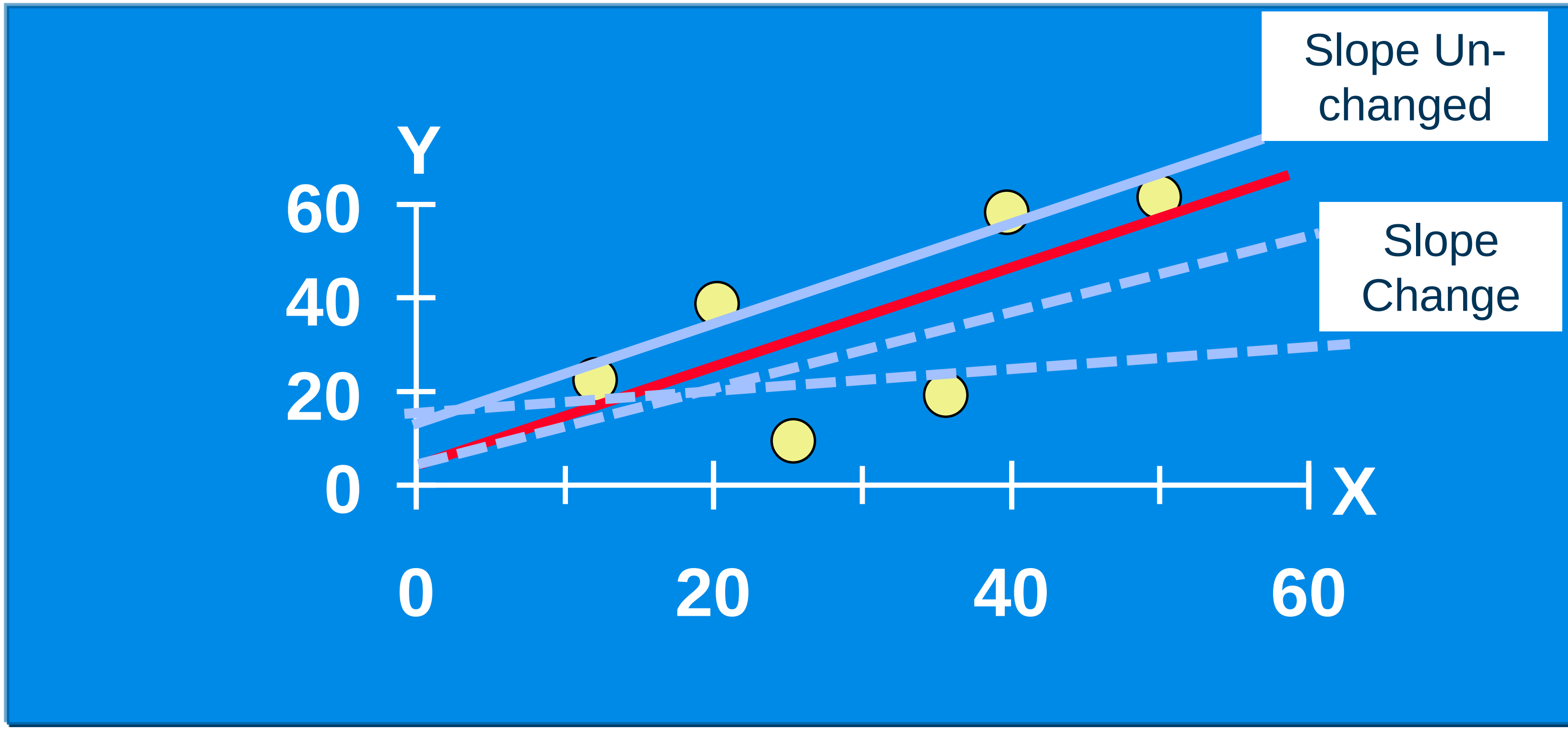
Scatter plot

- 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

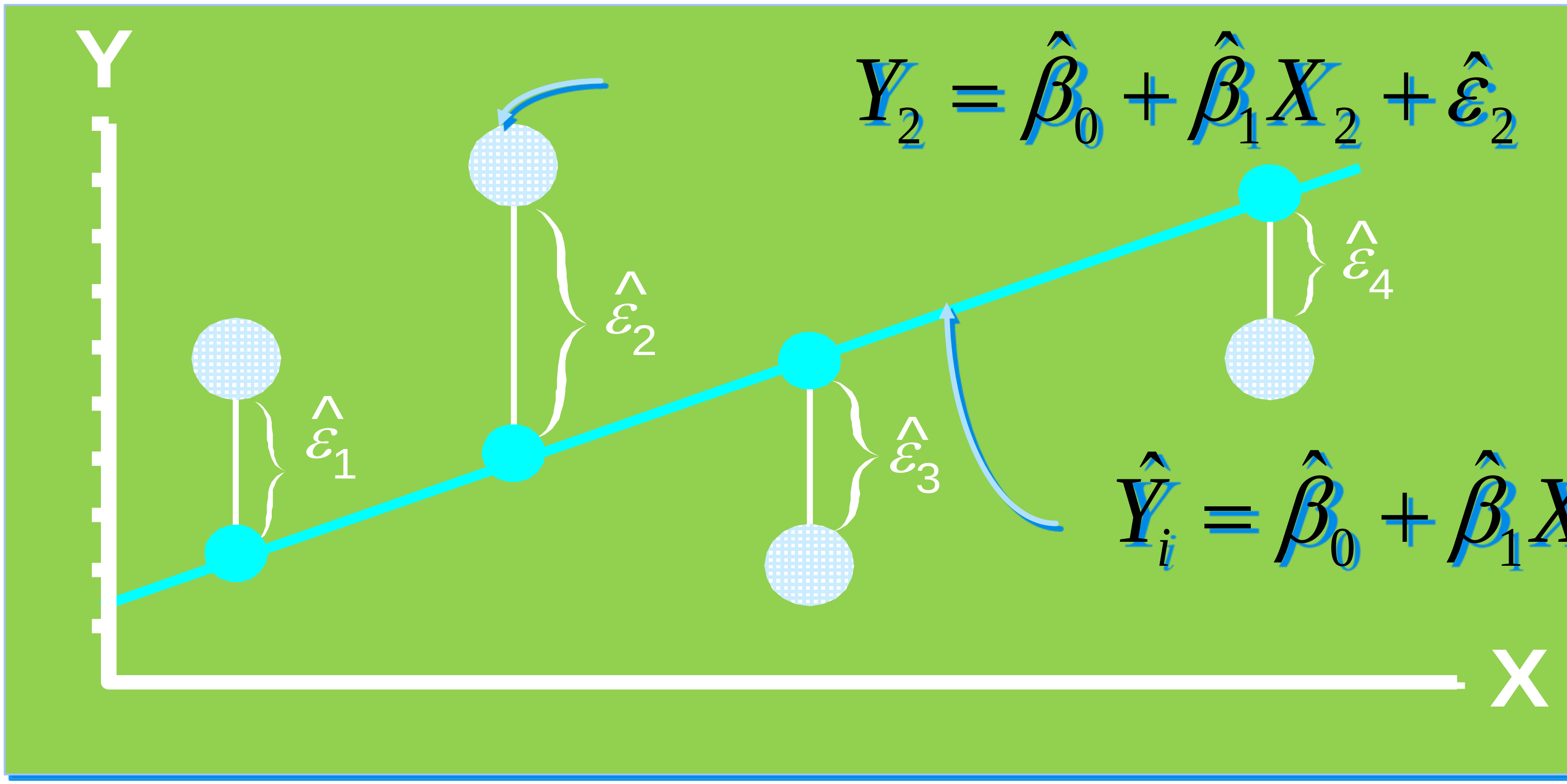
- 1. 'Best Fit' Means Difference Between Actual ***Y*** Values & Predicted $\hat{\boldsymbol{Y}}$ Values are a Minimum. *But* Positive Differences Off-Set Negative ones
- So square errors!

