Numerical Integration
Upper and Lower Sums
Trapezoid Method

CS3010

Numerical Methods

Dr. Amar Raheja

Section 5.1, 5.2, 5.3

Numerical Differentiation and Integration

- Calculus is the mathematics of change. Because scientists and engineers must continuously deal with systems and processes that change, calculus is an essential tool of science and engineering.

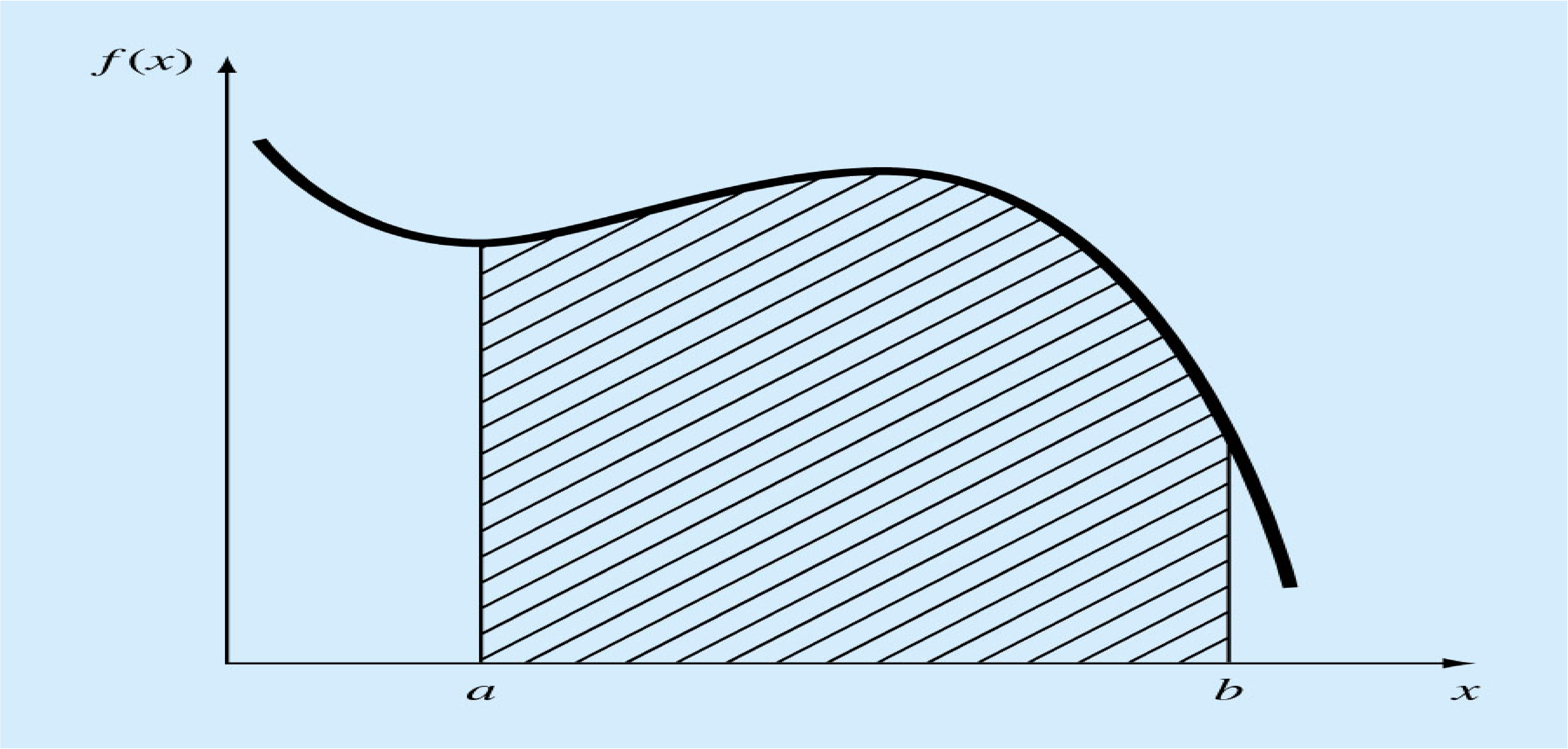
- Standing in the heart of calculus are the mathematical concepts of *differentiation* and *integration*:

