18.335 Problem Set 3

There are four problems below (Problem 1 - Problem 4). You may complete as many problems as you want, but please submit **only three** problems for grading. **Due November 23, 2025 at 11:59pm.** Late submission will only be accepted up to **three days** after the due date. You should submit your problem set **electronically** on the 18.335 Gradescope page. Submit **both** a *scan* of any handwritten solutions (I recommend an app like TinyScanner or similar to create a good-quality black-and-white "thresholded" scan) and **also** a *PDF printout* of the Julia notebook of your computer solutions.

`Problem 0: Pset Honor Code`

Include the following statement in your solutions:

> *I will not look at 18.335 pset solutions from previous semesters. I may discuss problems with my classmates or others, but I will write up my solutions on my own.* <*your signature*>

Problem 1: Pseudospectra

This problem is based on Exercise 26.1 in Trefenthen's book. Suppose we compute the eigenvalues of a matrix A numerically, and they are the exact eigenvalues of a matrix $A + \delta A$ with $\|\delta A\|/\|A\| = O(\gamma_n)$. How close must they be to the exact eigenvalues of A? One approach to this question is through pseudospectra. Given $A \in \mathbb{C}^{n\times n}$ with spectrum $\Lambda(A) \subset \mathbb{C}$ and a fixed parameter $\epsilon > 0$, we define the 2-norm ϵ-pseudospectrum of A, denoted $\Lambda_\epsilon(A)$, to be the set of $z \in \mathbb{C}$ satisfying any of the following conditions:

(a) z is an eigenvalue of $A + \delta A$ for some δA with $\|\delta A\|_2 \leqslant \epsilon$,

(b) there exists a $u \in \mathbb{C}^n$, $\|u\|_2 = 1$, with

$$\|(A - zI)u\|_2 \leqslant \epsilon\,,$$

(c) the smallest singular value $\sigma_n(zI - A) \leqslant \epsilon$,

(d) $\|(zI - A)^{-1}\|_2 \geqslant \epsilon^{-1}$ (with the convention that if z is an eigenvalue then $\|(zI-A)^{-1}\| = \infty$).

Show that these four conditions are equivalent.

Problem 2: Newton's Method for the Eigenvalue Problem

Consider Newton's method

$$u_+ = u - J[f(u)]^{-1} f(u)\,,$$

where J is the Jacobian, for finding a point $u \in \mathbb{R}^n$ such that $f(u) : \mathbb{R}^n \to \mathbb{R}^n$ equals zero. Apply Newton's method to the eigenvalue problem $Ax = \lambda x, x^\top x = 1$ for some $A \in \mathbb{R}^{n\times n}$. Derive an explicit update formula for one step of Newton's method, expressed as

$$\begin{pmatrix} x_+ \\ \lambda_+ \end{pmatrix} = F\left[\begin{pmatrix} x \\ \lambda \end{pmatrix}\right],$$

for an explicit function F depending only on x, λ and $(A - \lambda I)^{-1}$ (assuming $A - \lambda I$ is invertible). Use this update rule to construct an algorithm for computing eigenpairs, and compare it to the Rayleigh quotient iteration.
Hint: The two algorithms are similar in some aspects but not identical.

Problem 3: A Krylov Subspace Method with LU-based Recurrence

Let $A \in \mathbb{R}^{n\times n}$ be a real symmetric matrix, i.e., $A^\top = A$. Given an initial guess $x_0 \in \mathbb{R}^n$, Krylov subspace methods seek an approximate solution $x_k \in x_0 + \mathcal{K}_k$, where the Krylov subspace $\mathcal{K}_k$ is defined as:

$$\mathcal{K}_k(A, r_0) = \operatorname{span}\{r_0, Ar_0, \ldots, A^{k-1}r_0\}\,,$$

