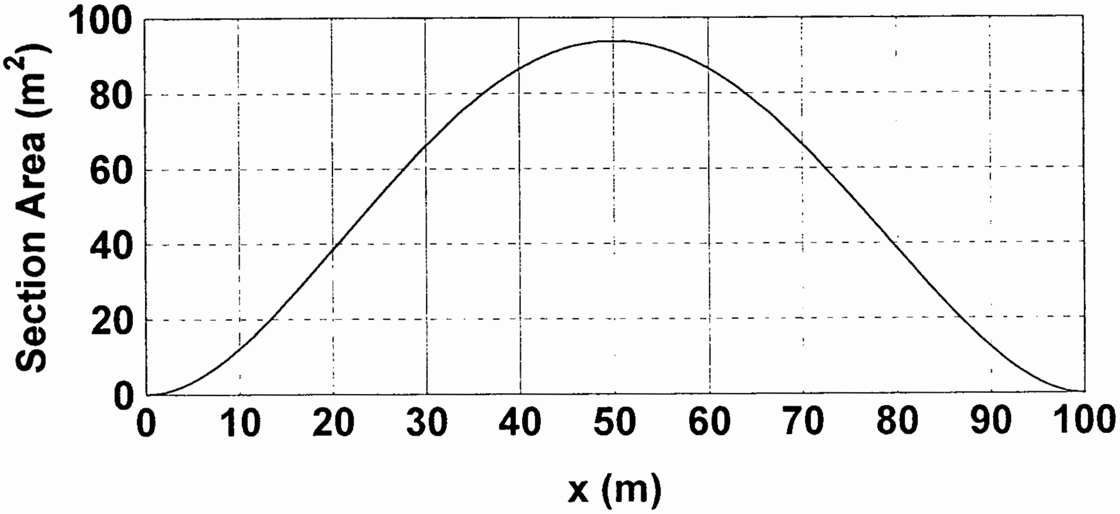
Numerical Integration

Numerical Integration

1. Used to integrate a function that we do not know how it integrate by quadrature. For example, suppose we seek $I = \int_{2.2}^{5.3} \exp(\sqrt{x + x^3} dx$
2. Used when we want to determine $\int_a^b f(x)dx$ and we have a set of pairs of values of $[x,\ f(x)]$

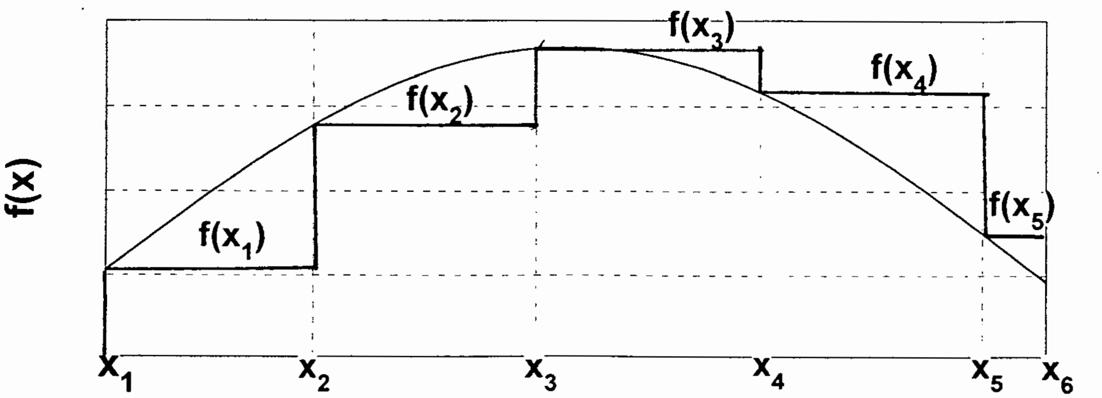


One approach, which we will not consider in detail here, is to fit a polynomial to the integrand and then to integrate the polynomial analytically.

The approach we follow here is to consider *integration rules* which provide a numerical approximation to the integral in terms of discrete values of the integrand for a set of values of x.

