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Phys 512 - Problem Set 1

Problem 1

Taylor series vs. roundoff errors to decide the step size to use on numerical derivatives calculations.

If evaluating a function f at four points (x±δ and x±2δ),

a) Give an estimate of the first derivative at x.
How to combine the derivative from x±δ with the derivative from x±2δ to cancel the next term in the Taylor series.

b) From the derivative operator, find optimal δ in terms of machine precision.
Show that the estimate for optimal δ is roughly correct for
- *f(x)* = e^x
- *f(x)* = $e^{0.01\,x}$

First I am Taylor expanding the function at the 4 evaluated points:

In[66]:=
$$f(x+\delta) = f(x) + f'(x)\,\delta + \frac{f''(x)}{2}\,\delta^2 + \frac{f^{(3)}(x)}{6}\,\delta^3 + \frac{f^{(4)}(x)}{24}\,\delta^4 + \frac{f^{(5)}(x)}{120}\,\delta^5 + g\,\epsilon\,f;$$
$$f(x-\delta) = f(x) - f'(x)\,\delta + \frac{f''(x)}{2}\,\delta^2 - \frac{f^{(3)}(x)}{6}\,\delta^3 + \frac{f^{(4)}(x)}{24}\,\delta^4 - \frac{f^{(5)}(x)}{120}\,\delta^5 - g\,\epsilon\,f;$$
$$f(x+2\,\delta) = f(x) + f'(x)\,2\,\delta + f''(x)\,2\,\delta^2 + \frac{f^{(3)}(x)}{3}\,4\,\delta^3 + \frac{f^{(4)}(x)}{3}\,2\,\delta^4 + \frac{f^{(5)}(x)}{15}\,4\,\delta^5 + g\,\epsilon\,f;$$
$$f(x-2\,\delta) = f(x) - f'(x)\,2\,\delta + f''(x)\,2\,\delta^2 - \frac{f^{(3)}(x)}{3}\,4\,\delta^3 + \frac{f^{(4)}(x)}{3}\,2\,\delta^4 - \frac{f^{(5)}(x)}{15}\,4\,\delta^5 - g\,\epsilon\,f;$$

Then I set the first derivative as a linear combination of the 4 equations above
$f'(x) = A\,f(\delta+x) + B\,f(x-\delta) + C\,f(x+2\,\delta) + D\,f(x-2\,\delta)$,
expand and collect the terms in f and its derivatives:

In[87]:= **Simplify[Expand[$A\, f(\delta + x) + B\, f(x - \delta) + C\, f(x + 2\,\delta) + D\, f(x - 2\,\delta)$]/$\delta$];**
expansion = Collect[%, {$f(x), f'(x), f''(x), f^{(3)}(x), f^{(4)}(x), f^{(5)}(x), g\, \epsilon\, f$}]

Out[88]= $$f\, g \left(\frac{A}{\delta} - \frac{B}{\delta} + \frac{C}{\delta} - \frac{D}{\delta}\right) \in + \frac{(A + B + C + D)\; f[x]}{\delta} + \frac{1}{6}\,(A - B + 8\,C - 8\,D)\;\delta^2\; f^3[x] + \left(\frac{A\,\delta^3}{24} + \frac{B\,\delta^3}{24} + \frac{2\,C\,\delta^3}{3} + \frac{2\,D\,\delta^3}{3}\right) f^4[x] + \left(\frac{A\,\delta^4}{120} - \frac{B\,\delta^4}{120} + \frac{4\,C\,\delta^4}{15} - \frac{4\,D\,\delta^4}{15}\right) f^5[x] + (A - B + 2\,C - 2\,D)\; f'[x] + \left(\frac{A\,\delta}{2} + \frac{B\,\delta}{2} + 2\,C\,\delta + 2\,D\,\delta\right) f''[x]$$

Since our goal here is to have an expression with the form
$f'(x) = f'(x) + \epsilon_{\text{truncation}} + \epsilon_{\text{roundoff}}$, where $\epsilon_{\text{truncation}} \sim f^{(5)}(x)$,
I can solve the system of equations by setting the coefficient of $f'(x)$ to one and the coefficients of $f(x)$, $f''(x)$ and $f^{(3)}(x)$ to zero, solve for {A, B, C, D}
and then substitute those in back in the expansion to find $f'(x)$:

In[89]:= $$\text{Solve}\left[\frac{(A + B + C + D)}{\delta} == 0\ \&\&\ (A - B + 2\,C - 2\,D) == 1\ \&\&\ \left(\frac{A\,\delta}{2} + \frac{B\,\delta}{2} + 2\,C\,\delta + 2\,D\,\delta\right) == 0\ \&\&\ \frac{1}{6}\,(A - B + 8\,C - 8\,D)\;\delta^2 == 0,\ \{A, B, C, D\}\right]$$

deriv = expansion /. %[[1]]

Out[89]= $$\left\{\left\{A \to \frac{2}{3},\ B \to -\frac{2}{3},\ C \to -\frac{1}{12},\ D \to \frac{1}{12}\right\}\right\}$$

Out[90]= $$\frac{7\, f\, g \in}{6\,\delta} - \frac{1}{30}\,\delta^4\, f^5[x] + f'[x]$$

So I have an expression $f'(x) = f'(x) + \epsilon_{\text{truncation}} + \epsilon_{\text{roundoff}}$ given by

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

To find the optimal step size δ, I have to minimize the error:

In[74]:= $f'(x) \to f'[x] - \frac{1}{30}\delta^4 f^5[x] + \frac{7\, f\, g\, \epsilon}{6\,\delta};$

$\text{error} = -\frac{1}{30}\delta^4 f^5[x] + \frac{7\, f\, g\, \epsilon}{6\,\delta};$
∂_δ **error**
Solve[% == 0, δ];
%[[2]]

Out[76]= $-\frac{7\, f\, g\, \epsilon}{6\,\delta^2} - \frac{2}{15}\delta^3\, f^5[x]$

Out[78]= $\left\{\delta \to -\frac{35^{1/5}\, f^{1/5}\, g^{1/5}\, \epsilon^{1/5}}{2^{2/5}\, f^5[x]^{1/5}}\right\}$

Let me rewrite this is a more reader-friendly way. The best choice of δ is:

$\delta \to -\sqrt[5]{\frac{35\, f\, g\, \epsilon}{2^2\, f^5(x)}};$

g is of order 1. Assuming that f and $f^{(5)}$ are of the same order-of-magnitude, we get

$\delta \sim -\sqrt[5]{\frac{35\,\epsilon}{4}};$

In[79]:= $\text{"single precision best } \delta\text{"} \to N\left[\sqrt[5]{\frac{35\,\epsilon}{4}} \;/.\; \epsilon \to 10^{-8}\right]$

$\text{"double precision best } \delta\text{"} \to N\left[\sqrt[5]{\frac{35\,\epsilon}{4}} \;/.\; \epsilon \to 10^{-16}\right]$

Out[79]= single precision best $\delta \to 0.0387616$

Out[80]= double precision best $\delta \to 0.000973647$

The fractional accuracy of the derivative is

In[81]:= $\text{"}\frac{\epsilon_{\text{truncation}} + \epsilon_{\text{roundoff}}}{f'(x)}\text{"} \to \text{Simplify}\left[\frac{1}{f'(x)}\left(-\frac{1}{30}\delta^4 f^5[x] + \frac{7\, f\, g\, \epsilon}{6\,\delta}\right) /.\; \delta \to -\sqrt[5]{\frac{35\,\epsilon}{4}}\right];$

$N\left[\text{Simplify}\left[\% \;/.\; \{f'(x) \to f,\, f^5[x] \to f,\, g \to 1\}\right]\right]$

Out[82]= $\frac{\epsilon_{\text{truncation}} + \epsilon_{\text{roundoff}}}{f'(x)} \to -0.945051\,\epsilon^{4/5}$

So the fractional accuracy of the calculated derivative is **$\sim\epsilon^{4/5}$**

In[83]:=
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"single precision frac accuracy" → N[ϵ^(4/5) /. ϵ → 10^-8]
"double precision frac accuracy" → N[ϵ^(4/5) /. ϵ → 10^-16]
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Out[83]= single precision frac accuracy → 3.98107×10^{-7}

Out[84]= double precision frac accuracy → 1.58489×10^{-13}

Python code results

Running the attached .py file "Phys512_PS1_P1_FCRM.py”,

- for $f(x) = e^x$:

→ Best delta = 0.0005623413251903491 , best accuracy = 2.873257187729905e-13

- for $f(x) = e^{0.01 x}$:

→ Best delta = 0.05623413251903491 , best accuracy = 2.96637714392034e-16

(Pretty good :D)