Numerical Methods

(MTH4002)

Lecture 03: Curve Fitting

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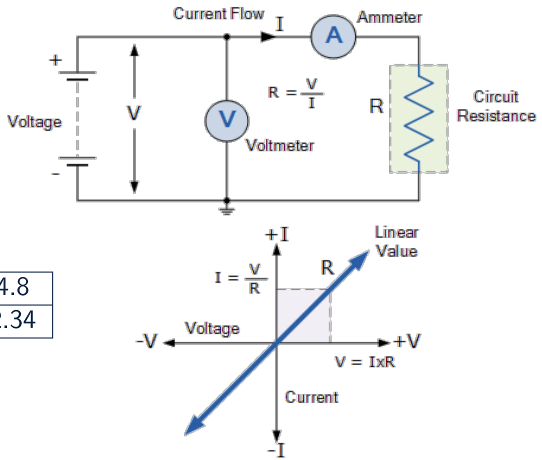
Outline

Introduction

- In many scientific and engineering experiments, observations of physical quantities are measured and recorded.
- For example, measuring the current through the circuit by changing the voltage across resistor.



V (volt)	0.8	1.4	2.0	2.7	3.8	4.8
I (amp)	0.69	1.00	1.6	2.02	2.39	2.34

- The experimental records are typically referred to as data points.

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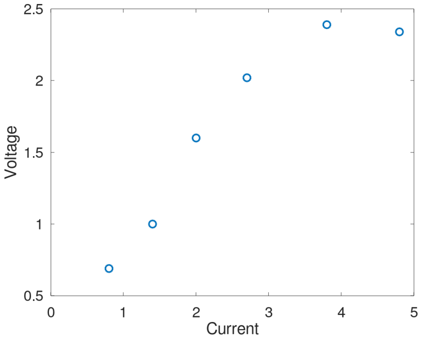

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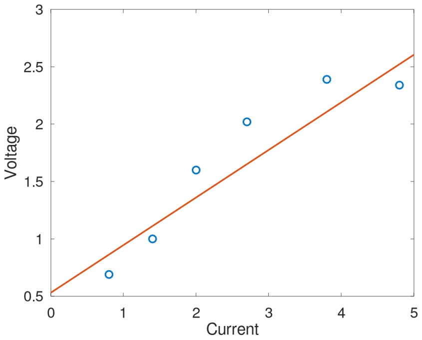


- The curve fits the general trend of the data but does not match any of the data points exactly.
- Generally, all experimental measurements have built-in errors or uncertainties, and requiring a curve fit to go through every data point is not beneficial.
- The objective is to find a function that fits the data points overall.

Introduction

- Often the data is used for developing or evaluating mathematical formulas (equations) that represent the data.
- This is done by curve fitting in which a specific form of an equation is assumed, or provided by a guiding theory, and then the parameters of the equation are determined such that the equation best fits the data points.
- Curve fitting can be carried out with many types of functions and with polynomials of various orders.
  - Linear function, e.g. $y = mx + c$
  - Nonlinear function, e.g. $y = cx^2$, $y = Ce^{Ax}$

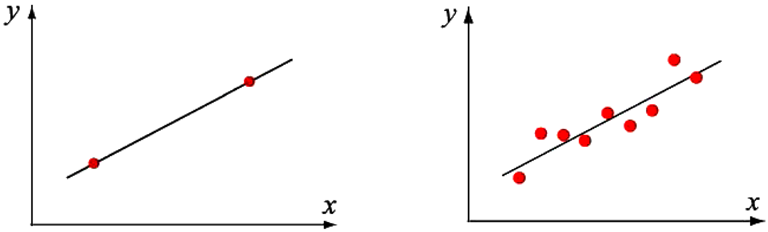
Curve fitting using linear function

Curve fitting with a linear function

- Curve fitting using a linear equation (first degree polynomial) is the process by which an equation of the form:

$$y = a_1 x + a_0$$

  is used to best fit given data points.
- This is done by determining the constants a_1 and a_0 that give the smallest error when the data points are substituted in the equation.

