

#### **Statistics and Probability**

### Regression

#### **Curve fitting**

- A line or curve that represents a number of data points
- There are two methods to find such line or curve
  - Regression
  - Interpolation
- Engineering applications
  - Trend analysis
  - Hypothesis testing

#### Regression vs interpolation

#### Regression

#### Interpolation

The data show significant errors or noise

The data are accurate

To find a single curve that represent general trend of the data

To find a curve or curves that encompass(es) every data point

Regression line (curve) does not need to pass every data point

To estimate values between data points

#### Regression and interpolation

- Extrapolation
  - Similar to interpolation but applied to outside range of data points
  - Not recommended

#### **Curve fitting to measured data**

- Trend analysis
  - Use of data trend (measurements, experiments) to estimate values
    - If the data are accurate, use interpolation technique
    - If the data show noise, use regression technique
- Hypothesis testing
  - Comparison between theoretical values with computed ones

#### Recall on statistical parameters

Arithmetic mean

$$\overline{Y} = \frac{1}{n} \sum y_i$$

Standard deviation

$$S_Y = \sqrt{\frac{S_t}{n-1}} \qquad S_t = \sum (y_i - \bar{Y})^2$$

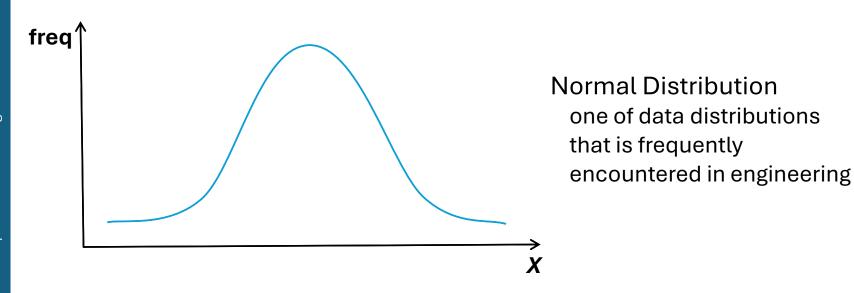
$$S_t = \sum (y_i - \bar{Y})^2$$

Variance

$$S_Y^2 = \frac{S_t}{n-1}$$

$$c_v = \frac{s_Y}{\bar{Y}} 100\%$$

#### **Probability distribution**



Regression

## Simple Linear Regression

#### Regression: least-square method

- To find a single curve or function (approximate) that represents the general trend of the data
  - The data show significant error
  - The curve does not need to pass every data point
- Methods
  - Linear regression (simple linear regression)
  - Linearized expressions
  - Polynomial regression
  - Multiple linear regression
  - Non-linear regression

#### Regression: least-square method

- How
  - Spreadsheet (Microsoft Excel)
  - Computer program
    - MatLab
  - Freeware
    - Octave
    - Scilab
    - Freemat
  - Self-made computer program

#### Simple linear regression

- To find a straight line that represents the general trend of data points:  $(x_0,y_0)$ ,  $(x_1,y_1)$ , ...,  $(x_n,y_n)$ 
  - $y_{reg} = a_0 + a_1 x$
  - $a_0$  intercept
  - $a_1$  slope
- Microsoft Excel
  - =INTERCEPT(*y*,*x*)
  - =SLOPE(y,x)

#### Simple Linear Regression

- Error or residual
  - Discrepancies between actual value of y (y data) and approximate value of y ( $y_{req}$ ) according to linear expression ( $a_0 + a_1 x$ )

$$e = y - y_{reg} = y - (a_0 + a_1 x)$$

Minimize the sum of squared residues

$$\min[S_r] = \min\left[\sum e_i^2\right] = \min\left[\sum (y - a_0 - a_1 x)^2\right]$$

