Elements of numerical integration

The need often arises for evaluating the definite integral of a function that has no explicit antiderivative or whose antiderivative is not easy to obtain. The basic method involved in approximation $\int_a^b f(x)\,dx$ is called Numerical quadrature. It uses a sum $\sum_{i=0}^{n} a_i f(x_i)$ to approximate $\int_a^b f(x)\,dx$.

The methods of quadrature are based on the interpolation polynomials. The basic idea is to select a set of distinct nodes $\{x_0, \ldots, x_n\}$, from the interval $[a,b]$. Then integrate the Lagrange interpolating polynomial

$$P_n(x) = \sum_{i=0}^{n} f(x_i)\, L_i(x)$$

and its trunction error term over $[a,b]$ to obtain

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

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

Where $\xi(x)$ is in $[a,b]$ for each x and

$$a_i = \int_a^b L_i(x)\,dx \qquad \text{for each } i = 0, 1, \dots, n$$

The quadrature formula is, therefore

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

With error given by

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

The Trapezoidal rule

To derive the Trapezoidal rule for approximating $\int_a^b f(x)\,dx$, let $x_0 = a$, $x_1 = b$, $h = b-a$ and use the linear Lagrange Polynomial:

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

Then

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_1} \left[\frac{(x-x_1)}{(x_0-x_1)} f(x_0) + \frac{(x-x_0)}{(x_1-x_0)} f(x_1) \right] dx$$

$$+ \frac{1}{2} \int_{x_0}^{x_1} f''(\xi(x))(x-x_0)(x-x_1)\,dx \quad \text{—— (1)}$$

The product $(x-x_0)(x-x_1)$ does not change sign on $[x_0, x_1]$, so the Weighted Mean Value Theorem for integrals can be applied to the error term to give, for some ξ in (x_0, x_1)

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

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

Consequently eq(1) implies that

$$\int_a^b f(x)\,dx = \left[\frac{(x-x_1)^2}{2(x_0-x_1)} f(x_0) + \frac{(x-x_0)^2}{2(x_1-x_0)} f(x_1)\right]_{x_0}^{x_1} - \frac{h^3}{12} f''(\xi)$$

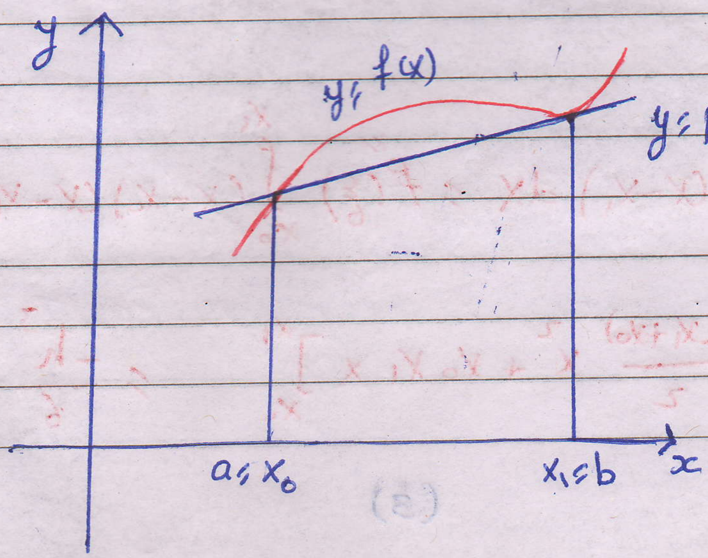
$$= \frac{(x_1-x_0)}{2}\left[f(x_0)+f(x_1)\right] - \frac{h^3}{12} f''(\xi)$$

Using the notation $h = x_1 - x_0$, gives the following r

Trapezoidal Rule:

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(x_0)+f(x_1)\right] - \frac{h^3}{12} f''(\xi)$$