with initial residual $r_0 = b - Ax_0$. Let $Q_k = \begin{bmatrix} q_1 & \ldots & q_k \end{bmatrix} \in \mathbb{R}^{n\times k}$ be an orthonormal basis for $\mathcal{K}_k$, constructed via the Arnoldi iteration. Let $\beta_1 = \|r_0\|_2$. The full orthogonalization method (FOM) seeks an approximate solution of the form $x_k = x_0 + Q_k y_k$ where y_k solves

$$H_k y_k = \beta_1 e_1\,, \tag{1}$$

and $H_k \in \mathbb{R}^{k\times k}$ is the tridiagonal matrix:

$$H_k = \begin{bmatrix} \alpha_1 & \beta_2 & & & \\ \beta_2 & \alpha_2 & \beta_3 & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{k-1} & \alpha_{k-1} & \beta_k \\ & & & \beta_k & \alpha_k \end{bmatrix}$$

The Lanczos recurrence gives:

$$Aq_j = \beta_{j+1} q_{j+1} + \alpha_j q_j + \beta_j q_{j-1}\,.$$

We now study a method that simultaneously constructs the vectors q_j and solves for y_k.

(a) Suppose the LU decomposition $H_k = L_k U_k$ exists. Show that L_k and U_k are both bidiagonal matrices. Let

$$L_k = \begin{bmatrix} 1 & & & & \\ \lambda_2 & 1 & & & \\ & \ddots & \ddots & & \\ & & \lambda_{k-1} & 1 & \\ & & & \lambda_k & 1 \end{bmatrix}$$

and

$$U_k = \begin{bmatrix} \eta_1 & \omega_2 & & & \\ & \eta_2 & \omega_3 & & \\ & & \ddots & \ddots & \\ & & & \eta_{k-1} & \omega_k \\ & & & & \eta_k \end{bmatrix}$$

Derive recurrence formulas for $\omega_k, \lambda_k, \eta_k$ in terms form $\eta_{k-1}, \alpha_k, \beta_k$.

(b) Define $D_k = Q_k U_k^{-1} \in \mathbb{R}^{n\times k}$, and let $z_k = L_k^{-1}\beta_1 e_1 \in \mathbb{R}^k$. Show that D_k and z_k can be computed recursively:

$$D_k = \begin{bmatrix} D_{k-1} & p_k \end{bmatrix} \text{ and } z_k = \begin{bmatrix} z_{k-1} \\ \zeta_k \end{bmatrix},$$

Derive a recurrence formula for p_k in terms of p_{k-1}, q_k and ω_k, η_k. Deirve a recurrence formula for ζ_k in terms of ζ_{k-1} and λ_k.

(c) Use the above relations to write an algorithm that compute x_k with $O(n)$ memory (independent of k). Compare this method to the Conjugate Gradient algorithm.

Hint: The two algorithms are the same.

Problem 4: Arnoldi Iteration in Action

This problem is based on Exercise 34.3 in Trefenthen's book. Let A be the $n \times n$ bidiagonal matrix with $A_{k,k} = A_{k,k+1} = k^{-1/2}$ and $n = 64$.

(a) Produce a plot showing the spectrum of A and contours showing the boundaries of the pseudospectra of A for $\epsilon = 10^{-i}$, $i = 1, 2, 3, 4$ (using the definition $\sigma_n(zI - A) \leqslant \epsilon$ is recommended; see Problem #1 for definition & details).

(b) Create an implementation of Arnoldi iteration and, starting from a random initial guess, run 20 steps of Arnoldi for A. Produce a plot illustrating the rate of convergence of the spectrum for $k = 1, \dots, 20$ to the largest, second-largest, and smallest eigenvalues of A. Comment on your results.

(c) For $k = 5, 10, 15, 20$, produce plots showing the spectrum of H_k and contours showing the boundaries of the pseudospectra of H_k for $\epsilon = 10^{-i}$, $i = 1, 2, 3, 4$. How well do they match the corresponding plot for A?

Feedback (optional)

Please let me know how you're finding the course and the first problem set. What are you hoping to get out of the class? How is the pace of lecture? Please rate the difficulty and volume of the first problem set. You can submit an anonymous survey here.