#### Simple linear regression

- How to find  $a_0$  and  $a_1$ ?
  - Differentiate the equation of  $S_r$  twice; firstly with respect to  $a_0$  and lastly with respect to  $a_1$
  - Set each of the two equations to zero
  - Solve the equations for  $a_0$  and  $a_1$

$$\frac{\partial S_r}{\partial a_0} = -2\sum (y_i - a_0 - a_1 x_i)$$

$$\frac{\partial S_r}{\partial a_1} = -2\sum (y_i - a_0 - a_1 x_i) x_i$$

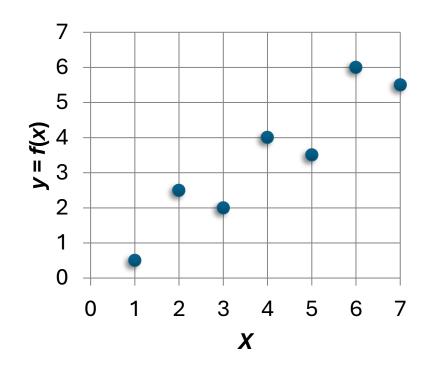
$$\frac{\partial S_r}{\partial a_0} = 0$$

$$\frac{\partial S_r}{\partial a_1} = 0$$

$$a_1 = \frac{n\sum x_i y_i - \sum x_i \sum y_i}{n\sum x_i^2 - (\sum x_i)^2}$$

$$a_0 = \bar{y} - a_1 \bar{x}$$

i	X <sub>i</sub>	$y_i = f(x_i)$
0	1	0.5
1	2	2.5
2	3	2
3	4	4
4	5	3.5
5	6	6
6	7	5.5



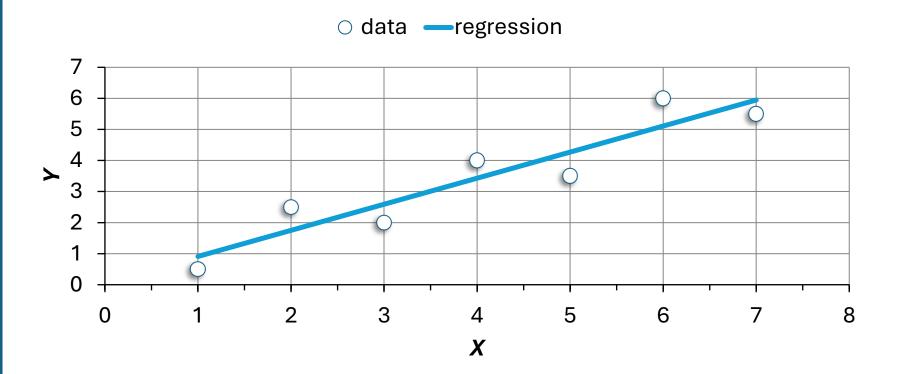
i i	X <sub>i</sub>	<b>y</b> i	$x_i y_i$	$x_i^2$	<b>y</b> reg	( <i>y<sub>i</sub></i> - <i>y<sub>reg</sub></i> ) <sup>2</sup>	(y <sub>i</sub> -y <sub>mean</sub> ) <sup>2</sup>
0	1	0.5	0.5	1	0.910714	0.168686	8.576531
1	2	2.5	5	4	1.75	0.5625	0.862245
2	3	2.0	6	9	2.589286	0.347258	2.040816
3	4	4.0	16	16	3.428571	0.326531	0.326531
4	5	3.5	17.5	25	4.267857	0.589605	0.005102
5	6	6.0	36	36	5.107143	0.797194	6.612245
6	7	5.5	38.5	49	5.946429	0.199298	4.290816
Σ	28	24.0	119.5	140	Σ	2.991071	22.71429

$$a_1 = \frac{n\sum x_i y_i - \sum x_i \sum y_i}{n\sum x_i^2 - (\sum x_i)^2} = \frac{7(119.5) - 28(24)}{7(140) - (28)^2} = 0.839286$$

$$\bar{y} = \frac{24}{7} = 3.4$$

$$\bar{x} = \frac{28}{7} = 4$$

$$a_0 = \bar{y} - a_1 \bar{x} = 3.4 - 0.839286(4) = 0.071429$$



#### **Error**

- Error
  - Standard error magnitude

$$s_{y/x} = \sqrt{\frac{S_r}{n-2}}$$
  $S_r = \sum (y_i - a_0 - a_1 x_i)^2$ 

Notice its similarity with standard deviation

$$s_y = \sqrt{\frac{S_t}{n-1}} \qquad S_t = \sum (y_i - \bar{y})^2$$

#### **Error**

 Diffrence between the two "errors" signifies an improvement of the prediction or a reduction of error

$$r = \frac{n\sum x_i y_i - (\sum x_i)(\sum y_i)}{\sqrt{n\sum x_i^2 - (\sum x_i)^2} \sqrt{n\sum y_i^2 - (\sum y_i)^2}} \longrightarrow \text{correlation coefficient}$$