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

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

Least Squares Graphically

$$\text{LS minimizes } \sum_{i=1}^{n} \hat{\varepsilon}_i^2 = \hat{\varepsilon}_1^2 + \hat{\varepsilon}_2^2 + \hat{\varepsilon}_3^2 + \hat{\varepsilon}_4^2$$



Coefficient Equations

Prediction equation

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

Sample slope

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

Sample Y - intercept

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

Derivation of Parameters

Least Squares (L-S):

Minimize squared error

$$\sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} \left(y_i - \beta_0 - \beta_1 x_i \right)^2$$

$$0 = \frac{\partial \sum \varepsilon_i^2}{\partial \beta_0} = \frac{\partial \sum \left(y_i - \beta_0 - \beta_1 x_i \right)^2}{\partial \beta_0}$$

$$= -2\left(n\bar{y} - n\beta_0 - n\beta_1 \bar{x} \right)$$

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

Derivation of Parameters…

Least Squares (L-S):

Minimize squared error

$$0 = \frac{\partial \sum \varepsilon_i^2}{\partial \beta_1} = \frac{\partial \sum \left(y_i - \beta_0 - \beta_1 x_i\right)^2}{\partial \beta_1}$$

$$= -2 \sum x_i \left(y_i - \beta_0 - \beta_1 x_i\right)$$

$$= -2 \sum x_i \left(y_i - \bar{y} + \beta_1 \bar{x} - \beta_1 x_i\right)$$

$$\beta_1 \sum x_i \left(x_i - \bar{x}\right) = \sum x_i \left(y_i - \bar{y}\right)$$

$$\beta_1 \sum \left(x_i - \bar{x}\right)\left(x_i - \bar{x}\right) = \sum \left(x_i - \bar{x}\right)\left(y_i - \bar{y}\right)$$

$$\hat{\beta}_1 = \frac{SS_{xy}}{SS_{xx}}$$

Computation Table

X_i	Y_i	X_i^2	Y_i^2	X_iY_i
X_1	Y_1	X_1^2	Y_1^2	X_1Y_1
X_2	Y_2	X_2^2	Y_2^2	X_2Y_2
:	:	:	:	:
X_n	Y_n	X_n^2	Y_n^2	X_nY_n
ΣX_i	ΣY_i	ΣX_i^2	ΣY_i^2	ΣX_iY_i

Interpretation of Coefficients

- $\beta_1 > 0 \Rightarrow$ Positive Association
- $\beta_1 < 0 \Rightarrow$ Negative Association
- $\beta_1 = 0 \Rightarrow$ No Association

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

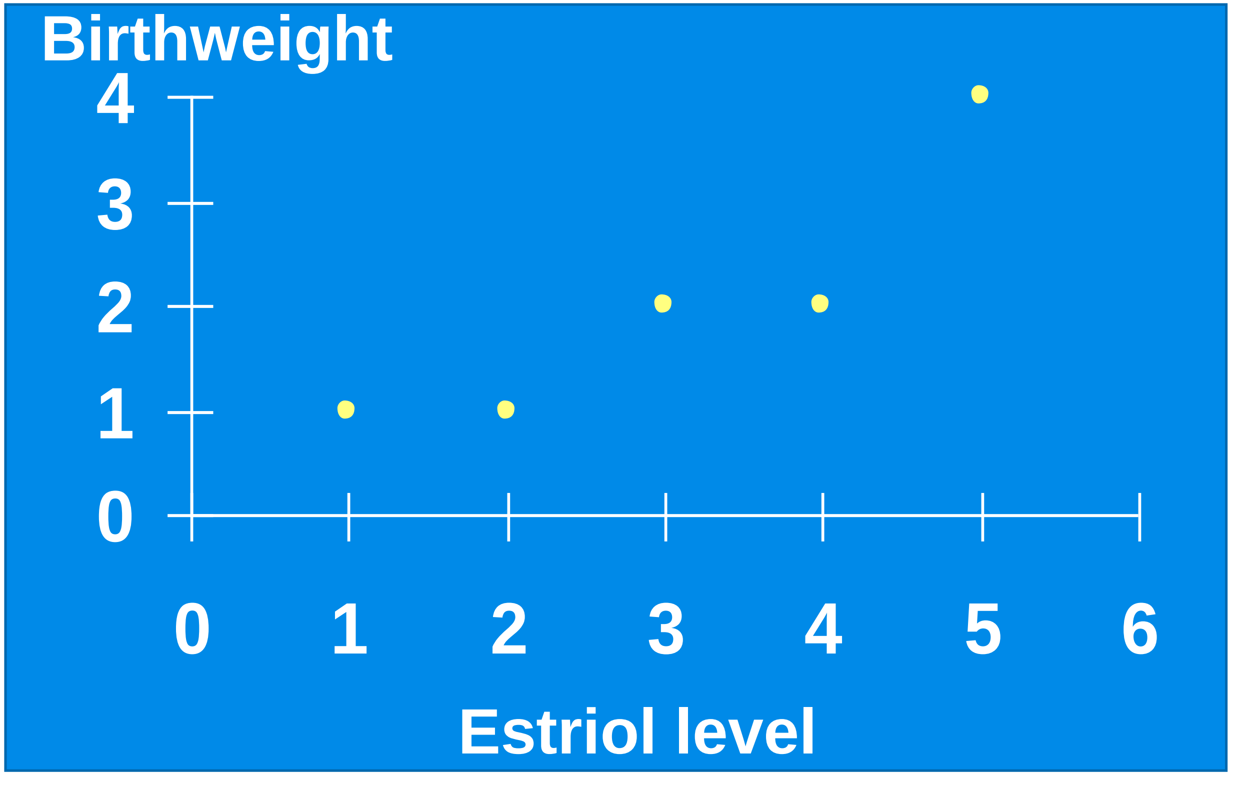
- Y-Intercept (β_0)
  - Average Value of Y When $X = 0$
    - If $\beta_0 = 4$, then Average Y is expected to be 4 When X is 0