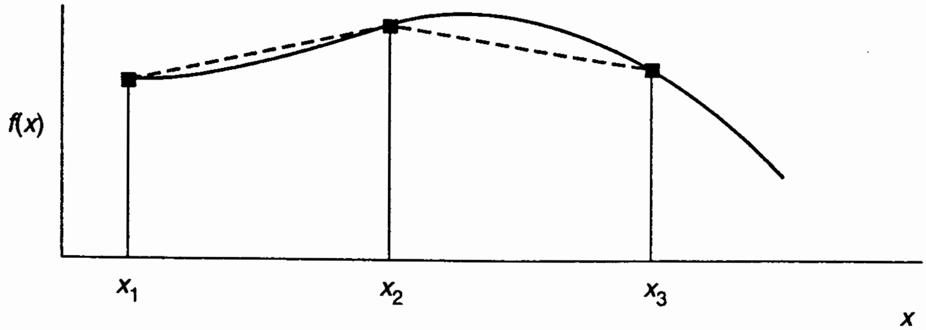
Rectangular Rule approximates the function by a set of rectangles and estimates the integral as the sum of the areas of the rectangles.

$$\int_{x_1}^{x_n} \approx \sum_{i=1}^{n-1} (x_{i+1} - x_i) f(x_i)$$

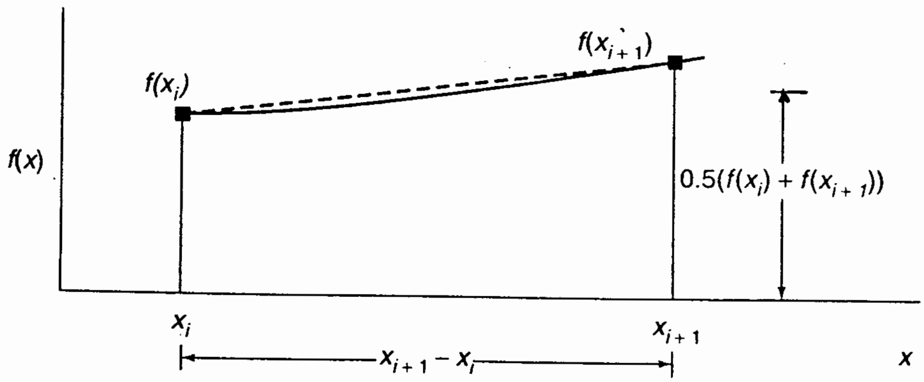


Trapezoidal Rule

The trapezoidal rule fits a trapezoid to each successive pair of values of $[x, f(x)]$ and estimates the integral as the sum of the areas of the trapezoids.



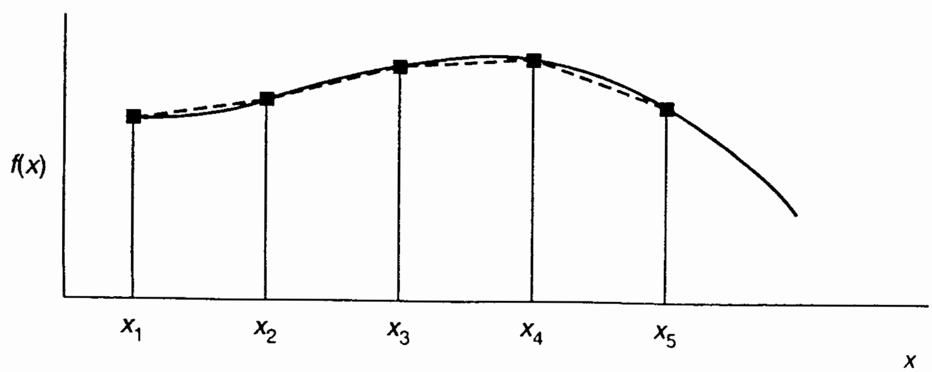
$$\int_{x_1}^{x_n} f(x)dx \approx \sum_{i=1}^{n-1} (x_{i-1} - x_i)\frac{1}{2}[f(x_{i+1} + f(x_i)]$$



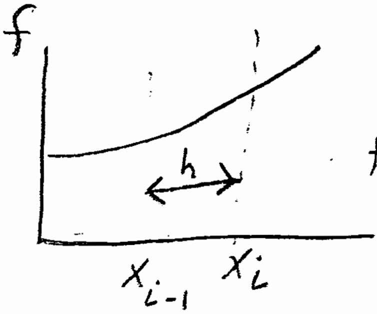
By expanding $f(x)$ in each interval as a Taylor series we find the error in the approximate integral, E_T is given by:

$$E_T = -\frac{h^3}{12}\sum_{i=1}^{n-1} f''(\eta_i)$$

where η_i is some value of x in the i^{th} interval. Since the number of terms in the sum is proportional to $1/h$, smaller intervals result in less error.