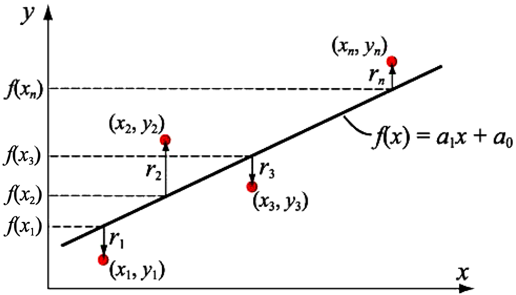


Measuring how good is a fit

- The fit between given data points and an approximating linear function is determined by first calculating the error, also called the residual, which is the difference between a data point and the value of the approximating function, at each point.

- Subsequently, the residuals are used for calculating a total error for all the points.
- The residual r_i at a point, (x_i, y_i), is the difference between the value y_i of the data point and the value of the function $f(x_i)$ used to approximate the data points:

$$\boxed{r_i = y_i - f(x_i)}$$



Measuring how good is a fit

- A criterion that measures how well the approximating function fits the given data can be obtained by calculating a total error E in terms of the residuals.

$$E = \sum_{i=1}^{n} r_i = \sum_{i=1}^{n} [y_i - (a_1 x_i + a_0)]$$

$$\text{or} \quad E = \sum_{i=1}^{n} |r_i| = \sum_{i=1}^{n} |y_i - (a_1 x_i + a_0)|$$

$$\text{or} \quad \boxed{E = \sum_{i=1}^{n} r_i^2 = \sum_{i=1}^{n} [y_i - (a_1 x_i + a_0)]^2}$$

- A smaller E indicates a better fit. This measure can be used to evaluate or compare proposed fits, and last equation can be used to calculate the coefficients a_1 and a_0 in the linear function.

Example

Question: Compare the maximum error, average error, and root-mean-square error for the linear approximation $f(x) = 8.6 - 1.6x$ to the data points $(-1, 10)$, $(0, 9)$, $(1, 7)$, $(2, 5)$, $(3, 4)$, $(4, 3)$, $(5, 0)$, and $(6, -1)$.

Linear least-squares regression

- An experiment produces a set of data points $(x_1, y_1), \ldots, (x_n, y_n)$, where are abscissas $\{x_k\}$ are distinct.
- One goal of numerical methods is to determine a formula $y = f(x)$ that relates these variables.

$$\boxed{y = f(x) = a_1 x + a_0}$$

- Linear least-squares regression is a procedure in which the coefficients a_1 and a_0 of a linear function $y = a_1 x + a_0$ are determined such that the function has the best fit to a given set of data points.
- The best fit is defined as the smallest possible total error that is calculated by adding the squares of the residuals.

$$\boxed{E = \sum_{i=1}^{n} [y_i - (a_1 x_i + a_0)]^2}$$

Linear least-squares regression

- Take the partial derivative of above equation, we get

$$\frac{\partial E}{\partial a_0} = -2\sum_{i=1}^{n}(y_i - a_1 x_i - a_0) = 0 \tag{1}$$

$$\frac{\partial E}{\partial a_1} = -2\sum_{i=1}^{n}(y_i - a_1 x_i - a_0)\, x_i = 0 \tag{2}$$

- Above two equations are a system of two linear equations for the unknows a_1 and a_0, and can be rewritten in the form as

$$n a_0 + \left(\sum_{i=1}^{n} x_i\right) a_1 = \sum_{i=1}^{n} y_i \tag{3}$$

$$\left(\sum_{i=1}^{n} x_i\right) a_0 + \left(\sum_{i=1}^{n} x_i^2\right) a_1 = \sum_{i=1}^{n} x_i y_i \tag{4}$$

Linear least-squares regression

- Solution can be written as

$$a_1 = \frac{n\sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2} \tag{5}$$

$$a_0 = \frac{\left(\sum_{i=1}^{n} x_i^2\right)\left(\sum_{i=1}^{n} y_i\right) - \left(\sum_{i=1}^{n} x_i y_i\right)\left(\sum_{i=1}^{n} x_i\right)}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2} \tag{6}$$

