Gaussian Quadrature (Integration).

Our previous formulas for numerical integration (Newton-Cotes rules) were all based on evenly spaced x-values; this means the x-values were predetermined. With a formula of three terms, then there were three parameters, the coefficients a_i (weights) applied to each of the function values. A formula with 3 parameters corresponds to a polynomial of the 2nd degree, one less than the number of parameters. Gauss (1777-1855) observed that if we remove the requirement that the function be evaluated at predetermined x-values, a 3-term formula will contain 6 parameters (the 3 x-values are now unknowns, and the three weights) and should correspond to a formula of degree 5. Formulas based on this principle are called *Gaussian Quadrature* formulas. They can be applied only when f(x) is explicitly known, so that it can be evaluated at any desired point x.

We shall determine the parameters in the simple case of a two term formula containing four unknown parameters:

$$\int_{-1}^{1} f(x)dx \approx af(x_1) + bf(x_2) \qquad (1)$$

The method is the same as that illustrated in the previous section, by determining unknown parameters. We use a symmetrical interval of integration to simplify the arithmetic, and call our variable t. Our formula is to be exact for any polynomial of degree 3, hence it will hold for f(x) = 1, x, x^2, x^3.

f(x)=1, $$\int_{-1}^{1} 1 = 2 = a + b \qquad (2a)$$

f(x)=x, $$\int_{-1}^{1} x = 0 = ax_1 + bx_2 \qquad (2b)$$

f(x)=x^2, $$\int_{-1}^{1} x^2 = \frac{2}{3} = ax_1^2 + bx_2^2 \qquad (2c)$$

f(x)=x^3, $$\int_{-1}^{1} x^3 = 0 = ax_1^3 + bx_2^3 \qquad (2d)$$

Multiplying the second equation by x_1^2, and subtracting from the third we have

$$0 = 0 + b(x_2^3 - x_2 x_1^2) = bx_2(x_2 - x_1)(x_2 + x_1) \qquad (3)$$

We can satisfy (3) by either b=0, $x_2 = 0$, $x_1 = x_2$, $x_2 = -x_1$.
Only the last possibility is satisfactory, the others being invalid ,or else reduce to a formula with only a single term, so we choose $x_1=-x_2$. We then find that

$$a = b = 1, x_2 = -x_1 = \sqrt{\frac{1}{3}} = 0.5773 .$$ Hence our formula is

$$\int_{-1}^{1} f(x) \approx f(-\sqrt{1/3}) + f(\sqrt{1/3}) \qquad (4)$$

This formula will integrate any cubic polynomial over the interval [-1,1] exactly.

In order to find the nodes $\{x_i\}_1^n$ for Gaussian formulas in general we need to understand the concept or **orthogonal polynomials.** These are polynomials which have special properties.

Orthogonal Polynomials.

The nodes $\{x_i\}_1^n$ are the zeros of the nth degree polynomial $p_n(x)$ having the orthogonality property

$$\int_a^b w(x)\,p_n(x)\,p_m(x)\,dx = 0 \qquad \text{for} \qquad m \neq n$$

$$\int_a^b w(x)\,p_n(x)\,p_n(x)\,dx \neq 0 (> 0)$$

These polynomials depend on the function w(x) and the interval [a,b]. The weighting function therefore influences both the weights $\{a_i\}_1^n$, and the nodes x_i, but does not appear explicitly in the Gaussian formula. Orthogonal polynomials therefore play a central role in Gaussian Integration.

Gauss-Legendre Formulas.

These occur when w(x) = 1, and the interval of integration is [-1,1]. The orthogonal polynomials are then the Legendre polynomials. These are given by

$$L_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n \qquad \text{with} \qquad L_0(x) = 1. \tag{5}$$

The $\{x_i\}_1^n$ are the zeros of these polynomials. Tables of $\{x_i\}_1^n$ and $\{a_i\}_1^n$ are available to be substituted into the Gauss-Legendre formula:

$$\int_{-1}^{1} f(x) \approx \sum_{i=1}^{n} a_i f(x_i)$$

Fortunately we do not need to use formula (5) to calculate these polynomials, as there exists a recurrence formula to compute them. The formula is given by:

$$(n+1)L_{n+1}(x) - (2n+1)xL_n(x) + nL_{n-1}(x) = 0 \tag{6}$$

with $L_0(x) = 1, L_1(x) = x.$ Then

$$L_2(x) = (3xL_1(x) - L_0(x))/2 = \frac{3}{2}x^2 - \frac{1}{2} \tag{7}$$

The roots of $L_2(x)$ are clearly $\pm\sqrt{\frac{1}{3}}$, i.e. the values for the 2-term formula already obtained earlier. By using the recursion, we find

$$L_3(x) = \frac{5}{2}x^3 - \frac{3}{2}x$$

$$L_4(x) = \frac{35x^4 - 30x^2 + 3}{8}, \quad \text{etc.}$$

The roots of $L_3(x)$ are the nodes for a 3-term formula. Clearly these roots are: $x_1 = 0, x_2 = \sqrt{3/5}, x_3 = -\sqrt{3/5}$.
The weights for the 3-term formula are 8/9, 5/9, 5/9 respectively.
Hence the complete formula is:

$$\int_{-1}^{1} f(x) \approx \frac{5}{9} f(-\sqrt{3/5}) + \frac{8}{9} f(0) + \frac{5}{9} f(\sqrt{3/5}) \qquad (8)$$

Gauss-Chebyshev Formulas.
These formulas take the form

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} dx \approx \sum_{i=1}^{n} \frac{\pi}{n} f(x_i) \qquad (10)$$

Here the weight function $w(x) = 1/\sqrt{1-x^2}$ and the nodes are the roots of the nth Chebyshev polynomial $T_n(x)$:

$T_n(x) = \cos(n \cos^{-1}(x)) = \cos(n\theta), x = \cos(\theta)$, i.e.
$\cos(n\theta) = T_n(\cos\theta)$, i.e., a polynomial in $\cos\theta$.

A recursion also exists for the Chebyshev polynomials. It is

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x) \qquad T_0(x) = 1, = T_1(x) = x \qquad (11)$$

From this we find that

$$T_2(x) = 2x^2 - 1, T_3(x) = 4x^3 - 3x, etc$$

These polynomials are orthogonal w.r.t. the weight function w(x).

Exercise: Find all the roots of $T_2(x), T_3(x)$. Note that these are the nodes for the Gauss-Chebyshev rules with n=2 and 3 respectively. Verify that these roots are given by $\cos(\theta)$, where

$$\theta = (2k+1)\pi / 2n, k = 0,1,\ldots,n-1.$$

Other orthogonal polynomials exist for other weight functions w(x) and intervals of integration. For example:

Interval	w(x)	Polynomials
[0,∞]	e^{-x}	Laguerre polynomials

For more info on Gauss see:
http://www-groups.dcs.st-and.ac.uk/~history/Mathematicians/Gauss.html