Ch 6 Numerical Differentiation

* In this chapter, we study formulas to approximate the derivatives $f'(x_0)$, $f''(x_0)$, $f'''(x_0)$, ...

* For example • We know $f'(x_0) = \lim_{h\to 0} \frac{f(x_0+h)-f(x_0)}{h}$

  • Here h is a step size

  • This limit gives exact value for $f'(x_0)$

  • We need to replace $\lim_{h\to 0} \frac{f(x_0+h)-f(x_0)}{h}$ by a Difference Formula (D.F) to approximate $f'(x_0)$.

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* We study three types of Difference Formulas:

  1. Central Difference formula (C.D.F)
  2. Backward Difference Formula (B.D.F)
  3. Forward Difference Formula (F.D.F)

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* Notation • $f_k = f(x_0 + kh)$, $k = 0, \pm 1, \pm 2, \pm 3, \ldots$

  • That is,

$$
\begin{aligned}
f_0 &= f(x_0)\\
f_1 &= f(x_0+h)\\
f_{-1} &= f(x_0-h)\\
f_2 &= f(x_0+2h)\\
f_{-2} &= f(x_0-2h)\\
&\vdots
\end{aligned}
$$

D.F for $f'(x_0)$

1 C.D.F of order $o(h^2)$:

$$f'(x_0) \approx \frac{f(x_0+h)-f(x_0-h)}{2h} + E_{trun}(f,h)$$

$$= \frac{f_1 - f_{-1}}{2h} + \frac{-h^2 f'''(c)}{6}$$

2 F.D.F of order $o(h^2)$:

$$f'(x_0) \approx \frac{-3f_0 + 4f_1 - f_2}{2h} + \frac{h^2 f'''(c)}{3}$$

3 B.D.F of order $o(h^2)$

$$f'(x_0) \approx \frac{3f_0 - 4f_{-1} + f_{-2}}{2h} + \frac{h^2 f'''(c)}{3}$$

4 C.D.F of order $o(h^4)$

$$f'(x_0) \approx \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h} + \frac{h^4 f^{(5)}(c)}{30}$$

Remark

- $E_{trun}(f,h)$ is called the truncation error.
- In case of 1, 2, 3 $\Rightarrow$ f is assumed to be $C^3[a,b]$
- In case of 4 $\Rightarrow$ f is assumed to be $C^5[a,b]$
- And so on ...

D.F for $f''(x_0)$

1. C.D.F of order $O(h^2)$:

$$f''(x_0) \approx \frac{f_1 - 2f_0 + f_{-1}}{h^2} + \frac{-h^2 f^{(4)}(c)}{12}$$

2. F.D.F of order $O(h^2)$:

$$f''(x_0) \approx \frac{2f_0 - 5f_1 + 4f_2 - f_3}{h^2} + \frac{11 h^2 f^{(4)}(c)}{12}$$

3. B.D.F of order $O(h^2)$

$$f''(x_0) \approx \frac{2f_0 - 5f_{-1} + 4f_{-2} - f_{-3}}{h^2} + \frac{11 h^2 f^{(4)}(c)}{12}$$

4. C.D.F of order $O(h^4)$:

$$f''(x_0) = \frac{-f_2 + 16f_1 - 30f_0 + 16f_{-1} - f_{-2}}{12h^2} + \frac{h^4 f^{(6)}(c)}{90}$$

Remark To derive any of these D.F's for $f'(x_0)$ and $f''(x_0)$, we use:

① Taylor's Expansion or

② Lagrange Interpolation or

③ Newton Interpolation.

D.F for $f'(x_0)$

$\boxed{1}$ C.D.F of order $o(h^2)$: $f'(x_0) = \dfrac{f_1 - f_{-1}}{2h} - \dfrac{h^2 f'''(c)}{6}$

$\boxed{2}$ F.D.F of order $o(h^2)$: $f'(x_0) = \dfrac{-3f_0 + 4f_1 - f_2}{2h} + \dfrac{h^2 f'''(c)}{3}$

$\boxed{3}$ B.D.F of order $o(h^2)$: $f'(x_0) = \dfrac{3f_0 - 4f_{-1} + f_{-2}}{2h} + \dfrac{h^2 f'''(c)}{3}$

$\boxed{4}$ C.D.F of order $o(h^4)$: $f'(x_0) = \dfrac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h} + \dfrac{h^4 f^{(5)}(c)}{30}$

D.F for $f''(x_0)$

$\boxed{1}$ C.D.F of order $o(h^2)$: $f''(x_0) = \dfrac{f_1 - 2f_0 + f_{-1}}{h^2} - \dfrac{h^2 f^{(4)}(c)}{12}$

$\boxed{2}$ F.D.F of order $o(h^2)$: $f''(x_0) = \dfrac{2f_0 - 5f_1 + 4f_2 - f_3}{h^2} + \dfrac{11 h^2 f^{(4)}(c)}{12}$

$\boxed{3}$ B.D.F of order $o(h^2)$: $f''(x_0) = \dfrac{2f_0 - 5f_{-1} + 4f_{-2} - f_{-3}}{h^2} + \dfrac{11 h^2 f^{(4)}(c)}{12}$

$\boxed{4}$ C.D.F of order $o(h^4)$: $f''(x_0) = \dfrac{-f_2 + 16f_1 - 30f_0 + 16f_{-1} - f_{-2}}{12h^2} + \dfrac{h^4 f^{(6)}(c)}{90}$

