Numerical Quadrature Rules

The idea: The definite integral $I[f;a,b] = \int_a^b f(x)\,dx$ is approximated with a numerical quadrature rule $Q[f;a,b]$.

Why? Fundamental reason: The fundamental theorem of calculus is not universal.

For instance arc lengths cannot be found in closed form in the general case.

Practical reason: Modern computers ...

Concepts: Points and weights

$$Q[f;a,b] = \sum_{i=0}^{n} w_i f(x_i),$$

where the quadrature points $x_i \in [a,b]$ and weights $w_i \in \mathbb{R}$.

Notice: $\sum_{i=0}^{n} w_i = b - a$.

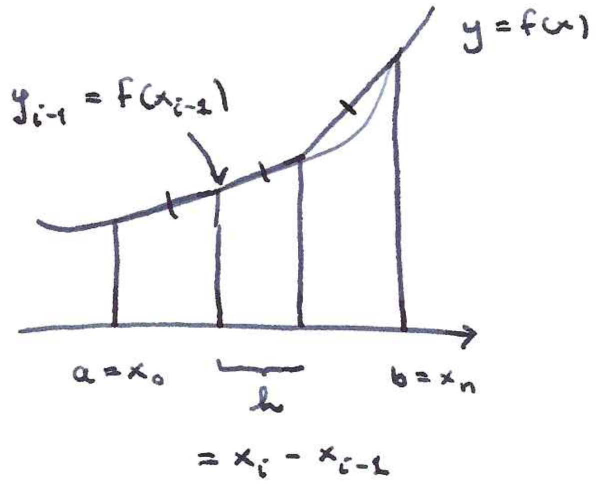
Rate of convergence

The error estimate relates the error to the number of intervals n (or points $n+1$).

For any convergent method the error decreases at some speed or rate.

There are many rules available and it is up to the engineer to select the appropriate one.

$T_n[f; a, b]$: The trapezoidal rule



The idea is to linearise the function f at every interval and then apply summation as in the definition of the definite integral.

One interval:

$$\int_{x_{j-1}}^{x_j} f(x)\,dx \simeq h \, \frac{y_{j-1} + y_j}{2}, \quad 1 \le j \le n.$$

Definition

$$T_n[f; a, b] = h \left(\frac{1}{2} y_0 + y_1 + y_2 + \dots + y_{n-1} + \frac{1}{2} y_n \right)$$

$$= \frac{h}{2} \left(y_0 + 2y_1 + 2y_2 + \dots + 2y_{n-1} + y_n \right)$$

Example $\quad I = \displaystyle\int_1^2 \frac{dx}{x}, \quad T_4 = ?$

$$h = \frac{2-1}{4} = \frac{1}{4}; \quad T_4 = \frac{1}{4} \left(\frac{1}{2} \cdot 1 + \frac{4}{5} + \frac{2}{3} + \frac{4}{7} + \frac{1}{2} \cdot \frac{1}{2} \right)$$

$$\simeq 0.697$$

$M_n[f; a, b]$: The midpoint rule

Let $h = \frac{b-a}{n}$. Choose the points $m_j = a + (j - \frac{1}{2})h$,
$1 \le j \le n$.

<u>Definition</u> $M_n[f; a, b] = h \sum_{j=1}^{n} f(m_j)$

Notice that this is just a special Riemann sum!

<u>Example</u> $I = \int_1^2 \frac{dx}{x}$; $M_4 = ?$

$$M_4 = \frac{1}{4}\left[\frac{8}{9} + \frac{8}{11} + \frac{8}{13} + \frac{8}{15}\right] \simeq 0.691$$

The exact solution : $I = \ln 2 \simeq 0.693$

So, it would appear that the midpoint rule wins in this case.

What can be said about the general case?

