Elements of Numerical Integration

We often need to evaluate the definite Integral of a function that has no explicit antiderivative (or its hard to find). The basic method to find $\int_a^b f(x)\,dx$ is called numerical quadrature and uses a sum of the form $\sum_{i=0}^{n} a_i f(x_i)$

We're going to use interpolating polynomials to get methods to approx integrals. If $P_n(x) = \sum_{i=0}^{n} f(x_i) L_i(x)$ is the Lagrange Interpolating polynomial, then

$$\int_a^b f(x)\,dx = \int_a^b \underbrace{\sum_{i=0}^{n} f(x_i) L_i(x)}_{P_n(x)}\,dx + \int_a^b \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^{n} (x-x_i)\,dx$$

$$= \sum_{i=0}^{n} f(x_i) \int_a^b L_i(x) \quad + \quad \frac{1}{\quad} \int^b f^{(n+1)}(\xi) \prod^{n} (x-x_i)$$

$$\sum_{i=0} f(x_i) \underbrace{\int_a L_i(x)}_{a_i} \qquad \qquad (n+1)! \int_a \qquad \qquad i=0$$

Simple case: $n=1$, Let $x_0=a$, $x_1=b$. Then

$$P_1(x) = \frac{x-x_1}{x_0-x_1} f(x_0) + \frac{x-x_0}{x_1-x_0} f(x_1)$$

Then

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_1} \frac{x-x_1}{x_0-x_1} f(x_0) + \frac{x-x_0}{x_1-x_0} f(x_1) \; dx + \frac{1}{2}\int_{x_0}^{x_1} f''(\xi)(x-x_0)(x-x_1)\,dx$$

$$= \frac{f(x_0)}{x_0-x_1}\left[\frac{(x-x_1)^2}{2}\right]_{x_0}^{x_1} + \frac{f(x_1)}{x_1-x_0}\left[\frac{(x-x_0)^2}{2}\right]_{x_0}^{x_1} + \text{error}$$

$$= -\frac{1}{2} f(x_0)\underbrace{(x_0-x_1)}_{-h} + \frac{1}{2} f(x_1)\underbrace{(x_1-x_0)}_{h} + \text{error}$$

If $h = x_1 - x_0$, then

$$= \frac{1}{2} h\left(f(x_0)+f(x_1)\right) + \text{error}$$

Because $(x-x_0)(x-x_1)$ does not change sign on $[x_0, x_1]$, then we can use the weighted MVT for integrals can be applied to the error term, and

$$\int_{x_0}^{x_1} f''(\xi(x))\,(x-x_0)(x-x_1) = f''(\xi)\int_{x_0}^{x_1}(x-x_0)(x-x_1)\,dx = f''(\xi)\int_{x_0}^{x_1} x^2-(x_1+x_0)x+x_0x_1$$

$$= \left[\frac{x^3}{3} - \frac{(x_1+x_0)x^2}{2} + x_0x_1x\right]_{x_0}^{x_1} f''(\xi)$$

$$= \left[\frac{x_1^3}{3} - \frac{(x_1+x_0)x_1^2}{2} + x_0x_1^2 - \frac{x_0^3}{3} + \frac{(x_1+x_0)x_0^2}{2} - x_0^2x_1\right] f''(\xi)$$

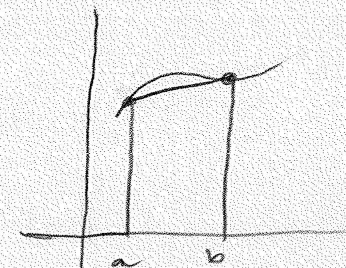
$$= \frac{1}{6}\left[2x_1^3 - 3(x_1+x_0)x_1^2 + 6x_0x_1^2 - 2x_0^3 + 3(x_1+x_0)x_0^2 - 6x_0^2x_1\right] f''(\xi)$$

$$= \frac{1}{6}\left[2x_1^3 - 3x_1^3 - \cancel{3x_0x_1^2} + \cancel{6x_0x_1^2} - \cancel{2x_0^3} + \cancel{3x_0^2x_1} + \cancel{3x_0^3} - \cancel{6x_0^2x_1}\right] f''(\xi)$$

$$\ldots 3] f''(\xi) = \frac{1}{\ }(x_0-x_1)^3 f''(\xi)$$

$$= \frac{1}{6}\left[x_0^3 - 3x_0^2 x_1 + 3x_0 x_1^2 - x_1^3\right] f''(\xi) = \frac{1}{6}(x_0 - x_1)^3 f''(\xi)$$

$$= -\frac{h^2}{6} f''(\xi)$$



Trapezoid Rule

$$\int_a^b f(x)dx = \frac{h}{2}\left[f(x_0) + f(x_1)\right] - \frac{h^2}{12} f''(\xi)$$

