AM 213A, Winter 2024
Homework 5 (100 points)

Posted on Thu, Feb 29, 2024
Due Fri, Mar 8, 2024

Submit your coding homework to Canvas
Submit your theory homework to Gradescope

- Use LaTeX or MS-words like text editors for homework. A scanned copy of handwritten solutions will be acceptable on an exceptional case-by-case only with permission from the instructor.
- Your report needs to have relevant discussions on each problem to describe what you demonstrate. In this coursework, do not simply copy and paste any screen outputs (e.g., screenshots) from your code execution and provide them as answers. Instead, discuss code results required for each problem and display them concisely with logical justification. For all coding problems, showing screen outputs only from your code execution is insufficient and will lose points.
- To disprove, you need to provide a counter-example.
- All homework submissions should meet the deadline. Late homework will be accepted under emergencies with permission from the instructor.
- Submit all code and reports using the following naming conventions:
  - The theory and computational report should be together in one PDF named as `LastnameFirstname_Report_hwX.pdf` where `X` is the homework number
  - The supporting code for each homework should be provided in a single compressed directory named as `LastnameFirstname_Code_hwX.tar.gz` or `LastnameFirstname_Code_hwX.zip`
    - Include only source files (e.g. `*.f90`, `*.c`, etc.) and the needed Makefile
    - Do **not** include object files, module files, executables, or data files.

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1. General Guidelines

1.1. Two parts

You have two parts in this homework set:

- **Part 1 (30 pts)**: Numerical coding problems (Make sure to use double precision unless you are told otherwise!!!)
- **Part 2 (70 pts)**: Theory problems

Your final set of answers should consist of

- For Part 1: a pdf file with your written answers. This pdf *must* be created using a word processor. Prepare a "README" file to give a short description of how to execute your code implementations, e.g., "To run the code, execute make first; run the executable file `hw5_exe`; the name of the driver routine – `hw5_QR.f90`". Each README file should be short and concise to provide first-hand guidelines to execute your codes.
- For Part 2: solutions to the theory problems. Use LeTeX or MS-words like text editors.
- For both Part 1 and Part 2: Please submit all your answers to Canvas. Submit two separate files named as
  - For Part1: `LastnameFirstname_Part1_hw5.tar.gz` or `LastnameFirstname_Part1_hw5.zip`
  - For Part 2: `LastnameFirstname_Part2_hw5.tar.gz` or `LastnameFirstname_Part2_hw5.zip`

Organize and present your solutions in the best possible way, in particular, for your Part 1 solutions:

- For any written material, be informative but concise. Mathematical derivations, if appropriate, should contain enough pertinent steps to show the reader how you proceeded. All included figures should be clearly annotated and have an informative caption. Each problem should be addressed in its own Section (e.g., "Section 1: Problem 1", "Section 2: Problem 2", etc.). References should be included if you are using any material as part of your discussions and/or calculations.
- For the codes: All codes must be written in Fortran 90 (or more recent Fortran, but not Fortran 77) or C, but *not* in any other language. MATLAB or Python is to be used only to (i) generate figures and/or (ii) perform simple analysis (e.g., calculating errors) of the data produced by your Fortran/C codes. Put all the codes relevant for each problem in separate directories called Prob1, Prob2, etc., as needed. Annotate your codes carefully so the reader knows what each part of the code does. For each routine and function in your Fortran/C, include a header (i.e., comment sections at the beginning of each code) explaining the inputs and outputs of the code and what the routine does. In the main program in each directory, include a header that contains (i) the command required to compile the code and (ii) the structure of the inputs and outputs of the main program.

Part 1: Coding Problems (30 points; 10 points each)

In your report, include inputs (e.g., initial guess) and outputs of your codes. Describe sufficiently the behaviors of your codes in each problem. Clarify what parts of your code implementations are corresponding to each individual problem (e.g., subroutines foo1 & foo2 in `LinAl.f90` are for Problem 1, etc.).

To debug your code, make sure you test your code to solve at least one of worked examples in the lecture note.

1. Write a program to reduce a symmetric matrix to tridiagonal form using Householder matrices for the similarity transformations. Use the program to reduce the following matrix to tridiagonal form:

$$\mathbf{A} = \begin{bmatrix} 5 & 4 & 1 & 1 \\ 4 & 5 & 1 & 1 \\ 1 & 1 & 4 & 2 \\ 1 & 1 & 2 & 4 \end{bmatrix}. \tag{1}$$

2. Write a program of the QR algorithm (i) without shift and (ii) with shift, to calculate the eigenvalues of

$$\mathbf{A} = \begin{bmatrix} 3 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 1 \end{bmatrix}. \tag{2}$$

3. Consider the matrix

$$\mathbf{A} = \begin{bmatrix} 2 & 1 & 3 & 4 \\ 1 & -3 & 1 & 5 \\ 3 & 1 & 6 & -2 \\ 4 & 5 & -2 & -1 \end{bmatrix}, \tag{3}$$

which has three eigenvalues $\lambda_1 = -8.0286, \lambda_2 = 7.9329, \lambda_3 = 5.6689$, and $\lambda_4 = -1.5732$. Write a program of the inverse iteration to calculate the corresponding eigenvectors.

