DTS104TC
NUMERICAL METHODS

LECTURE 4

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CONTENTS

- Curve Fitting [relates to syllabus (f)]
- Interpolation

CURVE FITTING

Describes techniques to fit curves (*curve fitting*) to discrete data to obtain intermediate estimates.

There are two general approaches two curve fitting:

Data exhibit a significant degree of scatter. The strategy is to derive a single curve that represents the general trend of the data.

Data is very precise. The strategy is to pass a curve or a series of curves through each of the points.

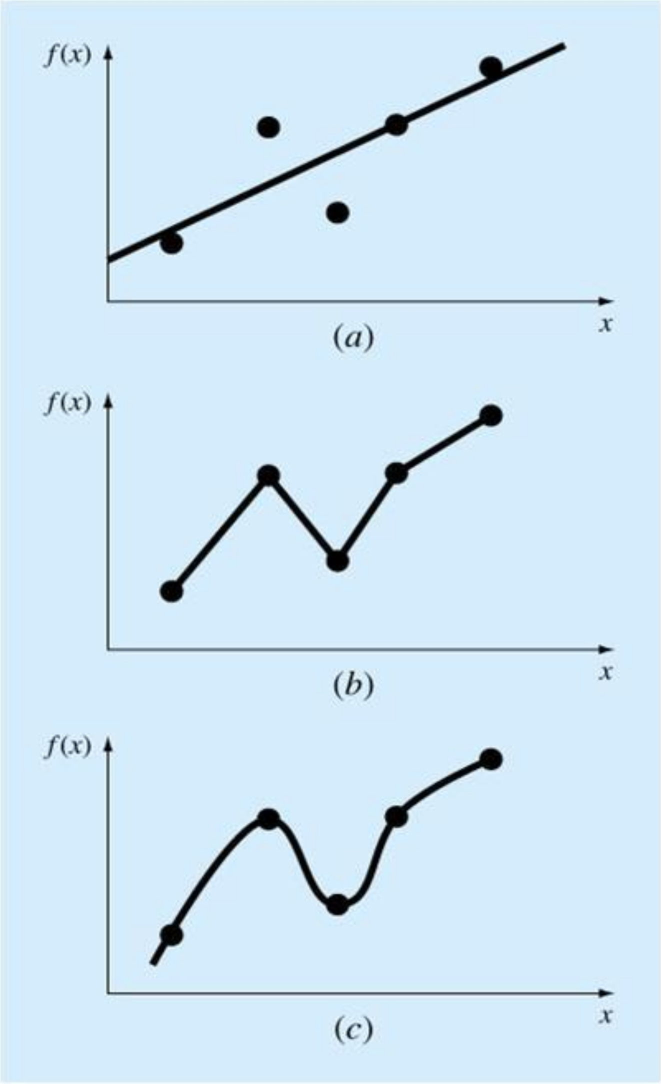
- Generally, two types of applications are encountered:
  - Trend analysis. Predicting values of dependent variable, may include extrapolation beyond data points or interpolation between data points.
  - Hypothesis testing. Comparing existing mathematical model with measured data.

THREE ATTEMPTS TO FIT A "BEST" CURVE THROUGH FIVE DATA POINTS

(a) **Least-squares regression.**

(b) **linear interpolation.**

(c) **curvilinear interpolation.**



MATHEMATICAL BACKGROUND

If several measurements are made of a particular quantity, additional insight can be gained by summarizing the data in one or more well chosen statistics that convey as much information as possible about specific characteristics of the data set.

These descriptive statistics are most often selected to represent,

- The location of the center of the distribution of the data,
- The degree of spread of the data.

DESCRIPTIVE STATISTICS

- *Arithmetic mean*. The sum of the individual data points (y_i) divided by the number of points (n).

$$\bar{y} = \frac{\sum y_i}{n}$$

$$i = 1, \ldots, n$$

- *Standard deviation*. The most common measure of a spread for a sample.

$$S_y = \sqrt{\frac{S_t}{n-1}} \quad \text{or} \quad S_y^2 = \frac{\sum y_i^2 - \left(\sum y_i\right)^2 / n}{n-1}$$

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

DESCRIPTIVE STATISTICS

- *Variance*. Representation of spread by the square of the standard deviation.

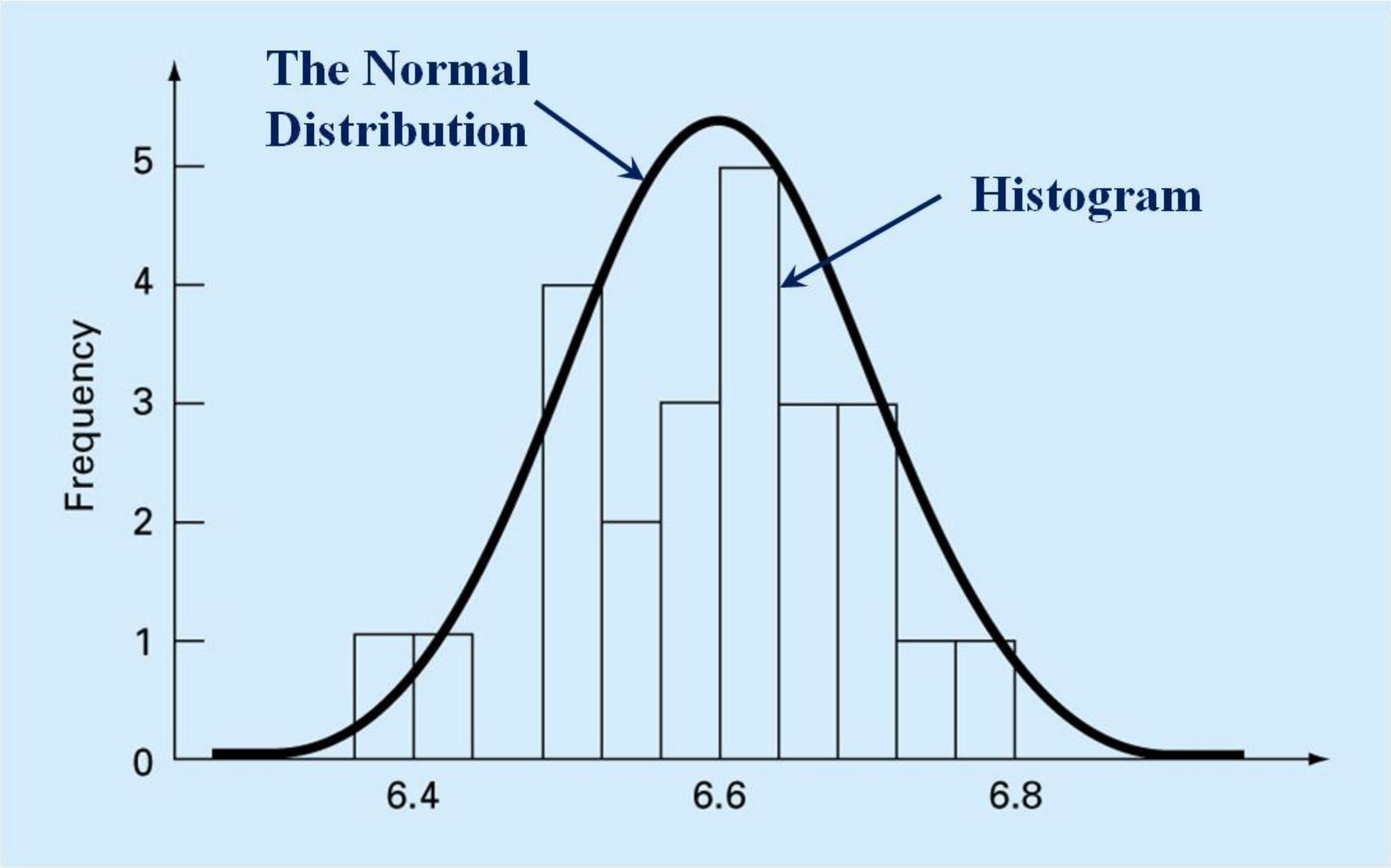
$$S_y^2 = \frac{\sum (y_i - \bar{y})^2}{n-1}$$

