Numerical Quadrature

For a function of one independent variable, the basic idea of a quadrature rule is to replace the definite integral by a sum of the integrand evaluated at certain points (quadrature points) multiplied by quadrature weights:

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

where n is the number of quadrature points.

Newton - Cotes quadrature formulas

The idea of Newton - Cotes quadrature rules is to use evenly spaced quadrature points, interpolate them and integrate to get quadrature weights. Thus Newton - Cotes formulas are interpolatory quadrature rules.

Once you choose the number of points in your Newton - Cotes formula and decide whether to use an open (don't use endpoints of the interval as quadrature points) or closed (use endpoints), then all that remains is to determine the weights w_i.

To do this, we simply use a Lagrange polynomial to interpolate $f(x)$ at the quadrature points. We then use this polynomial to approximate $f(x)$ and integrate it exactly.

Given a set of $k+1$ data points

$$(x_0, y_0), \ldots, (x_j, y_j), \ldots, (x_k, y_k)$$

where no two x_j are the same, the interpolation polynomial in the Lagrange form is a linear combination

$$L(x) := \sum_{j=0}^{k} y_j \ell_j(x)$$

of Lagrange basis polynomials

$$\ell_j(x) := \prod_{\substack{0 \le m \le k \\ m \ne j}} \frac{x - x_m}{x_j - x_m}$$

where $0 \le j \le k$.

Given the assumption that no two x_j are the same, $x_j - x_m \neq 0 \; \forall x_j$, so this expression is always well defined.

Furthermore, $\ell_{j \neq i}(x_i) = 0$ since the expansion for $\ell_j(x)$ includes $(x - x_{i \neq j})$ in the numerator.

The simplest open Newton-Cotes quadrature formula is the <u>Midpoint Rule</u>:

$$\int_a^b f(x)\,dx \approx (b-a)f\left(\frac{a+b}{2}\right)$$

The quadrature point $q_1 = \left(\frac{a+b}{2}\right)$ is the midpoint of $[a, b]$ and the weight $w_1 = (b-a)$, the length of the interval.

Derivation of this formula:

- approximate $f(x)$ on $[a,b]$ by f evaluated at the quadrature point:

$$f(x),\ x \in [a,b] \approx f\left(\frac{a+b}{2}\right)$$

- Now integrate approximate $f(x)$ to get the weight w_1:

$$\int_a^b f\left(\frac{a+b}{2}\right)dx = (b-a)f\left(\frac{a+b}{2}\right) = w_1 f(q_1)$$

$$\Rightarrow w_1 = (b-a)$$

The simplest closed Newton-Cotes formula is the <u>Trapezoidal Rule</u> which is a two-point rule: To determine the weights, we fit a linear polynomial through those two points:

Linear Lagrange polynomial through $(a, f(a))$ and $(b, f(b))$:

$$L(x) = \sum_{j=0}^{k} y_j \ell_j(x)$$ for $k+1$ data points $\Rightarrow k = 1$

$$\ell_j = \prod_{\substack{0 \le m \le k \\ m \neq j}} \frac{x - x_m}{x_j - x_m}$$

$x_0 = a, \; x_1 = b; \; y_0 = f(a), \; y_1 = f(b)$

$$\ell_0(x) = \frac{x - x_1}{x_0 - x_1} = \frac{x - b}{a - b}$$

$$\ell_1(x) = \frac{x - x_0}{x_1 - x_0} = \frac{x - a}{b - a}$$

$$L(x) = y_0 \ell_0 + y_1 \ell_1 = f(a)\frac{x-b}{a-b} + f(b)\frac{x-a}{b-a}$$

$$= \frac{f(a)(b - x + a - a) + f(b)(x-a)}{b-a}$$

$$= \frac{(f(b) - f(a))(x-a)}{b-a} + f(a) = \frac{x-a}{b-a}(f(b) - f(a)) + f(a)$$

Which we use to approximate $f(x)$ with in the integral to obtain the weights:

$$\int_a^b f(x)dx \approx \int_a^b L(x)dx = \int_a^b \left[\frac{x-a}{b-a}(f(b)-f(a)) + f(a)\right] dx$$

$$= \frac{f(b)-f(a)}{b-a} \left.\frac{(x-a)^2}{2}\right|_a^b + \left. x f(a)\right|_a^b$$

$$= \frac{f(b)-f(a)}{b-a} \frac{(b-a)^2}{2} + f(a)(b-a)$$

$$= \frac{(b-a)}{2}(f(b)+f(a))$$

$$= w_1 f(q_1) + w_2 f(q_2)$$

$$\Rightarrow w_1 = w_2 = \frac{b-a}{2}$$

The next closed rule would use three points; Since it is closed and we use evenly spaced points, we choose the endpoints and the midpoint of the interval.

