DDA 3005 — Numerical Methods

Exercise Sheet 4

Problem 1 (Power Iteration with Shift): (approx. *20* pts)
Let the matrix $\boldsymbol{A} \in \mathbb{R}^{4\times 4}$ and the initial point $\boldsymbol{x}^0 \in \mathbb{R}^4$ be given via

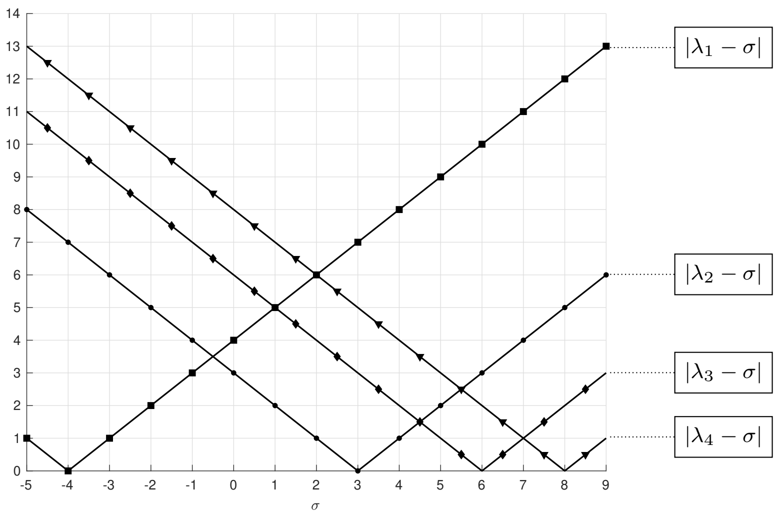
$$\boldsymbol{A} = \begin{bmatrix} 1 & 0 & 5 & 0 \\ 0 & 3 & 0 & 0 \\ 5 & 0 & 1 & 0 \\ 0 & 0 & 0 & 8 \end{bmatrix}, \qquad \tilde{\boldsymbol{x}}^0 = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}, \quad \boldsymbol{x}^0 = \frac{\tilde{\boldsymbol{x}}^0}{\|\tilde{\boldsymbol{x}}^0\|}. \tag{1}$$

In this problem, we want to apply the (normalized) power iteration with shift $\sigma \in \mathbb{R}$ to $\boldsymbol{A}$:

$$\tilde{\boldsymbol{x}}^k = (\boldsymbol{A} - \sigma \boldsymbol{I})\boldsymbol{x}^k, \quad \boldsymbol{x}^k = \tilde{\boldsymbol{x}}^k / \|\tilde{\boldsymbol{x}}^k\|, \quad \sigma_k = (\boldsymbol{x}^k)^\top \boldsymbol{A} \boldsymbol{x}^k, \quad k = 1, 2, \ldots$$

Let $(\lambda_i, \boldsymbol{v}_i)$, $i = 1, \ldots, 4$, further denote the corresponding eigenpairs of $\boldsymbol{A}$. It can be shown that $(\boldsymbol{x}^0)^\top \boldsymbol{v}_i \neq 0$ for all $i = 1, \ldots, 4$.

The plot below depicts the mappings $\sigma \mapsto |\lambda_i - \sigma|$, $i = 1, 2, 3, 4$ for the different eigenvalues of $\boldsymbol{A}$ and choices of σ.



a) State the eigenvalues $\lambda_1, \ldots, \lambda_4$ of $\boldsymbol{A}$.

b) Discuss which eigenpairs $(\lambda_i, \boldsymbol{v}_i)$ of $\boldsymbol{A}$ can be recovered by the (normalized) power iteration using suitable choices of the shift σ. Can all eigenpairs of $\boldsymbol{A}$ be recovered? Provide detailed explanations!

c) Derive the optimal choice of the shift σ for which the power iteration (1) converges with the fastest possible (optimal) convergence rate.

