Numeric Integration

Trying to approximate integrals via summations?

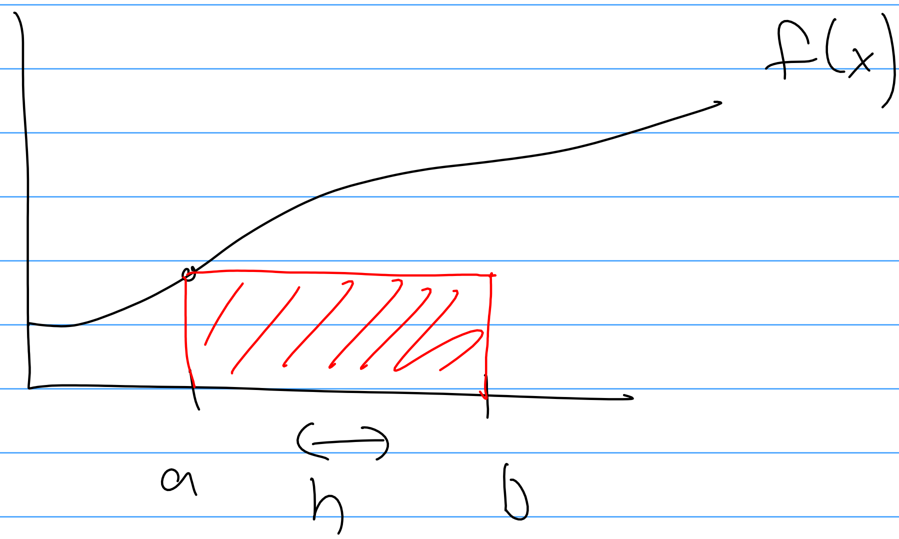
let $f(x)$ $x \in [a,b]$, then

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} c_i f(x_i)$$

for $x_i \in [a,b]$ and weights c_i.

Idea is to choose (x_i, c_i) in an appropriate manner,

- Left - Point Rule



$$\int_a^b f(x)\,dx \approx f(a)(b-a) = f(a)\,h$$

What is the error of this method?

To do that, integrate the Taylor series over the range $[0, h]$

$$\int_0^h \left(f(0) + x f'(0) + \tfrac{1}{2} x^2 f''(0) + \dots \right) dx$$

$$= h f(0) + \tfrac{1}{2} h^2 f'(0) + \tfrac{1}{6} h^3 f''(0) + \dots,$$

Error is then

$$E = \int_0^h f(x)\, dx - \underbrace{f(0)\, h}_{\text{the approximation}}$$

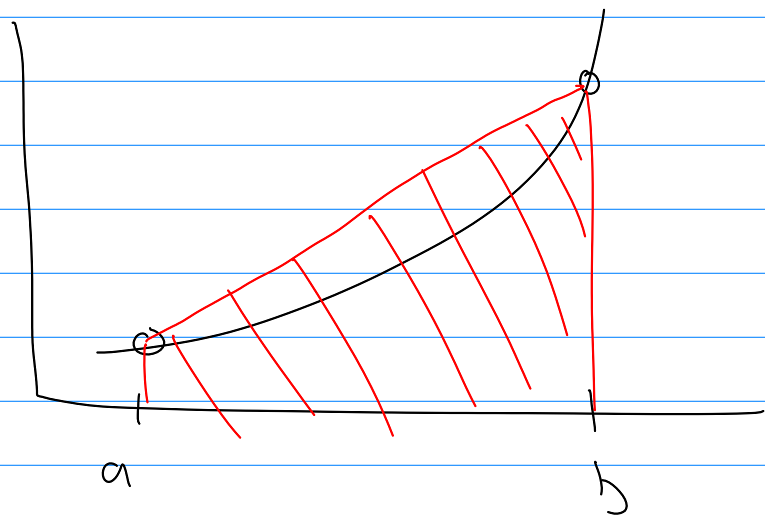
$$= h \cancel{f(0)} + \tfrac{1}{2} h^2 f'(0) + \text{H.O.T.} - h \cancel{f(0)}$$

$$= \tfrac{1}{2} h^2 f'(0) + \text{H.O.T.}$$

$\Rightarrow$ Error is thus $O(h^2)$

This scheme approximates $f(x)$ as a constant over $[a, b]$

- Midpoint Rule: Approximate $f(x)$ as a linear function.



