

Quadrature

$$\int_a^b f(x) dx = \sum_{i=1}^N \int_{x_{i-1}}^{x_i} f(x) dx$$

(where $x_i = a + i h$, $h = (b - a)/N$)

Simpson's local rule:

$$\begin{aligned} \int_0^h f(x) dx &\approx \int_0^h \left[\frac{(x-h/2)(x-h)}{(0-h/2)(0-h)} f(0) + \frac{(x-0)(x-h)}{(h/2-0)(h/2-h)} f(h/2) + \frac{(x-0)(x-h/2)}{(h-0)(h-h/2)} f(h) \right] dx \\ &= \frac{h}{6} f(0) + \frac{4h}{6} f(h/2) + \frac{h}{6} f(h) \end{aligned}$$

Simpson's composite rule:

$$\int_a^b f(x) dx \approx \sum_{i=1}^N \left[\frac{h}{6} f(x_{i-1} + 0) + \frac{4h}{6} f(x_{i-1} + h/2) + \frac{h}{6} f(x_{i-1} + h) \right]$$

Quadrature rule with sample points r_1, r_2, r_3, \dots and weights w_1, w_2, w_3, \dots :

$$\int_a^b f(x) dx \approx \sum_{i=1}^N [w_1 h f(x_{i-1} + r_1 h) + w_2 h f(x_{i-1} + r_2 h) + w_3 h f(x_{i-1} + r_3 h) + \dots]$$

Newton-Cotes formulas:

Name	r_1	r_2	r_3	r_4	r_5	w_1	w_2	w_3	w_4	w_5
Trapezoid	0	1				$\frac{1}{2}$	$\frac{1}{2}$			
Simpson	0	$\frac{1}{2}$	1			$\frac{1}{6}$	$\frac{4}{6}$	$\frac{1}{6}$		
—	0	$\frac{1}{3}$	$\frac{2}{3}$	1		$\frac{1}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{1}{8}$	
Boole	0	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{3}{4}$	1	$\frac{7}{90}$	$\frac{32}{90}$	$\frac{12}{90}$	$\frac{32}{90}$	$\frac{7}{90}$

Theorem: If a quadrature rule is exact for $f(x) = 1, x, x^2, \dots, x^m$, then the global error is bounded by $C_m \max_{(a,b)} |f^{(m+1)}(x)| h^{m+1}$

Proof: see chapter 5 video

MATLAB function implementing Simpson's rule

```
function int = simpson(f,a,b,n)
h = (b-a)/n;
w1 = 1./6.;
w2 = 4./6.;
w3 = 1./6.;
r1 = 0;
r2 = 0.5;
r3 = 1;
int = 0.0;
for i=1:n
    xim1 = a + (i-1)*h;
    int = int + w1*h*f(xim1+r1*h) ...
            + w2*h*f(xim1+r2*h) ...
            + w3*h*f(xim1+r3*h);
end
```

Experimental Order of Convergence

$$E(h) = I(h) - I = M h^\alpha$$

If exact integral I is known:

$$ratio_1 \equiv \frac{E(h)}{E(h/2)} = \frac{M h^\alpha}{M (h/2)^\alpha} = 2^\alpha$$

$$\text{so } \alpha = \frac{\ln(ratio_1)}{\ln(2)}$$

If exact integral is not known:

$$I(h) - I = M h^\alpha$$

$$I(h/2) - I = M (h/2)^\alpha$$

$$I(h/4) - I = M (h/4)^\alpha$$

and

$$I(h) - I(h/2) = M[h^\alpha - (h/2)^\alpha]$$

$$I(h/2) - I(h/4) = M[(h/2)^\alpha - (h/4)^\alpha] = M\frac{1}{2^\alpha}[h^\alpha - (h/2)^\alpha]$$

dividing gives:

$$ratio_2 \equiv \frac{I(h)-I(h/2)}{I(h/2)-I(h/4)} = 2^\alpha$$

$$\text{so } \alpha = \frac{\ln(ratio_2)}{\ln(2)}$$

Gauss Quadrature

Derivation of Gauss-3 point quadrature formula.

$$\int_a^b f(x) dx \approx \sum_{i=1}^N [w_i h f(x_{i-1} + r_i h) + w_2 h f(x_{i-1} + r_2 h) + w_3 h f(x_{i-1} + r_3 h)]$$

To make the algebra simpler, let's take $a = -1, b = 1, N = 1, h = 2$:

$$\int_{-1}^1 f(x) dx \approx [2w_1 f(-1 + 2r_1) + 2w_2 f(-1 + 2r_2) + 2w_3 f(-1 + 2r_3)]$$

By symmetry, we can assume:

$$\begin{aligned} -1 + 2r_1 &= -s, & 2w_1 &= A \\ -1 + 2r_2 &= 0, & 2w_2 &= B \\ -1 + 2r_3 &= s, & 2w_3 &= A \end{aligned}$$

that is,

$$\int_{-1}^1 f(x) dx \approx [Af(-s) + Bf(0) + Af(s)]$$

and we try to make this formula exact for $1, x, x^2, x^3, x^4, x^5$:

$$\begin{aligned} 2 &= \int_{-1}^1 1 dx &= A + B + A &= 2A + B \\ 0 &= \int_{-1}^1 x dx &= A(-s) + B(0) + A(s) &= 0 \\ \frac{2}{3} &= \int_{-1}^1 x^2 dx &= A(-s)^2 + B(0)^2 + A(s)^2 &= 2As^2 \\ 0 &= \int_{-1}^1 x^3 dx &= A(-s)^3 + B(0)^3 + A(s)^3 &= 0 \\ \frac{2}{5} &= \int_{-1}^1 x^4 dx &= A(-s)^4 + B(0)^4 + A(s)^4 &= 2As^4 \\ 0 &= \int_{-1}^1 x^5 dx &= A(-s)^5 + B(0)^5 + A(s)^5 &= 0 \end{aligned}$$

The solution is $s = \sqrt{0.6}$, $A = \frac{5}{9}$, $B = \frac{8}{9}$, which gives:

$$r_1 = \frac{1-s}{2} = \frac{1-\sqrt{0.6}}{2} = 0.112701665$$

$$r_2 = \frac{1}{2} = 0.5$$

$$r_3 = \frac{1+s}{2} = \frac{1+\sqrt{0.6}}{2} = 0.887298335$$

$$w_1 = \frac{1}{2}A = \frac{5}{18}$$

$$w_2 = \frac{1}{2}B = \frac{8}{18}$$

$$w_3 = \frac{1}{2}A = \frac{5}{18}$$

MATLAB function implementing Gauss 3-point formula

```
function int = gauss3(f,a,b,n)
h = (b-a)/n;
w1 = 5./18.;
w2 = 8./18.;
w3 = 5./18.;
r1 = (1-sqrt(0.6))/2.0;
r2 = 0.5;
r3 = (1+sqrt(0.6))/2.0;
int = 0.0;
for i=1:n
    xim1 = a + (i-1)*h;
    int = int + w1*h*f(xim1+r1*h) ...
           + w2*h*f(xim1+r2*h) ...
           + w3*h*f(xim1+r3*h);
end
```