Numerical Integration = Quadrature

1. Numerical integration plays key roles for computing, and some well-known functions are *definied* as integrals.
2. Numerical integration, also known as **quadrature**:

   Given a sample of n points for a function f, find an approximation of $\int_a^b f(x)dx$.

Numerical Integration = Quadrature

Interpolatory quadrature, also known as Newton-Cotes rules

let

$$f(x) = \sum_{i=1}^{n} a_i \phi_i(x)$$

where $\phi_i(x)$ *are basis functions (see Chapter 13 on Interpolation).*
Then the integral of f*:*

$$\int_a^b f(x) = \sum_{i=1}^{n} a_i \left(\int_a^b \phi_i(x) \right)$$

Numerical Integration = Quadrature

Newton-Cotes rules:

- $n = 1$, midpoint rule

$$\text{error} = O((b-a)^3)$$

- $n = 1$, trapezoidal rule

$$\text{error} = O((b-a)^3)$$

  Note: the same order as the midpoint rule

- $n = 2$, Simpson's rule

$$\text{error} = O((b-a)^5)$$

Numerical Integration = Quadrature

Composite rules: Let $[a, b]$ be subdivided into k intervals, say, take $\Delta x = \frac{b-a}{k}$, and $x_i = a + (i-1)\Delta x$.

- the composite trapezoidal rule is given by

$$\int_a^b f(x) \approx \sum_{i=1}^{k} \left(\frac{f(x_i) + f(x_{i+1})}{2} \right) \Delta x$$
$$= \left(\frac{1}{2} f(a) + f(x_2) + \cdots + f(x_k) + \frac{1}{2} f(b) \right) \Delta x$$

  error $= O((\Delta x)^3) \times \frac{b-a}{\Delta x} = O((\Delta x)^2)$.

- By a similar scheme, we can also derive a composite Simpson's rule. error $= O(\Delta x^5) \times \frac{b-a}{\Delta x} = O(\Delta x^4)$.

Numerical Integration = Quadrature

Adaptive Simpson's quadrature

- **Goal**: approx. $I = \int_a^b f(x)dx$ to within an error tolerance $\epsilon > 0$.
- step 1: Simpson's rule with $h = (b-a)/2$

$$I = S(a,b) - E_1 := S_1 - E_1$$

- step 2: Composite Simpson's rule with $h_1 = (b-a)/2^2$

$$I = S(a, \frac{a+b}{2}) + S(\frac{a+b}{2}, b) - E_2 := S_2 - E_2$$

- It can be shown that $E_1 \approx 16E_2$. Then

$$S_1 - S_2 = E_1 - E_2 \approx 15E_2.$$

which implies that

$$|I - S_2| = |E_2| \approx \frac{1}{15}|S_1 - S_2|.$$

Numerical Integration = Quadrature

Adaptive Simpson's quadrature, *cont'd*

- If $|S_1 - S_2|/15 < \epsilon$, then $|I - S_2| < \epsilon$. S_2 is sufficiently accuracy.
- Otherwise, apply the same error estimation procedure to the subintervals $[a, \frac{a+b}{2}]$ and $[\frac{a+b}{2}, b]$, respectively to determine if the approximation to the integral on each subinterval is within a tolerance of $\epsilon/2$
- **Recursive algorithm**
- MATLAB code: `quadtx.m`

Numerical Integration = Quadrature

1. Quadrature rules in a general form

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

   where x_i are *knots*, and w_i are *weights*.

2. The choices of $\{x_i\}$ and $\{w_i\}$ determine a quadrature rule.
3. *The method of undetermined coefficients*

   fix $\{x_i\}$, choose $\{w_i\}$ so that $Q(f)$ approximate the integral of f for reasonably smooth functions.

Numerical Integration = Quadrature

Example of *the method of undetermined coefficients*

- Let $x_1 = 0$, $x_2 = 1/2$ and $x_3 = 1$. pick $f_1(x) = 1$, $f_2(x) = x$ and $f_3(x) = x^2$ such that

$$\int_0^1 f_1(x)dx = w_1 f_1(x_1) + w_2 f_1(x_2) + w_3 f_1(x_3)$$
$$\int_0^1 f_2(x)dx = w_1 f_2(x_1) + w_2 f_2(x_2) + w_3 f_2(x_3)$$
$$\int_0^1 f_3(x)dx = w_1 f_3(x_1) + w_2 f_3(x_2) + w_3 f_3(x_3)$$

- Consequently, we have the Simplson's rule

$$\int_0^1 f(x)dx \approx Q(f) = \frac{1}{6}f(0) + \frac{2}{3}f(\frac{1}{2}) + \frac{1}{6}f(1)$$

- By the change of interval $[a, b] \to [0, 1]$, $x = a + (b-a)y$, we have the Simplson's rule on the interval $[a, b]$:

$$\int_a^b f(x)dx \approx Q(f) = (b-a)\left[\frac{1}{6}f(a) + \frac{2}{3}f(\frac{b+a}{2}) + \frac{1}{6}f(b)\right]$$