Thoughts on Num. Diff.

①

- Is generally not good to use if you can avoid it since you are taking differences of large numbers and dividing them by small numbers.

- Leads to round-off errors!

- Numerical integration is much better since roundoff errors it is more of a smoothing process.

Num. Integration

②

Will look at 3 approaches to deriving numerical integration formulas.

1) Geometric

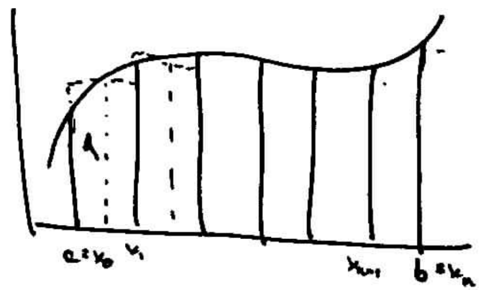
2) Poly. approximation to curves, then integrate the approximation

3) Matching of Taylor Series expansion.

Geometric

(3)

Rectangular Rule



Define $x_1^* = \frac{x_0+x_1}{2}$

$\vdots$

$x_n^* = \frac{x_n+x_{n-1}}{2}$

$A_1 \approx f(x_1^*)\cdot h$

Define $h = \frac{b-a}{n} = x_i - x_{i-1}$

Let $\int_a^b f(x)\,dx \approx A_1 + A_2 + \dots + A_n \approx h\cdot f(x_1^*) + h\,f(x_2^*) \dots + h\,f(x_n^*)$

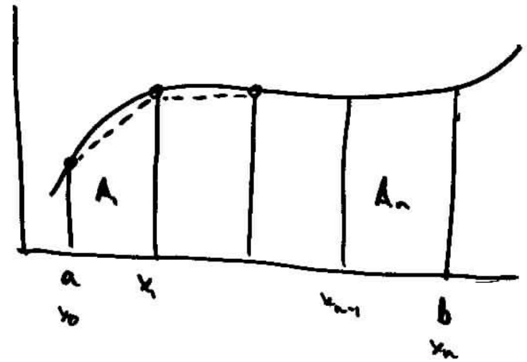
$$\boxed{\int_a^b f(x)\,dx = h\left[f(x_1^*) + \dots + f(x_n^*) \right]}$$

where $h = \frac{b-a}{n}$

Approximates the curve with a constant value!

(4)

Trapezoidal Rule



$A_1 \approx \frac{f(x_0)+f(x_1)}{2}\cdot h \quad \dots \quad A_n = \frac{f(x_{n-1})+f(x_n)}{2}\cdot h$

$$\int_a^b f(x)\,dx = A_1 + \dots + A_n$$

$$= \frac{h}{2}\Big[\big(f(x_0)+f(x_1)\big) + \big(f(x_1)+f(x_2)\big) + \dots \big(f(x_{n-2})+f(x_{n-1})\big) + \big(f(x_{n-1})+f(x_n)\big)\Big]$$

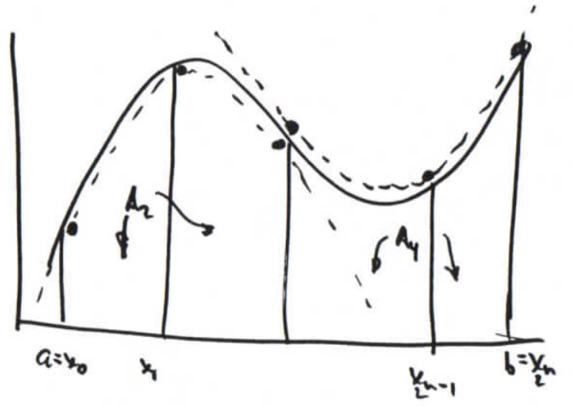
$$\boxed{\int_a^b f(x)\,dx = h\left[\tfrac{1}{2} f_0 + f_1 + f_2 + \dots + f_{n-1} + \tfrac{1}{2} f_n\right]}$$

Approximates the curve with a straight line segment.

