Computational Physics (6810): Session 3

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January 18, 2017

Questions about PS#1?

- Tell me about BuckeyeBox/Dropbox issues!
- Comments will be added to your BuckeyeBox/Dropbox folder.
- Check the online hints/suggestions!
- Don't panic if you have last-minute problems!
- Use the codes from class as examples.
- Need to *explain* for homework $1 + \frac{1}{2} + \cdots + \frac{1}{N}$ versus $\frac{1}{N} + \frac{1}{N-1} + \cdots + 1$; why is this like the example from class of $1 + a + \cdots + a$ versus $a + a + \cdots + 1$?
  E.g., is this an example of subtractive cancellation?
- Graphs *must* be labeled, both axes and different curves. "Column 1" and "Column 2" are *not* adequate labels.
- You don't need to explain the *values* of the slopes for the Bessel function problem, but you should understand the explanation in the (upcoming) Session 4 notes.

Session 2 follow-ups

- Finish through Bessel 1 in Session 2 then move on
- Make sure you can read slopes from log-log plots $\Longrightarrow$ ask!
- You can always upgrade a check to a plus
- $j_{10}(x)$ is a *spherical* Bessel function $\neq J_{10}(x)$
- Note the convenience of using a *plot file* for gnuplot
  - Type your plotting commands in a file instead of at `gnuplot>`
  - Save the file (e.g., `filename.plt`) but keep the editor open!
  - `load "filename.plt"` at `gnuplot>` after every change
- Learning about C++
  - For beginners: online tutorial `http://www.cplusplus.com/doc/tutorial/`
  - For comprehensive and advanced references, use Safari. See the 6810 info page.
  - Ask the instructors as we wander around!

Round-off versus Approximation errors

- Round-off errors from finite # of *significant figures*
  - about 7 for single precision (float)
  - about 15–16 for double precision (double)
- Sources of round-off errors
  - adding or subtracting very different size numbers, e.g., $(1 + a + a + \cdots)$
  - subtracting two similar numbers ("subtractive cancellation")
- Approximation error for a forward derivative (what if $h \ll x$?)

$$\frac{df}{dx} \approx \frac{f(x+h) - f(x)}{h} = \frac{\cancel{f(x)}^{a} + \cancel{h}^{b} f'(x) + \frac{\cancel{h^2}^{b}}{2} f''(x) + \cdots - \cancel{f(x)}^{a}}{\cancel{h}^{b}}$$

  - Frequently use *Taylor expansion* to derive algorithm *and* error
  - How big is the error? First term neglected: here $\frac{h}{2} f''(x)$
  - If you compare different h's at same x, result will *scale* as power law h^{α} with $\alpha = 1$. See section c.1 for optimal h.
  - What do you expect for *central difference* algorithm?

Numerical integration (or "quadrature")

- General form for approximation of integral:

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{N} f(x_i)w_i$$

  - the N x_i's are "nodes" and w_i's are "weights"
  - evenly spaced x_i's $\Longrightarrow$ "Newton-Cotes methods" (see notes)
  - unevenly spaced $\Longrightarrow$ Gaussian quadrature (see Hjorth-Jensen notes)
  - see Numerical Recipes for other discussions (new webpage)
- Error analysis for trapezoid and Simpson's rule in notes

Numerical Recipes

- Standard first reference for algorithms (for physicists)
- Like Wikipedia in many ways (good and bad :)
- Local pdf copies of chapters from 2nd edition now available from webpage
- Protected page with username: physics and password: 6810

Accumulation of errors

- If we multiply numbers, errors *add* (see notes)
- e.g., $0.5\epsilon_m + (-0.3)\epsilon_m + (-0.8)\epsilon_m + 0.02\epsilon_m + \cdots$
- This is like a *random walk*. What is sum of N such numbers?
- Sum *could* be $-N\epsilon_m$ to $N\epsilon_m$, but on *average* (e.g., many trials), the sum is $\sqrt{N}\epsilon_m$
- Learn the proof of this (see Session 3 notes for all steps)

$$\epsilon_{\text{total}}^2 = \epsilon_m^2(s_1 + s_2 + \cdots + s_N)^2 \approx N\epsilon_m^2$$

Comments on C++ programming

- Why make a function?
  - isolate the calculation, test separately, reuse code
  - first exposure to *pointers* (stay calm!)
- But how could you do it better?
  - What is bad about having a function *and* its derivative?
  - For the experts: what class could you define?
- Input/output formatting with C++ *manipulators*
  - adjust digits, spacing, fixed vs. scientific, . . .
  - see handout and discussion in Session 3 notes
- Output to a file (e.g., named `my_file.out`)
  1. put `#include <fstream>` at top
  2. associate file with name of a *stream* (e.g., `my_out`):
     `ofstream my_out ("my_file.out");`
  3. output using same conventions and manipulators as `cout`

```
my_out << "Answer: " << scientific << rel_error << endl;
```

Power laws: two ways to plot

If $y = Cx^{\alpha}$, where $\alpha = 1, 2, \ldots$ or -1 or $1/2$ or $-1/2$ or $\ldots$

then $\underbrace{\log_{10} y}_{z} = \log_{10} Cx^{\alpha} = \underbrace{\log_{10} C}_{D} + \alpha \underbrace{\log_{10} x}_{w}$

or $Z = D + \alpha w$