Chapter 3

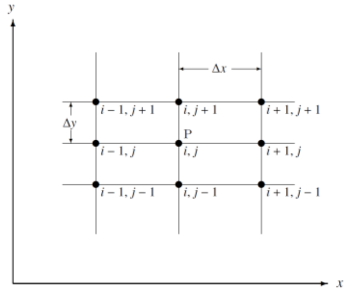
An Introduction to

Finite Difference Calculus

First Session Contents:

1) Approximation of Derivatives
2) Order Symbols
3) High-Order Derivatives
4) Richardson's Extrapolation (The deferred approach to the limit)

Discretization of Computational Domain



Taylor Series Expansion

Brook Taylor

Born: August 18, 1685
Municipal Borough of Edmonton

Died: November 30, 1731
London, United Kingdom

Education: St John's College, Cambridge,
University of Cambridge

Brook Taylor was an English mathematician who is best known for Taylor's theorem and the Taylor series

Taylor Series Expansion

If a function $f(x)$ is infinitely differentiable at $x = x_0$, we can express:

$$f(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)^2 + \dots = \sum_{n=0}^{\infty} a_n (x - x_0)^n$$

To find the coefficients, initially, we put $x = x_0$:

$$a_0 = f(x_0)$$

Taking the first derivative gives:

$$f'(x) = a_1 + 2a_2(x - x_0) + 3a_3(x - x_0)^2 + 4a_4(x - x_0)^3 + \dots$$

So,

$$a_1 = f'(x_0)$$

Taylor Series Expansion

Similarly, we take derivative again:

$$f''(x) = 2!a_2 + 3!a_3(x - x_0) + 4 \times 3 a_4 (x - x_0)^2 + \ldots$$

Putting $x = x_0$ results in:

$$a_2 = \frac{1}{2!} f''(x_0)$$

In this way, we may conclude:

$$a_n = \frac{1}{n!} f^{(n)}(x_0) \qquad \text{where} \qquad f^{(n)} = \frac{d^n f}{dx^n}$$

Eventually, we can write Taylor Series Expansion of $f(x)$ at $x = x_0$ as:

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n$$

5

Taylor Series Expansion

Now, we can write Taylor Series Expansion for other functions.

since

$$\frac{d}{dx}(\sin x) = \cos x, \qquad \frac{d}{dx}(\cos x) = -\sin x$$

So, we have:

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \ldots = \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n+1}}{(2n+1)!}$$

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \ldots = \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n}}{(2n)!}$$

As Taylor Series Expansion of $\sin(x)$ and $\cos(x)$ at $x = x_0$.

6

Taylor Series Expansion

Also, we already know

$$\frac{d}{dx}(e^x) = e^x$$

So, the its Taylor Series Expansion is:

$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \ldots = \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

To give another example, recall that:

$$\frac{d}{dx}[\ln(1 + x)] = (1 + x)^{-1} \qquad \frac{d}{dx}(1 + x)^{-n} = -n(1 + x)^{-n-1}$$

Hence:

$$\ln(1 + x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \ldots = \sum_{n=1}^{\infty} \frac{(-1)^{n+1} x^n}{n}$$

7

Order Symbols

Instead of saying that $\sin(x)$ tends to zero at the same rate that x tends to zero, we say:

Big "Oh"

$$\sin x = O(x) \qquad \text{as} \qquad x \to 0$$

In general:

$$f(x) = O[g(x)] \qquad \text{as} \qquad x \to 0$$

If

$$\lim_{x \to 0} \frac{f(x)}{g(x)} = A \qquad \text{and} \qquad 0 < |A| < \infty$$

$$\sin x = O(x) \qquad \text{as} \qquad x \to 0$$

8

Order Symbols

For example:

$$\sin x = O(x) \quad \text{as} \quad x \to 0$$

since $\lim_{x\to 0} \frac{\sin x}{x} = 1$

Other examples for $x \to 0$

$$\cos x = O(1) \qquad \tan x = O(x)$$

$$\cos x - 1 = O(x^2) \qquad \cot x = O(x^{-1})$$

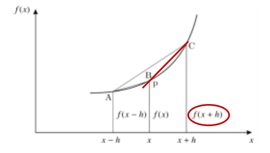
Finite Difference Calculus

Let's write Taylor Series Expansion for $f(x+h)$ at x

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \ldots$$

So,

$$f'(x) = \underbrace{\frac{f(x+h) - f(x)}{h}}_{\text{Finite Difference}} \underbrace{- \frac{h}{2!}f''(x) - \frac{h^2}{3!}f'''(x) + \ldots}_{\text{Truncation Error}}$$



