# VBM683 Machine Learning

Pinar Duygulu

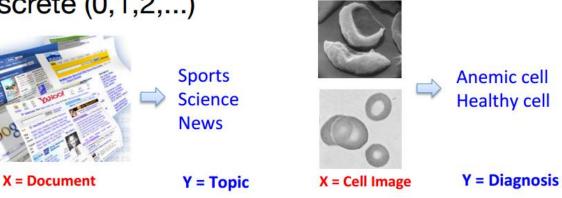
Slides are adapted from Dhruv Batra, Aarti Singh, Barnabas Poczos, Wenjiang Fu Aykut Erdem

#### Classification

- Input: X
  - Real valued, vectors over real.
  - Discrete values (0,1,2,...)
  - Other structures (e.g., strings, graphs, etc.)
- Output: Y

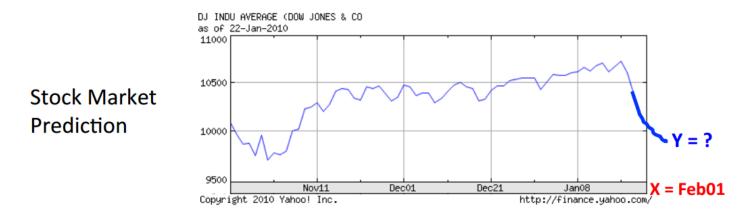
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- Discrete (0,1,2,...)



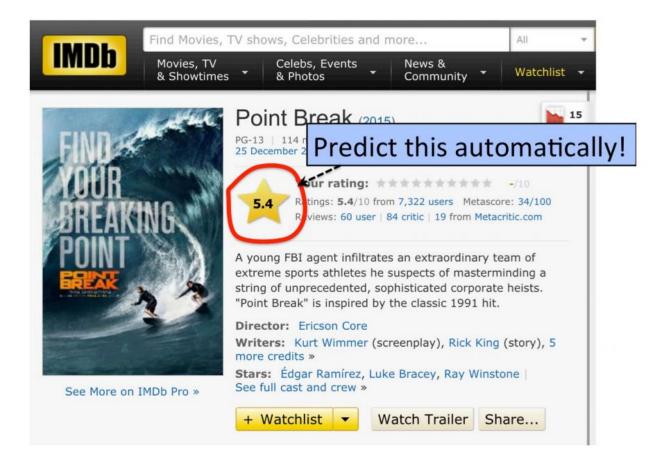
# Regression

- Input: X
  - Real valued, vectors over real.
  - Discrete values (0,1,2,...)
  - Other structures (e.g., strings, graphs, etc.)
- Output: Y
  - Real valued, vectors over real.

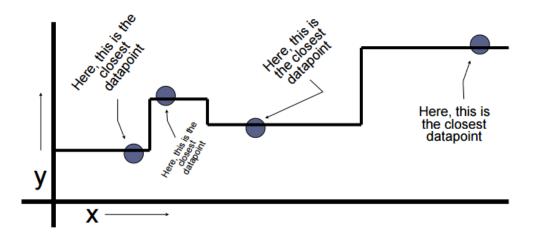


slide by Aarti Singh and Barnabas Poczo:

### What should I watch tonight?



### 1-NN for Regression

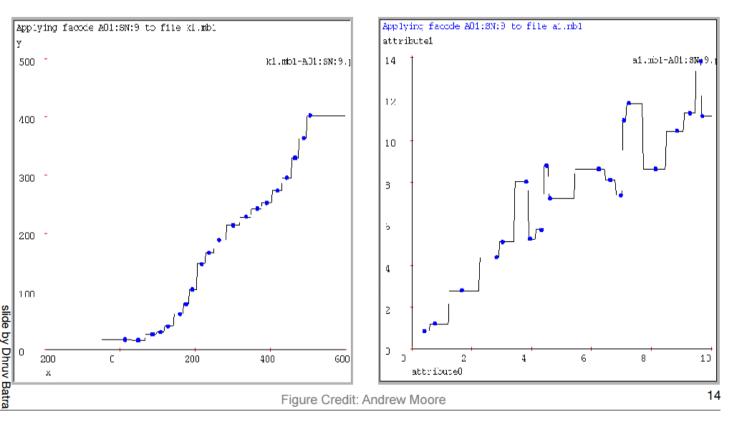


slide by Dhruv Batra

Figure Credit: Carlos Guestrin

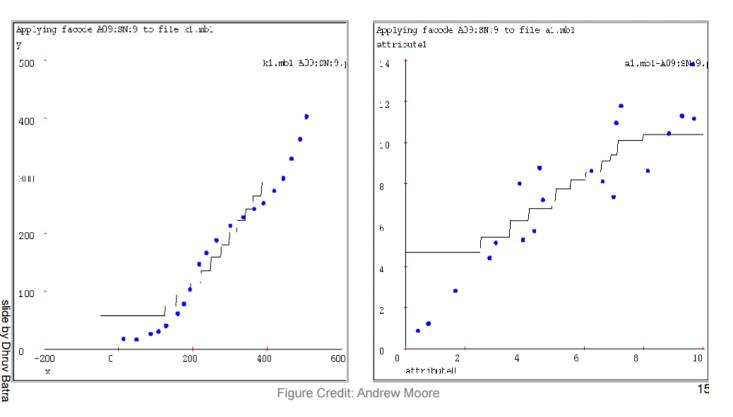
#### **1-NN for Regression**

• Often bumpy (overfits)

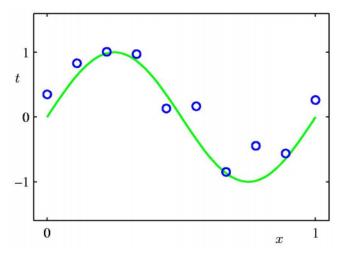


#### 9-NN for Regression

• Often bumpy (overfits)



# Simple 1-D Regression



- Circles are data points (i.e., training examples) that are given to us
- The data points are uniform in x, but may be displaced in y

$$t(x) = f(x) + \varepsilon$$

with  $\varepsilon$  some noise

In green is the "true" curve that we don't know

slide by Sanja Fidle

#### What is a Model?

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

Wenjiang Fu

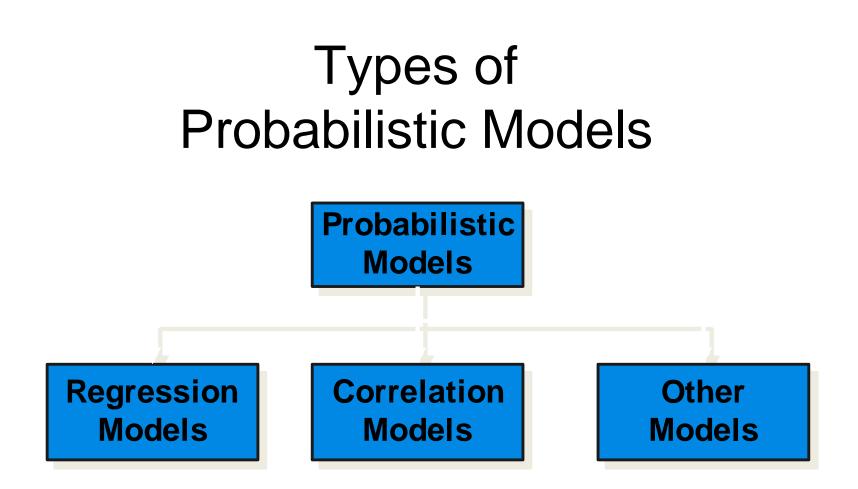
### **Deterministic Models**

- 1. Hypothesize Exact Relationships
- 2. Suitable When Prediction Error is Negligible
- 3. Example: Body mass index (BMI) is measure of body fat based

 $- BMI = \frac{Weight in Kilograms}{(Height in Meters)^2}$ 

## **Probabilistic Models**

- 1. Hypothesize 2 Components
  - Deterministic
  - Random Error
- 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. Birthweight)



#### Simple Regression

- Simple regression analysis is a statistical tool that gives us the ability to estimate the mathematical relationship between a dependent variable (usually called y) and an independent variable (usually called x).
- The dependent variable is the variable for which we want to make a prediction.
- While various non-linear forms may be used, simple linear regression models are the most common.

