4.3 Elements of Numerical Integration

1) General Statement of the problem

We need to compute $\int_a^b f(x)\,dx$ approximately

Def: The basic method involved in approximating

$$\int_a^b f(x)\,dx$$

is called <u>numerical quadrature</u>

Typically, we divide the interval into subintervals

$$a_0 = x_0 < x_1 < \dots < x_{n-1} < x_n = b$$

and write

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

In this and the next section, the main idea in generating the quadrature formula will be to approximate the function with, say, Lagrange interpolating polynomial

$$f(x) \approx P(x)$$

and then to integrate the polynomial instead

$$\int_a^b f(x)\,dx \approx \int_a^b P(x)\,dx$$

In particular, we select points $x_0, x_1, \ldots, x_n$ in $[a,b]$ and construct the Lagrange interpolating polynomial

$$P_n(x) = f(x_0)L_0(x) + \cdots + f(x_n)L_n(x)$$

Thus,
$$f(x) = P_n(x) + \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-x_0)\ldots(x-x_n)$$

We integrate both sides of this equation

$$\int_a^b f(x)\,dx = f(x_0)\int_a^b L_0(x)\,dx + \cdots + f(x_n)\int_a^b L_n(x)\,dx$$
$$+ \frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\xi)(x-x_0)\ldots(x-x_n)\,dx$$

Def: The quadrature formula then is
$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} a_i f(x_i)$$

where $a_i = \int_a^b L_i(x)\,dx$ and the error is given by
$$E(f) = \frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\xi(x))(x-x_0)\cdots(x-x_n)\,dx$$

Def: Formulas of this form are called closed Newton-Cotes formulas

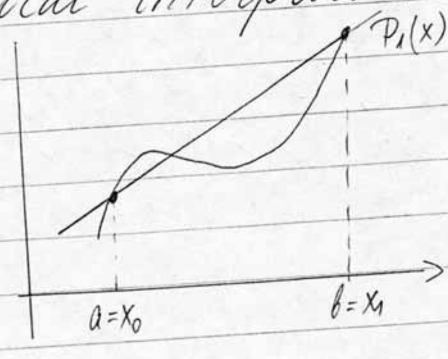
„Closed" because the endpoints of the interval: a & b participate in the formula. If only interior points participate in the formula, then it is called open Newton-Cotes formula.

Some specific Newton-Cotes formulas are.

α) The Trapezoidal Rule

To get the trapezoidal rule we approximate $f(x)$ with a linear Lagrange polynomial. If $x_0 = a$ $x_1 = b$, $h = b-a$ then we use $(x_0, f(x_0))$ and $(x_1, f(x_1))$ to write the linear Lagrange polynomial and integrate it instead.

Geometrical interpretation



We compute the area of the trapezoid instead of the arc under the curve.

The Trapezoidal Rule is

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

where ξ in (x_0, x_1) $\quad h = x_1 - x_0$

Thus,

$$\int_{x_0}^{x_1} f(x)\,dx \approx \frac{h}{2}\left[f(x_0)+f(x_1)\right]$$

Error: $E^T(f) = -\frac{h^3}{12} f''(\xi)$

Thus, the error of the trapezoidal rule is $O(h^3)$.

Ex #1b/2b/195 (a) Approximate the integral

$$\int_0^{0.5} \frac{2}{x-4}\,dx$$

using Trapezoidal rule.

(b) Find a bound for the error and compare with the actual error.

(a) $\int_0^{0.5} \frac{2}{x-4}\,dx \approx \frac{0.5-0}{2}\left[f(0)+f(0.5)\right]$

$= \frac{0.5}{2}\left[-\frac{1}{2}-\frac{4}{7}\right] = 0.25\left[-\frac{15}{14}\right]$

$= -0.267857$

Exact value $= -0.2670628$

Error $= 7.9421 \cdot 10^{-4} = 0.00079421$

(b) Error bound:

$f(x) = \frac{2}{x-4} \qquad f'(x) = \frac{-2}{(x-4)^2} \qquad f''(x) = \frac{4}{(x-4)^3}$

$|f''(x)| = \frac{4}{(4-x)^3}$ ← increasing in $[0, 0.5]$

$|f''(x)| = \frac{4}{(4-x)^3} \underset{\substack{\uparrow \\ \text{in } [0,0.5]}}{\leq} \frac{4}{(4-0.5)^3} = \frac{4}{(3.5)^3} = 0.093294$

$|E^T(f)| = \frac{(0.5)^3}{12}\,|f''(z)| \leq \frac{(0.5)^3}{12} \cdot 0.093294446 =$

$= 9.7181 \cdot 10^{-4}$

Error bound $= 9.7181 \cdot 10^{-4}$

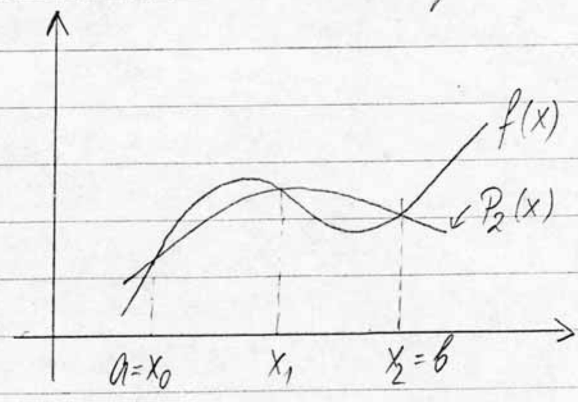
Note: Since the error depends on f'' it follows that the trapezoidal rule is exact for all functions for which $f''=0$. Thus, it is exact for polynomials of degree ≤ 1.