E.g. Parameter Estimation

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

Estriol (mg/24h)	**Birthweight** (g/1000)
1	1
2	1
3	2
4	2
5	4

Scatterplot
Birthweight vs. Estriol level



Parameter Estimation Solution Table

X_i	Y_i	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

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n} X_i Y_i - \frac{\left(\sum_{i=1}^{n} X_i\right)\left(\sum_{i=1}^{n} Y_i\right)}{n}}{\sum_{i=1}^{n} X_i^2 - \frac{\left(\sum_{i=1}^{n} X_i\right)^2}{n}} = \frac{37 - \frac{(15)(10)}{5}}{55 - \frac{(15)^2}{5}} = 0.70$$

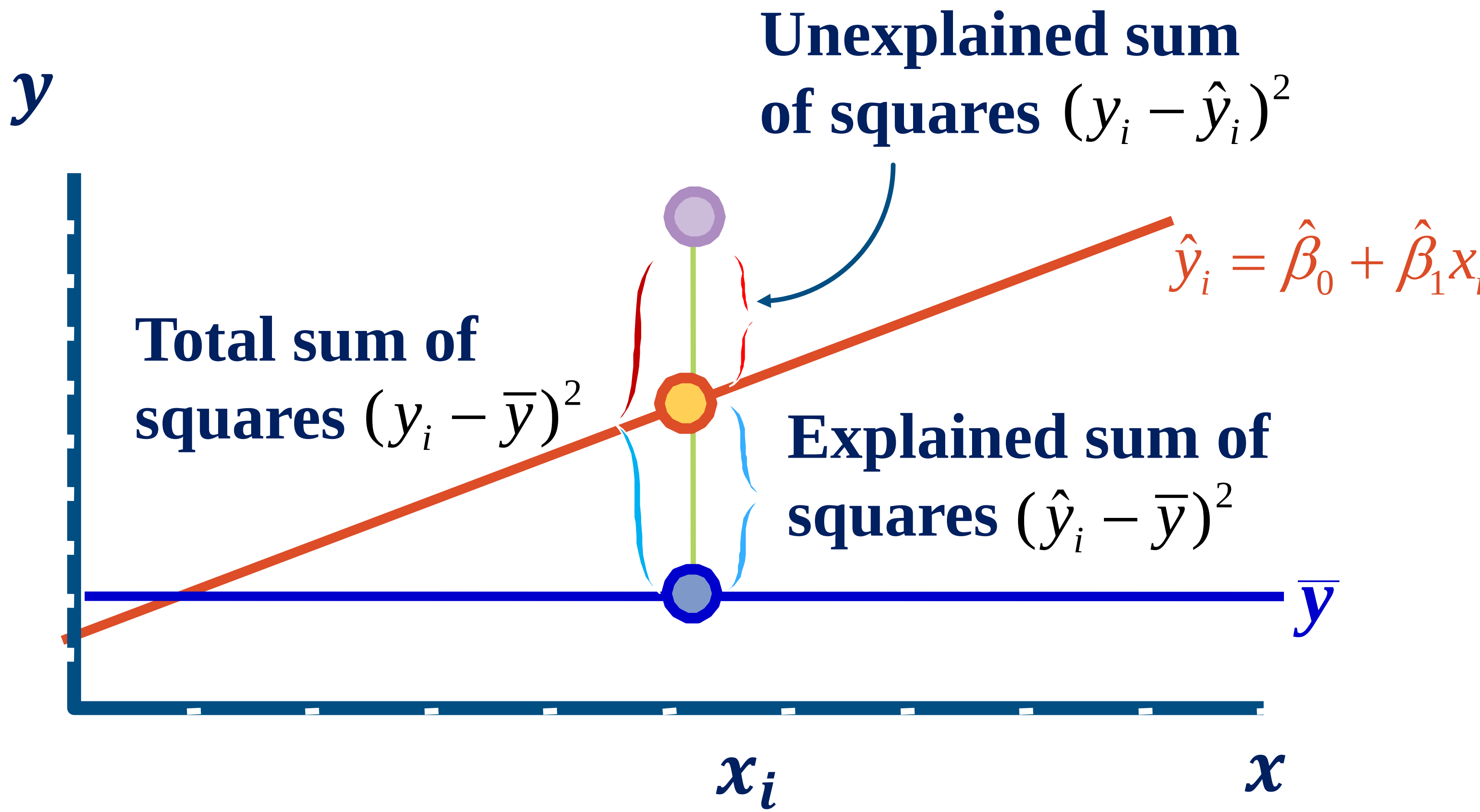
$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X} = 2 - (0.7)(3) = -0.1$$

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

Coefficient Interpretation Solution

- 1. Slope $(\hat{\beta}_1)$
  - Birthweight (Y) is Expected to Increase by .7 Units for Each 1 unit Increase in Estriol (X).
- 2. Intercept (β_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 σ²

$$s^2 = \frac{SSE}{n-2} \quad where \quad SSE = \sum \left(y_i - \hat{y}_i \right)^2$$

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

The subtraction of 2 can be thought of as the fact that we have estimated two parameters: β_0 and β_1

E.g. Compute SSE, s^2, s

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

Ad (₹)	Sales (Qty)
1	1
2	1
3	2
4	2
5	4

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

E.g. Solution: SSE, s^2, 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
				SSE=1.1

