Phys 512 PS 1

(a) Taylor series vs. round off errors

From points: $x+\delta$, $x-\delta$, $x+2\delta$, $x-\delta$

Taylor series: $f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \ldots + \frac{f^{(n)}}{n!}(x-a)^n + \ldots$

Thus,

$$f(x\pm\delta) = f(a) + f'(a)(x\pm\delta-a) + \frac{f''(a)}{2!}(x\pm\delta-a)^2 + \frac{f'''(x)}{3!}(x\pm\delta-a)^3 + \ldots + \frac{f^{(n)}}{n!}(x\pm\delta-a)^n + \ldots$$

$$= f(x) + f'(x)(\pm\delta) + \frac{f''(a)}{2!}(\pm\delta)^2 + \frac{f'''(x)}{3!}(\pm\delta)^3 + \ldots + \frac{f^{(n)}}{n!}(\pm\delta)^n + \ldots$$

$$f(x\pm\delta) = f(x) \pm f'(x)\delta + \frac{1}{2}f''(x)\delta^2 \pm \frac{1}{6}f'''(x)\delta^3 + \ldots + \frac{f^n}{n!}(\pm\delta)^n + \ldots$$

$$f(x\pm2\delta) = f(x) \pm 2f'(x)\delta + 2f''(x)\delta^2 \pm \frac{4}{3}f'''(x)\delta^3 + \ldots + \frac{f^n}{n!}(\pm2\delta)^n + \ldots$$

Multiply coefficients: $c_1 f(x+\delta)$, $c_2 f(x-\delta)$, $c_3 f(x+2\delta)$, $c_4 f(x-2\delta)$

| | $f(x)$ | $f'(x)\delta$ | $f''\delta^2$ | $f'''\delta^3$ |
|---|---|---|---|---|
| $c_1$ | 1 | 1 | 1/2 | 1/6 |
| $c_2$ | 1 | -1 | 1/2 | -1/6 |
| $c_3$ | 1 | 2 | 2 | 4/3 |
| $c_4$ | 1 | -2 | 2 | -4/3 |
| | 0 | 1 | 0 | 0 |

$$c_1 + c_2 + c_3 + c_4 = 0$$
$$c_1 - c_2 + c_3 - c_4 = 0$$
$$\frac{1}{2}c_1 + \frac{1}{2}c_2 + 2c_3 + 2c_4 = 0$$
$$\frac{1}{6}c_1 - \frac{1}{6}c_2 + \frac{8}{3}c_3 - \frac{4}{3}c_4 = 0$$

$$Ax = B$$

$$x = A^{-1}B$$

$$\begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1/2 & 1/6 \\ 1 & -1 & 1/2 & -1/6 \\ 1 & 2 & 2 & 4/3 \\ 1 & -2 & 2 & -4/3 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

Thus, $c_1 = \frac{2}{3}$

$c_2 = -\frac{2}{3}$

$c_3 = \frac{-1}{12}$

$c_4 = \frac{1}{12}$

$$f'(x)\delta = \frac{2}{3}f(x+\delta) - \frac{2}{3}f(x-\delta) - \frac{1}{12}f(x+2\delta) + \frac{1}{12}f(x-2\delta)$$

$$f'(x) = \left\{\frac{2}{3}\left[f(x+\delta) - f(x-\delta)\right] - \frac{1}{12}\left[f(x+2\delta) - f(x-2\delta)\right]\right\}\frac{1}{\delta}$$

(b)

From the def'n of $f(x\pm\delta)$ and $f(x\pm 2\delta)$, inspecting it w/ respect to $f'(x)$, even-primed derivatives cancel each other leaving us at max, 5th order term:

$$\frac{2}{3}\left[2\frac{f^5(x)}{5!}\delta^5 - \frac{1}{12}\left[2\frac{f^5(x)}{5!}(2\delta)^5\right]\right]$$

$$= \frac{4}{3}\frac{f^5(x)}{5!}\delta^5 - \frac{1}{6}2^5\frac{f^5(x)}{5!}\delta^5 = \left[\frac{4}{3} - \frac{16}{3}\right]\frac{f^5(x)}{5!}\delta^5 = \frac{-12}{3}\frac{f^5(x)}{5(4\cdot 3)\cdot 2\cdot 1}\delta^5$$

$$= -\frac{f^5(x)}{30}\delta^5$$

Trunc error, therefore, $R = \left|\frac{f^5(x)}{30}\delta^5\right|$ but $f'(x)$ has a factor of $\frac{1}{\delta}$

Thus, $R = \left|\frac{f^5(x)}{30}\delta^4\right|$

Round-off error: Since $f'(x)$ is defined in terms of $f(x)$, let's say that error can be quantified as $\frac{g\epsilon}{\delta}|f(x)|$ with $\epsilon$ as the machine precision error and $g$ as some factor. Thus, $E = \frac{g\epsilon}{\delta}|f(x)|$

Total error: $E_T = R + E = \frac{\delta^4}{30}|f^5| + \frac{g\epsilon}{\delta}|f|$

Optimizing: $\frac{d}{d\delta}E = 0 \rightarrow \frac{d}{d\delta}\left[\frac{\delta^4}{30}|f^5| + \frac{g\epsilon}{\delta}|f|\right] = \frac{2}{15}\delta^3|f^5| - \frac{g\epsilon}{\delta^2}|f| = 0$

Therefore, $\delta^5 = \frac{15}{2}g\epsilon\frac{|f|}{|f^5|}$ or $\delta = \left(\frac{15}{2}g\epsilon\frac{|f|}{|f^5|}\right)^{1/5}$

For $f = e^x$: $\delta = \left(\frac{15}{2}g\right)^{1/5}(\epsilon = 10^{-16})^{1/5}\left(\frac{e^x}{e^x}\right)^{1/5} \approx \underline{\left(\frac{15}{2}g\right)^{1/5}\cdot 10^{-3}}$

64-bit machine

For $f = e^{0.01x}$: $\delta \approx \left(\frac{15}{2}g\right)^{1/5}(10^{-16})^{1/5}\left(\frac{e^x}{(0.01)^5 e^x}\right)^{1/5} \approx \left(\frac{15}{2}g\right)^{1/5}(10^{-3})\left(\frac{1}{(10^{-2})^5}\right)^{1/5} = \underline{\left(\frac{15}{2}g\right)^{1/5}\cdot 10^{-1}}$