

# Regression

# Models

- Representation of some phenomenon
- Mathematical model is a mathematical expression of some phenomenon
- Often describe relationships between variables
- Types
  - Deterministic models
  - Probabilistic models

# Deterministic Models

- Hypothesize exact relationships
- Suitable when prediction error is negligible
- Example: force is exactly mass times acceleration
  - $F = m \cdot a$

# Probabilistic Models

Hypothesize two components

Deterministic

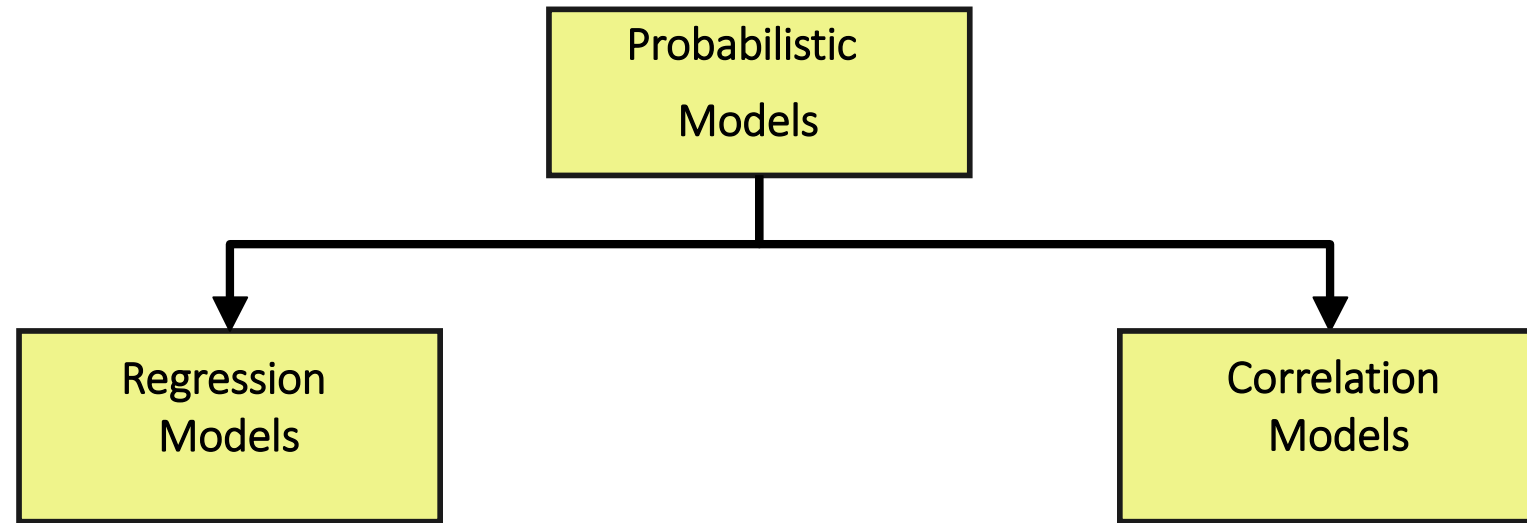
Random error

**Example:** sales volume ( $y$ ) is 10 times advertising spending ( $x$ ) + random error

$$y = 10x + \varepsilon$$

Random error may be due to factors other than advertising

# Types



# Regression Models

- Answers ‘What is the relationship between the variables?’
- Equation used
  - One numerical dependent (response) variable
    - What is to be predicted
  - One or more numerical or categorical independent (explanatory) variables
- Used mainly for prediction and estimation

# 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

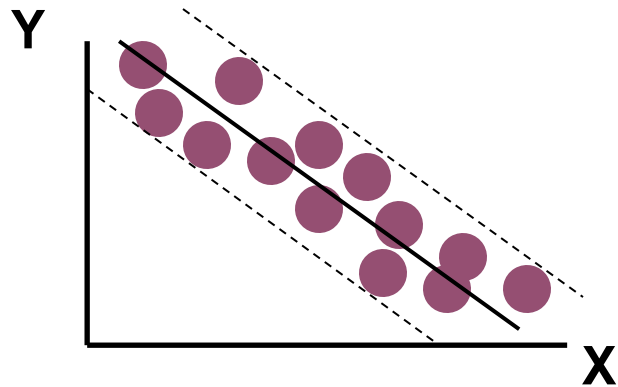
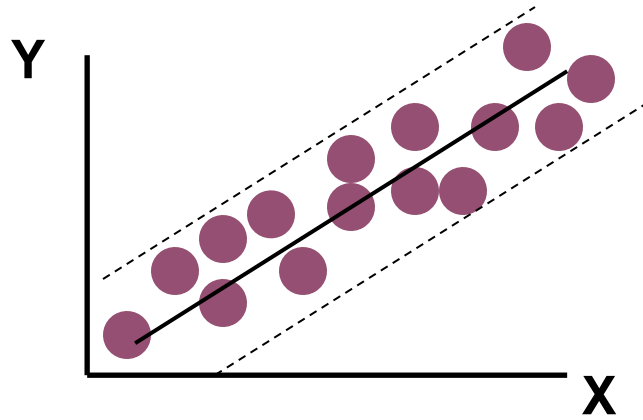
# Specifying the Model

1. Define variables
  1. Conceptual (e.g., Advertising, price)
  2. Empirical (e.g., List price, regular price)
  3. Measurement (e.g., \$, Units)
2. Hypothesize nature of relationship
  1. Expected effects (i.e., Coefficients' signs)
  2. Functional form (linear or non-linear)
  3. Interactions

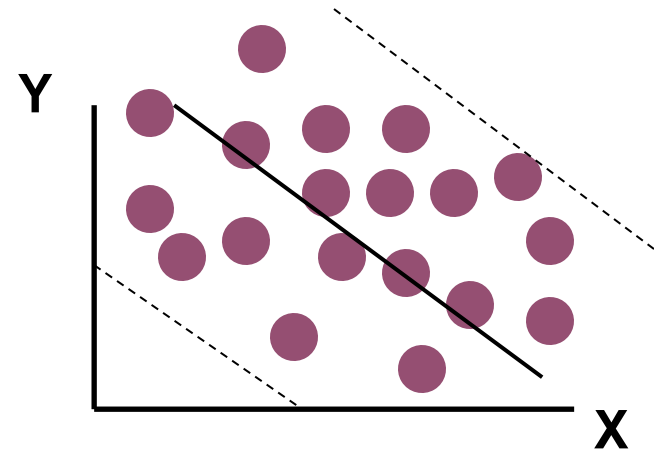
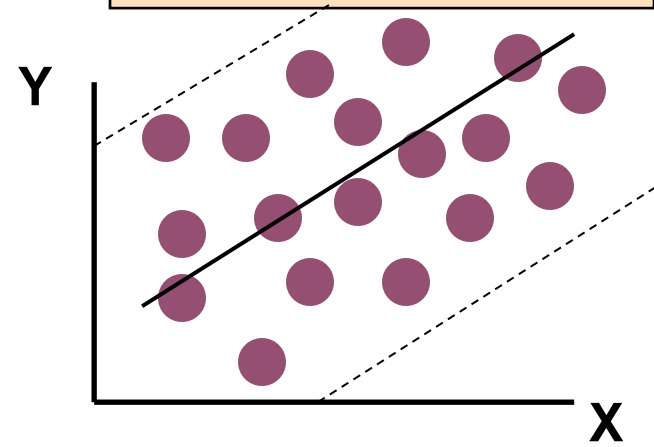