(5)

2^{nd} order Poly

Even number of points!



Let $P_2(x) = a_2 x^2 + a_1 x + a_0$ pass through x_0, x_1, x_2

then $A_2 = \int_{x_0}^{x_2} P_2(x)\,dx = h\left[\frac{1}{3}f_0 + \frac{4}{3}f_1 + \frac{1}{3}f_2\right]$

$\vdots$

$A_{2n} = \int_{x_{2n-2}}^{x_{2n}} P_{2n}(x)\,dx = h\left[\frac{1}{3}f_{2n-2} + \frac{4}{3}f_{2n-1} + \frac{1}{3}f_{2n}\right]$

$$\cancel{\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f_0 + 4f_1 + f_2\right] + \frac{h}{3}\left[f_1 + 4f_2 + f_3\right] + \frac{h}{3}\left[f_{2n-3} + 4f_{2n-2} + f_{2n-1}\right] + \frac{h}{3}\left[f_{2n-2} + 4f_{2n-1} + f_{2n}\right]}$$

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$$\int_a^b f(x)\,dx = A_2 + A_4 + \cdots + A_{2n-2} + A_{2n}$$

$$= \frac{h}{3}\left(f_0 + 4f_1 + f_2\right) + \frac{h}{3}\left(f_2 + 4f_3 + f_4\right) + \cdots + \frac{h}{3}\left(f_{2n-4} + 4f_{2n-3} + f_{2n-2}\right) + \frac{h}{3}\left(f_{2n-2} + 4f_{2n-1} + f_{2n}\right)$$

$$\simeq \frac{h}{3}\left[f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots 2f_{2n-2} + 4f_{2n-1} + f_{2n}\right]$$

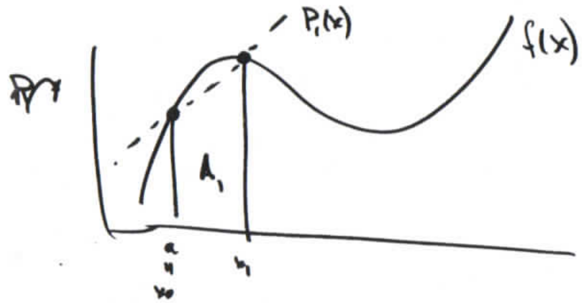
$$= \frac{h}{3}\left[f_0 + f_{2n} + 4\sum_{i=1}^{n/2} f_{2i-1} + 2\sum_{j=1}^{\frac{n}{2}-1} f_{2j}\right]$$

$$\boxed{\int_a^b f\,dx = \frac{h}{3}\left[f_0 + 4\sum f_{odds} + 2\sum f_{evens} + f_{2n}\right]}$$

Now with Poly Approx for all

(7)

Trapezoidal



$$P_1(x) = \frac{x-x_1}{x_0-x_1} f_0 + \frac{x-x_0}{x_1-x_0} f_1 + \text{error} \approx f(x)$$

↑ will ignore for now.

$$A_1 \approx \int_{x_0}^{x_1} P_1(x)\,dx$$

$$= \frac{f_0}{x_0-x_1}\int_{x_0}^{x_1}(x-x_1)\,dx + \frac{f_1}{x_1-x_0}\int_{x_0}^{x_1}(x-x_0)\,dx$$

$$= \frac{f_0}{x_0-x_1}\left(\frac{(x-x_1)^2}{2}\right)\Bigg|_{x_0}^{x_1} + \frac{f_1}{x_1-x_0}\left(\frac{(x-x_0)^2}{2}\right)\Bigg|_{x_0}^{x_1}$$

$$= \frac{f_0}{x_0-x_1}\left(-\frac{(x_0-x_1)^2}{2}\right) + \frac{f_1}{x_1-x_0}\left(\frac{(x_1-x_0)^2}{2}\right)$$

$$= -\frac{f_0(x_0-x_1)}{2} + \frac{f_1(x_1-x_0)}{2}$$

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$$A_1 \approx \frac{x_1-x_0}{2}(f_0+f_1)$$