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

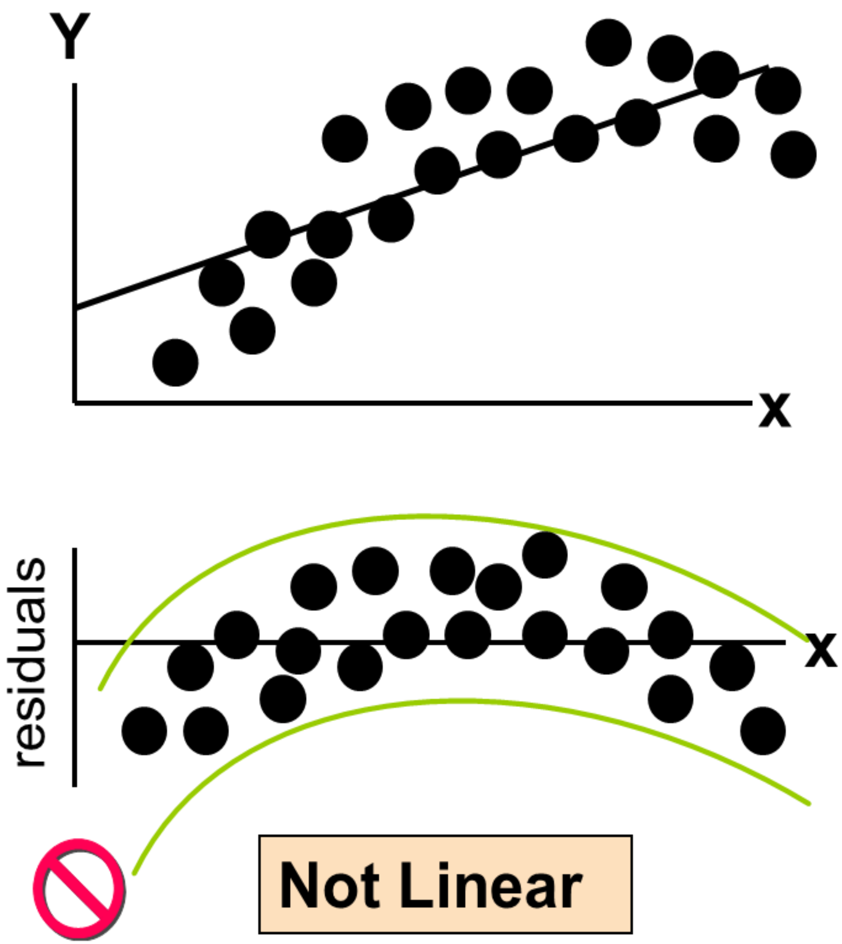
$$s = \sqrt{.36667} = .6055$$

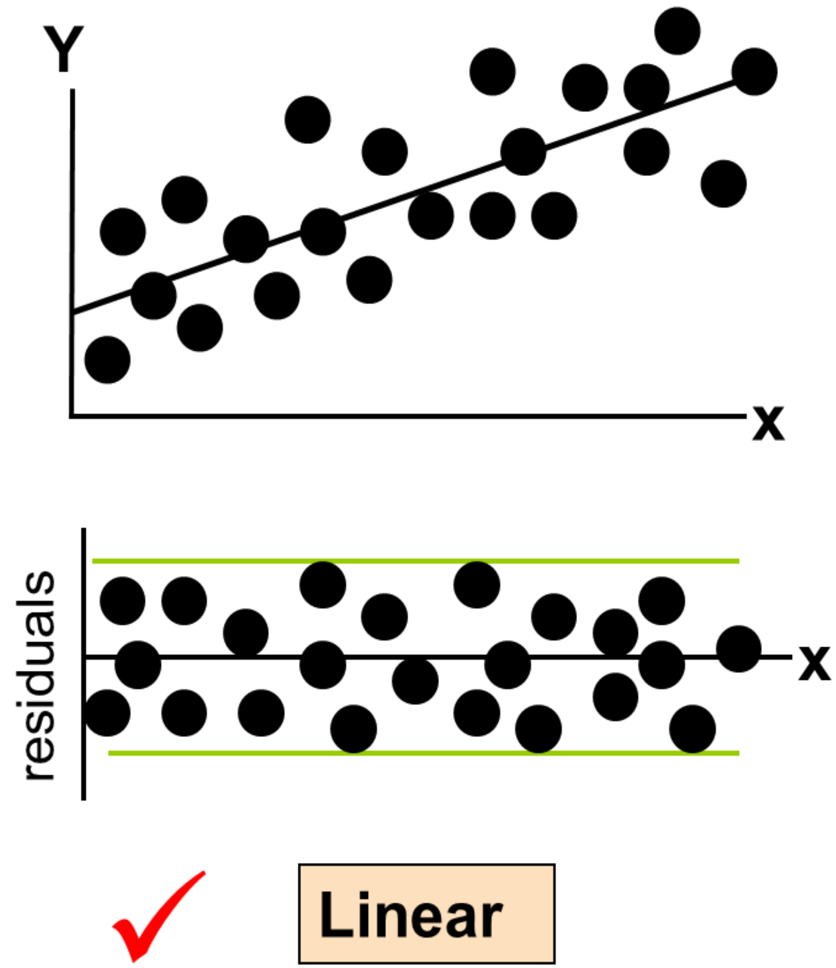
Residual Analysis

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

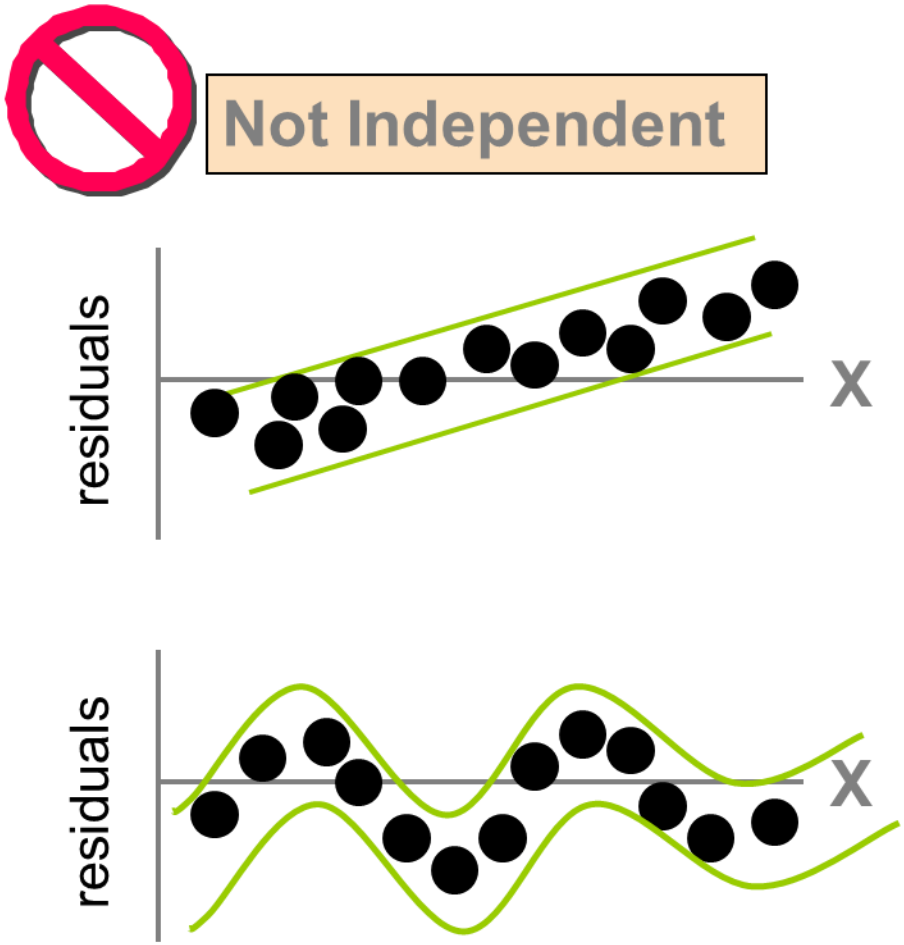
- The residual for observation i, e_i, is the difference between its observed and predicted value
- Check the assumptions of regression by examining the residuals
  - Examine for linearity assumption
  - Evaluate independence assumption
  - Evaluate normal distribution assumption
  - Examine for constant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

