數值分析

Chapter 4
Curve Fitting and Interpolation

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Outline

- Curve fitting with a linear/nonlinear equation (4.2 4.3)
- Curve fitting with quadratic/higher order polynomials (4.4)
- Interpolation using a single polynomial (4.5)
  - Lagrange polynomials (4.5.1)
  - Newton's polynomials (4.5.2)
- Piecewise (spline)interpolation (4.6)
- MATLAB built-in functions (4.7)

4.1 Background

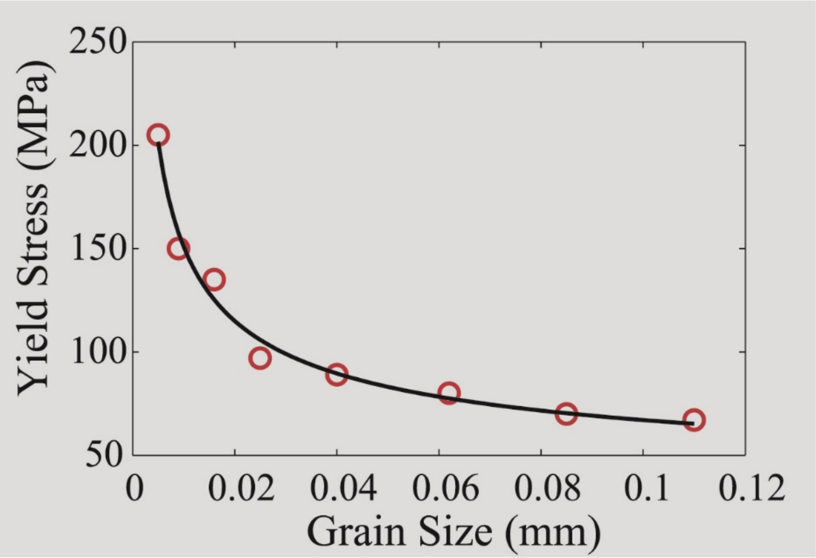
- Experimental data is used for developing, or evaluating, mathematical formulas (equations) – **curve fitting**

- Find the equation that *best fit* the data

- The data points are used for
  - estimating the expected values between the known point (**interpolation**)
  - predicting how the data might extend beyond the range (**extrapolation**)

Curve-Fitting

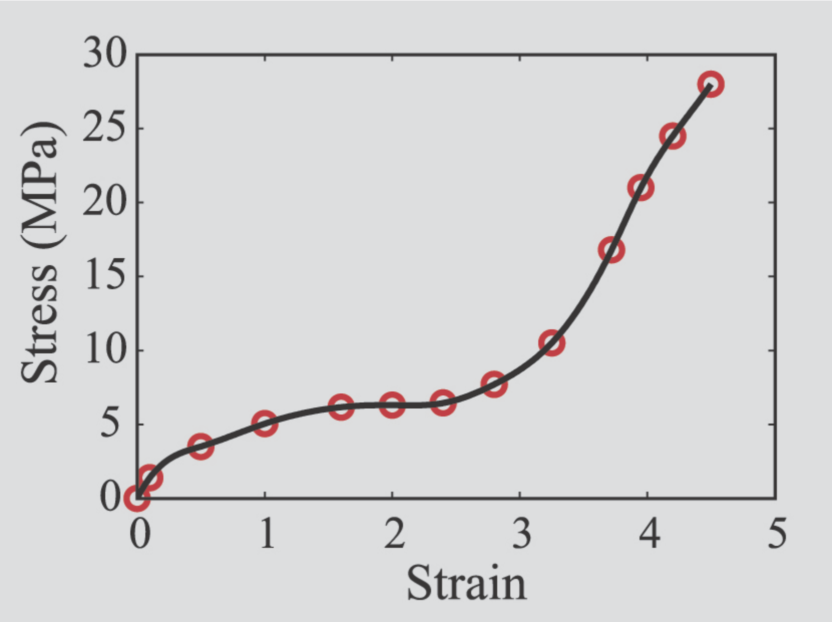
- A procedure in which a mathematical formula is used to best fit a given set of data points
- The function does not have to give the exact value at any single point (but fits the data well overall)
- Curve fitting is typically used when the values of the data points have some error, or scatter.



