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NUMERICAL METHODS & OPTIMISATION

Part I: Curve Fitting

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Chapter Description

- Aims
  - Apply numerical methods in solving engineering problem and optimisation

- Expected Outcomes
  - Estimate the first and higher-order of mathematical model that represents the experimental data by using different kinds of curve fitting methods
  - Estimate the regression coefficient, standard deviation and standard error of experimental data by using different kinds of curve fitting methods
  - Apply the curve fitting methods to solve engineering problems

- References
  - Steven C. Chapra and Raymond P. Canale (2009), Numerical Methods for Engineers, McGraw-Hill, 6th Edition

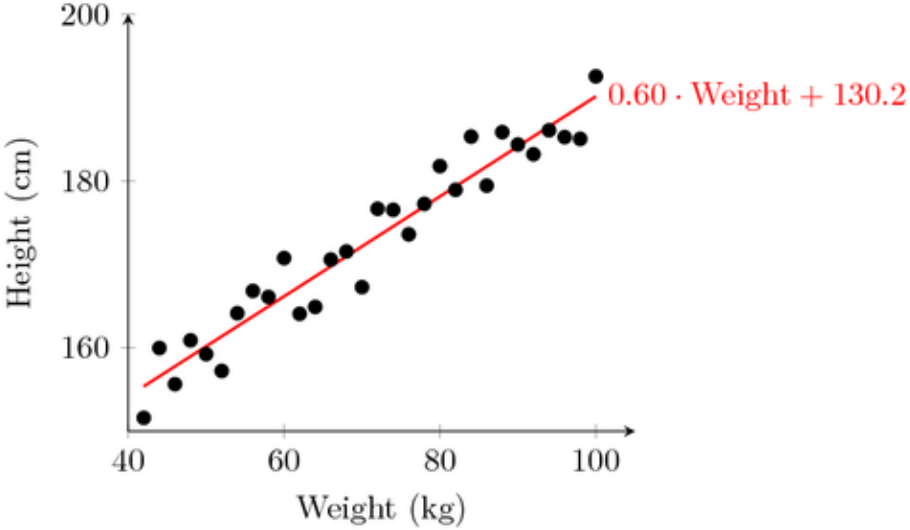
Overview of Curve Fitting

- Data are always presented in discrete values along a continuum
- Estimates are required between the discrete values – curve fitting
- Curve fitting can be achieved by computing values of the function at a number of discrete values along the range of interest
- Two general approaches:
  - Least-squares regression: derive a single curve that represents the general trend of the data
  - Interpolation: very precise, fitting a curve that passes directly through each points

Overview of Curve Fitting (cont'd)

- In curve fitting, the intermediate values are determined from tabulated data
- Curve fitting is used in engineering for
  - **Trend analysis**: predictions are made based on the pattern of data
  - **Hypothesis testing**: the measured data are compared to the existing mathematical model

Overview of Curve Fitting (cont'd)



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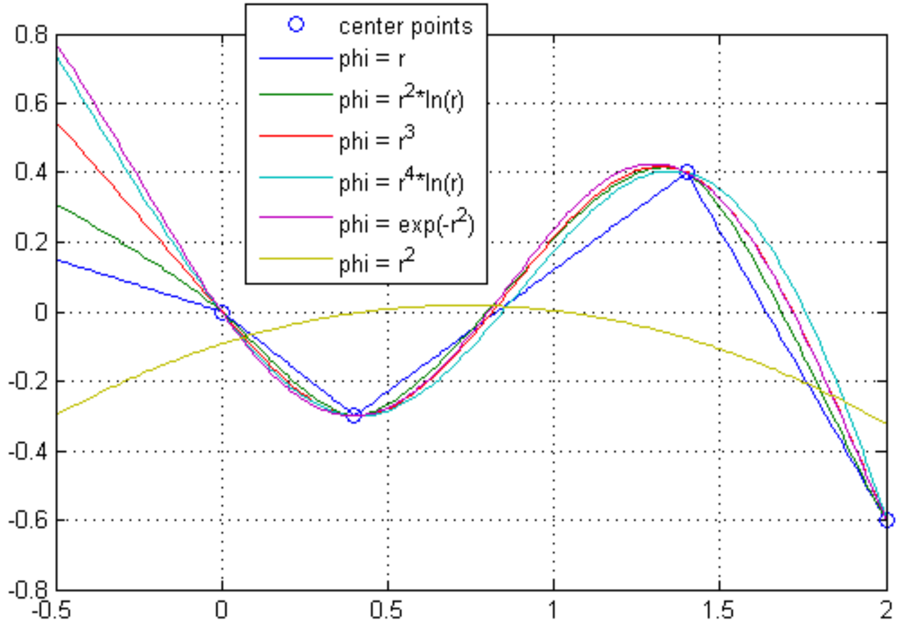