#### **Error**

$$S_r = \sum (y_i - a_0 - a_1 x_i)^2 = 2.991071$$

$$S_t = \sum (y_i - \bar{y})^2 = 22.71429$$

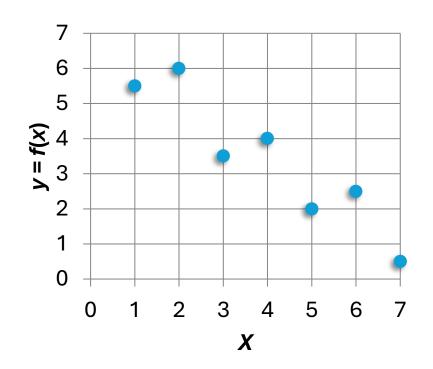
$$S_t = S_t - S_t = 22.714$$

$$r^2 = \frac{S_t - S_r}{S_t} = \frac{22.71429 - 2.991071}{22.71429} = 0.868318$$

$$r = 0.931836$$

 $-1 \le r \le +1$ 

i	<b>x</b> <sub>i</sub>	$y_i = f(x_i)$
0	1	5.5
1	2	6
2	3	3.5
3	4	4
4	5	2
5	6	2.5
6	7	0.5



Regression

## Polynomial Regression

#### Polynomial regression

- Some engineering data, although exhibiting a marked pattern, is poorly represented by a straight line
  - Method 1: coordinate transformation (linearized non-linear eq.)
  - Method 2: polynomial regression
    - The mth-degree polynomial

$$y = a_0 + a_1 x + a_2 x^2 + \dots + a_m x^m$$

The sum of the squares of the residuals

$$S_r = \sum_{i=1}^n e_i^2 = \sum_{i=1}^n (y_i - a_0 - a_1 x_i - a_2 x_i^2 - \dots - a_m x_i^m)^2$$

#### Polynomial regression

- The least-square method extended to fit the data to an mth-degree polynomial
- These equations can be set equal to zero and rearranged to develop a set of normal equations

$$\frac{\partial S_r}{\partial a_0} = -2\sum \left(y_i - a_0 - a_1 x_i - a_2 x_i^2 - \dots - a_m x_i^m\right)$$

$$\frac{\partial S_r}{\partial a_1} = -2\sum_i x_i \left( y_i - a_0 - a_1 x_i - a_2 x_i^2 - \dots - a_m x_i^m \right)$$

$$\frac{\partial S_r}{\partial a_2} = -2\sum_{i} x_i^2 (y_i - a_0 - a_1 x_i - a_2 x_i^2 - \dots - a_m x_i^m)$$

•

•

•

$$\frac{\partial S_r}{\partial a_m} = -2\sum_i x_i^m \left( y_i - a_0 - a_1 x_i - a_2 x_i^2 - \dots - a_m x_i^m \right)$$

#### Polynomial regression

$$a_{0}n + a_{1} \sum_{i=1}^{n} x_{i} + a_{2} \sum_{i=1}^{n} x_{i}^{2} + \dots + a_{m} \sum_{i=1}^{n} x_{i}^{m} = \sum_{i=1}^{n} y_{i}$$

$$a_{0} \sum_{i=1}^{n} x_{i} + a_{1} \sum_{i=1}^{n} x_{i}^{2} + a_{2} \sum_{i=1}^{n} x_{i}^{3} + \dots + a_{m} \sum_{i=1}^{n} x_{i}^{m+1} = \sum_{i=1}^{n} x_{i}y_{i}$$

$$a_{0} \sum_{i=1}^{n} x_{i}^{2} + a_{1} \sum_{i=1}^{n} x_{i}^{3} + a_{2} \sum_{i=1}^{n} x_{i}^{4} + \dots + a_{m} \sum_{i=1}^{n} x_{i}^{m+2} = \sum_{i=1}^{n} x_{i}^{2}y_{i}$$

$$a_0 \sum_{i=1}^{n} x_i^m + a_1 \sum_{i=1}^{n} x_i^{m+1} + a_2 \sum_{i=1}^{n} x_i^{m+2} + \dots + a_m \sum_{i=1}^{n} x_i^{2m} = \sum_{i=1}^{n} x_i^m y_i$$

- There are m+1linear equations having m+1unknowns, i.e.  $a_0, a_1, a_2, \dots, a_m$
- These linear equations can be simultaneously solved by using methods such as
  - Gauss elimination
  - Gauss-Jordan
  - Jacobi iteration
  - Matrix inversion

