Chapter 5: Numerical Differentiation and Integration Approximation

I) Numerical Differentiation

The need for numerical differentiation arises from the fact that either:

1. $f(x)$ is not explicitly given and only the values of $f(x)$ at certain points are known
2. $f'(x)$ is difficult to compute

$$\text{slope} = \frac{y_2 - y_1}{x_2 - x_1}$$

let's denote the difference between the two x-coordinates as h

$h \longrightarrow$ step size $\qquad h \longrightarrow +ve$

$$\text{slope} = \frac{y_2 - y_1}{h}$$

The value of the function at the first point $(y_1) = f(x)$, and the value of the function at the second point is $f(x+h)$

$$\text{slope} = \frac{f(x+h) - f(x)}{h}$$

$\text{slope} = f'(x)$

$$\boxed{f'(x) = \frac{f(x+h) - f(x)}{h}}$$

The aim is to calculate $f'(x)$ at a given x

<u>Example</u>

$$f(x) = x^2 - 4x + 5$$

$$f'(x) = 2x - 4$$

$$f'(x) = 0 \quad \text{at } x = 2$$

at $x = 2$ $\quad f(2) = 2^2 - 4(2) + 5$

$f(2) = 1$

$$f'(x) = \frac{f(x+h) - f(x)}{h}$$

at $h = 2$

$$\frac{f(2+2) - f(2)}{2} = \frac{f(4) - f(2)}{2} = \frac{5 - 1}{2} = 2$$

However, that is completely wrong bc we Know that the value of the derivative at $x = 2$ is equal to <u>zero</u>

at $h = 1$

$$f'(x) = \frac{f(2+1) - f(2)}{1} = \frac{2 - 1}{1} = 1 \longrightarrow \text{closer to zero}$$

So as h decreases, the closer we will be to reach the <u>ACTUAL</u> value of the derivative

at $h = 0.001$

$$f'(x) = \frac{f(2.001) - f(2)}{0.001} = \frac{1.000001 - 1}{0.001} = 0.001$$

We conclude that

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$ Sub $f(x) = x^2 - 4x + 5$

$$f'(x) = \frac{(x+h)^2 - 4(x+h) + 5 - x^2 + 4x - 5}{h}$$

$$f'(x) = \frac{\cancel{x^2} + 2xh + h^2 \cancel{-4x} - 4h + 5 \cancel{-x^2} \cancel{+4x} - 5}{h}$$

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

$$f'(x) = \lim_{h \to 0} 2x - 4 + h$$

So as h approaches 0

$$f'(x) = 2x - 4$$

In this approach we approximate the derivative based on values of the points in the neighbourhood of the point we wold like to approximate the derivative at.

The accuracy of the finite difference method depends on the accuracy of the points, spacing between the points.

[1] Backward difference

$$f'(x) = \frac{f(x) - f(x-h)}{h}$$

[2] Forward difference

$$f'(x) = \frac{f(x+h) - f(x)}{h}$$

[3] Central difference (uses points that surround x from both sides)

$$f'(x) = \left[\text{Forward} + \text{Backward}\right] \cdot \frac{1}{2}$$

$$\Rightarrow \frac{1}{2}\left[\frac{f(x+h) - f(x)}{h} + \frac{f(x) - f(x-h)}{h}\right] = \frac{f(x+h) - f(x-h)}{2h}$$

2^{nd} Order Numerical Differentiation

$$f''(x) = \frac{f(x_1+h) - 2f(x_1) + f(x_1-h)}{h^2} \qquad x = x_1$$

Example: $f(x) = x\ln(x) + x$ and $x = 0.9, 1.3, 2.1, 2.5, 3.2$. find the approximate of $f''(x) = \frac{1}{x}$ at $x = 1.9$. Also, compute the absolute error.

$$f''(x_1) = \frac{f(x_1+h) - 2f(x_1) + f(x_1-h)}{h^2}$$

Taking the ~~#~~ three points 1.3, 1.9, 2.5 that are equally spaced

$$h = \begin{cases} 1.9 - 1.3 = 0.6 \\ 2.5 - 1.9 = 0.6 \end{cases}$$

$h = 0.6$

$$f''(1.9) = \frac{f(2.5) - 2f(1.9) + f(1.3)}{(0.6)^2}$$

$$= \frac{4.7907 - 6.2391 + 1.6411}{0.36} = 0.5353$$

$$f''(1.9) = \frac{1}{1.9} = 0.5263$$

$$|E| = |0.5263 - 0.5353| = 0.009$$

2] Numerical Integration

I] Simpson's Rule

let f be continous on $[a,b]$ and let n be an even integer.

$$\int_a^b f(x)\,dx = \frac{b-a}{3n}\Big[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) \dots + 4f(x_{n-1}) + f(x_n)\Big]$$

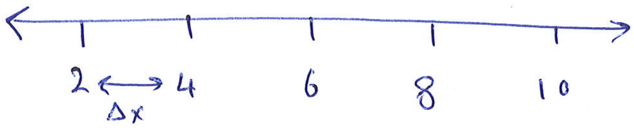
as n approaches ∞, the R.H.S approaches $\int_a^b f(x)\,dx$.

Example: $\int_2^{10} x^3\,dx \qquad n = 4$

$$\Delta x = \frac{b-a}{n}$$

$$\Delta x = \frac{10-2}{4} = 2$$

$$S_n = \frac{\Delta x}{3}\Big[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + f(x_4)\Big]$$



$$S_4 = \frac{2}{3}\Big[f(2) + 4f(4) + 2f(6) + 4f(8) + f(10)\Big]$$

$$= \frac{2}{3}\Big[2^3 + 4(4)^3 + 2(6)^3 + 4(8)^3 + (10)^3\Big]$$

$$= 2496$$

Error bound for simpson's Rule

(6)

$$|E| \le \frac{(b-a)^5}{180\underbrace{n^4}_{\text{number of intervals}}}\Big[\underbrace{\max|f^{4}(x)|}_{K}\Big]$$

$$K \ge |f^{(4)}(x)|$$

for $a \le x \le b$

(1) can be asked to find n

(2) can be asked to find E at given n

Example: How large should we take n in order to guarantee that the Simpson's Rule approximation for $\int_1^2 (1/x)$ is accurate to within 0.0001?

$f(x) = 1/x$

$f'(x) = -\frac{1}{x^2}$

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

$f'''(x) = -6x^{-4}$

$f^{4}(x) = \frac{24}{x^5}$

$1 \le x \le 2$

$K = |f^{4}(x)|$

when choosing K, always choose the maximum possible value

at $x = 1$

$$\boxed{f^{4}(1) = \frac{24}{(1)^5} = 24} \rightarrow \text{max value}$$

at $x = 2$

$$f^{4}(2) = \frac{24}{2^5} = \frac{3}{4}$$

$K = 24$

$$|E| \le \frac{(b-a)^5}{180n^4}(K)$$

$$0.0001 \le \frac{(2-1)^5 \cdot 24}{180n^4}$$

$$n^4 \ge \frac{24(2-1)^5}{180(0.0001)}$$

$$n^4 \ge \frac{4000}{3} \quad \sqrt[4]{\ }$$

$n \ge 6.04$

(1) first round up to the next whole number $= 7$

Therfore $n = 8$

(2) Take the first even number after 7

2 Trapezoidal Rule

let f be continous on $[a, b]$. The Trapezoidal Rule for approximating $\int_a^b f(x)\,dx = \frac{b-a}{2n}\left[f(x_0) + 2f(x_1) + 2f(x_2) + \cdots\right.$ $\left. 2f(x_{n-1}) + f(x_n)\right]$ as $n \to \infty$, the R.H.S approaches

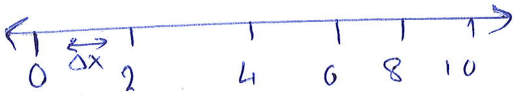
$$\int_a^b f(x)\,dx$$

$$\Delta x = \frac{b-a}{n}$$

$$T_n = \frac{\Delta x}{2}\left[f(x_0) + 2f(x_1) + 2f(x_3) + \cdots + 2f(x_{n-1}) + f(x_n)\right]$$