$$A_1 = \frac{h}{2}(f_0+f_1)$$

And then will find that

$$A_2 = \frac{h}{2}(f_1+f_2)$$

$\vdots$

$$A_n = \frac{h}{2}(f_{n-1}+f_n)$$

then

$$\int_a^b f(x)\,dx = h\left[\frac{f_0+f_1}{2} + \frac{f_1+f_2}{2} + \dots + \frac{f_{n-2}+f_{n-1}}{2} + \frac{f_{n-1}+f_n}{2}\right]$$

$$\boxed{\int_a^b f(x)\,dx = h\left[\tfrac{1}{2}f_0 + f_1 + \dots + f_{n-1} + \tfrac{1}{2}f_n\right]}$$

Same as before!

Can also get an estimate of the error associated with this. $\boxed{O(h^3)}$

2nd order Poly - Simpsons rule!

- Was published by self-taught English mathematician Thomas Simpson (1710 - 1761)
- Was actually used 100 years earlier by Torricelli and Newton (1676).

$$P_2 = \frac{(x-x_1)(x-x_2)}{\underbrace{(x_0-x_1)(x_0-x_2)}_{2h^2}} f_0 + \frac{(x-x_0)(x-x_2)}{\underbrace{(x_1-x_0)(x_1-x_2)}_{-h^2}} f_1 + \frac{(x-x_0)(x-x_1)}{\underbrace{(x_2-x_0)(x_2-x_1)}_{2h^2}} f_2$$

Want to integrate but is easier to transform first

$$\boxed{s \equiv \frac{x-x_1}{h}} \Rightarrow \begin{aligned} x-x_0 &= (s+1)h \\ x-x_1 &= sh \\ x-x_2 &= (s-1)h \end{aligned} \quad \Bigg\| \quad \int_{x_0}^{x_2} f\,dx = \int_{-1}^{1} f \cdot h\,ds$$

so $P_2(x) = \frac{1}{2} s(s-1) f_0 - (s+1)(s-1) f_1 + \frac{1}{2}(s+1) s f_2$

So

$$\frac{1}{h}\int_{x_0}^{x_2} P_2(x)\,dx = \frac{f_0}{2}\int_{-1}^{1}(s^2-s)\,ds - f_1\int_{-1}^{1}(s^2-1)\,ds + \frac{f_2}{2}\int_{-1}^{1}(s^2+s)\,ds$$

$$= \frac{f_0}{2}\left(\frac{s^3}{3} - \frac{s^2}{2}\right|_{-1}^{1} - f_1\left(\frac{s^3}{3} - s\right|_{-1}^{1} + \frac{f_2}{2}\left(\frac{s^3}{3} + \frac{s^2}{2}\right|_{-1}^{1}$$

$$= \frac{f_0}{2}\left(\frac{1-(-1)}{3} - \frac{1-1}{2}\right) - f_1\left(\frac{1-(-1)}{3} - \frac{1-(-1)}{1}\right) + \frac{f_2}{2}\left(\frac{1-(-1)}{3} + \frac{1-1}{2}\right)$$

$$= \frac{1}{3} f_0 + \frac{4}{3} f_1 + \frac{1}{3} f_2$$

So $A_1 = \frac{h}{3}\left(f_0 + 4f_1 + f_2\right)$

It follows that

$A_2 = \frac{h}{3}\left(f_2 + 4f_3 + f_4\right)$ $\qquad \mathcal{O}(h^4)$ easily shown

$\vdots$ $\qquad \mathcal{O}(h^5)$ error. is more diff. to show but is correct.