- Degrees of freedom

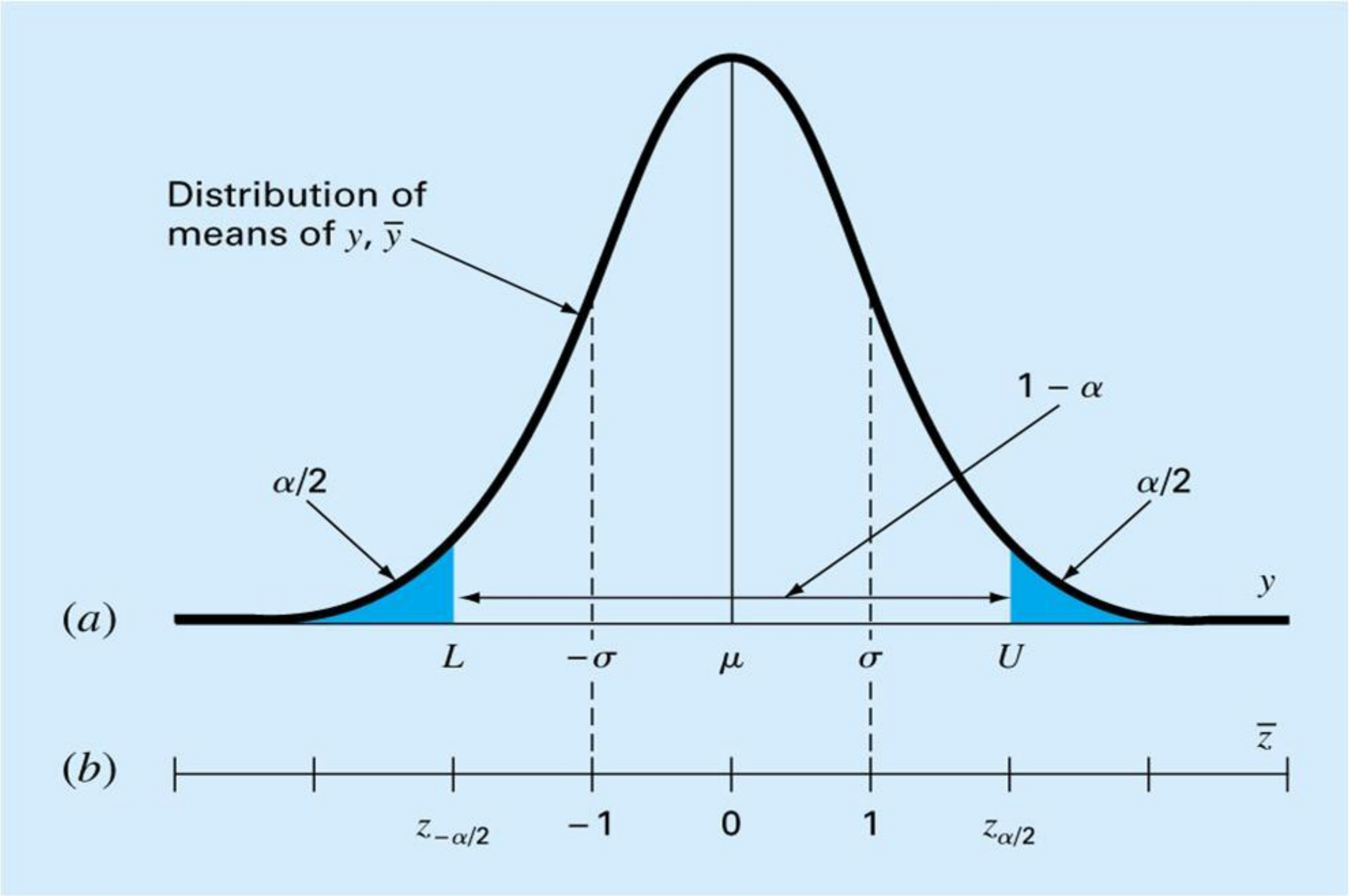
- *Coefficient of variation*. Has the utility to normalize the spread of data.

$$c.v. = \frac{S_y}{\bar{y}} 100\%$$

HISTOGRAM: DEPICTS THE DISTRIBUTION OF DATA



THE NORMAL DISTRIBUTION



LEAST SQUARES REGRESSION

Linear Regression

- Fitting a straight line to a set of paired observations: $(x_1, y_1), (x_2, y_2),\ldots,(x_n, y_n)$,

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

- a_1: slope
- a_0: intercept
- e: error, or residual, between the model and the observations

CRITERIA FOR A "BEST" FIT

- Minimize the sum of the residual errors for all available data:

$$\sum_{i=1}^{n} e_i = \sum_{i=1}^{n} (y_i - a_o - a_1 x_i)$$

- where n = total number of points.

- However, this is an inadequate criterion, so is the sum of the absolute values,

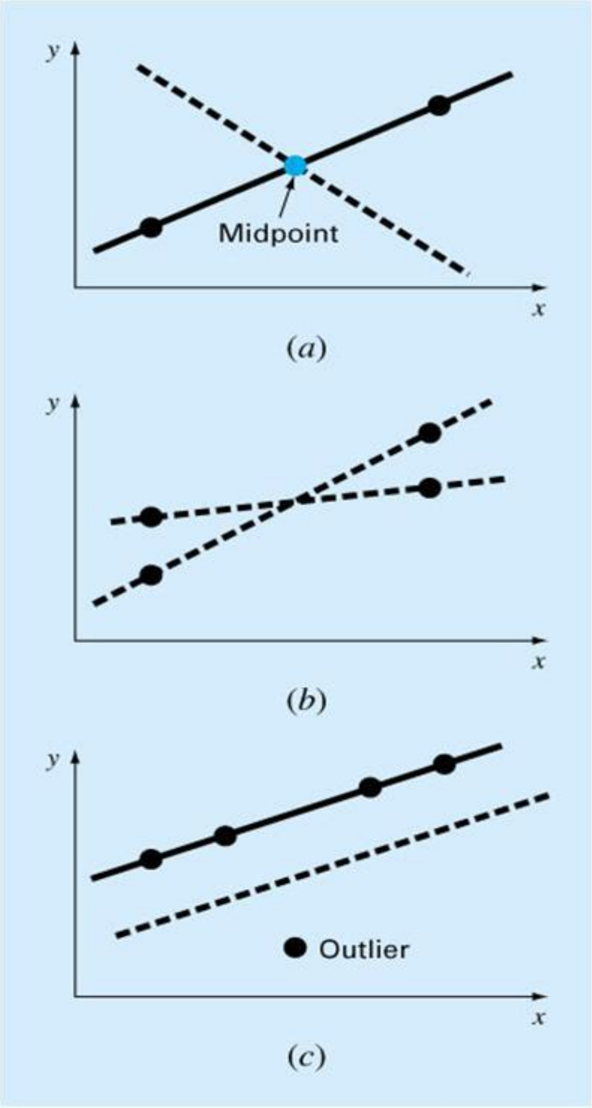
$$\sum_{i=1}^{n} |e_i| = \sum_{i=1}^{n} |y_i - a_0 - a_1 x_i|$$

3 INADEQUATE DEFINITIONS OF A "BEST FIT"

(a) minimize the sum of the residuals.