Collecting all terms of $O(h)$:

$$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h) \quad \text{Forward Difference}$$

Let's re-write based on index notation:$(h \to 0)$

$$f_i'(x) = \frac{f_{i+1} - f_i}{h} + O(h) \qquad f_{i+1} = f(x+h), \qquad f_i = f(x)$$

Finite Difference Calculus

Defining "Forward Difference" Operator:

$$\Delta f_i = f_{i+1} - f_i$$

We have:

$$f_i' = \frac{\Delta f_i}{h} + \text{T.E.}$$

Truncation Error

NOTE:

Truncation error is the difference between the derivative and its finite difference Approximation.

For the "Forward Difference":

$$\text{T.E.} = O(h) = O(\Delta x) \quad \text{as} \quad x \to 0$$

$$\lim_{\Delta x \to 0} \frac{\text{T.E.}}{\Delta x} = \text{Limited}$$

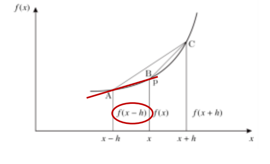
Finite Difference Calculus

Similarly for $f(x-h)$ at P we have

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \ldots$$

So,

$$f'(x) = \underbrace{\frac{f(x) - f(x-h)}{h}}_{\text{Finite Difference}} \underbrace{+ \frac{h}{2!}f''(x) - \frac{h^2}{3!}f'''(x) + \ldots}_{\text{Truncation Error}}$$



Collecting all terms of $O(h)$:

$$f'(x) = \frac{f(x) - f(x-h)}{h} + O(h) \quad \textbf{Backward}\text{ Difference}$$

Let's re-write based on index notation:$(h \to 0)$

$$f_i'(x) = \frac{f_i - f_{i-1}}{h} + O(h)$$

Finite Difference Calculus

Defining “**Backward** Difference” Operator:

$$\nabla f_i = f_i - f_{i-1}$$

We have: Truncation Error

$$f_i' = \frac{\nabla f_i}{h} + O(h)$$

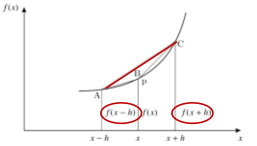
13

Finite Difference Calculus

Let's re-write both Taylor Series Expansion at P

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \dots$$

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \dots$$



So,

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3}f'''(x) + \dots$$

We may write $f'(x)$ explicitely:

$$f'(x) = \underbrace{\frac{f(x+h) - f(x-h)}{2h}}_{\text{Finite Difference}} \underbrace{- \frac{h^2}{6}f'''(x) + \dots}_{\text{Truncation Error}}$$

14

Finite Difference Calculus

$$f'(x) = \underbrace{\frac{f(x+h) - f(x-h)}{2h}}_{\text{Finite Difference}} \underbrace{- \frac{h^2}{6}f'''(x) + \dots}_{\text{Truncation Error}}$$

Collecting all terms of $O(h^2)$:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$ **Central** Difference

Based on index notation we have: $f_i' = \dfrac{f_{i+1} - f_{i-1}}{2h} + O(h^2)$

15

Higher-Order Derivatives

Let's take a look at these two Taylor Series:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \dots \times(-2)$$

$$f(x+2h) = f(x) + 2hf'(x) + \frac{(2h)^2}{2!}f''(x) + \frac{(2h)^3}{3!}f'''(x) + \dots$$

So, we have:

$$-2f(x+h) + f(x+2h) = -f(x) + h^2 f''(x) + h^3 f'''(x) + \dots$$

Solving for $f''(x)$ yields:

$$f''(x) = \frac{f(x+2h) - 2f(x+h) + f(x)}{h^2} + O(h) \quad \text{or} \quad f_i'' = \frac{f_{i+2} - 2f_{i+1} + f_i}{h^2} + O(h)$$

