Scientific Computing II, Semester I

Walter Mudzimbabwe

Presentation Outline

Motivation

The following data was recorded during a chemical reaction.

t, min	0	15	30	45	60	90	120
V, barrels	0.5	0.65	0.73	0.88	1.03	1.14	1.30

At what rate is V growing? i.e., Calculate $\dfrac{dV}{dt}$.

Definition of derivative

The derivative of $y = f(x)$ is:

$$\frac{dy}{dx} = f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}. \tag{1}$$

Taylor series expansion of "$f(x+h)$ **about** x":

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2}h^2 + \frac{f'''(x)}{6}h^3 + \ldots, \tag{2}$$

Therefore

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{f''(x)}{2}h + \ldots \approx \frac{f(x+h) - f(x)}{h}, \tag{3}$$

which is the **Forward Difference Formula**.
This approximation is **first-order** $\mathcal{O}(h)$ and the truncation error is $-\frac{h}{2}f''(\epsilon)$ for $x < \epsilon < x + h$.

Definition of derivative

Again Taylor series expansion of "$f(x-h)$ **about** x":

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)}{2}h^2 - \frac{f'''(x)}{6}h^3 + \dots. \quad (4)$$

Therefore

$$f'(x) = \frac{f(x) - f(x-h)}{h} + \frac{f''(x)}{2}h + \dots \approx \frac{f(x) - f(x-h)}{h}, \quad (5)$$

which is the **Backward Difference Formula**.
This approximation is also $\mathcal{O}(h)$ and the truncation error is $\frac{h}{2}f''(\epsilon)$ for $x - h < \epsilon < x$.

Central difference

Subtracting (4) from (2) gives the **Central Difference Formula**:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{f'''(x)}{6}h^2 + \dots$$
$$\approx \frac{f(x+h) - f(x-h)}{2h}, \qquad (6)$$

which is second order accurate, i.e. $\mathcal{O}(h^2)$ since the truncation error is $-\frac{h^2}{6}f'''(\epsilon)$ for $x - h < \epsilon < x + h$. This approximation is a two-point formula.

$f''(x)$

Adding (2) to (4) gives the **Central Difference Formula** for $f''(x)$:

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{f^4(x)}{12}h^2 + \dots$$

$$\approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}, \qquad (7)$$

which is second order accurate $\mathcal{O}(h^2)$ and the truncation error here is $-\frac{h^2}{12}f^{iv}(\epsilon)$. This approximation is a three-point formula.

Example

Problem: Approximate $f'(1)$ for $f(x) = x^2\cos(x)$ using the central difference formula using $h = 0.1, 0.05, 0.025, 0.0125$.
Solution:

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

So if $h = 0.1$ and $x = 1$ then

$$f'(1) \approx \frac{f(1+0.1) - f(1-0.1)}{2(0.1)}$$
$$= 0.2267361631$$

Repeat for $h = 0.05, 0.025, 0.0125$.
True solution: $f'(x) = -x^2\sin(x) + 2x\cos(x)$ so $f'(1) = -\sin(1) + 2\cos(1) = 0.2391336269$.

Richardson's Extrapolation 1

Suppose we have some initial approximation $F_n(h)$, of order n, then we can obtain a general $(n+1)^{th}$ order formula $F_{n+1}(h)$:

$$F_{n+1}(h) = \frac{2^n F_n(h/2) - F_n(h)}{2^n - 1}.$$

Example: Suppose $F_1(h) = f'(x) = \dfrac{f(x+h) - f(x)}{h}$. Then

$$\begin{aligned} F_2(h) &= \frac{2F_1(h/2) - F_1(h)}{2-1} \\ &= 2\frac{f(x+h/2) - f(x)}{h/2} - \frac{f(x+h) - f(x)}{h} \\ &= \frac{4f(x+h/2) - 3f(x) - f(x+h)}{h}, \quad \mathcal{O}(h^2) \end{aligned}$$

Execise: Verify that the formula above is $\mathcal{O}(h^2)$

Richardson's Extrapolation 2

Richardson's Extrapolation can be written as:

$$F_j^i = \frac{1}{4^j - 1}\left(4^j F_{j-1}^i - F_{j-1}^{i-1}\right), \; j = 1, 2, \dots m, \;\; i = 1, 2, \dots, n.$$

Here j denotes iteration of the extrapolation and i the particular stepsize.

Example: Build a Richardson's extrapolation table for $f(x) = x^2 \cos(x)$ to evaluate $f'(1)$ for $h = 0.1, 0.05, 0.025, 0.0125$.

From the formula:

$$F_j^i = \frac{1}{4^j - 1}\left(4^j F_{j-1}^i - F_{j-1}^{i-1}\right)$$

we have

$$\begin{aligned}
F_1^2 &= \frac{1}{3}(4F_0^2 - F_0^1) \\
F_1^3 &= \frac{1}{3}(4F_0^3 - F_0^2) \\
F_1^4 &= \frac{1}{3}(4F_0^4 - F_0^3) \\
F_2^3 &= \frac{1}{15}(16F_1^3 - F_1^2) \\
F_2^4 &= \frac{1}{15}(16F_1^4 - F_1^3) \\
F_3^4 &= \frac{1}{63}(64F_2^4 - F_2^3)
\end{aligned}$$

ctd

i	h_i	F_0^i	F_1^i	F_2^i	F_3^i
1	0.1	0.226736			
2	0.05	0.236031	0.239129		
3	0.025	0.238358	0.239134	0.239134	
4	0.0125	0.238940	0.239134	0.239134	0.239134

F_0^i is initial approximation (central difference in your notes).