Part 2: Theory Problems (70 points)

1. [15 pts] Consider the Householder matrix defined by

$$\mathbf{H} = \mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}. \tag{4}$$

a. [3 pts] Show that for any nonzero vector $\mathbf{v}$, the matrix is orthogonal and symmetric.

b. [3 pts] Let $\mathbf{a}$ be any nonzero vector and let $\mathbf{v} = \mathbf{a} + \alpha\mathbf{e}_1$, where $\alpha = \text{sign}(a_{11})||\mathbf{a}||_2$. Show that $\mathbf{Ha} = -\alpha\mathbf{e}_1$ by direct calculation.

c. [3 pts] Determine $\mathbf{v}$ and α that transforms

$$\mathbf{H}\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} \alpha \\ 0 \\ 0 \\ 0 \end{bmatrix}. \tag{5}$$

d. [3 pts] Given the vector $\mathbf{a} = (2, 3, 4)^T$, specify a Householder transformation that annihilates the third component of $\mathbf{a}$.

e. [3 pts] What are the eigenvalues of $\mathbf{H}$ for any nonzero vector $\mathbf{x}$?

2. [8 pts] The Schur decomposition theorem states that every square matrix $\mathbf{A} \in \mathbb{C}^{m\times m}$ has a Schur decomposition, $\mathbf{A} = \mathbf{QUQ}^*$, where Q is unitary and T is upper-triangular. Use this theorem to prove that, for an arbitrary norm $||\cdot||$,

$$\lim_{n\to\infty} ||\mathbf{A}^n|| = 0 \iff \rho(\mathbf{A}) < 1. \tag{6}$$

(Note: Show the claim first with the 2-norm or the Frobenius norm and use the fact that all norms are equivalent in a finite vector space.)

3. [8 pts] Let $\mathbf{A}$ be $m \times n$ and $\mathbf{B}$ be $n \times m$. Show that the matrices $\begin{bmatrix} \mathbf{AB} & 0 \\ B & 0 \end{bmatrix}$ and $\begin{bmatrix} 0 & 0 \\ \mathbf{B} & \mathbf{BA} \end{bmatrix}$ have the same eigenvalues.

4. [8 pts] Show that for a real-valued square matrix the Gerschgorin theorem also holds with the bounds r_i which are given by the partial column sums (instead of the partial row sums):

$$r_i = \sum_{i=1, i\neq j}^{m} |a_{i,j}|, \quad i = 1, \ldots, m. \tag{7}$$

5. [7 pts] Use the Gerschgorin theorem to show that the matrix

$$\mathbf{A} = \begin{bmatrix} 1.0 & 0.3 & 0.1 & 0.4 \\ 0.0 & 2.0 & 0.0 & 0.1 \\ 0.0 & 0.4 & 3.0 & 0.0 \\ 0.1 & 0.0 & 0.0 & 4.0 \end{bmatrix} \tag{8}$$

has exactly one eigenvalue in each of the four circles

$$|z - k| \leq 0.1, \quad k = 1, 2, 3, 4. \tag{9}$$

6. [8 pts] Let $\mathbf{A} \in \mathbb{R}^{m \times m}$ be real and symmetric that is positive definite. Let $y \in \mathbb{R}^m$ be nonzero. Prove that the limit

$$\lim_{k \to \infty} \frac{y^T \mathbf{A}^{k+1} y}{y^T \mathbf{A}^k y} \tag{10}$$

exists and is an eigenvalue of $\mathbf{A}$.

7. [8 pts] Let $\mathbf{A} \in \mathbb{R}^{m \times m}$ be real with nonnegative enties such that

$$\sum_{j=1}^{m} a_{ij} = 1 \ \ (1 \leq i \leq m). \tag{11}$$

Prove that no eigenvalue of $\mathbf{A}$ has an absolute value greater than 1.

8. [8 pts] Let $\mathbf{A} \in \mathbb{R}^{m \times m}$ be a non-defective matrix with its eigenvalues $\{\lambda_i\}_{i=1}^m$ and its singular values $\{\sigma_i\}_{i=1}^m$, satisfying

$$|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_m|, \tag{12}$$

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_m. \tag{13}$$

Let $\rho(\mathbf{A})$ be the spectral radius of $\mathbf{A}$ and $\text{cond}(\mathbf{A}) = ||\mathbf{A}||_2 ||\mathbf{A}^{-1}||_2$ be the condition number of $\mathbf{A}$. Let $\mathbf{A}$ be normal, i.e., $\mathbf{A}^T\mathbf{A} = \mathbf{A}\mathbf{A}^T$. Show that:

(a) $\sigma_i = |\lambda_i|$, $1 \leq i \leq m$.

(b) $||\mathbf{A}||_2 = |\lambda_1| = \rho(\mathbf{A})$.