Numerical Integration.

Newton-Cotes formulae for $n=2$

We are trying to compute $\int_a^b f(x)\,dx$

We will interpolate a quadratic polynomial, using three (equispaced) points.

Say $c = \frac{a+b}{2}$

our points are $(a, f(a))$, $(c, f(c))$, $(b, f(b))$

The polynomial is given by

$$p_2(x) = f(a)\frac{(x-c)(x-b)}{(a-c)(a-b)} + f(c)\frac{(x-a)(x-b)}{(c-a)(c-b)}$$

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

We can then integrate $p_2(x)$ over $[a,b]$ to get the formula.

This can get messy!

We know that the integral has the form:

$$\int_a^b f(x)\,dx = A_1 f(a) + A_2 f(c) + A_3 f(b)$$

We also know that this formula is exact for all polynomials of degree 2 or less. So we can test with polynomials to determine A_1, A_2 and A_3

$$\int_a^b 1\,dx = b-a = (A_1 + A_2 + A_3) \quad \text{— } (1)$$

$$\int_a^b x\,dx = \frac{b^2-a^2}{2} = A_1 a + A_2 \frac{(a+b)}{2} + A_3 b \quad \text{— } (2)$$

$$\int_a^b x^2\,dx = \frac{b^3-a^3}{3} = A_1 a^2 + A_2\left(\frac{(a+b)}{2}\right)^2 + A_3 b^2 \quad \text{— } (3)$$

Solving (1), (2) & (3), we get

$$A_1 = A_3 = \frac{b-a}{6}, \quad A_2 = \frac{4(b-a)}{6}$$

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

It turns out this formula is also exact for polynomials of degree 3

$$\int_a^b x^3\,dx = \frac{1}{4}(b^4 - a^4) = \frac{1}{4}(b-a)(b^3 + ab^2 + a^2b + a^3)$$

and

$$\frac{b-a}{6}\left(a^3 + 4\left(\left(\frac{a+b}{2}\right)\right)^3 + b^3\right) = \frac{1}{4}(b-a)(b^3 + ab^2 + a^2b + b^3)$$

Error analysis:

$$f\left(\frac{a+b}{2}\right) = f(a) + \frac{b-a}{2} f'(a) + \frac{(b-a)^2}{8} f''(a) + \frac{(b-a)^3}{48} f'''(a)$$
$$+ \frac{(b-a)^4}{384} f''''(a) + \cdots$$

$$f(b) = f(a) + (b-a) f'(a) + \frac{(b-a)^2}{2} f''(a) + \frac{(b-a)^3}{6} f'''(a)$$
$$+ \frac{(b-a)^4}{24} f''''(a) + \cdots$$

$$\therefore \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] = (b-a) f(a) + \frac{(b-a)^2}{2} f''(a)$$
$$+ \frac{(b-a)^3}{6} f'''(a) + \frac{(b-a)^4}{24} f'''(a)$$
$$+ \frac{5(b-a)^5}{576} f''''(a)$$

Define $F(x) \equiv \int_a^x f(t)\,dt$

we know that $F'(x) = f(x)$

$$\int_a^b f(t)\,dt = F(b)$$

Expanding $F(b)$, we have (since $F(a)=0$)

$$F(b) = (b-a)\,F'(a) + \frac{(b-a)^2}{2} F''(a) + \cdots$$

$$= (b-a)\,f(a) + \frac{(b-a)^2}{2} f'(a) + \frac{(b-a)^3}{6} f''(a) + \frac{(b-a)^4}{24} f'''(a) + \frac{(b-a)^5}{120} f''''(a)$$

Comparing these two equations, we have the error as

$$\frac{1}{2880}(b-a)^5 f''''(a) + O((b-a)^6)$$

$$= \frac{1}{2880}(b-a)^5 f''''(\xi) \qquad \xi \in [a,b]$$

Ex

Using Simpson's rule, approximate

$$\int_0^2 e^{-x^2}\,dx$$

$$= \frac{1}{3}\left(e^0 + 4e^{-1} + e^{-4}\right) \simeq 0.8299.$$

The error is $\dfrac{2^5}{2880} f''''(\xi) \quad \xi \in [0,2]$

Max $f''''(\xi) \leq 12$

$$\therefore \text{error} \leq \frac{2^5 \times 12}{2880} \approx 0.1333$$

Piecewise Polynomial Interpolation.

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

for degree 1 interpolant, we get

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} (x - x_i) \cdot \frac{f(x_i) + f(x_{i+1})}{2}$$

$$\approx \frac{h}{2}\left(f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n \right).$$

for degree 2 interpolant, we get

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

$$= \frac{h}{6}\left[f_0 + 4f_{\frac{1}{2}} + 2f_1 + \cancel{4f}_3 + \cdots + 4f_{n-\frac{1}{2}} + f_n \right]$$

Gauss Quadrature.

Suppose
$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} A_i f(x_i)$$

Now we want to choose both A_i & x_i

for $n=0$
$$\int_a^b f(x)\,dx \approx A f(x_0)$$

for higher order polynomials
$$\int_a^b 1\,dx = b-a = A_0$$

$$\int_a^b x\,dx = \frac{b^2-a^2}{2} = A_0 x_0 = (b-a)\,x_0$$

$$\text{or} \quad x_0 = \frac{b+a}{2}.$$

Choosing A_0 & x_0 in this manner is exact for degree $= 0, 1$

This does not work for degree 2.