3) Simpson's rule

In Simpson's rule we work with the points

$$x_0 = a \qquad \underset{\substack{\uparrow \\ \text{midpoint}}}{x_1} \qquad x_2 = b\,, \qquad h = \frac{b-a}{2}$$

and we approximate $f(x)$ with a quadratic Lagrange polynomial constructed on these 3 points.



We approximate the area under $f(x)$ with the area under $P_2(x)$.

Simpson's Rule: $h = \frac{b-a}{2}$

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

Thus,

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f(x_0)+4f(x_1)+f(x_2)\right]$$

and the error of Simpson's rule is

$$E^S(f) = -\frac{h^5}{90} f^{IV}(\xi)$$

where ξ in (a,b).

The error of Simpson's rule is $O(h^5)$. Thus, Simpson's rule is much more accurat than trapezoidal rule.

Note: Since the error term involves f^{IV}, it will be zero if $f^{IV}=0$. Thus, Simpson's rule is exact (gives the exact value) when applied to polynomials of degree ≤ 3.

Ex (a) Use the Simpson's rule to approximate
3c/4c the integral
195

$$\int_1^{1.5} x^2 \ln x\,dx$$

(b) Find the bound for the error and compare to the actual error.

Solution:

(a) We divide the interval by the points $x_0 = 1 \quad x_1 = 1.25 \quad x_2 = 1.5 \quad h = 0.25$

Then

$$\int_1^{1.5} x^2 \ln x \, dx \approx \frac{0.25}{3}\left[1 \cdot \ln 1 + 4(1.25)^2 \ln 1.25 + (1.5)^2 \ln 1.5\right]$$
$$= 0.1922453$$

Exact value: $= 0.19225935777332$

Error $= 1.405 \cdot 10^{-5}$

(b) Error bound

$f'(x) = 2x \ln x + x$

$f''(x) = 2 \ln x + 3$

$f'''(x) = \frac{2}{x}$

$f^{IV}(x) = -\frac{2}{x^2} \Rightarrow |f^{IV}(x)| = \frac{2}{x^2} \leftarrow$ decr. in $[1, 1.5]$

$$|f^{IV}(x)| \underset{\substack{\uparrow \\ \text{in } [1, 1.5]}}{\leq} \frac{2}{1^2} \leq 2$$

$$|E^S(f)| = \frac{h^5}{90}|f^{IV}(\xi)| \le \frac{(0,25)^5}{90}\cdot 2 = 2,17\cdot 10^{-5}$$

Error bound $= 2.17\cdot 10^{-5}$

Ex #7/195 The Trapezoidal rule applied to

$$\int_0^2 f(x)\,dx$$

gives value 4, and Simpson's rule gives the value 2. What is $f(1)$?

Solution:

Trapezoidal rule:

$$\frac{2}{2}[f(0)+f(2)] = 4$$

Simpson's rule:

$$\frac{1}{3}[f(0)+4f(1)+f(2)] = 2$$

Thus, from the first equation

$$f(0)+f(2) = 4$$

From the second equation

$$f(0)+4f(1)+f(2) = 6$$

$$4f(1) + 4 = 6$$

$$4f(1) = 2 \Rightarrow \boxed{f(1) = \frac{1}{2}}$$

4) Simpson's 3/8 rule:

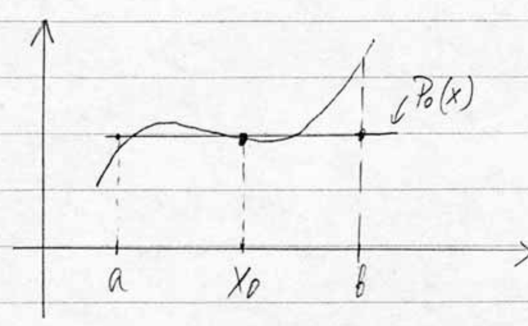
If we divide the interval by 4 points $x_0 = a \quad x_1 \quad x_2 \quad x_3 = b$ we can write Simpson's 3/8 rule

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

where ξ is in (a, b).

The error is again $O(h^5)$ and this formula is exact for polynomials of degree ≤ 3.

5) Midpoint rule - open Newton-Cotes.