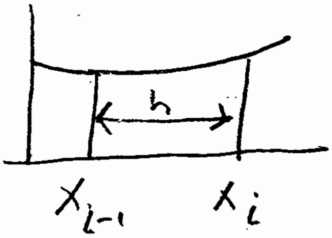


TRAPEZOIDAL Rule Error



$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) + \cdots$$

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + \frac{h}{2}f''(x_i) + \cdots$$



$$I = \int_{x_{i-1}}^{x_i} f(x)dx = F(x_i) - F(x_{i-1}) \quad \text{where } \frac{dF}{dx} = F'(x) = f(x)$$

$$F(x_{i-1}) = F(x_i) - hF'(x_i) + \frac{h^2}{2}F''(x_i) - \frac{h^3}{6}F'''(x_i) + \cdots$$

$$I = F(x_i) - F(x_{i-1}) = hF'(x_i) - \frac{h^2}{2}F''(x_i) + \frac{h^3}{6}F'''(x_i) + \cdots$$

Since $F'(x_i) = f(x_i)$,

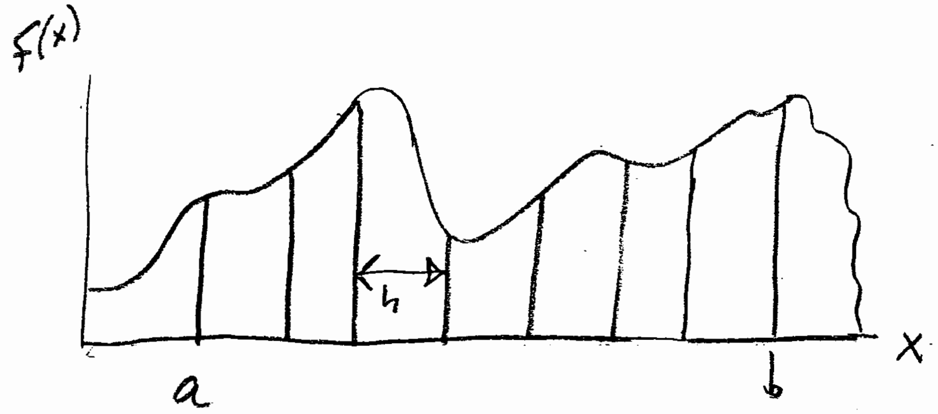
$$I = hf(x_i) - \frac{h^2}{2}f'(x_i) + \frac{h^3}{3}f''(x_i) + \cdots$$

$$I = hf(x_i) - \frac{h^2}{2}\left[\frac{f(x_i) - f(x_{i-1})}{h} + \frac{h}{2}f''(x_i) + \cdots\right] + \frac{h^3}{3}f''(x_i) + \cdots$$

$$I = hf(x_i) - \frac{h}{2}f(x_i) + \frac{h}{2}f(x_{i-1}) - \frac{h^3}{4}f''(x_i) + \frac{h^3}{3}f''(x_i) + \cdots$$

