數值分析

Chapter 6
Numerical Integration

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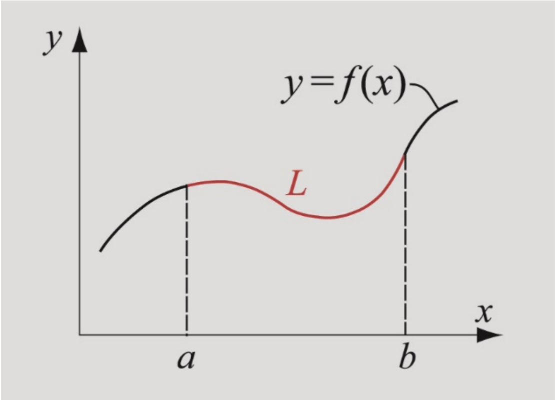
Outline

- Background (6.1)
- Rectangle and midpoint method (6.2)
- Trapezoidal method (6.3)
- Simpson’s method (6.4)
- Gauss quadrature (6.5)
- Evaluation of multiple integrals (6.6)
- MATLAB built-in functions (6.7)
- Complementary topics (6.8 - 6.11)

6.1 Background

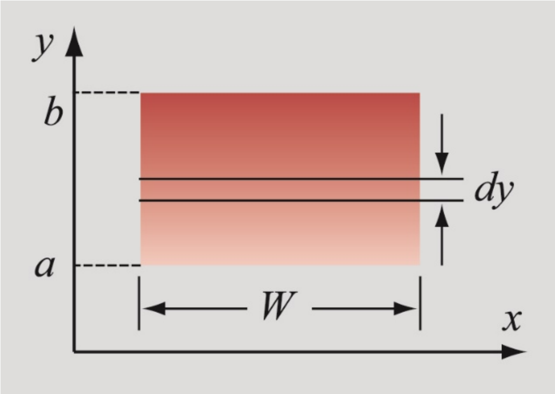
- Calculate the length of a curve:

$$L = \int_a^b \sqrt{1+\left[f'(x)\right]^2}\,dx$$



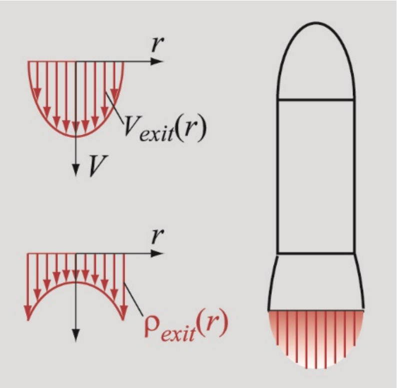
- Heat flux through a rectangular cross section:

$$\dot{Q} = \int_{y=a}^{y=b} \dot{q}'' W dy$$



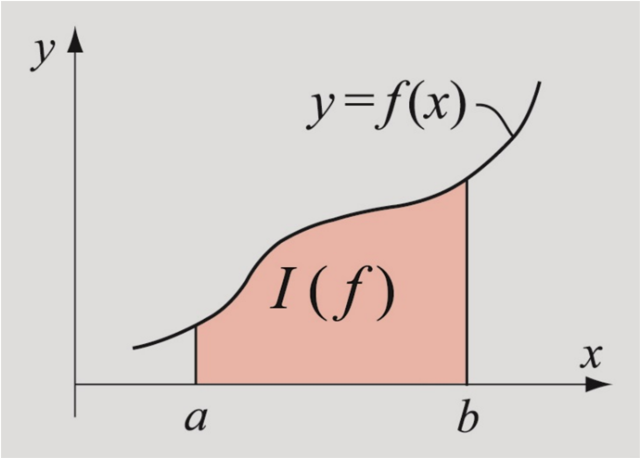
- Exhaust of a rocket engine thrust (T):

$$T = \int_0^R 2\pi\rho(r)V_{exit}^2(r)rdr$$

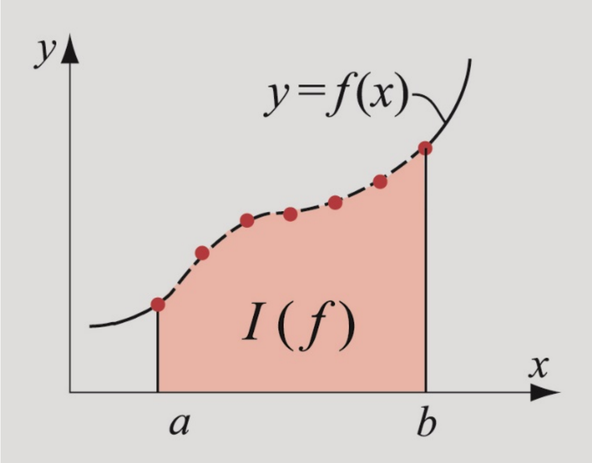


Overview of Numerical Integration

- The numerical integration is needed when
  - analytical integration is difficult or not possible
  - the integrand is given as a set of discrete points
- Calculate the integral over each **subinterval** and added together
- Numerical integration can also be done with discrete points



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



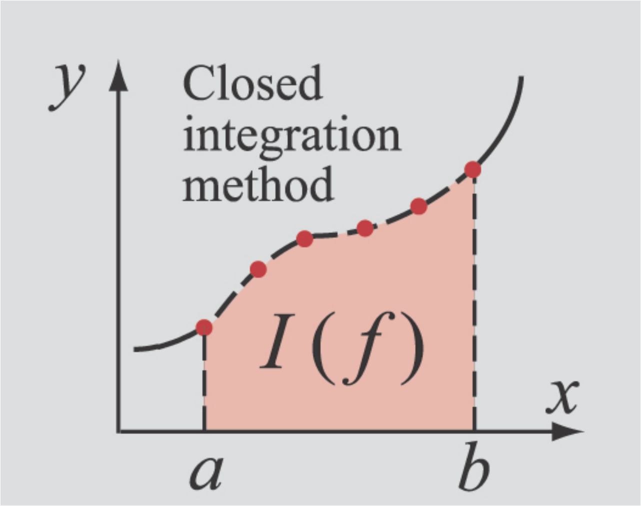
Definition integral of f(x) between a and b