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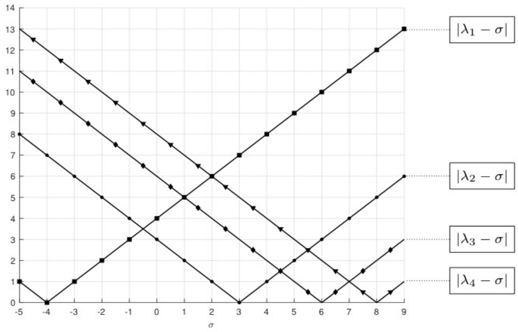

a) State the eigenvalues $\lambda_1, \ldots, \lambda_4$ of $\boldsymbol{A}$.

(a) from the graph,
They're $-4, 3, 6, 8$

b) Discuss which eigenpairs $(\lambda_i, \boldsymbol{v}_i)$ of $\boldsymbol{A}$ can be recovered by the (normalized) power iteration using suitable choices of the shift σ. Can all eigenpairs of $\boldsymbol{A}$ be recovered? Provide detailed explanations!

(b) $(A+4I)V_1 = 0 \Rightarrow \begin{bmatrix} 5 & 0 & 5 & 0 \\ 0 & 7 & 0 & 0 \\ 5 & 0 & 5 & 0 \\ 0 & 0 & 0 & 12 \end{bmatrix}\begin{bmatrix} \\ \\ \\ \end{bmatrix} = 0 \Rightarrow V_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ -\frac{1}{\sqrt{2}} \\ 0 \end{bmatrix}$

$(A-3I)V_2 = 0 \Rightarrow \begin{bmatrix} -2 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 \\ 5 & 0 & -2 & 0 \\ 0 & 0 & 0 & 5 \end{bmatrix}\begin{bmatrix} \\ \\ \\ \end{bmatrix} = 0 \Rightarrow V_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$

$(A-6I)V_3 = 0 \Rightarrow \begin{bmatrix} -5 & 0 & 5 & 0 \\ 0 & -3 & 0 & 0 \\ 5 & 0 & -5 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}\begin{bmatrix} \\ \\ \\ \end{bmatrix} = 0 \Rightarrow V_3 = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ -\frac{1}{\sqrt{2}} \\ 0 \end{bmatrix}$

$(A-8I)V_4 = 0 \Rightarrow \begin{bmatrix} -7 & 0 & 5 & 0 \\ 0 & -5 & 0 & 0 \\ 5 & 0 & -7 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} \\ \\ \\ \end{bmatrix} = 0 \Rightarrow V_4 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$

If $\sigma \in (-\infty, +2)$, the $(8, V_4)$ will be recovered
If $\sigma \in (2, +\infty)$, the $(-4, V_1)$ will be recovered

Proof: $(A - \sigma I)^k X^0 = S \Lambda^k S^{-1} \cdot S \begin{bmatrix} C_1 \\ \vdots \\ C_4 \end{bmatrix}$, where $\Lambda_{ii}^k = (\lambda_i - \sigma)^k$

$= S\Lambda^k \begin{bmatrix} C_1 \\ \vdots \\ C_4 \end{bmatrix} = (\lambda_1 - \sigma)^k C_1 V_1 + \cdots + (\lambda_4 - \sigma)^k C_4 V_4$

when $\sigma \in (-\infty, 2)$, $|(\lambda_4-\sigma)^k| >> |(\lambda_i-\sigma)^k|$ when $k \to \infty$

$\therefore$ $(\lambda_4=8, V_4)$ will be recovered

when $\sigma \in (2, +\infty)$, $|(\lambda_1-\sigma)^k| >> |(\lambda_i-\sigma)^k|$ when $k \to \infty$

$\therefore$ $(\lambda_1=-4, V_1)$ will be recovered

c) Derive the optimal choice of the shift σ for which the power iteration (1) converges with the fastest possible (optimal) convergence rate.

$-4 \qquad 3 \qquad 6 \qquad 8$

when $\sigma < 1$, the converge rate is $O(|\frac{6-\sigma}{8-\sigma}|^k)$, the optimal converge rate is $O(|\frac{5}{7}|^k)$.

when $1 < \sigma < 2$, the converge rate is $O(|\frac{-4-\sigma}{8-\sigma}|^k)$. the optimal converge rate is $O(|\frac{5}{7}|^k)$

when $2 < \sigma < 5.5$, the converge rate is $O(|\frac{8-\sigma}{-4-\sigma}|^k)$, the optimal converge rate is $O(|\frac{2.5}{9.5}|^k)$

when $\sigma \geq 5.5$, the Converge rate is $O(|\frac{3-\sigma}{-4-\sigma}|^k)$, the optimal converge rate is $O(|\frac{2.5}{9.5}|^k)$.

Overall, the optimal converge rate is at $\sigma = 5.5$

Problem 2 (Power Methods): (approx. *30* pts)

In this exercise, we want to calculate eigen-pairs of the 5×5 matrix using power methods:

$$\boldsymbol{A} = \begin{bmatrix} 46 & 99 & 45 & 24 & -27 \\ -6 & -32 & -6 & 4 & 18 \\ 18 & 18 & 19 & 6 & 0 \\ -9 & -90 & -9 & -47 & 27 \\ 12 & 39 & 12 & 28 & 19 \end{bmatrix}.$$

a) Implement the power method and compute the largest eigenvalue and the corresponding eigenvector of $\boldsymbol{A}$, e.g., using the initial point $\boldsymbol{x}^0 = \boldsymbol{e}_1 = [1, 0, 0, 0, 0]^\top$.

Choose a proper stopping criterion for the power method and state how many iterations your algorithm requires to recover the largest eigenvalue (using modest or high accuracy). Explain the choice of your termination criterion.

b) Implement the inverse iteration (with shift σ) to calculate the remaining eigen-pairs of the matrix $\boldsymbol{A}$ (again using $\boldsymbol{x}^0 = \boldsymbol{e}_1$ as initial point). Possible choices for the shift σ are $\sigma \in \{0, 46, -32, 19, -47\}$.

c) Implement the Rayleigh Quotient iteration using the five initial points $\boldsymbol{x}^0 \in \{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3, \boldsymbol{e}_4, \boldsymbol{e}_5\}$ and state the respective obtained eigen-pairs. Compare the performance of the Rayleigh Quotient iteration and the power iterations tested in part a) and b).

θ between x^{k+1} and x^k

(a) I choose to use $|\cos\theta| \to 1$ as the stopping criterion, but It's not accurate enough compared to use $|x^{k+1} - x^k| < \varepsilon$ or $|x^{k+1} - x^k| < \varepsilon$ in 5-dimension vector case.

At the end, I changed to use $|\lambda^{k+1} - \lambda^k| < \varepsilon$ as criterion, because it's accurate enough with better stability compared to computations on eigenvectors.

my ε is set to be 1e-12, and it takes 844 iterations

(b)

Converged after 10 iterations with shift 0.
Eigenvalue with shift 0: 1.000000000000016
Corresponding Eigenvector with shift 0: [7.07106781e-01 8.73963191e-16 -7.07106781e-01 -4.99799766e-15 -7.26855813e-16]

Converged after 43 iterations with shift 46.
Eigenvalue with shift 46: 54.99999999999984
Corresponding Eigenvector with shift 46: [8.16496581e-01 1.54220071e-14 4.08248290e-01 -0.00000000e+00 4.08248290e-01]

Converged after 26 iterations with shift -32.
Eigenvalue with shift -32: -25.999999999999826
Corresponding Eigenvector with shift -32: [-2.04964251e-15 3.01511345e-01 -2.03834218e-17 -9.04534034e-01 3.01511345e-01]

Converged after 45 iterations with shift 19.
Eigenvalue with shift 19: 28.00000000000022
Corresponding Eigenvector with shift 19: [3.01511345e-01 -3.01511345e-01 2.56562789e-14 -3.75715719e-17 -9.04534034e-01]

Converged after 26 iterations with shift -47.
Eigenvalue with shift -47: -53.00000000000018
Corresponding Eigenvector with shift -47: [-3.01511345e-01 2.20284202e-15 8.71030337e-18 9.04534034e-01 -3.01511345e-01]

(c)

Converged after 5 iterations
Eigenvalue with initial vector [1 0 0 0 0]:55.00000000000001
Corresponding Eigenvector: [−8.16496581e−01 1.23358114e−17
−4.08248290e−01 −1.49217005e−18
 −4.08248290e−01]

Converged after 7 iterations
Eigenvalue with initial vector [0 1 0 0 0]:−25.999999999999996
Corresponding Eigenvector: [0.00000000e+00 −3.01511345e−01
7.24709226e−18 9.04534034e−01
 −3.01511345e−01]

Converged after 8 iterations
Eigenvalue with initial vector [0 0 1 0 0]:1.000000000000003
Corresponding Eigenvector: [−7.07106781e−01 −1.66999388e−17
7.07106781e−01 2.32606290e−17
 −7.75354301e−18]

Converged after 6 iterations
Eigenvalue with initial vector [0 0 0 1 0]:−53.000000000000014
Corresponding Eigenvector: [−3.01511345e−01 7.25739331e−17
8.69832854e−18 9.04534034e−01
 −3.01511345e−01]

Converged after 6 iterations
Eigenvalue with initial vector [0 0 0 0 1]:27.999999999999996
Corresponding Eigenvector: [3.01511345e−01 −3.01511345e−01
2.92170706e−32 1.09564015e−32
 −9.04534034e−01]

Converge rate is much faster

Problem 3 (Computing Roots of Polynomials): (approx. *50* pts)

For given degree $n \in \mathbb{N}$ and coefficients $a_i \in \mathbb{R}$, $i = 0, \dots, n-1$, let us consider the univariate polynomial

$$p(x) := x^n + a_{n-1}x^{n-1} + \cdots + a_2x^2 + a_1x + a_0.$$

In this exercise, we want to develop an algorithm that allows computing all roots of the polynomial p using eigenvalues and QR iterations.

a) The so-called companion matrix associated with the polynomial p is given by

$$\boldsymbol{C}_p := \begin{bmatrix} 0 & 0 & \cdots & 0 & -a_0 \\ 1 & 0 & \cdots & 0 & -a_1 \\ 0 & 1 & \cdots & 0 & -a_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & -a_{n-1} \end{bmatrix}.$$

Show that $\det(\boldsymbol{C}_p - \lambda \boldsymbol{I}) = (-1)^n p(\lambda)$ for all λ.

(a) $\det(C_p - \lambda I) = \begin{vmatrix} -\lambda & 0 & \cdots & 0 & -a_0 \\ 1 & -\lambda & \cdots & 0 & -a_1 \\ 0 & 1 & \cdots & 0 & -a_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & -a_{n-1}-\lambda \end{vmatrix}$

Similar pattern

$= \begin{vmatrix} 0 & 0 & \cdots & 0 & -a_0 \\ 1 & -\lambda & \cdots & 0 & -a_1 \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & \cdots & 1 & -a_{n-1}-\lambda \end{vmatrix} + \begin{vmatrix} -\lambda & & & \\ 1 & -\lambda & & -a_1 \\ & \ddots & -\lambda & \vdots \\ & & 1 & -a_{n-1}-\lambda \end{vmatrix}$

$= (-1)^{n+1}(-a_0) \begin{vmatrix} 1 & -\lambda & 0 & \cdots & 0 \\ 0 & 1 & -\lambda & & \\ 0 & 0 & 1 & \ddots & \\ 0 & 0 & 0 & \ddots & -\lambda \\ 0 & \cdots & & & 1 \end{vmatrix} + (-\lambda) \begin{vmatrix} -\lambda & & -a_1 \\ 1 & \ddots & \vdots \\ & 1 & -a_{n-1}-\lambda \end{vmatrix}$

$= (-1)^n (a_0) \begin{vmatrix} 1 & -\lambda & & \\ & \ddots & \ddots & \\ & & & -\lambda \\ & & & 1 \end{vmatrix} +$

I always decompose it using cofactor for the first column, repeat and repeat again, at the end, I get 1

$$= (-1)^n a_0 + (-\lambda) \det(C_p^1 - \lambda I)$$

$$= (-1)^n a_0 + (-1)^n a_1 \lambda + \det(C_p^2 - \lambda I)(-\lambda)^2$$

$$= \cdots$$

$$= (-1)^n a_0 + (-1)^n a_1 \lambda + (-1)^n a_2 \lambda^2 + \cdots$$
$$+ (-1)^n \alpha_{n-2} \lambda^{n-2} + \underbrace{\det(C_p^{n-1} - \lambda I)}_{-a_{n-1} - \lambda} (-\lambda)^{n-1}$$

$$= (-1)^n \left[\alpha_0 + \alpha_1 \lambda + \cdots + \alpha_{n-2} \lambda^{n-2} + \alpha_{n-1} \lambda^{n-1} + \lambda^n \right]$$

$$= (-1)^n P(\lambda)$$

(b) see code output

(c) see code output and the comment I write in code.

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   Show that $\det(\boldsymbol{C}_p - \lambda \boldsymbol{I}) = (-1)^n p(\lambda)$ for all λ.

b) Implement the QR algorithm (with shift) discussed in the lecture to calculate the eigenvalues of the companion matrix $\boldsymbol{C}_p$.

   In order to improve the performance of your algorithm, you can utilize the following deflation strategy: let $\boldsymbol{X}^k \in \mathbb{R}^{n \times n}$ be the current iterate of the QR iteration. We can terminate the iteration, if $\|\boldsymbol{X}^k(\mathtt{n}, \mathtt{1:n-1})\| \leq \mathtt{tol}$, i.e., if the norm of the first $n-1$ entries of the last row of $\boldsymbol{X}^k$ is small. This ensures that the last row of $\boldsymbol{C}_p$ has been reduced to upper triangular form and $\boldsymbol{X}^k(\mathtt{n}, \mathtt{n}) = \boldsymbol{X}^k_{nn}$ should be a good eigenvalue approximation. We can then continue the QR algorithm with the smaller (deflated) matrix $\boldsymbol{B} = \boldsymbol{X}^k(\mathtt{1:n-1}, \mathtt{1:n-1}) \in \mathbb{R}^{(n-1)\times(n-1)}$ (or $\mathbb{C}^{(n-1)\times(n-1)}$) as new initial point. This process continues until we have recovered all eigenvalues of $\boldsymbol{C}_p$. Suitable choices for $\mathtt{tol}$ are 10^{-12} or 10^{-13}. You can also use a shifted

QR iteration to further enhance performance (e.g., the Rayleigh quotient or Wilkinson shift can be a good strategy).

Test your implementation and find all roots of the polynomials:

- $p(x) = x^4 - 324x^3 + 7175x^2 + 8100x - 180000$.
- $q(x) = x^{10} - 167x^9 + 10081x^8 - 251447x^7 + 1676815x^6 + 17367175x^5 - 66421125x^4 - 352378125x^3 + 454612500x^2 + 1949062500x$.

Report all found roots of p and q (you can order the roots from smallest to largest).

c) What happens if the coefficients a_2, a_1, and a_0 in the polynomial p are changed to $a_2 = 7225$, $a_1 = -8100$, and $a_0 = 180000$? Can you explain your observations?

Hint: Use a Wilkinson shift or plot the adjusted polynomial p.

Acknowledgements: This question is motivated by a conversation and discussion with Xiuyuan Wang.