Exp Consider the following points:

$(2,-1), (2.1, 2), (2.2, -1.5), (2.3, 0), (2.4, 2)$

1. Estimate $f'(2.1)$ using C.D.F of order $O(h^2)$
2. Estimate $f'(2.2)$ using F.D.F of order $O(h^2)$

Clearly $h = 0.1$

$\boxed{1}$ $$f'(2.1) \approx \frac{f_1 - f_{-1}}{2h} = \frac{f(2.1+0.1) - f(2.1-0.1)}{2(0.1)}$$

$$= \frac{f(2.2) - f(2)}{0.2} = \frac{-1.5 - -1}{0.2} = \frac{-0.5}{0.2} = -2.5$$

$\boxed{2}$ $$f'(2.2) \approx \frac{-3f_0 + 4f_1 - f_2}{2h} = \frac{-3f(2.2) + 4f(2.3) - f(2.4)}{2(0.1)}$$

$$= \frac{-3(-1.5) + 4(0) - 2}{0.2} = \frac{2.5}{0.2} = 12.5$$

Exp Let $f(x) = e^x$. Estimate $f'(1)$ using B.D.F of order $O(h^2)$ with $\boxed{i}$ $h = 0.01$ $\boxed{ii}$ $h = 0.001$

$$f'(1) \approx \frac{3f_0 - 4f_{-1} + f_{-2}}{2h} = \frac{3f(1) - 4f(1-h) + f(1-2h)}{2h}$$

$\boxed{i}$ $$f'(1) = \frac{3f(1) - 4f(0.99) + f(0.98)}{0.02} = \frac{3e - 4e^{0.99} + e^{0.98}}{0.02}$$

$$= 2.7181918955$$

$\boxed{ii}$ $$f'(1) = \frac{3f(1) - 4f(0.999) + f(0.998)}{0.02} = \frac{3e - 4e^{0.999} + e^{0.998}}{0.002}$$

$$= 2.718280923$$

Exp Let $f(x) = \sin x$

1. Estimate $f'(0)$ using C.D.F of order $O(h^4)$ with step size $h = 0.01$
2. Estimate $f'(3)$ using B.D.F of order $O((0.1)^2)$.

1. $$f'(0) \approx \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h}$$

$$= \frac{-f(0.02) + 8f(0.01) - 8f(-0.01) + f(-0.02)}{12(0.01)}$$

$$= \frac{-2\sin(0.02) + 16\sin 0.01}{0.12} \approx \frac{0.120061199}{0.12} = 1.00051$$

2. $h = 0.1$, $x_0 = 3$ $\Rightarrow$ $$f'(3) \approx \frac{3f_0 - 4f_{-1} + f_{-2}}{2h}$$

$$= \frac{3f(3) - 4f(2.9) + f(2.8)}{2(0.1)}$$

$$= \frac{3\sin 3 - 4\sin(2.9) + \sin(2.8)}{0.2}$$

$$= -0.9939715075$$

Note that the true values are:

$f'(x) = \cos x$

$f'(0) = \cos 0 = 1$

$f'(3) = \cos 3 = -0.9902072488$

Exp Consider the following table:

t	1	1.3	1.6	1.9
D	10	30	60	100

where t : time
D : distance

1. Estimate the velocity at $t=1.6$ using C.D.F of $O(h^2)$
2. Estimate the acceleration at $t=1.3$ using C.D.F of $O(h^2)$
3. Estimate the velocity at $t=1.6$ using F.D.F of $O(h^2)$.

$h = 0.3 \Rightarrow$

1. $$v(t_0) = D'(t_0) \approx \frac{D_1 - D_{-1}}{2h} = \frac{D(t_0+h) - D(t_0-h)}{2h}$$

$t_0 = 1.6$

$$D'(1.6) \approx \frac{D(1.6+0.3) - D(1.6-0.3)}{2(0.3)} = \frac{D(1.9) - D(1.3)}{0.6}$$

$$= \frac{100-30}{0.6} = \frac{70}{0.6} = 116.67$$

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2. $$a(t_0) = D''(t_0) \approx \frac{D_1 - 2D_0 + D_{-1}}{h^2} = \frac{D(1.6) - 2D(1.3) + D(1)}{(0.3)^2}$$

$t_0 = 1.3$

$$= \frac{60 - 2(30) + 10}{0.09} = 111.11$$

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3. $$v(t_0) = D'(t_0) \approx \frac{-3\overset{\checkmark}{D_0} + 4\overset{\checkmark}{D_1} - \overset{\times}{D_2}}{2h}$$ not possible

$t_0 = 1.6$

Derivation of D.F's

Bak to Remark page 127

- Recall Taylor's expansion of $f(x)$ about x_0:

$$f(x) = f(x_0) + f'(x_0)(x-x_0) + \frac{f''(x_0)}{2!}(x-x_0)^2 + \frac{f'''(x_0)}{3!}(x-x_0)^3 + \cdots$$