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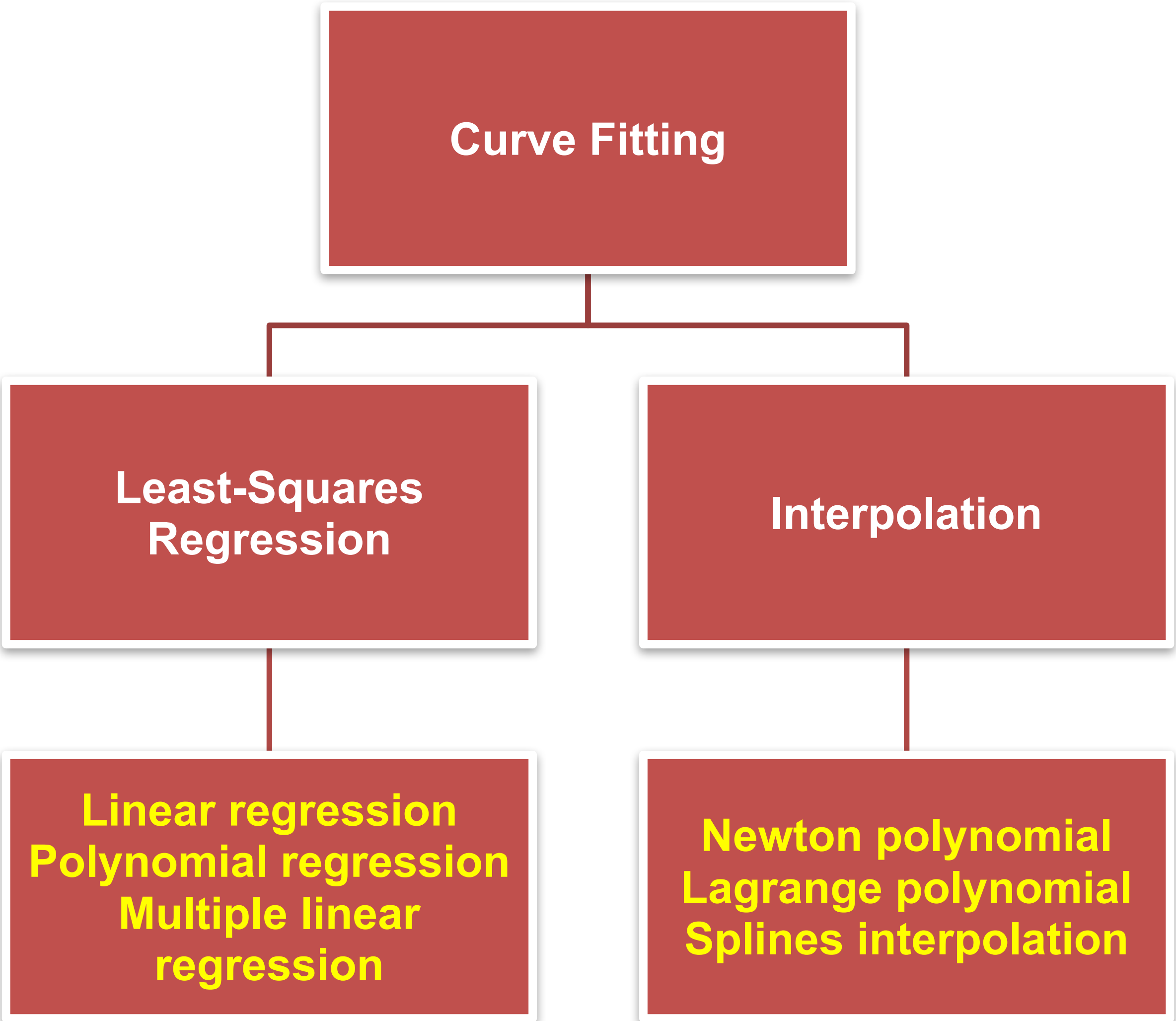
Least-square regression