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

$$I = \int_a^b f(x)dx$$

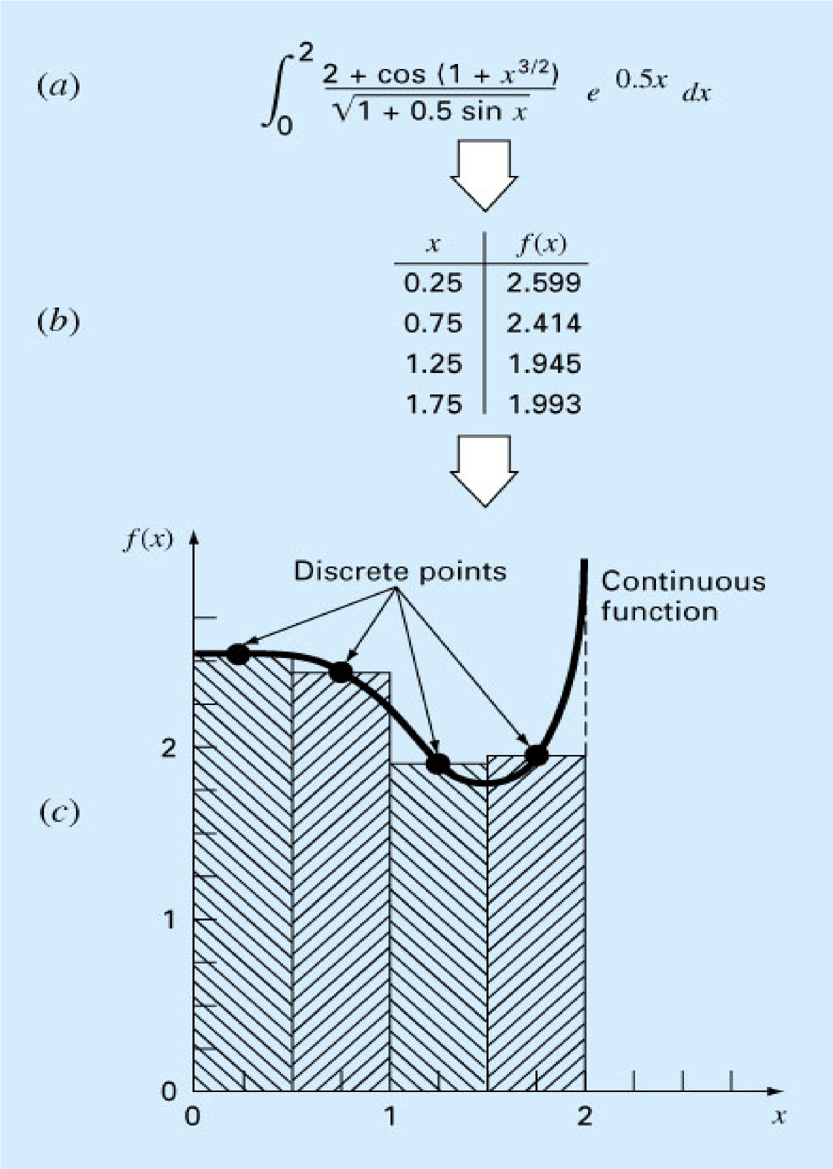
Integral of f(x) between x=a and x=b



Noncomputer Methods for Differentiation and Integration

- The function to be differentiated or integrated will typically be in one of the following three forms:
  - A simple continuous function such as polynomial, an exponential, or a trigonometric function.
  - A complicated continuous function that is difficult or impossible to differentiate or integrate directly.
  - A tabulated function where values of x and $f(x)$ are given at a number of discrete points, as is often the case with experimental or field data.

Use of Grid to Approximate Integral



Theorem on Riemann-Integral

- $\sup_P L(f;P)$: Least upper bound (supremum) of the set of all numbers L(f;P) obtained when P is allowed to range over all partitions of interval [a,b]
- $\inf_P U(f;P)$: Greatest lower bound (infimum) of the set of all numbers $L(f;P)$ obtained when P is allowed to range over all partitions of interval [a,b]
- If $\sup_P L(f;P) = \inf_P U(f;P)$, then the function f is Riemann-integrable on [a,b] and defined to be the common value obtained above.