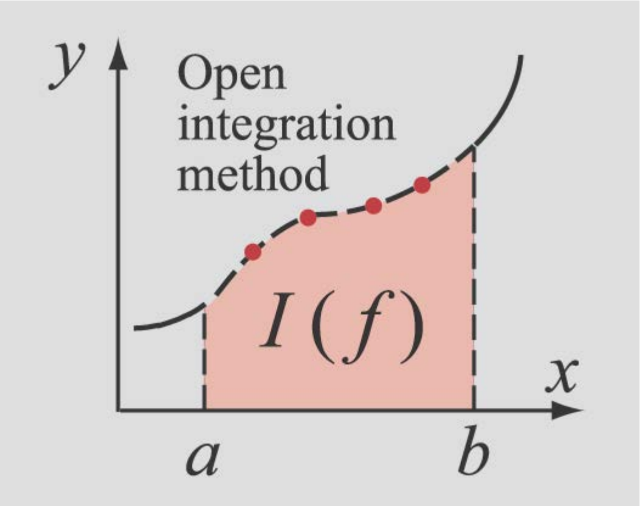
Finite number of points are used in numerical integration

Closed and Open Method

- Closed method:
  - the **endpoints** of the interval are used in the formula
  - Trapezoidal (6.3) and Simpson's method (6.4)

- Open method:
  - the interval of integration extends beyond the range of the endpoints
  - midpoint method (6.2) and Gauss quadrature(6.5)

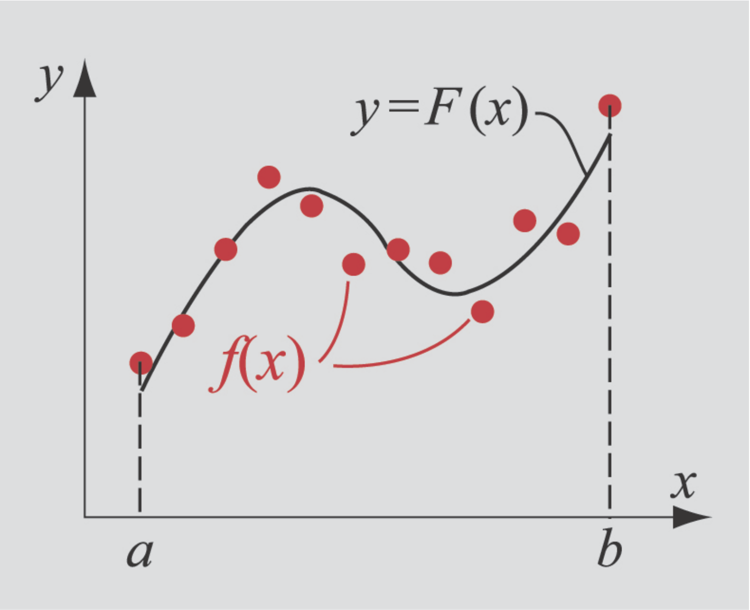




Newton-Cotes Integration Formulas

- Estimate the integrands between the discrete points using a function that can be integrated
  - For analytical function: replaced with a simpler function
  - For data points: interpolates the integrand between the points

$$I_f = \int_a^b f(x)dx \approx \int_a^b F(x)dx$$

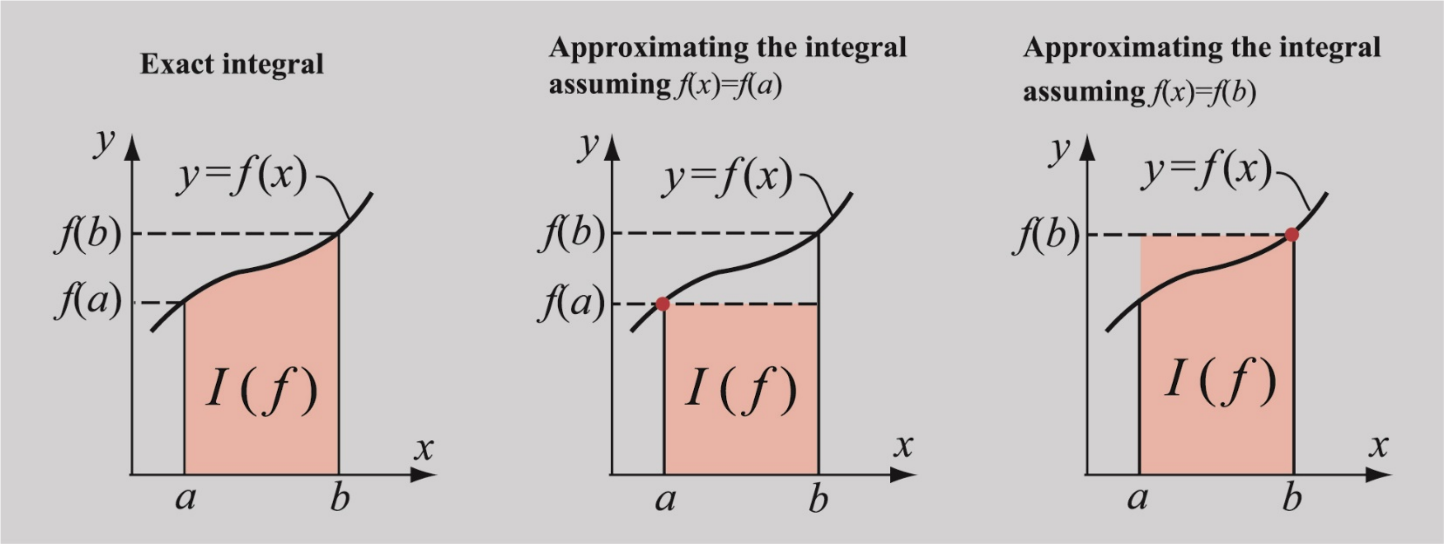


6.2 Rectangle and Midpoint Methods

- Take the value of f(x) over the interval [a,b] as a constant equal to the value of f(a) or f(b)

$$I_f = \int_a^b f(x)dx = f(a)(b-a) \qquad\qquad I_f = \int_a^b f(x)dx = f(b)(b-a)$$

