

Physics 780.20: Assignment #3

These exercises are follow-ups to class and background-note discussion of Richardson extrapolation (session 4), eigensystems (session 5), and adaptive numerical routines (the last one is a bonus problem). These involve modifications to the `derivative_test.cpp` code and the `eigen_basis.cpp` code. Please ask questions! It is due at the end of the day (midnight) on Friday, February 19.

To “hand in” the assignment, email me (at `furnstahl.1@osu.edu`) a zip archive (see below) with your makefiles and programs (with the answers to any questions in the comments at the top) and postscript files of any plots. Comment your codes with your name, etc., as in the sample codes from class. *Check the 780.20 webpage for suggestions and hints.* Please ask questions and give feedback early and often.

1. It’s time to start thinking about a 780.20 project. Please send email (as soon as you can, separate from the rest of the homework) to `furnstahl.1@osu.edu` with a (brief!) description of your ideas for a project. They can be very vague at this point; we will refine them as the quarter progresses! See the 780 webpage for some past project descriptions.
2. Add a subroutine to take the Richardson extrapolation used in the “`extrap_diff`” subroutine one step further. That is, `extrap_diff` calls `central_diff` with two different values of h and then combines them to extrapolate to smaller h (leading to an error proportional to h^4). Now write a new routine (called `extrap_diff2`) that calls `extrap_diff` with two different values of h and combines them appropriately to get a still steeper dependence of the error on h . Verify the result by making an error plot (you may want to increase the starting value of h to 0.5). [A new version of `derivative_test.cpp` with `extrap_diff` explicitly written with `central_diff` is available from the hints.]
3. Modify `eigen_basis.cpp` so that you can print out (to a file is best!) the approximate wave function corresponding to a given state (e.g., the ground state or the first excited state). Plot the exact ground state wave function and the approximate wave function (as a function of r) for one of the potentials (your choice; I like the Coulomb best!) with a fixed b (your choice) for basis sizes of 1, 5, 10, and 20. Comment on the nature of the convergence and speculate about choosing b based on your plots. Make sure that the wave functions are normalized.
4. (BONUS) Make the calculation using the central difference method *adaptive*. That is, you specify the function but don’t specify the value of h . Instead, your program determines (or,

more precisely, estimates) the optimal value of h automatically and uses that. Compare the h chosen by your program for the function described above to the value you would select based on the error plot.

5. (BONUS) Devise a measure of how close the approximate wave function is to the exact wave function and determine how this measure scales with the basis size D .