16

Higher-Order Derivatives

Recall:

$$\Delta f_i = f_{i+1} - f_i$$

So,

$$\Delta(\Delta f_i) = \Delta f_{i+1} - \Delta f_i \quad = f_{i+2} - f_{i+1} - (f_{i+1} - f_i) = f_{i+2} - 2f_{i+1} + f_i$$

Therefore, we can write forward difference for $f''(x)$ in operator notation

$$f_i'' = \frac{\Delta^2 f_i}{h^2} + O(h)$$

Similarly, backward difference for $f''(x)$ in operator notation would be:

$$f_i'' = \frac{\nabla^2 f_i}{h^2} + O(h)$$

17

Higher-Order Forward and Backward Difference

Recall:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \dots$$

Solving for $f'(x)$ gives:

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2}\left[\frac{f(x+2h) - 2f(x+h) + f(x)}{h^2} + O(h)\right] + O(h^2)$$

Simplifying of this equation results in:

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

or:

$$f_i' = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h} + O(h^2)$$

18

Finite Difference Discretization

Forward Difference $O(h)$

	f_i	f_{i+1}	f_{i+2}	f_{i+3}	f_{i+4}
$hf'(x_i) =$	-1	1			
$h^2f''(x_i) =$	1	-2	1		
$h^3f'''(x_i) =$	-1	3	-3	1	
$h^4f^{iv}(x_i) =$	1	-4	6	-4	1

$+ O(h)$

Backward Difference $O(h)$

	f_{i-4}	f_{i-3}	f_{i-2}	f_{i-1}	f_i
$hf'(x_i) =$				-1	1
$h^2f''(x_i) =$			1	-2	1
$h^3f'''(x_i) =$		-1	3	-3	1
$h^4f^{iv}(x_i) =$	1	-4	6	-4	1

$+ O(h)$

Central Difference $O(h^2)$

	f_{i-2}	f_{i-1}	f_i	f_{i+1}	f_{i+2}
$2hf'(x_i) =$		-1	0	1	
$h^2f''(x_i) =$		1	-2	1	
$2h^3f'''(x_i) =$	1	-2	0	2	-1
$h^4f^{iv}(x_i) =$	1	-4	6	-4	1

$+ O(h^2)$

19

Finite Difference Discretization

Forward Difference $O(h)$

	f_i	f_{i+1}	f_{i+2}	f_{i+3}	f_{i+4}	f_{i+5}
$2hf'(x_i) =$	-3	4	-1			
$h^2f''(x_i) =$	2	-5	4	-1		
$2h^3f'''(x_i) =$	-5	18	-24	14	-3	
$h^4f^{iv}(x_i) =$	3	-14	26	-24	11	-2

$+ O(h^2)$

Backward Difference $O(h)$

	f_{i-5}	f_{i-4}	f_{i-3}	f_{i-2}	f_{i-1}	f_i
$2hf'(x_i) =$				1	-4	3
$h^2f''(x_i) =$			-1	4	-5	2
$2h^3f'''(x_i) =$		3	-14	24	-18	5
$h^4f^{iv}(x_i) =$	-2	11	-24	26	-14	3

$+ O(h^2)$

Central Difference $O(h^4)$

	f_{i-3}	f_{i-2}	f_{i-1}	f_i	f_{i+1}	f_{i+2}	f_{i+3}
$12hf'(x_i) =$		1	-8	0	8	-1	
$12h^2f''(x_i) =$		-1	16	-30	16	-1	
$8h^3f'''(x_i) =$	1	-8	13	0	-13	8	-1
$6h^4f^{iv}(x_i) =$	-1	12	-39	56	-39	12	-1

$+ O(h^4)$

20

Example1

If $f(x) = e^x$ find $f'(1)$ using forward difference, choosing $h = 0.1$

$$f'(۱) = \frac{e^{۱٫۱} - e^{۱٫۰}}{۰٫۱} + O(۰٫۱) = \frac{۳٫۰۰۴۱۶۶ - ۲٫۷۱۸۲۸۲}{۰٫۱} + O(۰٫۱)$$