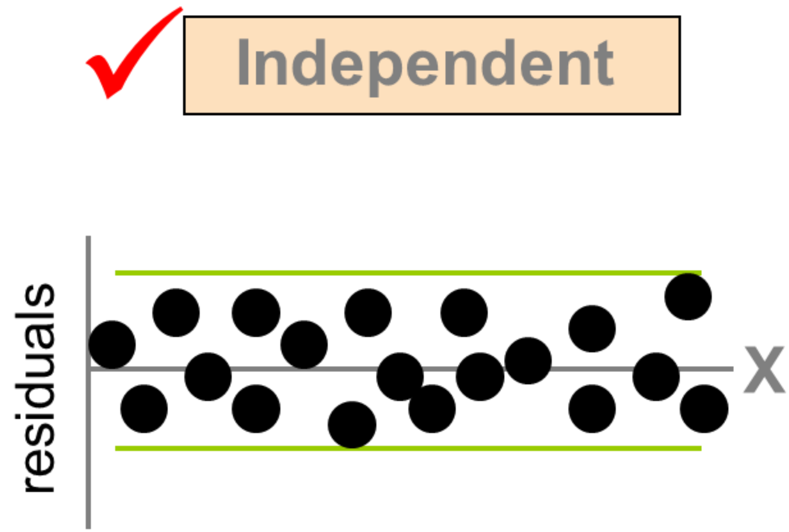
Residual Analysis for Linearity



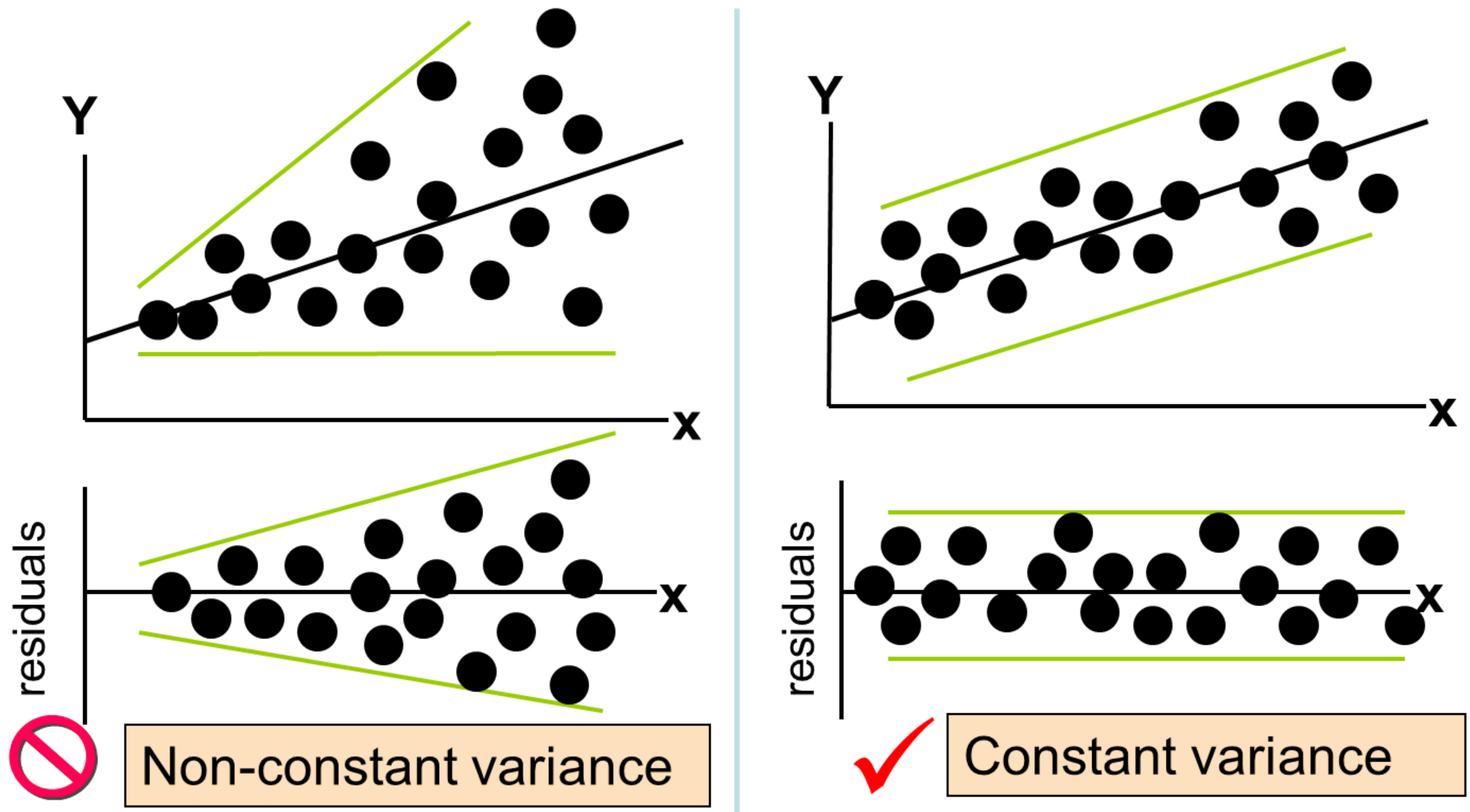


Residual Analysis for Independence





RA for Equal Variance



Evaluating the Model

Testing for Significance

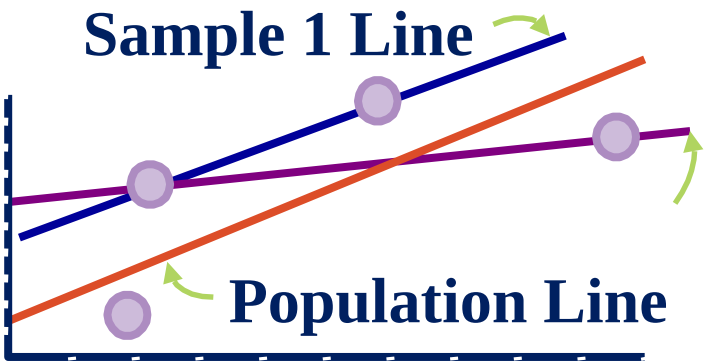
Regression Modeling Steps

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

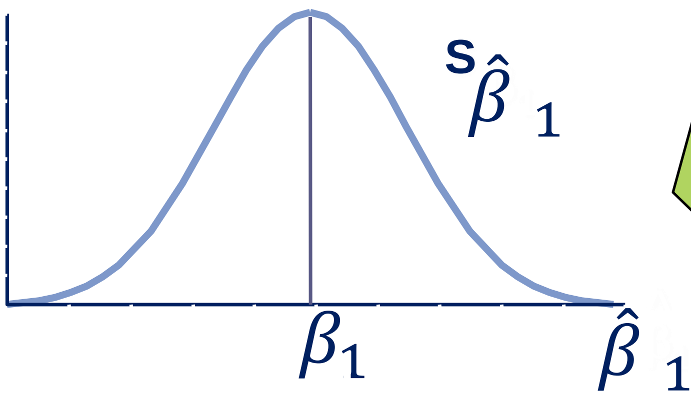
Test of Slope Coefficient

- Shows if there is a linear relationship between x and y
- Involves population slope β_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



Sampling Distribution



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

$$t = \frac{\hat{\beta}_1}{S_{\hat{\beta}_1}} = \frac{\hat{\beta}_1}{s \big/ \sqrt{SS_{xx}}} \qquad df = n - 2$$

where

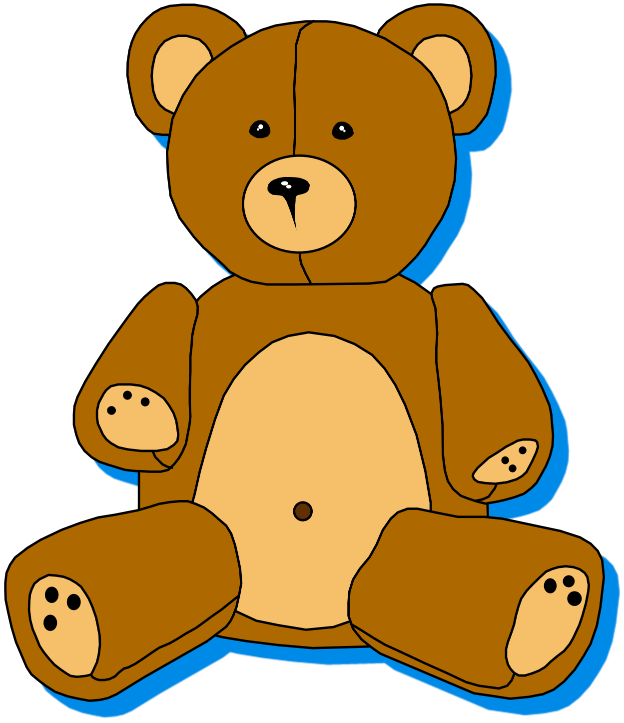