#### Introduction

- The primary goal of quantitative analysis is to use current information about a phenomenon to predict its future behavior.
- Current information is usually in the form of a set of data.
- In a simple case, when the data form a set of pairs of numbers, we may interpret them as representing the observed values of an independent (or predictor or explanatory) variable X and a dependent ( or response or outcome) variable Y.

lot size	Man-hours	
30	73	
20	50	
60	128	
80	170	
40	87	
50	108	
60	135	
30	69	
70	148	
60	132	

#### Introduction

Statistical relation between Lot size and Man-Hour

The goal of the analyst who studies 180 the data is to find a functional 160 relation 140 8 between the response variable y 120 and the predictor variable x. 00 Man-Hour 80 y = f(x)60 . 40 20

0 + 0

10

20

30

40

Lot size

50

60

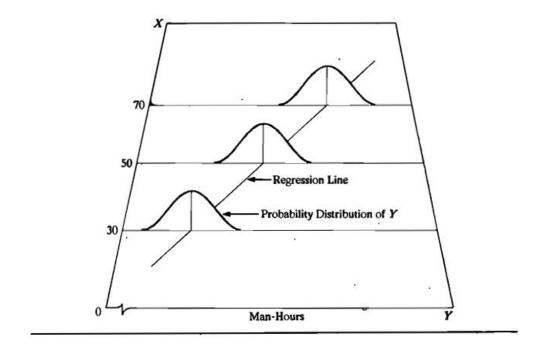
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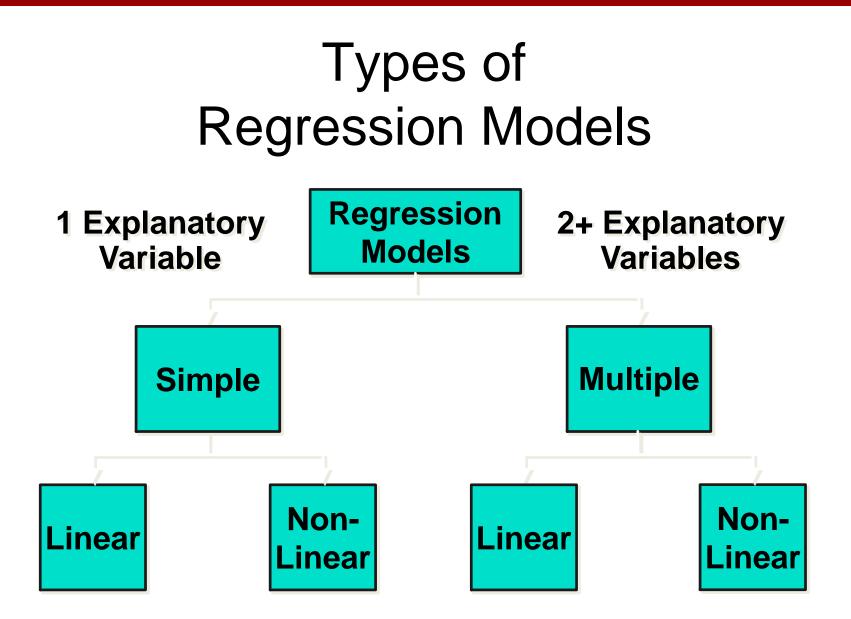
80

90

٠

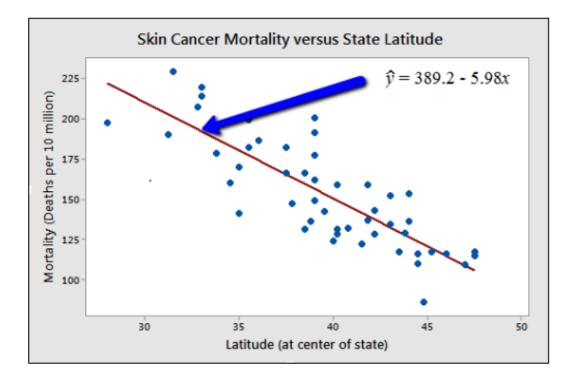
#### Pictorial Presentation of Linear Regression Model





# Linear Regression Model

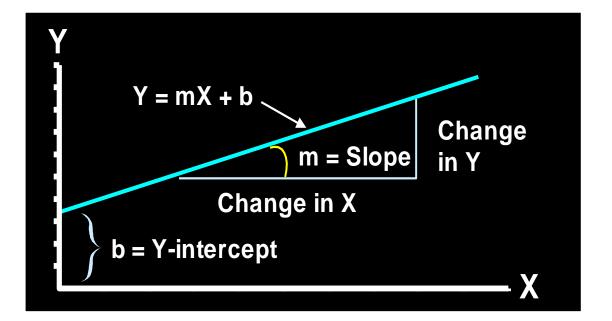
Wenjiang Fu



#### Assumptions

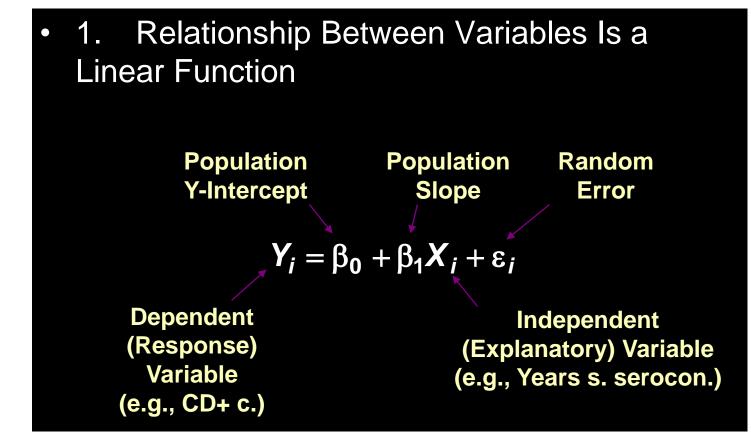
- Linear regression assumes that...
  - The relationship between X and Y is linear
  - 2. Y is distributed normally at each value of X
  - 3. The variance of Y at every value of X is the same (homogeneity of variances)
  - 4. The observations are independent