Every continuous function defined on a closed and bounded interval of the real line is Riemann-integrable.

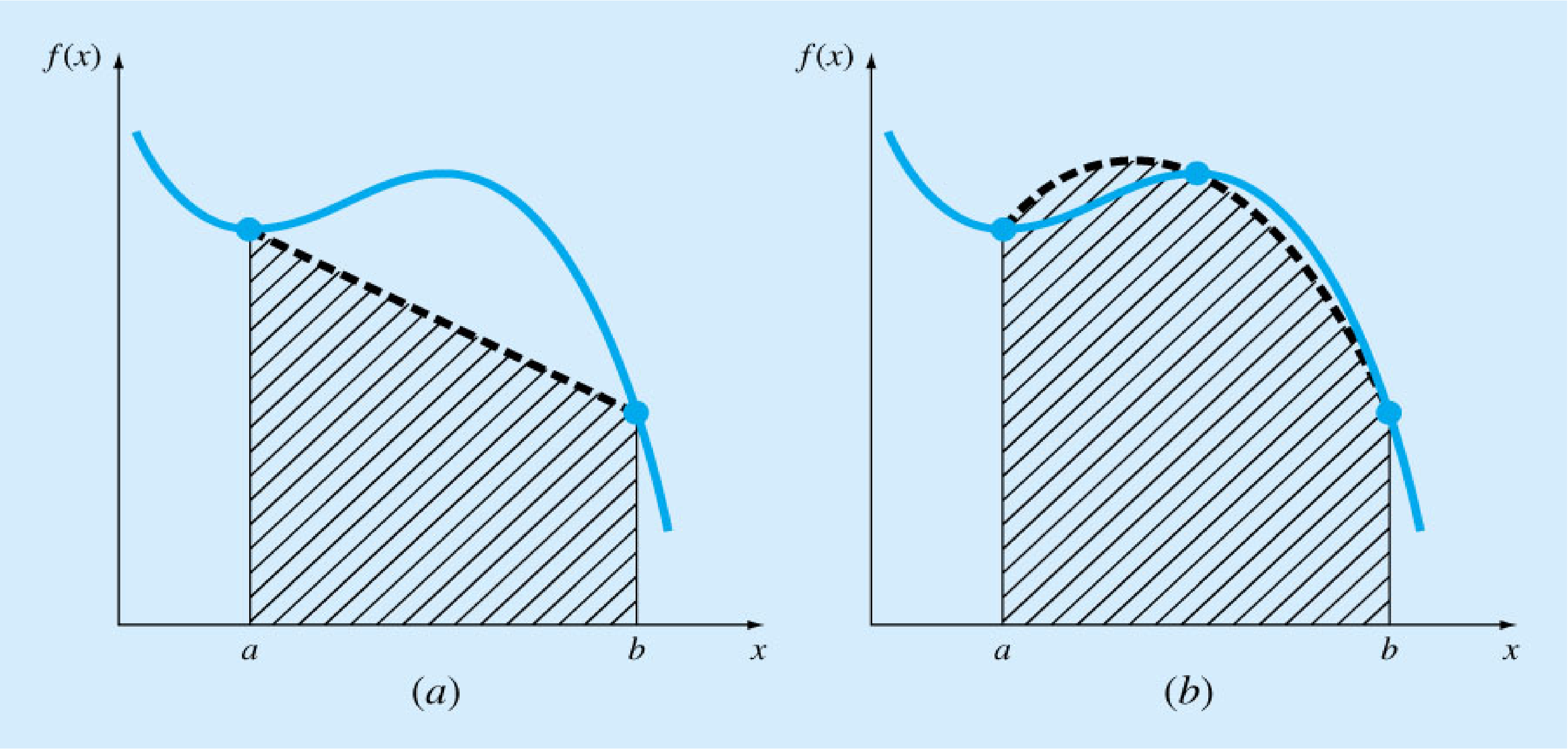
Newton-Cotes Integration Formulas

- The *Newton-Cotes formulas* are the most common numerical integration schemes.
- They are based on the strategy of replacing a complicated function or tabulated data with an approximating function that is easy to integrate:

$$I = \int_a^b f(x)dx \cong \int_a^b f_n(x)dx$$

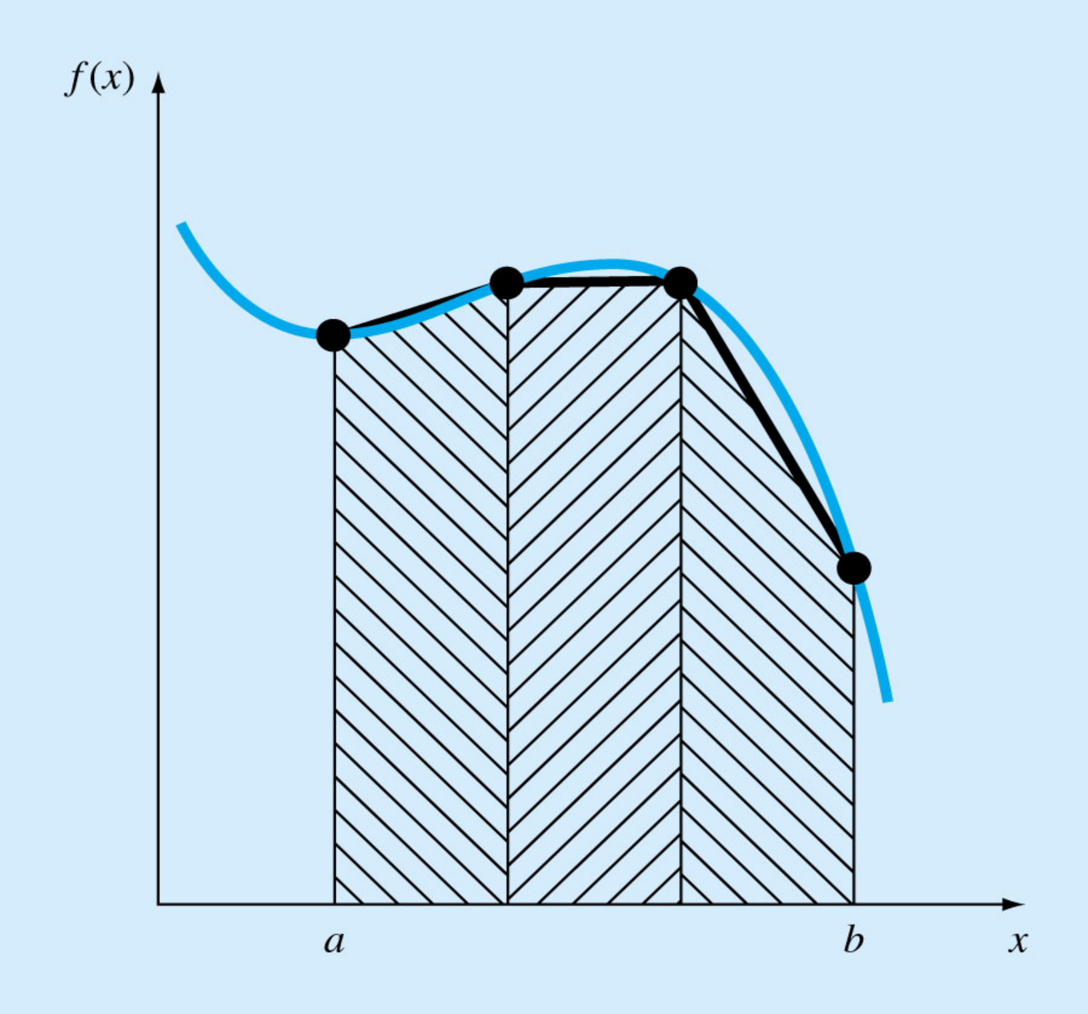
$$f_n(x) = a_0 + a_0 x + \cdots + a_{n-1}x^{n-1} + a_n x^n$$

Approximation of an Integral



- (a) linear interpolation between a and b
- (b) quadratic interpolation between a and b