$$SS_{xx} = \sum_{i=1}^{n} x_i^2 - \frac{\left(\sum_{i=1}^{n} x_i\right)^2}{n}$$

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 $s = .6055$.

Ad (₹)	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	16	4	8
5	4	25	16	20
15	10	55	26	37

Slope Coefficient Test Statistic

$$t = \frac{\hat{\beta}_1}{S_{\hat{\beta}_1}} = \frac{\hat{\beta}_1}{s \big/ \sqrt{SS_{xx}}} \qquad df = n - 2$$

where

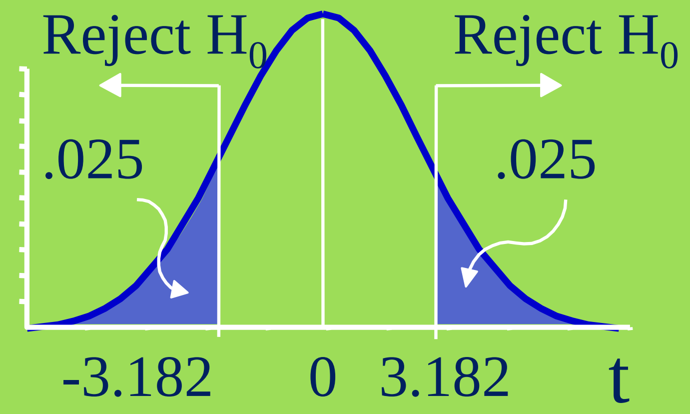
$$SS_{xx} = \sum_{i=1}^{n} x_i^2 - \frac{\left(\sum_{i=1}^{n} x_i\right)^2}{n}$$

$$S_{\hat{\beta}_1} = \frac{S}{\sqrt{SS_{xx}}} = \frac{.6055}{\sqrt{55 - \frac{(15)^2}{5}}} = .1914$$

$$t = \frac{\hat{\beta}_1}{S_{\hat{\beta}_1}} = \frac{.70}{.1914} = 3.657$$

Test of Slope Coefficient Solution

- **H_0: $\beta_1 = 0$**
- **H_a: $\beta_1 \neq 0$**
- **$\alpha = .05$**
- **df = 5 - 2 = 3**
- **Critical Value(s):**