#### **Example**

 Fit a second-order polynomial to the data in the table on the right

$$y = a_0 + a_1 x + a_2 x^2$$

Answer

$$y = 2.47857 + 2.35929x + 1.86071x^2$$

$$r^2 = 1 - \frac{S_r}{S_t} = 1 - \frac{3.74657}{2513.39} = 0.9985$$

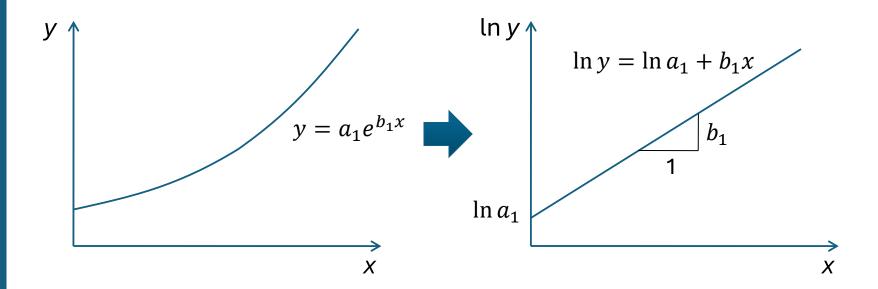
$$r = 0.9993$$

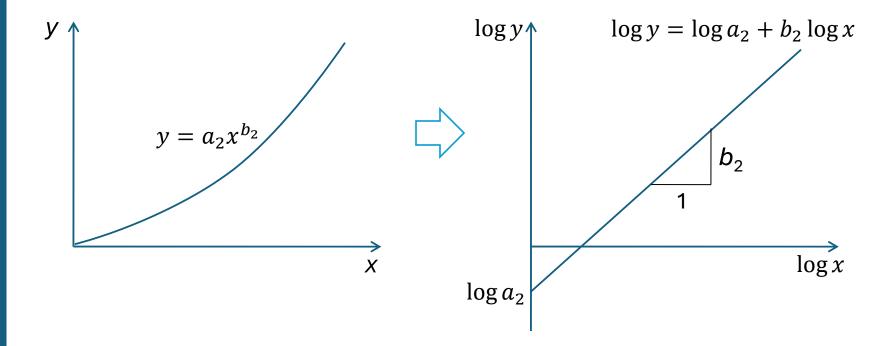
<b>x</b> <sub>i</sub>	y <sub>i</sub>
0	2.1
1	7.7
2	13.6
3	27.2
4	40.9
5	61.1

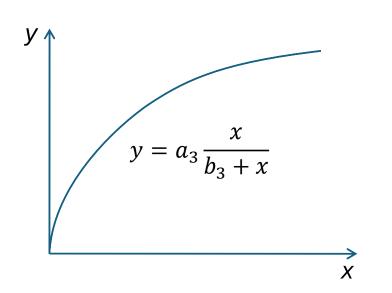
#### Regression

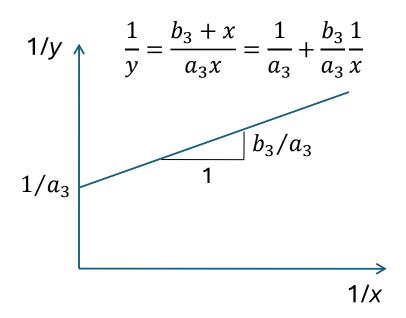
# Regression of Linearized Expression

- Linearized non-linear equations
  - Logarithmic eq. → linear eq.
  - Exponential eq.  $\rightarrow$  linear eq.
  - n-th order polynomial eq.  $(n > 1) \rightarrow$  linear eq.
  - etc.









Regression

## Multiple Linear Regression

■ Suppose the dependent variable y is a linear function of two independent variables  $x_1$  and  $x_2$ 

$$y = a_0 + a_1 x_1 + a_2 x_2$$

 The best values of the coefficients are determined by setting up the sum of the squares of the residuals

$$S_r = \sum_{i=1}^n (y_i - a_0 1 a_1 x_{1i} - a_2 x_{2i})^2$$

 Differentiating this equation with respect to each of the unknown coefficients

$$\frac{\partial S_r}{\partial a_0} = -2 \sum_{i=1}^n (y_i - a_0 - a_1 x_{1i} - a_2 x_{2i})$$

$$\frac{\partial S_r}{\partial a_1} = -2 \sum_{i=1}^n x_{1i} (y_i - a_0 - a_1 x_{1i} - a_2 x_{2i})$$

$$\frac{\partial S_r}{\partial a_2} = -2 \sum_{i=1}^n x_{2i} (y_i - a_0 - a_1 x_{1i} - a_2 x_{2i})$$