- The values of a_1 and a_0 in the equation $y = a_1 x + a_0$ that has the best fit to n data points (x_i, y_i)

$$a_1 = \frac{nS_{xy} - S_x S_y}{nS_{xx} - (S_x)^2} \qquad a_0 = \frac{S_{xx} S_y - S_{xy} S_x}{nS_{xx} - (S_x)^2}$$

where,

$$S_x = \sum_{i=1}^{n} x_i, \quad S_y = \sum_{i=1}^{n} y_i, \quad S_{xy} = \sum_{i=1}^{n} x_i y_i, \quad S_{xx} = \sum_{i=1}^{n} x_i^2$$

Example

Question: Find the least-squares line for the data points $(-1, 10)$, $(0, 9)$, $(1, 7)$, $(2, 5)$, $(3, 4)$, $(4, 3)$, $(5, 0)$, and $(6, -1)$.

Algorithm for the linear least-square regression

Algorithm 1: Algorithm for Linear Least-Square Regression

Result: Find the linear function $f(x) = a_1 x + a_0$ which best fit the given data points (x_i, y_i), i.e., find the parameter a_0 and a_1 for which the Sum-of-Squared Error is minimum.

Initialization: Initialize the values of x, y.

1. Compute the length of x and y.
2. If the length of x and y is not equal then terminate the program.
3. Compute the value of s_x, s_y, s_{xx}, and s_{xy} as

$$S_x = \sum_{i=1}^{n} x_i, \quad S_y = \sum_{i=1}^{n} y_i, \quad S_{xy} = \sum_{i=1}^{n} x_i y_i, \quad S_{xx} = \sum_{i=1}^{n} x_i^2$$

Algorithm for the linear least-square regression

4. Compute a_0 and a_1

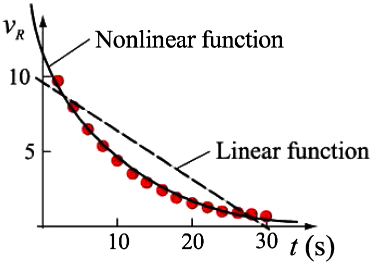
$$a_1 = \frac{nS_{xy} - S_x S_y}{nS_{xx} - (S_x)^2} \qquad a_0 = \frac{S_{xx} S_y - S_{xy} S_x}{nS_{xx} - (S_x)^2}$$

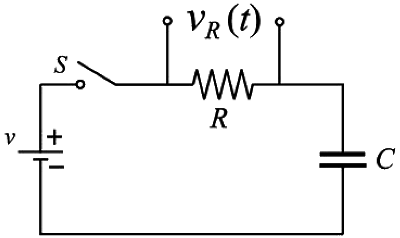
5. Plot the data points and the linear function.

Curve Fitting with Nonlinear Equation

Curve fitting with nonlinear equation

- Many situations in science and engineering show that the relationship between the quantities that are being considered is not linear.
- For example, the data points meansured in RC circuit.





- It is obvious from the plot that curve fitting the data points with a nonlinear function gives a much better fit than curve fitting with a linear function.

Curve fitting with nonlinear equation

- There are many kinds of nonlinear functions which can be used with linear-squares regression method to determine the coefficients that gives the best fit. For examples

$$y = bx^m \qquad \text{(power function)} \tag{7}$$

$$y = be^{mx} \text{ or } y = b10^{mx} \qquad \text{(exponential function)} \tag{8}$$

$$y = \frac{1}{mx+b} \qquad \text{(reciprocal function)} \tag{9}$$

- In order to be able to use linear regression, the form of a nonlinear equation of two variables is changed such that the new form is linear with terms that contain the original variables.