$$\sigma = Cd^{m}$$

Interpolation

- A procedure for estimating a value between know values of data points.
  - (1) first determining a polynomial that gives the exact value at the data points
  - (2) using the polynomial for calculating values between the points

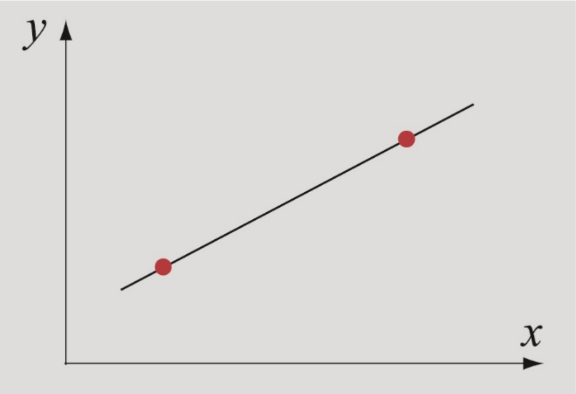


4.2 Curve Fitting with a Linear Equation

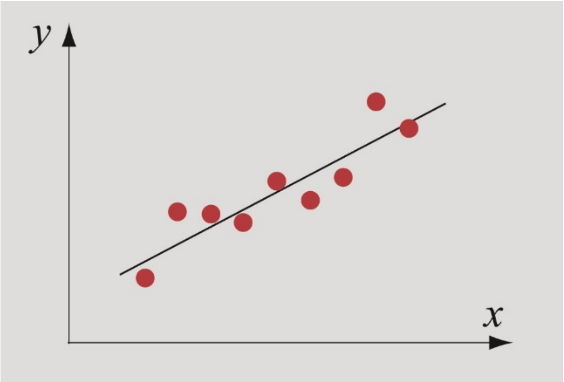
- Using a linear equation:

$$y = a_1 x + a_0$$

- Determine the constants (a_1 and a_0) that give the **smallest error**



Two data points

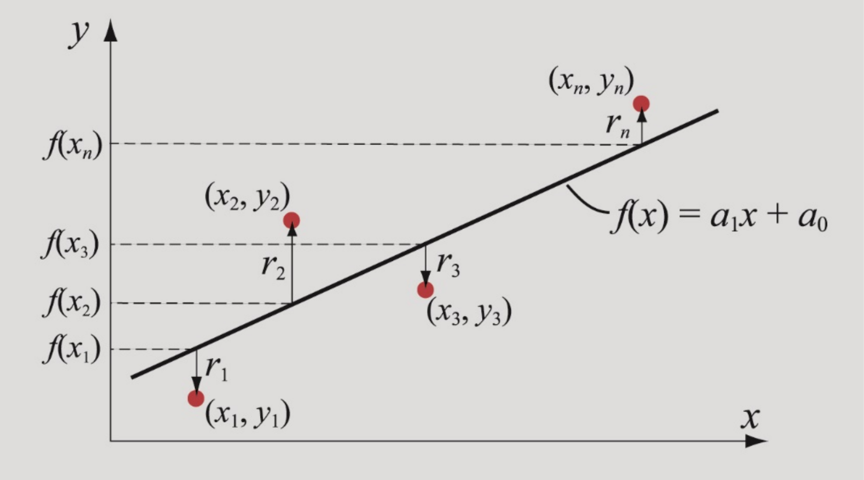


Many data points

Measuring how good is a fit

- Calculate a number that quantifies the overall agreement between the points and the function
  - To compare two different functions that are used for fitting the same data points
  - The criterion itself is used for determining the coefficients of the function
- Determine the error (residual): the difference between a data point and the value of the approximating function at each point