- Clearly $\Rightarrow$ when $x = x_0 + h \Rightarrow x - x_0 = h \Rightarrow$

$$f_1 = f(x_0+h) = f(x_0) + h f'(x_0) + \frac{h^2}{2!} f''(x_0) + \frac{h^3}{3!} f'''(x_0) + \cdots$$

$$f_{-1} = f(x_0-h) = f(x_0) - h f'(x_0) + \frac{h^2}{2!} f''(x_0) - \frac{h^3}{3!} f'''(x_0) + \cdots$$

$$f_2 = f(x_0+2h) = f(x_0) + 2h f'(x_0) + \frac{(2h)^2}{2!} f''(x_0) + \frac{(2h)^3}{3!} f'''(x_0) + \cdots$$

$$f_{-2} = f(x_0-2h) = f(x_0) - 2h f'(x_0) + \frac{(2h)^2}{2!} f''(x_0) - \frac{(2h)^3}{3!} f'''(x_0) + \cdots$$

$$\vdots$$

$$f_k = f(x_0+kh) = f_0 + kh f'(x_0) + \frac{(kh)^2}{2!} f''(x_0) + \frac{(kh)^3}{3!} f'''(x_0) + \cdots \quad \text{where } k = 0, \pm 1, \pm 2, \ldots$$

Exp Derive the C.D.F of order $O(h^2)$ for $f'(x_0)$ using Taylor's Expansion.

- $f'(x_0) \approx \dfrac{f_1 - f_{-1}}{2h} + \dfrac{-h^2 f'''(c)}{6}$
- Note that $f_1 = f_0 + h f'(x_0) + \dfrac{h^2}{2} f''(x_0) + \dfrac{h^3}{3!} f'''(c)$ and

$$f_{-1} = f_0 - h f'(x_0) + \frac{h^2}{2} f''(x_0) - \frac{h^3}{3!} f'''(c)$$

- Hence, $f_1 - f_{-1} = 2h f'(x_0) + \dfrac{2h^3}{6} f'''(c)$
- That is $\Rightarrow$ $f'(x_0) = \dfrac{f_1 - f_{-1}}{2h} - \dfrac{h^2 f'''(c)}{6}$

Exp Derive the C.D.F of order $O(h^2)$ for $f''(x)$ using Taylor's expansion.

$$f''(x_0) \doteq \frac{f_1 - 2f_0 + f_{-1}}{h^2} + \frac{-h^2 f^{(4)}(c)}{12}$$

- Note that

$$f_1 = f_0 + \cancel{h f'(x_0)} + \frac{h^2}{2!} f''(x_0) + \cancel{\frac{h^3}{3!} f'''(x_0)} + \frac{h^4}{4!} f^{(4)}(c)$$

$$f_{-1} = f_0 - \cancel{h f'(x_0)} + \frac{h^2}{2!} f''(x_0) - \cancel{\frac{h^3}{3!} f'''(x_0)} + \frac{h^4}{4!} f^{(4)}(c)$$

- Adding these equations $\Rightarrow$

$$f_1 + f_{-1} = 2f_0 + h^2 f''(x_0) + \frac{h^4}{12} f^{(4)}(c)$$

- Solving for $f''(x_0) \Rightarrow$

$$f''(x_0) = \frac{f_1 - 2f_0 + f_{-1}}{h^2} - \frac{h^2 f^{(4)}(c)}{12}$$

Exercise $\boxed{1}$ Derive the F.D.F of order $O(h^2)$ for $f''(x)$ using Taylor's Expansion

we need to show:

$$f''(x_0) = \frac{2f_0 - 5f_1 + 4f_2 - f_3}{h^2} + \frac{11}{12} h^2 f^{(4)}(c)$$

$$f_1 = f_0 + h f'(x_0) + \frac{h^2}{2!} f''(x_0) + \frac{h^3}{3!} f'''(x_0) + \frac{h^4}{4!} f^{(4)}(c)$$

$$f_2 = f_0 + 2h f'(x_0) + \frac{(2h)^2}{2!} f''(x_0) + \frac{(2h)^3}{3!} f'''(x_0) + \frac{(2h)^4}{4!} f^{(4)}(c)$$

$$f_3 = f_0 + 3h f'(x_0) + \frac{(3h)^2}{2!} f''(x_0) + \frac{(3h)^3}{3!} f'''(x_0) + \frac{(3h)^4}{4!} f^{(4)}(c)$$

$$-5f_1 + 4f_2 - f_3 = \left(-5f_0 + 4f_0 - f_0\right) +$$

$$f'(x_0)\left(-5h + 8h - 3h\right) +$$

$$f''(x_0)\left(-\frac{5h^2}{2} + \frac{16h^2}{2} - \frac{9h^2}{2}\right) +$$

$$f'''(x_0)\left(\frac{-5h^3}{6} + \frac{4(8)h^3}{6} - \frac{27h^3}{6}\right) +$$

$$f^{(4)}(c)\left(\frac{-5h^4}{24} + \frac{4(16)}{24}h^4 - \frac{81h^4}{24}\right)$$

$$= -2f_0 + 0 + h^2 f''(x_0) + 0 - \frac{22}{24} h^4 f^{(4)}(c)$$

Hence, $$2f_0 - 5f_1 + 4f_2 - f_3 + \frac{11}{12} h^4 f^{(4)}(c) = h^2 f''(x_0)$$

$$f''(x_0) = \frac{2f_0 - 5f_1 + 4f_2 - f_3}{h^2} + \frac{11}{12} h^2 f^{(4)}(c)$$

Exercise Derive the B.D.F of order $o(h^2)$ for $f''(x)$ using Taylor's Expansion. $\boxed{13\,2.2}$