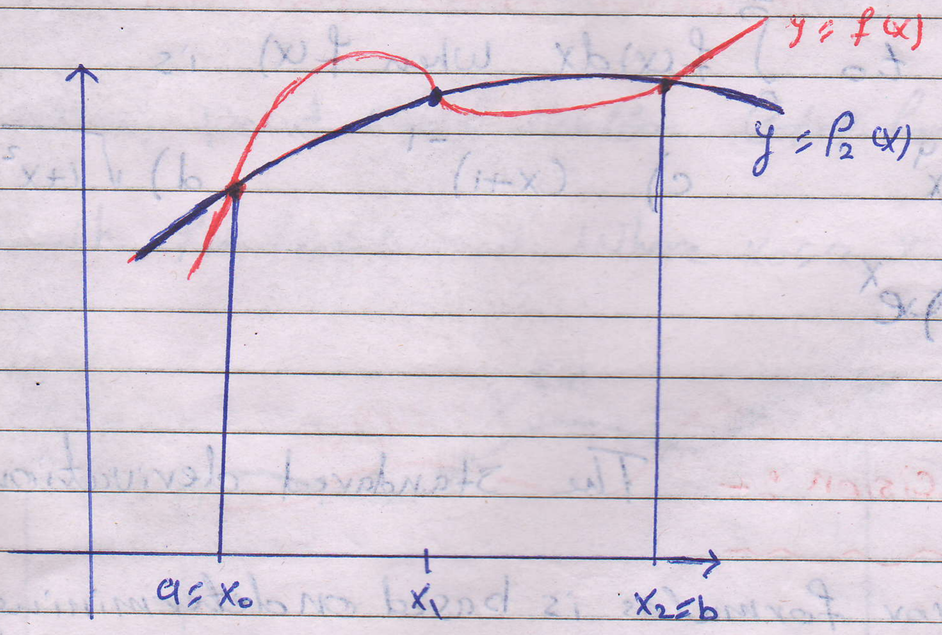
This is called the Trapezoidal rule because whe f is a function with positive values, $\int_a^b f(x)dx$ is approximated by the area under or in a trapezoid as shown



The error term for the Trapezoidal rule involves f'', so the rule gives the exact result when applied to any function whose second derivative is identically zero, that is any polynomial of degree one or less

Simpson's Rule :-

Simpson's rule results from integrating over $[a,b]$ the second Lagrange Polynomial with equally spaced nodes $x_0 = a$, $x_2 = b$, and $x_1 = a+h$, where $h = \frac{b-a}{2}$



There fore

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx + \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\xi(x))\,dx$$

Simpson's Rule:

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

Ex:- Compare the Trapezoidal rule and Simpson's rule approximations to $\int_0^2 f(x)\,dx$ when $f(x)$ is

a) x^2 b) x^4 c) $(x+1)^{-1}$ d) $\sqrt{1+x^2}$

e) $\sin x$ f) e^x

Measuring Precision:- The standard derivation of quadrature error formulas is based on determining class of polynomials for which these formulas produce exact results

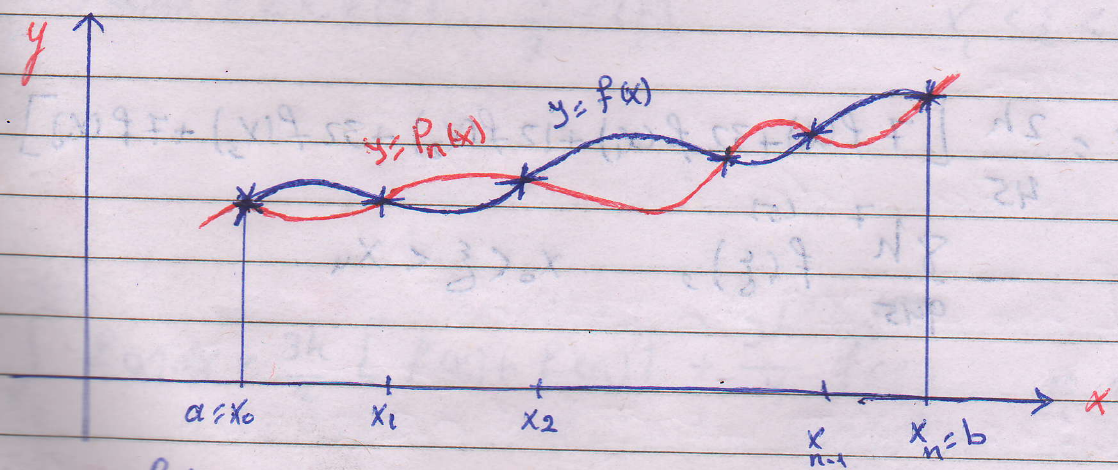
Definition:- The degree of accuracy, or precision of quadrature formula is the largest positive integer n such the formula is exact for x^k for each $k=0,1,\dots,$

* The degree of precision of a quadrature formula is n if and if the error is zero for all polynomials of degree $k=0,1,$ but is not zero for some polynomial of degree $n+1$.