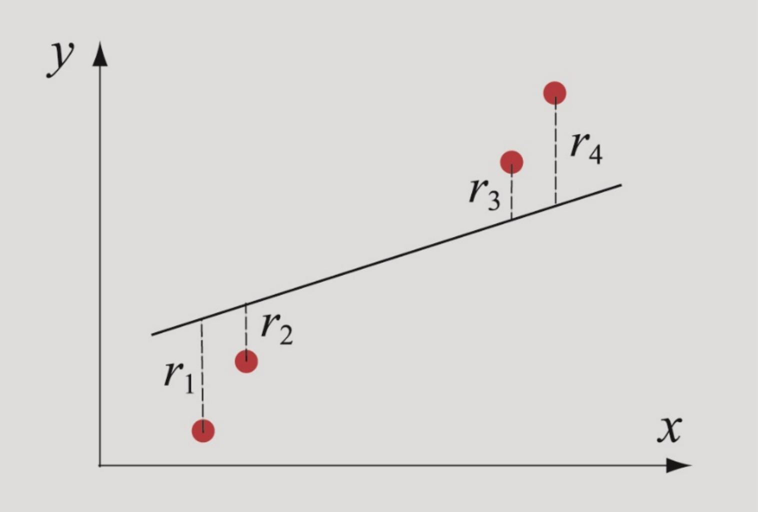
$$r_i = y_i - f(x_i)$$



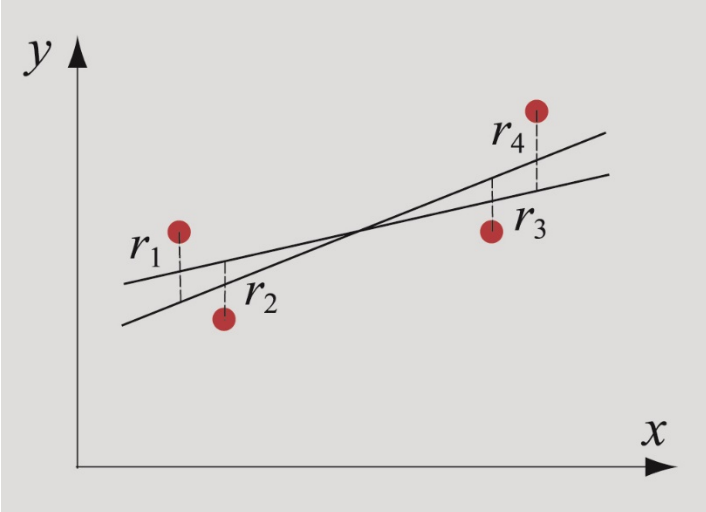
Measuring how good is a fit

- Define a total error (E):

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



Fit with no error according to Eq. (4.3)



Two fits with the same error according to Eq. (4.4)

Linear Least-Square Regression

- A procedure to determined the coefficient of a linear function such that the function has the best fit

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

- The function E has a minimum at the values of a_1 and a_0 where the **partial derivative** of E with respect to each variable is equal to zero

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

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

Linear Least-Square Regression

$$na_0 + \left(\sum_{i=1}^{n} x_i\right)a_1 = \sum_{i=1}^{n} y_i \qquad \left(\sum_{i=1}^{n} x_i\right)a_0 + \left(\sum_{i=1}^{n} x_i^2\right)a_1 = \sum_{i=1}^{n} x_i y_i$$

The solution of the system is:

$$a_1 = \frac{n\sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2} \qquad a_0 = \frac{\left(\sum_{i=1}^{n} x_i^2\right)\left(\sum_{i=1}^{n} y_i\right) - \left(\sum_{i=1}^{n} x_i y_i\right)\left(\sum_{i=1}^{n} x_i\right)}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

It is convenient to calculate the summations and substitute into equations:

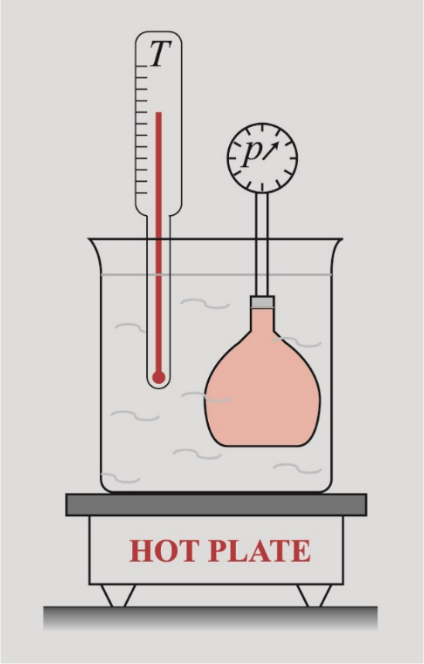
$$\boxed{a_1 = \frac{nS_{xy} - S_x S_y}{nS_{xx} - (S_x)^2} \qquad a_0 = \frac{S_{xx} S_y - S_{xy} S_x}{nS_{xx} - (S_x)^2}}$$