#### **Linear Equations**



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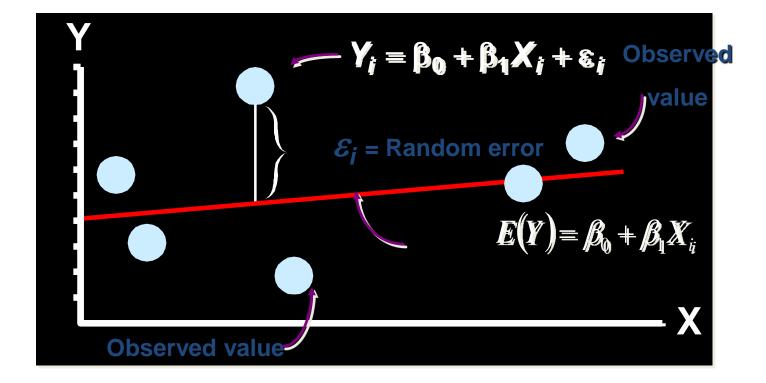
#### **Linear Regression Model**



#### Meaning of Regression Coefficients

- General regression model
  - 1.  $\beta_0$ , and  $\beta_1$  are parameters
  - 2. X is a known constant
  - 3. Deviations  $\varepsilon$  are independent N(o,  $\sigma^2$ )
- The values of the regression parameters  $\beta_0$ , and  $\beta_1$  are not known. We estimate them from data.
- $\beta_1$  indicates the change in the mean response per unit increase in X.

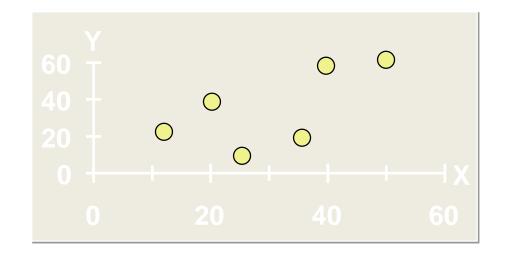
Population Linear Regression Model



Estimating Parameters: Least Squares Method

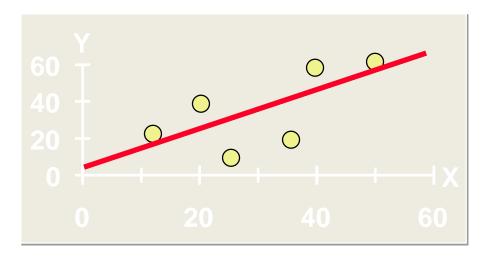
#### Scatter plot

- 1. Plot of All  $(X_i, Y_j)$  Pairs
- 2. Suggests How Well Model Will Fit

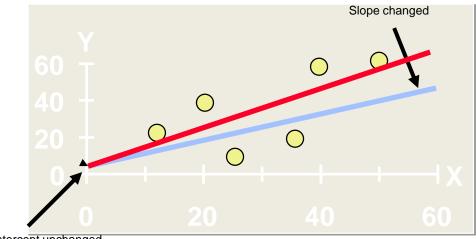


#### Thinking Challenge

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



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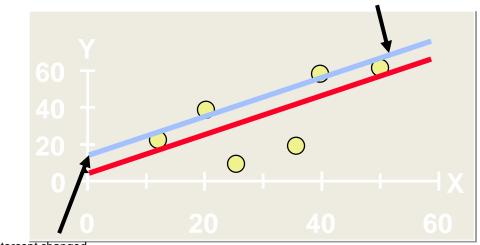


Intercept unchanged

### Thinking Challenge

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

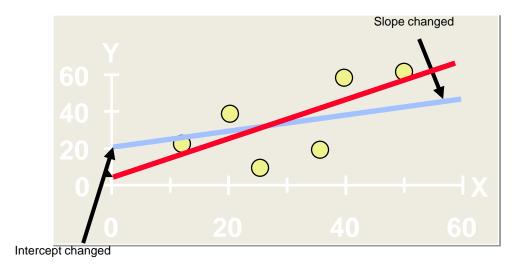
Slope unchanged



Intercept changed

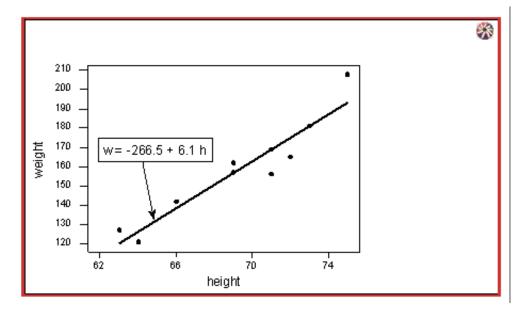
#### Thinking Challenge

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



#### What is the best fitting line

i	$x_i$	$y_i$	$\hat{y}_i$	
1	63	127	120.1	
2	64	121	126.3	
3	66	142	138.5	
4	69	157	157.0	
5	69	162	157.0	
6	71	156	169.2	
7	71	169	169.2	
8	72	165	175.4	
9	73	181	181.5	
10	75	208	193.8	



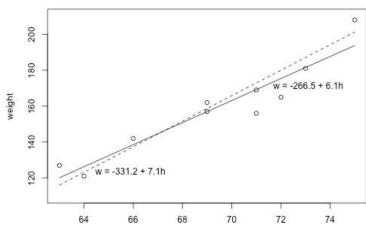
- y<sub>i</sub> denotes the observed response for experimental unit i
- x<sub>i</sub> denotes the predictor value for experimental unit i
- $\hat{y}_i$  is the predicted response (or fitted value) for experimental unit *i*

 $\hat{y}_i = b_0 + b_1 x_i$ 

#### **Prediction Error**

1						
	w = -331.2 + 7.1 h (the dashed line)					
	i	$x_i$	$y_i$	$\hat{y}_i$	$(y_i - \hat{y}_i)$	$(y_i - {\hat y}_i)^2$
	1	63	127	116.1	10.9	118.81
	2	64	121	123.2	-2.2	4.84
	3	66	142	137.4	4.6	21.16
	4	69	157	158.7	-1.7	2.89
	5	69	162	158.7	3.3	10.89
0	6	71	156	172.9	-16.9	285.61
	7	71	169	172.9	-3.9	15.21
	8	72	165	180.0	-15.0	225.00
6.1h	9	73	181	187.1	-6.1	37.21
	10	75	208	201.3	6.7	44.89
						766.5

w = -266.53 + 6.1376 h (the solid line)					
i	$x_i$	$y_i$	$\hat{y}_i$	$(y_i - \hat{y}_i)$	$(y_i - {\hat y}_i)^2$
1	63	127	120.139	6.8612	47.076
2	64	121	126.276	-5.2764	27.840
3	66	142	138.552	3.4484	11.891
4	69	157	156.964	0.0356	0.001
5	69	162	156.964	5.0356	25.357
6	71	156	169.240	-13.2396	175.287
7	71	169	169.240	-0.2396	0.057
8	72	165	175.377	-10.3772	107.686
9	73	181	181.515	-0.5148	0.265
10	75	208	193.790	14.2100	201.924
					597.4





 $e_i = y_i - \hat{y}_i$ 

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

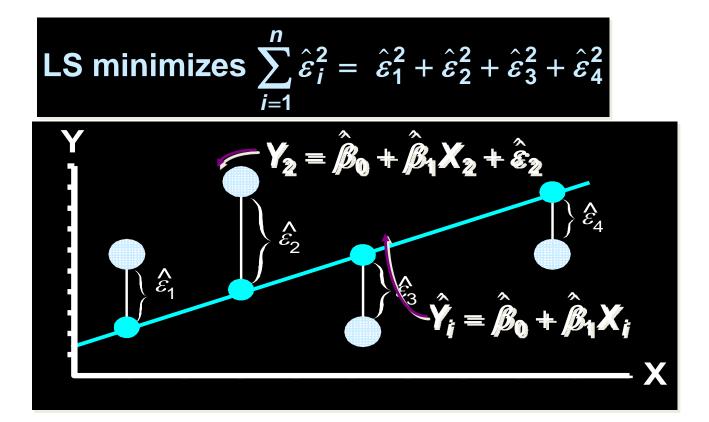
## Least Squares

 1. 'Best Fit' Means Difference Between Actual Y Values & Predicted Y Values Are a Minimum. *But* Positive Differences Off-Set Negative. So square errors!