$A_{2n} = \frac{h}{3}\left(f_{2n-2} + 4f_{2n-1} + f_{2n}\right)$

or

$$\boxed{\int_a^b f(x)\,dx = \frac{h}{3}\left[f_0 + 4f_1 + 2f_2 + 4f_3 \cdots 2f_{2n-2} + 4f_{2n-1} + f_{2n}\right]}$$

Some additional expressions

$$\int_{x_0}^{x_3} f(x)dx \approx \frac{3}{8}h\left(f_0 + 3f_1 + 3f_2 + f_3\right) + O(h^5)\, f''''(\xi(x))$$

$$\int_{x_0}^{x_4} f(x)dx \approx \frac{2}{45}h\left(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4\right) + O(h^7)$$

$$\vdots$$

$$\int_{x_0}^{x_8} f(x)dx = \frac{4h}{14175}\left(989f_0 + 5888f_1 - 928f_2 + 10496f_3 - 4540f_4 + \dots 989f_8\right) + O(h^{11})$$

Taylor Series Method

Look for $\int_0^1 f(x)dx = a f(0) + b f(1)$ (*)

$\xi = \frac{x - x_0}{h}$ $\int_{x_0}^{x_1} (\ )dx \to \int_0^1 (\ )dx$

Write $f(x) = \underbrace{f(0) + x f'(0) + \frac{x^2}{2} f''(0)}_{\text{use these}} + \frac{x^3}{6} f'''(0) + \dots$

And substitute on each side of (*)

$$\int_0^1 \left[f(0) + x f'(0) + \frac{x^2}{2} f''(0) + \dots\right]dx = a\left[f(0) + \dots\right] + b\left[f(0) + f'(0) + \frac{1}{2}f''(0) + \dots\right]$$

$$f(0)\left(x\Big|_0^1 + f'(0)\left(\frac{x^2}{2}\Big|_0^1 + f''(0)\left(\frac{x^3}{6}\Big|_0^1 + \dots = a[\ ] + b[\ ]\right.\right.\right.$$

$$f(0) + \frac{1}{2}f'(0) + \frac{1}{6}f''(0) + \dots = a f(0) + b f(0) + b f'(0) + \frac{b}{2} f''(0) + \dots$$

Want to match as many terms as possible to maximize the # of functions that this is valid for.

$$\left.\begin{array}{ll} f(0) & 1 = a + b \\ f'(0) & \frac{1}{2} = b \end{array}\right\} \Rightarrow a = b = \frac{1}{2}$$

$\textcircled{f''(0)}$ $\frac{1}{6} = \frac{b}{2} + \text{error}$ $\text{error} = \frac{1}{6} - \frac{1}{4} = \frac{4-6}{24}$

$= -\frac{1}{12}$

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occurs from the $\frac{x^3}{6}\Big|_0^1$ term $\Rightarrow O(h^3)$

$\therefore$

$$\boxed{\int_{x_0}^{x_1} f(x)dx = h\left(\tfrac{1}{2}f_0 + \tfrac{1}{2}f_1\right) + O(h^3) \text{ error.}}$$

Trapezoidal

$$\boxed{\mathcal{E} = \left| -\frac{h^3}{12} f''(\xi) \right|}$$

Now try <u>Simpsons</u> 1/3 rule (14)

$$\int_{-1}^{1} f(x)dx = a f(-1) + b f(0) + c f(1)$$

$$f(x) = f(0) + x f'(0) + \frac{x^2}{2}f''(0) + \frac{x^3}{6}f'''(0) + \frac{x^4}{24}f''''(0) + \cdots$$

use all of these

$$\int_{-1}^{1}\left[f(0) + x f'(0) + \frac{x^2}{2}f''(0) + \frac{x^3}{6}f'''(0) + \cdots + \frac{x^4}{24}f''''(0)\right]dx$$

$$= f(0)\left[x\Big|_{-1}^{1} + f'(0)\left[\frac{x^2}{2}\Big|_{-1}^{1} + \frac{f''(0)}{2}\left[\frac{x^3}{3}\Big|_{-1}^{1} + \frac{f'''(0)}{6}\left[\frac{x^4}{4}\Big|_{-1}^{1} + \cdots\right.\right.\right.\right.$$

$$= f(0)\cdot(1-(-1)) + f'(0)\left(\frac{1-1}{2}\right) + \frac{f''(0)}{2}\left(\frac{1-(-1)}{3}\right) + \frac{f'''(0)}{6}\left(\frac{1-1}{4}\right) + \cdots$$