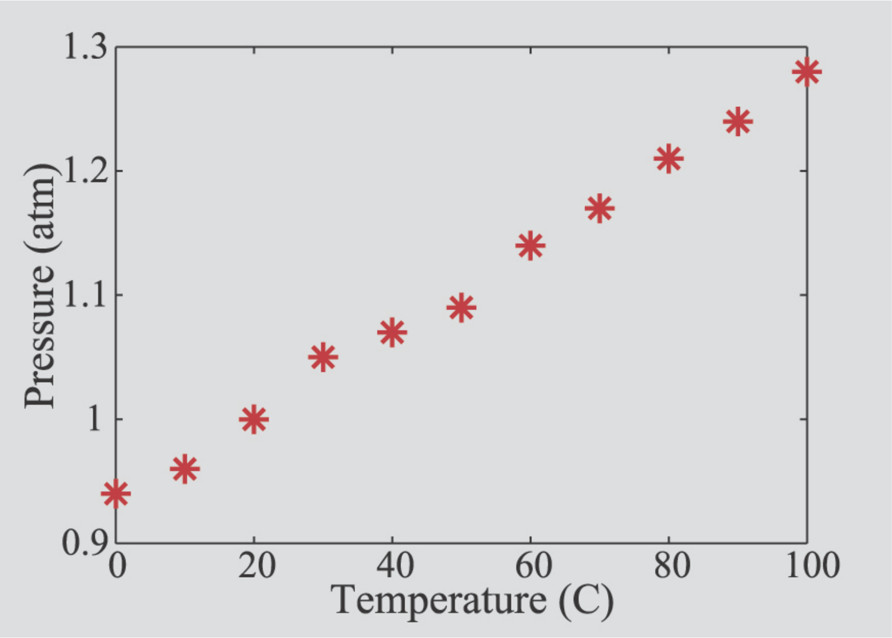
$$S_x = \sum_{i=1}^{n} x_i \qquad S_y = \sum_{i=1}^{n} y_i \qquad S_{xy} = \sum_{i=1}^{n} x_i y_i \quad S_{xx} = \sum_{i=1}^{n} x_i^2$$

Example 4.1

- Determine the relationship between pressure and temperature using linear least-square regression

p (atm)	0.94	0.96	1.0	1.05	1.07	1.09	1.14	1.17	1.21	1.24	1.28
T (˚C)	0	10	20	30	40	50	60	70	80	90	100





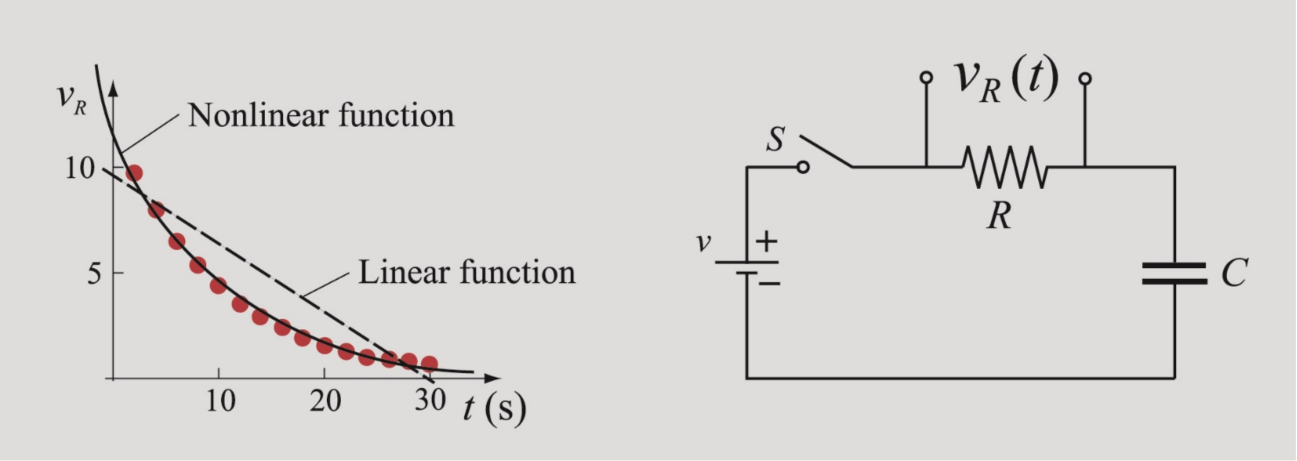
4.3 Curve Fitting with Nonlinear Equation by Writing the Equation in a Linear Form

- Nonlinear function that gives a better fit
- This section considers the nonlinear function that can be written in a **form** for which linear least-square regression method can be used

$$y = bx^m$$ Power function

$$y = be^{mx}$$ Exponential function

$$y = \frac{1}{mx+b}$$ Reciprocal function



Writing a nonlinear equation in linear form

- By changing the variables into a new linear form that contain the original variable

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

- This equation is linear for **ln(y)** in terms of **ln(x)**

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

$$Y = a_1 X + a_0$$

- The linear least-square regression can be used

$$m = a_1$$

$$b = e^{a_0}$$

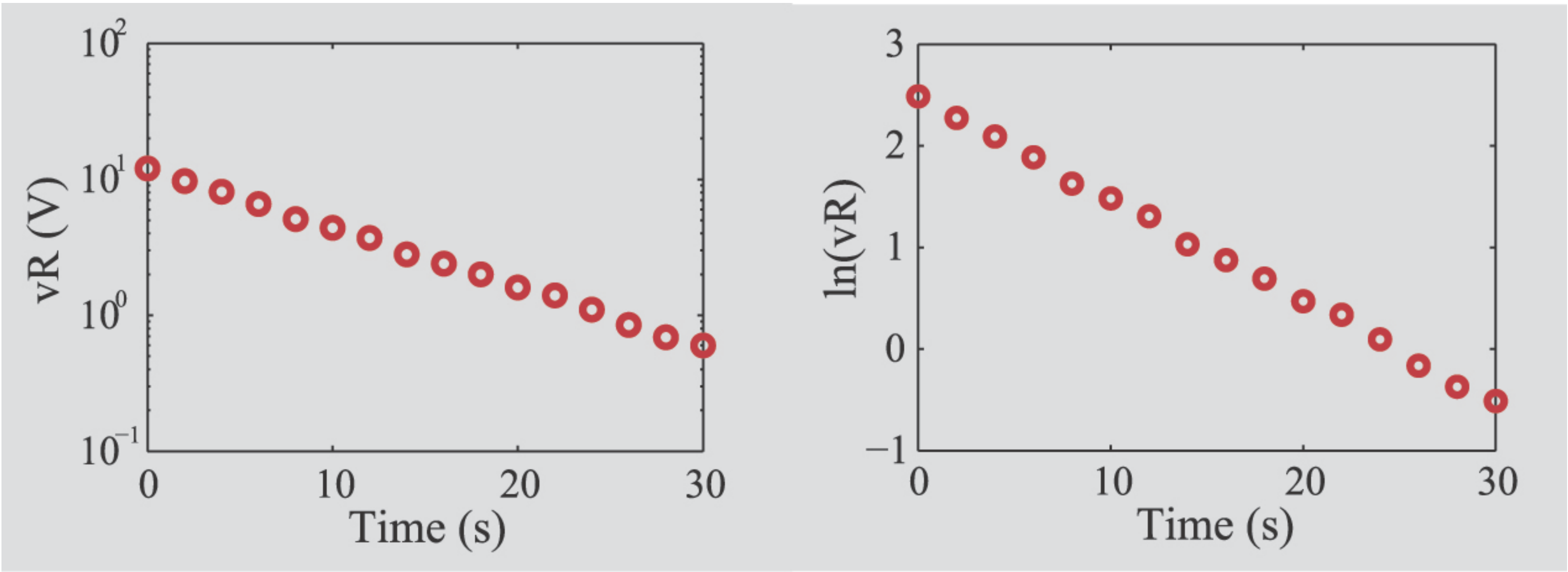
Writing a nonlinear equation in linear form

Table 4-2: 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 $\ln(y_i)$	y vs. x plot on logarithmic y and linear x axes. $\ln(y)$ vs. x plot on linear x and y axes.
$y = \dfrac{1}{mx + b}$	$\dfrac{1}{y} = mx + b$	$Y = \dfrac{1}{y}$, $X = x$ $a_1 = m$, $a_0 = b$	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.