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

Error in interval x_{i-1} to x_i is $\frac{h^3}{12}f''(x_i) + O(h^4)$



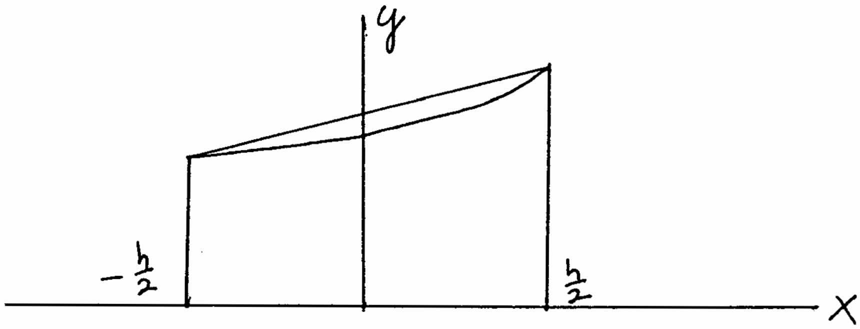
Number of intervals is $\frac{b-a}{h}$

If $|f''(x)| \leq M$ in $a<x<b$

Total error $\leq \frac{b-a}{h}\left[\frac{h^3}{12}M + O(h^4)\right]$

Total error $\leq (b-a)\left[\frac{h^2}{12}M + O(h^3)\right]$

Estimate 3 - Usual Trapezoidal Rule



$$y = f(x) = a + bx + cx^2 + \cdots$$

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

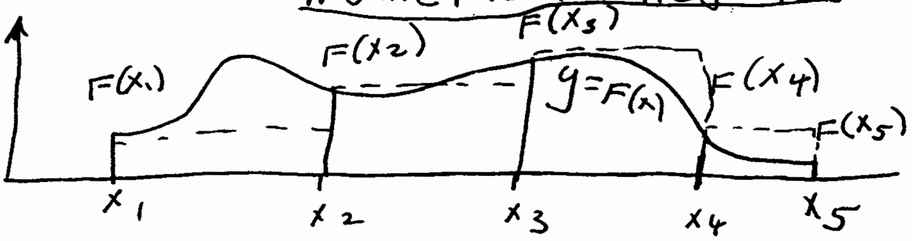
$$c = \frac{1}{2}f''(\beta) \qquad -\frac{h}{2} \le \beta \le \frac{h}{2}$$

$$I = ah + c\frac{h^3}{12} + \cdots = \frac{h}{2}\left[f\left(-\frac{h}{2}\right) + f\left(\frac{h}{2}\right)\right] + \frac{1}{2}f''(\beta)\frac{h^3}{12} + \cdots$$

$$I_{\text{trap}} = \frac{h}{2}\left[f\left(-\frac{h}{2}\right) + f\left(\frac{h}{2}\right)\right]$$

$$\text{Error} = \frac{h^3}{24}f''(\beta) + O(h^4)$$

Numerical Integration



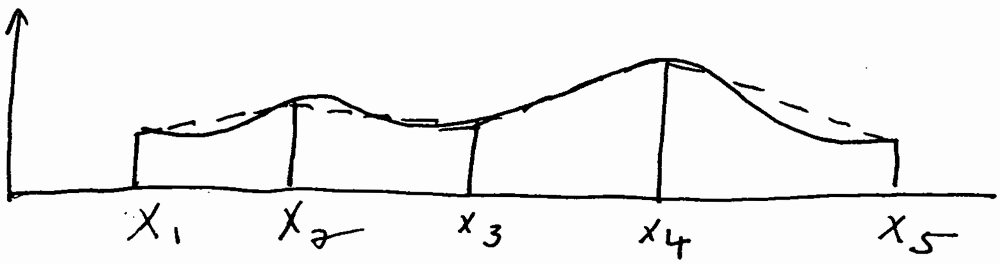
$$I = \int_{x_1}^{x_5} f(x)\,dx$$

Rectangular Rule Abbreviation $F(x_i) \equiv F_i$

$$I = F(x_1)(x_2 - x_1) + F(x_2)(x_3 - x_2) + F(x_3)(x_4 - x_3) + F(x_4)(x_5 - x_4)$$

$$= x_2 F_1 - x_1 F_1 + x_3 F_2 - x_2 F_2 + x_4 F_3 - x_3 F_3 + x_5 F_4 - x_4 F_4$$

Trapezoidal Rule



$$I = \left(\frac{F_1 + F_2}{2}\right)(x_2 - x_1) + \left(\frac{F_2 + F_3}{2}\right)(x_3 - x_2) + \left(\frac{F_3 + F_4}{2}\right)(x_4 - x_3) + \left(\frac{F_4 + F_5}{2}\right)(x_5 - x_4)$$

$$= \frac{1}{2}\left\{ F_1 x_2 - F_1 x_1 + \cancel{F_2 x_2} - F_2 x_1 + F_2 x_3 - \cancel{F_2 x_2} + \cancel{F_3 x_3} - F_3 x_2 + F_3 x_4 - \cancel{F_3 x_3} + \cancel{F_4 x_4} - F_4 x_3 + F_4 x_5 - \cancel{F_4 x_4} + F_5 x_5 - F_5 x_4 \right\}$$