(b) minimize the sum of the absolute values of the residuals.

(c) minimize the maximum error of any individual point.



MINIMIZE THE SUM OF THE SQUARES OF THE RESIDUALS

- Best strategy is to minimize the sum of the squares of the residuals between the measured *y* and the *y* calculated with the linear model:

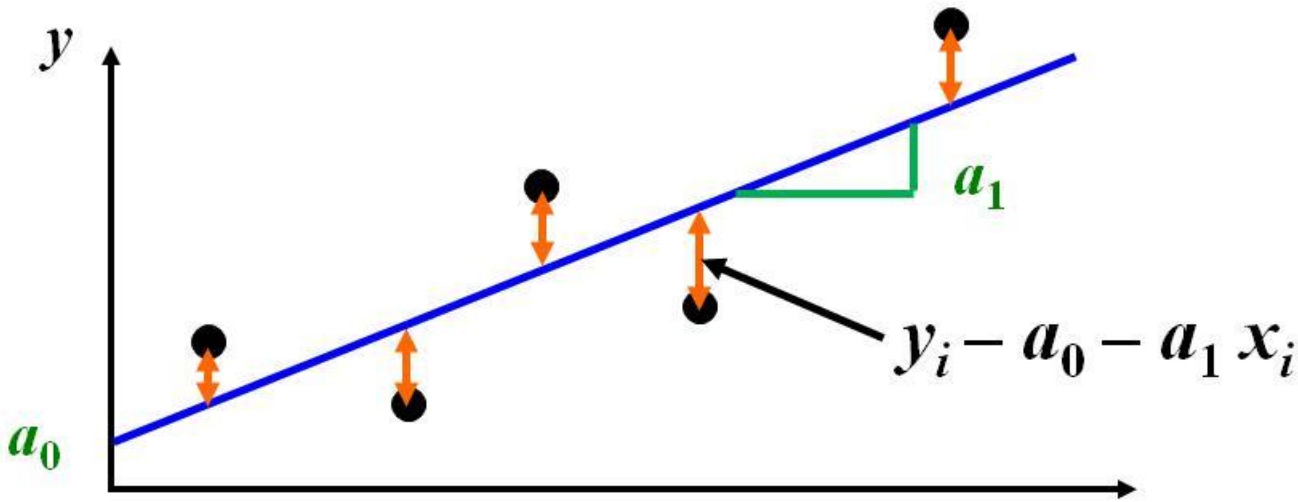
$$S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i, \text{measured} - y_i, \text{model})^2 = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i)^2$$

- Yields a unique line for a given set of data.

SUM OF THE SQUARES OF THE RESIDUALS

$$S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} \left(y_{i,\text{measured}} - y_{i,\text{model}} \right)^2$$

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



MINIMIZE S_r

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

$$\frac{\partial S_r}{\partial a_0} = -2 \sum \left(y_i - a_0 - a_1 x_i \right) = 0$$

$$\frac{\partial S_r}{\partial a_1} = -2 \sum \left[\left(y_i - a_0 - a_1 x_i \right) x_i \right] = 0$$

$$0 = \sum y_i - \sum a_0 - \sum a_1 x_i$$

$$0 = \sum y_i x_i - \sum a_0 x_i - \sum a_1 x_i^2$$

MINIMIZE S_r

$$0 = \sum y_i - \sum a_0 - \sum a_1 x_i$$

$$0 = \sum y_i x_i - \sum a_0 x_i - \sum a_1 x_i^2$$

$$\boxed{\begin{aligned} n a_0 \quad &+ \left(\sum x_i\right) a_1 = \sum y_i \\ \left(\sum x_i\right) a_0 &+ \left(\sum x_i^2\right) a_1 = \sum x_i y_i \end{aligned}}$$

Normal Equations

NORMAL EQUATIONS

$$na_0 + \left(\sum x_i\right)a_1 = \sum y_i$$

$$\left(\sum x_i\right)a_0 + \left(\sum x_i^2\right)a_1 = \sum x_i y_i$$

Matrix form:

$$\begin{bmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \end{Bmatrix} = \begin{Bmatrix} \sum y_i \\ \sum x_i y_i \end{Bmatrix}$$