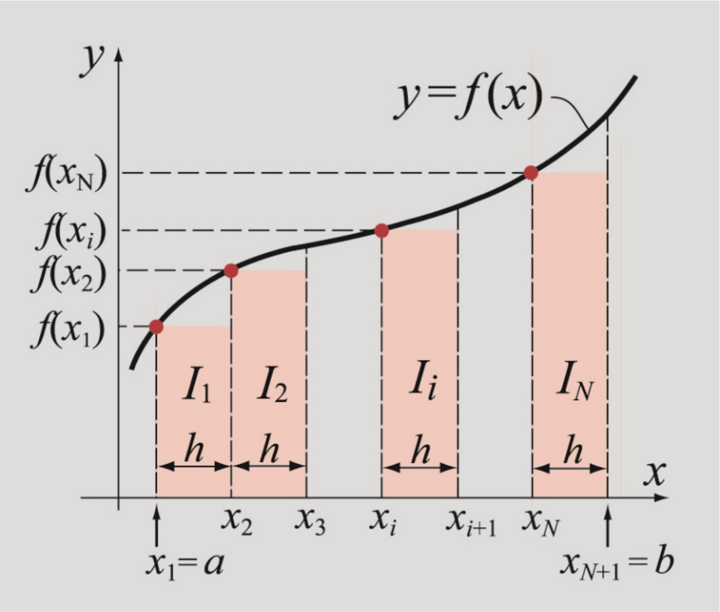
- The integral is approximated by an area of a rectangle
- The error can be large



Composite Rectangle Method

- When the analytical function is given, the error can be reduced with composite rectangle method
  - Divide the domain [a,b] into N subintervals
  - Calculate the integrand in each subinterval with rectangle method, and added together
- Smaller intervals can be used in regions where the integrand changes rapidly

$$
\begin{aligned}
I_f &= \int_a^b f(x)dx \approx I_1 + I_2 + \ldots + I_N \\
&= f(x_1)(x_2 - x_1) + f(x_2)(x_3 - x_2) + \ldots \\
&+ f(x_N)(x_{N+1} - x_N)
\end{aligned}
$$



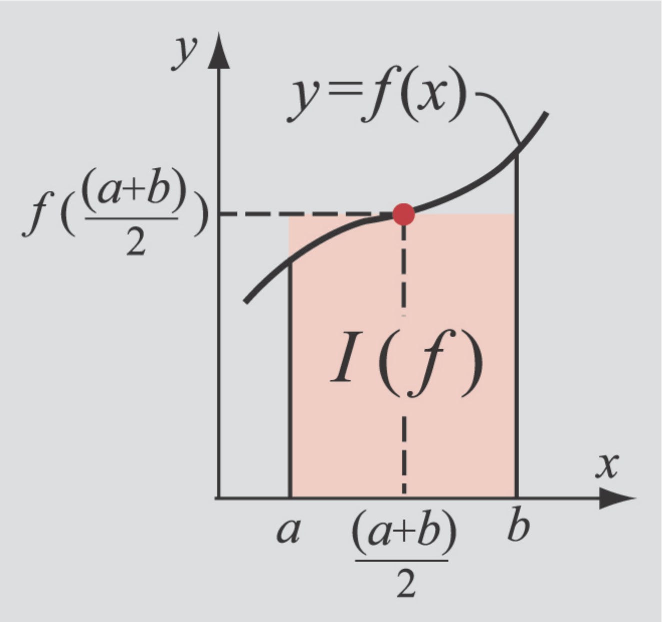
- If the intervals have the same h

$$I_f = \int_a^b f(x)dx \approx h\sum_{i=1}^{N} f(x_i)$$

Midpoint Method

- An improve method over the rectangle method by using the value of the midpoint (a+b)/2
- This may still be not accurate enough
- The accuracy can be increased using a **composite midpoint method**

$$I_f = \int_a^b f(x)dx \approx \int_a^b f(\frac{a+b}{2})dx = f(\frac{a+b}{2})(b-a)$$



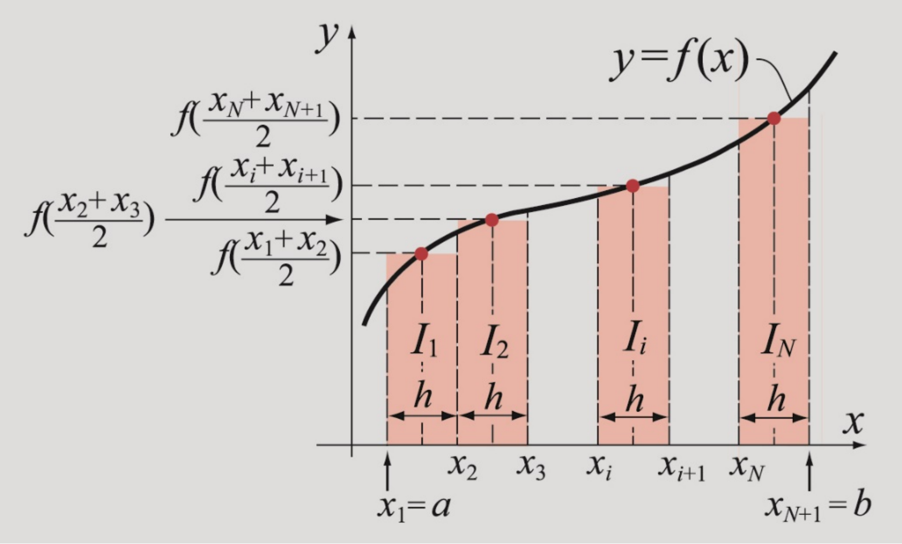
Composite Midpoint Method

- Divide the domain [a,b] into N subintervals
- Calculate the integrand in each subinterval with midpoint method, and added together

$$I_f = \int_a^b f(x)dx \approx I_1 + I_2 + \ldots + I_N$$

$$= f\left(\frac{x_1 + x_2}{2}\right)(x_2 - x_1) + f\left(\frac{x_2 + x_3}{2}\right)(x_3 - x_2) + \ldots + f\left(\frac{x_N + x_{N+1}}{2}\right)(x_{N+1} - x_N)$$