$$+ \frac{f''''(0)}{24}\left(\frac{1-(-1)}{5}\right)$$

$$\text{LHS} = 2f(0) + \frac{1}{3}f''(0) + \frac{1}{60}f''''(0) + \cdots$$

$$\text{RHS} = a\left[f(0) - f'(0) + \frac{1}{2}f''(0) - \frac{1}{6}f'''(0) + \frac{1}{24}f''''(0) + \cdots\right]$$

$$+ b\left[f(0)\right]$$

$$+ c\left[f(0) + f'(0) + \frac{1}{2}f''(0) + \frac{1}{6}f'''(0) + \frac{1}{24}f^{(4)}(0) + \cdots\right]$$

LHS = RHS

$$f(0) \qquad 2 = a+b+c$$
$$f'(0) \qquad 0 = -a+c$$
$$f''(0) \qquad \tfrac{1}{3} = \tfrac{1}{2}a + \tfrac{1}{2}c$$
$$f'''(0) \qquad 0 = -\tfrac{1}{6}a + \tfrac{1}{6}c$$
$$f''''(0) \qquad \tfrac{1}{60} = \tfrac{a}{24} + \tfrac{c}{24}$$

$$\Rightarrow \left.\begin{aligned} 2 &= a+b+c \\ 0 &= -a+c \\ \tfrac{2}{3} &= a+c \end{aligned}\right\} \text{Solve these}$$

$$\left. 0 = -a+c \right\} \text{ is ok}$$

$$\tfrac{2}{5} = a+c + \text{error}$$

Soln is $a = \frac{1}{3}$ $b = \frac{4}{3}$ $c = \frac{1}{3}$

error $= \frac{2}{5} - \frac{2}{3} = \frac{6-10}{15} = -\frac{4}{15}$ occurs in the $\left.\frac{x^5}{5}\right|_{-1}^{1}$ term $\Rightarrow O(h^5)$ error. $\boxed{-\frac{h^5}{90} f''''(\xi)}$

So

$$\boxed{\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}\left[f_0 + 4f_1 + f_2\right] + O(h^5)}$$ Simpson

EXAMPLE Consider $\int_0^1 e^{-x^2}\,dx$ $n=10$ $h=0.1$

i	x_i	e^{-x^2}		
0	0	1.000 000		
1	0.1		0.990 050	
2	0.2			0.960 789
3	0.3		0.913 931	
4	0.4			0.852 144
5	0.5		0.778 801	
6	0.6			0.697 676
7	0.7		0.612 626	
8	0.8			0.527 292
9	0.9		0.444 858	
10	10	0.367 879		
		1.367 879	3.740 266	3.037 901

Using Trapezoidal rule

$$\int_0^1 e^{-x^2}\,dx \approx h\left[\tfrac{1}{2}f_0 + f_1 + f_2 + \cdots f_8 + f_9 + \tfrac{1}{2}f_{10}\right]$$

$$= 0.1\left[\tfrac{1}{2}(1 + 0.367\,879) + (3.740\,266 + 3.037\,901)\right]$$

$$\approx 0.746\,211$$

$$(= 0.746\,824 \quad \text{real})$$

error $\sim 6\times10^{-4} < (0.1)^3$

Using Simpsons rule

$$\int_0^1 e^{-x^2}\,dx \approx \frac{h}{3}\left[(f_0 + f_{2n}) + 4\sum f_{odd} + 2\sum f_{even}\right)$$

$$= \frac{0.1}{3}\left[(1 + 0.367\,879) + 4(3.740\,266) + 2\,(3.037\,901)\right]$$

$$= 0.746\,825$$

error $\sim 10^{-6} < (0.1)^5$

Handbook of Mathematical Functions

Abramowitz + Stegun

Dover

Table of Integrals, Series and Products

Gradshteyn Ryzhik

Academic Press 2nd ed w corrections