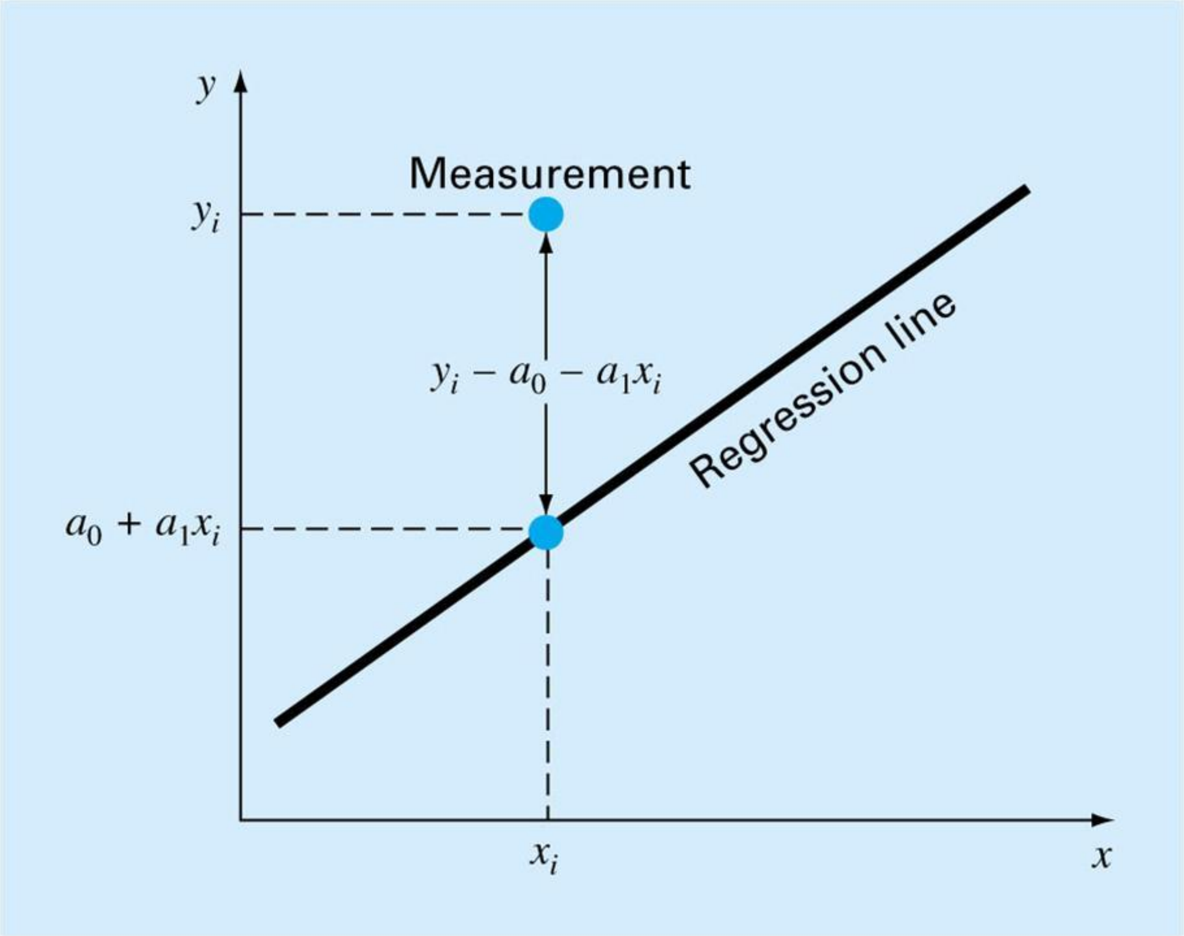
SOLUTION FOR SLOPE AND INTERCEPT

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

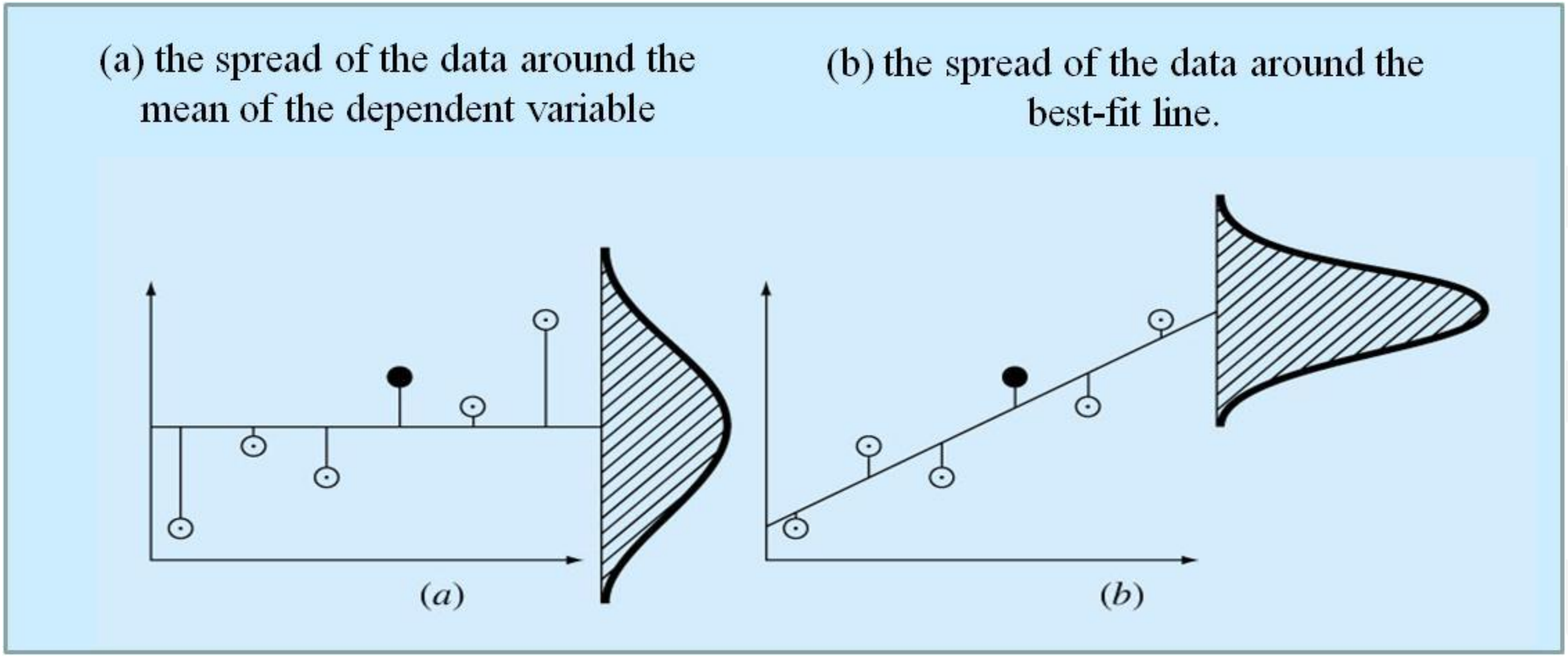
$$a_0 = \bar{y} - a_1\bar{x}$$

Mean values

THE RESIDUAL

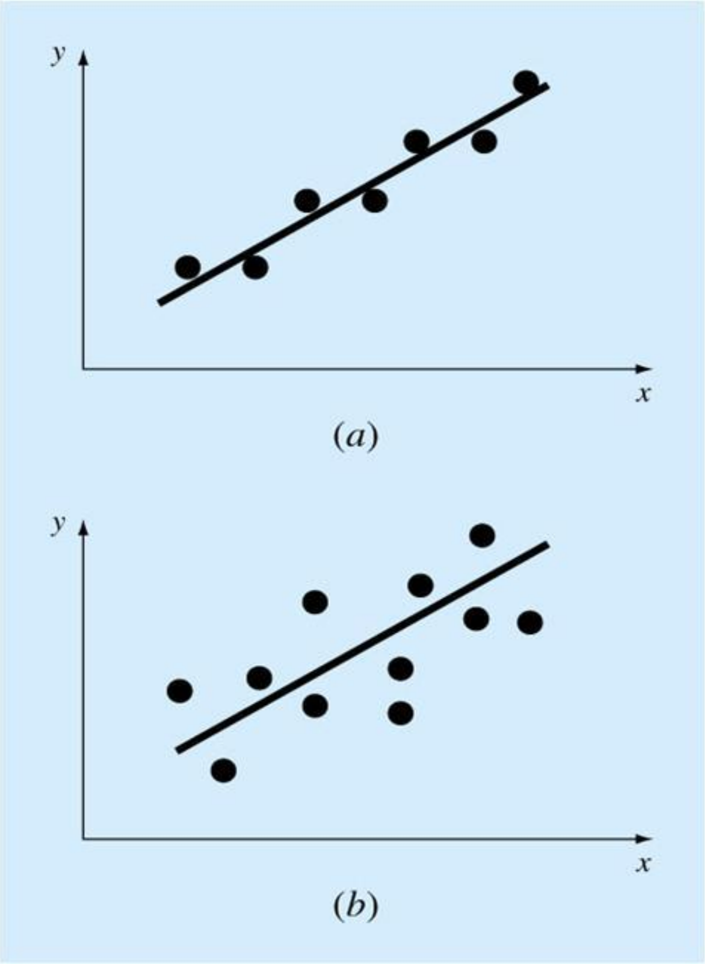


SPREAD OF DATA AROUND THE MEAN & THE REGRESSION



The reduction of spread in going from (a) to (b), as indicated by the bell-shaped curves at the right, represents the improvement due to linear regression.

