4.3. Elements of numerical integration.

The basic method to approximate $\int_a^b f(x)dx$ is called numerical quadrature.

We will use interpolating polynomials. The Lagrange polynomial is given by

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

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

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

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

$a_i = \int_a^b L_i(x)dx; \quad i = 0,1, \dots, n-1,$

and the error

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

The Trapezoidal Rule.

Let $x_0 = a, x_1 = b, h = b - a$. This rule uses 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

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

$$\frac{1}{2}\int_a^b f''\big(\xi(x)\big)(x-x_0)(x-x_1)dx \qquad (4.23)$$

Recall weighted mean value theorem for integrals:

Thm. 1.13. Suppose $f \in C[a,b]$, g is integrable on $[a,b]$, and $g(x)$ doesn't change its sign on $[a,b]$. Then there exists $c \in [a,b]$ such that

$\int_a^b f(x)g(x)dx = f(c)\int_a^b g(x)dx$.

Note that $(x-x_0)(x-x_1)$ doesn't change sign on $[x_0,x_1]$;

apply Thm. 1.13 to the error term in (4.23):

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

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

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

$-\frac{h^3}{6}f''(\xi)$.

Then Eq. (4.23) turns into

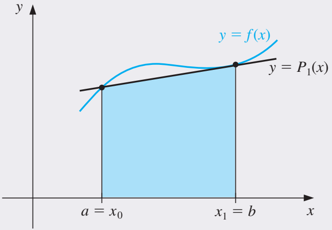
$$\int_a^b f(x)dx = \left[\frac{(x-x_1)^2}{2(x_0-x_1)}f(x_0) + \frac{(x-x_0)^2}{2(x_1-x_0)}f(x_1)\right]_{x_0}^{x_1}$$

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

Trapezoidal Rule

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

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



Simpson's Rule

Let $x_0 = a, x_2 = b,\ x_1 = a + h, where\ h = \frac{b-a}{2}$.

Use $P_2(x)$ to interpolate (x) :

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

This leads to the error term that is $O(h^4)$.

Alternative method: expand $f(x)$ about x_1 using third-order Taylor polynomial:

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

So

$$\int_{x_0}^{x_2} f(x)dx = \left[f(x_1)(x-x_1) + f'(x_1)\frac{(x-x_1)^2}{2} + f''(x_1)\frac{(x-x_1)^3}{6} + f'''(x_1)\frac{(x-x_1)^4}{24} \right] \Big|_{x_0}^{x_2} + \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}\big(\xi(x)\big)(x-x_1)^4 dx \qquad (4.24)$$

Note that $(x-x_1)^4 \geq 0$ on $[x_0, x_2]$.

By Thm. 1.13,

$$\frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x-x_1)^4 dx = \frac{f^{(4)}(\xi_1)}{24}\int_{x_0}^{x_2}(x-x_1)^4 dx =$$

$\frac{f^{(4)}(\xi_1)}{24}(x-x_1)^5 \,|_{x_0}^{x_2}$.

Here $\xi_1 \in (x_0, x_2)$. Since $h = x_2 - x_1 = x_1 - x_0$;

$$(x_2-x_1)^2-(x_0-x_1)^2=(x_2-x_1)^4-(x_0-x_1)^4=0,$$

While

$(x_2-x_1)^3-(x_1-x_0)^3=2h^3;\ (x_2-x_1)^5-(x_0-x_1)^5=2h^5.$

Eq. (4.24) turns into

$$\int_{x_0}^{x_2} f(x)dx = 2hf(x_1)+\frac{h^3}{3}f''(x_1)+\frac{2f^{(4)}(\xi_1)}{120}h^5 \qquad (*)$$

We will now use (4.9) (midpoint formula for the second derivative) to approximate $f''(x_1)$ (second term in (*)):

$$\int_{x_0}^{x_2} f(x)dx = 2hf(x_1) + \frac{h^3}{3}\left\{\frac{1}{h^2}[f(x_1-h)-2f(x_1)+f(x_1+h)]-\frac{h^2}{12}f^{(4)}(\xi_2)\right\} + \frac{f^{(4)}(\xi_1)}{60}h^5 =$$

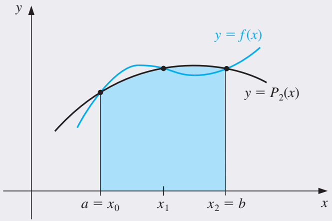
$$\frac{h}{3}[f(x_0)+4f(x_1)+f(x_2)]-\frac{h^5}{12}\left[\frac{f^{(4)}(\xi_2)}{3}-\frac{f^{(4)}(\xi_1)}{5}\right].$$

The values ξ_1 and ξ_2 can be replaced by a common value $\xi \in (x_0, x_2)$.

