

Assignment #1

Due Date: F Sep 20, 2024

1 Problem Description and Questions

For this first assignment I want you to reproduce some results from one of my papers. Consequently, you will have something to compare against and should know if your answer is incorrect.

The paper in question is “Superconvergent functional estimates from summation-by-parts finite-difference discretizations,” published in the SIAM Journal on Scientific Computing in 2011. The problem is described in Section 5.1 of the paper, but I will provide the necessary details below.

1.1 PDE and Functional Description

The PDE is of Poisson type and is defined on the square domain $\Omega = [0, 1]^2$ with Dirichlet boundary conditions:

$$\begin{aligned} -\nabla \cdot (\gamma \nabla u) &= f, & \forall (x, y) \in \Omega, \\ u(x, y) &= u_{\partial\Omega}(x, y), & \forall (x, y) \in \partial\Omega, \end{aligned} \quad (1)$$

where $\partial\Omega$ denotes the boundary of Ω .

You will determine the source term, $f(x, y)$, and boundary function, $u_{\partial\Omega}(x, y)$, using the method of manufactured solutions. That is, you will adopt the analytical solution, u , and diffusion coefficient, γ , defined below and substitute these into the PDE and boundary condition to find f and $u_{\partial\Omega}$. The solution and diffusion coefficient are, respectively,

$$u(x, y) = e^y \sin\left(\frac{\pi(e^x - 1)}{e - 1}\right), \quad \text{and} \quad \gamma(x) = \frac{\pi e^x}{e - 1}.$$

The functional for this problem is defined as a weighted integral of the normal derivative of u over the lower boundary, $\partial\Omega_1 = \{(x, y) \mid x \in [0, 1], y = 0\}$. More precisely, the functional is given by

$$\mathcal{J}(u) = \int_{\partial\Omega_1} \beta \gamma (\hat{n} \cdot \nabla u) \, dx, \quad (2)$$

where \hat{n} is the outward pointing unit normal on $\partial\Omega$. A couple different functions will be considered for the weighting $\beta(x)$. These are defined below in the questions.

1.2 Questions

1. Derive the adjoint PDE for (1) and (2). I am more interested in the derivation than the result (which is available in the paper), so show your work!
2. Choose and implement an adjoint consistent discretization for (1) and (2). The discretization must yield errors with a higher than second-order rate of convergence in the L^2 norm (for sufficiently smooth solutions). See Section 3 for suggested methods and libraries.

Verify the accuracy and rate of convergence of your discretization by plotting the L^2 and/or L^∞ solution error norm versus mesh size h .

3. For this question, use $\beta(x) = 1$, i.e. the constant one. With this choice for β the functional's value is $\mathcal{J}(u) = -2$.
 - (a) Solve for the adjoint using the discrete adjoint approach, and plot the contours of the adjoint solution you obtain.
 - (b) Plot the function error versus mesh size h ; is the functional superconvergent? Why or why not?
4. For this question, use

$$\beta(x) = \frac{\pi^2(e^x - 1)(e - e^x)}{(e - 1)^2}, \quad (3)$$

which produces $\mathcal{J}(u) = 4$ for the exact solution.

- (a) Solve for the adjoint using the discrete adjoint approach, and plot the contours of the adjoint solution you obtain.
- (b) Plot the function error versus mesh size h ; is the functional superconvergent? Why or why not?

2 Report and Code Expectations

As mentioned in class, I expect all reports to be L^AT_EX'ed. If you have not used L^AT_EX before, I recommend that you try overleaf.com, which provides some templates and other resources.

The report should be fewer than 10 pages if you use a 12 point font. This is a “soft” page limit, but please do not be overly verbose.

The following should be included in the report.

- An abstract that summarizes the discretization that you used and the results of your study.
- Provide a separate section or subsection in which you answer each question in the above list of questions.
- In your answer to Question 2, be sure to clearly describe the discretization that you used for (1) and (2), as well as how you generated the meshes.

You do not need to include an introduction, since your audience (me!) knows the background. You can include the results of additional studies that you performed out of interest.

The report will include several figures as requested in the questions. Please use an adequate font size on the figures! It should be legible if printed.

Please provide the code for your project as a separate zip file. You do not need to include the code in the report itself. If the code needs to be compiled, please provide instructions for how to compile it. All code should have adequate commenting.

3 Notes on the Discretization

You are welcome to use whatever discretization satisfies the greater-than-second-order requirement mentioned in Question 2. Here are some possible options.

Use the one in the paper: You can use the same finite-difference method described in the paper. I can point you toward some other papers where the necessary summation-by-parts (SBP) operators are defined. These methods are relatively easy to implement, although the notation is sometimes a bit of a pain in the neck.

Use MFEM: If you are comfortable with C++, the MFEM library may be a good option to consider. The bilinear forms you will need are mostly ready to use “off the shelf.” There is also a Python version, if you prefer that.

Use FEniCS: If you are familiar with finite-element methods and Python, FEniCS may be a great option (fenicsproject.org). FEniCS can even help you get the adjoint and there is lots of documentation available.

Use SummationByParts.jl: `SummationByParts.jl` is a Julia (<https://www.julialang.org>) package that can be used to construct element-based discretizations on line, triangular, and tetrahedral elements. *Note that I may rely on this package for assignments 2, 3, and 4.*

Collaboration

You are permitted and encouraged to discuss the assignment with each other, provided each of you writes your own code and report. A good policy to follow in order to avoid academic misconduct is to not take notes or exchange files with one another; i.e. exchange information verbally and you should be fine. Please acknowledge any help you receive.

AI Use

The current generation of large-language models (e.g. LLMs such as ChatGPT) can be helpful to experts, because experts can detect errors and correct the answers given. On the other hand, LLMs are **not** as helpful for novices, because novices cannot detect errors.

Keeping the above comment in mind, LLMs are permitted for two use case in this course.

- You may use AI to help write your initial code.
- You may use AI to help correct grammar in any narrative you have written.

In both cases, **the use of AI must be acknowledged**. Failure to acknowledge AI assistance will be treated as a breach of academic integrity.

Please note that overly verbose reports and writing with excessive superlatives will not receive full credit. Be concise.