Test Statistic: $$t = \frac{\hat{\beta}_1}{S_{\hat{\beta}_1}} = \frac{.70}{.1914} = 3.657$$

Decision: **Reject 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

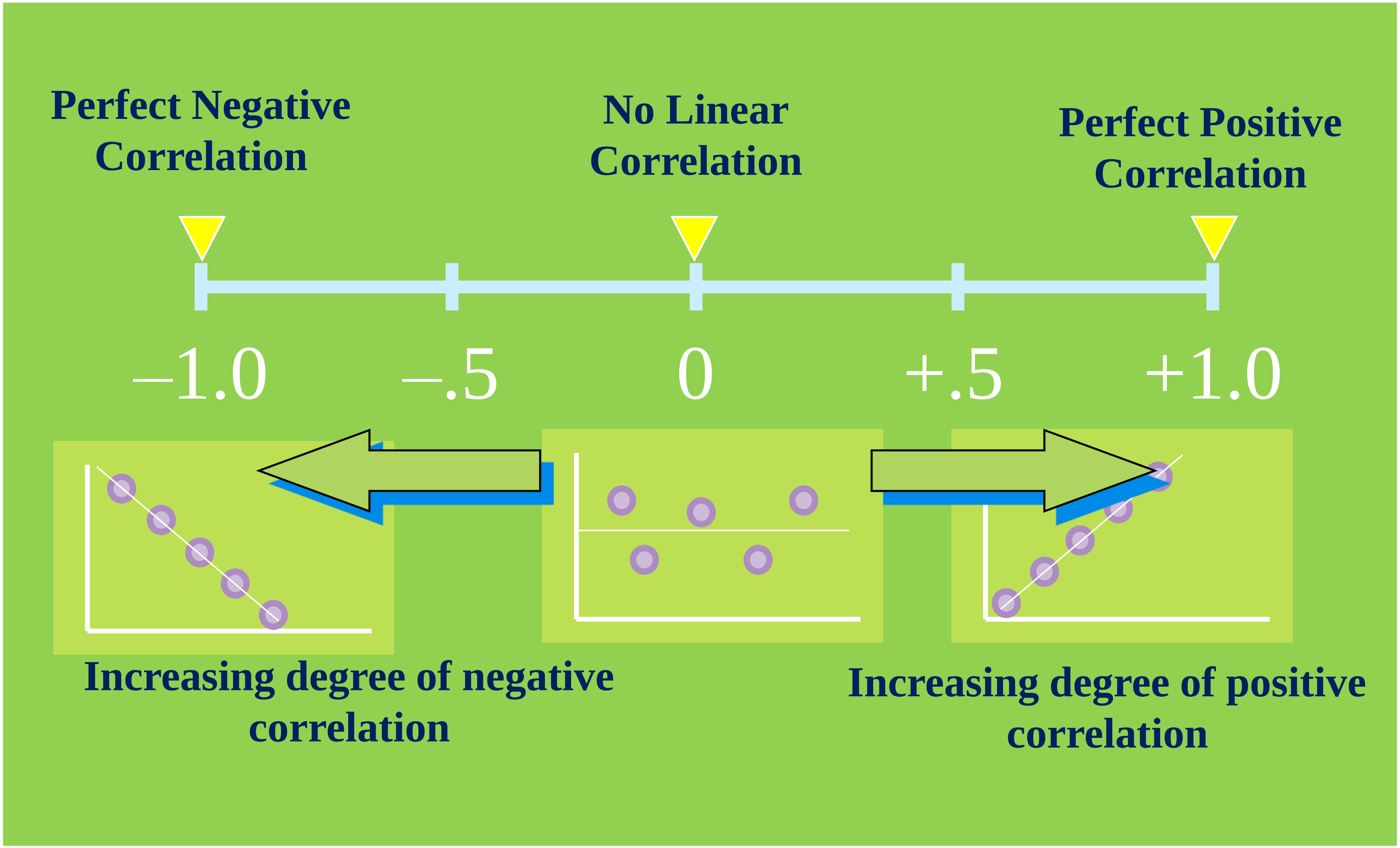
$$r = \frac{SS_{xy}}{\sqrt{SS_{xx}SS_{yy}}}$$

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

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

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

Correlation Coefficient Values

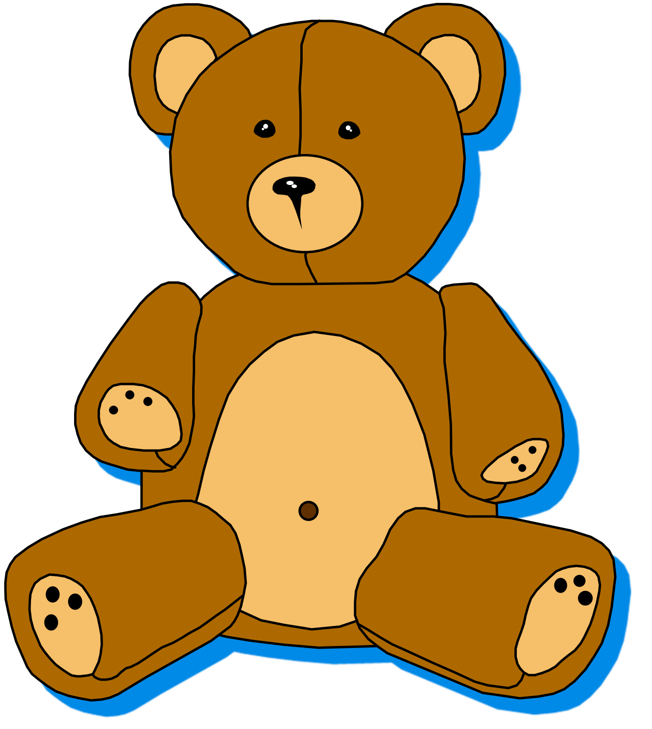


E.g. Coefficient of Correlation

You're a marketing analyst for any Toys.