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

• 2. LS Minimizes the Sum of the Squared Differences (errors) (SSE)

#### Least Squares Graphically



### **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 (1)

Least Squares (L-S):

Minimize squared error

$$\sum_{i=1}^{n} \varepsilon_{i}^{2} = \sum_{i=1}^{n} (y_{i} - \beta_{0} - \beta_{1} x_{i})^{2}$$

$$0 = \frac{\partial \sum \varepsilon_i^2}{\partial \beta_0} = \frac{\partial \sum (y_i - \beta_0 - \beta_1 x_i)^2}{\partial \beta_0}$$
$$= -2(n\overline{y} - n\beta_0 - n\beta_1 \overline{x})$$

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

# Derivation of Parameters (1)

 Least Squares (L-S): Minimize squared error

$$0 = \frac{\partial \sum \varepsilon_i^2}{\partial \beta_1} = \frac{\partial \sum (y_i - \beta_0 - \beta_1 x_i)^2}{\partial \beta_1}$$
$$= -2\sum x_i (y_i - \beta_0 - \beta_1 x_i)$$
$$= -2\sum x_i (y_i - \overline{y} + \beta_1 \overline{x} - \beta_1 x_i)$$

$$\beta_{1}\sum_{x_{i}} x_{i} (x_{i} - \overline{x}) = \sum_{x_{i}} x_{i} (y_{i} - \overline{y})$$
$$\beta_{1}\sum_{x_{i}} (x_{i} - \overline{x}) (x_{i} - \overline{x}) = \sum_{x_{i}} (x_{i} - \overline{x}) (y_{i} - \overline{y})$$
$$\hat{\beta}_{1} = \frac{SS_{xy}}{SS_{xx}}$$

EPI 809/Spring 2008

# **Computation Table**

Xi	Y <sub>i</sub>	<b>X</b> <sup>2</sup>	$Y_i^2$	<b>X</b> <sub>i</sub> Υ <sub>i</sub>
<b>X</b> <sub>1</sub>	<b>Y</b> <sub>1</sub>	$X_1^2$	$Y_1^2$	$X_1 Y_1$
<b>X</b> <sub>2</sub>	Y <sub>2</sub>	$X_2^2$	$Y_2^2$	$X_2Y_2$
:	:	:	:	:
Xn	Y <sub>n</sub>	$X_n^2$	$Y_n^2$	$X_n Y_n$
$\Sigma X_i$	$\Sigma \mathbf{Y}_{i}$	$\Sigma X_i^2$	$\Sigma Y_i^2$	$\Sigma X_i Y_i$

# Interpretation of Coefficients

- 1. Slope  $(\beta_1)$ 
  - Estimated Y Changes by  $\beta_1$  for Each 1 Unit Increase in X
    - If  $\beta_1 = 2$ , then Y Is Expected to Increase by 2 for Each 1 Unit Increase in X
- 2. 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

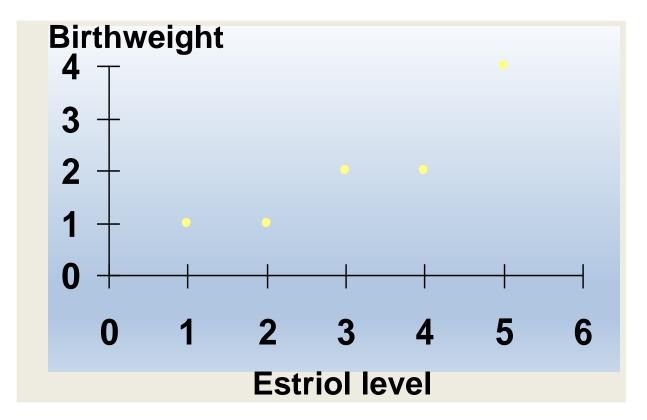
# Parameter Estimation Example

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

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



# Scatterplot Birthweight vs. Estriol level



# Parameter Estimation Solution Table

Xi	Y <sub>i</sub>	<b>X</b> <sup>2</sup>	$Y_i^2$	X <sub>i</sub> Y <sub>i</sub>
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**

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

$$\hat{\beta}_0 = \overline{Y} - \hat{\beta}_1 \overline{X} = 2 - (0.70)(3) = -0.10$$

#### How to estimate parameters

#### We minimize the equation for the sum of the squared prediction errors:

$$Q = \sum_{i=1}^n (y_i - (b_0 + b_1 x_i))^2$$

(that is, take the derivative with respect to  $b_0$  and  $b_1$ , set to 0, and solve for  $b_0$  and  $b_1$ ) and get the "least squares estimates" for  $b_0$  and  $b_1$ :

$$b_{1} = \frac{\sum_{i=1}^{n} (x_{i} - \bar{x})(y_{i} - \bar{y})}{\sum_{i=1}^{n} (x_{i} - \bar{x})^{2}}$$

$$b_{0} = \bar{y} - b_{1}\bar{x}$$

$$s_{15} = \frac{1}{5}$$

the least squares line passes through the point  $(\bar{x}, \bar{y})$ , since when  $x = \bar{x}$ , then  $y = b_0 + b_1 \bar{x} = \bar{y} - b_1 \bar{x} + b_1 \bar{x} = \bar{y}$ .

# Estimating the intercept and slope: least squares estimation

\*\* Least Squares Estimation

A little calculus....