$$\int_a^b f(x)\,dx \approx \int_a^b \left(f(a) + \frac{f(b)-f(a)}{b-a}(x-a) \right) dx$$

$$= f(a)(b-a) + \frac{f(b)-f(a)}{2}(b-a)$$

$$= \left(\frac{f(a)+f(b)}{2} \right)(b-a)$$

$$\Rightarrow \int_a^b f(x) = \sum_{i=1}^{n} c_i f(x_i) = \sum_{i=1}^{2} c_i f(x_i)$$

$x_1 = a \qquad c_1 = \frac{b-a}{2}$

$x_2 = b \qquad c_2 = \frac{b-a}{2}$

Error for midpoint:

$$|E| = \frac{1}{2} f''(\eta)(b-a)^3 = \frac{1}{2} f''(\eta) h^3$$

for some $\eta \in [a, b]$

- Simpson's Rule: Model $f(x)$ as a quadratic polynomial

Set $x_1 = a$, $x_2 = \frac{a+b}{2}$, $x_3 = b$

Recall the Lagrange Polynomial

$$f(x) \approx \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)} f(x_1) + \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)} f(x_2)$$

$$+ \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)} f(x_3)$$

Take this & integrate from $[a, b]$

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left(f(x_1) + 4f(x_2) + f(x_3)\right)$$

$$\Rightarrow c_1 = c_3 = \frac{b-a}{6} \qquad c_2 = \frac{2(b-a)}{3}$$

$$|E| = \frac{(b-a)^5}{90} f^{(4)}(\eta) \quad \text{for } \eta \in [a,b]$$

$$= \frac{h^5}{90} f^{(4)}(\eta)$$

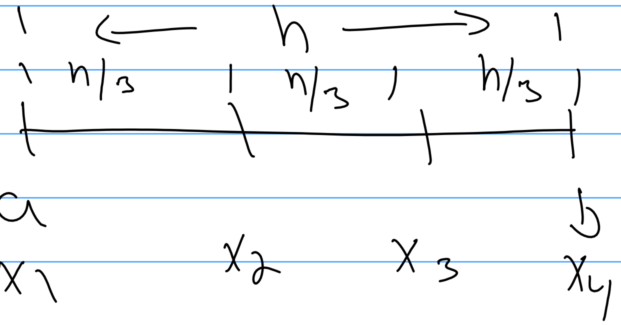
Each of these are part of the Newton-Cotes Quadrature Rules.

There are integration schemes based uniform point distributions.

Specifically, these are Closed Newton-Cotes Quadratures

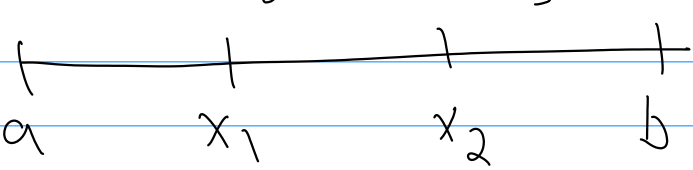
Closed $\Rightarrow$ You use the end points.

Closed:



Open Newton-Cotes do not use the end points.