Note: Since $f''(\xi)$ is in the error term, trap rule gives exact answers for functions where $f^{(2)}(x) = 0$ (Linear & const functions)

Let $n=2$ $\Rightarrow$ derives Simpson's Rule. Using Lagrange Rule doesn't lead to the best error term. Possible. To do that, we use Taylor Series expanded about $x = x_1$

$$x_0 \quad x_1 \quad x_2$$

$$f(x) = f(x_1) + f'(x_1)(x-x_1) + \frac{f''(x_1)}{2}(x-x_1)^2 + \frac{f'''(x_1)}{6}(x-x_1)^3 + \frac{f^{(4)}(\xi)(x-x_1)^4}{24}$$

Integrating yields

$$\int_{x_0}^{x_2} f(x)\,dx = \int_{x_0}^{x_2} f(x_1)\,dx + \int_{x_0}^{x_2} f'(x_1)(x-x_1)\,dx + \int_{x_0}^{x_2} \frac{f''(x_1)(x-x_1)^2}{2} + \int_{x_0}^{x_2} \frac{f^{(3)}(x-x_1)^3}{6} + \int_{x_0}^{x_2} \frac{f^{(4)}(\xi)(x-x_1)^4}{24}$$

$$= f(x_1)\underbrace{(x_2-x_0)}_{2h} + f'(x_1)\left[\frac{(x-x_1)^2}{2}\right]_{x_0}^{x_2} + f''(x_1)\left[\frac{(x-x_1)^3}{6}\right]_{x_0}^{x_2} + f^{(3)}(x_1)\left[\frac{(x-x_1)^4}{24}\right]_{x_0}^{x_2} + \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi)(x-x_1)^4$$

$$= 2hf(x_1) + f'(x_1)\underbrace{\left[\frac{(x_2-x_1)^2}{2} - \frac{(x_0-x_1)^2}{2}\right]}_{0} + f''(x_1)\left[\frac{(\overbrace{x_2-x_1}^{h})^3}{6} - \frac{(\overbrace{x_0-x_1}^{-h})^3}{6}\right] + 0 + \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi)(x-x_1)^4\,dx$$

$$= 2hf(x_1) + f''(x_1)\frac{h^3}{3} + \frac{1}{24}f^{(4)}(\xi)\int_{x_0}^{x_2}(x-x_1)^4\,dx$$

$$= 2hf(x_1) + \frac{h^3}{3}f''(x_1) + \underbrace{\frac{1}{24}f^{(4)}(\xi)\underbrace{\left[\frac{(x-x_1)^5}{5}\right]_{x_0}^{x_2}}_{\frac{2h^5}{5}}}_{\frac{h^5}{60}}$$

Let's approx $f''(x_1)$ by using

$$f''(x_1) = \frac{1}{h^2}\left[f(\underbrace{x_1 - h}_{x_0}) - 2f(x_1) + f(\underbrace{x_1 + h}_{x_2})\right] - \frac{h^2}{12} f^4(\xi_2)$$

$$= 2hf(x_1) + \frac{h^3}{3}\left[\frac{1}{h^2}[f(x_0) - 2f(x_1) + f(x_2)] - \frac{h^2}{12} f^{(4)}(\xi_2)\right] + \frac{h^5}{60} f^{(4)}(\xi)$$

$$= 2hf(x_1) + \frac{h}{3} f(x_0) - \frac{2hf(x_1)}{3} + \frac{h^3}{3} f(x_2) - \frac{h^5}{36} f^{(4)}(\xi_2) + \frac{h^5}{60} f^{(4)}(\xi)$$

$$= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{36} f^{(4)}(\xi_2) + \frac{h^5}{60} f^{(4)}(\xi)$$

It can be show that a common value for ξ_2 & ξ can be used.

$$= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \left[\frac{h^5}{36} + \frac{h^5}{60}\right] f^{(4)}(\xi)$$

$$\boxed{= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi)}$$

Do an example

Note: It is exact for all polys of degree $\underline{\underline{3}}$ or less!!

DEF Degree of accuracy (or precision), of a quadrature formula is the positive int, n, such that Error term of $P_k = 0$ $(E(P_k)=0)$ for all poly P_k of degree less than or equal to n, but for which $E(P_{n+1}) \neq 0$ for poly of degree $n+1$.