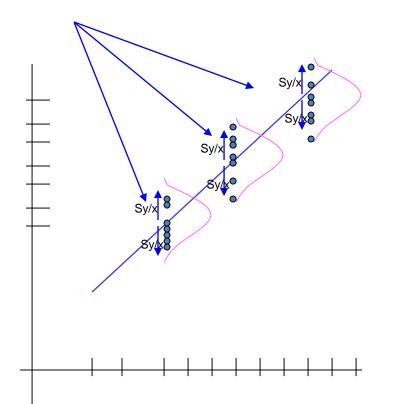
What are we trying to estimate?  $\beta$ , the slope, from

What's the constraint? We are trying to minimize the squared distance (hence the "least squares") between the observations themselves and the predicted values , or (also called the "residuals", or leftover unexplained variability)

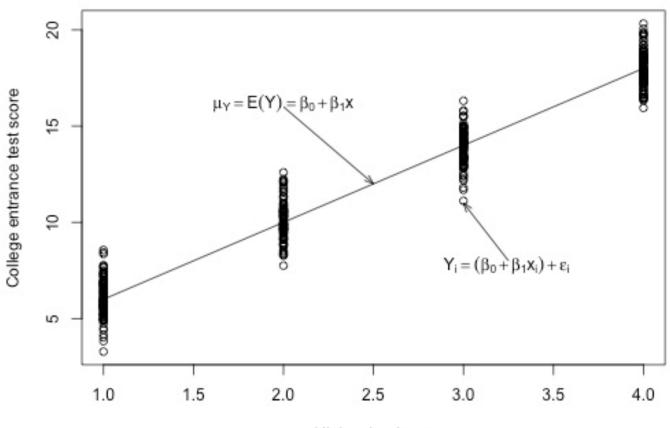
Differencei =  $yi - (\beta x + \alpha)$  Differencei<sup>2</sup> =  $(yi - (\beta x + \alpha))^2$ 

Find the *β* that gives the minimum sum of the squared differences. How do you maximize a function? Take the derivative; set it equal to zero; and solve. Typical max/min problem from calculus....

$$\frac{d}{d\beta} \sum_{i=1}^{n} (y_i - (\beta x_i + \alpha))^2 = 2(\sum_{i=1}^{n} (y_i - \beta x_i - \alpha)(-x_i))$$
$$= 2(\sum_{i=1}^{n} (-y_i x_i + \beta x_i^2 + \alpha x_i)) = 0...$$

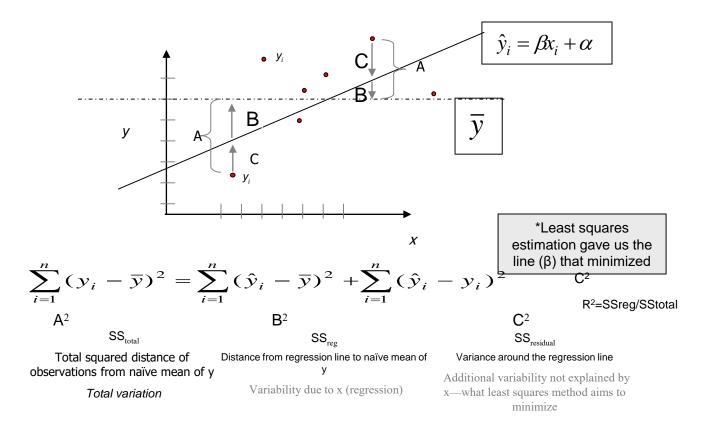


The standard error of Y given X is the average variability around the regression line at any given value of X. It is assumed to be equal at all values of X.



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#### **Regression Picture**



### **Regression Line**

• If the scatter plot of our sample data suggests a linear relationship between two variables i.e.

we can summarize the relationship by drawing a straight line on the plot.  $y = \beta_0 + \beta_1 x$ 

• Least squares method give us the "best" estimated line for our set of sample data.

#### **Regression Line**

- We will write an estimated regression line based on sample data as
- The method of least squares chooses the values for  $b_0$ , and  $b_1$  to minimize the sum of squared errors

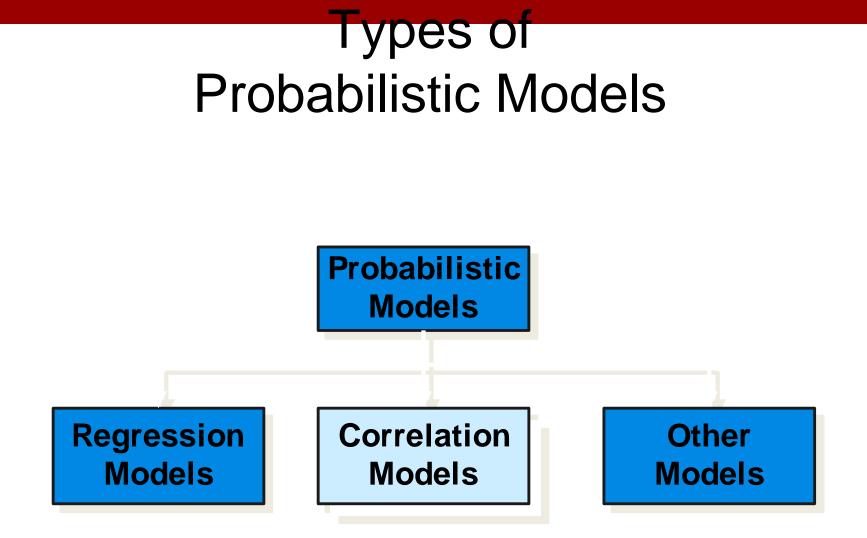
$$SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} (y - b_0 - b_1 x)^2$$

#### **Regression Line**

• Using calculus, we obtain estimating formulas:

or

$$b_{1} = \frac{\sum_{i=1}^{n} (x_{i} - \bar{x})(y_{i} - \bar{y})}{\sum_{i=1}^{n} (x_{i} - \bar{x})^{2}} = \frac{n \sum_{i=1}^{n} x_{i} y_{i} - \sum_{i=1}^{n} x_{i} \sum_{i=1}^{n} y_{i}}{n \sum_{i=1}^{n} x_{i}^{2} - (\sum_{i=1}^{n} x_{i})^{2}}$$
$$b_{1} = r \frac{S_{y}}{S_{x}}$$
$$b_{0} = \bar{y} - b_{1} \bar{x}$$



# Correlation vs. regression

- Both variables are treated the same in correlation; in regression there is a predictor and a response
- In regression the x variable is assumed non-random or measured without error
- Correlation is used in looking for relationships, regression for prediction

# **Correlation Models**

- 1. Answer '**How Strong** Is the Linear Relationship Between 2 Variables?'
- 2. Coefficient of Correlation Used
  - Population Correlation Coefficient Denoted  $\rho$  (Rho)
  - Values Range from -1 to +1
  - Measures Degree of Association
- 3. Used Mainly for Understanding

# Covariance

$$cov(x, y) = \frac{\sum_{i=1}^{n} (x_i - \overline{X})(y_i - \overline{Y})}{n-1}$$

#### **Interpreting Covariance**

 $cov(X,Y) > 0 \longrightarrow X$  and Y are positively correlated  $cov(X,Y) < 0 \longrightarrow X$  and Y are inversely correlated  $cov(X,Y) = 0 \longrightarrow X$  and Y are independent

#### **Correlation coefficient**

Pearson's Correlation Coefficient is standardized covariance (unitless):

$$r = \frac{\operatorname{cov} ariance(x, y)}{\sqrt{\operatorname{var} x} \sqrt{\operatorname{var} y}}$$