How to Choose an Appropriate nonlinear function

- **What kind of nonlinear function** is selected for curve fitting?
- Choose the function from the knowledge from a guiding theory of the physical phenomena
- Plotting the data points in a specific way to examine



Example 4.2

- Curve fitting with a nonlinear function

t (s)	2	4	6	8	10	12	14	16	18	20	22	24	26	28	30
V_R (V)	9.7	8.1	6.6	5.1	4.4	3.7	2.8	2.4	2.0	1.6	1.4	1.1	0.85	0.69	0.6

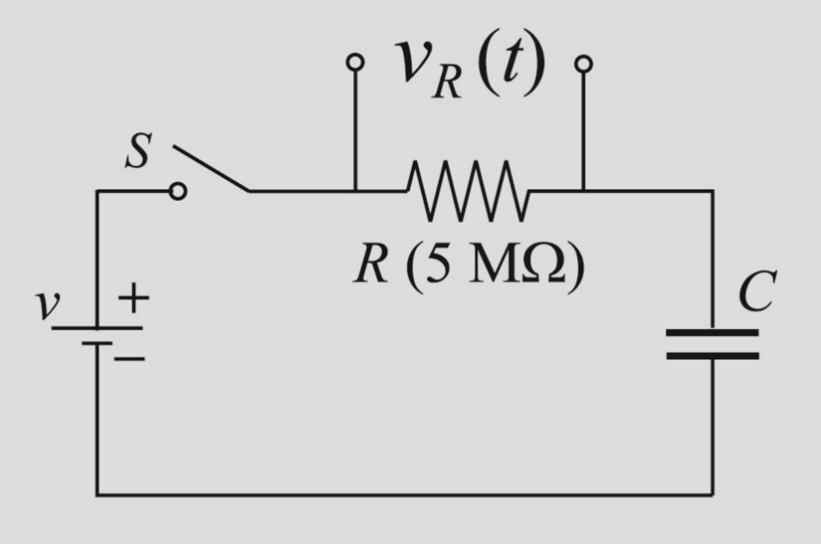
- Curve fitting using the exponential function