Approximation of an Integral using multipartition with linear interpolation



- Area under 3 straight line segments

The Trapezoidal Rule

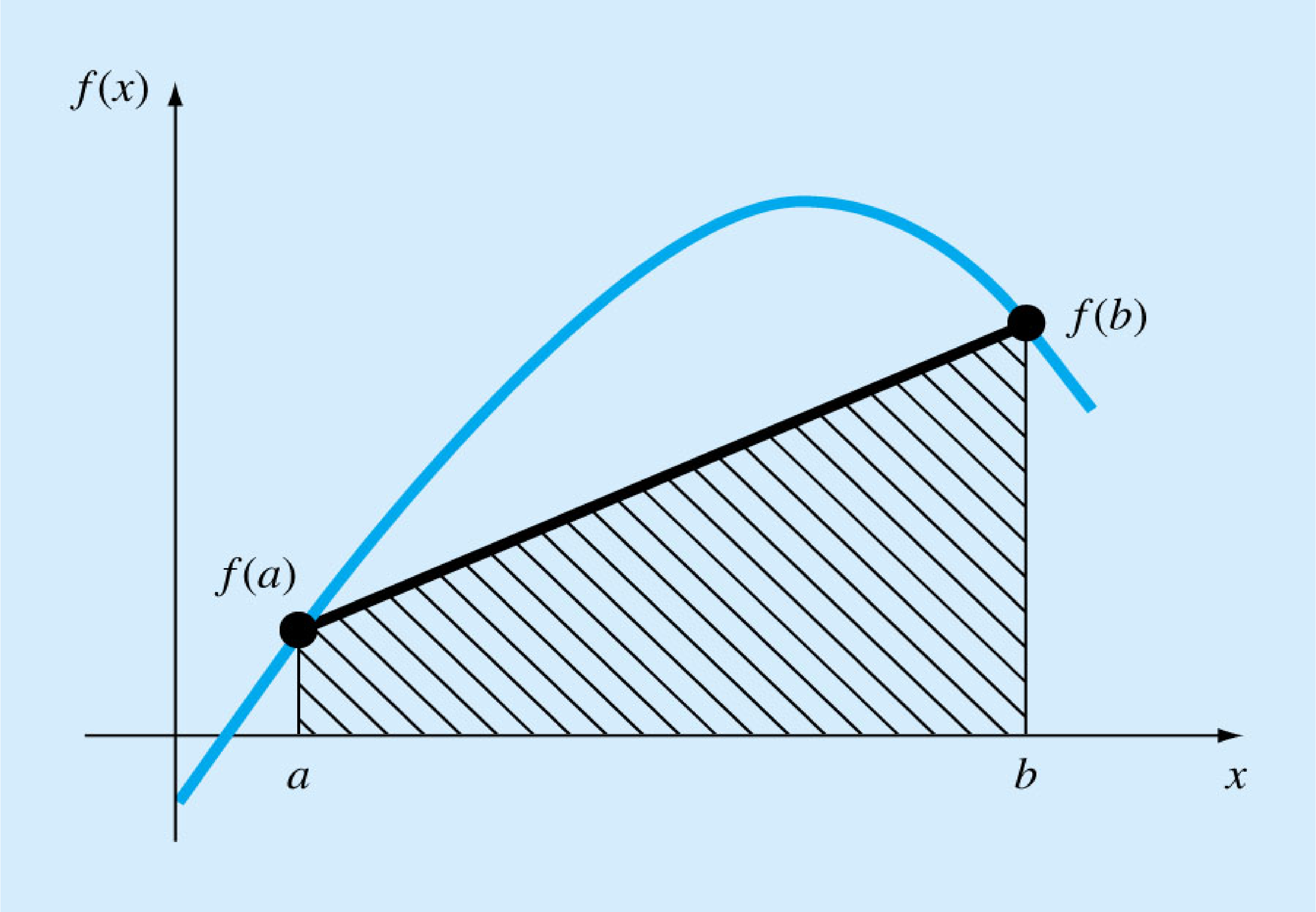
- The *Trapezoidal rule* is the first of the Newton-Cotes closed integration formulas, corresponding to the case where the polynomial is first order:

$$I = \int_a^b f(x)dx \cong \int_a^b f_1(x)dx$$

- The area under this first order polynomial is an estimate of the integral of *f(x)* between the limits of *a* and *b*:

$$I = (b-a)\left[\frac{f(a)+f(b)}{2}\right]$$

Application Trapezoidal Rule



Multiple Application Trapezoidal Rule

- One way to improve the accuracy of the trapezoidal rule is to divide the integration interval from a to b into a number of segments and apply the method to each segment.
- The areas of individual segments can then be added to yield the integral for the entire interval.