LINEAR REGRESSIONS WITH (A) SMALL AND (B) LARGE RESIDUAL ERRORS



GOODNESS" OF FIT

- If total sum of the squares around the mean for the dependent variable, *y*, is S_t.
- Sum of the squares of residuals around the regression line is S_r.
- $S_t - S_r$ quantifies the improvement or error reduction due to describing data in terms of a straight line rather than as an average value.

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

r^2 = coefficient of determination

$r = \sqrt{r^2}$ = correlation coefficient

GOODNESS" OF FIT

- For a perfect fit $S_r = 0$ and $r = r^2 = 1$,
- signifying that
- the line explains 100 % 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 is poorly represented by a straight line. For these cases a curve is better suited to fit the data. The least squares method can readily be extended to fit the data to higher order polynomials

GENERAL LINEAR LEAST SQUARES

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

$$\text{If } z_0 = 1,\ z_1 = x,\ z_2 = x^2, \ldots, z_m = x^m :$$

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

Polynomial Regression!

GENERAL LINEAR LEAST SQUARES

$$\text{If } z_0 = 1, z_1 = x_1, z_2 = x_2, \ldots, z_m = x_m :$$

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

Multiple Linear Regression!

$$\text{If } z_0 = 1, z_1 = \cos(x), z_2 = \sin(x), z_3 = \cos(2x), \ldots$$

$$y = a_0 + a_1 \cos(\omega t) + a_2 \sin(\omega t) + a_3 \cos(2\omega t) + \ldots$$

- **Fourier Series!**

GENERAL LINEAR LEAST SQUARES SOLUTION

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

Write in matrix form:

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

- **Sum of squares:**

$$S_r = \sum_{i=1}^{n} \left(y_i - \sum_{j=0}^{m} a_j z_{ji} \right)^2$$

- **Differentiating and setting to zero yields normal equations:**

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

GENERAL LINEAR LEAST SQUARES SOLUTION

Normal equations:

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

- **Solution for coefficients by matrix inverse:**

$$\{A\} = \underbrace{\left[[Z]^T[Z]\right]}_{\text{Elements: } \mathrm{Z}_{i,j}^{-1}}^{-1}\left\{[Z]^T\{Y\}\right\}$$

$$\operatorname{var}\left(a_{i-1}\right) = z_{i,i}^{-1} s_{y/x}^{2}$$

$$\operatorname{cov}\left(a_{i-1}, a_{j-1}\right) = z_{i,j}^{-1} s_{y/x}^{2}$$

Interpolation

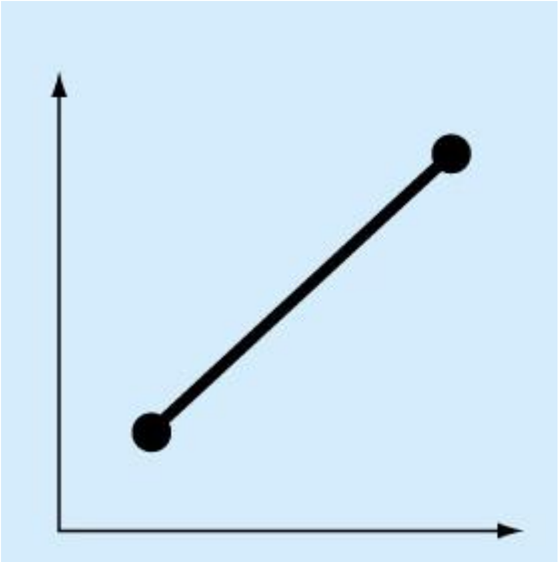
INTERPOLATION

Estimation of intermediate values between precise data points. The most common method is:

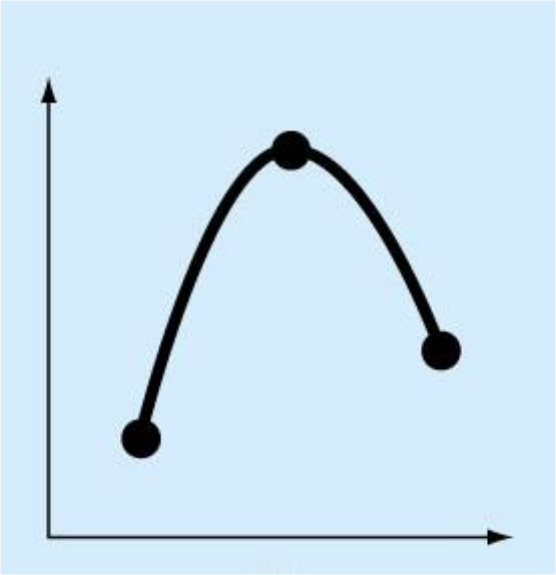
$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

- Although there is one and only one n^{th}-order polynomial that fits $n + 1$ points, there are a variety of mathematical formats in which this polynomial can be expressed:
  - The Newton polynomial.
  - The Lagrange polynomial.

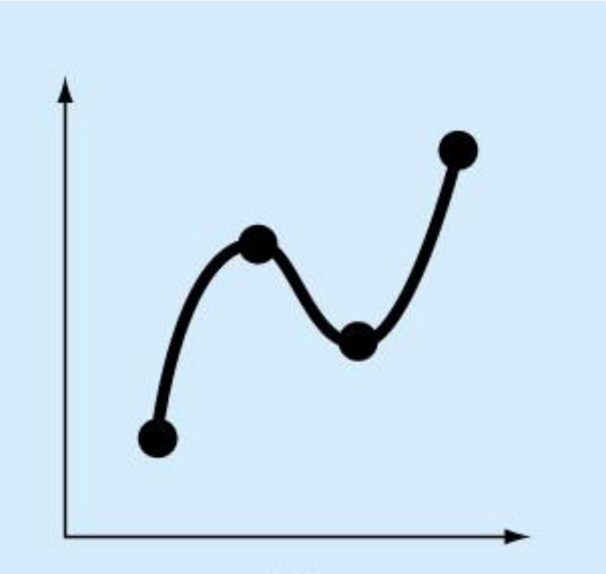
EXAMPLES OF INTERPOLATING POLYNOMIALS



(a) 1st-order (linear) connecting 2 points



(b) 2nd-order (quadratic /parabolic) connecting 3 points



(c) 3rd-order (cubic) connecting 4 points.