# Relationships

Strong relationships

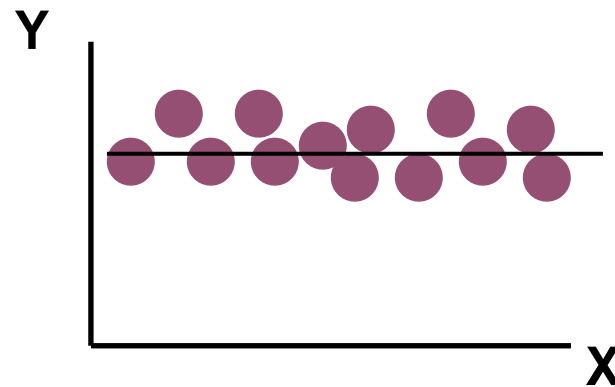
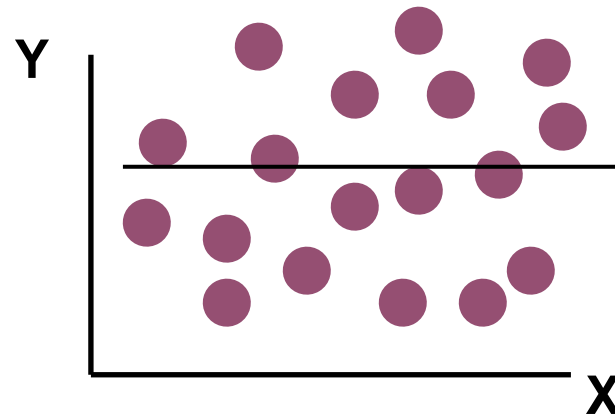


Weak relationships

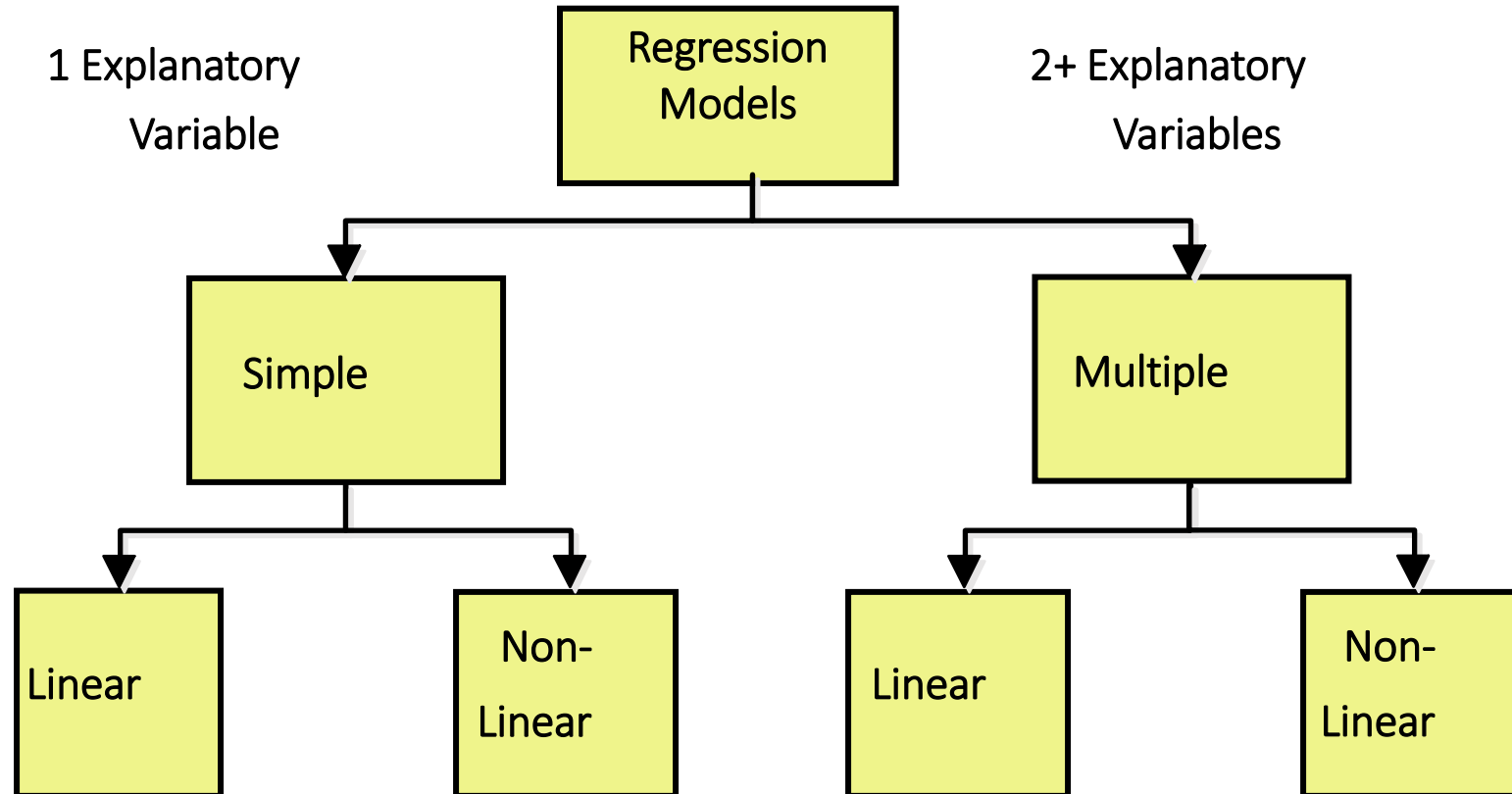


# Relationships

No relationship



# Types of Regression Models



# The Model

Relationship between variables is a linear function

The diagram illustrates the linear regression model equation  $y = \beta_0 + \beta_1 x + \epsilon$ . The equation is written in a dark red font. Five green arrows point from descriptive labels to the corresponding parts of the equation: 

- An arrow from "Dependent (Response) Variable" points to  $y$ .
- An arrow from "Population y-intercept" points to  $\beta_0$ .
- An arrow from "Population Slope" points to  $\beta_1$ .
- An arrow from "Independent (Explanatory) Variable" points to  $x$ .
- An arrow from "Random Error" points to  $\epsilon$ .