$f'(۱) \simeq ۲٫۸۵۸۸۴$ **Forward Difference**

Using Central Difference:

$$f'(۱) = \frac{e^{۱٫۱} - e^{۰٫۹}}{۲(۰٫۱)} + O[(۰٫۱)^۲] = \frac{۳٫۰۰۴۱۶۶ - ۲٫۴۵۹۶۰۳}{۰٫۲} + O[(۰٫۱)^۲]$$

$f'(۱) \simeq ۲٫۷۲۲۸۲$ **Central Difference**

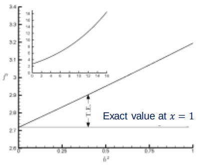
	Exact	Forward Difference	Central Difference
Value	2.718282	2.85844	2.72282
Relative Error	-	5.15%	0.17%

Example1

Now, let's choose $h = 0.05$

$$f'(۱) = \frac{e^{۱٫۰۵} - e^{۰٫۹۵}}{۲(۰٫۰۵)} =$$

$$= \frac{۲٫۸۵۷۶۵۱ - ۲٫۸۵۷۱۰}{۰٫۱} = ۲٫۷۱۹۴۱۵$$



Slope of line in f'- h^2 coordinate system is:

$$m = \frac{f'_۲ - f'_۱}{h_۲^۲ - h_۱^۲} = \frac{f'_۱ - f'_e}{h_۱^۲ - ۰}$$

So, we can find exact value of $f'(x = 1)$:

$$f'_e = f'_۱ - mh_۱^۲ = ۲٫۷۱۸۲۸۲$$

Example2

If $f(x) = \sin(x)$ find $f'(1)$ using central difference, choosing $h = 0.2$

$$f'(۱) = \frac{\sin(۱٫۲) - \sin(۰٫۸)}{۲(۰٫۲)} + O[(۰٫۲)^۲]$$

$$f'(۱) = \frac{۰٫۹۳۲۰۳۹ - ۰٫۷۱۷۳۵۶}{۰٫۴} = ۰٫۵۳۶۷۱$$

Let's choose $h = 0.1$

$$f'(۱) = \frac{\sin(۱٫۱) - \sin(۰٫۹)}{۲(۰٫۱)} + O[(۰٫۱)^۲]$$

$$f'(۱) = \frac{۰٫۸۹۱۲۰۷ - ۰٫۷۸۳۳۲۷}{۰٫۲} = ۰٫۵۳۹۴۰$$

Let's choose $h = 0.05$

$$f'(۱) = \frac{\sin(۱٫۰۵) - \sin(۰٫۹۵)}{۲(۰٫۰۵)} + O[(۰٫۰۵)^۲]$$

$$f'(۱) = \frac{۰٫۸۶۷۴۲۳ - ۰٫۸۱۳۴۱۶}{۰٫۱} = ۰٫۵۴۰۰۷$$

Example2

The exact answer is:

$$f'(۱) = \cos(۱) = ۰٫۵۴۰۳۰$$

Using the method introduced in previous example:

$$m = \frac{f'_۲ - f'_۱}{h_۲^۲ - h_۱^۲} = \frac{f'_۱ - f'_e}{h_۱^۲ - ۰}$$

Which gives:

$$f'_e = f'_۱ - mh_۱^۲ = ۰٫۵۴۰۲۹$$

Example3

Consider $f(x) = \sin(10\pi x)$, find $f'(0)$ by choosing $h = 0.2$

The exact answer is:

$$f'(x) = 10\pi \cos 10\pi x$$

So,

$$f'(0) = 10\pi \cos 10\pi(0) = 31.41593$$

Forward Difference

$$f'(0) = \frac{f(0.2) - f(0)}{0.2} + O(0.2)$$
$$= \frac{\sin 10\pi(0.2) - \sin 10\pi(0)}{0.2} + O(0.2) = \frac{\sin 2\pi - 0}{0.2} = 0$$

Central Difference

$$f'(0) = \frac{f(0.2) - f(-0.2)}{2(0.2)} + O[(0.2)^2]$$
$$= \frac{\sin 10\pi(0.2) - \sin 10\pi(-0.2)}{0.4} + O[(0.2)^2] = 0$$