- For example, the power function $y = bx^m$ can be put into linear form by taking the natural logarithm (ln) of both sides:

$$\ln(y) = \ln\left(bx^m\right) = m\ln(x) + \ln(b)$$

Writing a nonlinear equation in linear form

- The equation is linear for $\ln(y)$ in terms $\ln(x)$.
- The equation is in the form

$$\underbrace{\ln(y)}_{Y} = \underbrace{m}_{a_1}\,\underbrace{\ln(x)}_{X} + \underbrace{\ln(b)}_{a_0}$$

- This means that linear least-squares regression can be used for curve fitting an equation of the form $y = bx^m$ to a set of data points (x_i, y_i).
- Once a_1 and a_0 are known, the constants b and m in the exponential equation are calculated by:

$$m = a_1 \qquad \text{and} \qquad b = e^{a_0}$$

Transforming nonlinear equations to linear form

Nonlinear equation	Linear form	Relationship to $Y = a_1X + a_0$	Values for linear least-squares regression	Plot where data points appear to fit a straight line
$y = bx^m$	$\ln(y) = m\ln(x) + \ln(b)$	$Y = \ln(y)$, $X = \ln(x)$ $a_1 = m$, $a_0 = \ln(b)$	$\ln(x_i)$ and $\ln(y_i)$	y vs. x plot on logarithmic y and x axes. $\ln(y)$ vs. $\ln(x)$ plot on linear x and y axes.
$y = be^{mx}$	$\ln(y) = mx + \ln(b)$	$Y = \ln(y)$, $X = x$ $a_1 = m$, $a_0 = \ln(b)$	x_i and $\ln(y_i)$	y vs. x plot on logarithmic y and linear x axes. $\ln(y)$ vs. x plot on linear x and y axes.
$y = b10^{mx}$	$\log(y) = mx + \log(b)$	$Y = \log(y)$, $X = x$ $a_1 = m$, $a_0 = \log(b)$	x_i and $\log(y_i)$	y vs. x plot on logarithmic y and linear x axes. $\log(y)$ vs. x plot on linear x and y axes.
$y = \dfrac{1}{mx+b}$	$\dfrac{1}{y} = mx + b$	$Y = \dfrac{1}{y}$, $X = x$ $a_1 = m$, $a_0 = b$	x_i and $1/y_i$	$1/y$ vs. x plot on linear x and y axes.
$y = \dfrac{mx}{b+x}$	$\dfrac{1}{y} = \dfrac{b}{m}\dfrac{1}{x} + \dfrac{1}{m}$	$Y = \dfrac{1}{y}$, $X = \dfrac{1}{x}$ $a_1 = \dfrac{b}{m}$, $a_0 = \dfrac{1}{m}$	$1/x_i$ and $1/y_i$	$1/y$ vs. $1/x$ plot on linear x and y axes.

Example

Question: Use the least-squares method and determine the exponential fit $y = Ce^{Ax}$ for the five data points $(0, 1.5)$, $(1, 2.5)$, $(2, 3.5)$, $(3, 5.0)$, and $(4, 7.5)$.

Choose an appropriate nonlinear function for curve fitting

- A plot of the given data points can give an intuitive relationship between the quantities whether the relationship is linear or nonlinear.
- Prior knowledge from a guiding theory of the physical phenomena and the form of the mathematical equation associated with the data points.
- Other fundamental concepts can be used
  - Exponential functions cannot pass through the origin.
  - Exponential functions can only fit data with all positive ys, or all negative ys.
  - Logarithmic functions cannot include $x = 0$ or negative values of x.
  - For power function $y = 0$ when $x = 0$.
  - The reciprocal equation cannot include $y = 0$.

Example

Question: Students collected the experimental data points (t,d) at different instance of time as (0.200,0.1960), (0.400,0.7850), (0.600,1.7665), (0.8,3.1405), and (1,4.9075). The relation is $d = \frac{1}{2}gt^2$, where d is distance in meters and t is time in seconds. Find the gravitational constant g.

