Numerical Methods

DS288 and UMC201

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August-December 2025

Numerical Integration

Why Numerical Integration

- For evaluating the definite integral of a function that has no explicit antiderivative or whose antiderivative is not easy to get.
- The basic idea involved inapproximating $\int_a^b f(x)dx$ is called numerical quadrature.
- It uses a sum $\sum_{i=0}^{n} f(x_i)$ 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 $\{x_0, \cdots, x_n\}$ from the interval $[a, b]$. Then integrate the Lagrange interpolating polynomial

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

Elements of numerical integration

Now truncation error term over $[a, b]$

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

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

$$a_i = \int_a^b L_i(x)dx, \qquad \forall i = 0, 1, \cdots, n.\text{and} \quad \zeta \in [a, b]$$

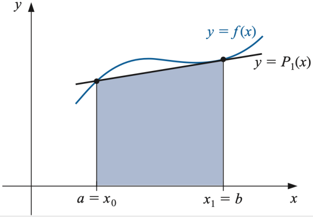
- The quadrature formula thus: $\int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i)$.
- Error: $\mathrm{E(f)} = \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^{n} (x - x_i) f^{(n+1)}(\zeta(x)) dx$

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 linear Lagrange polynomial:
- Use $P_1(x) = \dfrac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \dfrac{(x - x_0)}{(x_1 - x_0)} f(x_1)$.

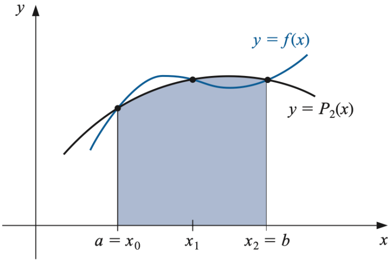
  We get
$$\int_a^b f(x)dx = \int_a^b \left[\frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_1)}{(x_0 - x_1)} f(x_1) \right] dx$$
$$= \frac{h}{2}\left[f(x_0) + f(x_1)\right] - \frac{h^3}{12} f''(\zeta).$$

- Error: $-\dfrac{h^3}{12} f''(\zeta)$.



Simpson's Rule

- Simpson's rule can be derived using the second Lagrange polynomial.
- Integrate over $[a, b]$ with equally spaced nodes $x_0 = a$, $x_2 = b$ and $x_1 = a + h$, where $h = \frac{b-a}{2}$
- We get $\displaystyle\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] - \frac{h^5}{90}f^{(4)}(\zeta)$.
- Error term in Simpson's rule involves the fourth derivative of f(x).
- It gives exact results for polynomial of degree 3 or less.



Simppson's rule

Consider three equally spaced points:

$$x_0, \quad x_1 = x_0 + h, \quad x_2 = x_0 + 2h \tag{1}$$

where h is the spacing between points.
Let $f(x_0)$, $f(x_1)$, $f(x_2)$ be the function values at these points.
The Lagrange interpolating polynomial $P_2(x)$ that passes through these three points is:

$$P_2(x) = f(x_0)L_0(x) + f(x_1)L_1(x) + f(x_2)L_2(x) \tag{2}$$

where the Lagrange basis polynomials are:

$$L_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} \tag{3}$$

$$L_1(x) = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} \tag{4}$$

$$L_2(x) = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} \tag{5}$$

Simppson's rule

Substituting the values: $x_1 - x_0 = h$, $x_2 - x_0 = 2h$ and $x_2 - x_1 = h$, We get:

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(-h)(-2h)} = \frac{(x-x_1)(x-x_2)}{2h^2} \tag{6}$$

$$L_1(x) = \frac{(x-x_0)(x-x_2)}{(h)(-h)} = -\frac{(x-x_0)(x-x_2)}{h^2} \tag{7}$$

$$L_2(x) = \frac{(x-x_0)(x-x_1)}{(2h)(h)} = \frac{(x-x_0)(x-x_1)}{2h^2} \tag{8}$$