To obtain the weights, we first again need the Lagrange interpolating polynomial which passes through $\{(a, f(a)), (\frac{a+b}{2}, f(\frac{a+b}{2})), (b, f(b))\}$

$$L(x) = \sum_{j=0}^{k} y_j \, l_j(x) \qquad \text{with } k = 2$$

$$l_j(x) = \prod_{\substack{0 \le m \le k \\ m \ne j}} \frac{x - x_m}{x_j - x_m}$$

$$l_0 = \frac{x - x_1}{x_0 - x_1} \, \frac{x - x_2}{x_0 - x_2}$$

$$l_1 = \frac{x - x_0}{x_1 - x_0} \, \frac{x - x_2}{x_1 - x_2}$$

$$l_2 = \frac{x - x_0}{x_2 - x_0} \, \frac{x - x_1}{x_2 - x_1}$$

$$\Rightarrow L(x) = y_0 \frac{x - x_1}{x_0 - x_1} \, \frac{x - x_2}{x_0 - x_2} + y_1 \frac{x - x_0}{x_1 - x_0} \, \frac{x - x_2}{x_1 - x_2} + $$
$$+ y_2 \frac{x - x_0}{x_2 - x_0} \, \frac{x - x_1}{x_2 - x_1}$$

Since we have equal distances:

Let $x_1 - x_0 = \frac{a+b}{2} - a = x_2 - x_1 = b - \frac{a+b}{2} \equiv h/2$

$x_2 - x_0 = b - a \equiv h$

$$\Rightarrow L(x) = f(a) \frac{x - \frac{a+b}{2}}{-h/2} \, \frac{x - b}{-h} + f\left(\frac{a+b}{2}\right) \frac{x - a}{h/2} \, \frac{x - b}{-h/2} + $$
$$+ f(b) \frac{x - a}{h} \, \frac{x - \frac{a+b}{2}}{h/2}$$

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

$$-2f\left(\frac{a+b}{2}\right)(x-a)(x-b) + \qquad (2)$$

$$+ f(b)(x-a)\left(x - \frac{a+b}{2}\right)\Big] \qquad (3)$$

(1) $$w_1 = \int_a^b \frac{2}{h^2}\left(x - \frac{a+b}{2}(x-b)\right)dx =$$

$$= \frac{2}{h^2}\int_0^b \left[x^2 - x\left(\frac{a}{2} + \frac{3}{2}b\right) + \frac{ab}{2} + \frac{b^2}{2}\right]dx$$

$$= \frac{2}{h^2}\left[\frac{x^3}{3} - \frac{x^2}{2}\left(\frac{a+3b}{2}\right) + x\left(\frac{ab+b^2}{2}\right)\right]dx$$

$$= \frac{2}{h^2}\left[\frac{b^3-a^3}{3} - \frac{(b^2-a^2)}{2}\left(\frac{a+3b}{2}\right) + (b-a)\left(\frac{ab+b^2}{2}\right)\right]$$

$$= \frac{2}{h^2}\,\frac{4b^3-4a^3-3ab^2-9b^3+3a^3+9a^2b+6ab^2+6b^3-6a^2b-6ab^2}{12}$$

$$= \frac{2}{h^2}\,\frac{b^3-3ab^2+3a^2b-a^3}{12}$$

$$= \frac{2}{h^2}\,\frac{(b-a)^3}{12} = \frac{2}{h^2}\,\frac{h^3}{12} = \underline{\underline{\frac{h}{6}}}$$

Similarly, $w_2 = \frac{2h}{3}$, $w_3 = \frac{h}{6}$

This gives us <u>Simpson's Rule</u>:

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

Further rules for more quadrature points can be derived in the same manner both for open and closed families of rules.

