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Phys. 512 - Comp. Phys. with Applications
PS #1:

1.a) Using the same notation as in class where $f(x)$ is the true evaluation of f at x & $\bar{f}$ is the "computer evaluation" of f at x, & where $\bar{f}(x) = f(x)\cdot(1+g\varepsilon)$ ε: error brought on by machine precision
g: gaussian noise element of order 1

Again, following the same vein as seen in class we Taylor expand $\bar{f}(x\pm\delta)$, but this time to the 5^{th} order term in δ:

$$\bar{f}(x\pm\delta) \approx f(x)\cdot(1+g_\pm\varepsilon) \pm f'(x)\delta + \frac{f''(x)\delta^2}{2} \pm \frac{f'''(x)\delta^3}{6} + \frac{f^{(4)}(x)\delta^4}{24} \pm \frac{f^{(5)}(x)\delta^5}{120} + O(\delta^6)$$

& the same with $f(x\pm 2\delta)$:

$$\bar{f}(x\pm 2\delta) \approx f(x)\cdot(1+g_\pm\varepsilon) \pm 2f'(x)\delta + 2f''(x)\delta^2 \pm \frac{4}{3}f'''(x)\delta^3 + \frac{2}{3}f^{(4)}(x)\delta^4 \pm \frac{4}{15}f^{(5)}(x)\delta^5 + O(\delta^6)$$

g_+ & g_- are the gaussian noise elements encurred when evaluating $f(x+n\delta)$ & $f(x-n\delta)$ respectively.
We use these to generate two different derivatives at x:

$$\bar{f}_1'(x) \equiv \frac{\bar{f}(x+\delta)-\bar{f}(x-\delta)}{2\delta} \approx \frac{1}{2\delta}\Big[f(x)\underbrace{(g_+-g_-)}_{g_1}\varepsilon + 2f'(x)\delta + \frac{1}{3}f'''(x)\delta^3 + \frac{1}{60}f^{(5)}(x)\delta^5 + O(\delta^7)\Big]$$

$$= f'(x) + \frac{f(x)g_1\varepsilon}{2\delta} + \frac{1}{6}f'''(x)\delta^2 + \frac{1}{120}f^{(5)}(x)\delta^4 + O(\delta^6)$$

$$\bar{f}_1'(x) - f'(x) \approx \frac{1}{2\delta}f(x)g_1\varepsilon + \frac{1}{6}f'''(x)\delta^2 + \frac{1}{120}f^{(5)}(x)\delta^4 + O(\delta^6)$$

$$\bar{f}_2'(x) \equiv \frac{\bar{f}(x+2\delta)-\bar{f}(x-2\delta)}{4\delta} \approx \frac{1}{4\delta}\Big[f(x)\cdot\underbrace{(g_+-g_-)}\varepsilon + 4f'(x)\delta + \frac{8}{3}f'''(x)\delta^3 + \frac{8}{15}f^{(5)}(x)\delta^5 + O(\delta^7)\Big]$$

$$= f'(x) + \frac{1}{4\delta}f(x)g_2\varepsilon + \frac{2}{3}f'''(x)\delta^2 + \frac{2}{15}f^{(5)}(x)\delta^4 + O(\delta^6)$$

$$\bar{f}_2'(x) - f'(x) \approx \frac{1}{4\delta}f(x)g_2\varepsilon + \frac{2}{3}f'''(x)\delta^2 + \frac{2}{15}f^{(5)}(x)\delta^4 + O(\delta^6)$$

$$(\bar{f}_2'(x) - f'(x)) - 4(\bar{f}_1'(x) - f'(x)) \approx \frac{f(x)\varepsilon}{\delta}\left(\frac{1}{4}g_2 - 2g_1\right) + \cancelto{0}{\left(\frac{4}{6}-\frac{2}{3}\right)}f'''(x)\delta^2 - \frac{3}{30}f^{(5)}(x)\delta^4 + O(\delta^6)$$

$$(\bar{f}_2'(x) - 4\bar{f}_1'(x)) + 3f'(x) \approx \frac{f(x)\varepsilon}{\delta}\left(\frac{1}{4}g_2 - 2g_1\right) - \frac{1}{10}f^{(5)}(x)\delta^4 + O(\delta^6)$$

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$$\underbrace{\left(\frac{4\bar{f}_1'(x) - \bar{f}_2'(x)}{3}\right) - f'(x)}_{\Delta f'(x)} \approx \frac{2}{3}\frac{f(x)\varepsilon}{\delta}\underbrace{\left(\frac{1}{8}g_2 - g_1\right)}_{g} - \frac{1}{30}f^{(5)}(x)\delta^4 + O(\delta^6)$$

$$\frac{\partial\Delta f'(x)}{\partial\delta} = \frac{2}{3}\frac{f(x)g\varepsilon}{\delta^2} - \frac{2}{15}f^{(5)}(x)\delta^3 = 0 \longrightarrow \delta = \sqrt[5]{5g\varepsilon\frac{f(x)}{f^{(5)}(x)}}$$

$\Rightarrow$ Optimal δ to minimize difference between numerical & true derivative.

So $\frac{4\bar{f}_1'(x) - \bar{f}_2'(x)}{3}$ seems like a good choice to minimize the difference between the computed derivative & the true derivative as the leading roundoff error term is of order δ^4 (to which the machine-precision error is added.)

b) Using $\delta = \sqrt[5]{5 \cdot 9\varepsilon \frac{f(x)}{f^{(5)}(x)}}$ is the optimal value to minimize said difference without augmenting the numerical-precision error to a counter-productive degree.

For $y = \exp(x)$ float 32 ($\varepsilon \simeq 10^{-7}$) $\rightarrow \delta \approx 0.055$
float 64 ($\varepsilon \simeq 10^{-16}$) $\rightarrow \delta \approx 0.00087$

$y = \exp(0.01x)$ float 32 $\rightarrow \delta \approx 5.5$
float 64 $\rightarrow \delta \approx 0.087$