Population y-intercept

Population Slope

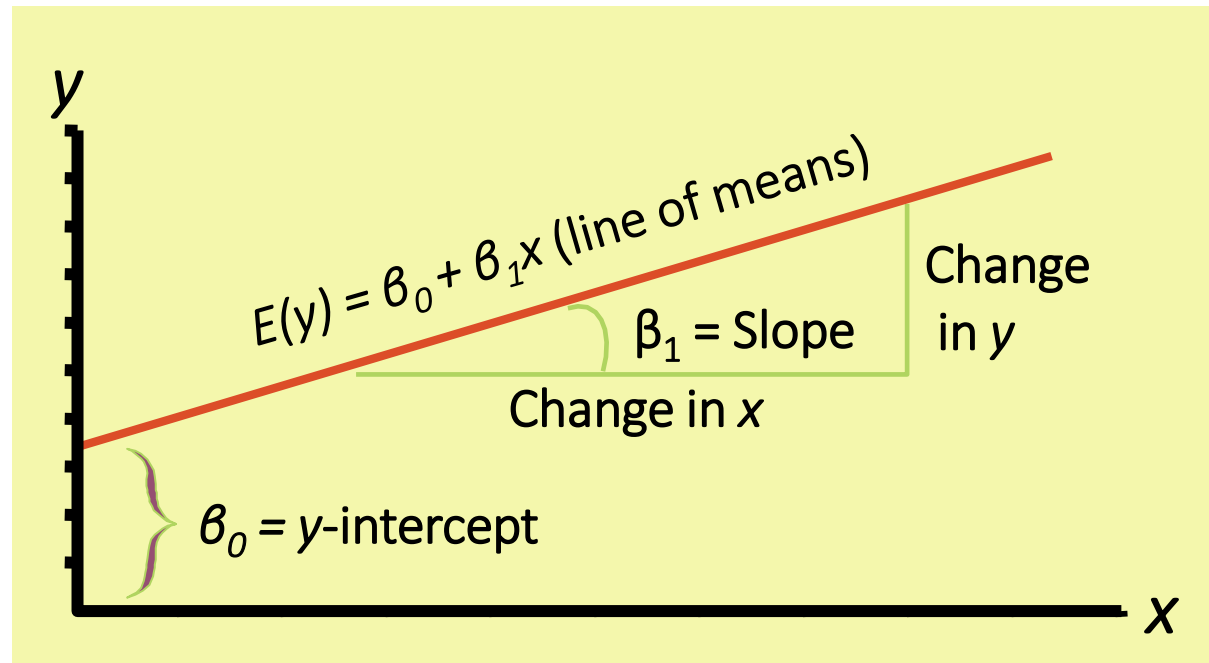
Random Error

Dependent (Response) Variable

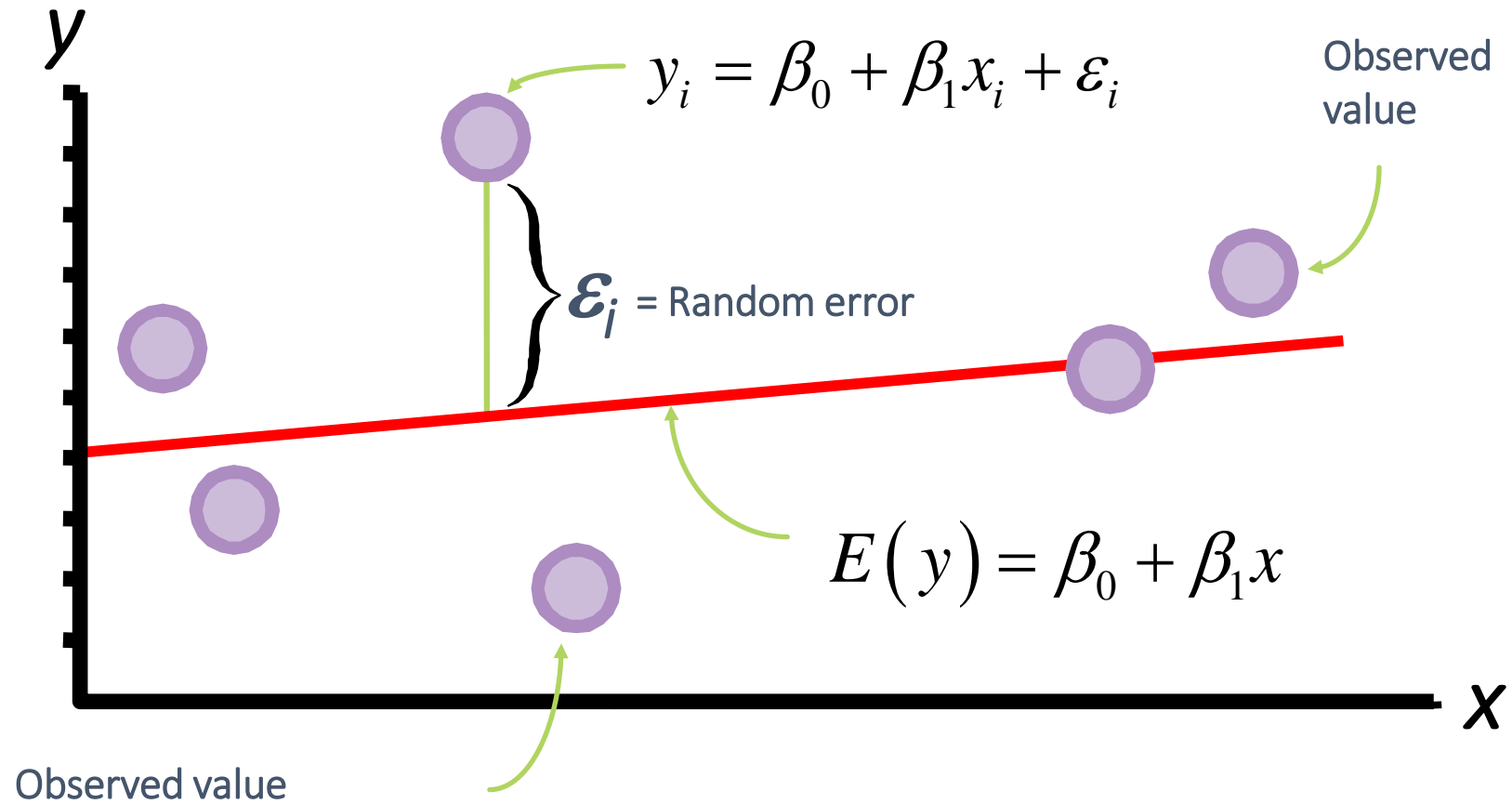
Independent (Explanatory) Variable

$$y = \beta_0 + \beta_1 x + \epsilon$$

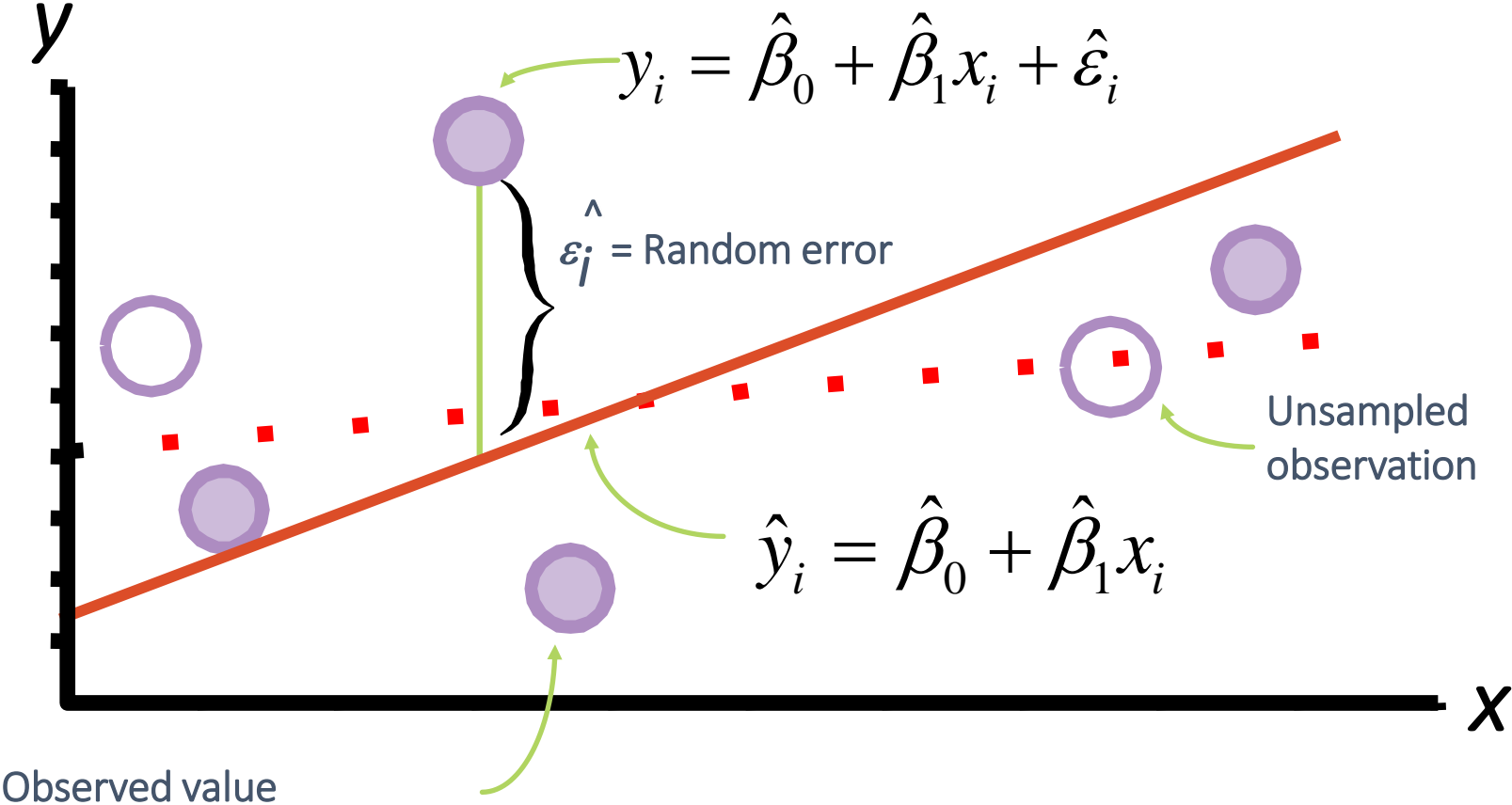
# The Model



# The Model

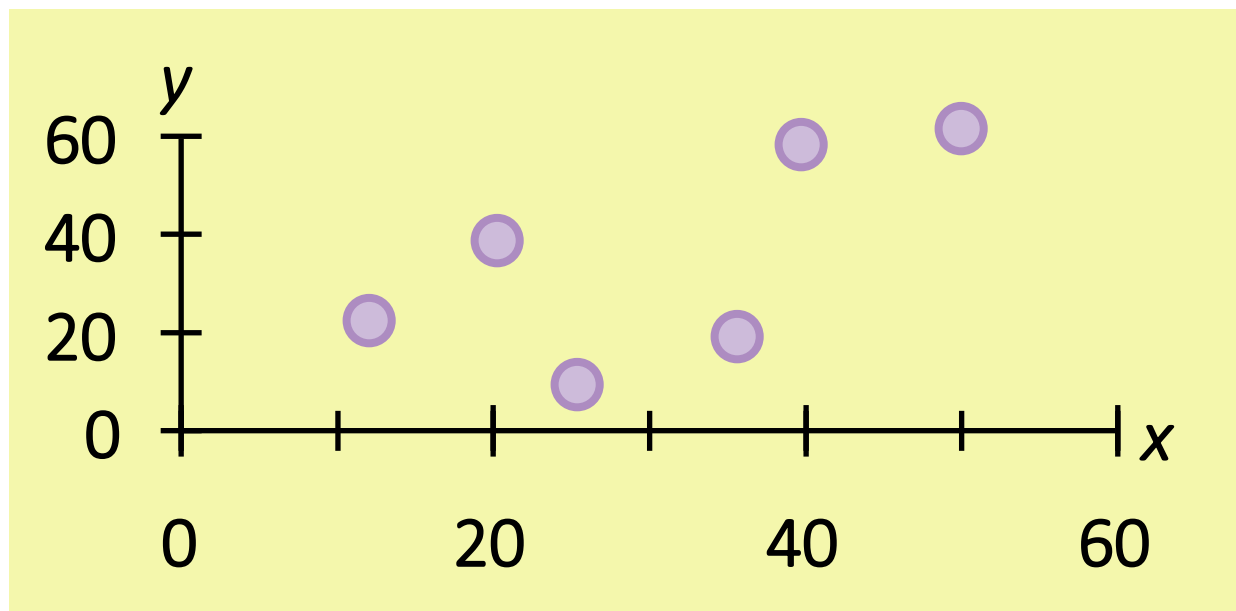


# The Model



# Estimating Parameters

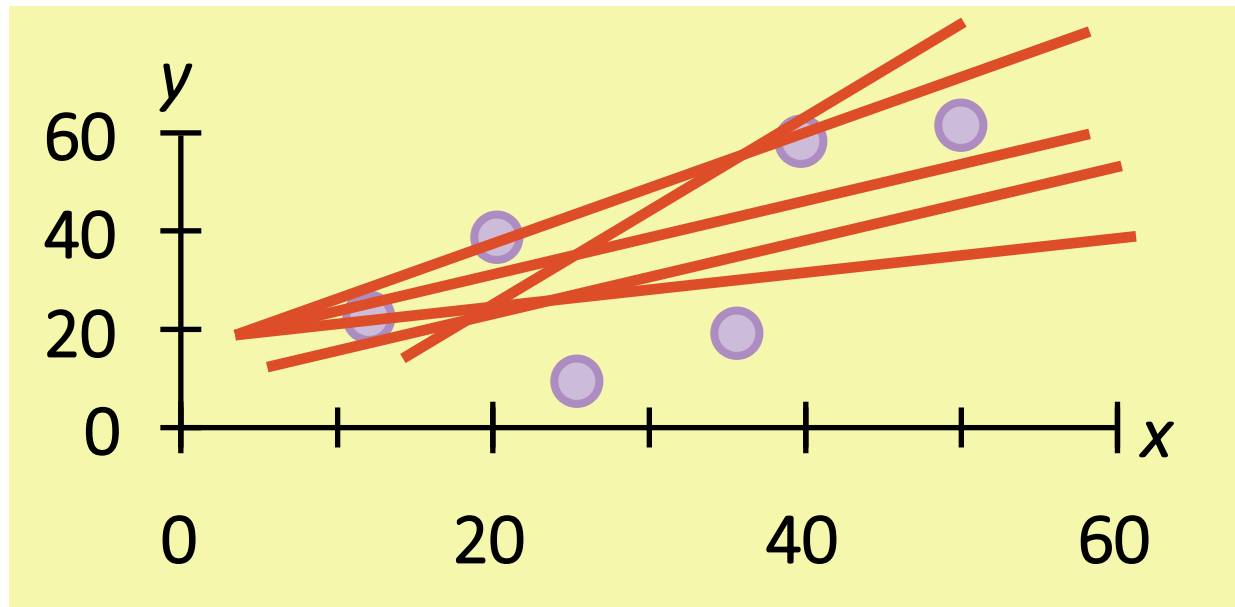