To derive Simpson's rule, we integrate $P_2(x)$ from x_0 to x_2:

$$\int_{x_0}^{x_2} f(x)\,dx \approx \int_{x_0}^{x_2} P_2(x)\,dx = \int_{x_0}^{x_2} [f(x_0)L_0(x) + f(x_1)L_1(x) + f(x_2)L_2(x)]\,dx \tag{9}$$

This gives us:

$$\int_{x_0}^{x_2} f(x)\,dx \approx f(x_0)\int_{x_0}^{x_2} L_0(x)\,dx + f(x_1)\int_{x_0}^{x_2} L_1(x)\,dx + f(x_2)\int_{x_0}^{x_2} L_2(x)\,dx \tag{10}$$

Simppson's rule

- Computing Each Integral For convenience, let $u = x - x_0$, so when $x = x_0$, $u = 0$ and when $x = x_2$, $u = 2h$.
- For $L_0(x)$

$$\int_0^{2h} \frac{(u-h)(u-2h)}{2h^2}\,du = \frac{1}{2h^2}\int_0^{2h}\left[u^2 - 3hu + 2h^2\right]du \tag{11}$$

$$= \frac{1}{2h^2}\left[\frac{u^3}{3} - \frac{3hu^2}{2} + 2h^2u\right]_0^{2h} \tag{12}$$

$$= \frac{1}{2h^2}\left[\frac{8h^3}{3} - 12h^3 + 4h^3\right] \tag{13}$$

$$= \frac{1}{2h^2}\cdot\frac{2h^3}{3} = \frac{h}{3} \tag{14}$$

Simppson's rule

- For $L_1(x)$:

$$\int_0^{2h} -\frac{u(u-2h)}{h^2}\,du = -\frac{1}{h^2}\int_0^{2h}\left[u^2 - 2hu\right]du \tag{15}$$

$$= -\frac{1}{h^2}\left[\frac{u^3}{3} - hu^2\right]_0^{2h} \tag{16}$$

$$= -\frac{1}{h^2}\left[\frac{8h^3}{3} - 4h^3\right] \tag{17}$$

$$= -\frac{1}{h^2}\cdot\left(-\frac{4h^3}{3}\right) = \frac{4h}{3} \tag{18}$$

Simppson's rule

- For $L_2(x)$:

$$\int_0^{2h} \frac{u(u-h)}{2h^2}\,du = \frac{1}{2h^2}\int_0^{2h}\left[u^2 - hu\right] du \tag{19}$$

$$= \frac{1}{2h^2}\left[\frac{u^3}{3} - \frac{hu^2}{2}\right]_0^{2h} \tag{20}$$

$$= \frac{1}{2h^2}\left[\frac{8h^3}{3} - 2h^3\right] \tag{21}$$

$$= \frac{1}{2h^2}\cdot\frac{2h^3}{3} = \frac{h}{3} \tag{22}$$

- Simpson's Rule (Combining these results):

$$\boxed{\int_{x_0}^{x_2} f(x)\,dx \approx \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]} \tag{23}$$

Example

Example

Compare the Trapezoidal rule and Simpson's rule approximations to $\int_0^2 f(x)dx$, when $f(x) = x^2$ and x^4.

- Trapezoid rule: $\int_0^2 f(x)dx \approx f(0) + f(2) =\approx 0^2 + 2^2 = 4$
- Simpson's rule:

$$\int_0^2 f(x)dx \approx \frac{1}{3}\left[f(0) + 4f(1) + f(2)\right] = \frac{1}{3}\left[0^2 + 4 \cdot 1^2 + 2^2\right] = \frac{8}{3}$$

Method	$f(x) = x^2$	$f(x) = x^4$
Using Trapezoidal	4	16.000
Using Simpson's	2.667	6.667
Exact integration value	2.667	6.400

Degree of Accuracy

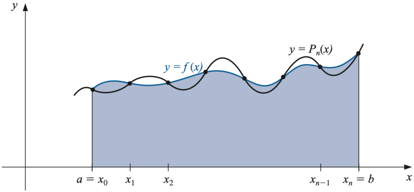
Definition

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 $k = 0, 1, \cdots n$.