We need to show that:

$$f''(x_0) = \frac{2f_0 - 5f_{-1} + 4f_{-2} - f_{-3}}{h^2} + \frac{11}{12}h^2 f^{(4)}(c)$$

$$f_{-1} = f_0 - hf'(x_0) + \frac{h^2}{2!}f''(x_0) - \frac{h^3}{3!}f'''(x_0) + \frac{h^4}{4!}f^{(4)}(c)$$

$$f_{-2} = f_0 - 2hf'(x_0) + \frac{(-2h)^2}{2!}f''(x_0) + \frac{(-2h)^3}{3!}f'''(x_0) + \frac{(-2h)^4}{4!}f^{(4)}(c)$$

$$f_{-3} = f_0 - 3hf'(x_0) + \frac{(-3h)^2}{2!}f''(x_0) + \frac{(-3h)^3}{3!}f'''(x_0) + \frac{(-3h)^4}{4!}f^{(4)}(c)$$

$$-5f_{-1} + 4f_{-2} - f_{-3} = (-5f_0 + 4f_0 - f_0) +$$

$$f'(x_0)\left(5h - 8h + 3h\right) +$$

$$f''(x_0)\left(-\frac{5h^2}{2} + \frac{16h^2}{2} - \frac{9h^2}{2}\right) +$$

$$f'''(x_0)\left(\frac{5h^3}{6} - \frac{4(8)h^3}{6} + \frac{27h^3}{6}\right) +$$

$$f^{(4)}(c)\left(-\frac{5h^4}{24} + \frac{4(16)h^4}{24} - \frac{81h^4}{24}\right)$$

$$= -2f_0 + 0 + h^2 f''(x_0) + 0 - \frac{22}{24}h^4 f^{(4)}(c)$$

Hence, $2f_0 - 5f_{-1} + 4f_{-2} - f_{-3} + \frac{11}{12}h^4 f^{(4)}(c) = h^2 f''(x_0)$

$\Rightarrow$

$$f''(x_0) = \frac{2f_0 - 5f_{-1} + 4f_{-2} - f_{-3}}{h^2} + \frac{11}{12}h^2 f^{(4)}(c)$$

Exercise Derive the C.D.F of order $o(h^4)$ for $f''(x)$ using Taylor's Expansion

We need to show that

$$f''(x_0) = \frac{-f_2 + 16 f_1 - 30 f_0 + 16 f_{-1} - f_{-2}}{12 h^2} + \frac{h^4}{90} f^{(6)}(c)$$

$$f_1 = f_0 + h f'(x_0) + \frac{h^2}{2!} f''(x_0) + \frac{h^3}{3!} f'''(x_0) + \frac{h^4}{4!} f^{(4)}(x_0) + \frac{h^5}{5!} f^{(5)}(x_0) + \frac{h^6}{6!} f^{(6)}(c)$$

$$f_{-1} = f_0 - h f'(x_0) + \frac{h^2}{2!} f''(x_0) - \frac{h^3}{3!} f'''(x_0) + \frac{h^4}{4!} f^{(4)}(x_0) - \frac{h^5}{5!} f^{(5)}(x_0) + \frac{h^6}{6!} f^{(6)}(c)$$

$$f_2 = f_0 + 2h f'(x_0) + \frac{(2h)^2}{2!} f''(x_0) + \frac{(2h)^3}{3!} f'''(x_0) + \frac{(2h)^4}{4!} f^{(4)}(x_0) + \frac{(2h)^5}{5!} f^{(5)}(x_0) + \frac{(2h)^6}{6!} f^{(6)}(c)$$

$$f_{-2} = f_0 - 2h f'(x_0) + \frac{(2h)^2}{2!} f''(x_0) - \frac{(2h)^3}{3!} f'''(x_0) + \frac{(2h)^4}{4!} f^{(4)}(x_0) - \frac{(2h)^5}{5!} f^{(5)}(x_0) + \frac{(2h)^6}{6!} f^{(6)}(c)$$

$$\begin{aligned}
16 f_1 + 16 f_{-1} - f_2 - f_{-2} = {} & (16 f_0 + 16 f_0 - f_0 - f_0) + \\
& f'(x_0)\left(16h - 16h - 2h + 2h\right) + \\
& f''(x_0)\left(8h^2 + 8h^2 - 2h^2 - 2h^2\right) + \\
& f'''(x_0)\left(\frac{16h^3}{6} - \frac{16h^3}{6} - \frac{8h^3}{6} + \frac{8h^3}{6}\right) + \\
& f^{(4)}(x_0)\left(\frac{16h^4}{24} + \frac{16h^4}{24} - \frac{16h^4}{24} - \frac{16h^4}{24}\right) + \\
& f^{(5)}(x_0)\left(\frac{16h^5}{5!} - \frac{16h^5}{5!} - \frac{32h^5}{5!} + \frac{32h^5}{5!}\right) + \\
& f^{(6)}(c)\left(\frac{16h^6}{720} + \frac{16h^6}{720} - \frac{64h^6}{720} - \frac{64h^6}{720}\right)
\end{aligned}$$

$$= 30 f_0 + 0 + 12h^2 f''(x_0) + 0 + 0 + 0 - \frac{\cancel{96}^{\,2}}{\cancel{720}_{\,15}} h^6 f^{(6)}(c)$$

$$\Rightarrow f''(x_0) = \frac{-f_2 + 16 f_1 - 30 f_0 + 16 f_{-1} - f_{-2}}{12 h^2} + \frac{h^4}{90} f^{(6)}(c)$$

Exp Derive the B.D.F of order $o(h^2)$ with its truncation error using Newton's Polynomial.