$$V_R = ve^{(-t/(RC))}$$

- Determine the constants

$$V = be^{mt}$$

$$\frac{-1}{RC} = m$$

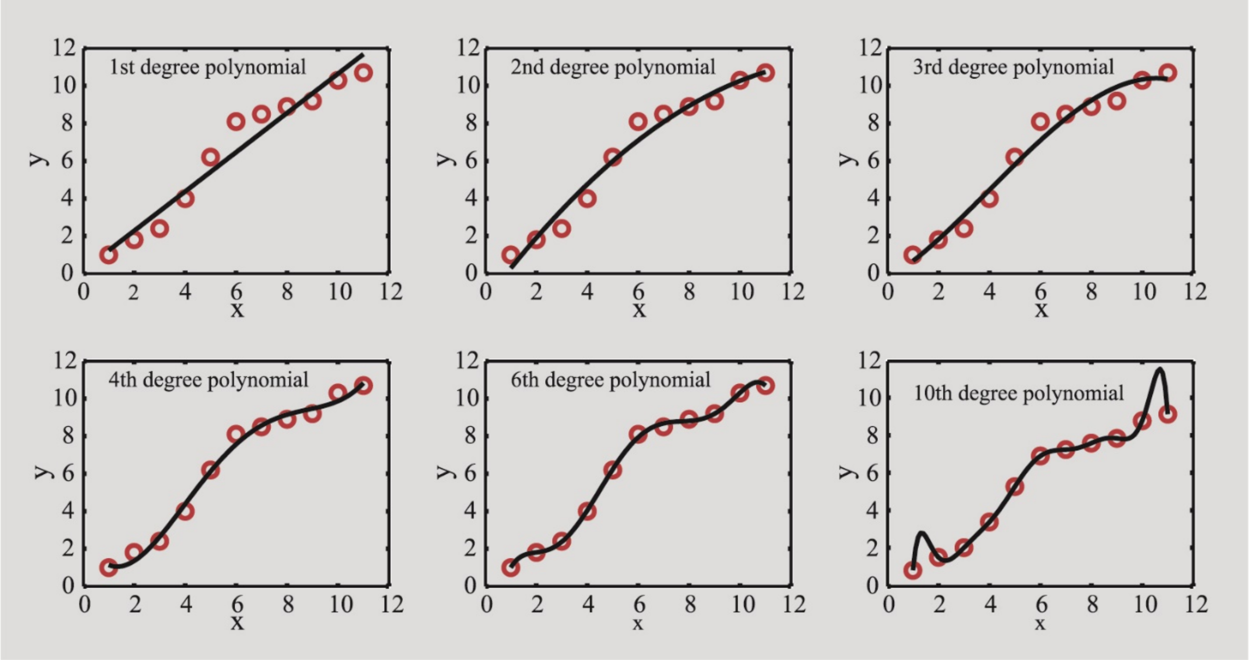


4.4 Curve Fitting with Higher Order Polynomials

- Polynomials are functions that have the form:

$$f(x) = a_n x^n + a_{n-1} x^{n-1} + \ldots + a_1 x + a_0$$

- In general, higher order polynomials have more ‘bends’
- A given set of **n data points** can be curve-fit with polynomials of different order up to an order of **n-1**
- Although higher order polynomial gives the exact values at the data points, often the polynomial deviates **between** some of the points



Polynomial Regression

- Polynomial regression is a procedure for determining the coefficients of a polynomial such that the polynomial gives a best fit
- If the polynomial of order m that is used for fitting:

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

- For a given set of n data points(x_i, y_i), the total error is:

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

- The function has a minimum at the values of a_0 through a_m where the partial derivative of E with respect to each variable is zero
- For the case of m=2 (quadratic polynomial):

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

Polynomial Regression

- Take the partial derivative with respect to a_0, a_1 and a_2:

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

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

- The system of three linear equations can be written as:

$$na_0 + \left(\sum_{i=1}^{n} x_i\right)a_1 + \left(\sum_{i=1}^{n} x_i^2\right)a_2 = \sum_{i=1}^{n} y_i$$

$$\left(\sum_{i=1}^{n} x_i\right)a_0 + \left(\sum_{i=1}^{n} x_i^2\right)a_1 + \left(\sum_{i=1}^{n} x_i^3\right)a_2 = \sum_{i=1}^{n} x_i y_i$$

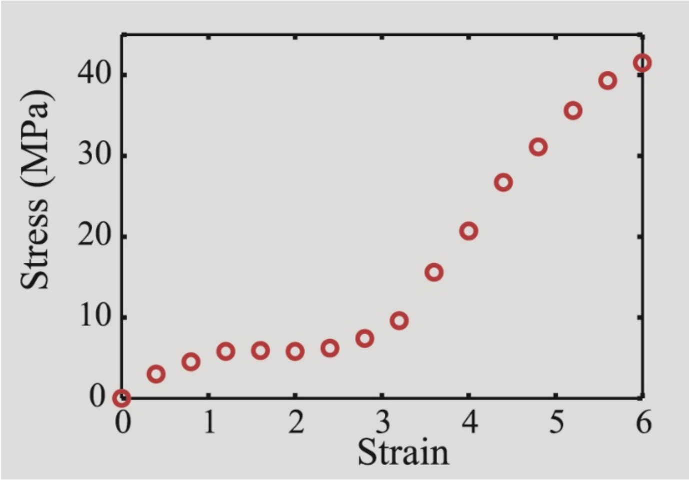
$$\left(\sum_{i=1}^{n} x_i^2\right)a_0 + \left(\sum_{i=1}^{n} x_i^3\right)a_1 + \left(\sum_{i=1}^{n} x_i^4\right)a_2 = \sum_{i=1}^{n} x_i^2 y_i$$