- 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 $k = 0, 1, \cdots, n$, 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.

Closed Newton-cotes formula

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



- The formula assumes the form: $\displaystyle\int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i)$.
- Error: $E(f) = \dfrac{h^{n+3} f^{(n+2)}(\zeta)}{(n+2)!} \displaystyle\int_0^n t^2(t-1)\cdots(t-n)dt$ (n is even)
- Error: $E(f) = \dfrac{h^{n+2} f^{(n+1)}(\zeta)}{(n+1)!} \displaystyle\int_0^n t(t-1)\cdots(t-n)dt$ (n is odd)

Closed Newton-Cotes formulae

- **Trapezoidal rule** **($n = 1$)**

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

- **Simpson's rule** **($n = 2$)**

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

- **Simpson's Three-Eighths rule** **($n = 3$)**

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

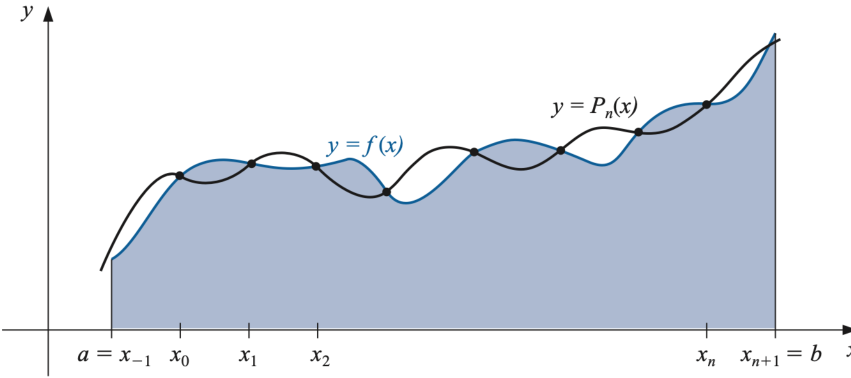
- **$n = 4$:**

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

where $x_0 < \zeta < x_4$.

Open Newton-cotes formula

- The open Newton-Cotes formulas do not include the endpoints of $[a, b]$. It use nodes $x_i = x_0 + ih$, for $i = 0, 1, \cdots, n$, where $x_0 = a + h, x_n = b - h$ and $h = (b - a)/(n + 2)$.



Open Newton-cotes formula

The formula: $\int_a^b f(x)dx = \int_{x_{-1}}^{x_{n+1}} f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i).$

Theorem

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 $f \in C^{n+1}[a,b]$.

Open Newton-Cotes formulae

- **Midpoint rule** $(n = 0)$

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

- $n = 1$:

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

- $n = 2$:

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

- $n = 3$:

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

where $x_{-1} < \zeta < x_4$.

Example

Compare the of the closed and open Newton-Cotes formulas approximations to $\int_0^{\pi/4} \sin x dx = 1 - \sqrt{2}/2 \approx 0.29289322$.

- For the closed formulas we have (n=1)

$$\int_0^{\pi/4} \sin x dx \approx \frac{\pi/4}{2}\left[\sin 0 + \sin\frac{\pi}{4}\right] = 0.27768018$$

- For the open formulas we have (n=0)

$$\int_0^{\pi/4} \sin x dx \approx 2\frac{\pi/8}{2}\left[\sin\frac{\pi}{8}\right] = 0.30055887$$

n	0	1	2	3	4
Closed formulas		0.27768018	0.29293264	0.29291070	0.29289318
Error		0.01521303	0.00003942	0.00001748	0.00000004
Open formulas	0.30055887	0.29798754	0.29285866	0.29286923	
Error	0.00766565	0.00509432	0.00003456	0.00002399	


ANY
QUESTIONS?