- Recall that : $f(t) = P_n(t) + E_n(t)$ with
  $f'(t) = P_n'(t) + E_n'(t)$ where

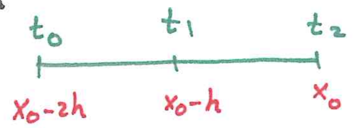
$P_n(t)$ is the Newton poly. given by

$$P_n(t) = a_0 + a_1(t-t_0) + a_2(t-t_0)(t-t_1) + \cdots + a_n(t-t_0)\cdots(t-t_{n-1})$$

with $a_0 = f[t_0] = y_0$ and $a_1 = f[t_0, t_1]$, $a_2 = f[t_0, t_1, t_2]$ ...

- We need to show $f'(x_0) = \dfrac{3f_0 - 4f_{-1} + f_{-2}}{2h} + \dfrac{h^2 f'''(c)}{3}$

since $o(h^2) \Rightarrow n = 2 \Rightarrow$ find $f'(t_2)$:
(B.D.F)



$f(t) = P_2(t) + E_2(t)$

$f'(t) = P_2'(t) + E_2'(t)$ but $f'(x_0) = f'(t_2) = P_2'(t_2) + E_2'(t_2)$

- $P_2(t) = a_0 + a_1(t-t_0) + a_2(t-t_0)(t-t_1)$

$P_2'(t) = 0 + a_1 + a_2(t-t_0) + a_2(t-t_1) = a_1 + a_2\left[2t - t_0 - t_1\right]$

$P_2'(t_2) = a_1 + a_2(2t_2 - t_0 - t_1) = \boxed{a_1 + 3h\,a_2}$

- $a_1 = f[t_0, t_1] = \dfrac{f(t_1) - f(t_0)}{t_1 - t_0} = \dfrac{f_{-1} - f_{-2}}{h}$

$$a_2 = f[t_0, t_1, t_2] = \frac{f[t_1, t_2] - f[t_0, t_1]}{t_2 - t_0} = \frac{\dfrac{f[t_2] - f(t_1)}{t_2 - t_1} - \dfrac{f_{-1} - f_{-2}}{h}}{t_2 - t_0}$$

$$= \frac{\dfrac{f_0 - f_{-1}}{h} - \dfrac{f_{-1} - f_{-2}}{h}}{2h} = \frac{f_0 - 2f_{-1} + f_{-2}}{2h^2}$$

- Hence, $P_2'(t_2) = a_1 + 3h\,a_2 = \dfrac{f_{-1} - f_{-2}}{h} + 3\cancel{h}\left(\dfrac{f_0 - 2f_{-1} + f_{-2}}{2h^{\cancel{2}}}\right)$

$$= \frac{3f_0 - 4f_{-1} + f_{-2}}{2h}$$

• To find the error $E_2'(t_2)$ $\Rightarrow$

$\Rightarrow$ Recall the error term $E_2(t) = \dfrac{f'''(c)\,(t-t_0)(t-t_1)(t-t_2)}{3!}$

$\Rightarrow$ Now $E_2'(t) = \dfrac{f'''(c)}{6}\Big[(t-t_0)(t-t_1) + (t-t_2)\big((t-t_0)+(t-t_1)\big)\Big]$

$$E_2'(t_2) = \frac{f'''(c)}{6}\Big[(t_2-t_0)(t_2-t_1)\Big]$$

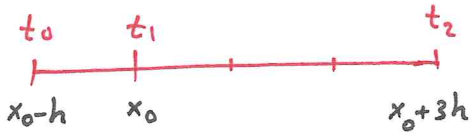
$$= \frac{f'''(c)\,(2h)(h)}{6} = \frac{h^2 f'''(c)}{3}$$

Exp Derive the D.F $f''(x_0) = \dfrac{f_3 - 4f_0 + 3f_{-1}}{6h^2} - \dfrac{2h\,f'''(c)}{3}$

using Lagrange polynomial.

• $n=2 \Rightarrow$ $f(t) = P_2(t) + E_2(t)$

$f''(t) = P_2''(t) + E_2''(t)$



• $f''(x_0) = f_2''(t_1) = P_2''(t_1) + E_2''(t_1)$ where $P_2(t)$ is Lagrange's poly. given by

$$P_2(t) = y_0\frac{(t-t_1)(t-t_2)}{(t_0-t_1)(t_0-t_2)} + y_1\frac{(t-t_0)(t-t_2)}{(t_1-t_0)(t_1-t_2)} + y_2\frac{(t-t_0)(t-t_1)}{(t_2-t_0)(t_2-t_1)}$$

$$= f_{-1}\frac{(t-t_1)(t-t_2)}{(-h)(-4h)} + f_0\frac{(t-t_0)(t-t_2)}{(h)(-3h)} + f_3\frac{(t-t_0)(t-t_1)}{(4h)(3h)}$$

$$P_2'(t) = \frac{f_{-1}}{4h^2}\left(t-t_1+t-t_2\right) - \frac{f_0}{3h^2}\left(t-t_0+t-t_2\right) + \frac{f_3}{12h^2}\left(t-t_0+t-t_1\right)$$

$$P_2''(t) = \frac{2f_{-1}}{4h^2} - \frac{2f_0}{3h^2} + \frac{2f_3}{12h^2}$$

$$= \frac{2f_3 - 8f_0 + 6f_{-1}}{12h^2}$$

$$= \frac{f_3 - 4f_0 + 3f_{-1}}{6h^2}$$

- To find the error $E_2''(t_1) \Rightarrow$

$\Rightarrow$ Recall the error term $E_2(t) = \dfrac{f'''(c)(t-t_0)(t-t_1)(t-t_2)}{3!}$