$$= h\sum_{i=1}^{N} f\left(\frac{x_i + x_{i+1}}{2}\right)$$



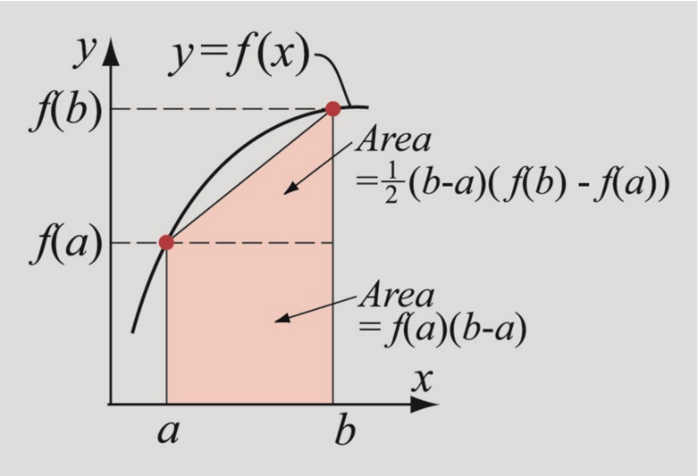
6.3 Trapezoidal Method

- A refinement over the simple rectangular and midpoint methods is to use a linear function to approximate the integrand over the interval

$$f(x) \approx f(a) + (x-a) f[a,b] = f(a) + (x-a)\frac{f(b)-f(a)}{b-a}$$

$$I_f \approx \int_a^b \left\{ f(a) + (x-a)\frac{f(b)-f(a)}{b-a} \right\} dx = f(a)(b-a) + \frac{1}{2}\left[f(b)-f(a)\right](b-a)$$

$$I_f \approx \frac{f(a)+f(b)}{2}(b-a)$$



Composite Trapezoidal Method

- Divide the domain [a,b] into N subintervals
- Calculate the integrand in each subinterval with trapezoidal method, and added together

$$I_f = \int_a^b f(x)dx \approx I_1 + I_2 + \ldots + I_N = \sum_{i=1}^{N} \int_{x_i}^{x_{i+1}} f(x)dx$$

- Using the trapezoidal method:

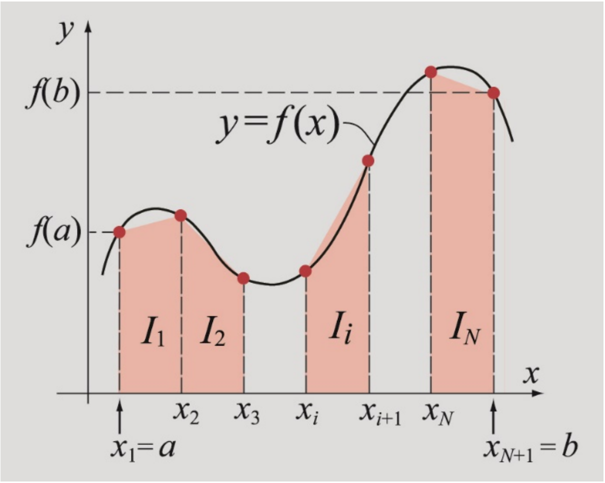
$$I_f = \int_a^b f(x)dx \approx \frac{1}{2}\sum_{i=1}^{N}\left[f(x_i) + f(x_{i+1})\right](x_{i+1} - x_i)$$

- For the same subinterval h

$$I_f \approx \frac{h}{2}\sum_{i=1}^{N}\left[f(x_i) + f(x_{i+1})\right]$$

$$= \frac{h}{2}\left[f(a) + 2f(x_2) + 2f(x_3) + \ldots + 2f(x_N) + f(b)\right]$$

$$= \frac{h}{2}\left[f(a) + f(b)\right] + h\sum_{i=2}^{N} f(x_i)$$



Example 6-1

- Calculate the distance traveled by a decelerating airplane from v = 93m/s to 40 m/s:

$$mv\frac{dv}{dx} = -5v^2 - 570000$$

m = 97,000 kg

- This can be solved by the separation of variables

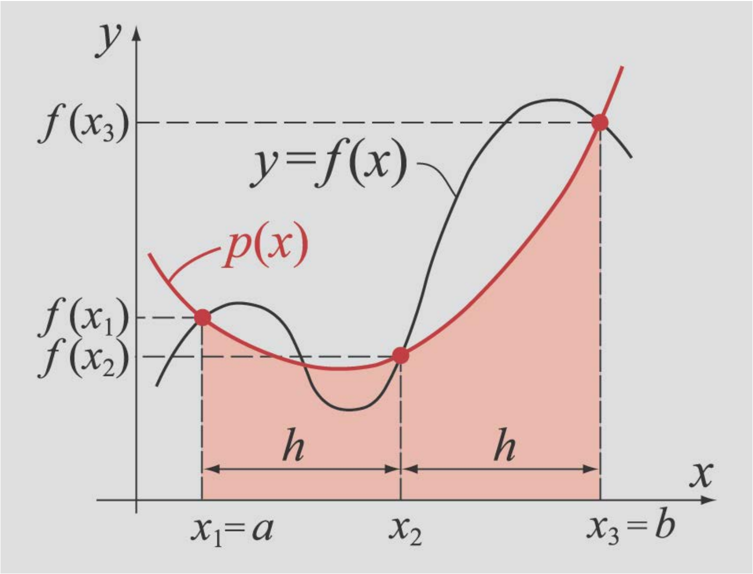
$$\frac{97000vdv}{-5v^2 - 570000} = dx$$

$$\int_0^x dx = -\int_{93}^{40} \frac{97000vdv}{5v^2 + 570000}$$

$$x = 574.1494m$$

6.4 Simpson's Method

- The trapezoidal method relies on approximating the integrand by a straight line
- A better approximation can be possibly obtained by approximating the integrand with a nonlinear function that can be easily integrated
  - Quadratic (Simpson's 1/3 method)
  - Cubic (Simpson's 3/8 method)