$x_{-1} = a$

$x_1 = b$

x_0 - midpoint

$h = \frac{b-a}{2}$

We approximate the function with the constant equal to $f(x_0)$

$$\int_a^b f(x)\,dx = 2h f(x_0) + \frac{h^3}{3} f''(\xi)$$

Thus,

$$\int_a^b f(x)\,dx \approx 2h f(x_0)$$

and the error is

$$E^M(f) = \frac{h^3}{3} f''(\xi)$$

Hence, the error is $O(h^3)$. Since the error contains f'', if $f''=0$ then the formula is exact. Therefore the Midpoint rule is exact for polynomials of degree ≤ 1.

Ex. Use the Midpoint rule to approximate

$$\int_{0.5}^{1} x^4\,dx$$

Solution: Midpoint: $x_0 = 0.75$ $h = 0.25$

$$\int_{0.5}^{1} x^4\,dx \approx 2\cdot(0.25)\cdot(0.75)^4 = 0.1582$$

Exact value $= 0.19375$
Actual error $= -0.035547$

6) Degree of accuracy or precision

The Trapezoidal rule and the Midpoint rule will give exact value for polynomials of degree 0 and 1. In particular they will give exact value of

$$\int_a^b 1\,dx, \quad \int_a^b x\,dx$$

Therefore, we say that the Trapezoidal and Midpoint rule have degree of accuracy (precision) equal to one.
Simpson's rule will give exact value for all polynomials of degree ≤ 3. In particular, Simpson's rule will give exact value of

$$\int_a^b 1\,dx, \int_a^b x\,dx, \int_a^b x^2\,dx, \int_a^b x^3\,dx$$

Therefore, we say the Simpson's rule has degree of precision equal to 3.

Def: The <u>degree of accuracy (precision)</u> of a quadrature formula is the largest positive integer n such that the formula is exact for $\int_a^b x^k\,dx$ for each $k = 0, 1, \dots, n$.

Note: If a formula has a degree of precision n, then it is exact (no error) for all polynomials of degree $\le n$.

Ex. #9/195 Find the degree of precision of the quadrature formula

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

Solution:

$$\int_{-1}^{1} 1\,dx = x\Big|_{-1}^{1} = 2 \qquad f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) = 1+1 = 2$$

$\Rightarrow$ exact

$$\int_{-1}^{1} x\,dx = \frac{x^2}{2}\Big|_{-1}^{1} = 0 \qquad f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) = -\frac{\sqrt{3}}{3} + \frac{\sqrt{3}}{3} = 0$$

$\Rightarrow$ exact

$$\int_{-1}^{1} x^2\,dx = \frac{x^3}{3}\Big|_{-1}^{1} = \frac{2}{3} \qquad f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) = \left(\frac{\sqrt{3}}{3}\right)^2 + \left(\frac{\sqrt{3}}{3}\right)^2$$

$$= \frac{3}{9} + \frac{3}{9} = \frac{2}{3} \Rightarrow \text{exact}$$

$$\int_{-1}^{1} x^3\,dx = \frac{x^4}{4}\Big|_{-1}^{1} = 0 \qquad f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) = \left(-\frac{\sqrt{3}}{3}\right)^3 + \left(\frac{\sqrt{3}}{3}\right)^3 = 0$$

$\Rightarrow$ exact

$$\int_{-1}^{1} x^4\,dx = \frac{x^5}{5}\Big|_{-1}^{1} = \frac{2}{5} \qquad f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) = \left(-\frac{\sqrt{3}}{3}\right)^4 + \left(\frac{\sqrt{3}}{3}\right)^4 = \frac{2}{9}$$

$\Rightarrow$ not exact

$\Rightarrow$ Degree of precision is 3.

Ex #13/195

Find constants c_0, c_1, x_1 so that the quadrature formula

$$\int_0^1 f(x)\,dx = c_0 f(0) + c_1 f(x_1)$$

has the highest possible degree of precision

Solution:

$$\int_0^1 1\,dx = x\Big|_0^1 = 1 \qquad \Rightarrow \boxed{c_0 + c_1 = 1}$$

$$\int_0^1 x\,dx = \frac{x^2}{2}\Big|_0^1 = \frac{1}{2} \qquad \Rightarrow c_0 \cdot 0 + c_1 \cdot x_1 = \frac{1}{2}$$

$$\Rightarrow \boxed{c_1 x_1 = \frac{1}{2}}$$

$$\int_0^1 x^2\,dx = \frac{x^3}{3}\Big|_0^1 = \frac{1}{3} \qquad c_0 \cdot 0^2 + c_1 (x_1)^2 = \frac{1}{3}$$

$$\boxed{c_1 (x_1)^2 = \frac{1}{3}}$$

The three equations in boxes are a system for the unknowns c_0, c_1, x_1. Solving it we have: from the second and third equation we have

$$\frac{c_1 (x_1)^2}{c_1 x_1} = \frac{\frac{1}{3}}{\frac{1}{2}} \Rightarrow x_1 = \frac{2}{3}$$

From the second equation: $c_1 = \frac{\frac{1}{2}}{x_1} = \frac{3}{4}$

From the first equation: $c_0 = 1 - c_1 = 1 - \frac{3}{4} = \frac{1}{4}$