 Equating the differentials to zero and expressing the resulted equation as a set of simultaneous linear equations yield

$$a_0 n + a_1 \sum_{i=1}^{n} x_{1i} + a_2 \sum_{i=1}^{n} x_{2i} = \sum_{i=1}^{n} y_i$$

$$a_0 \sum_{i=1}^{n} x_{1i} + a_1 \sum_{i=1}^{n} x_{1i}^2 + a_2 \sum_{i=1}^{n} x_{1i} x_{2i} = \sum_{i=1}^{n} x_{1i} y_i$$

$$a_0 \sum_{i=1}^{n} x_{2i} + a_1 \sum_{i=1}^{n} x_{1i} x_{2i} + a_2 \sum_{i=1}^{n} x_{2i}^2 = \sum_{i=1}^{n} x_{2i} y_i$$

Written in matrix form

$$\begin{bmatrix} n & \sum_{i=1}^{n} x_{1i} & \sum_{i=1}^{n} x_{2i} \\ \sum_{i=1}^{n} x_{1i} & \sum_{i=1}^{n} x_{1i}^{2} & \sum_{i=1}^{n} x_{1i} x_{2i} \\ \sum_{i=1}^{n} x_{2i} & \sum_{i=1}^{n} x_{1i} x_{2i} & \sum_{i=1}^{n} x_{2i}^{2} \end{bmatrix} \begin{Bmatrix} a_{0} \\ a_{1} \\ a_{2} \end{Bmatrix} = \begin{Bmatrix} \sum_{i=1}^{n} x_{1i} y_{i} \\ \sum_{i=1}^{n} x_{2i} y_{i} \end{Bmatrix}$$

#### Example

- Find the best linear equation that fits to the data in the table on the right
- Answer

$$y = 5 + 4x_1 - 3x_2$$
$$r^2 = 1$$

<b>x</b> <sub>1</sub>	X <sub>2</sub>	у
0	0	5
2	1	10
2.5	2	9
1	3	0
4	6	3
7	2	27

 Multiple linear regression can be useful in the derivation of power equations of the general form

$$y = a_0 x_1^{a_1} x_2^{a_2} \dots x_m^{a_m}$$

- Such equations are extremely useful when fitting experimental data
- In order to use the multiple linear regression, the equation is transformed by taking its logarithm to yield

$$\log y = \log a_0 + a_1 \log x_1 + a_2 \log x_2 + \dots + a_m \log x_m$$

Regression

## General Linear Least Squares

#### General linear least squares

■ The three types of regression that have been presented, i.e. simple linear, polynomial, and multiple linear can be expressed in a general least-squares model

$$y = a_0 z_0 + a_1 z_1 + a_2 z_2 + \dots + a_m z_m$$

- where  $z_0, z_1, ..., z_m$  are m + 1 different functions
- m+1 is the number of independent variables
- n+1 is the number of data points
- The above expression can be written in a matrix form

$$\{Y\} = [Z]\{A\}$$

#### General linear least squares

$${Y} = [Z]{A} \longrightarrow [Z]^T[Z]{A} = [Z]^T{Y}$$

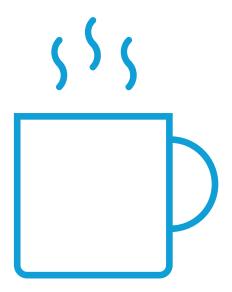
$$S_r = \sum_{i=1}^n \left( y_i - \sum_{j=1}^m a_j z_{ji} \right)^2$$

- {Y} contains the observed values of the dependent variables
- [Z] is a matrix of the observed values of the independent variables
- {A} contains the unknown coefficients

#### **General Linear Least Squares**

$$[Z]^T[Z]{A} = [Z]^T{Y}$$

- Solution strategy
  - LU decomposition
  - Cholesky's method
  - Matrix inverse approach  $\longrightarrow$   $\{A\} = \left[ [Z]^T [Z] \right]^{-1} [Z]^T \{Y\}$



#### **Statistics and Probability**

Regression