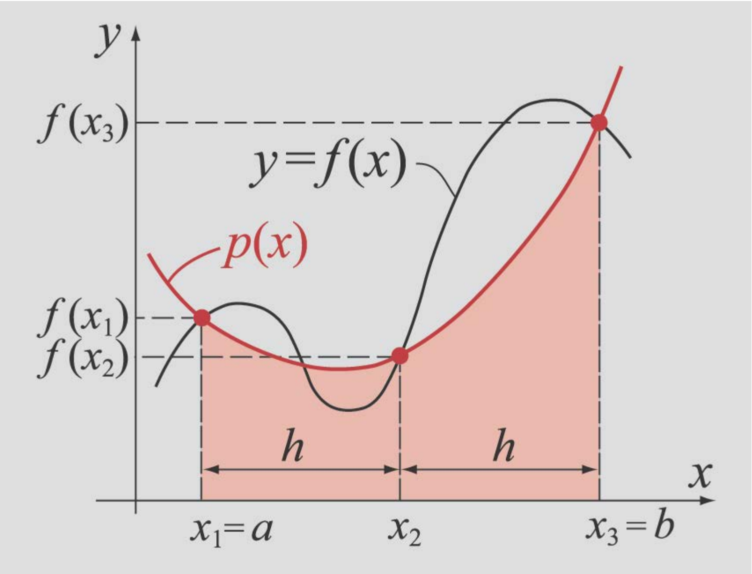


Simpson’s 1/3 Method

- A quadratic (2nd order) polynomial is used to approximate the integrand
- The coefficients of a quadratic polynomial can be determined from **three** points x = a, x = b, and x = (a+b)/2

$$p(x) = \alpha + \beta(x - x_1) + \gamma(x - x_1)(x - x_2)$$

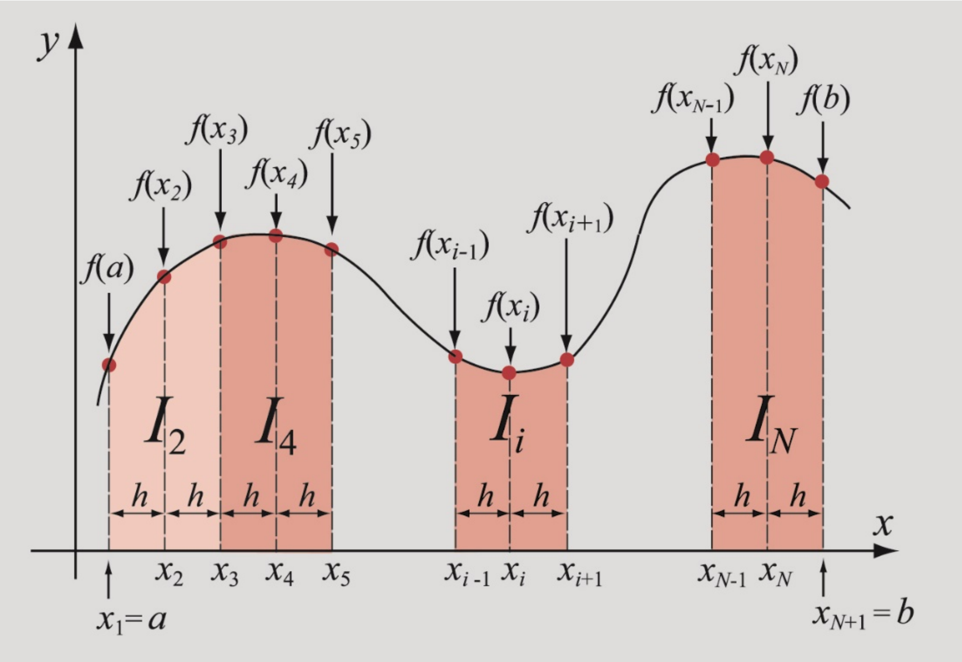
$$I = \int_{x_1}^{x_3} f(x)dx \approx \int_{x_1}^{x_3} p(x)dx = \frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$