$$a = x_0 \text{ and } b = x_n$$

$$I = \int_a^b f(x)dx \cong \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \ldots + \int_{x_{n-1}}^{x_n} f(x)dx$$

- Substituting the trapezoidal rule for each integral yields:

$$I = (x_1 - x_0)\left[\frac{f(x_0) + f(x_1)}{2}\right] + (x_2 - x_1)\left[\frac{f(x_1) + f(x_2)}{2}\right] + \cdots (x_n - x_{n-1})\left[\frac{f(x_{n-1}) + f(x_n)}{2}\right]$$

Multiple Application Trapezoidal Rule to Equidistant Partitions

- One way to improve the accuracy of the trapezoidal rule is to divide the integration interval from a to b into a number of segments and apply the method to each segment.
- The areas of individual segments can then be added to yield the integral for the entire interval.

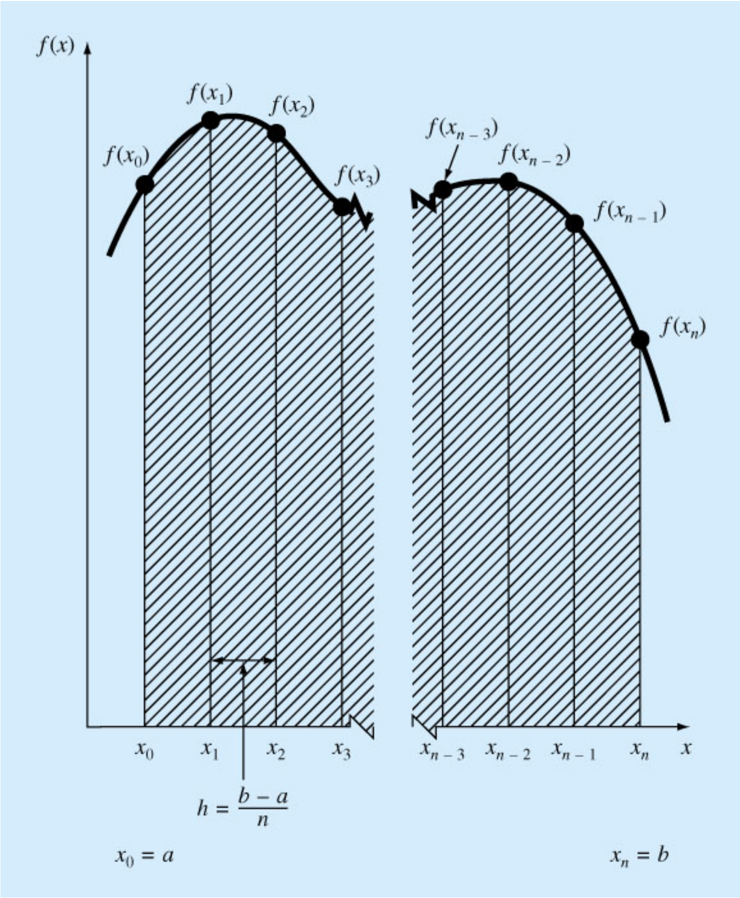
$$\mathrm{h} = \frac{b-a}{n} \; where \; a = x_0 \text{ and } b = x_n$$

$$I = \int_a^b f(x)dx \cong \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \ldots + \int_{x_{n-1}}^{x_n} f(x)dx +$$

- Substituting the trapezoidal rule for each integral yields:

$$I = h\left[\frac{f(x_0) + f(x_1)}{2}\right] + h\left[\frac{f(x_1) + f(x_2)}{2}\right] + \cdots h\left[\frac{f(x_{n-1}) + f(x_n)}{2}\right] = \frac{h}{2}\sum_{i=0}^{n-1}[f(x_i) + f(x_{i+1})]$$

Trapezoid Rule for Integration



Class Exercise 1

- What is the numerical value of the composite trapezoid rule applied to the reciprocal function $f\ (x) = x^{-1}$ using the points 1, 4/3 and 2?
- Compute two approximate values for $\int_1^2 \frac{dx}{x^2}$ using h = 1/2 with lower sums and the composite trapezoid rule.