Open: $x_1 = \frac{2a+b}{3}$ $\quad x_2 = \frac{a+2b}{3}$



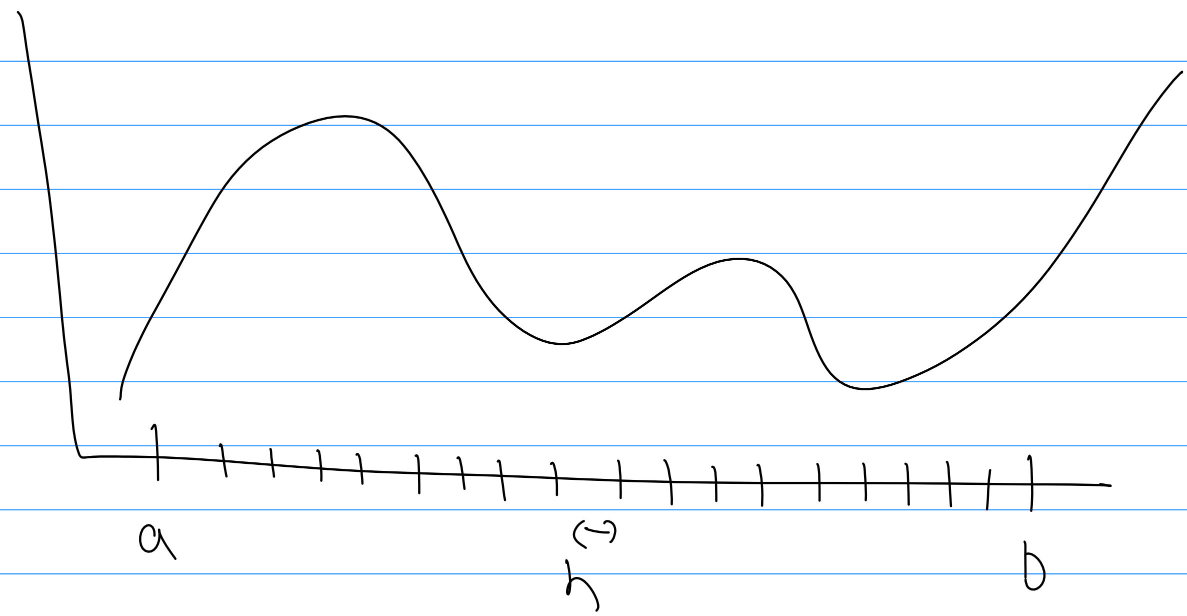
Open 2-point $\int_a^b f(x)\,dx \approx \frac{b-a}{2}\left[f(x_1) + f(x_2)\right]$

$$|E| = \frac{(b-a)^3}{36} f''(\eta)$$

Usually you do <u>not</u> integrate over $[a,b]$ in one step.

You usualy break it up into smaller chunks & sum up.

Called Composite Rules



Do integration over a distance $h \ll b-a$

Then $\int_a^b f(x) = \sum_{i=1}^{N} \underbrace{\sum_{j=1}^{n} c_{ij} f(x_{ij})}_{\text{Integral from } x_i \text{ to } x_{i+1}}$

Summation of all integrals

If you use N intervals over $[a,b]$, then

$N \sim 1/h$

Then $\int_a^b f(x)\,dx \simeq \sum_{i=1}^{N} \sum_{j=1}^{n} c_{ij} f(x_{ij})$

$= \sum_{i=1}^{N} O(h^p)$ ← Order of the Newton-Cote Quadrature,

Midpoint: $p=3$ Simpson: $p=5$

$\sum_{i=1}^{N} O(h^p) = N\,O(h^p) = \frac{1}{h} O(h^p)$

$= O(h^{p-1})$

⇒ Typically midpoint is called $O(h^2)$ & Simpson is $O(h^4)$

Newton - Cotes is useful, but it does have limitations,

It can not integrate polynomials exactly past 1^{st} - order,

$\Rightarrow$ Gauss Quadrature: let x_i exist on a non-uniform grid to minimize errors,

ex,) Let $f(x)$ be given & set $x_1 = a$, $x_2 = b$

Then $\int_a^b f(x) = \underbrace{c_1 f(x_1) + c_2 f(x_2)}_{}$

2 unknowns

Condition #1: Integrate $f(x) = 1$ exactly

Condition #2: Integrate $f(x) = x$ exactly

$$\int_a^b 1\, dx = b - a = c_1 + c_2 \quad (a,\ f(x) = 1)$$

$$\int_a^b x\, dx = \frac{b^2 - a^2}{2} = c_1 a + c_2 b \quad (a,\ f(x) = x)$$

$$\Rightarrow c_1 = c_2 = \frac{b-a}{2} \quad (\text{Mid point Rule})$$

Gauss Quadrature: What if c_1, x_1, c_2 & x_2 are all unknowns?