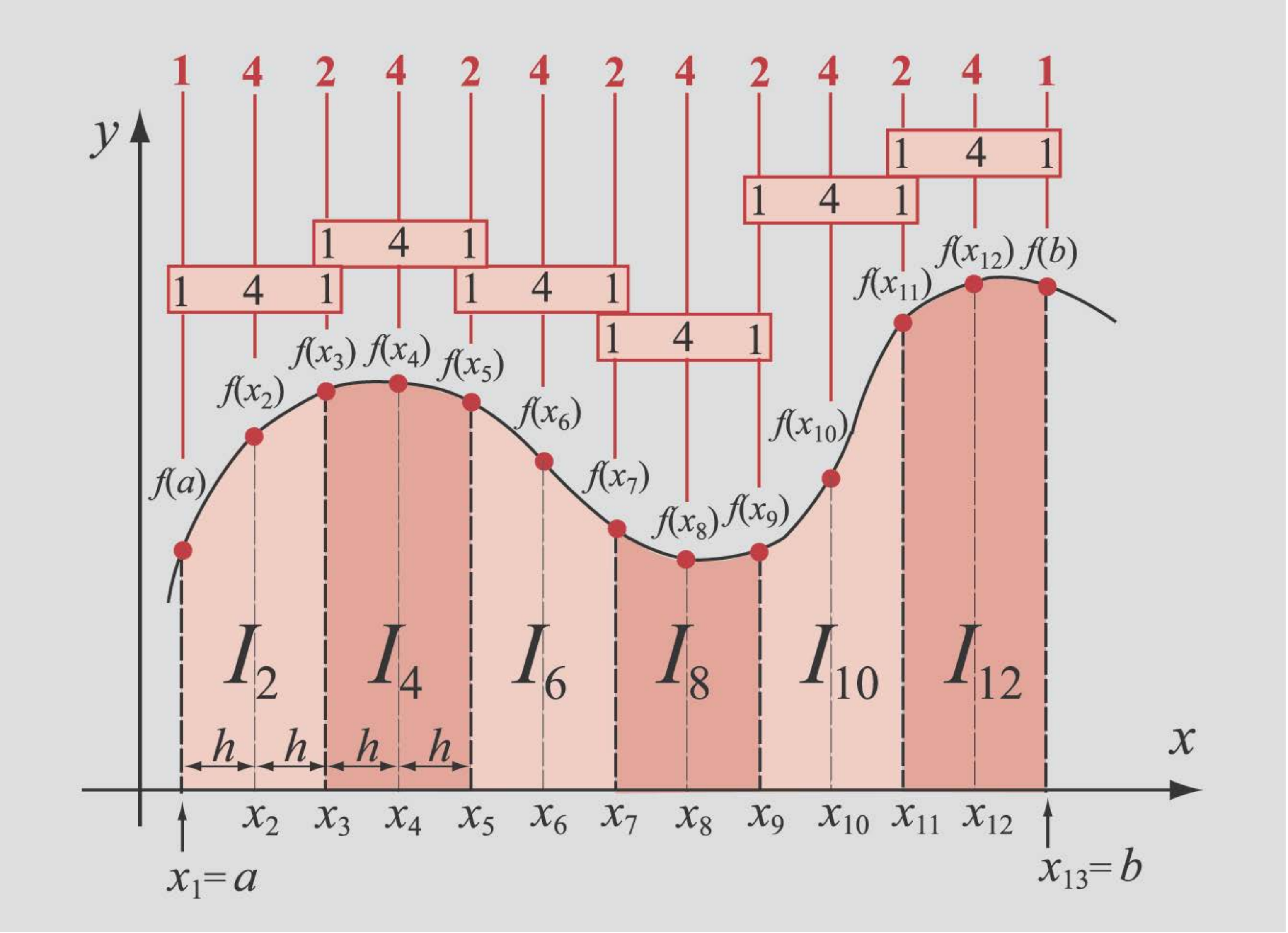
Composite Simpson's 1/3 Method

- The whole interval has to be divided into an even number of subintervals (since three points are required for each interval)
- For equally spaced interval h:

$$I = \int_a^b f(x)dx \approx \frac{h}{3}\left[f(a) + 4\sum_{i=2,4,6}^{N} f(x_i) + 2\sum_{j=3,5,7}^{N-1} f(x_j) + f(b) \right]$$



Weighted Addition with the Composite Simpson's 1/3 Method

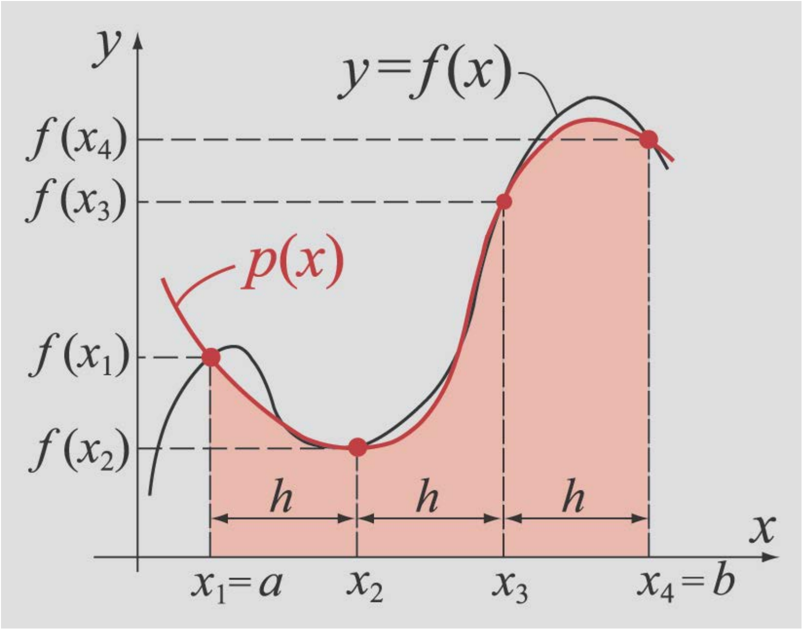


Simpson's 3/8 Method

- A cubic (3rd order) polynomial is used to approximate the integrand
- The coefficients of a quadratic polynomial can be determined from **four** points $x_1 = a$, x_2, x_3, and $x_4 = b$

$$p(x) = c_3 x^3 + c_2 x^2 + c_1 x + c_0$$

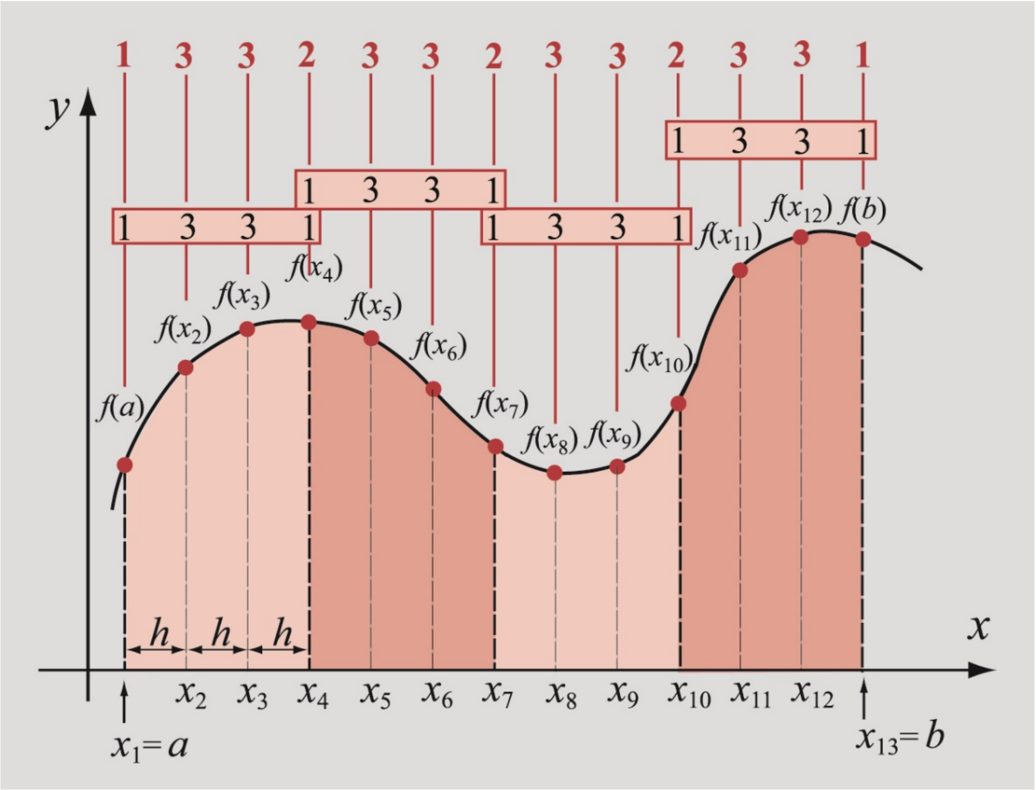
$$I = \int_a^b f(x)dx \approx \int_{x_1}^{x_3} p(x)dx = \frac{3h}{8}\left[f(a) + 3f\left(x_2\right) + 3f\left(x_3\right) + f(b)\right]$$