Error Analysis

- Theorem on Precision of Trapezoidal Rule

  If f" exists and is continuous on the interval [a,b], and if the composite trapezoidal rule T with uniform spacing h is used to estimate the integral $I = \int_a^b f(x)dx$, then for some ζ in (a,b),

$$I - T = \frac{1}{12}(b-a)h^2 f''(\zeta) = O(h^2)$$

- Error for the composite trapezoidal rule can be calculated by first finding error for a subinterval (assume *n* equal subintervals)

$$I = \frac{h}{2}[f(x_i) - f(x_{i+1})] - \frac{h^3}{12} f''(\xi_i)$$

where $x_i < \xi_i < x_{i+1}$

Error for Composite Trapezoid Rule

$$\int_a^b f(x)dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)dx = \frac{h}{2}\sum_{0}^{n-1}[f(x_i) + f(x_{i+1})] - \frac{h^3}{12}\sum_{i=0}^{n-1} f''(\xi_i)$$

- Final term in the equation above is the error term and can be simplified by using $h = \frac{b-a}{n}$

$$-\frac{h^3}{12}\sum_{i=0}^{n-1} f''(\xi_i) = -\frac{b-a}{12}h^2\left[\frac{1}{n}\sum_{i=0}^{n-1} f''(\xi_i)\right] = -\frac{b-a}{12}h^2 f''(\zeta)$$

- Reasoning is that the average value of $[{}^1/_n]\sum_{i=0}^{n-1} f''(\xi_i)$ lies between the least and greatest values of f'' on the interval (a, b). Hence by Intermediate-Value Theorem of continuous functions, it is $f''(\zeta)$ for some point ζ in (a, b)

Example: Applying Error Formula

- If we Compute $\int_0^1 e^{-x^2} dx$ with an error at most 1/2x10^{-4} , how many points are needed?

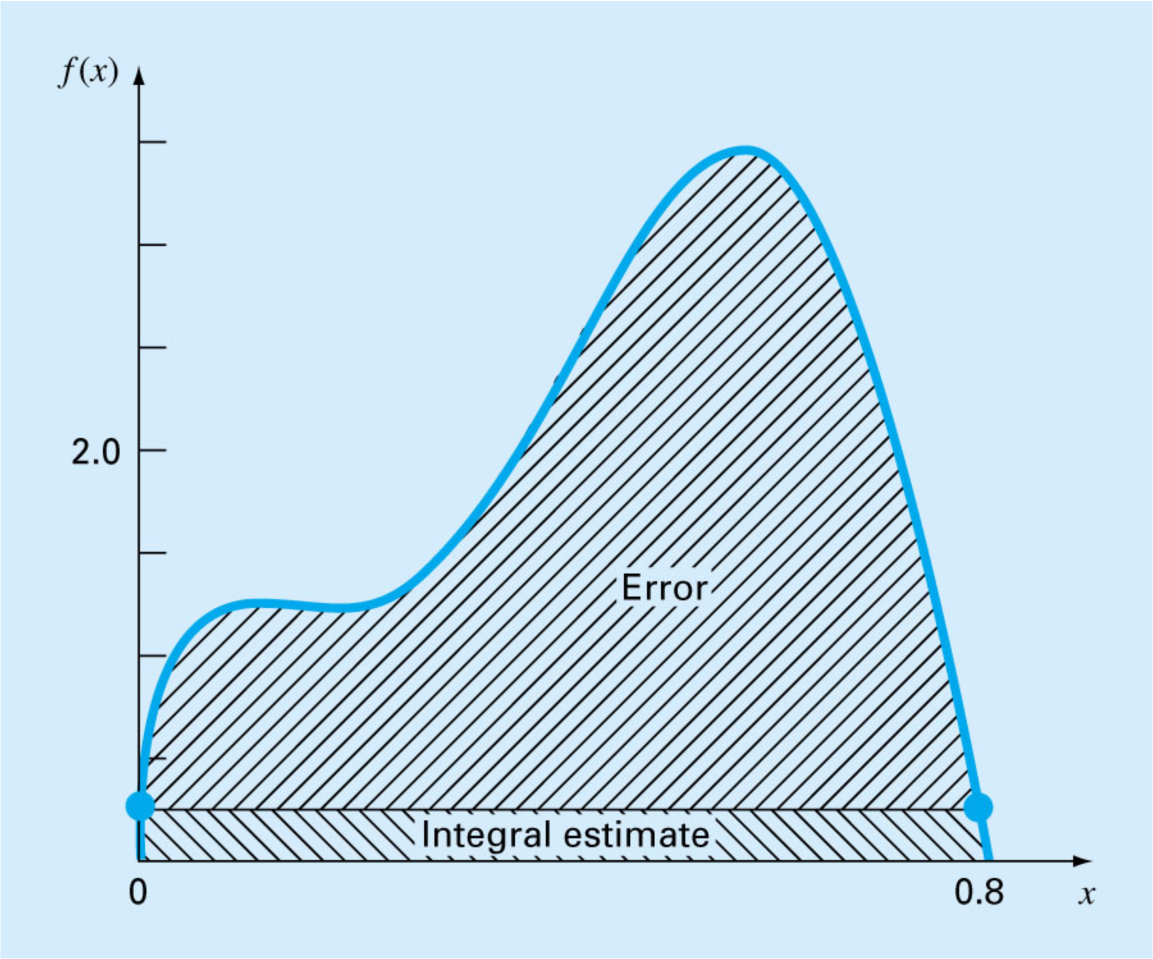
$$Error = -\frac{b-a}{12} h^2 f''(\zeta)$$