# Correlation

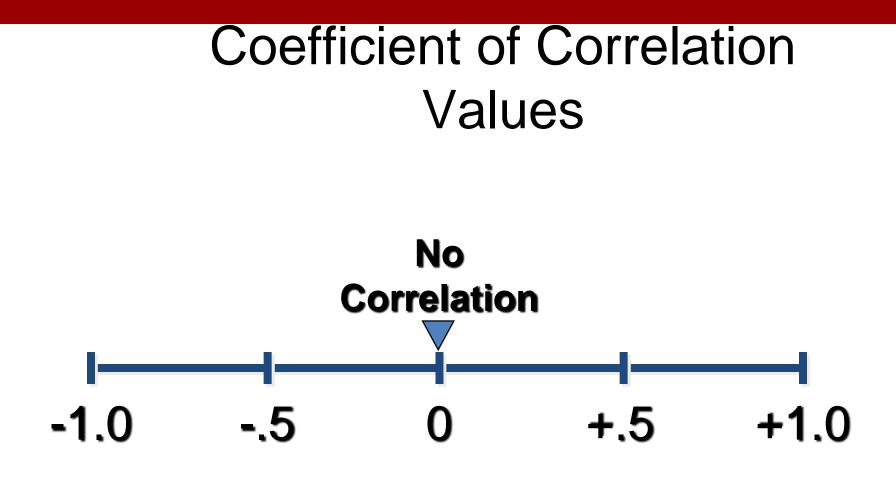
- Measures the relative strength of the *linear* relationship between two variables
- Unit-less
- Ranges between -1 and 1
- The closer to -1, the stronger the negative linear relationship
- The closer to 1, the stronger the positive linear relationship
- The closer to 0, the weaker any positive linear relationship

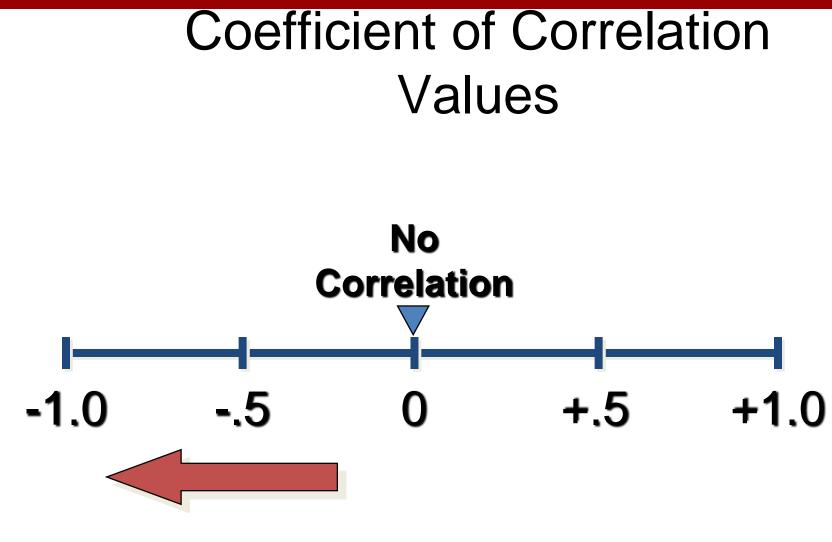
# Sample Coefficient of Correlation

 Pearson Product Moment Coefficient of Correlation between x and y:

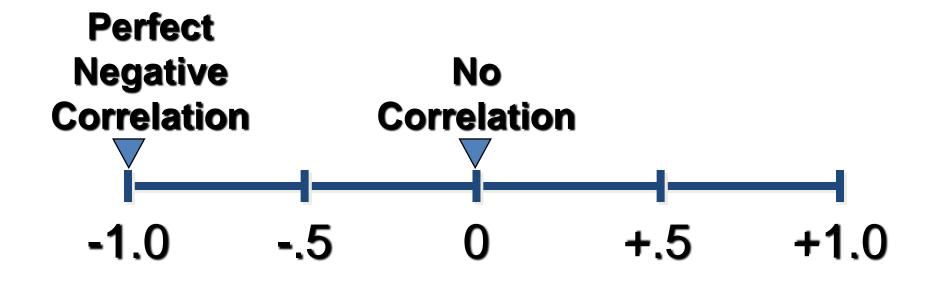
$$r = \frac{\sum_{i=1}^{n} (X_i - \overline{X})(Y_i - \overline{Y})}{\sqrt{\sum_{i=1}^{n} (X_i - \overline{X})^2} \cdot \sqrt{\sum_{i=1}^{n} (Y_i - \overline{Y})^2}} = \frac{SS_{xy}}{\sqrt{SS_{xx}}SS_{yy}}$$

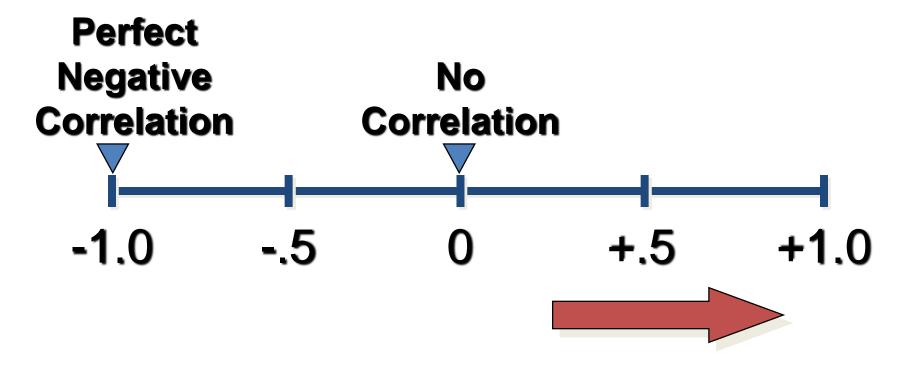




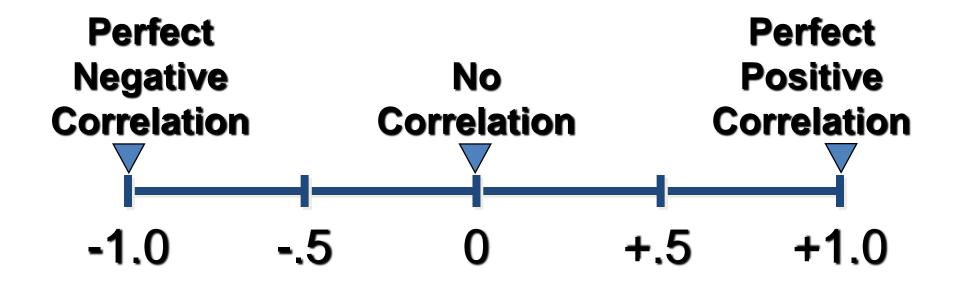


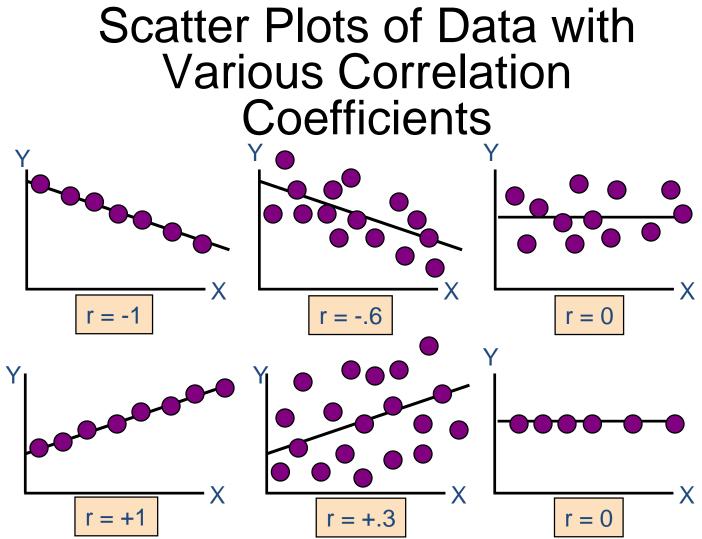
#### Increasing degree of negative correlation