Linear & polynomial interpolation

Overview of Curve Fitting (cont'd)



Least squares regression

- Polynomial interpolation is inappropriate for data associated with large error – originates from experiments

- Types of least squares regression:
  - Linear regression
  - Polynomial regression
  - Multiple linear regression

Linear Regression: Example 17.1

- Fitting a straight line to a set of paired observation $(x_1, y_1), (x_2, y_2),\ldots,(x_n, y_n)$ by using the following equations:

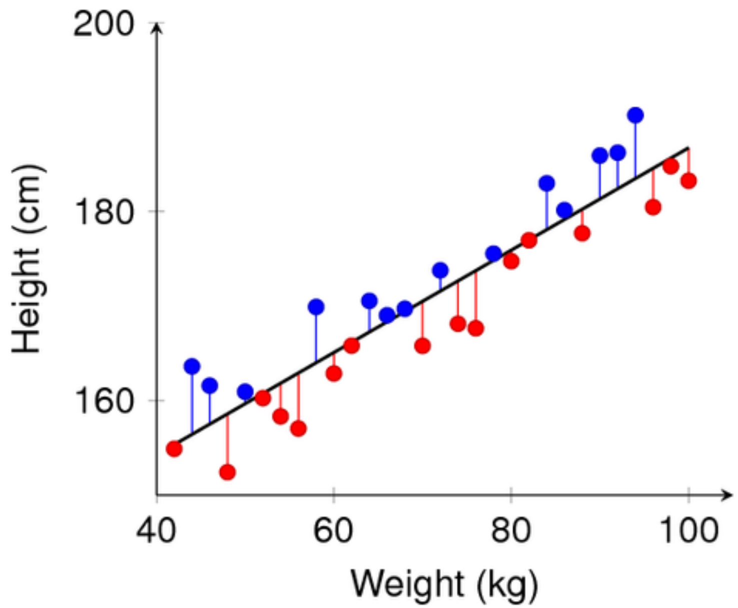
$$y = a_0 + a_1 x + e$$

$$a_1 = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{n \sum x_1^2 - (\sum x_i)2}$$

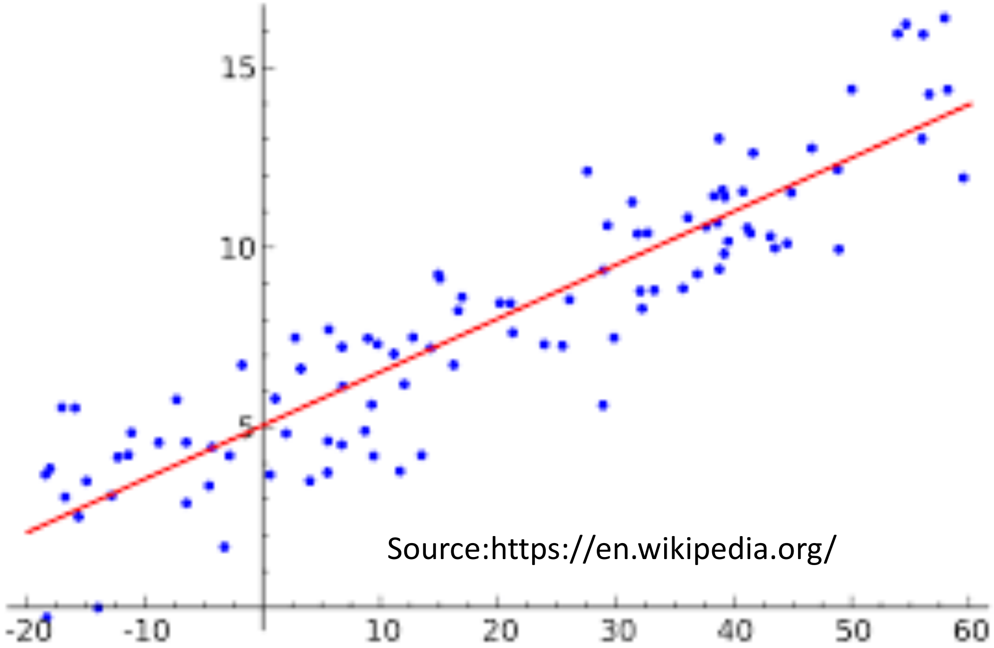
Linear Regression: Error

- The error or residual represent the vertical distance between the measured data and the straight line.