1. Plot of all  $(x_i, y_i)$  pairs
2. Suggests how well model will fit





# Estimating Parameters

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



# Estimating Parameters

‘Best fit’ means difference between actual  $y$  values and predicted  $y$  values are a minimum

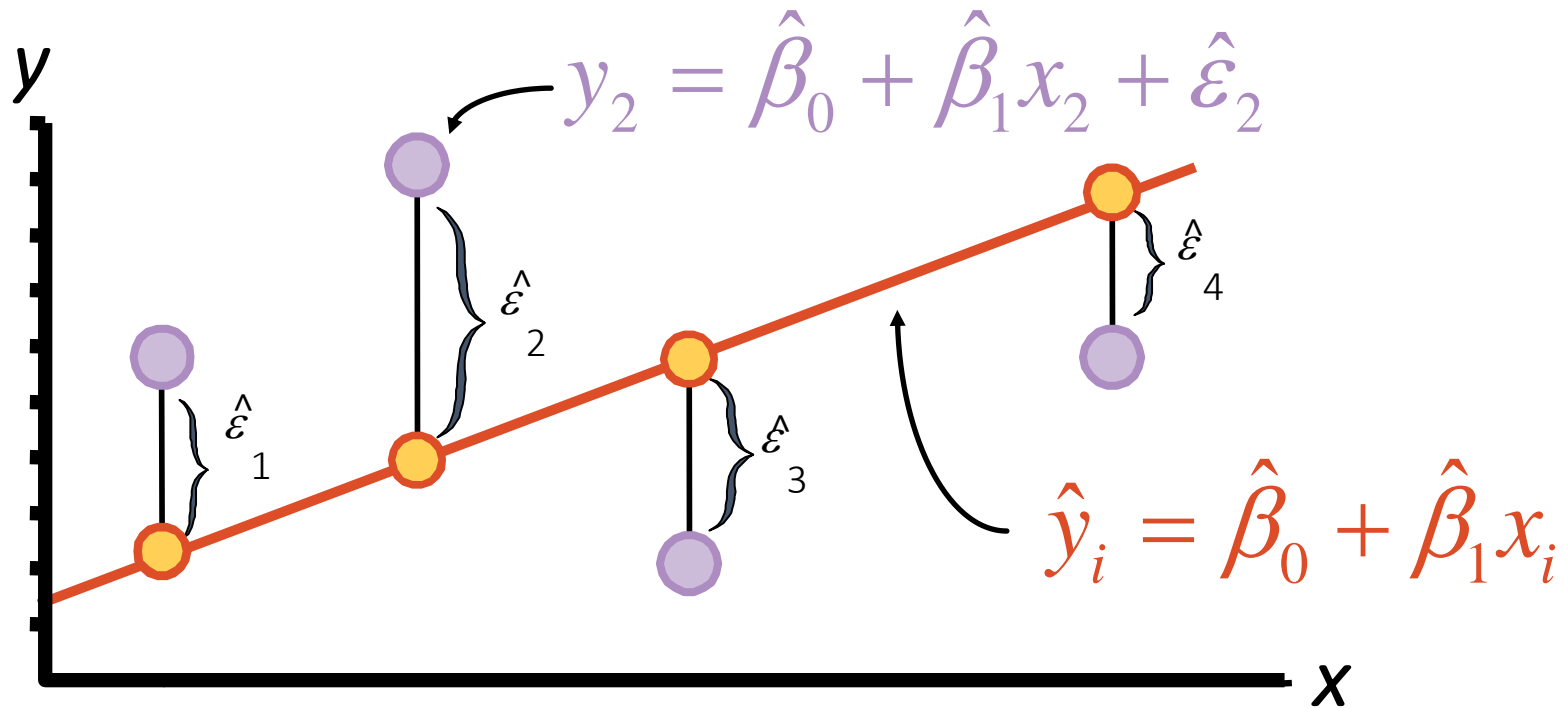
*But* positive differences off-set negative

$$\sum_{i=1}^n (y_i - \hat{y}_i)^2 = \sum_{i=1}^n \hat{\epsilon}_i^2$$

Least Squares minimizes the Sum of the Squared Differences (SSE)

# Estimating Parameters

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



# Estimating Parameters

Prediction Equation  $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$

Slope 
$$\hat{\beta}_1 = \frac{SS_{xy}}{SS_{xx}} = \frac{\sum_{i=1}^n x_i y_i - \frac{\left(\sum_{i=1}^n x_i\right)\left(\sum_{i=1}^n y_i\right)}{n}}{\sum_{i=1}^n x_i^2 - \frac{\left(\sum_{i=1}^n x_i\right)^2}{n}}$$