Example $\int_0^{10} x^2\,dx \qquad n = 5$

$$\frac{\Delta x}{n} = \frac{b-a}{n} = \frac{10-0}{5} = 2$$



$$T_5 = \frac{2}{2}\left[f(0) + 2f(2) + 2f(4) + 2f(6) + 2f(8) + f(10)\right]$$

$$T_5 = \left[0 + 2(4) + 2(16) + 2(36) + 2(64) + 100\right]$$

$$= 340$$

Error bound for Trapezoidal Rule

$$|E| \le \frac{(b-a)^3}{\underset{\text{number of intervals}}{12\underline{n}^2}}\left[\underbrace{\max|f''(x)|}_{K}\right]$$

$$K \ge \left| f^{(2)}(x) \right| \quad \text{for } a \le x \le b$$

$$|E| \le \frac{nKh^3}{12} = \frac{K(b-a)^3}{12n^2} \qquad h = \frac{b-a}{n}$$

$$|E| \le \frac{nK\frac{(b-a)^3}{n^3}}{12} \Longrightarrow |E| \le \frac{K(b-a)^3}{12n^2}$$

Or $|E| \le \frac{h^2(b-a)}{12} f''(x)$

Example: find the number of intervals to $\int_0^2 \frac{dx}{1+x^2}$

$$f(x) = \frac{1}{1+x^2} \qquad (1+x^2)^{-1}$$

$$f'(x) = \frac{-1(2x)}{(1+x^2)^2} = -2x(1+x^2)^{-2} \Longrightarrow$$

$$f''(x) \Rightarrow \cancel{4x(2x)} \qquad u = -2x \quad u' = -2 \qquad v = (1+x^2)^{-2} \quad v' = -2(2x)(1+x^2)^{-3}$$

$$\frac{-2(1+x^2)^{-2} - \cancel{16}\, 8x^2(1+x^2)^{-3}}{(1+x^2)^{-4}}$$

$$\frac{(1+x^2)^{-2}\left(-2 - 8x^2(1+x^2)^{-1}\right)}{(1+x^2)^{-4}}$$

Example: find the number of intervals for $\int_0^2 \frac{dx}{1+x^2}$

$f(x) = (1+x^2)^{-1}$

$E = 5 \times 10^{-6}$

$f'(x) = \frac{-2x}{(1+x^2)^2}$

$f''(x) \Rightarrow \quad u = -2x \quad v = (1+x^2)^2$

$u' = -2 \quad v' = 2(2x)(1+x^2)$

$$\frac{-2(1+x^2)^2 + 8x^2(1+x^2)}{((1+x^2)^2)^2}$$

$$\frac{\cancel{(1+x^2)}(-2(1+x^2) + 8x^2)}{(1+x^2)^{\cancel{4}\,3}}$$

$\boxed{K=2}$

$f''(x) = \frac{-2 - 2x^2 + 8x^2}{(1+x^2)^3}$

$f''(x) = \frac{6x^2 - 2}{(1+x^2)^3}$

at $x = 0$

$|f''(0)| = \left|\frac{6(0)^2 - 2}{(1+0^2)^3}\right|$

max value

$= |-2| = 2$

$f''(1) = \frac{6(1)^2 - 2}{(1+1)^3}$

$= 1/2$

$f''(2) = \frac{6(2)^2 - 2}{(1+2)^3}$

$= \frac{22}{7}$

$|E| \geq \frac{h^2(b-a)}{12} \cdot \cancel{2} f''(x)$

$|E| \geq \frac{h^2(2-0)}{12} \cdot 2 \longrightarrow K$

$|E| \geq \frac{2h^2}{6}$

$|E| \geq \frac{1}{3}h^2$

$\frac{1}{3}h^2 \geq 5 \times 10^{-6}$

$h^2 \geq 1.5 \times 10^{-5}$

$h \geq 0.003873$

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

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

$n = \frac{2}{0.003873}$

$n \geq 516.39$

$n = 517$

OR

$$|E| \geq \frac{K(b-a)^3}{12n^2}$$

$$5\times10^{-6} \geq \frac{2(2-0)^3}{12n^2}$$

$$n^2 \geq \frac{2(2-0)^3}{12(5\times10^{-6})}$$

$$n^2 \geq \frac{800000}{3} \quad \sqrt{\ }$$

$$n \geq 516.39$$

$$\boxed{n = 517}$$