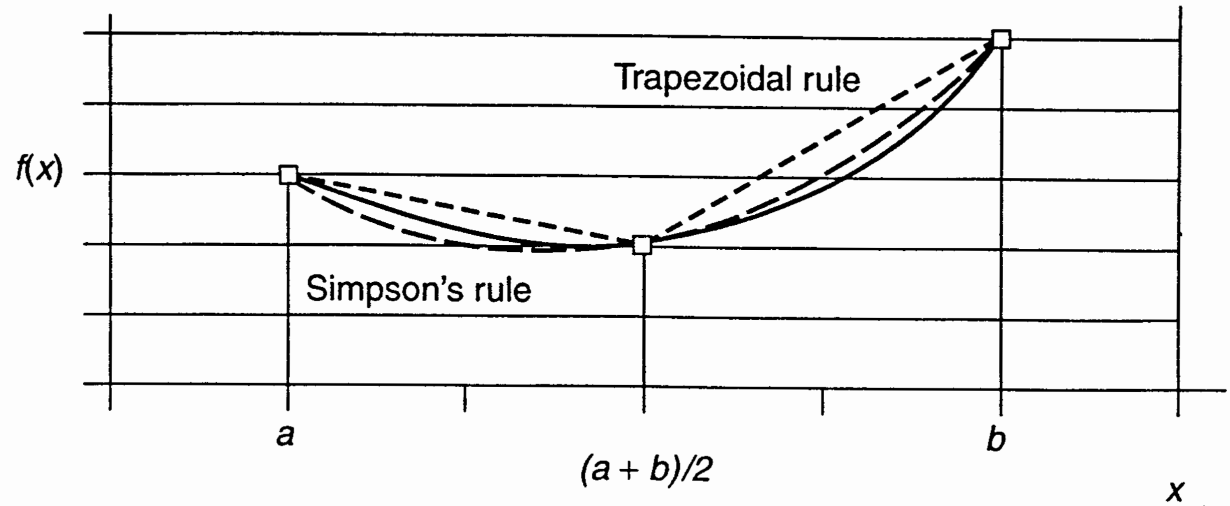
$$= \frac{1}{2}\left\{ F_1(x_2 - x_1) + F_2(x_3 - x_1) + F_3(x_4 - x_2) + F_4(x_5 - x_3) + F_5(x_5 - x_4) \right\}$$

If $x_{n+2} - x_n = 2(x_{n+2} - x_{n+1}) \Leftrightarrow$ equal spacing

$$I = \tfrac{1}{2} F_1 (x_2 - x_1) + F_2 (x_3 - x_2) + F_3 (x_4 - x_3) + F_4 (x_5 - x_4) + \tfrac{1}{2} F_5 (x_5 - x_4)$$

Simpson's Rule

Simpson's rule fits a parabola (2^{nd} order polynomial) to each interval between $[x_i, f(x_i)]$ and $[x_{i+2}, f(x_{i+2})]$ and estimates the integral as the sum of the areas under the parabolas.



For Simpson's Rule, the intervals $[x_{i+1} - x_i]$ and $[x_{i+2} - x_{i+1}]$ must be equal and the x-distance interval length is called Δx. For three values of x_i; $a, a + \Delta x, b$ the integral is

$$\int_a^b f(x)dx \approx \frac{\Delta x}{3}[f(a) + 4f(a + \Delta x) + f(b)]$$

Simpson's Rule requires that there be an even number of intervals which means that there are an odd number of data pairs $[x_i, f(x_i)]$ Then the integral is approximated by the sum of the areas under the approximating parabolas as

$$\int_{x_1}^{x_n} f(x)dx \approx \sum_{i=1,3,5,\ldots}^{n-2} \frac{x_{i+1} - x_i}{3}[f(x_i) + 4f(x_{i+1}) + f(x_{i+2})]$$

For the usual case of equal spacing, Δx, of all the x_i's, Simpson's Rule can be expressed as:

$$\int_{x_1}^{x_n} f(x)dx \approx \frac{\Delta x}{3}\left[f(x_1) + f(x_n) + 4\sum_{i=2,4,6,\ldots}^{n-1} f(x_i) + 2\sum_{i=3,5,7,\ldots}^{n-2} f(x_i)\right]$$