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 $h = (b - a)/2$.

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



Definition

4.1 The **degree of accuracy**, or **precision**, of a quadrature formula is the largest positive integer n such that the formula is exact for x^k, for each $k = 0, 1, \ldots, n$.

- Definition 4.1 implies that the Trapezoidal and Simpson's rules have degrees of precision one and three, respectively.
- The degree of precision of a quadrature formula is n if and only if the error is zero for all polynomials of degree $k = 0, 1, \ldots, n$, but is not zero for some polynomial of degree $n + 1$.
- The Trapezoidal and Simpson's rules are examples of a class of methods known as Newton-Cotes formulas. There are two types of Newton-Cotes formulas, open and closed.

Newton-Cotes formulas.

Closed Newton-Cotes formula uses nodes $x_i = x_0 + ih, i = 0,1, \dots, n,$

where $x_0 = a, x_n = b, h = \frac{b-a}{n}$. The end points of the interval $[a, b]$ are included as the nodes.

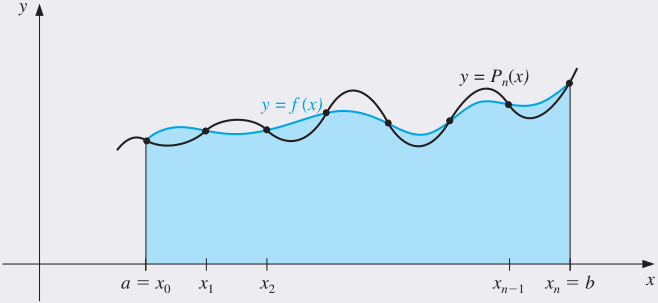
The formula assumes the form

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

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

Closed Newton-Cotes Formulas

The $(n+1)$-*point closed Newton-Cotes formula* uses nodes $x_i = x_0 + ih$, for $i = 0, 1, \ldots, n$, where $x_0 = a$, $x_n = b$ and $h = (b-a)/n$. (See Figure) It is called closed because the endpoints of the closed interval $[a, b]$ are included as nodes.



Theorem (4.2: Closed Newton-Cotes Formulas)

Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ *denotes the* $(n+1)$*-point closed Newton-Cotes formula with* $x_0 = a$, $x_n = b$, *and* $h = (b-a)/n$. *There exists* $\xi \in (a, b)$ *for which*

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

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

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

if n *is odd and* $f \in C^{n+1}[a, b]$.

Common Closed Newton-Cotes Formulas

- $n = 1$: Trapezoidal rule where $x_0 < \xi < x_1$

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

- $n = 2$: Simpson's rule where $x_0 < \xi < x_2$

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

- $n = 3$: Simpson's Three-Eighths where $x_0 < \xi < x_3$

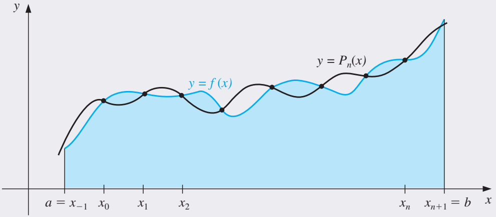
$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] - \frac{3h^5}{80} f^{(4)}(\xi).$$

- $n = 4$: where $x_0 < \xi < x_4$

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

Open Newton-Cotes Formulas

The *open Newton-Cotes formulas* do not include the endpoints of $[a, b]$ as nodes. They use the nodes $x_i = x_0 + ih$, for each $i = 0, 1, \ldots, n$, where $h = (b - a)/(n + 2)$ and $x_0 = a + h$. This implies that $x_n = b - h$, so we label the endpoints by setting $x_{-1} = a$ and $x_{n+1} = b$, as shown in the figure. Open formulas contain all the nodes used for the approximation within the open interval (a, b).