Degrees of Precision

For Newton-Cotes rules:

if N even $\rightarrow$ DoP $= N-1$

if N odd $\rightarrow$ DoP $= N$

The degree of precision is the highest order polynomial that the rule integrates exactly.

Computing the Error of an Integration Rule

The error can be computed as

$$E = \left| \int_a^b f(x)\,dx - \sum_i w_i f(q_i) \right|$$

by expanding the approximate expressions using Taylor series and representing the integral in terms of $f(x)$ and its derivatives.

From the fundamental theorem of calculus:

$$\int_a^x f(s)\,ds = F(x) \qquad \text{with } F(a) = 0$$

Now expand:

$$\int_a^{a+h} f(s)\,ds = F(a+h)$$

$$= \Big[F(a) + F'(a)h + F''(a)\frac{h^2}{2} + F'''(a)\frac{h^3}{6} + \mathcal{O}(h$$

$$= \Big[0 + f(a)h + f'(a)\frac{h^2}{2} + f''(a)\frac{h^3}{6} + \mathcal{O}(h^4) \Big]$$

For the midpoint rule, we expand

$$f\left(\frac{a+b}{2}\right) = f\left(a+\frac{h}{2}\right) = f(a) + \frac{h}{2}f'(a) + \frac{h^2}{8}f''(a) + \frac{h^3}{48}f''' + O(h^4)$$

This gives us the error for the midpoint rule:

$$E_{mid} = \left| \int_a^b f(x)dx - \sum_i w_i f(q_i) \right| =$$

$$= \left| \int_a^b f(x)dx - h f\left(\frac{a+b}{2}\right) \right| =$$

$$= \left| \left[f(a)h + f'(a)\frac{h^2}{2} + f''(a)\frac{h^3}{6} + O(h^4) \right] - h\left[f(a) + \frac{h}{2}f'(a) + \frac{h^2}{8}f''(a) + \frac{h^3}{48}f''' + O(h^4) \right] \right|$$

$$= \left| f''(a)\left(\frac{h^3}{6} - \frac{h^3}{8}\right) + O(h^4) \right|$$

$$= \left| -f''(a)\frac{h^3}{24} \right| = |f''(a)|\frac{h^3}{24} = \underline{\underline{O(h^3)}}$$

This can be repeated analoguely for the Trapezoid and Simpson's rule:

$$E_{trap} = O(h^3)$$

$$E_{Simpson} = O(h^5)$$

Gauss-Legendre Quadrature

In Newton-Cotes formulas we fixed the quadrature points as uniformly spaced in the intervals and then used an interpolation polynomial to determine the weights.

If we let the quadrature points and the weights be variable, we could derive a quadrature formula which has a higher degree of precision than Newton-Cotes formulas.

The most commonly used of these rules is Gauss-Legendre quadrature or just Gauss quadrature. One way to derive Gauss quadrature is to determine the quadrature points and weights such that the rule integrates as high a degree polynomial as possible, i.e. we optimize the rule. Hence the Gauss-Legendre rules are not interpolatory like the Newton-Cotes rules. If we use N quadrature points then we can integrate a polynomial of degree 2N-1 exactly with these rules.

The first Gauss rule is the Midpoint rule.
Let's derive the two-point Gauss rule directly:

Let the two quadrature points and weights be

$$(q_i, w_i), \quad i = 1, 2$$

Then a two point quadrature rule for an integral I is of the form

$$I \approx f(q_1) w_1 + f(q_2) w_2$$

We have four variables, so we can satisfy four different conditions. Thus we should be able to choose the points and weights such that a cubic polynomial is integrated exactly.
Then the following relationship must hold:

$$\int_{-1}^{1} (a_0 + a_1 x + a_2 x^2 + a_3 x^3)\, dx = w_1 [a_0 + a_1 q_1 + a_2 q_1^2 + a_3 q_1^3] + w_2 [a_0 + a_1 q_2 + a_2 q_2^2 + a_3 q_2^3]$$

$$= \left[a_0 x + \frac{a_1 x^2}{2} + \frac{a_2 x^3}{3} + \frac{a_3 x^4}{4} \right]_{-1}^{1}$$

$$= 2a_0 + \frac{2}{3} a_2$$

the Gauss quadrature rule is usually given on the interval $[-1, 1]$. How to expand to any interval will be discussed later.