Ad (₹)	Sales (Qty)
1	1
2	1
3	2
4	2
5	4

Calculate the **coefficient of correlation**.



Solution Table

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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

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

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

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

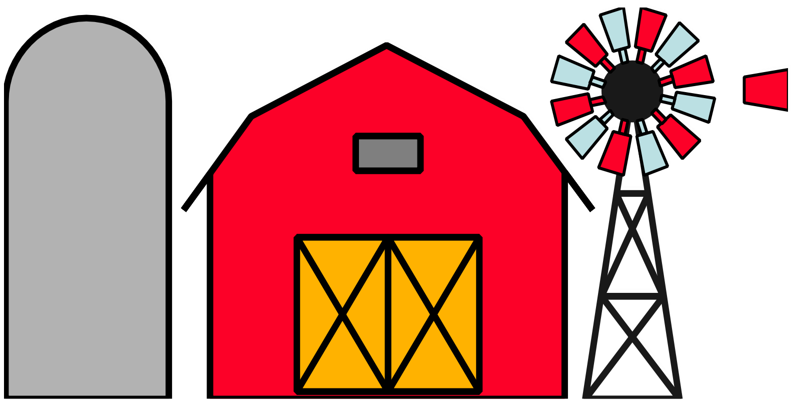
$$r = \frac{SS_{xy}}{\sqrt{SS_{xx} SS_{yy}}} = \frac{7}{\sqrt{10 \cdot 6}} = .904$$

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
12	9.0



Find the **coefficient of correlation**.

Solution Table*

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*

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

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

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

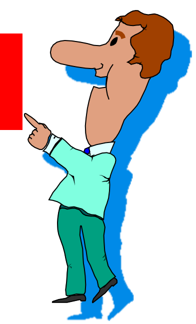
$$r = \frac{SS_{xy}}{\sqrt{SS_{xx} SS_{yy}}} = \frac{26}{\sqrt{40 \cdot 18.5}} = .956$$

Coefficient of Determination

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

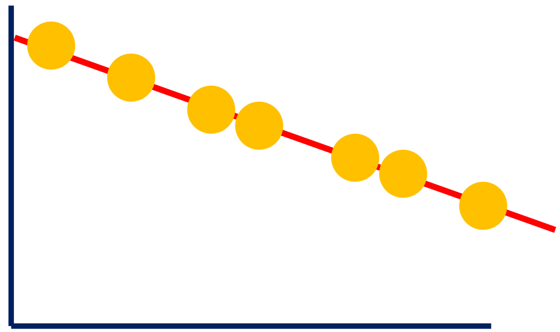
$$r^2 = \frac{\text{Explained Variation}}{\text{Total Variation}} = \frac{SS_{yy} - SSE}{SS_{yy}}$$

$\mathbf{0 \le r^2 \le 1}$

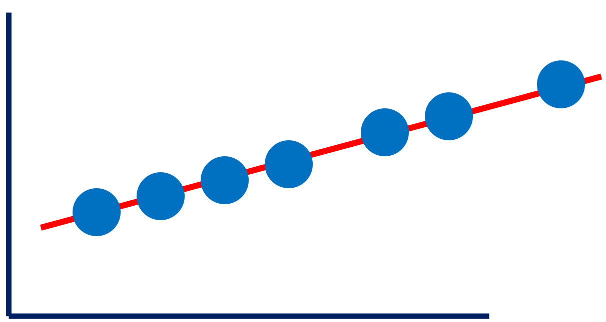


r^2 = (coefficient of correlation)^2

E.g. Approximate r^2 Values



$r^2 = 1$



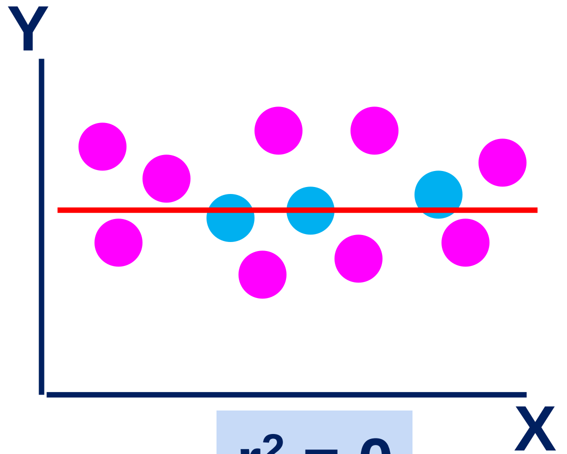
$r^2 = 1$

$r^2 = 1$

Perfect linear relationship between X and Y:

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

E.g. Approximate r^2 Values…



$r^2 = 0$

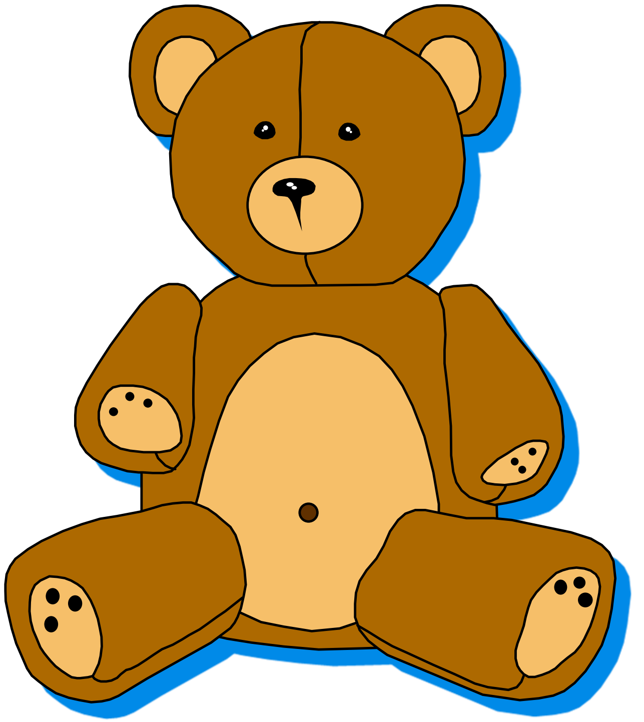
$r^2 = 0$

- 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 $r = .904$.

Ad (₹)	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)^2
$r^2 = (.904)^2$
$r^2 = .817$

Interpretation: About 81.7% of the sample variation in Sales (y) can be explained by using Ad ₹ (x) to predict Sales (y) in the linear model.

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