$$\Rightarrow E_2'(t) = \frac{f'''(c)}{6}\Big[(t-t_0)(t-t_1) + (t-t_2)\big((t-t_0)+(t-t_1)\big)\Big]$$

$$E_2''(t) = \frac{f'''(c)}{6}\Big[(t-t_0) + (t-t_1) + (t-t_2) + (t-t_0) + (t-t_1) + (t-t_2)\Big]$$

$$= \frac{f'''(c)}{3}\Big[(t-t_0) + (t-t_1) + (t-t_2)\Big]$$

$$\Rightarrow E_2''(t_1) = \frac{f'''(c)}{3}\Big[(t_1-t_0) + 0 + (t_1-t_2)\Big]$$

$$= \frac{f'''(c)}{3}\big[h - 3h\big]$$

$$= \frac{-2h\, f'''(c)}{3}$$

Error Analysis and Optimal step Size

- In any D.F. $\Rightarrow$

Total Error = Round off Error + Truncation Error

$$\boxed{E_{Total}(f,h) = E_{round}(f,h) + E_{trun}(f,h)}$$

- The Round off Error $E_{round}(f,h)$ in any D.F :

$$f_k = y_k + e_k \quad , \quad k = 0, \pm 1, \pm 2, \dots$$

$$\Rightarrow f_0 = y_0 + e_0 \quad , \quad f_1 = y_1 + e_1 \quad , \quad f_2 = y_2 + e_2$$

$$f_{-1} = y_{-1} + e_{-1} \quad , \quad f_{-2} = y_{-2} + e_{-2} \quad \dots$$

- **Remark**: The magnitude of the round off error is

$$|e_k| \leq \epsilon = 5 \times 10^{-10}$$

- The truncation error $E_{trun}(f,h)$ depends on the form of the D.F.
- To find the optimal step size h for a given D.F, we differentiate $E_{Total}(f,h)$ w.r.t h and find the critical value.

*Exp • Let $f(x) = \sin x$

• Estimate $f'(1)$ using the C.D.F of order $O(h^2)$ with $h = 0.01$ and $h = 0.001$ and $h = 0.0001$ and compare with the true value.

• True Value : $f'(x) = \cos x \Rightarrow f'(1) = \boxed{0.5403023059}$

• $f'(x_0) \approx \dfrac{f(x_0+h) - f(x_0-h)}{2h}$

• $h = 0.01 \Rightarrow f'(1) = \dfrac{f(1.01) - f(0.99)}{2(0.01)} = 0.5402933009$

• $h = 0.001 \Rightarrow f'(1) = \dfrac{f(1.001) - f(0.999)}{2(0.001)} = 0.5403022158$

• $\boxed{h = 0.0001} \Rightarrow f'(1) = \dfrac{f(1.0001) - f(0.9999)}{2(0.0001)} = \boxed{0.540302305}$

optimal

since it gives zero error

Exp Find the optimal step size h for the C.D.F of order $O(h^2)$ using to estimate $f'(x_0)$.

• $f'(x_0) = \dfrac{f(x_0+h) - f(x_0-h)}{2h} + E_{trun}(f,h)$

$$= \frac{f_1 - f_{-1}}{2h} - \frac{h^2 f'''(c)}{6}$$

$$= \frac{y_1 + e_1 - (y_{-1} + e_{-1})}{2h} - \frac{h^2 f'''(c)}{6}$$

$$= \frac{y_1 - y_{-1}}{2h} + \underbrace{\frac{e_1 - e_{-1}}{2h}}_{\text{Roundoff Error}} + \underbrace{\frac{-h^2 f'''(c)}{6}}_{\text{Truncation Error}}$$

- Hence, the total error is

$$E_{total}(f,h) = E_{round\,off}(f,h) + E_{trun}(f,h)$$

$$= \frac{e_1 - e_{-1}}{2h} + \frac{-h^2 f'''(c)}{6}$$

- Now $$|E_{total}| \leq \left|\frac{e_1 - e_{-1}}{2h}\right| + \left|\frac{h^2 f'''(c)}{6}\right|$$

$$\leq \left|\frac{e_1}{2h}\right| + \left|\frac{e_{-1}}{2h}\right| + \frac{h^2 M_3}{6}$$

$$\leq \frac{\epsilon}{2h} + \frac{\epsilon}{2h} + \frac{h^2 M_3}{6} \quad \text{by Remark page 136}$$

$$= \frac{\epsilon}{h} + \frac{h^2 M_3}{6}$$

$$= \phi(h)$$

- Now set $\phi'(h) = 0$ and find the critical value h^*

$$-\frac{\epsilon}{h^2} + \frac{h M_3}{3} = 0 \iff h^3 M_3 = 3\epsilon$$

$$\iff h^* = \left(\frac{3\epsilon}{M_3}\right)^{\frac{1}{3}}$$

- Note that in *Exp $\Rightarrow M_3 = \max |f'''(c)| = 1$ since $f(x) = \sin x$

$$\Rightarrow h^* = (3\epsilon)^{\frac{1}{3}} = (3 \times 5 \times 10^{-10})^{\frac{1}{3}} \simeq 0.001145 > 0.001 \checkmark$$

$$\Rightarrow h^* \approx 0.0001 \checkmark \text{ better}$$

- Remember that for C.D.F of order $O(h^2)$ to estimate $f'(x_0) \Rightarrow$ we have $f'(x_0) = \frac{f_1 - f_{-1}}{2h} - \frac{h^2 f'''(c)}{6}$ with

$$\phi(h) = \frac{\epsilon}{h} + \frac{h^2 M_3}{6} \quad \text{and} \quad h^* = \left(\frac{3\epsilon}{M_3}\right)^{\frac{1}{3}}$$

Exp Find the optimal step size h for the C.D.F of order $O(h^2)$ in estimating $f''(x_0)$.