Now try $n = 1$

$$\therefore \int_a^b f(x)\,dx \approx A_0 f(x_0) + A_1 f(x_1)$$

$$\int_a^b 1\,dx = b - a = A_0 + A_1$$

$$\int_a^b x\,dx = \frac{b^2 - a^2}{2} \Rightarrow A_0 x_0 + A_1 x_1 = \frac{b^2 - a^2}{2}$$

$$\int_a^b x^2\,dx = \frac{b^3 - a^3}{3} \Rightarrow A_0 x_0^2 + A_1 x_1^2 = \frac{b^3 - a^3}{3}$$

$$\vdots$$

These equations become hard to solve!

Orthogonal Polynomials.

Two polynomials p & q are orthogonal on $[a, b]$

if $$\langle p, q \rangle = \int_a^b \cancel{x}\, p(x)\, q(x)\, dx = 0$$

They are orthonormal if $\langle p, p \rangle = \langle q, q \rangle = 1$

Starting from a linearly independent set

$1, x, x^2 \ldots$, we can construct an orthonormal

basis using Gram Schmidt orthogonalization.

Set $$q_0 = \frac{1}{\left(\int_a^b 1^2\, dx \right)^{1/2}} = \frac{1}{\sqrt{b-a}}$$

For $j = 1, 2, 3 \ldots$

$$\tilde{q}_j = x\, q_{j-1}(x) - \sum_{i=0}^{j-1} \langle x\, q_{j-1}(x), q_i(x) \rangle\, q_i(x)$$

$$q_j = \frac{\tilde{q}_j(x)}{\| \tilde{q}_j(x) \|}$$

q_{j-1} is orthogonal to all poly. of degree $j-1$ or less

$$\therefore \tilde{q}_j(x) = x\, q_{j-1}(x) - \langle x\, q_{j-1}(x), q_{j-1}(x) \rangle\, q_{j-1}(x)$$
$$- \langle x\, q_{j-1}(x), q_{j-2}(x) \rangle\, q_{j-2}(x)$$

It then follows that

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} A_i f(x_i)$$

$$A_i = \int_a^b \ell_i(x)\,dx \qquad \ell_i(x) \equiv \prod_{\substack{i=0 \\ j\neq i}}^{n} \frac{x-x_j}{x_i-x_j}$$

$x_0, x_1 \dots x_n$ are zeros of $q_{n+1}(x)$.

This formula is exact for polynomials of degree $2n+1$ or less.

Proof. Say f is a polynomial of degree $2n+1$ or less

divide f by q_{n+1} to write

$$f = q_{n+1} p_n + r_n.$$ (p_n & r_n are degree n polynomials).

$$\int_a^b f(x)\,dx = \underbrace{\int_a^b q_{n+1}(x)\,p_n(x)\,dx}_{0} + \int_a^b r_n(x)\,dx$$

0 since q_{n+1} is orthogonal to polynomials of degree n or less

$$\therefore \int_a^b f(x)\,dx = \int_a^b r_n(x)\,dx.$$ (This is exact).

Example.

Find the Gauss Quadrature formula for

$$\int_{-1}^{1} f(x)\,dx \approx A_0 f(x_0) + A_1 f(x_1)$$

Construct $\tilde{q}_0, \tilde{q}_1, \tilde{q}_2$ on $[-1,1]$.

The roots of q_2 are $x_0\ x_1$

$$\tilde{q}_0 = 1.$$

$$\tilde{q}_1 = x - \frac{\langle x, 1\rangle}{\langle 1, 1\rangle}\cdot 1 = x - \frac{\int_{-1}^{1} x\,dx}{\int_{-1}^{1} 1\,dx}\cdot 1 = x$$

$$\tilde{q}_2 = x^2 - \frac{\langle x^2, 1\rangle}{\langle 1, 1\rangle}\cdot 1 - \frac{\langle x^2, x\rangle}{\langle x, x\rangle}\cdot x$$

$$= x^2 - \frac{\int_{-1}^{1} x^2\,dx}{\int_{-1}^{1} 1\,dx} - \frac{\int_{-1}^{1} x^3\,dx}{\int_{-1}^{1} x^2\,dx}\cdot x$$

$$= x^2 - \frac{1}{3}$$

Roots are $x = \pm \frac{1}{\sqrt{3}}$.

We have:

$$\int_{-1}^{1} f(x)\,dx = A_0 f\left(-\frac{1}{\sqrt{3}}\right) + A_1 f\left(\frac{1}{\sqrt{3}}\right).$$

$$\int_{-1}^{1} 1\,dx = 2 = A_0 + A_1 \qquad \int_{-1}^{1} x\,dx = 0 = A_0\left(-\frac{1}{\sqrt{3}}\right) + A_1\left(\frac{1}{\sqrt{3}}\right)$$

$$\therefore \quad A_0 = A_1 = 1$$

$$\therefore \quad \int_{-1}^{1} f(x)\,dx = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right).$$

This is also exact for x^2 and x^3.

However, it is not exact for x^4