Example3

Consider $f(x) = \sin(10\pi x)$, find $f'(0)$ by choosing $h = 0.2$

The exact answer is:

$$f'(x) = 10\pi \cos 10\pi x$$

So,

$$f'(0) = 10\pi \cos 10\pi(0) = 31.41593$$

Problem?
$T = h$

Forward Difference

$$f'(0) = \frac{f(0.2) - f(0)}{0.2} + O(0.2)$$
$$= \frac{\sin 10\pi(0.2) - \sin 10\pi(0)}{0.2} + O(0.2) = \frac{\sin 2\pi - 0}{0.2} = 0$$

Central Difference

$$f'(0) = \frac{f(0.2) - f(-0.2)}{2(0.2)} + O[(0.2)^2]$$
$$= \frac{\sin 10\pi(0.2) - \sin 10\pi(-0.2)}{0.4} + O[(0.2)^2] = 0$$

Richardson Extrapolation

Lewis Fry Richardson

Born: October 11, 1881
Newcastle upon Tyne, United Kingdom

Died: September 30, 1953
Kilmun, United Kingdom

Education: Bootham School, Newcastle University, King's College, Cambridge, University of London, Durham University

He was an English mathematician, physicist, meteorologist, psychologist and pacifist who pioneered modern mathematical techniques of weather forecasting.

Question Is it possible to obtain the exact solution from numerical solution?

Richardson Extrapolation

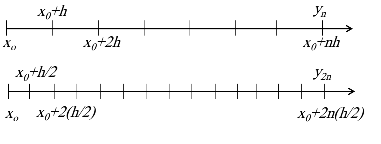
$$\begin{cases} y' = F(x, y) \\ y(x_0) = f_0 \end{cases} \Rightarrow y = f(x)$$

$$\underbrace{f(x)}_{\text{Analytical Solution}} = \underbrace{y_n(h)}_{\text{Numerical Solution}} + O(h) = y_n(h) + \underbrace{Ch + M(h)}_{\text{T.E.}}$$

$M(h) \propto h^2$

C is constant

$$h \longrightarrow h/2 \qquad f(x) = y_{2n}(h/2) + Ch/2 + M(h/2)$$



Richardson Extrapolation

$$f(x) = y_n(h) + O(h) = y_n(h) + Ch + M(h)$$

Regardless of h^2 terms, C can be obtained as $\boxed{C = \frac{f - y_n}{h}}$

By Replacing, C in

$$f(x) = y_{2n}(h/2) + Ch/2$$

we have

$$f(x) = y_{2n}(h/2) + \left[y_{2n}(h/2) - y_n(h)\right]$$

Consequently, the error for step size of $h/2$ can be determined as

$$\boxed{f(x) - y_{2n}(h/2) \cong y_{2n}(h/2) - y_n(h)}$$

29

Richardson Extrapolation

Second order approximation

$$f(x) = y_n + Ch^2 \longrightarrow C = \frac{f - y_n}{h^2} \longrightarrow f(x) = y_{2n} + C(h^2/4)$$

$$f = y_{2n} + \frac{f - y_n}{h^2}\frac{h^2}{4} = y_{2n} + \frac{f - y_n}{4}$$

$$f = \frac{4}{3}y_{2n} - \frac{1}{3}y_n = \frac{1}{3}(4y_{2n} - y_n)$$

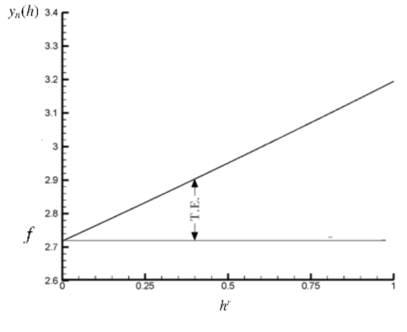
Higher order approximation

$$f(x) = y_n(h) + Ch^r \longrightarrow C = \frac{f - y_n}{h^r} \longrightarrow f(x) = y_{2n}(h/2) + C(h/2)^r$$

$$f = y_{2n} + \frac{f - y_n}{h^r}\frac{h^r}{2^r} = y_{2n} + \frac{1}{2^r}f - \frac{1}{2^r}y_n$$

$$f = \frac{2^r}{2^r - 1}y_{2n} - \frac{1}{2^r - 1}y_n$$

30



31