Trapezoidal and Simpson's rules are examples of a class Methods known as Newton-Cotes formulas

- Closed Newton-Cotes formulas

The $(n+1)$-point closed Newton-Cotes formula uses nod $x_i = x_0 + ih$, for $i=0,1,\dots,n$ Where $x_0 = a$, $x_n = b$, $h = \frac{b-a}{n}$



Some of the common closed Newton-Cotes formulas with error terms are listed Note that in each case the unknown valu ξ lies in (a,b)

n = 1 : Trapezoidal rule

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

n = 2 : Simpson's rule

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

n = 3 : Simpson's rule Three - Eights

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

$$x_0<\xi<x_3$$

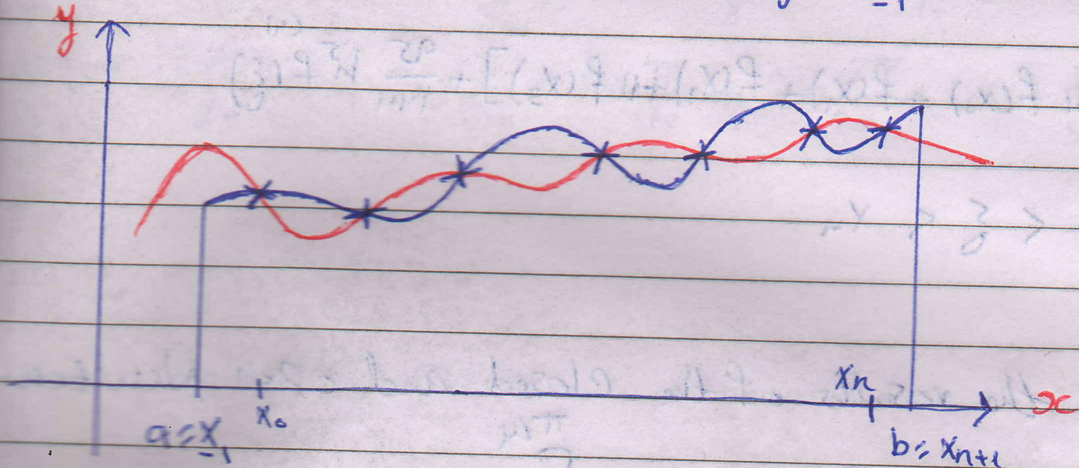
n = 4

$$\int_{x_0}^{x_4} f(x)\,dx = \frac{2h}{45}\left[7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)\right]$$

$$-\frac{8h^7}{945} f^{(5)}(\xi), \quad x_0<\xi<x_4$$

Open Newton-Cotes formulas

The open Newton-Cotes formulas do not include the endpoints of $[a,b]$. They use the nodes $x_i = x_0 + ih$, $\forall i = 0, 1, \ldots, n$ where $h = \frac{b-a}{n+2}$ and $x_0 = a+h$. This implies that $x_n = b-h$, So we label the endpoints by ~~setn~~ setting $x_{-1} = a$ and $x_{n+1} = b$



$n=0$: Midpoint rule

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

$n=1$

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

$n=2$:

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

$$x_{-1} < \xi < x_3$$

$n=3$

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

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

Ex:- Compaire the results of the closed and open Newt Cotes formulas to approximate $\int_0^{\pi/4} \sin x\, dx$

Sol $\int_0^{\frac{\pi}{4}} \sin x\, d = -\cos x \Big|_0^{\frac{\pi}{4}} \Rightarrow -\left(\cos\frac{\pi}{4} - \cos 0\right) = 1 - \frac{\sqrt{2}}{2}$

≈ 0.29289322

for closed Newton-Cotes formula

$n=1$; $\frac{\pi/4}{2}\left[\sin 0 + \sin\frac{\pi}{4}\right] \approx 0.27768018$

$n=2$; $\frac{\pi/8}{3}\left[\sin 0 + 4\sin\frac{\pi}{8} + \sin\frac{\pi}{4}\right] \approx 0.29293264$

$n=3$; $\frac{3\pi/12}{8}\left[\sin 0 + 3\sin\frac{\pi}{12} + 3\sin\frac{\pi}{6} + \sin\frac{\pi}{4}\right] \approx 0.29291070$

$n=4$; $\frac{2\pi/16}{45}\left[7\sin 0 + 32\sin\frac{\pi}{16} + 12\sin\frac{\pi}{8} + 32\sin\frac{3\pi}{16} + 7\sin\right.$

≈ 0.29289318

for ~~closed~~ open Newton - Cotes formulas

$n=0: 2\pi/8 \left[\sin\frac{\pi}{8}\right] \approx 0.30055887$

$n=1: \frac{3\pi/12}{2}\left[\sin\frac{\pi}{12}+\sin\frac{\pi}{6}\right] \approx 0.29798754$

$n=2: \frac{4\pi/16}{3}\left[2\sin\frac{\pi}{16}-\sin\frac{\pi}{8}+2\sin\frac{3\pi}{16}\right] \approx 0.29285866$

$n=3: \frac{5\pi/20}{24}\left[11\sin\frac{\pi}{20}+\sin\frac{\pi}{10}+\sin\frac{3\pi}{20}+11\sin\frac{\pi}{5}\right] \approx 0.292869$