Numerical Integration (Quadrature)

We wish to approximate the value of integrals of the form

$$I(f) \equiv \int_a^b f(x)w(x)dx \qquad (1)$$

where the interval of the integration, $\Omega = [a,b]$, may be bounded or unbounded and w(x) is a nonnegative function on Ω, and is called a weight function. Often w(x) =1. We assume that the integral exists and we seek approximations to I(f) of the form

$$I_n(f) = \sum_{j=1}^{n} a_j f(x_j) \qquad (2)$$

where we assume that the points in the set $\{x_j\}_1^n$, called the nodes are real numbers and that the coefficients or weights $\{a_j\}_1^n$ are real numbers not necessarily non-negative.

Definition. We say that the numerical integration rule (2) is *exact of degree m* or is of degree m if

$$\int_a^b p(x)w(x)dx = \sum_{j=1}^{n} a_j p(x_j) \qquad \forall\ p \in P_m(\Omega).$$

That is, the formula is exact for all polynomials of degree m, and is not exact for at least one polynomial of degree m+1.

The number of degrees of freedom available to us in the construction of rules of the form (2) is at most 2n, namely the choice of the nodes $\{x_j\}_1^n$ and of the coefficients $\{a_j\}_1^n$. Frequently some or all of the nodes are specified in advance, because for example the values of the function f may be known only at certain points. In this case the number of degrees of freedom is reduced to n. We state the following theorem which shows us that the degree of such rules is n-1.

Theorem. Let $\{x_j\}_1^n$ be n given distinct, but otherwise arbitrary nodes. Then there exist coefficients $\{a_j\}_1^n$ such that the integration rule

$$I_n(f) = \sum_{j=1}^{n} a_j f(x_j)$$

is of degree at least n-1.

To find the weights $\{a_j\}_1^n$ we let $p_{n-1}(x)$ be the Lagrange interpolant of f(x) at the nodes $\{x_j\}_1^n$, then

$$p_{n-1}(x) = \sum_{j=1}^{n} f(x_j)l_j(x) \qquad (3)$$

where $l_j(x)$ are the basic Lagrange polynomials. Then $f(x) = p_{n-1}(x) + E(x)$.

$$\int_a^b f(x)w(x)dx = \int_a^b \sum_{j=1}^{n} f(x_j)l_j(x)w(x)dx + \int_a^b E(x)w(x)dx$$

$$= \sum_{j=1}^{n} f(x_j)\int_a^b l_j(x)w(x)dx + \int_a^b E(x)w(x)dx$$

$$= \sum_{j=1}^{n} a_j f(x_j) + \int_a^b E(x)w(x)dx = \sum_{j=1}^{n} a_j p_{n-1}(x_j) + \ldots..$$

where the coefficients are given by

$$a_j = \int_a^b l_j(x)w(x)dx \qquad j = 1,\ldots,n \tag{4}$$

If f(x) is a polynomial of degree <= n-1, the interpolation is exact, i.e. E(x) = 0, and the integration formula is exact if the coefficients are chosen according to (4).

A more direct way to compute the coefficients is to choose the formula so that it integrates exactly the functions (monomials) f(x):

$$f(x) = 1, x, x^2, x^3, \ldots, x^{n-1}.$$

This gives a system of n equations for the n unknowns (degrees of freedom) $\{a_j\}_1^n$, which can be solved to find these weights. Since integration is a *linear operator*, the formula holds for all polynomials of degree <= n-1. That is

$$\int (f(x) + g(x))dx = \int f(x)dx + \int g(x)dx$$

$$\int af(x) = a\int f(x)$$

Newton-Cotes Formulas.

When the nodes are equally spaced, the formulae derived are called the Newton-Cotes formulas. There are various ways to derive these formulas.
The first of the Newton-Cotes formulas, n = 2, based on approximating f(x) on (x_1,x_2) by a straight line, is also called the **Trapezoidal Rule**. It is given by

$$\int_{x_1}^{x_2} f(x)dx = \frac{h}{2}(f_1 + f_2), \ldots\ldots.error = -\frac{1}{12}h^3 f''(\xi), \qquad x_1 < \xi < x_2 \tag{5}$$

and for an interval [a,b] subdivided into subintervals of size h,

$$\int_a^b f(x)dx = \frac{h}{2}(f_1 + 2f_2 + 2f_3 + \ldots + 2f_{n-1} + f_n) \tag{6}$$

Simpson's 1/3 Rule (n = 3).
The second Newton-Cotes formula (n = 3) is for a quadratic integrand over two intervals that are of uniform width, i.e. with 3 nodes. Such intervals are often called panels. It is given by

$$\int_{x1}^{x_3} f(x)dx = \frac{h}{3}(f_1 + 4f_2 + f_3), \ldots error = -\frac{h^5}{90} f^{iv}(\xi), \qquad x_1 < \xi < x_3 \tag{7}$$

If we apply this to a succession of pairs of panels, to evaluate the integral, we get:

$$\int_a^b f(x)dx = \frac{h}{3}(f_1 + 4f_2 + 2f_3 + 4f_4 + \ldots + 2f_{n-2} + 4f_{n-1} + f_n) - \frac{(b-a)}{180}h^4 f^{iv}(\xi), \qquad x_1 < \xi < x_n \tag{8}$$

Simpson's 3/8 Rule (n = 4)

The third Newton-Cotes formula that finds frequent use is obtained by integrating a cubic interpolating polynomial over its range of fit, i.e. 4 nodes. This rule is given by:

$$\int_{x_1}^{x_4} f(x)dx = \frac{3h}{8}(f_1 + 3f_2 + 3f_3 + f_4) - \frac{3h^5}{80} f^{iv}(\xi), x_1 < \xi < x_4 \tag{9}$$

The value of the coefficient 3h/8 gives this rule its common name. To apply this rule to a general interval [a,b], the interval must be divided into a multiple of three panels. I will not write down the general formula for n points here.

Other rules can be derived in a similar way for n = 5, 6,…etc. These are tabulated in mathematical tables.

The global error for each of these formulas is given by:

Trapezoidal Rule:

Error = $-\frac{(b-a)}{12}h^2 f''(\xi), \qquad a \le \xi \le b.$ (10)

Simpson's 1/3 Rule.

Error = $-\frac{(b-a)}{180}h^4 f^{iv}(\xi), \qquad a \le \xi \le b.$ (11)

Simpson's 3/8 Rule.

Error = $-\frac{(b-a)}{80}h^4 f^{iv}(\xi), \qquad a \le \xi \le b$ (12)

The Trapezoidal Rule (n = 2) is of degree 1.
Both the Simpson's 1/3 and 3/8 (n = 3 and 4 respectively) Rules are of degree 3. So there is no advantage gained in using the 3/8 Rule over the 1/3 rule.

In general the **n-node** Newton-Cotes rules are of degree: n-1, if n = even
n, if n = odd.