Numerical Integration

- Not all functions have closed-form anti-derivatives. Thus not all integrals can be evaluated by the Fundamental Theorem of Calculus.
- For special functions, such as the error function
$$\frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt,$$
efforts can be taken to tabulate values once for all. But this practice is too limited.
- One better approach is to approximate the integral by *quadratures*.
  - ◇ Given a function $f(t)$ defined on $[a,b]$, a formula of the form
$$Q_n(f) := \sum_{i=1}^{n} \alpha_i f(x_i) \tag{1}$$
with $\alpha_i \in R$ and $x_i \in [a,b]$ is called a quadrature rule for the integral $I(f) := \int_a^b f(t)dt$.
    - ▷ The points x_i are called the quadrature points (abscissas)
    - ▷ The values α_i are called the quadrature coefficients (weights).
    - ▷ The quadrature error is defined to be $E_n(f) := I(f) - Q_n(f)$.
  - ◇ A quadrature rule is said to have *degree of precision* m if $E_n(x^k) = 0$ for $k = 0, \ldots, m$ and $E_n(x^{m+1}) \neq 0$.
    - ▷ If a quadrature rule has degree of precision m, then $E_n(p_k) = 0$ for all polynomials $p_k(x)$ of degree $\leq m$.
  - ◇ The trapezoidal rule,
$$Q_2(f) = \frac{b-a}{2}[f(a) + f(b)], \tag{2}$$
is a quadrature rule with degree of precision $m = 1$.

More on Trapezoidal Rule

- Recall the linear interpolant of $f(t)$ and the corresponding error:

$$f(t) = f(a) + \frac{f(b) - f(a)}{b - a}(t - a) + \frac{f''(\xi_t)}{2}(t - a)(t - b).$$

- Integrate both side of the above, we obtain

$$I(f) \approx Q_2(f) = \frac{b - a}{2}[f(a) + f(b)]$$

  and

$$E_2(f) = \int_a^b \frac{f''(\xi_t)}{2}(t - a)(t - b)dt.$$

  - ◇ Recall the Mean Value Theorem for integrals (?): *If f is continuous and g is nondecreasing in the interval $[a, b]$, then there exists $\xi \in [a, b]$ such that*

$$\int_a^b f dg = f(\xi) \int_a^b dg.$$

  - ◇ We may rewrite

$$E_2(f) = \frac{f''(\eta)}{2} \int_a^b (t - a)(t - b)dt = -\frac{f''(\eta)}{12}(b - a)^3. \qquad (3)$$

  - ◇ If $|f''(t)|$ is not too large and if $b - a$ is small, the trapezoidal rule gives an approximation with errors around $O(h^3)$.

- Over a large interval, the trapezoidal rule should be applied by summing the results of many applications of the rule over smaller intervals. This is called *composite trapezoidal rule.*
  - ◇ Divide $[a, b]$ into n equally spaced intervals with step size $h = \frac{b-a}{n}$ and nodes $x_i = a + ih$ for $i = 0, 1, \ldots, n$.
  - ◇ Use the trapezoidal rule to approximate

$$\int_{x_{i-1}}^{x_i} f(x)dx \approx \frac{h}{2}[f(x_{i-1}) + f(x_i)]$$

    over each subinterval $[x_{i=1}, x_i]$.
  - ◇ Sum these approximations together:

$$\int_a^b \approx h\left[\frac{f(x_0)}{2} + f(x_1) + \ldots + f(x_{n-1}) + \frac{f(x_n)}{2}\right]. \qquad (4)$$

    This is called the *composite trapezoidal rule.*
  - ◇ Error formula:

$$E_n(f) = -\frac{h^3}{12}\sum_{i=1}^{n} f''(\eta_i) = -\frac{h^2}{12}\frac{b-a}{n}\sum_{i=1}^{n} f''(\eta_i) = -\frac{(b-a)h^2}{12}f''(\eta).$$