Composite Simpson's 3/8 Method

- The number of subintervals that must be divisible by **3**

$$I \approx \frac{3h}{8}\left[f(a) + 3\sum_{i=2,5,8}^{N-1}[f(x_i) + f(x_{i+1})] + 2\sum_{j=4,7,10}^{N-2} f(x_j) + f(b) \right]$$



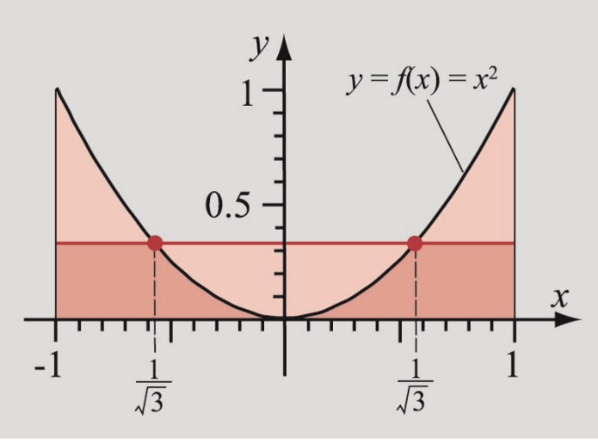
6.5 Gauss Quadrature

- The integral is also evaluated by using weighted addition of the values of f(x) at different points (Gauss points) within [a,b]
- The Gauss points are **not** equally spaced and do **not** include the end points
- General form:

$$\int_a^b f(x)dx \approx \sum_{i=1}^{n} C_i f(x_i)$$

C_i: weights
x_i: points

- The value of the coefficients (C_i) and the location of points x_i depend on the values of n, a, and b



Gauss Quadrature

- For n = 2 and the domain [-1,1], f(x) = 1, x, x^2, x^3,…

$$\int_{-1}^{1} f(x)dx \approx C_1 f(x_1) + C_2 f(x_2)$$

- There are four cases:

$$f(x) = 1 \qquad \int_{-1}^{1} (1)dx = 2 = C_1 + C_2$$

$$f(x) = x \qquad \int_{-1}^{1} xdx = 0 = C_1 x_1 + C_2 x_2$$

$$f(x) = x^2 \qquad \int_{-1}^{1} x^2 dx = \frac{2}{3} = C_1 x_1^2 + C_2 x_2^2$$

$$f(x) = x^3 \qquad \int_{-1}^{1} x^3 dx = 0 = C_1 x_1^3 + C_2 x_2^3$$

- Solve to get: $C_1 = 1 \quad C_2 = 1 \quad x_1 = -\frac{1}{\sqrt{3}} \quad x_2 = \frac{1}{\sqrt{3}}$

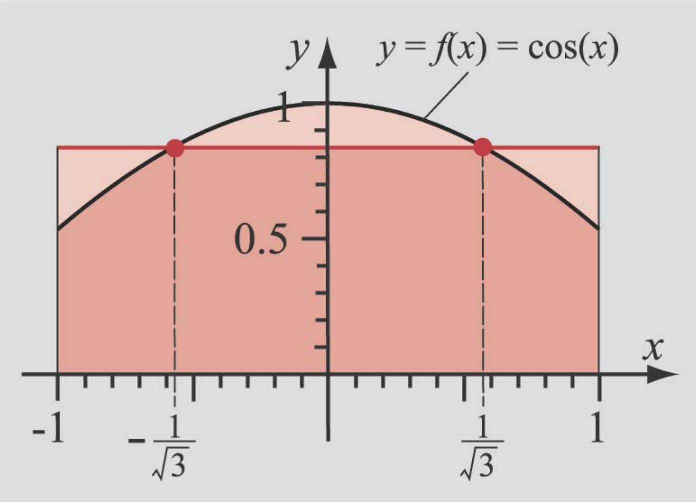
- For n=2, $\int_{-1}^{1} f(x)dx \approx f(-\frac{1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}})$

Gauss Quadrature

- Then f(x) is a function that is different from f(x) = 1, x, x^2, x^3, or any linear combination of these, Gauss quadrature gives an **approximate** value for the integral
- The accuracy of Gauss quadrature can be increased by using a higher value for n (**Table 6-1**)
- The interval can have any domain [a,b] by using a transformation

$$\int_a^b f(x)dx = \int_{-1}^{1} f(t)dt$$

$$\int_a^b f(x)dx = \int_{-1}^{1} f\left(\frac{(b-a)t+a+b}{2}\right)\left(\frac{b-a}{2}\right)dt$$



Example 6.2

- Evaluate the following equations using four-pint Gauss quadrature

$$\int_0^3 e^{-x^2}\,dx$$

- Transform the equation into: $\int_{-1}^{1} f(t)dt$

$$x = \frac{1}{2}[t(b-a)+a+b] = \frac{1}{2}[t(3-0)+0+3] = \frac{3}{2}(t+1)$$

$$dx = \frac{1}{2}(b-a)dt = \frac{1}{2}(3-1)dt = \frac{3}{2}dt$$

- Therefore

$$I = \int_0^3 e^{-x^2}dx = \int_{-1}^{1} f(t)dt = \int_{-1}^{1} \frac{3}{2} e^{-[\frac{3}{2}(t+1)]^2}\,dt$$

$$I = \int_{-1}^{1} f(t)dt \approx C_1 f(t_1) + C_2 f(t_2) + C_3 f(t_3) + C_4 f(t_4)$$