Curve fitting with quadratic and higher order polynomials

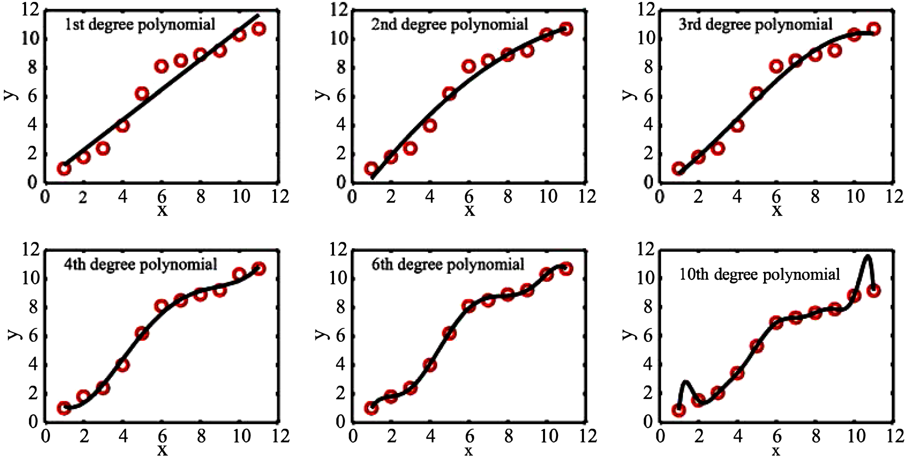
Curve fitting with quadratic and higher order polynomials

- Polynomials are functions that have the form

$$f(x) = a_m x^m + a_{m-1} x^{m-1} + \cdots + a_0.$$

  The coefficients $a_m, a_{m-1}, \ldots, a_1, a_0$ are real numbers and m is a non-negative integer called degree or order of the polynomial.
- A plot of the polynomial is a curve. A first-order polynomial is a linear function, and its plot is a straight line. Higher-order polynomials are nonlinear functions, and their plots are curves.
- A quadratic (second-order) polynomial is a curve that is either concave up or down (parabola).
- A third-order polynomial has an inflection point such that the curve can be concave up (or down) in one region, and concave down (or up) in another.

Curve fitting with polynomials of different order



Curve fitting with quadratic and higher order polynomials

- A given set of n data points can be curve-fit with polynomials of different order up to an order of $(n-1)$.
- The coefficients of a polynomial can be determined such that the polynomial best fits the data by minimizing the error in a least squares sense.
- For n points, the polynomial that passes through all of the points is one of order $(n-1)$.

Polynomial regression

- Polynomial regression is a procedure for determining the coefficients of a polynomial of a second degree, or higher, such that the polynomial best fits (minimizing the total error) a given set of data points.
- If the polynomial of order m, that is used for curve fitting is

$$f(x) = a_m x^m + a_{m-1} x^{m-1} + \ldots + a_1 x + a_0.$$

- Then, for a given set of n data points $\{(x_i, y_i)\}_{i=1}^{n}$ (m is smaller than $n-1$), the total error is given by

$$E = \sum_{i=1}^{n} \left[y_i - (a_m x_i^m + a_{m-1} x_i^{m-1} + \ldots + a_1 x_i + a_0) \right]^2$$

- The function E has a minimum at the values of a_0 through a_m, where the partial derivatives of E with respect to each of the variables is equal to zero.

Polynomial regression

- For the simplicity, let us consider the case of $m = 2$ (Quadratic polynomial)

$$E = \sum_{i=1}^{n} \left[y_i - (a_2 x_i^2 + a_1 x_i + a_0)\right]^2$$

- Taking the partial derivatives with respect to a_0, a_1, and a_2 , and setting them equal to zero gives:

$$\frac{\partial E}{\partial a_0} = -2 \sum_{i=1}^{n} \left(y_i - a_2 x_i^2 - a_1 x_i - a_0\right) = 0 \tag{10}$$

$$\frac{\partial E}{\partial a_1} = -2 \sum_{i=1}^{n} \left(y_i - a_2 x_i^2 - a_1 x_i - a_0\right) x_i = 0 \tag{11}$$

$$\frac{\partial E}{\partial a_2} = -2 \sum_{i=1}^{n} \left(y_i - a_2 x_i^2 - a_1 x_i - a_0\right) x_i^2 = 0 \tag{12}$$