Common Open Newton-Cotes Formulas

- $n = 0$: Midpoint rule $\int_{x_{-1}}^{x_1} f(x)\,dx = 2hf(x_0) + \frac{h^3}{3} f''(\xi), \quad x_{-1} < \xi < x_1.$
- $n = 1$: $\int_{x_{-1}}^{x_2} f(x)\,dx = \frac{3h}{2}[f(x_0) + f(x_1)] + \frac{3h^3}{4} f''(\xi), \quad x_{-1} < \xi < x_2.$
- $n = 2$:

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

- $n = 3$:

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

Theorem (4.3)

Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ *denotes the* $(n+1)$*-point open Newton-Cotes formula with* $x_{-1} = a$, $x_{n+1} = b$, *and* $h = (b-a)/(n+2)$. *There exists* $\xi \in (a, b)$ *for which*

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

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

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

if n *is odd and* $f \in C^{n+1}[a, b]$.

1(a). Approximate the following integral using the Trapezoidal Rule.

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

$$x_0 = a = 0.5, x_1 = b = 1; h = 1 - 0.5 = 0.5$$

$$\int_{0.5}^{1} x^4 dx \approx \frac{0.5}{2}[0.5^4 + 1] = 0.25 * 1.0625 = 0.265625$$

3(a). Find an error bound in 1(a) using the error formula and compare this to the actual error.

$$f(x) = x^4, f'(x) = 4x^3, f''(x) = 12x^2$$

$$\max_{x \in [0.5,1]} |f''(x)| = 12 * 1 = 12$$

$$E \leq \frac{0.5^3}{12} * 12 = 0.125$$

Exact value of the integral.

$$\int_{0.5}^{1} x^4 dx = \frac{x^5}{5}\Big|_{0.5}^{1} = \frac{1}{5}(1 - 0.5^5) = 0.193750$$

Actual error=$|0.265625 - 0.193750| = 0.07185$

5(a). Repeat 3(a) using Simpson's rule.

$$x_0 = a = 0.5, x_1 = 0.75, x_2 = b = 1; h = 0.25$$

$$f'''(x) = 24x, f^{(4)}(x) = 24$$

$$\int_{0.5}^{1} x^4 dx \approx \frac{0.25}{3}[1^4 + 4 * 0.75^4 + 0.5^4] = 0.1940104$$

7(a). Repeat 3(a) using Simpson's rule and the results of 5(a).

$$E \leq \frac{0.25^5}{90} * 24 = 0.00026042$$

Actual error $|0.1937500 - 0.1940104| = 0.0002604$

9(a). Repeat 1(a) using the Midpoint rule.

$$x_{-1} = 0.5, x_0 = 0.75, x_1 = 1; h = \frac{1 - 0.5}{2} = 0.25$$

$$\int_{0.5}^{1} x^4 dx \approx 2 * 0.25 * 0.75^4 = 0.1582031$$

11(a). Repeat 3(a) using the Midpoint rule and the results of 9(a).

$$E \leq \frac{0.25^3}{3} * 12 = 0.0625$$

Actual error $|0.1937500 - 0.1582031| = 0.0355469$

#23. Find the constants c_0, c_1 and 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.

$f(x) = 1$: $\quad 1 = c_0 + c_1$

$$f(x) = x: \quad \frac{1}{2} = 0 + c_1 x_1, c_1 = \frac{1}{2x_1}$$

$f(x) = x^2$: $\frac{1}{3} = 0 + c_1 {x_1}^2, c_1 = \frac{1}{3{x_1}^2}$

$$\frac{1}{2x_1} = \frac{1}{3{x_1}^2} \quad x_1 = \frac{2}{3}, c_1 = \frac{3}{4}, c_0 = \frac{1}{4}$$

#1(e) $\int_1^{1.6} \frac{2x}{x^2-4} dx = \ln|x^2 - 4|_1^{1.6} = \ln 1.44 - \ln 3 = -0.733969$

Trapezoidal rule:

$$\int_1^{1.6} \frac{2x}{x^2 - 4} dx \approx \frac{0.6}{2}[f(1) + f(1.6)] = -0.866667$$

#3(e) Find an error bound in 1(a) using the error formula and compare this to the actual error.

$$f(x) = \frac{2x}{x^2 - 4}, f'(x) = -2\frac{x^2 + 4}{(x^2 - 4)^2}$$

$f''(x) = 4\frac{x(x^2+12)}{(x^2-4)^3}$.

$$\max_{1 \le x \le 1.6} |f''(x)| = |f''(1.6)| = 31.2071$$

$$E \le \frac{0.6^3}{12} * 31.2071 = 0.561728$$

Actual error = $|-0.733969 + 0.866667| = 0.132698$.