NEWTON'S DIVIDED-DIFFERENCE INTERPOLATING POLYNOMIALS

Linear Interpolation

- The simplest form of interpolation, connecting two data points with a straight line.

$$\frac{f_1(x) - f(x_0)}{x - x_0} = \frac{f(x_1) - f(x_0)}{x - x_0}$$

- Slope and a finite divided difference approximation to 1st derivative

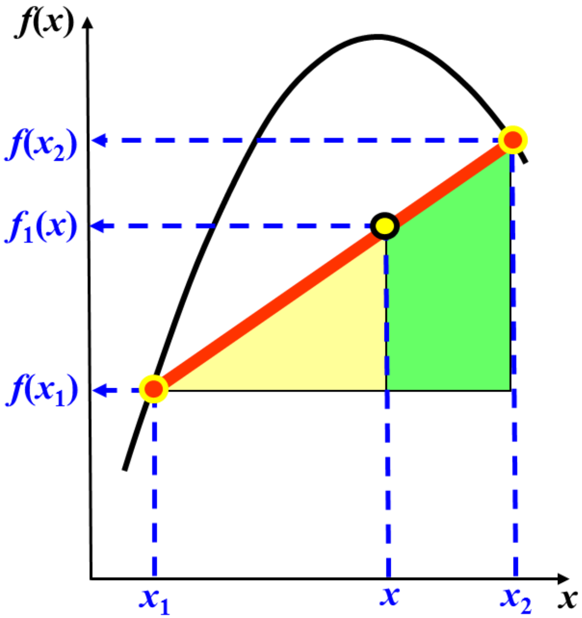
$$\boxed{f_1(x) = f(x_0) + \boxed{\frac{f(x_1) - f(x_0)}{x - x_0}}(x - x_0)}$$

- Linear-interpolation formula

- $f_1(x)$ designates that this is a first-order interpolating polynomial.

NEWTON'S DIVIDED-DIFFERENCE INTERPOLATING POLYNOMIALS

- ***Linear Interpolation*:**



$$\frac{f_1(x) - f(x_1)}{x - x_1} = \frac{f(x_2) - f(x_1)}{x_2 - x_1}$$

$$f_1(x) = f(x_1) + \frac{f(x_2) - f(x_1)}{x_2 - x_1}(x - x_1)$$

$$\textbf{Prediction} = \textbf{Constant value} + \textbf{Slope} \times \textbf{Distance}$$

QUADRATIC INTERPOLATION

- If three data points are available, the estimate is improved by introducing some curvature into the line connecting the points.

$$f_2(x) = b_0 + b_1(x - x_0) + b_2(x - x_0)(x - x_1)$$

- A simple procedure can be used to determine the values of the coefficients.

$$x = x_0 \qquad b_0 = f(x_0)$$

$$x = x_1 \qquad b_1 = \frac{f(x_1) - f(x_0)}{x - x_0}$$

$$x = x_2 \qquad b_2 = \frac{\dfrac{f(x_2) - f(x_1)}{x_2 - x_1} - \dfrac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0}$$

COMPARISON WITH TAYLOR SERIES

$$f_2(x) = f(x_1) + \frac{f(x_2) - f(x_1)}{x_2 - x_1}(x - x_1)$$

$$+ \frac{\dfrac{f(x_3) - f(x_2)}{x_3 - x_2} - \dfrac{f(x_2) - f(x_1)}{x_2 - x_1}}{x_3 - x_1}(x - x_1)(x - x_2)$$

Taylor Series

$$f(x_{i+1}) \cong f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2$$

GENERAL NTH-ORDER INTERPOLATING POLYNOMIAL

$$f_n(x) = b_1 + b_2(x - x_1) + \cdots + b_n(x - x_1)(x - x_2)\cdots(x - x_{n-1})$$

$$b_1 = f(x_1)$$

$$b_2 = f[x_2,\ x_1] \qquad f[x_i,\ x_j] = \frac{f(x_i) - f(x_j)}{x_i - x_j}$$

$$b_3 = f[x_3, x_2, x_1] \qquad f[x_i, x_j, x_k] = \frac{f[x_i, x_j] - f[x_j, x_k]}{x_i - x_k}$$

ERRORS OF NEWTON'S INTERPOLATING POLYNOMIALS

- Structure of interpolating polynomials is similar to the Taylor series expansion in the sense that finite divided differences are added sequentially to capture the higher order derivatives.
- For an n^{th}-order interpolating polynomial, an analogous relationship for the error is:

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-x_0)(x-x_1)\cdots(x-x_n)$$

ξ is somewhere in the interval containing the unknown and the data

- For non differentiable functions, if an additional point $f(x_{n+1})$
- is available, an alternative formula can be used that does not require prior knowledge of the function:

$$R_n \cong f[x_{n+1}, x_n, x_{n-1}, \ldots, x_0](x-x_0)(x-x_1)\cdots(x-x_n)$$

RECURSIVE NATURE OF FINITE DIVIDED DIFFERENCES

i	x_i	$f(x_i)$	First	Second	Third
0	x_1	$f(x_1)$	$f[x_2,x_1]$	$f[x_3,x_2,x_1]$	$f[x_4,x_3,x_2,x_1]$
1	x_2	$f(x_2)$	$f[x_3,x_2]$	$f[x_4,x_3,x_2]$	
2	x_3	$f(x_3)$	$f[x_4,x_3]$		
3	x_4	$f(x_4)$			

$$f(x) = f(x_1) + f[x_2, x_1](x - x_1)$$
$$+ f[x_3, x_2, x_1](x - x_1)(x - x_2)$$
$$+ f[x_4, x_3, x_2, x_1](x - x_1)(x - x_2)(x - x_3)$$

LAGRANGE INTERPOLATING POLYNOMIALS

- The Lagrange interpolating polynomial is simply a reformulation of the Newton's polynomial that avoids the computation of divided differences:

$$f_n(x) = \sum_{i=0}^{n} L_i(x)\, f(x_i)$$

$$L_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

LAGRANGE SECOND-ORDER POLYNOMIAL

$$f_1(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)$$

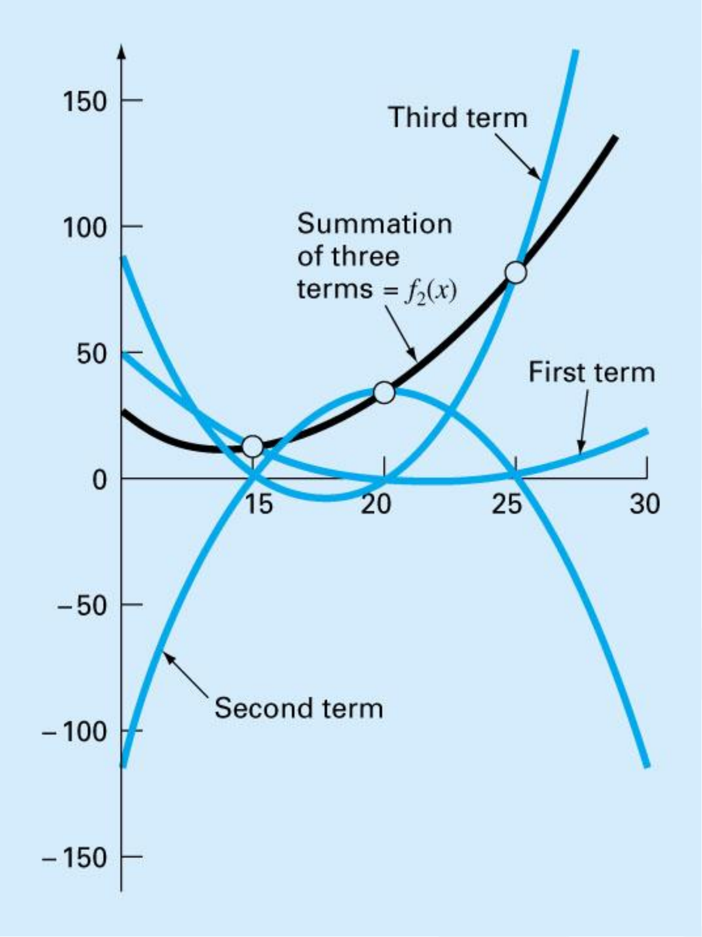
$$f_2(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

- As with Newton's method, the Lagrange version has an estimated error of:

$$R_n = f[x, x_n, x_{n-1}, \ldots, x_0] \prod_{i=0}^{n} (x - x_i)$$

A VISUAL DEPICTION OF THE RATIONALE BEHIND THE LAGRANGE POLYNOMIAL

This figure shows a second-order case. Each of the three terms is a parabola that passes through one of the data points and is zero at the other two. The summation of the three terms must, therefore, be the unique second-order polynomial $f_2(x)$ that passes exactly through the three points.