$$f(x) = e^{-x^2}, f'(x) = -2xe^{-x^2}, f''(x) = (4x^2 - 2)e^{-x^2}$$

Thus, maximum absolute value of $f''(x)$ is 2 in the interval [0,1] and using that in the error

$$\frac{h^2}{6} < \frac{1}{2} \times 10^{-4} \; or \; h \leq 0.01732 \; \; or \; \; \frac{1}{n} \leq 0.01732 \; or \; n \geq 58$$

Error Estimate



Trapezoid Rule: 2^n Equal Intervals

- Find the recursive trapezoid formula for 2^n equal subintervals for $\int_a^b f(x)dx$
- Start with n = 0 and then do n = 1,2 and 3 and see if you can generalize for n
- Romberg Algorithm produces a triangular array of numbers, all of which are estimates of the definite integral

$$
\begin{array}{l|llllll}
R(0,0) & & & & & & \\
R(1,0) & R(1,1) & & & & & \\
R(2,0) & R(2,1) & R(2,2) & & & & \\
R(3,0) & R(3,1) & R(3,2) & R(3,3) & & & \\
\bullet & \bullet & \bullet & \bullet & \bullet & & \\
\bullet & \bullet & \bullet & \bullet & & \bullet & \\
\bullet & \bullet & \bullet & \bullet & & & \bullet \\
R(n,0) & R(n,1) & R(n,2) & R(n,3) & \bullet\ \bullet & \bullet & R(n,n)
\end{array}
$$

Romberg Algorithm

- The first column contains estimates of integral obtained by recursive trapezoid formula with decreasing values of step size. *R*(*n*,0) is got by applying trapezoid rule with 2^n subintervals. *R*(0,0) is obtained with just using one trapezoid.

$$R(0,0) = \frac{1}{2}(b-a)[f(a) + f(b)]$$

R(1,0) is obtained by using two trapezoids

$$R(1,0) = \frac{1}{4}(b-a)\left[f(a) + f\left(\frac{a+b}{2}\right)\right] + \frac{1}{4}(b-a)\left[f\left(\frac{a+b}{2}\right) + f(b)\right]$$

$$= \frac{1}{4}(b-a)[f(a) + f(b)] + \frac{(b-a)}{2} f\left(\frac{a+b}{2}\right)$$

$$= \frac{1}{2}R(0,0) + \frac{(b-a)}{2} f\left(\frac{a+b}{2}\right)$$

$$R(n,0) = \frac{1}{2}R(n-1,0) + h\sum_{k=1}^{2^{n-1}} f[a + (2k-1)h]$$

where $h = \frac{b-a}{2^n}$ and $n \geq 1$