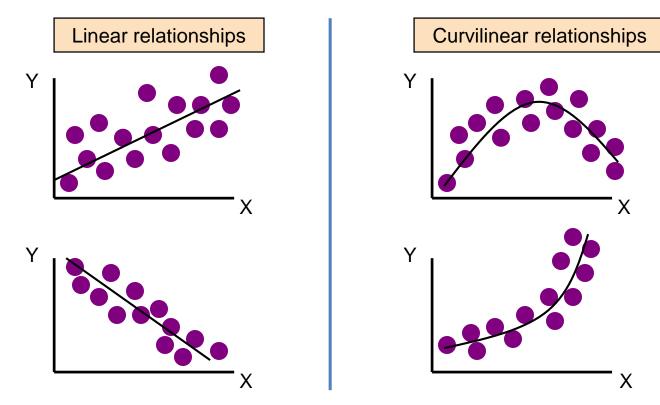
# Increasing degree of positive correlation





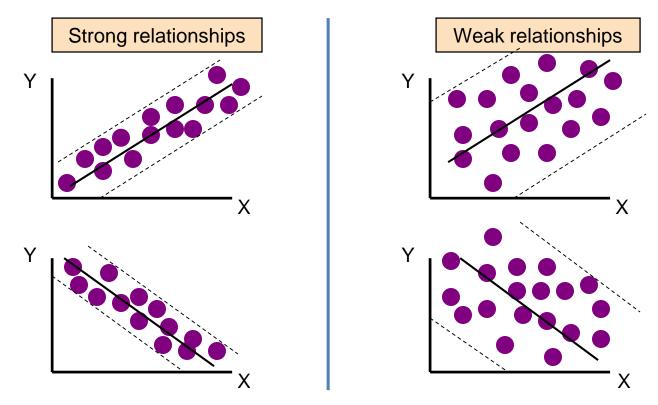
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#### **Linear Correlation**



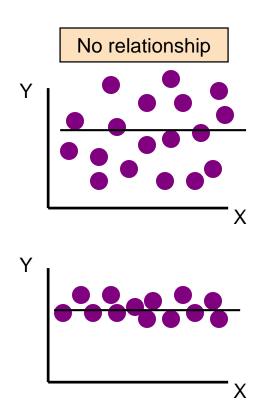
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### **Linear Correlation**



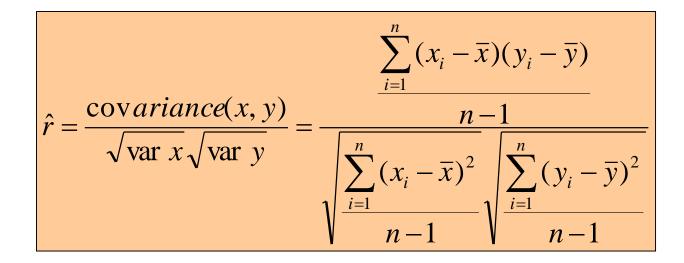
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### **Linear Correlation**

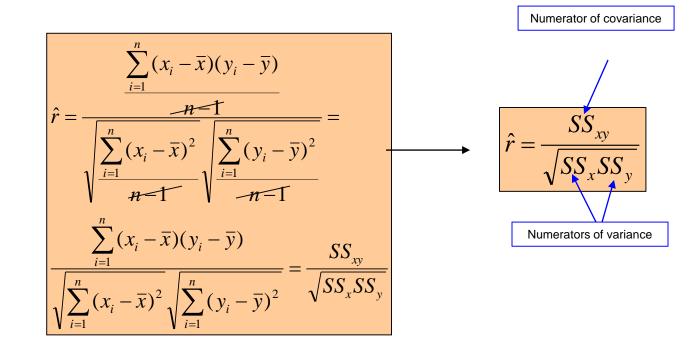


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#### Calculating by hand...



#### Simpler calculation formula...



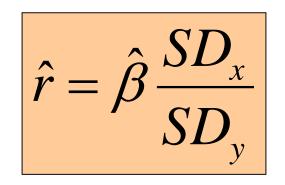
#### Least Square estimation

Slope (beta coefficient 
$$\hat{\beta} = \frac{Cov(x, y)}{Var(x)}$$

Intercept= Calculate : 
$$\hat{\alpha} = \overline{y} - \hat{\beta}\overline{x}$$

Regression line always goes throught the point:

### Relationship with correlation



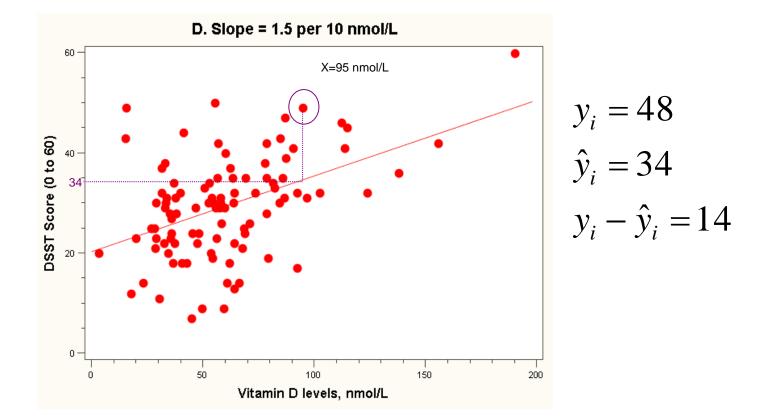
In correlation, the two variables are treated as equals. In regression, one variable is considered independent (=predictor) variable (X) and the other the dependent (=outcome) variable Y.

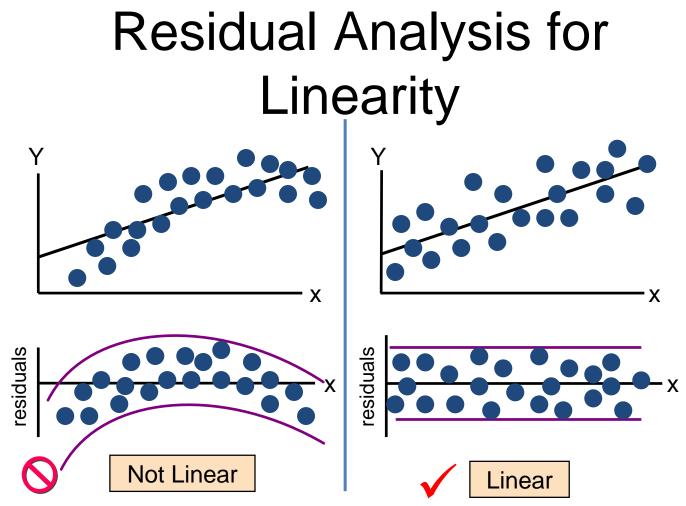
## Residual Analysis: check assumptions

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

- The residual for observation i, e<sub>i</sub>, is the difference between its observed and predicted value
- Residuals are highly useful for studying whether a given regression model is appropriate for the data at hand.
- Check the assumptions of regression by examining the residuals
  - Examine for linearity assumption
  - Examine for constant variance for all levels of X (homoscedasticity)
  - Evaluate normal distribution assumption
  - Evaluate independence assumption
- Graphical Analysis of Residuals
  - Can plot residuals vs. X