COEFFICIENTS OF AN INTERPOLATING POLYNOMIAL

- Although both the Newton and Lagrange polynomials are well suited for determining intermediate values between points, they do not provide a polynomial in conventional form:

$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_x x^n$$

- Since n+1 data points are required to determine n+1 coefficients, simultaneous linear systems of equations can be used to calculate “a”s.

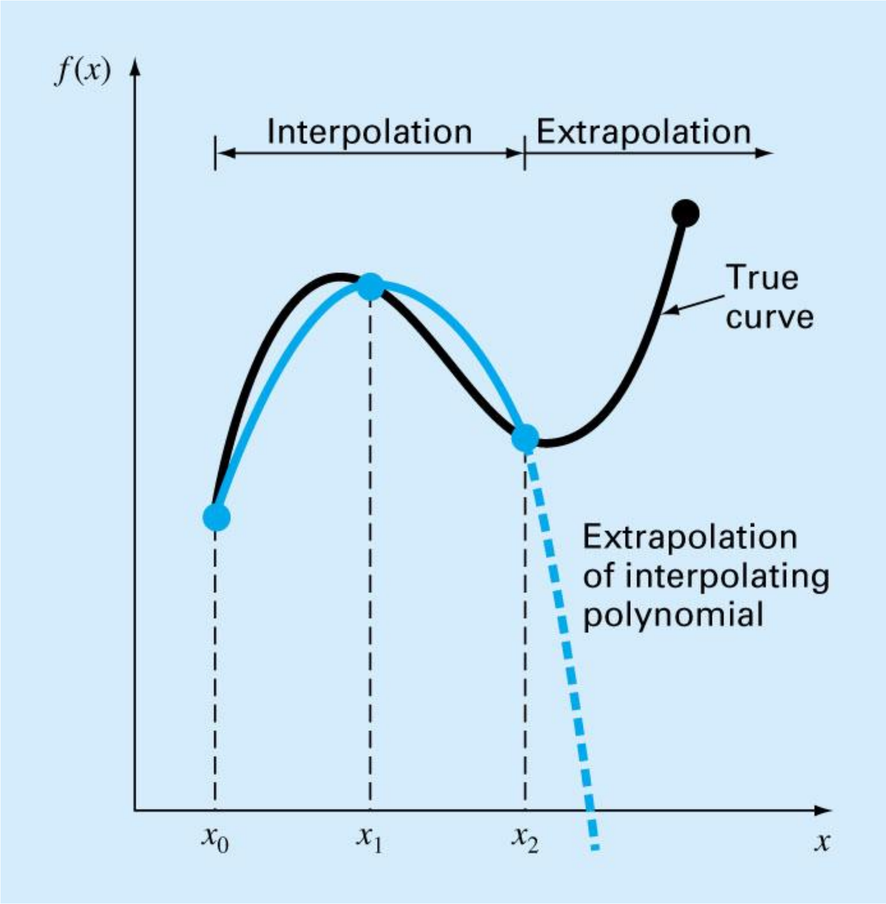
COEFFICIENTS OF AN INTERPOLATING POLYNOMIAL

$$f(x_0) = a_0 + a_1 x_0 + a_2 x_0^2 \cdots + a_n x_0^n$$
$$f(x_1) = a_0 + a_1 x_1 + a_2 x_1^2 \cdots + a_n x_1^n$$
$$\vdots$$
$$f(x_n) = a_0 + a_1 x_n + a_2 x_n^2 \cdots + a_n x_n^n$$

Where "*x*"s are the knowns and "*a*"s are the polynomial's coefficients.

- **CAUTION: This approach is ill-conditioned so is subject to large roundoff errors, especially for higher-order polynomials.**

THE DANGER OF USING AN INTERPOLATING POLYNOMIAL FOR EXTRAPOLATION



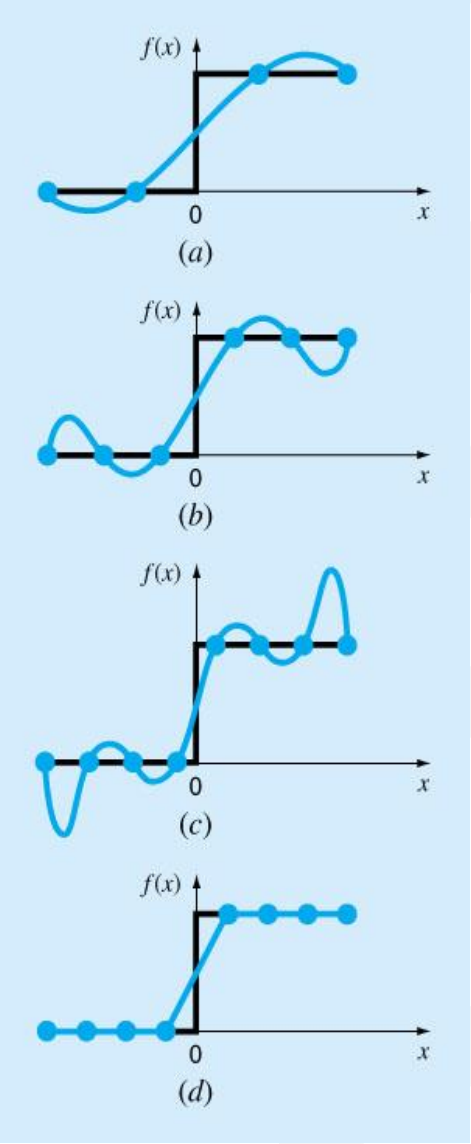
SPLINE INTERPOLATION

- There are cases where polynomials can lead to erroneous results because of round off error and overshoot.
- Alternative approach is to apply lower-order polynomials to subsets of data points. Such connecting polynomials are called spline functions.

