FYS-4096 Computational Physics: Exercise 3

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Week 4

General:

- You should have access to help files on teacher's repo. If not, please provide your username and associated email to the teacher.
- There, in folder ex3_help, you will find files linear_interp.py, spline_class.py, and matrix_eigs.py that are needed or can be useful in these exercises.
- **Deadline always before noon on Monday the following week!** That is, for these problems before noon on Monday February 1.
- Better to send/push unfinished in time, than finished, but past deadline.

Problem 1: 2D integral revisited

• Calculate the integral below using scipy's Simpson rule:

$$\int_{-2}^{2} \int_{x_0}^{x_1} f(x, y) dx dy,$$

where $f(x,y) = (x+y)^2 \exp(-\sqrt{x^2+y^2})$ with $x_0 = 0$ and $x_1 = 2$.

- Note: from scipy.integrate import simps.
- Estimate the accuracy by using a couple of different grids.

Problem 2: 2D interpolation revisited

• Generate your "experimental data" using the function

$$f(x,y) = (x+y) \exp(-\sqrt{x^2 + y^2})$$

on a 30 by 30 linear grid with $x \in [-2, 2]$ and $y \in [-2, 2]$.

- Use the "experimental data" in estimating values along a path given by $y = 2x^2$, where $x \ge 0$. In the path there should be 100 uniformly spaced grid points for the x-values.
- Plot the 1D values from your interpolation as well as from the exact function. Use different line styles, legend, etc. to straightforwardly distinct the interpolated and exact solutions.

Problem 3: Power method

- Code a function called largest_eig and apply it to find the largest eigenvalue and corresponding eigenvector of the matrix given in matrix_eigs.py
- Compare the eigenvalue and the eigenvector with scipy's solver (provided in the example file).

Extra If time permits after problem 4 (on next page), read about inverse power method as well as Arnoldi iteration from, e.g., wikipedia.

Problem 4: Electric field

- Consider a charged 1D rod that is on x-axis from -L/2 to L/2, where L is the length of the rod.
- A positive charge Q is evenly distributed along the rod, and thus, its line charge density is given as $\lambda = Q/L$.
- The differential electric field at any point in space is given as

$$d\mathbf{E} = \frac{1}{4\pi\varepsilon_0} \frac{\lambda dx}{r^2} \hat{\mathbf{r}},\tag{1}$$

where r is the distance from a point (i.e., charge element) in the rod to a point in space, and $\hat{\mathbf{r}}$ is a corresponding unit vector.

- Since the net field is given by integration, i.e., $E = \int dE$, use Simpson rule for the integration.
- First, implement a code that calculates the electric field by the charged rod at any point in space. Test your numerical implementation against the electric field at $\mathbf{r} = (L/2 + d, 0) = (x, y)$ for which the analytical answer is

$$\mathbf{E} = \frac{\lambda}{4\pi\varepsilon_0} \left[\frac{1}{d} - \frac{1}{d+L} \right] \hat{\mathbf{i}}.$$
 (2)

• Second, calculate numerically the electric field in xy-plane, and visualize your vector field result with matplotlib's quiver function (or something similar). (Notes: Avoid y = 0 in your grid. A 20 by 20 grid should be good enough.)

Returning your exercise

- 1. Make a new folder called "exercise3" into your existing Computational Physics repo.
- 2. Create a file solvedProblems.txt at the root of your "exercise3" folder. Inside it, write a comma separated list of problems you have solved, e.g., 1,2,3x.
- 3. Make sure all your source files are under version control and push them to GitLab.
- 4. Push your commits (and possible tags) to GitLab before noon on Monday February 1: