Computational Physics (6810): Session 11

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Comments on PS#3

Random recaps and followups

Turing Award from ACM

Still working on Problem Set 3? Read the hints!

1. Remember: send me email about your project ideas!
2. Richardson extrapolation: Note that `extrap_diff` calls `central_diff` with two different *h*'s. Your function `extrap_diff2` should call `extrap_diff` twice (and NOT `central_diff` twice).
3. Plotting the wave function for different basis sizes and *b*
   - Write $u(r) = \sum_{i=0}^{D-1} c_i\phi_i(r)$ where $\phi_i(r)$ is a harmonic oscillator wave function, which depends on *b*
   - The c_i's come from your eigenvector for the state of interest
   - The $\phi_i(r)$'s come from evaluating a function you are provided with (`harmonic_oscillator`). Be careful of what "*i*" to call it with!

Numerical derivatives and Richardson extrapolations

- If you know the precise *form* of the error . . .
- Consider the central difference derivative (function `central_diff`)

$$D_c[f,h] \equiv \frac{f(x_0+h/2)-f(x_0-h/2)}{h} = f'(x_0) + \frac{1}{24}h^2 f^{(3)}(x_0) + Ch^4 f^{(5)}(x_0) + \cdots$$

- The only h dependence in the error is explicit. What if $h \to 2h$?

$$D_c[f,2h] = \frac{f(x_0+h)-f(x_0-h)}{2h} = f'(x_0) + \frac{1}{24}4h^2 f^{(3)}(x_0) + 16Ch^4 f^{(5)}(x_0) + \cdots$$

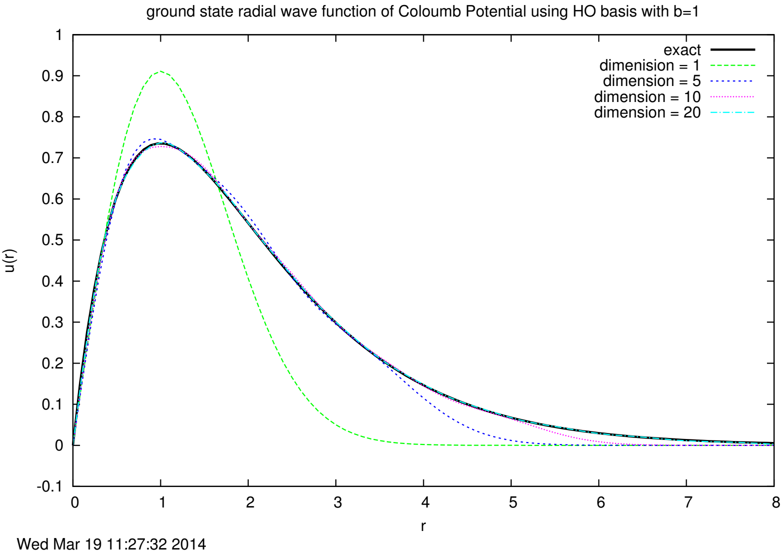
- Richardson: consider the error term as an unknown and eliminate:

$$\frac{4D_c[f,h]-D_c[f,2h]}{3} = \frac{1}{3}\left\{\left[4f'(x_0) + \cancel{\frac{4}{24}f^{(3)}(x_0)}\right] - \left[f'(x_0) + \cancel{\frac{4}{24}f^{(3)}(x_0)}\right]\right\}$$

$$= f'(x_0) - 4Ch^4 f^{(5)}(x_0) = f'(x_0) + \mathcal{O}(h^4)\ !$$

- `extrap_diff` does this calculation. Your job: call `extrap_diff` twice from `extrap_diff2` to eliminate the $\mathcal{O}(h^4)$ term.
  - You *only* need to know the last line!

An example plot for problem 3 for one value of b



- This is not such an interesting choice of *b* (converges too quickly)

Random recaps and follow-ups

- Power spectrum (Fourier transform)
  - How is the power (energy per time) distributed among different frequencies?
  - What does a peak at zero frequency mean? How can you get rid of it?
  - See Session 11 handout for examples (to intepret!)
- Using classes makes it easier to generalize
  - e.g., GSL adaptive ODE solver for Van der Pol oscillator with different parameters
- Interpolation vs. least-squares fitting
  - When do you do each?
  - What is different between linear and non-linear fitting?
- Set up your code to be able to use multiple algorithms
  - for integration, interpolation, minimization, . . .
  - GSL allows this, but there are other options

Random recaps and follow-ups (cont.)

- Lessons from Session 9
  - Use GDB (or equivalent) to find segmentation faults
  - Compiler optimization is your (great!) friend, but don't turn it on until the program is debugged
  - Write first for correctness and clarity, then for speed (but only where you need speed!)
  - Why use `set` and `get` functions?
  - `rsync` is awesome!
- Python scripts to run C++ programs
  - Here: set up input, run a C++ code, and process output
  - Replace interactive input with command-line arguments
    - conventional: `main (int argc, char *argv[])`
    - `argc` is # of arguments, including program name
    - `argv[i]` is i'th argument (0 is name)
  - Python by example! Use generic scripts and adapt to needs
- Multidimenstional minimization is hard!
  - Session 11: try out some GSL algorithms for *local* minima
  - Coming: global methods (we'll do simulated annealing)

Chaos

- Characteristics of chaos (see Session 8 notes)
  - past behavior not repeated (not periodic)
  - deterministic but not predictable, because uncertainty (or imprecision) in initial conditions grows exponentially in time
  - system has distributed power spectrum (see Mathematica notebooks)
- Necessary conditions for chaos
  - $\geq$ 3 independent variables and the equations have nonlinear terms coupling
  - Three equations for the pendulum (with $\phi = \omega_{\text{ext}} t$)

$$\frac{d\theta}{dt} = \omega \qquad \frac{d\omega}{dt} = -\alpha\omega \underbrace{- \omega_0^2 \sin\theta - f_{\text{ext}} \cos\phi}_{\text{nonlinear couplings}} \qquad \frac{d\phi}{dt} = \omega_{\text{ext}}$$

- Session 10: Mathematica notebook `pendulum.nb`
  - gives results for Session 8 “Looking for Chaos”
  - power spectrum: what frequencies are in the $\theta(t)$ plot?

2013 Turing Award winner: Dr. Leslie Lamport

- ACM (Association for Computing Machinery) webpage with details
  - "The A.M. Turing Award, the ACM's most prestigious technical award, is given for major contributions of lasting importance to computing. . . . The award is also accompanied by a cash prize of $250,000, which in recent years has been underwritten by the Intel Corporation and Google, Inc."
- Citation:

  For fundamental contributions to the theory and practice of distributed and concurrent systems, notably the invention of concepts such as causality and logical clocks, safety and liveness, replicated state machines, and sequential consistency.

- In part for applying concepts familiar from special relativity to computer networks! (see this link to "Time, Clocks and the Ordering of Events in Distributed Systems")
- You may also know Dr. Lamport as the creator of LaTeX, which is a widely used macro package built on Donald Knuth's TeX.