6.6 Evaluation of Multiple Integrals

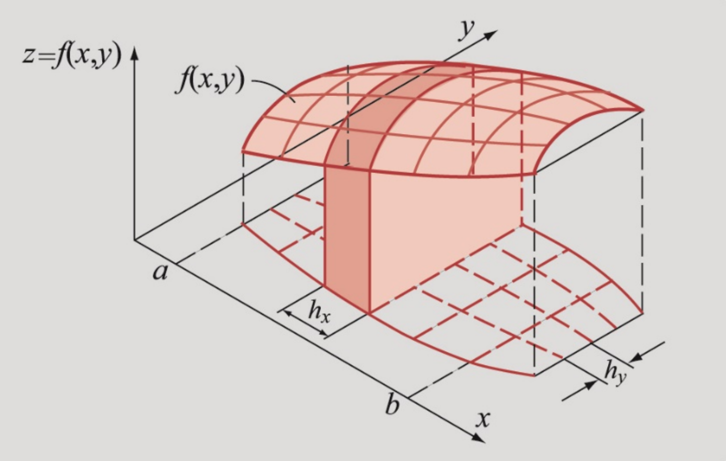
- The double integration can be separated into two parts:

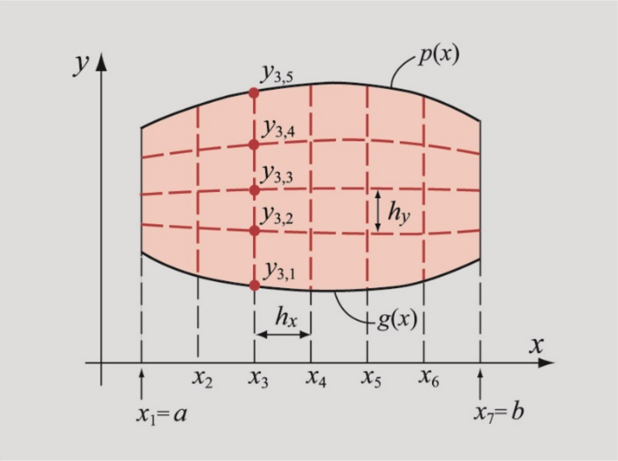
$$G(x)=\int_{y=g(x)}^{y=p(x)} f(x,y)dy \qquad I=\int_a^b G(x)dx$$

- The outer integral can be evaluated (ex. 1/3 Simpson's method):

$$I(G)\approx \frac{h_x}{3}\left\{G(a)+4\left[G(x_2)+G(x_4)+G(x_6)\right]+2\left[G(x_3)+G(x_5)\right]+G(b)\right\}$$

$$h_x=(b-a)/6$$





6.7 MATLAB Built-inFunctions

- Command **quad**:
  - I = quad(function,a,b)

- Command **quadl**:
  - I = quadl(function,a,b)

- Command **trapz**:
  - q=trapz(x,y)

- Command **dblquad**:
  - I=dblquad(function,xmin,xmax,ymin,ymax)

6.8 Estimation of Error

- As an example from the rectangle method, the error E is:

$$E = \int_a^b f(x)dx - f(a)(b-a)$$

- Using one-term Taylor series expansion

$$f(x) = f(a) + f'(\xi)(x-a)$$

- Using this in the calculation:

$$E = \int_a^b f(x)dx - f(a)(b-a) = \frac{1}{2} f'(\xi)(b-a)^2$$

- The error can be reduced with the composite method and when the small subinterval is used

Estimation of Error

- For the case where h is the same:

$$E = \frac{1}{2} h^2 \sum_{i=1}^{N} f'(\xi_i)$$

and the average value of the derivative

$$\overline{f'} \approx \frac{\sum_{i=1}^{N} f'(\xi_i)}{N}$$

- Since h = (b-a)/N, the above equation can be reduced to:

$$E = \frac{b-a}{2} h \overline{f'} = O(h)$$

- The error in the other methods can also be estimated:

Composite midpoint method: $E = \frac{b-a}{24} h^2 \overline{f''} = O(h^2)$

Composite trapezoidal method: $E = -\frac{b-a}{12} h^2 \overline{f''} = O(h^2)$

Composite Simpson’s 1/3 method: $E = -\frac{b-a}{180} h^4 \overline{f''''} = O(h^4)$

Composite Simpson’s 3/8 method: $E = -\frac{b-a}{80} h^4 \overline{f''''} = O(h^4)$

6.9 Richardson's Extrapolation

- Obtain a more accurate estimate of an integral from **two** less accurate estimates
- If the integral I(f) with the error $O(h^2)$is written as:

$$I(f) = I(f)_h + Ch^2 + Dh^4 + ...$$

- Two estimated using different intervals:

$$I(f) = I(f)_{h1} + Ch_1^2 \qquad I(f) = I(f)_{h2} + Ch_2^2$$

- The I(f) can be solved with the error $O(h^4)$:

$$I(f) = \frac{I(f)_{h1} - \left(\frac{h_1}{h_2}\right)^2 I(f)_{h_2}}{1 - \left(\frac{h_1}{h_2}\right)^2}$$

Richardson's Extrapolation

- Similarly, two estimates with error $O(h^4)$ can be used to calculate the estimate with the error $O(h^6)$:

$$I(f) = \frac{I(f)_{h1} - \left(\frac{h_1}{h_2}\right)^4 I(f)_{h_2}}{1 - \left(\frac{h_1}{h_2}\right)^4}$$

- The Richardson's general extrapolation formula:

$$I = \frac{2^p I_{2n} - I_n}{2^p - 1}$$

- where
  - I_n is an estimate using n subintervals with error order h^p
  - I_{2n} is an estimate using 2n subintervals with error order h^p
  - The new estimate of the integral has the error order $h^{(p+2)}$

6.10 Romberg Integration

- Improving the accuracy by successive application of Richardson's extrapolation formula