<u>Theorem</u> The error estimates

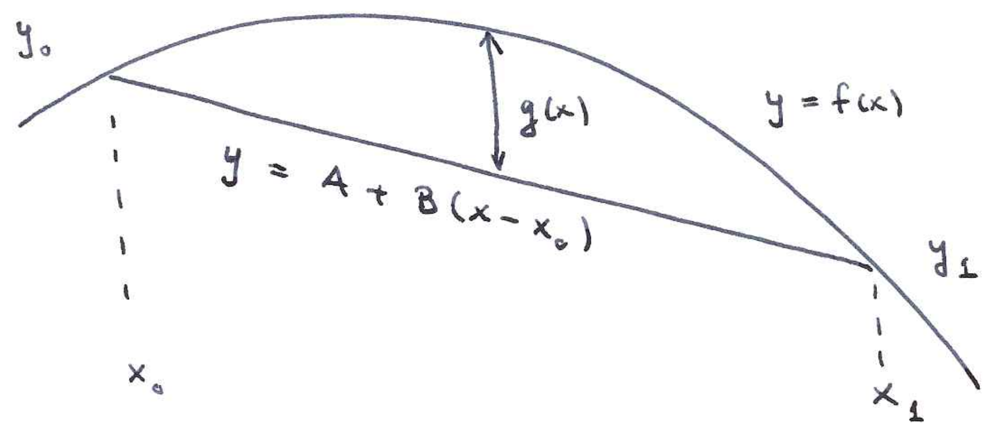
Let f'' be continuous and bounded from above over $[a,b]$, that is, $|f''(x)| \leq K$, K = constant. Then, with $h = \frac{b-a}{n}$, we have

$$\left| \int_a^b f(x)\,dx - T_n \right| \leq \frac{K(b-a)}{12} h^2 = \frac{K(b-a)^3}{12 n^2}$$

$$\left| \int_a^b f(x)\,dx - M_n \right| \leq \frac{K(b-a)}{24} h^2 = \frac{K(b-a)^3}{24 n^2}$$

Both methods are quadratic, i.e., for the error $\sim \Theta\left(\frac{1}{n^2}\right)$.

<u>Proof</u> (Trapezoid)



The error $g(x) = f(x) - A - B(x - x_0)$

$$= f(x) - y_0 - \frac{1}{h}(y_1 - y_0)(x - x_0)$$

By the definition of the definite integral:

$$\int g(x)\,dx = \int f(x)\,dx - h\,\frac{y_0 + y_1}{2} \quad \text{over } [x_0, x_1]$$

Now : $g''(x) = f''(x)$, $g(x_0) = g(x_1) = 0$

Also : $$\int_{x_0}^{x_1} (x - x_0)(x_1 - x)\, g''(x)\, dx = -2 \int_{x_0}^{x_1} g(x)\, dx$$

Triangle inequality :

$$\left| \int_{x_0}^{x_1} f(x)\,dx - h\,\frac{y_0 + y_1}{2} \right| \leq \frac{1}{2} \int_{x_0}^{x_1} (x - x_0)(x_1 - x)\, |f''(x)|\, dx$$

$$\leq \frac{K}{2} \int_{x_0}^{x_1} \left(-x^2 + (x_0 + x_1)\, x - x_0 x_1 \right) dx$$

$$= \frac{K}{12} (x_1 - x_0)^3 = \frac{K}{12} h^3$$

The whole interval :

$$\left| \int_a^b f(x)\,dx - T_n \right| = \left| \sum_{j=1}^{n} \left(\int_{x_{j-1}}^{x_j} f(x)\,dx - h\,\frac{y_{j-1} + y_j}{2} \right) \right|$$

$$\leq \sum_{j=1}^{n} \left| \int_{x_{j-1}}^{x_j} f(x)\,dx - h\,\frac{y_{j-1} + y_j}{2} \right| = \sum_{j=1}^{n} \frac{K}{12} h^3$$

$$= K \cdot \frac{1}{12} \cdot n \cdot h^3 = \frac{K(b-a)}{12} h^2$$

$(nh = b - a)$ $\square$