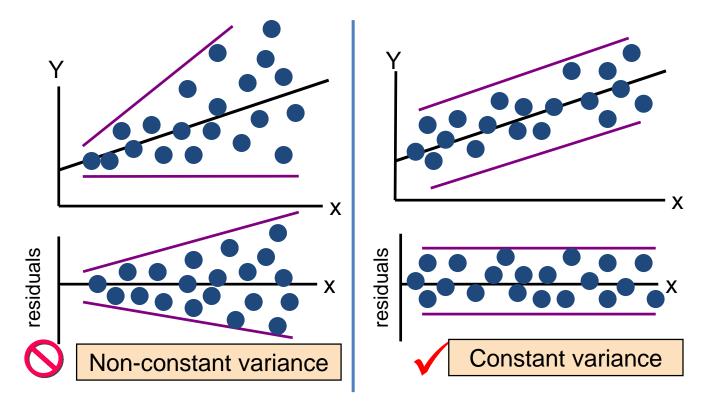
# Residual = observed - predicted





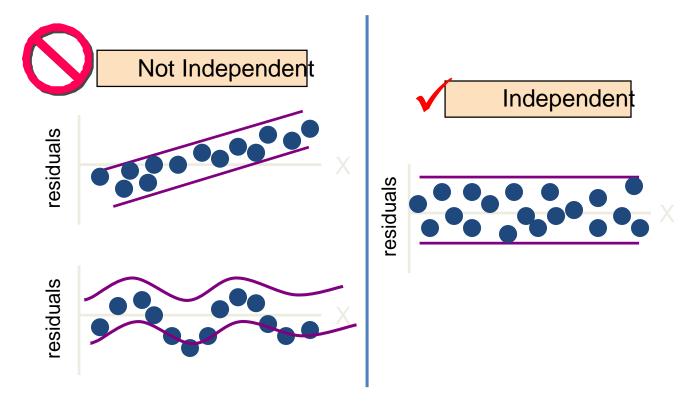
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#### Residual Analysis for Homoscedasticity



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#### Residual Analysis for Independence



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#### Example: weekly advertising expenditure

у	Х	y-hat	Residual (e)
1250	41	1270.8	-20.8
1380	54	1411.2	-31.2
1425	63	1508.4	-83.4
1425	54	1411.2	13.8
1450	48	1346.4	103.6
1300	46	1324.8	-24.8
1400	62	1497.6	-97.6
1510	61	1486.8	23.2
1575	64	1519.2	55.8
1650	71	1594.8	55.2

Estimation of the variance of the error terms,  $\sigma^2$ 

- The variance  $\sigma^2$  of the error terms  $\varepsilon_i$  in the regression model needs to be estimated for a variety of purposes.
  - It gives an indication of the variability of the probability distributions of y.
  - It is needed for making inference concerning regression function and the prediction of y.

### **Regression Standard Error**

- To estimate  $\sigma$  we work with the variance and take the square root to obtain the standard deviation.
- For simple linear regression the estimate of  $\sigma^2$  is the average squared residual.

• To estimate 
$$\sigma$$
,  $u \ddot{s} \dot{e}^2 = \frac{1}{n-2} \sum e_i^2 = \frac{1}{n-2} \sum (y_i - \hat{y}_i)^2$ 

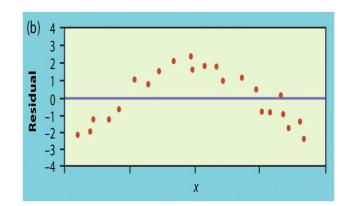
• s estimates the standard deviation  $\sigma$  of the error term  $\varepsilon$  in the statistical model for simple linear regression.

#### **Regression Standard Error**

У	×	y-hat	Residual (e)	square(e)
1250	41	1270.8	-20.8	432.64
1380	54	1411.2	-31.2	973.44
1425	63	1508.4	-83.4	6955.56
1425	54	1411.2	13.8	190.44
1450	48	1346.4	103.6	10732.96
1300	46	1324.8	-24.8	615.04
1400	62	1497.6	-97.6	9525.76
1510	61	1486.8	23.2	538.24
1575	64	1519.2	55.8	3113.64
1650	71	1594.8	55.2	3047.04
y-hat = 828+10.8X			total	36124.76
			S <sub>y.x</sub>	67.19818

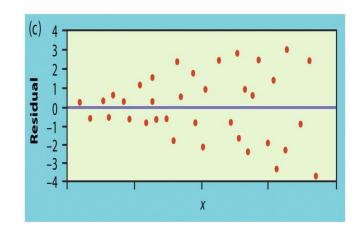
### Residual plots

• The points in this residual plot have a curve pattern, so a straight line fits poorly



## Residual plots

• The points in this plot show more spread for larger values of the explanatory variable *x*, so prediction will be less accurate when *x* is large.

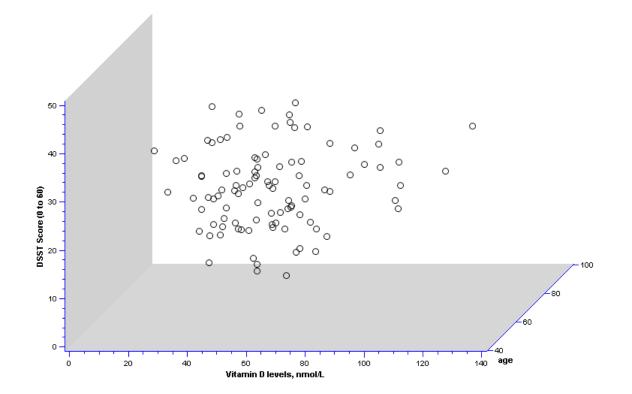


#### Variable transformations

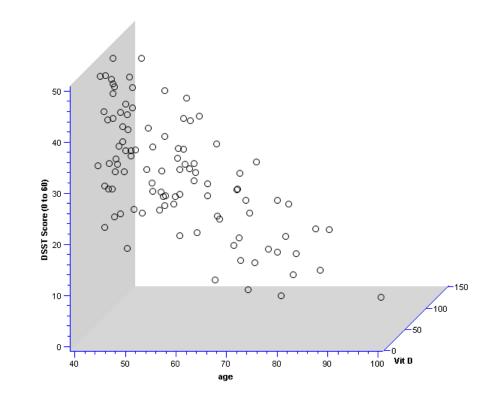
- If the residual plot suggests that the variance is not constant, a transformation can be used to stabilize the variance.
- If the residual plot suggests a non linear relationship between x and y, a transformation may reduce it to one that is approximately linear.
- Common linearizing transformations are:
- Variance stabilizing  $\frac{1}{t}$  ransformations are:

$$\frac{1}{y}$$
,  $\log(y)$ ,  $\sqrt{y}$ ,  $y^2$ 

### 2 predictors: age and vit D...



#### Different 3D view...



#### Fit a plane rather than a line...

