

SI231 - Matrix Computations, Fall 2020-21

Homework Set #4

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Acknowledgements:

- 1) Deadline: **2020-11-20 23:59:00**
- 2) Submit your homework at **Gradescope**. Homework #4 contains two parts, the theoretical part and the programming part.
- 3) About the theoretical part:
 - (a) Submit your homework in **Homework 4** in gradescope. Make sure that you have correctly select pages for each problem. If not, you probably will get 0 point.
 - (b) Your homework should be uploaded in the **PDF** format, and the naming format of the file is not specified.
 - (c) No handwritten homework is accepted. You need to use \LaTeX in principle.
 - (d) Use the given template and give your solution in English. Solution in Chinese is not allowed.
- 4) About the programming part:
 - (a) Submit your codes in **Homework 4 Programming part** in gradescope.
 - (b) When handing in your homework in gradescope, package all your codes into `your_student_id+hw4_code.zip` and upload. In the package, you also need to include a file named `README.txt/md` to clearly identify the function of each file.
 - (c) Make sure that your codes can run and are consistent with your solutions.
- 5) **Late Policy details can be found in the bulletin board of Blackboard.**

STUDY GUIDE

This homework concerns the following topics:

- Eigenvalues, eigenvectors & eigenspaces
- Algebraic multiplicity & geometric multiplicity
- Eigendecomposition (Eigenvalue decomposition) & Eigendecomposition for Hermitian matrices
- Similar transformation, Schur decomposition & Diagonalization
- Variational characterizations of eigenvalues
- Power iteration & Inverse iteration
- QR iteration & Hessenberg QR iteration
- Givens QR & Householder QR (from previous lectures)

I. UNDERSTANDING EIGENVALUES AND EIGENVECTORS

Problem 1. (6 points + 4 points)

Consider the 2×2 matrix

$$\mathbf{A} = \begin{bmatrix} -4 & -3 \\ 6 & 5 \end{bmatrix}.$$

- 1) Determine whether \mathbf{A} can be diagonalized or not. Diagonalize \mathbf{A} by $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}$ if the answer is "yes" or give the reason if the answer is "no".
- 2) Give the eigenspace of \mathbf{A} . And then consider: is there a matrix being similar to \mathbf{A} but have different eigenspaces with it. If the answer is "yes", show an example (here you are supposed to give the specific matrix and its eigenspaces), or else explain why the answer is "no" .

Remarks:

- In 1), if \mathbf{A} can be diagonalized, you are supposed to present not only the specific diagonalized matrix but also how do you get the similarity transformation. If not, you should give the necessary derivations of the specific reason.
- In 2), if your answer is "yes", you are supposed to give the specific matrix and its eigenspaces. If "no", you should give the necessary derivations of the specific reason.

Solution.

- 1) By computing $|A - \lambda \cdot I| = 0$, we can easily get $\lambda_1 = -1, \lambda_2 = 2$. For $\lambda_i = -1$, we can get $A - \lambda_1 \cdot I = \begin{bmatrix} -3 & -3 \\ 6 & 6 \end{bmatrix}$, $\therefore x_1 + x_2 = 0$, the eigenvector of λ_1 is $v_1 = [-1, 1]^T$, similarly, we get the eigenvector of λ_2 , which is $v_2 = [-1, 2]^T$. Therefore, we can let $V = \begin{bmatrix} -1 & -1 \\ 1 & 2 \end{bmatrix}$, $V^{-1} = \begin{bmatrix} -2 & -1 \\ 1 & 1 \end{bmatrix}$ and $\mathbf{\Lambda} = \begin{bmatrix} -1 & 0 \\ 0 & 2 \end{bmatrix}$. The matrix A can be diagonalized.
- 2) The eigenspace of A are: For $\lambda_1, \varepsilon_{\lambda_1} = \text{span}\{v_1\}$, for $\lambda_2, \varepsilon_{\lambda_2} = \text{span}\{v_2\}$. And the answer is yes. We can simply choose a matrix B that $B = \begin{bmatrix} -1 & 0 \\ 0 & 2 \end{bmatrix}$. The eigenvalues of B are $\lambda'_1 = -1, \lambda'_2 = 2$, and the corresponding eigenvectors are $v'_1 = [1, 0]^T, v'_2 = [0, 1]^T$. Therefore, the eigenspaces are: For $\lambda'_1 = -1, \varepsilon'_{\lambda_1} = \text{span}\{v'_1\}$, for $\lambda'_2 = 2, \varepsilon'_{\lambda_2} = \text{span}\{v'_2\}$. Since v'_1 is linear independent to v_1 , therefore ε'_{λ_1} is different from ε_{λ_1} , similar to ε'_{λ_2} and ε_{λ_2} , therefore, there exists a matrix being similar to A but have different eigenspaces with it.

Problem 2. (6 points \times 5)

For a matrix $\mathbf{A} \in \mathbb{C}^{n \times n}$, $\lambda_1, \lambda_2, \dots, \lambda_n$ are its n eigenvalues (though some of them may be the same). Prove that:

- 1) The matrix \mathbf{A} is singular if and only if 0 is an eigenvalue of it.
- 2) $\text{rank}(\mathbf{A}) \geq$ number of nonzero eigenvalues of \mathbf{A} .
- 3) If \mathbf{A} admits an eigendecomposition (eigenvalue decomposition), $\text{rank}(\mathbf{A}) =$ number of nonzero eigenvalues of \mathbf{A} .
- 4) If \mathbf{A} is Hermitian, then all of eigenvalues of \mathbf{A} are real.
- 5) If \mathbf{A} is Hermitian, then eigenvectors corresponding to different eigenvalues are orthogonal.

Solution

- 1) if \mathbf{A} is singular, then $\|\mathbf{A}\| = 0$, which means that $\|\mathbf{A} - 0 \cdot \mathbf{I}\| = 0$, $\therefore 0$ is an eigenvalue of \mathbf{A} .
if 0 is an eigenvalue of \mathbf{A} , then $\|\mathbf{A} - 0 \cdot \mathbf{I}\| = 0 = \|\mathbf{A}\|$, $\therefore \mathbf{A}$ is singular. Q.E.D.
- 2) Using the schur decomposition, we can find that $\mathbf{A} = \mathbf{Q}\mathbf{T}\mathbf{Q}^H$, \mathbf{T} is an upper triangular matrix and its diagonal entries are eigenvalue of \mathbf{A} , $\mathbf{Q} \in \mathbb{C}^{n \times n}$ is an invertible matrix, $\text{rank}(\mathbf{Q}) = n$.

$$\begin{aligned}
 \therefore \text{rank}(\mathbf{A}) &= \text{rank}(\mathbf{Q}\mathbf{T}\mathbf{Q}^H) \geq \text{rank}(\mathbf{Q}) + \text{rank}(\mathbf{T}\mathbf{Q}^H) - n \\
 &\geq \text{rank}(\mathbf{Q}) + \text{rank}(\mathbf{Q}^H) - 2n + \text{rank}(\mathbf{T}) \\
 &= \text{rank}(\mathbf{T}) \\
 &\geq \text{number of non-zero eigenvalues of } \mathbf{A}
 \end{aligned}$$

Q.E.D.

- 3) Since \mathbf{A} admits eigen decomposition, $\therefore \mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}$, $\mathbf{\Lambda} \in \mathbb{C}^{n \times n}$ is a diagonal matrix which diagonal entries are the eigenvalues of \mathbf{A} , $\mathbf{V} \in \mathbb{C}^{n \times n}$ is an invertible matrix, $\text{rank}(\mathbf{V}) = n$.
 $\text{rank}(\mathbf{A}) = \text{rank}(\mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}) \geq \text{rank}(\mathbf{\Lambda})$, like shown in 2).
 $\text{rank}(\mathbf{A}) = \text{rank}(\mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}) \leq \min(\text{rank}(\mathbf{\Lambda}\mathbf{V}^{-1}), \text{rank}(\mathbf{V})) = \text{rank}(\mathbf{\Lambda}\mathbf{V}^{-1}) \leq \min(\text{rank}(\mathbf{\Lambda}), \text{rank}(\mathbf{V}^{-1})) = \text{rank}(\mathbf{\Lambda})$
 $\therefore \text{rank}(\mathbf{A}) = \text{rank}(\mathbf{\Lambda}) = \text{number of non-zeros eigenvalues of } \mathbf{A}$. Q.E.D.

- 4) \mathbf{A} is hermitian matrix means that $\mathbf{A} = \mathbf{A}^H$, let (λ, x) be an eigenpair of \mathbf{A}

$$\begin{aligned}
 \therefore \lambda x &= \mathbf{A}x, \bar{\lambda}x^H = x^H \mathbf{A}^H \\
 \therefore \lambda x^H x &= x^H \mathbf{A}x, \bar{\lambda}x^H x = x^H \mathbf{A}^H x \\
 \therefore (\lambda - \bar{\lambda})x^H x &= x^H \mathbf{A}^H x - x^H \mathbf{A}x = 0 \\
 \therefore \lambda &= \bar{\lambda}, \text{ which means that } \mathbf{A} \text{ is real.}
 \end{aligned}$$

Q.E.D.

- 5) Let $(\lambda_i, v_i), (\lambda_j, v_j)$ be two eigenpairs of \mathbf{A} , $\lambda_i \neq \lambda_j$, then we have $\lambda_i v_i = \mathbf{A}v_i, \lambda_j v_j = \mathbf{A}v_j$
(1) if $\lambda_i = 0, \lambda_j \neq 0$, then we have $\mathbf{A}v_i = 0, \lambda_j v_j = \mathbf{A}v_j, \therefore \lambda_j v_j^H v_i = v_j^H \mathbf{A}^H v_i = v_j^H \mathbf{A}v_i = 0, \therefore v_j^H v_i = 0$.

In this case, v_i, v_j are orthogonal.

(2)if $\lambda_i \neq 0$ and $\lambda_j \neq 0$, then $\lambda_j v_j^H \lambda_i v_i = \lambda_i \lambda_j v_j^H v_i = v_j^H A^H A v_i = \lambda_i^2 v_j^H v_i$, $\therefore v_j^H v_i \cdot (\lambda_i^2 - \lambda_i \lambda_j) = 0$, which means that if $\lambda_i \neq \lambda_j$, then $v_j^H v_i = 0$. In this case, v_i, v_j are orthogonal. Q.E.D.

II. UNDERSTANDING THE EIGENVALUES OF REAL SYMMETRIC MATRICES

Problem 3. (12 points) Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be a symmetric matrix, \mathcal{S}_k denote a subspace of \mathbb{R}^n of dimension k , and $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ represent the eigenvalues of \mathbf{A} . For any $k \in \{1, 2, 3, \dots, n\}$, prove that

$$\lambda_k = \min_{\mathcal{S}_{n-k+1} \subseteq \mathbb{R}^n} \max_{\mathbf{x} \in \mathcal{S}_{n-k+1}, \|\mathbf{x}\|_2=1} \mathbf{x}^T \mathbf{A} \mathbf{x}.$$

Solution.

Using schur decomposition we can find that $D = U^T \mathbf{A} U$, $D^T = U^T \mathbf{A}^T U = U^T \mathbf{A} U = D$. $\therefore D$ is a diagonal matrix, $D = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$. \therefore the original proposition is equal to $\lambda_k = \min_{\mathcal{S}_{n-k+1} \subseteq \mathbb{R}^n} \max_{y \in \mathcal{S}_{n-k+1}, \|y\|_2=1} y^T D y$, $y = U^T x$. For a subspace ν of dimension $n - k + 1$, let $S_\nu = \{y \in \nu, \|y\|_2 = 1\}$ and let $S'_\nu = \{y \in \nu \cap F\}$, where $F = \text{span}\{e_1, e_2, \dots, e_n\}$. We find that $\nu \cap F \neq \emptyset$, or otherwise $\dim(\nu + F) = \dim(\nu) + \dim(F) = n + 1$, which is impossible.

Therefore, we find that S'_ν contains these vectors of S_ν of the form: $y = [y_1, y_2, \dots, y_k, 0, 0, \dots, 0]^T$ with $\sum_{j=1}^k |y_j|^2 = 1$, \therefore for all $y \in S'_\nu$, $y^T D y = \sum_{j=1}^k \lambda_j |y_j|^2 \geq \lambda_k \sum_{j=1}^k |y_j|^2 = \lambda_k$. Since $S'_\nu \subseteq S_\nu$, it follows that $\max_{y \in S_\nu} y^T D y \geq \max_{y \in S'_\nu} y^T D y \geq \lambda_k$. $\therefore \min_{\nu \subseteq \mathbb{R}^n} \max_{y \in \nu, \|y\|_2=1} y^T D y \geq \lambda_k$.

However, the inequality is reversible because if $\nu_2 = \{e_1, e_2, \dots, e_k\}^\perp$, then every $y \in \nu_2$ has the form: $y = [0, 0, \dots, 0, y_k, y_{k+1}, \dots, y_n]^T$. \therefore for all $y \in S_{\nu_2}$, $y^T D y = \sum_{j=k}^n \lambda_j |y_j|^2 \leq \lambda_k \sum_{j=k}^n |y_j|^2 = \lambda_k$. $\therefore \min_{\nu \subseteq \mathbb{R}^n} \max_{y \in \nu, \|y\|_2=1} y^T D y \leq \max_{y \in S_{\nu_2}} y^T D y \leq \lambda_k$.

In general, we can get $\min_{\nu \subseteq \mathbb{R}^n} \max_{y \in \nu, \|y\|_2=1} y^T D y = \lambda_k$, where the dimension of ν is $n - k + 1$. Q.E.D.

Problem 4. (5 points+8 points+10 points) To assist the understanding of this problem, we first provide some **basic concepts of graph theory**:

① A *simple graph* G is a pair (V, E) , such that

- V is the set of vertices;
- E is the set of edges and every edge is denoted by an *unordered* pair of its two *distinct* vertices.

② If i, j are two distinct vertices and (i, j) is an edge, we then say that i and j are *adjacent*. A graph is called *d-regular graph* if every vertex in the graph is adjacent to d vertices, where d is a positive integer.

③ Given two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, if $V_1 \subset V_2$ and $E_1 \subset E_2$, we call G_1 the *subgraph* of G_2 . Furthermore, we call G_1 the *connected component* of G_2 if

- any vertex in G_1 is only connected to vertices in G_1 .
- any two vertices in G_1 are connected either directly or via some other vertices in G_1 ;

Suppose $G = (V, E)$ is a simple graph with n vertices indexed by $1, 2, \dots, n$ respectively. The adjacency matrix of G is a matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ given by

$$\mathbf{A}_{i,j} = \begin{cases} 1, & \text{if vertex } i \text{ and vertex } j \text{ are adjacent;} \\ 0, & \text{otherwise.} \end{cases} \quad (1)$$

Besides, if G is a d -regular graph, its *normalized Laplacian matrix* \mathbf{L} is defined as $\mathbf{L} \triangleq \mathbf{I} - \frac{1}{d}\mathbf{A}$, where \mathbf{I} is the identity matrix. Let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ denote the eigenvalues of \mathbf{L} . Please prove the following propositions:

1) For any vector $\mathbf{x} \in \mathbb{R}^n$, it follows that

$$\mathbf{x}^T \mathbf{L} \mathbf{x} = \frac{1}{d} \sum_{(i,j) \in E} (\mathbf{x}_i - \mathbf{x}_j)^2, \quad (2)$$

where i, j represent two distinct vertices and $(i, j) \in E$ represents an edge between i and j in the graph G .

2) $\lambda_n = 0$ and $\lambda_1 \leq 2$.

3) (**Bonus Problem**) the graph G has at least $(n - k + 1)$ connected components if and only if $\lambda_k = 0$.

Hint: The matrix \mathbf{L} is real and symmetric. You can directly utilize Courant-Fischer Theorem without proof. Particularly, you may need to utilize the min-max form of the Courant-Fischer Theorem for the Bonus Problem.

Solution

1)

$$\begin{aligned}
x^T Lx &= \frac{1}{d} x^T (dI - A)x \\
&= \frac{1}{d} (x^T dTx - x^T Ax) \\
&= \frac{1}{d} \left[\sum_{i=1}^n dx_i^2 - \sum_{\{i,j\} \in E} 2x_i x_j \right] \\
&= \frac{1}{d} \left[\sum_{i=1}^n \sum_{\{i,j\} \in E} x_i^2 - \sum_{\{i,j\} \in E} 2x_i x_j \right] \\
&= \frac{1}{d} \left[\sum_{\{i,j\} \in E} (x_i^2 + x_j^2 - 2x_i x_j) \right] \\
&= \frac{1}{d} \sum_{\{i,j\} \in E} (x_i - x_j)^2
\end{aligned}$$

Q.E.D.

2) It is easy to find that L is a SPD matrix, therefore for rayleigh-ritz theorem, we find that $\lambda_n = \min_{x \in R^n - \{0\}} \frac{x^T Lx}{\|x\|_2^2} =$

$\min_{x \in R^n - \{0\}} \frac{\frac{1}{d} \sum_{\{i,j\} \in E} (x_i - x_j)^2}{\sum_{k=1}^n x_k^2}$, $\therefore \lambda_n \geq 0$, let $x = \{1, 1, \dots, 1\} \in R^n$, we can get $\lambda_n = 0$.

Also, we can get $\lambda_1 = \max_{x \in R^n - \{0\}} \frac{x^T Lx}{\|x\|_2^2}$, since we can easily get $2x^T x - x^T Lx = x^T 2Ix - x^T Lx =$

$x^T (I + \frac{1}{d} A)x = \frac{1}{d} \sum_{\{i,j\} \in E} (x_i + x_j)^2$, therefore, $\frac{x^T Lx}{x^T x} = 2 - \frac{\frac{1}{d} \sum_{\{i,j\} \in E} (x_i + x_j)^2}{\sum_{k=1}^n x_k^2}$, $\therefore \lambda_1 = \max_{x \in R^n - \{0\}} \frac{x^T Lx}{\|x\|_2^2} \leq 2$.

Q.E.D.

3) From Problem 3, we get $\lambda_k = \min_{S_{n-k+1} \subseteq \mathbb{R}^n} \max_{x \in S_{n-k+1}, \|x\|_2=1} x^T A x$. If $\lambda_k = 0$, there must exist a space S with dimension $n - k + 1$ and for all $x \in S$, all $\{i, j\} \in E$, satisfies $x_i = x_j$, which means that any i, j , are in the same connected component. Since every $x \in S$ satisfies this constraint, we find that $x \in S$ is constant within each connected component of G , $\therefore k = \dim(S) = n - k + 1 \leq \text{number of connected components of } G$.

On the contrary, if the number of connected components of $G \geq n - k + 1$, then we can let S be the space of vectors that are constant on each component; and this S has dimension larger or equal than $n - k + 1$. Therefore, we have $\sum_{\{i,j\} \in E} (x_i - x_j)^2$, which means that, by the conclusion of Problem 3, we get $\lambda_k = 0$, Q.E.D.

III. EIGENVALUE COMPUTATIONS

A. Power Iteration

Problem 5. (20 points)

Consider the 2×2 matrix \mathbf{A}

$$\mathbf{A} = \begin{bmatrix} 0 & \alpha \\ \beta & 0 \end{bmatrix}, \quad \text{with } \alpha, \beta > 0.$$

- 1) Find the eigenvalues and eigenvectors of \mathbf{A} by hand. (5 points)
- 2) Program **the power iteration** (See Algorithm 1) and **the inverse iteration** (See Algorithm 2) respectively and report the output of two algorithms for \mathbf{A} (you can determine α, β by yourself), do the two algorithms converge or not? Report what you have found (you can use plots to support your analysis). (10 points: programming takes 5 points and the analysis takes 5 points) After a few iterations, the sequence given by the power iteration fails to converge, explain why. (5 points) (**After-class exercise:** If you want, you can study the case for other randomly generated matrices.)

Remarks: Programming languages are not restricted. In `Matlab`, you are free to use `[v,D] = eig(A)` to generate the eigenvalues and eigenvectors of \mathbf{A} as a reference to study the convergence.

Algorithm 1: Power iteration

Input : $\mathbf{A} \in \mathbb{C}^{n \times n}$

1 **Initialization:** random choose $\mathbf{q}^{(0)}$.

2 **for** $k = 1, \dots$, **do**

3 $\mathbf{z}^{(k)} = \mathbf{A}\mathbf{q}^{(k-1)}$

4 $\mathbf{q}^{(k)} = \mathbf{z}^{(k)} / \|\mathbf{z}^{(k)}\|_2$

5 $\lambda^{(k)} = (\mathbf{q}^{(k)})^H \mathbf{A} \mathbf{q}^{(k)}$

6 **end**

Output: $\lambda^{(k)}$

Algorithm 2: Inverse iteration

Input : $\mathbf{A} \in \mathbb{C}^{n \times n}$, μ

1 **Initialization:** random choose $\mathbf{q}^{(0)}$.

2 **for** $k = 1, \dots$, **do**

3 $\mathbf{z}^{(k)} = (\mathbf{A} - \mu\mathbf{I})^{-1} \mathbf{q}^{(k-1)}$

4 $\mathbf{q}^{(k)} = \mathbf{z}^{(k)} / \|\mathbf{z}^{(k)}\|_2$

5 $\lambda^{(k)} = (\mathbf{q}^{(k)})^H \mathbf{A} \mathbf{q}^{(k)}$

6 **end**

Output: $\lambda^{(k)}$

Solution

1)

$$A = \begin{bmatrix} 0 & \alpha \\ \beta & 0 \end{bmatrix}, \alpha, \beta > 0, \therefore \|A - \lambda I\| = \begin{bmatrix} -\lambda & \alpha \\ \beta & -\lambda \end{bmatrix} = \lambda^2 - \alpha\beta, \therefore \lambda = \pm\sqrt{\alpha\beta}$$

$$(1) \lambda_1 = \sqrt{\alpha\beta}, A - \lambda_1 = \begin{bmatrix} -\sqrt{\alpha\beta} & \alpha \\ \beta & -\sqrt{\alpha\beta} \end{bmatrix} \therefore \beta x_1 - \sqrt{\alpha\beta} x_2 = 0, v_1 = [\sqrt{\alpha}, \sqrt{\beta}]^T$$

$$(2) \lambda_2 = -\sqrt{\alpha\beta}, A - \lambda_2 = \begin{bmatrix} \sqrt{\alpha\beta} & \alpha \\ \beta & \sqrt{\alpha\beta} \end{bmatrix} \therefore \beta x_1 + \sqrt{\alpha\beta} x_2 = 0, v_2 = [\sqrt{\alpha}, -\sqrt{\beta}]^T$$

2) The code is shown in **HW4_5.m**, and figures of of Power Iteration and Inverse Iteration are shown below, from which we can find that, 1) the Power Iteration cannot converge, which is lost in oscillation, and 2) the Inverse Iteration converge to a right value which represents the largest eignevalue of A .

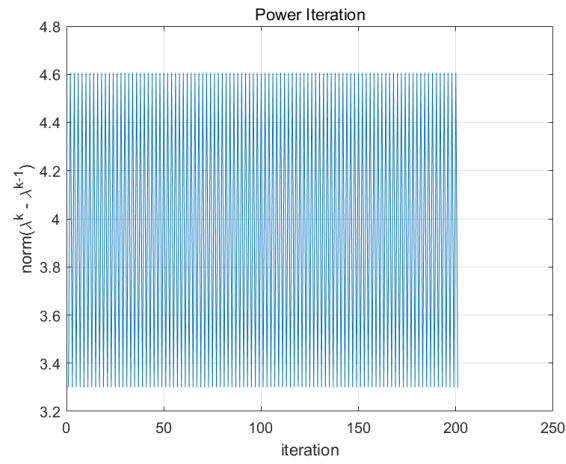


Figure 1. Power iteration

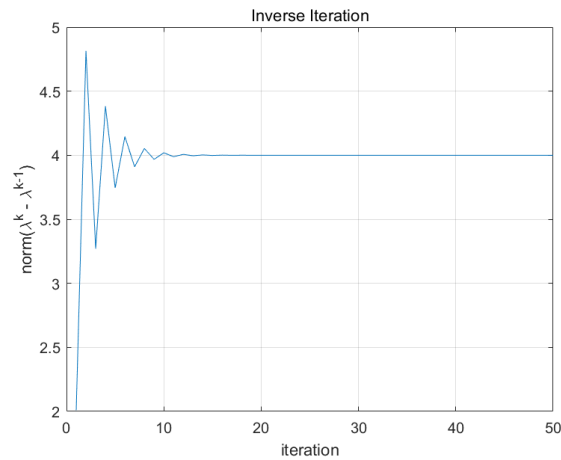


Figure 2. Inverse iteration

- 3) The reason why the Power Iteration cannot converge is that, in this case, the absolute values of these two eigenvalues of A are the same, which means that the convergence rate is always equal to $\frac{|\lambda_1|}{|\lambda_2|} = 1$, therefore, this algorithm cannot converge. From the program we can find, the absolute values in iteration $[1, 3, 5, \dots, 2n+1]$ are the same, and also, the absolute values in iteration $[2, 4, 6, \dots, 2n]$ are the same.

B. QR iteration and Hessenberg QR iteration

Recap. For $\mathbf{A} \in \mathbb{C}^{n \times n}$, consider the QR iteration (See Algorithm 3) for finding all the eigenvalues and eigenvectors of \mathbf{A} . In each iteration, $\mathbf{A}^{(k)}$ is similar to \mathbf{A} in that

Algorithm 3: QR iteration

Input : $\mathbf{A} \in \mathbb{C}^{n \times n}$

```

1 Initialization:  $\mathbf{A}^{(0)} = \mathbf{A}$ .
2 for  $k = 1, \dots$ , do
3    $\mathbf{Q}^{(k)}\mathbf{R}^{(k)} = \mathbf{A}^{(k-1)}$   % Perform QR for  $\mathbf{A}^{(k-1)}$ 
4    $\mathbf{A}^{(k)} = \mathbf{R}^{(k)}\mathbf{Q}^{(k)}$ 
5 end
```

Output: $\mathbf{A}^{(k)}$

$$\begin{aligned} \mathbf{A}^{(k)} &= \mathbf{R}^{(k)}\mathbf{Q}^{(k)} = (\mathbf{Q}^{(k)})^H \mathbf{Q}^{(k)} \mathbf{R}^{(k)} \mathbf{Q}^{(k)} = (\mathbf{Q}^{(k)})^H \mathbf{A}^{(k-1)} \mathbf{Q}^{(k)} = \dots \\ &= (\mathbf{Q}^{(1)}\mathbf{Q}^{(2)} \dots \mathbf{Q}^{(k)})^H \mathbf{A} (\mathbf{Q}^{(1)}\mathbf{Q}^{(2)} \dots \mathbf{Q}^{(k)}) \Rightarrow \mathbf{A}^{(k)} \text{ is similar to } \mathbf{A}. \end{aligned}$$

Suppose the Schur decomposition of \mathbf{A} is $\mathbf{A} = \mathbf{U}\mathbf{T}\mathbf{U}^H$, then under some mild assumptions, $\mathbf{A}^{(k)}$ converges to \mathbf{T} . Therefore, we can compute all the eigenvalues of \mathbf{A} by taking the diagonal elements of $\mathbf{A}^{(k)}$ for sufficiently large k . However, each iteration requires $\mathcal{O}(n^3)$ flops to compute QR factorization which is computationally expensive. One possible solution is: first perform similarity transform \mathbf{A} to an upper Hessenberg form (Step 1 in Algorithm

Algorithm 4: Hessenberg QR iteration

Input : $\mathbf{A} \in \mathbb{C}^{n \times n}$

```

1 Initialization:  $\mathbf{H} = \mathbf{Q}^H \mathbf{A} \mathbf{Q}$ ,  $\mathbf{A}^{(0)} = \mathbf{H}$ .  % Hessenberg reduction for  $\mathbf{A}$ 
2 for  $k = 1, \dots$ , do
3    $\mathbf{Q}^{(k)}\mathbf{R}^{(k)} = \mathbf{A}^{(k-1)}$   % Perform QR for  $\mathbf{A}^{(k-1)}$  using Givens QR
4    $\mathbf{A}^{(k)} = \mathbf{R}^{(k)}\mathbf{Q}^{(k)}$   % Matrix computation
5 end
```

Output: $\mathbf{A}^{(k)}$

4), then perform QR iteration (Algorithm 3) over new $\mathbf{A}^{(0)} = \mathbf{H}$. By using Givens rotations, the QR step 3 only takes $\mathcal{O}(n^2)$ flops.

Problem 6. (15 points +10 points)

- 1) Complete the Algorithm 5 (corresponding to the step 3-4 of Algorithm 4) first (7 points), then show **the detailed derivation** of the computational complexity of in Algorithm 5 ($\mathcal{O}(n^2)$). (8 points) (Derivation is for the computational complexity of the algorithm.)

To be more specific, we can present the process of performing QR for $\mathbf{A}^{(k)}$ using Givens rotations as:

- (a) First, overwrite $\mathbf{A}^{(k)}$ with upper-triangular $\mathbf{R}^{(k)}$

$$\mathbf{A}^{(k)} = (\mathbf{G}_m^H \mathbf{G}_{m-1}^H \cdots \mathbf{G}_1^H) \mathbf{A}^{(k)} = \mathbf{R}^{(k)},$$

where $\mathbf{G}_1, \dots, \mathbf{G}_m$ is a sequence of Givens rotations for some m (In your algorithm, you need to clearly specify what \mathbf{G}_i is), and $\mathbf{R}^{(k)} = \mathbf{G}_1 \cdots \mathbf{G}_m$.

- (b) Perform matrix multiplication such that $\mathbf{A}^{(k)}$ is of Hessenberg form,

$$\mathbf{A}^{(k)} = \mathbf{R}^{(k)} \mathbf{Q}^{(k)} = \mathbf{A}^{(k)} \mathbf{G}_1 \cdots \mathbf{G}_m.$$

2) **(Bouns Problem) Implicit QR iteration**

Another way to implement step 3-4 in Algorithm 4 is through *implicit QR iteration*. The idea is as follows, for $\mathbf{A}^{(0)} \in \mathbb{R}^{n \times n}$ which is of Hessenberg form,

- (a) First, compute a Givens rotation \mathbf{G}_1 such that $(\mathbf{G}_1^H \mathbf{A}^{(0)})_{2,1} = 0$ and update $\mathbf{A}^{(1)} = \mathbf{G}_1^H \mathbf{A}^{(0)} \mathbf{G}_1$. However, the entry $\mathbf{A}_{3,1}^{(1)}$ may be nonzero (known as "bulge").
- (b) Compute another Givens rotation \mathbf{G}_2 such that $(\mathbf{G}_2 \mathbf{A}^{(1)})_{3,1} = 0$ (i.e., nulling out the "bulge") and update $\mathbf{A}^{(2)} = \mathbf{G}_2^H \mathbf{A}^{(1)} \mathbf{G}_2$ which is analogous with step (a). Note that the entry $\mathbf{A}_{4,2}^{(2)}$ will now be nonzero.
- (c) Then, we try to find \mathbf{G}_3 such that $(\mathbf{G}_3 \mathbf{A}^{(2)})_{4,2} = 0$. The procedure of iterating nulling out the "bulges" to reset in a upper Hessenberg form is known as "bulge chasing".

This algorithm *implicitly* computed QR factorization at the cost of $\mathcal{O}(n^2)$, and this is why the algorithm is called the *Implicit QR iteration*. Consider a 4×4 Hessenberg matrix

$$\mathbf{A}^{(0)} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 3 & 1 & 2 \\ 0 & 1 & 3 & 2 \\ 0 & 0 & 2 & 1 \end{bmatrix}.$$

Carry out the implicit QR iteration (show the detailed derivation) (To simplify the computation, you can use [Matlab](#) to do the matrix multiplications. Specifically, explicitly show \mathbf{G}_i , $\mathbf{G}_i^H \mathbf{A}^{(i-1)}$ and $\mathbf{A}^{(i)}$ for each step but when computing the matrix multiplication such as $\mathbf{G}_i^H \mathbf{A}^{(i-1)}$, $\mathbf{G}_i^H \mathbf{A}^{(i-1)} \mathbf{G}_i$, you are free to use [Matlab](#) . But be careful with the precision issue during the process of computing.), and observe where does the so-called "bulge" appears. (5 points: including the detailed derivation of the implicit QR iteration and pointing out the "bulge") Based on your observations, explain why the implicit QR iteration is indeed equivalent to the Algorithm 5. (5 points)

Solution

Algorithm 5: Step 3-4 in Hessenberg QR iteration

Input : $\mathbf{A}^{(k-1)} \in \mathbb{C}^{n \times n}$ which is of upper Hessenberg form % corresponding to $\mathbf{A}^{(k-1)}$ in step 3 of Algorithm 4

```

1  % Perform QR for  $\mathbf{A}^{(k)}$  using Givens rotations
2   $\hat{G} = \text{zeros}(n-1, 2, 2)$ ,  $B = A^{k-1}$ 
3  for  $i = 1 : n-1$  do
4       $\hat{G}[i, :, :] = \text{givens}(A(i, i), A(i+1, i), \theta)$ ; %  $\hat{G}[i, :, :]$  is a  $2 \times 2$  matrix, and this step
        contains  $6n$  flops
5       $\text{tmp} = \hat{G}[i, :, :] * A^{k-1}[i : i+1, :]$ ; % contains  $6n$  flops
6       $B[i : i+1, :] = \text{tmp}$ ;
7  end
8  % Matrix computation
9   $C = B$ ;
10 for  $i = 1 : n-1$  do
11      $\text{tmp} = G[i, :, :]^H$ ; % tmp is a  $2 \times 2$  matrix
12      $C[:, i : i+1] = C[:, i : i+1] * \text{tmp}$ ; % contains  $6n$  flops
13 end
14  $A^k = C$ 

Output:  $\mathbf{A}^{(k)}$     % corresponding to  $\mathbf{A}^{(k)}$  in step 4 of Algorithm 4

```

1) The flops of each step of this algorithm is shown in the annotation of algorithm 5, and we can find that the computational complexity of this algorithm is $[(6n + 6n) + 6n] * (n - 1) = 18n^2 - 18n \approx O(n^2)$

2) I have finished the whole procedure but do not have time to write it by latex.

The reason why it is similar to algorithm 5 is that, the implicit QR using $O(n)$ times givens QR iteration, which means that the mainly computational part is $O(n) \times 6n \approx O(n^2)$, therefore, it is equal to the algorithm 5.