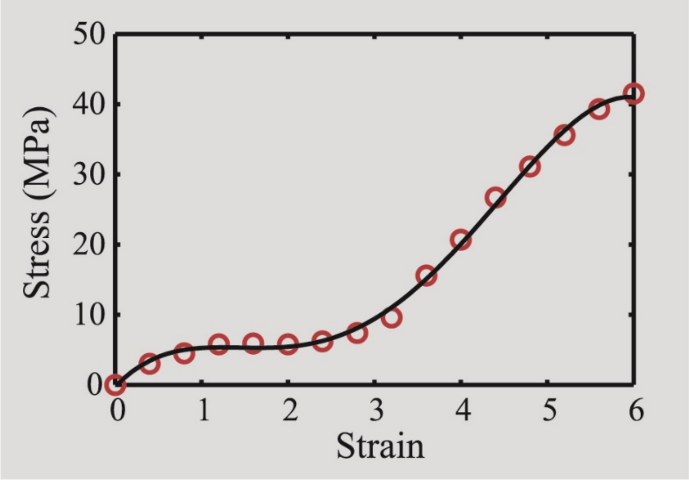
- The coefficients for higher-order polynomials can be determined by the similar procedure

Example 4-3: Polynomial regression

- Curve-fit the stress-strain curve with the fourth order polynomial

$$f(x) = a_4 x^4 + a_3 x^3 + a_2 x^2 + a_1 x + a_0$$





Strain	0	0.4	0.8	1.2	1.6	2.0	2.4	2.8	3.2	3.6	4.0	4.4	4.8	5.2	5.6	6.0
Stress	0	3.0	4.5	5.8	5.9	5.8	6.2	7.4	9.6	15.6	20.7	26.7	31.1	35.6	39.3	41.5

Example 4-3: Polynomial regression

- The coefficients (a_0, a_1, a_2, a_3, a_4) are obtained by solving a system of five linear equations

$$na_0 + \left(\sum_{i=1}^{n} x_i\right)a_1 + \left(\sum_{i=1}^{n} x_i^2\right)a_2 + \left(\sum_{i=1}^{n} x_i^3\right)a_3 + \left(\sum_{i=1}^{n} x_i^4\right)a_4 = \sum_{i=1}^{n} y_i$$

$$\left(\sum_{i=1}^{n} x_i\right)a_0 + \left(\sum_{i=1}^{n} x_i^2\right)a_1 + \left(\sum_{i=1}^{n} x_i^3\right)a_2 + \left(\sum_{i=1}^{n} x_i^4\right)a_3 + \left(\sum_{i=1}^{n} x_i^5\right)a_4 = \sum_{i=1}^{n} x_i y_i$$

$$\left(\sum_{i=1}^{n} x_i^2\right)a_0 + \left(\sum_{i=1}^{n} x_i^3\right)a_1 + \left(\sum_{i=1}^{n} x_i^4\right)a_2 + \left(\sum_{i=1}^{n} x_i^5\right)a_3 + \left(\sum_{i=1}^{n} x_i^6\right)a_4 = \sum_{i=1}^{n} x_i^2 y_i$$

$$\left(\sum_{i=1}^{n} x_i^3\right)a_0 + \left(\sum_{i=1}^{n} x_i^4\right)a_1 + \left(\sum_{i=1}^{n} x_i^5\right)a_2 + \left(\sum_{i=1}^{n} x_i^6\right)a_3 + \left(\sum_{i=1}^{n} x_i^7\right)a_4 = \sum_{i=1}^{n} x_i^3 y_i$$

$$\left(\sum_{i=1}^{n} x_i^4\right)a_0 + \left(\sum_{i=1}^{n} x_i^5\right)a_1 + \left(\sum_{i=1}^{n} x_i^6\right)a_2 + \left(\sum_{i=1}^{n} x_i^7\right)a_3 + \left(\sum_{i=1}^{n} x_i^8\right)a_4 = \sum_{i=1}^{n} x_i^4 y_i$$

Example 4-3: Polynomial regression

- Procedure
  - Step 1: create vectors x and y with data points
  - Step 2: create a vector *xsum* to calculate summation terms

$$xsum(4) = \sum_{i=1}^{n} x_i^4$$

  - Step 3: set up the system of five linear equations [a][p]=[b]
  - Step 4: solve the system of five linear equations
  - Step 5: plot the data points and the curve-fitting polynomial