Polynomial regression

$$
\begin{aligned}
na_0 + \left(\sum_{i=1}^{n} x_i\right) a_1 + \left(\sum_{i=1}^{n} x_i^2\right) a_2 &= \sum_{i=1}^{n} y_i \\
\left(\sum_{i=1}^{n} x_i\right) a_0 + \left(\sum_{i=1}^{n} x_i^2\right) a_1 + \left(\sum_{i=1}^{n} x_i^3\right) a_2 &= \sum_{i=1}^{n} x_i y_i \\
\left(\sum_{i=1}^{n} x_i^2\right) a_0 + \left(\sum_{i=1}^{n} x_i^3\right) a_1 + \left(\sum_{i=1}^{n} x_i^4\right) a_2 &= \sum_{i=1}^{n} x_i^2 y_i
\end{aligned} \tag{13}
$$

- The solution of the system of equations gives the values of the coefficients a_0, a_1, and a_2 of the polynomial $y = a_2 x_i^2 + a_1 x_i + a_0$ that best fits then data points $\{(x_i, y_i)\}_{i=1}^{n}$.
- The coefficients for higher-order polynomials are derived in the same way.

Examples

Example: Find the least-squares parabola for the four points $(-3, 3)$, $(0, 1)$, $(2, 1)$, and $(4, 3)$.

Polynomial of higher order

- A polynomial of the fourth order can be written as

$$f(x) = a_4x^4 + a_3x^3 + a_2x^2 + a_1x + a_0$$

- The values of the five coefficients a_0, a_1, a_2, a_3, and a_4 are obtained by solving a system of five linear equations.

$$\begin{aligned}
na_0 + \left(\sum_{i=1}^{n} x_i^1\right) a_1 + \left(\sum_{i=1}^{n} x_i^2\right) a_2 + \left(\sum_{i=1}^{n} x_i^3\right) a_3 + \left(\sum_{i=1}^{n} x_i^4\right) a_4 &= \sum_{i=1}^{n} x_i y_i \\
\left(\sum_{i=1}^{n} x_i\right) a_0 + \left(\sum_{i=1}^{n} x_i^2\right) a_1 + \left(\sum_{i=1}^{n} x_i^3\right) a_2 + \left(\sum_{i=1}^{n} x_i^4\right) a_3 + \left(\sum_{i=1}^{n} x_i^5\right) a_4 &= \sum_{i=1}^{n} x_i y_i \\
\left(\sum_{i=1}^{n} x_i^2\right) a_0 + \left(\sum_{i=1}^{n} x_i^3\right) a_1 + \left(\sum_{i=1}^{n} x_i^4\right) a_2 + \left(\sum_{i=1}^{n} x_i^5\right) a_3 + \left(\sum_{i=1}^{n} x_i^6\right) a_4 &= \sum_{i=1}^{n} x_i^2 y_i \\
\left(\sum_{i=1}^{n} x_i^3\right) a_0 + \left(\sum_{i=1}^{n} x_i^4\right) a_1 + \left(\sum_{i=1}^{n} x_i^5\right) a_2 + \left(\sum_{i=1}^{n} x_i^6\right) a_3 + \left(\sum_{i=1}^{n} x_i^7\right) a_4 &= \sum_{i=1}^{n} x_i^3 y_i \\
\left(\sum_{i=1}^{n} x_i^4\right) a_0 + \left(\sum_{i=1}^{n} x_i^5\right) a_1 + \left(\sum_{i=1}^{n} x_i^6\right) a_2 + \left(\sum_{i=1}^{n} x_i^7\right) a_3 + \left(\sum_{i=1}^{n} x_i^8\right) a_4 &= \sum_{i=1}^{n} x_i^4 y_i
\end{aligned}$$

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Thank you!