- For the best fit: Minimize the total sum of the squares of the residuals (error) between the measured *y* and *y* calculated with the linear model



Linear Regression: Error (cont'd)



- Linear regression with small and large errors
- Standard deviation, S_y is normally used to measure the spread of data:

$$S_r = \sum_{i=1}^{n} (y_1 - a_0 - a_1 x_1)^2$$

Linear Regression: Error (cont'd)

- Least squares regression provides the best fit if the following criteria are met – maximum likelihood principle:
  - The spread of the point along the line is of similar magnitude along the entire range of data
  - The distribution of these points about the line is normal

$$S_{y/x} = \sqrt{\frac{S_r}{n-2}}$$

- If these criteria are met, the standard deviation for the regression line can be determined as:
- The standard deviation is called standard error
- y/x: the error is for a predicted value of y corresponding to a particular value of x

Linear Regression: Error (cont'd)

- The following equation quantifies the improvement or error reduction due to describing the data in terms of a straight line than as an average value
- Because the magnitude of this quantity is scale-dependent, the coefficient of determination and r is the correlation coefficient:

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

- For a perfect fit: S_r=0 and $r = r^2 = 1$, the line explains 100 percent of the variability of the data.
- For $r = r^2$=0, $S_r = S_t$, the fit represents no improvement.

Polynomial Regression

- Some engineering data generated from experiments can be poorly represented by a straight line
- For this case, curve would be a better option to fit the data
- Alternatives:
  - To transform the data into straight line
  - To fit polynomials to the data using polynomial regression
- The following equation is used as a model to fit the data:

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

- With a0, a1 and a2 are determined by the following simultaneous equations:

$$(n)a_0 + (\sum x_i)a_1 + (\sum x_i^2)a_2 = \sum y_i$$

$$(\sum x_i)a_0 + (\sum x_i^2)a_1 + (\sum x_i^3)a_2 = \sum x_i y_i$$

$$(\sum x_i^2)a_0 + (\sum x_i^3)a_1 + (\sum x_i^4)a_2 = \sum x_i^2 y_i$$

Polynomial Regression (cont'd)

- The standard error can be calculated by using the following equation:

$$s_{y/x} = \sqrt{\frac{S_r}{n-(m+1)}}$$

- m is the order of polynomial

Polynomial Regression: Exercise

Use polynomial regression to fit a **parabola** to the data:

x	1	2	3	4	5	6	7	8	9
y	1	1.5	2	3	4	5	8	10	13

Multiple Linear Regression

- In multiple linear regression, y is a linear function of two or more independent variables (x_1, x_2, x_3), and is given by:

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

- a_0, a_1 and a_2 can be calculated by using gauss elimination method as follows:

$$\begin{bmatrix} n & \sum x_{1i} & \sum x_{2i} \\ \sum x_{1i} & \sum x_{1i}^{2} & \sum x_{1i}x_{2i} \\ \sum x_{2i} & \sum x_{1i}x_{2i} & \sum x_{2i}^{2} \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} \sum y_i \\ \sum y_i x_{1i} \\ \sum y_i x_{2i} \end{Bmatrix}$$

- The standard error is given by:

$$s_{y/x} = \sqrt{\frac{S_r}{n-(m+1)}}$$

Multiple Linear Regression: Exercise

Use multiple linear regression to fit:

x_1	1	2	3	4	5	6	7	8	9
x_2	0	2	2	4	4	6	6	2	1
y	1	1.5	2	3	4	5	8	10	13

Compute the coefficients, standard error of the estimate, and the correlation coefficient.

Conclusion

- First and higher-order of mathematical model that represents the experimental data can be estimated by using different kinds of curve fitting methods
- Regression coefficient, standard deviation and standard error of experimental data can be estimated by using different kinds of curve fitting methods

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Main Reference

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