Trap: degree of Precision one

Simpsons: degree of Precision two.

Trap & Simpsons are examples of a class of methods known as Newton-Cotes formulas. There are two types Closed Newton-cotes formulas and Open Newton-cotes

For closed, we divide the interval $[a,b]$ equally

$$a = x_0 < x_1 < x_2 \ldots < x_{n-1} < x_n = b \quad , \text{ where } \quad x_i = x_0 + ih$$
$$h = \frac{(b-a)}{n}$$

The formula is

$$\int_a^b f(x)\,dx \;\hat{=}\; \sum_{i=0}^{n} a_i f(x_i)\text{, where}$$

$$a_i = \int_{x_0}^{x_n} L_i(x)\,dx = \int_{x_0}^{x_n} \prod_{\substack{j=0\\ j\neq i}}^{n} \frac{x-x_j}{x_i-x_j}\,dx$$

Error Analysis: closed Newton-cotes formula, with $x_0=a, x_n=b, \; x_i = x_0 + ih, \; h=\frac{b-a}{n}$. There exists $\xi \in [a,b]$

If n is even, and $f \in C^{n+2}[a,b]$, then

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2(t-1)\cdots(t-n)\,dt$$

If n is odd, and $f \in C^{n+1}[a,b]$, then

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1)\cdots(t-n)\,dt.$$

Note you get free degree of precision for even degrees!

Some examples of Closed Newton-Cotes

$n=1$: Trapezoid Rule

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}[f(x_0)+f(x_1)] - \frac{h^3}{12} f''(\xi), \text{ where } x_0 < \xi < x_1$$

$n=2$: Simpson's Rule

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}[f(x_0)+4f(x_1)+f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi), \text{ where } x_0 < \xi < x_2$$

$n=3$: Simpson's three-eighths Rule

$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3h}{8}[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)] - \frac{3h^5}{80} f^{(4)}(\xi), \ x_0 < \xi < x_3$$

$n=4$: (No name)

$x_0 < \xi < x_4$

$$\int^{x_4} f(x)\,dx = \frac{2h}{45}[7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)] - \frac{8h^7}{945} f^{(6)}(\xi)$$

x_0

Open Newton Cotes (use open intervals)

Idea: (don't use left & right endpts for evaluation)

$$a = x_{-1} < x_0 < x_1 < \cdots < x_n < x_{n+1} = b$$

This means that

$$x_0 = a + h, \quad x_n = b - h, \quad x_i = x_0 + ih \; (i = -1, \cdots, n+1), \quad h = \frac{b-a}{n+2})$$

The function $f(x)$ is never evaluated at x_{-1} or x_{n+1}. This is what makes it "open". The formulas are the same

$$\int_a^b f(x)dx = \int_{x_{-1}}^{x_{n+1}} f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i), \text{ where } a_i = \int_a^b L_i(x)\,dx$$

Error Analysis for Open Newton-Cotes

$x_{-1} = a, \quad x_0 = a+h, \quad x_i = x_0 + ih, \quad x_{n+1} = b, \quad h = \dfrac{b-a}{n+2}$

There exists $\xi \in (a,b)$ such that

If n is even and $f \in C^{n+2}[a,b]$, then

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_{-1}^{n+1} t^2 (t-1)\cdots(t-n)\,dt$$

If n is odd and $f \in C^{(n+1)}[a,b]$, then

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_{-1}^{n+1} t(t-1)\cdots(t-n)\,dt$$

Common Open Newton-Cotes

$n=0$: Midpoint Rule

$$\int^{x_1} f(x)\,dx = 2hf(x_0) + \frac{h^3}{\ } f''(\xi), \quad x_{-1} < \xi < x_1$$

n = 1: (No-name)

$$\int_{x_{-1}}^{x_2} f(x)\,dx = \frac{3h}{2}\left[f(x_0) + f(x_1)\right] + \frac{3h^3}{4} f''(\xi), \quad x_{-1} < \xi < x_2$$

n = 2: (No-name)

$$\int_{x_{-1}}^{x_3} f(x)\,dx = \frac{4h}{3}\left[2f(x_0) - f(x_1) + 2f(x_2)\right] + \frac{14h^5}{45} f^{(4)}(\xi), \quad x_{-1} < \xi < x_3$$

n = 3: (No-name)

$$\int_{x_{-1}}^{x_4} f(x)\,dx = \frac{5h}{24}\left[11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)\right] + \frac{95h^5}{144} f^{(4)}(\xi)$$

$$x_{-1} < \xi < x_4$$