FYS-4096 Computational Physics: Exercise 3

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General:

- You should have access to `exercise3_help_files` on teacher's repo. If not, please provide your username and associated email to the teacher.
- There you will find files `linear_interp.py`, `spline_class.py`, and `matrix_eigs.py` that are needed or can be useful in these exercises.

Problem 1: 2D integral revisited

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

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

where $f(x,y) = (x+y)\exp(-(x^2+y^2))$ with $x_0 = 0$ and $x_1 = 2$. Note: `from scipy.integrate import simps`.

Problem 2: 2D interpolation revisited

- Generate your "experimental data" using the function

$$f(x,y) = (x+y)\exp(-(x^2+y^2)) \tag{1}$$

on a 40 by 40 grid with $x \in [-2,2]$ and $y \in [-2,2]$.

- Your task is to estimate values on a straight line $y = \sqrt{2}x$ for $x \geq 0$ from the "experimental data". For the straight line the x-values should be linearly spaced for all the acceptable values using 100 grid points.
- Plot the 1D values from your interpolation and from the exact function.

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

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

- Test your numerical implementation by computing the electric field at $\mathbf{r} = (L/2+d, 0) = (x, y)$ for which the analytical answer is

$$\mathbf{E} = \frac{\lambda}{4\pi\varepsilon_0}\left[\frac{1}{d} - \frac{1}{d+L}\right]\hat{\mathbf{i}}. \tag{3}$$

- Calculate numerically the electric field in xy-plane, and visualize your vector field result with matplotlib's quiver function. (Note: avoid $y = 0$ in your grid).

Returning your exercise

1. Create a new git repo or make new folder to your existing Computational Physics repo.
2. Create a file problems_solved.txt at the root of your "exercise3" git repo. Inside it, write a comma separated list of problems you have solved, e.g., 1,2,3.
3. Make sure all your source files are under version control and push them to GitLab.
4. Tag your final solution (git commit) with "final" tag: `git tag final`
5. Push your commits and the final tag to GitLab before Friday 11 am:
   `git push --all && git push --tags`
6. Remember to share your GitLab project with the teacher before or right after the final git push. Be careful in providing proper permissions, so that the teacher can also access the data. (Teacher's GitLab account: kylanpaait, ilkka.kylanpaa@tuni.fi).
7. **If you are using the same repo for all exercises, send the teacher an email once you are done with the weeks exercise!**