- $$f''(x_0) = \frac{f_1 - 2f_0 + f_{-1}}{h^2} + E_{trun}(f,h)$$

$$= \frac{y_1 + e_1 - 2(y_0 + e_0) + y_{-1} + e_{-1}}{h^2} + \frac{-h^2 f^{(4)}(c)}{12}$$

$$= \frac{y_1 - 2y_0 + y_{-1}}{h^2} + \underbrace{\frac{e_1 - 2e_0 + e_{-1}}{h^2}}_{\text{Round off Error}} + \underbrace{\frac{-h^2 f^{(4)}(c)}{12}}_{\text{Truncation Error}}$$

- Hence, $E_{total}(f,h) = E_{roundoff}(f,h) + E_{trun}(f,h)$

$$= \frac{e_1 - 2e_0 + e_{-1}}{h^2} + \frac{-h^2 f^{(4)}(c)}{12}$$

- Now $|E_{total}| \le \left|\frac{e_1 - 2e_0 + e_{-1}}{h^2}\right| + \left|\frac{h^2 f^{(4)}(c)}{12}\right|$

$$\le \frac{\epsilon + 2\epsilon + \epsilon}{h^2} + \frac{h^2 M_4}{12}$$

$$= \frac{4\epsilon}{h^2} + \frac{h^2 M_4}{12}$$

$$= \phi(h)$$

- $\phi'(h) = 0 \iff \frac{-8\epsilon}{h^3} + \frac{h M_4}{6} = 0 \iff$

$$h^* = \left(\frac{48\epsilon}{M_4}\right)^{\frac{1}{4}}$$

Exp
- Let $f(x) = \ln x$ where $0.1 \leq x \leq 0.5$
- Find the best step size h for the C.D.F of order $o(h^2)$ in estimating $f''(x_0)$

- Using the previous Exp $\Rightarrow h^* = \left(\dfrac{48\epsilon}{M_4}\right)^{\frac{1}{4}}$
- To find $M_4 \Rightarrow f'(x) = \dfrac{1}{x} \Rightarrow f''(x) = \dfrac{-1}{x^2}$

$$\Rightarrow f'''(x) = \frac{2}{x^3} \Rightarrow f^{(4)}(x) = \frac{-6}{x^4}$$

$$M_4 = \underset{0.1 \leq x \leq 0.5}{Max} \left| f^{(4)}(x) \right| = \underset{0.1 \leq x \leq 0.5}{Max} \frac{6}{x^4} = \frac{6}{(0.1)^4} = 60000$$

- $h^* = \left(\dfrac{48 \times 5 \times 10^{-10}}{60000}\right)^{\frac{1}{4}} = \left(4 \times 10^{-13}\right)^{\frac{1}{4}} = 0.0007952707$

Exp Find the optimal h for $f(x) = e^{-x}$, $1 \leq x \leq 2$ if the C.D.F of order $o(h^4)$ is used to estimate $f'(x_0)$.

- $f'(x_0) = \dfrac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h} + \dfrac{h^4 f^{(5)}(c)}{30}$
- Similarly to what have been done befor, we could arrive:

$$\phi(h) = \frac{18\epsilon}{12h} + \frac{h^4 M_5}{30} = \frac{3\epsilon}{2h} + \frac{h^4 M_5}{30}$$

- $\phi'(h) = \dfrac{-3\epsilon}{2h^2} + \dfrac{2h^3 M_5}{15} = 0 \Leftrightarrow h^* = \left(\dfrac{45\epsilon}{4M_5}\right)^{\frac{1}{5}}$
- To find $M_5 \Rightarrow f' = -e^{-x} = f''' = f^{(5)} \Rightarrow M_5 = \underset{1 \leq x \leq 2}{Max} \left| f^{(5)}(x) \right| = \left. \dfrac{1}{e^x} \right|_{x=1}$

$$= \frac{1}{e} = 0.3678794412$$

- Hence, $h^* = \left(\dfrac{45 \times 5 \times 10^{-10}}{4(0.3678794412)}\right)^{\frac{1}{5}}$

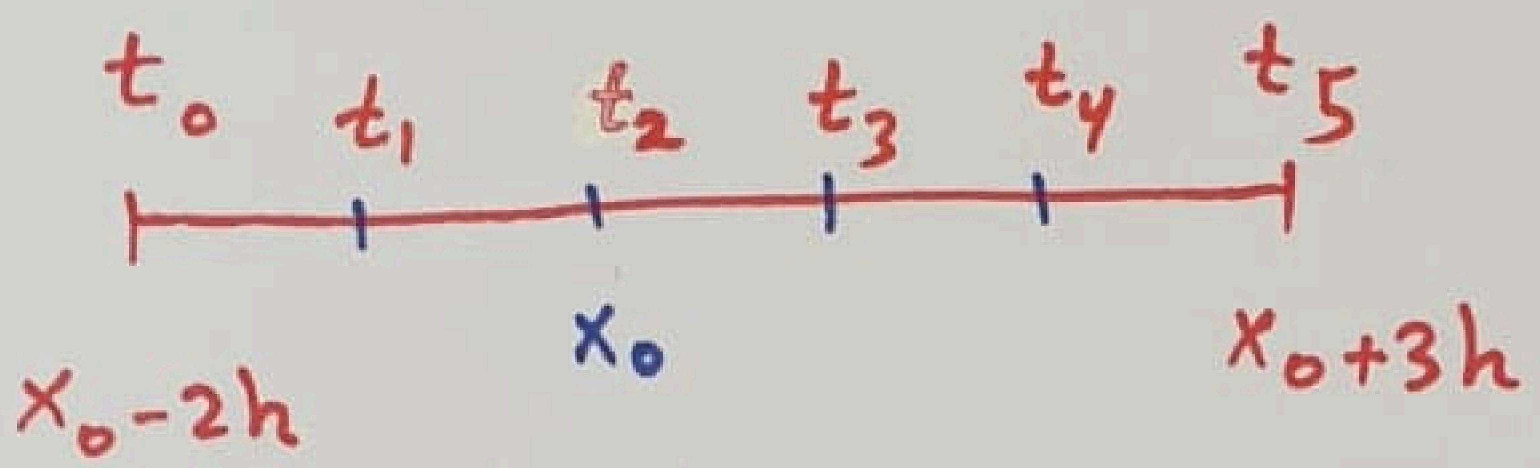
$= $ [redacted]

2.7345344669

Exp Use the points: $x_0 - 2h$, $x_0 + 3h$ to estimate $f'(x_0)$ with its truncation error using Newton's Interpolation.

- $n = 1 \Rightarrow$ Newton's Poly. is $P_1(t) = a_0 + a_1(t - t_0)$

$$P_1'(t) = a_1 = f[t_0, t_5]$$



$$= \frac{f(t_5) - f(t_0)}{t_5 - t_0}$$

$$= \frac{f_3 - f_{-2}}{5h}$$

$$= P_1'(x_0)$$

- $f(t) = P_1(t) + E_1(t)$

$$f'(t) = P_1'(t) + E_1'(t)$$

$$f'(x_0) = P_1'(x_0) + E_1'(x_0)$$

- Note that $E_1(t) = \dfrac{f''(c)(t - t_0)(t - t_5)}{2}$

$$E_1'(t) = \frac{f''(c)}{2}\left[(t - t_0) + (t - t_5)\right]$$

$$E_1'(t_2) = E_1'(x_0) = \frac{f''(c)}{2}\left[2h + (-3h)\right]$$

$$= -\frac{h f''(c)}{2}$$

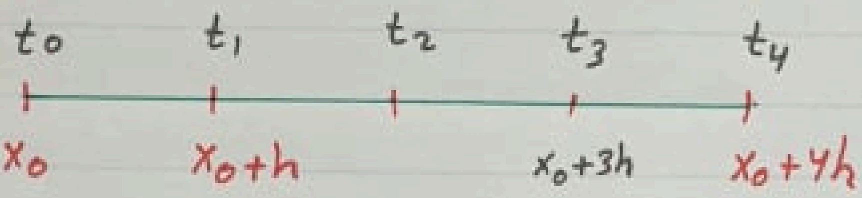
- Hence, $f'(x_0) = P_1'(x_0) + E_1'(x_0)$

$$= \frac{f_3 - f_{-2}}{5h} - \frac{h f''(c)}{2}$$

Exp Given the nodes x_0, x_0+h, x_0+4h.
Use Newton Polynomial to find the Difference formula that estimates $f'(x_0+3h)$

- Three points $\Rightarrow n=2 \Rightarrow P_2(t) = a_0 + a_1(t-t_0) + a_2(t-t_0)(t-t_1)$

$$P_2'(t) = a_1 + a_2\left[(t-t_0)+(t-t_1)\right]$$



$$a_1 = f[t_0,t_1] = \frac{f(t_1)-f(t_0)}{t_1-t_0} = \frac{f_1-f_0}{h}$$

$$a_2 = f[t_0,t_1,t_4] = \frac{f[t_1,t_4]-f[t_0,t_1]}{t_4-t_0} = \frac{\dfrac{f_4-f_1}{t_4-t_1} - \dfrac{f_1-f_0}{t_1-t_0}}{t_4-t_0}$$

$$= \frac{\dfrac{f_4-f_1}{3h} - \dfrac{f_1-f_0}{h}}{4h} = \frac{f_4-4f_1+3f_0}{12h^2}$$

$$f(t) = P_2(t) + E_2(t)$$

$$f'(t) \approx P_2'(t)$$

$$f'(t_3) \approx P_2'(t_3) = a_1 + a_2\left((t_3-t_0)+(t_3-t_1)\right) = a_1 + a_2(3h+2h)$$

$$f'(x_0+3h) = \frac{f_1-f_0}{h} + 5\cancel{h}\left(\frac{f_4-4f_1+3f_0}{12h^{\cancel{2}}}\right)$$

$$= \frac{12f_1-12f_0}{12h} + \frac{5f_4-20f_1+15f_0}{12h}$$

$$= \frac{5f_4-8f_1+3f_0}{12h}$$