Scientific Computation
Autumn 2024
Project 2

Due: Friday December 13th, 1pm

In addition to this project description, there are 2 files for this assignment:

- project2.py: a Python file which you will complete and submit on Blackboard (see below for details)
- report2.tex: a Latex template file for the short report which you will submit. The discussion and figure(s) described below should be placed in this report.

Part 1

In Part 1, you will answer questions related to the following system of n ODEs:

$$\frac{dx_i}{dt} = x_i\left(1 - x_i - \gamma\left(x_{i-2} + x_{i+1}\right)\right), \quad i = 2, 3 \ldots, n-2,$$

$$\frac{dx_0}{dt} = x_0\left(1 - x_0 - \gamma\left(x_{n-2} + x_1\right) + \mu x_{n-3}\right),$$

$$\frac{dx_1}{dt} = x_1\left(1 - x_1 - \gamma\left(x_{n-1} + x_2\right)\right),$$

$$\frac{dx_{n-1}}{dt} = x_{n-1}\left(1 - x_{n-1} - \gamma\left(x_{n-3} + x_0\right)\right).$$

Here, μ and γ are model parameters, and an initial condition must also be specified at $t = 0$. You have been provided with the function *simulate1* which computes numerical solutions for this problem using `solve_ivp`.

1. (6 points) Let $\bar{\mathbf{x}}$, be a non-trivial equilibrium solution for the system, and consider the behavior of infinitesimal perturbations to such an equilibrium, $\mathbf{x} = \bar{\mathbf{x}} + \tilde{\mathbf{x}}$ with the magnitudes of all elements of $\tilde{\mathbf{x}}$ much smaller than one. Define the perturbation energy at time t as, $e(t) = \tilde{\mathbf{x}}(t)^T\tilde{\mathbf{x}}(t)$.

   (a) Complete the function *part1q1a* so that it: 1) computes and returns a non-trivial equilibrium solution and 2) computes and returns an initial perturbation vector $\tilde{\mathbf{x}}_0 = \tilde{\mathbf{x}}(t = 0)$ which maximizes $e(t = T)/e(t = 0)$. Here, T is an input parameter for the function and the maximum $e(t = T)/e(t = 0)$ should also be returned. See the function docstring for more details. In your report, provide a 2-3 sentence description of the general approach you have taken.

   (b) Set $n = 19$, $\gamma = 1.2$, $\mu = 2.5$, and $T = 50$. Design a numerical test that compares results for the perturbation energy produced by *part1q1a* with simulation results for the full problem (computed with *simulation1*). The test should be designed to show consistency between the results, though you are not expected to show perfect consistency. Place your test code in *part1q1b*. In your report, provide a clear and concise description of your test design and your test results.

(c) Now set $\gamma = 2$ and $\mu = 0$ while keeping $n = 19$. Analyze how $\max\left(e(t=T)/e(t=0)\right)$ varies with T for $0 < T \leq 50$. You should describe the observed behavior carefully and also attempt to draw connections to properties of the model system. Place your discussion and any supporting figures in your report. Place the code for your analysis in *part1q1c*.

2. (8 points) Set $\gamma = 1$ and $\mu = 0$, and consider the following three cases: case A: $n = 9$, case B: $n = 20$, and case C: $n = 59$. Analyze simulation results for these three cases. Typically simulations contain an initial transient as the system responds to the initial conditions followed by a relatively settled dynamical state. Discard the transient in your analysis, and focus on the subsequent dynamics of $\mathbf{x}$ and the variation of its elements with time (you should vary Nt and tf as needed for the different cases). Also consider the global qualitative dynamics (e.g. no time-dependence, simple sinusoidal oscillations, components are synchronized, ...). Carefully analyze if/to what degree chaotic dynamics are present. Qualitative observations should be supported by quantitative results obtained using the simulation results. You should provide a careful and thorough analysis of all three cases supporting your discussion with well-designed figures. Add the code used in your analysis to the function, *part1q2*, and add the discussion of your findings along with supporting figures to your report.
Note: For this question, you should use the initial condition set within *simulate1* though it's fine to also consider other initial conditions if it helps your analysis.

Part 2

(6 points) Often, when simulating nonlinear systems, both the first and second derivatives of the dependent variables are needed. In this question, you will analyze an implicit finite difference method which simultaneously computes both derivatives. The derivatives, $\frac{du}{dx}$, and $\frac{d^2u}{dx^2}$ should be computed on a two-dimensional Cartesian grid with the grid defined as follows:

$$x_j = j\Delta x, \;\; j = 0, 1, 2, ..., n-1, \;\; \Delta x = \frac{1}{n-1}, \tag{1}$$

$$y_i = i\Delta y, \;\; i = 0, 1, 2, ..., m-1, \;\; \Delta y = \frac{1}{m-1}, \tag{2}$$

and the data at location (x_j, y_i) is $u_{i,j}$. We will use $u'_{i,j}$ and $u''_{i,j}$ as shorthand for first and second derivatives of u with respect to x at (x_j, y_i). For each $j \in \{1, 2, ..., n-2\}$ and any y_i, we have two equations for the two unknowns $u'_{i,j}$ and $u''_{i,j}$:

$$7u'_{i,j-1} + 16u'_{i,j} + 7u'_{i,j+1} + h\left(u''_{i,j-1} - u''_{i,j+1}\right) = \frac{15}{h}\left(u_{i,j+1} - u_{i,j-1}\right),$$

$$9\left(u'_{i,j+1} - u'_{i,j-1}\right) - h\left(u''_{i,j-1} - 8u''_{i,j} + u''_{i,j+1}\right) = \frac{24}{h}\left(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}\right),$$

where $h = \Delta x$. Different equations are needed at the boundaries, $j = 0$, and $j = n-1$. For $j = 0$:

$$u'_{i,j} + 2u'_{i,j+1} - hu''_{i,j+1} = \frac{1}{h}\left[-3.5u_{i,j} + 4u_{i,j+1} - 0.5u_{i,j+2}\right],$$
$$-6u'_{i,j+1} + h\left(u''_{i,j} + 5u''_{i,j+1}\right) = \frac{1}{h}\left[9u_{i,j} - 12u_{i,j+1} + 3u_{i,j+2}\right],$$

and for $j = n-1$:

$$u'_{i,j} + 2u'_{i,j-1} + hu''_{i,j-1} = -\frac{1}{h}\left[-3.5u_{i,j} + 4u_{i,j-1} - 0.5u_{i,j-2}\right],$$
$$-6u'_{i,j-1} - h\left(u''_{i,j} + 5u''_{i,j-1}\right) = -\frac{1}{h}\left[9u_{i,j} - 12u_{i,j-1} + 3u_{i,j-2}\right].$$

Code that implements this method for the special case where $m = 1$ has been provided for reference in the function, *dualfd1*, however note that the implementation is not efficient.

1. Complete *part2q1* so that it efficiently implements this scheme to compute first and second derivatives along the m rows of a two-dimensional m x n array provided to the function as input. Each row of the input array should contain data, $r(x_j),\ j = 0, 1, 2, ..., n-1$, which should be differentiated. In your report, briefly describe why your Python implementation of the given method should be considered to be efficient.

2. Design a set of computational tests that support a critical comparison of the methods implemented in *part2q1* and *fd2*. Assume that m is comparable to n, and assess the effectiveness of these methods for multiscale problems. Ultimately, your analysis should reflect a clear understanding of the cost and accuracy of the implicit method and your implementation. It is sufficient for analysis of the accuracy to only consider results for the first derivative and to focus on the portion of the domain away from the horizontal boundaries. Add your analysis and accompanying figures to your pdf. Place the code used for the analysis in *part2q2*.

You may use numpy, scipy, matplotlib, time, and timeit as needed for this assignment. Please do not use other packages without permission.

Further guidance

- You should submit both your completed python file (*project2.py*),a pdf containing your discussion and figure(s) (*report2.pdf*). You are not required to use the provided latex template, any well-organized pdf is fine. To submit your assignment, go to the module Blackboard page and click on"Project 2". There will be an option to attach your files to your submission. (these should be named *project2.py* and *report2.pdf*). After attaching the files, submit your assignment.

- Please do not modify the input/output of the provided functions without permission. You may use numpy, scipy, matplotlib, networkx, time, timeit, collections, and heapq as needed. Otherwise, please do not import any modules without permission. You may create additional functions as needed, and you may use any code that I have provided during the term. Some functions have input variables with specified default values. You are not required to use these values unless the relevant question explicitly states that you are.

- Marking will be based on the correctness of your work and the degree to which your submission reflects a good understanding of the material covered up through lecture 17. Excluding figures, you should aim to keep the pdf version of your report to less than 8 pages of text (if you take all the text in your report excluding figures, title, references, it should fit in 6 pages).
- You may use chatgpt-4o, claude 3.5 sonnet, or claude haiku for the assignment without restriction (other llms and code-generation tools are not allowed). Any submitted llm-generated code must be clearly referenced with comments indicating what is llm-generated and which specific llm was used (e.g. chatgpt-4o). Prompts used to generate submitted code should be included in an appendix of the submitted report. Similarly, submitted discussion which draws substantially on llm-generated content should be clearly referenced and relevant prompts should be included in a report appendix. Note that both chatgpt-4o and claude 3.5 sonnet are free but have usage limits, and it is your responsibility to manage your usage appropriately.
- Open-ended questions require sensible time-management on your part. If you are concerned that your approach to the assignment may require an excessive amount of time, please get in touch with the instructor.
- Questions on the assignment should be asked in private settings. This can be a "private" question on Ed (which is distinct from "anonymous") or by arrangement with the instructor.
- Please regularly backup your work. For example, you could keep an updated copy of your files on OneDrive and use Overleaf for your report.
- In order to assign partial credit, we need to understand what your code is doing, so please add comments to the code to help us.
- You have been asked to submit code in Python functions, but it may be helpful to initially develop code outside of functions so that you can easily check the values of variables in a Python terminal.
- Your project2.py module should not run anything when it is imported in a Python terminal (e.g. it should not call any functions or generate any output or figures).
- Your submission should be your own work, you should not collaborate with other students, and you should clearly and completely cite external sources which are used in your work (detailed citations of slides/labs from the module are not needed).