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

# Calculations

$$f(a, b) = a + b x,$$

$$R^2 \equiv \sum [y_i - f(x_i, a_1, a_2, \dots, a_n)]^2$$

$$R^2(a, b) \equiv \sum_{i=1}^n [y_i - (a + b x_i)]^2 \quad \frac{\partial(R^2)}{\partial a_i} = 0$$

$$\frac{\partial(R^2)}{\partial a} = -2 \sum_{i=1}^n [y_i - (a + b x_i)] = 0$$

$$\frac{\partial(R^2)}{\partial b} = -2 \sum_{i=1}^n [y_i - (a + b x_i)] x_i = 0.$$

# Calculations

$$\frac{\partial(R^2)}{\partial a} = -2 \sum_{i=1}^n [y_i - (a + b x_i)] = 0$$

$$\frac{\partial(R^2)}{\partial b} = -2 \sum_{i=1}^n [y_i - (a + b x_i)] x_i = 0.$$

$$n a + b \sum_{i=1}^n x_i$$
$$a \sum_{i=1}^n x_i + b \sum_{i=1}^n x_i^2$$

$$\begin{bmatrix} n & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^n y_i \\ \sum_{i=1}^n x_i y_i \end{bmatrix},$$

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} n & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 \end{bmatrix}^{-1} \begin{bmatrix} \sum_{i=1}^n y_i \\ \sum_{i=1}^n x_i y_i \end{bmatrix}.$$

# Calculations

$$\mathbf{A} \equiv \begin{bmatrix} a & b \\ c & d \end{bmatrix},$$

$$\mathbf{A}^{-1} = \frac{1}{|\mathbf{A}|} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

$$= \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}.$$

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} n & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 \end{bmatrix}^{-1} \begin{bmatrix} \sum_{i=1}^n y_i \\ \sum_{i=1}^n x_i y_i \end{bmatrix}.$$

$$\begin{bmatrix} a \\ b \end{bmatrix} = \frac{1}{n \sum_{i=1}^n x_i^2 - (\sum_{i=1}^n x_i)^2} \begin{bmatrix} \sum_{i=1}^n y_i \sum_{i=1}^n x_i^2 - \sum_{i=1}^n x_i \sum_{i=1}^n x_i y_i \\ n \sum_{i=1}^n x_i y_i - \sum_{i=1}^n x_i \sum_{i=1}^n y_i \end{bmatrix},$$

# Calculations

$$\begin{bmatrix} a \\ b \end{bmatrix} = \frac{1}{n \sum_{i=1}^n x_i^2 - (\sum_{i=1}^n x_i)^2} \begin{bmatrix} \sum_{i=1}^n y_i \sum_{i=1}^n x_i^2 - \sum_{i=1}^n x_i \sum_{i=1}^n x_i y_i \\ n \sum_{i=1}^n x_i y_i - \sum_{i=1}^n x_i \sum_{i=1}^n y_i \end{bmatrix}$$

$$\begin{aligned} a &= \frac{\sum_{i=1}^n y_i \sum_{i=1}^n x_i^2 - \sum_{i=1}^n x_i \sum_{i=1}^n x_i y_i}{n \sum_{i=1}^n x_i^2 - (\sum_{i=1}^n x_i)^2} \\ &= \frac{\bar{y} (\sum_{i=1}^n x_i^2) - \bar{x} \sum_{i=1}^n x_i y_i}{\sum_{i=1}^n x_i^2 - n \bar{x}^2} \\ b &= \frac{n \sum_{i=1}^n x_i y_i - \sum_{i=1}^n x_i \sum_{i=1}^n y_i}{n \sum_{i=1}^n x_i^2 - (\sum_{i=1}^n x_i)^2} \\ &= \frac{(\sum_{i=1}^n x_i y_i) - n \bar{x} \bar{y}}{\sum_{i=1}^n x_i^2 - n \bar{x}^2} \end{aligned}$$



# Calculations

$x_i$	$y_i$	$x_i^2$	$y_i^2$	$x_i y_i$
$x_1$	$y_1$	$x_1^2$	$y_1^2$	$x_1 y_1$
$x_2$	$y_2$	$x_2^2$	$y_2^2$	$x_2 y_2$
:	:	:	:	:
$x_n$	$y_n$	$x_n^2$	$y_n^2$	$x_n y_n$
$\Sigma x_i$	$\Sigma y_i$	$\Sigma x_i^2$	$\Sigma y_i^2$	$\Sigma x_i y_i$

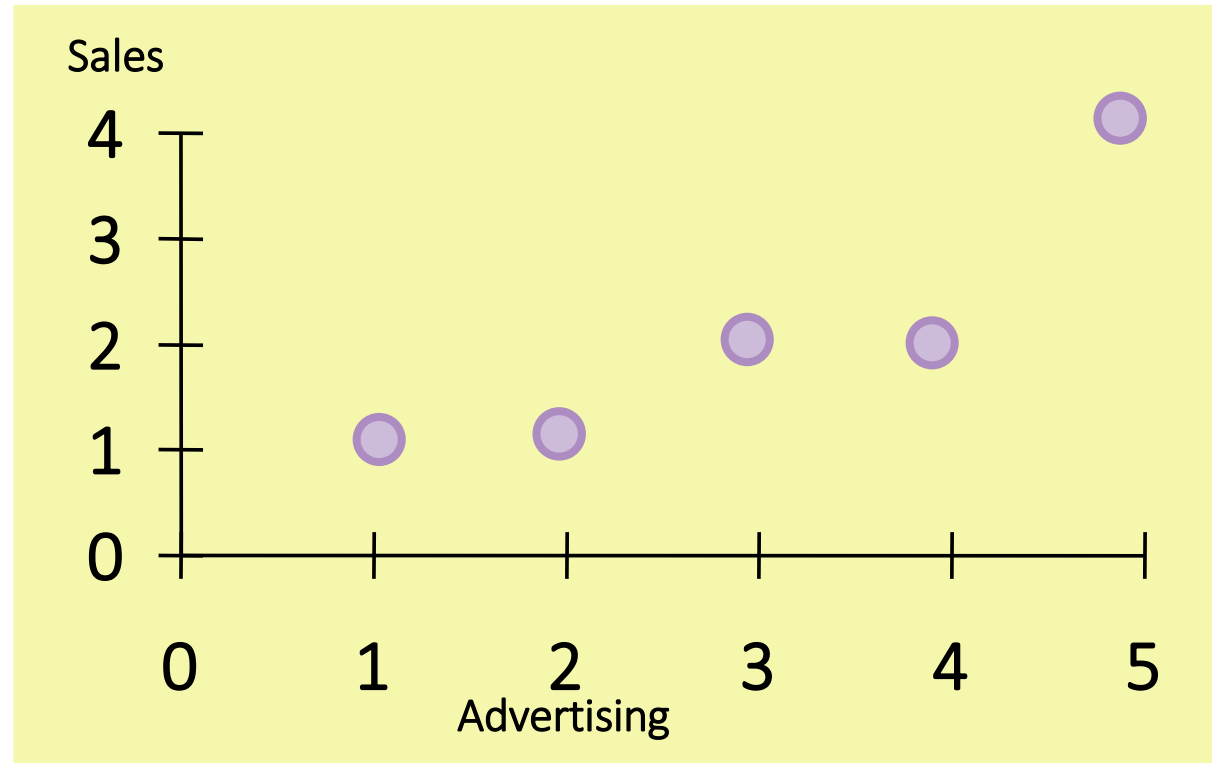
# Example

You gather the following data:

<u>Ad \$</u>	<u>Sales (Units)</u>
1	1
2	1
3	2
4	2
5	4

Find the **least squares line** relating sales and advertising

# Example



# Example

$x_i$	$y_i$	$x_i^2$	$y_i^2$	$x_i y_i$
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

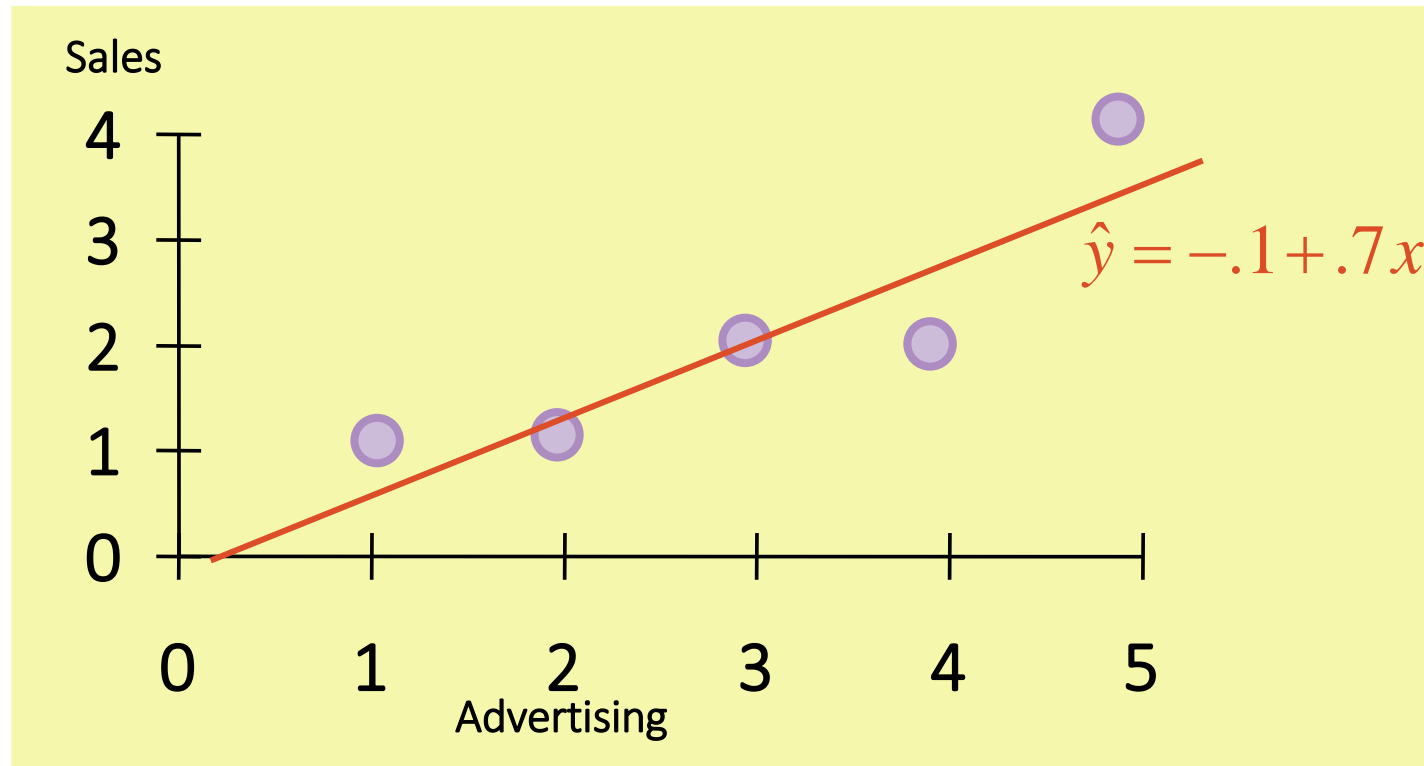
# Example

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n x_i y_i - \frac{\left(\sum_{i=1}^n x_i\right)\left(\sum_{i=1}^n y_i\right)}{n}}{\sum_{i=1}^n x_i^2 - \frac{\left(\sum_{i=1}^n x_i\right)^2}{n}} = \frac{37 - \frac{(15)(10)}{5}}{55 - \frac{(15)^2}{5}} = .70$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} = 2 - (.70)(3) = -.10$$

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

# Example



# Bayesian Learning

# Introduction

- A statistical classifier: performs *probabilistic prediction, i.e.*, predicts class membership probabilities
- Foundation: Based on Bayes' Theorem.
- Performance: A simple Bayesian classifier, *naïve Bayesian classifier*, has comparable performance with decision tree and selected neural network classifiers
- Incremental: Each training example can incrementally increase/decrease the probability that a hypothesis is correct — prior knowledge can be combined with observed data
- Standard: Even when Bayesian methods are computationally intractable, they can provide a standard of optimal decision making against which other methods can be measured



# The Model

A good strategy is to predict:

$$\arg \max_Y P(Y | X_1, \dots, X_n)$$

(for example: what is the probability that the image represents a 5 given its pixels?)

# The Model

Total probability Theorem: 
$$P(B) = \sum_{i=1}^M P(B|A_i)P(A_i)$$

Bayes' Theorem: 
$$P(H|\mathbf{X}) = \frac{P(\mathbf{X}|H)P(H)}{P(\mathbf{X})} = P(\mathbf{X}|H) \times P(H) / P(\mathbf{X})$$

- Let  $\mathbf{X}$  be a data sample (“*evidence*”): class label is unknown
- Let  $H$  be a *hypothesis* that  $X$  belongs to class  $C$
- Classification is to determine  $P(H|\mathbf{X})$ , (i.e., *posteriori probability*): the probability that the hypothesis holds given the observed data sample  $\mathbf{X}$
- $P(H)$  (*prior probability*): the initial probability
  - E.g.,  $\mathbf{X}$  will buy computer, regardless of age, income, ...
- $P(\mathbf{X})$ : probability that sample data is observed
- $P(\mathbf{X}|H)$  (*likelihood*): the probability of observing the sample  $\mathbf{X}$ , given that the hypothesis holds
  - E.g., Given that  $\mathbf{X}$  will buy computer, the prob. that  $X$  is 31..40, medium income

# The Model

- Given training data  $\mathbf{X}$ , *posteriori probability of a hypothesis*  $H$ ,  $P(H|\mathbf{X})$ , follows the Bayes' theorem

$$P(H|\mathbf{X}) = \frac{P(\mathbf{X}|H)P(H)}{P(\mathbf{X})} = P(\mathbf{X}|H) \times P(H) / P(\mathbf{X})$$

- Informally, this can be viewed as  
**posteriori = likelihood x prior/evidence**
- Predicts  $\mathbf{X}$  belongs to  $C_i$  iff the probability  $P(C_i|\mathbf{X})$  is the highest among all the  $P(C_k|\mathbf{X})$  for all the  $k$  classes
- Practical difficulty: It requires initial knowledge of many probabilities, involving significant computational cost

# The Model

- Let  $D$  be a training set of tuples and their associated class labels, and each tuple is represented by an  $n$ -D attribute vector  $\mathbf{X} = (x_1, x_2, \dots, x_n)$
- Suppose there are  $m$  classes  $C_1, C_2, \dots, C_m$ .
- Classification is to derive the maximum posteriori, i.e., the maximal  $P(C_i | \mathbf{X})$
- This can be derived from Bayes' theorem

$$P(C_i | \mathbf{X}) = \frac{P(\mathbf{X} | C_i)P(C_i)}{P(\mathbf{X})}$$

- Since  $P(\mathbf{X})$  is constant for all classes, only
  - needs to be maximized  $P(C_i | \mathbf{X}) = P(\mathbf{X} | C_i)P(C_i)$

# The Model

- A simplified assumption: attributes are conditionally independent (i.e., no dependence relation between attributes):

$$P(\mathbf{X} | C_i) = \prod_{k=1}^n P(x_k | C_i) = P(x_1 | C_i) \times P(x_2 | C_i) \times \dots \times P(x_n | C_i)$$

- This greatly reduces the computation cost: Only counts the class distribution
- If  $A_k$  is categorical,  $P(x_k | C_i)$  is the # of tuples in  $C_i$  having value  $x_k$  for  $A_k$  divided by  $|C_{i,D}|$  (# of tuples of  $C_i$  in  $D$ )
- If  $A_k$  is continuous-valued,  $P(x_k | C_i)$  is usually computed based on Gaussian distribution with a mean  $\mu$  and standard deviation  $\sigma$

and  $P(x_k | C_i)$  is

$$g(x, \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

$$P(\mathbf{X} | C_i) = g(x_k, \mu_{C_i}, \sigma_{C_i})$$

# Example

Class:

C1:buys\_computer = 'yes'

C2:buys\_computer = 'no'

Data to be classified:

X = (age <=30,

Income = medium,

Student = yes

Credit\_rating = Fair)

age	income	student	credit_rating	comp
<=30	high	no	fair	no
<=30	high	no	excellent	no
31...40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31...40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31...40	medium	no	excellent	yes
31...40	high	yes	fair	yes
>40	medium	no	excellent	no

# Example

$$P(C_i): P(\text{buys\_computer} = \text{"yes"}) = 9/14 = 0.643$$
$$P(\text{buys\_computer} = \text{"no"}) = 5/14 = 0.357$$

Compute  $P(X|C_i)$  for each class

$$P(\text{age} = \text{"<=30"} \mid \text{buys\_computer} = \text{"yes"}) = 2/9 = 0.222$$

$$P(\text{age} = \text{"<= 30"} \mid \text{buys\_computer} = \text{"no"}) = 3/5 = 0.6$$

$$P(\text{income} = \text{"medium"} \mid \text{buys\_computer} = \text{"yes"}) = 4/9 = 0.444$$

$$P(\text{income} = \text{"medium"} \mid \text{buys\_computer} = \text{"no"}) = 2/5 = 0.4$$

$$P(\text{student} = \text{"yes"} \mid \text{buys\_computer} = \text{"yes"}) = 6/9 = 0.667$$

$$P(\text{student} = \text{"yes"} \mid \text{buys\_computer} = \text{"no"}) = 1/5 = 0.2$$

$$P(\text{credit\_rating} = \text{"fair"} \mid \text{buys\_computer} = \text{"yes"}) = 6/9 = 0.667$$

$$P(\text{credit\_rating} = \text{"fair"} \mid \text{buys\_computer} = \text{"no"}) = 2/5 = 0.4$$

**$X = (\text{age} \leq 30, \text{income} = \text{medium}, \text{student} = \text{yes}, \text{credit\_rating} = \text{fair})$**

$$P(X|C_i): P(X \mid \text{buys\_computer} = \text{"yes"}) = 0.222 \times 0.444 \times 0.667 \times 0.667 = 0.044$$

$$P(X \mid \text{buys\_computer} = \text{"no"}) = 0.6 \times 0.4 \times 0.2 \times 0.4 = 0.019$$

$$P(X|C_i) * P(C_i): P(X \mid \text{buys\_computer} = \text{"yes"}) * P(\text{buys\_computer} = \text{"yes"}) = 0.028$$

$$P(X \mid \text{buys\_computer} = \text{"no"}) * P(\text{buys\_computer} = \text{"no"}) = 0.007$$

Therefore,  $X$  belongs to class (**"buys\_computer = yes"**)

age	income	student	credit_rating	com
<=30	high	no	fair	no
<=30	high	no	excellent	no
31...40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31...40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31...40	medium	no	excellent	yes
31...40	high	yes	fair	yes
>40	medium	no	excellent	no

# Avoiding Zero Probability

- Naïve Bayesian prediction requires each conditional prob. be **non-zero**. Otherwise, the predicted prob. will be zero

$$P(X | C_i) = \prod_{k=1}^n P(x_k | C_i)$$

- Ex. Suppose a dataset with 1000 tuples, income=low (0), income=medium (990), and income = high (10)
- Use **Laplacian correction** (or Laplacian estimator)
  - *Adding 1 to each case*
    - Prob(income = low) = 1/1003
    - Prob(income = medium) = 991/1003
    - Prob(income = high) = 11/1003
  - The “corrected” prob. estimates are close to their “uncorrected” counterparts



# Comments

- Advantages
  - Easy to implement
  - Good results obtained in most of the cases
- Disadvantages
  - Assumption: class conditional independence, therefore loss of accuracy
  - Practically, dependencies exist among variables
    - E.g., hospitals: patients: Profile: age, family history, etc.
      - Symptoms: fever, cough etc., Disease: lung cancer, diabetes, etc.
    - Dependencies among these cannot be modeled by Naïve Bayes Classifier