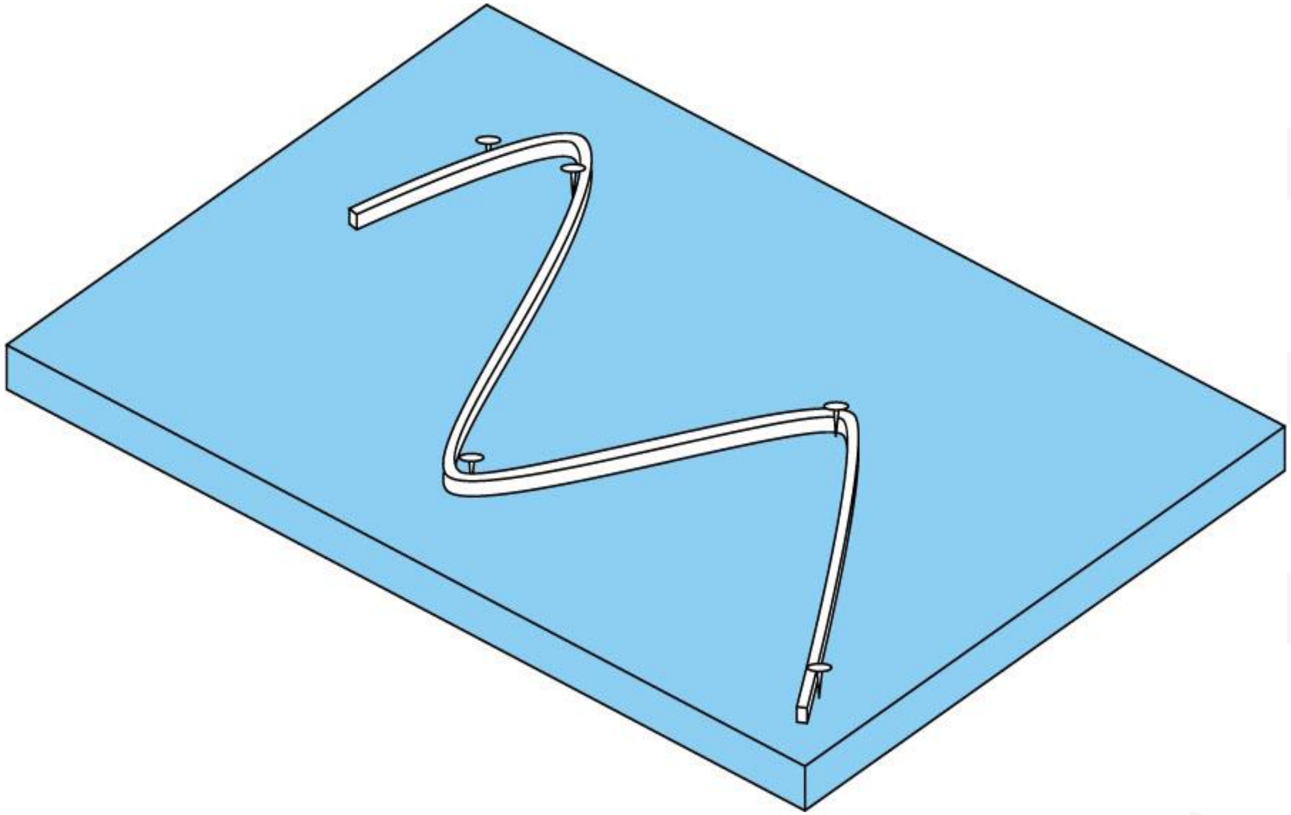
SUPERIORITY OF SPLINE INTERPOLATION

- A visual representation of a situation where the splines are superior to higher-order interpolating polynomials. The function to be fit undergoes an abrupt increase at $x = 0$. Parts (a) through (c) indicate that the abrupt change induces oscillations in interpolating polynomials.

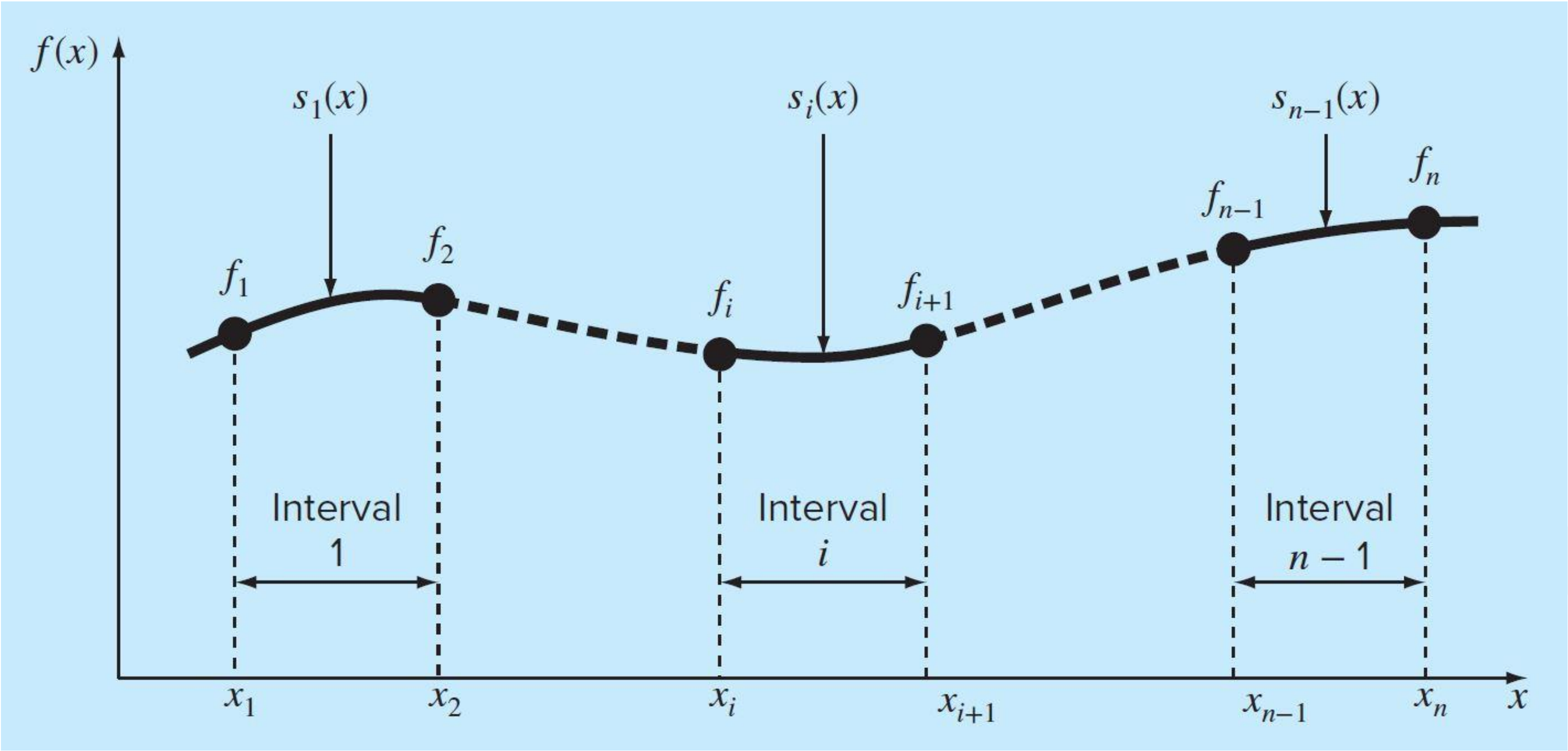
- In contrast, because it is limited to third-order curves with smooth transitions, a linear spline (d) provides a much more acceptable approximation.



ORIGIN OF SPLINES IN PRE-COMPUTER DRAFTING



NOTATION USED TO DERIVE SPLINES



SPLINE FITS OF FOUR POINTS