For Simplicity compute over $[-1, 1]$

$$\int_{-1}^{-1} f(x)\,dx = c_1 f(x_1) + c_2 f(x_2) \leftarrow 4 \text{ unknowns}$$

$$f(x) = 1: \int_{-1}^{1} 1\,dx = 2 = c_1 + c_2$$

$$f(x) = x: \int_{-1}^{1} x\,dx = 0 = c_1 x_1 + c_2 x_2$$

$$f(x) = x^2: \int_{-1}^{1} x^2\,dx = \frac{2}{3} = c_1 x_1^2 + c_2 x_2^2$$

$$f(x) = x^3: \int_{-1}^{1} x^3\,dx = 0 = c_1 x_1^3 + c_2 x_3^3$$

from $f(x) = x$ we get $c_2 = \frac{-c_1 x_1}{x_2}$

Use in $f(x) = x^3$ to get $\cancel{c_1} x_1^{\cancel{3}\,2} - \frac{\cancel{c_1} \cancel{x_1}}{\cancel{x_2}} x_2^{\cancel{3}\,2} = 0$

$$\Rightarrow x_1^2 = x_2^2$$

Since $x_1 \neq x_2 \Rightarrow x_1 = -x_2$

$$\Rightarrow C_2 = -\frac{C_1 x_1}{x_2} = -\frac{C_1(-x_2)}{x_2} = C_1 \Rightarrow C_1 = C_2$$

Use $f(x)=1$ & $f(x)=x^2$ w/ this to get

$$C_1 = C_2 = 1 \qquad x_1 = \frac{1}{\sqrt{3}} \qquad x_2 = -\frac{1}{\sqrt{3}}$$

$\Rightarrow$ If I use

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

then polynomials up to 3rd-order are evaluated exactly,

ex.) $f(x) = 2 + 3x - 9x^2 + 10x^3$

$$\int_{-1}^{1} f(x)\,dx = -2$$

$$f\left(-\frac{1}{\sqrt{3}}\right) = -1 - \frac{10}{3\sqrt{3}} - \sqrt{3}$$

$$f\left(+\frac{1}{\sqrt{3}}\right) = -1 + \frac{10}{3\sqrt{3}} + \sqrt{3}$$

-2

This is called the two-point rule as $n=2$.

In general an n-point Gauss Quadrature will integrate polynomials up to order

$$2n-1$$

exactly over $[-1, 1]$

n	x_i	c_i
2	$\pm 1/\sqrt{3}$	1
3	0	8/9
	± 0.77459	5/9
4	± 0.339981	0.652145
	± 0.86136	0.347855
$\vdots$		

What if $x \notin [-1, 1]$?

Do a change of variables:

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f(g(t))\, g'(t)\, dt$$

w/ $g(t) = a_1 + a_2 t$

We need $g(-1) = a = q_1 - q_2$

$g(1) = b = q_1 + q_2$

$\Rightarrow q_1 = \frac{a+b}{2} \qquad q_2 = \frac{b-a}{2}$

$$\Rightarrow \int_a^b f(x)\,dx = \int_{-1}^{1} f\left[\frac{(b-a)t + (b+a)}{2}\right] \frac{b-a}{2}\,dt$$

Other Gauss-Like Quadratures

- Gauss - Kronrod
- Gauss - Chebyshev
- Gauss - Lobatto

Matlab Methods for integration

- trapz → Trapezoidal rule for a single interval.
- cumtrapz → Composite / Cumulative trapezoid over larger range.
- integral → Numeric integration over a function (or vector?)