$$\Rightarrow 0 = a_0\left[w_1 + w_2 - 2\right] + a_1\left[w_1 q_1 + w_2 q_2\right] + a_2\left[w_1 q_1^2 + w_2 q_2^2 \pm \frac{2}{3}\right] + a_3\left[w_1 q_1^3 + w_2 q_2^3 \ldots\right.$$

$$\Rightarrow w_1 + w_2 = 2 \qquad (1)$$

$$w_1 q_1 + w_2 q_2 = 0 \qquad (2)$$

$$w_1 q_1^2 + w_2 q_2^2 = 0 \qquad (3)$$

$$w_1 q_1^3 + w_2 q_2^3 = 0 \qquad (4)$$

(1) $w_1 = 2 - w_2$

(2) $(2 - w_2) q_1 + w_2 q_2 = 0$

$$q_1 = \frac{w_2 q_2}{w_2 - 2}$$

(3) $$(2 - w_2)\frac{w_2^2 q_2^2}{(w_2 - 2)^2} + w_2 q_2^2 = \frac{2}{3} = w_2 q_2^2\left(\frac{w_2}{2 - w_2} + 1\right) =$$

$$= w_2 q_2^2 \frac{2}{2 - w_2} = \frac{2}{3} \qquad \Rightarrow w_2 q_2^2 = \frac{2 - w_2}{3}$$

(4) $$w_1 q_1^3 + w_2 q_2^3 = 0 = (2 - w_2)\frac{w_2^3 q^3}{(w_2 - 2)^3} + w_2 q_2^3 =$$

$$= w_2 q_2^3\left(\frac{-w_2^2}{(w_2 - 2)^2} + 1\right) = w_2 q_2^3\left(\frac{-w_2^2 + w_2^2 - 4w_2 + 4}{(w_2 - 2)^2}\right)$$

$$= 4 w_2 q_2^3\left(\frac{1 - w_2}{(w_2 - 2)^2}\right) = 0$$

$$\Rightarrow w_2 = 1, \quad w_1 = 2 - w_2 = 1$$

$$w_2 q_2^2 = \frac{2 - w_2}{3} \quad \Rightarrow \quad q_2 = \sqrt{\frac{2 - w_2}{3 w_2}} = \sqrt{1/3}$$

$$q_1 = \frac{w_2 q_2}{w_2 - 2} = -\sqrt{1/3}$$

This gives us

$$\int_{-1}^{1} f(x)\,dx \approx f(-1/\sqrt{3}) + f(1/\sqrt{3})$$

It turns out that the n quadrature points are given by the roots of the n-th Legendre polynomial:

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n}\left[(x^2-1)^n\right]$$

The weights can again be computed by integration and the constraint that a polynomial of degree $2n-1$ is integrated exactly.

Transforming a Gauss Rule to an arbitrary Interval

Gauss quadrature rules are always given on the interval $[-1, 1]$. If the domain of integration is different, then a change of variables is needed:

$$x \in [-1, 1] \longrightarrow \hat{x} = a + \frac{b-a}{2}(x+1) \in [a, b]$$

With this change of variables, we have

$$\int_a^b f(\hat{x})\, d\hat{x} = \frac{b-a}{2} \int_{-1}^{1} f\left(a + \frac{b-a}{2}(x+1)\right) dx$$

with $d\hat{x} = \frac{b-a}{2} dx$

This effectively maps the quadrature points to $[a, b]$ and we have modified the quadrature weight in the given rule by $\frac{b-a}{2}$.

Explicitly, to approximate the integral, you need to:

$$\int_a^b f(\hat{x})\, d\hat{x} = \sum_i \hat{w}_i f(\hat{q}_i)$$

$$\hat{w}_i = \frac{b-a}{2} w_i \quad , \quad \hat{q}_i = a + \frac{b-a}{2}(q_i + 1)$$