CSE 6643 Homework 7

Karl Hiner, Spring 2023

1 Convergence of Lanczos iteration [60 pts]

Consider the Lanczos process for a symmetric matrix $\boldsymbol{A} \in \mathbb{R}^{m \times m}$, with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m$. We denote by $\boldsymbol{T}_k$ the $k \times k$ tri-diagonal matrix computed by the Lancczos process starting with the vector $\boldsymbol{q}_1$. Recall that

$$\boldsymbol{T}_k = \boldsymbol{Q}_k^T \boldsymbol{A} \boldsymbol{Q}_k. \tag{1}$$

The largest eigenvalue μ_k of $\boldsymbol{T}_k$ satisfies

$$\mu_k = \max_{\boldsymbol{y} \neq \boldsymbol{0}} \frac{\boldsymbol{y}^T \boldsymbol{T}_k \boldsymbol{y}}{\boldsymbol{y}^T \boldsymbol{y}}. \tag{2}$$

You can use (or prove, for bonus points, in problem 3) that

$$\mu_k \leq \lambda_1. \tag{3}$$

In this exercise you will also need the Chebychev polynomials $T_k(x)$ satisfying

$$T_k(\cos \theta) = \cos(k\theta), \tag{4}$$

$$T_k(\cosh y) = \cosh(ky). \tag{5}$$

Using the Chebychev polynomials, we define

$$p_k(x) = T_{k-1}\left(-1 + 2\frac{x - \lambda_m}{\lambda_2 - \lambda_m}\right). \tag{6}$$

(a) [10 pts]
Consider a polynomial $p(x)$ of degree $k - 1$. Show that

$$\mu_k \geq \frac{\boldsymbol{q}_1^T p(\boldsymbol{A}) \boldsymbol{A} p(\boldsymbol{A}) \boldsymbol{q}_1}{\boldsymbol{q}_1^T p(\boldsymbol{A})^2 \boldsymbol{q}_1} \tag{7}$$

$$
\begin{aligned}
\mu_k &= \max_{\boldsymbol{y} \neq \boldsymbol{0}} \frac{\boldsymbol{y}^T \boldsymbol{T}_k \boldsymbol{y}}{\boldsymbol{y}^T \boldsymbol{y}} && \text{(given)} \\
&= \max_{\boldsymbol{y} \neq \boldsymbol{0}} \frac{\boldsymbol{y}^T \boldsymbol{Q}_k^T \boldsymbol{A} \boldsymbol{Q}_k \boldsymbol{y}}{\boldsymbol{y}^T \boldsymbol{y}} && \text{(substitute } \boldsymbol{T}_k = \boldsymbol{Q}_k^T \boldsymbol{A} \boldsymbol{Q}_k) \\
&= \max_{\boldsymbol{y} \neq \boldsymbol{0}} \frac{(\boldsymbol{Q}_k \boldsymbol{y})^T \boldsymbol{A} (\boldsymbol{Q}_k \boldsymbol{y})}{\boldsymbol{y}^T \boldsymbol{y}} && \text{(rearrange numerator)} \\
&= \max_{\boldsymbol{x} \in \mathcal{K}(A, q, k) \setminus \emptyset} \frac{\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}}{\boldsymbol{x}^T \boldsymbol{x}} && (\boldsymbol{x} := \boldsymbol{Q}_k \boldsymbol{y}, \ \mathcal{K} \text{ is the Krylov subspace of } \boldsymbol{A})
\end{aligned}
$$

The last step follows since $\boldsymbol{Q}_k$ is obtained by applying the Gram-Schmidt process to the Krylov subspace $\mathcal{K}(A, q, k)$, and thus $\boldsymbol{Q}_k$ is an orthonormal basis for $\mathcal{K}(A, q, k)$.

Since $\boldsymbol{x}$ is in the Krylov space of $\boldsymbol{A}$, we can (by the definition of the Krylov space) express it as $\boldsymbol{x} = p(\boldsymbol{A})\boldsymbol{b}$, where p is a polynomial of degree $k - 1$, and we have

$$\mu_k = \max_{p \text{ of deg } k-1} \frac{\boldsymbol{b}^T p(\boldsymbol{A})^T \boldsymbol{A} p(\boldsymbol{A}) \boldsymbol{b}}{\boldsymbol{b}^T f(\boldsymbol{A})^2 \boldsymbol{b}}.$$

Since the starting vector $\boldsymbol{q}_1$ is arbitrary, we can choose $\boldsymbol{b} = \boldsymbol{q}_1$, which completes the proof.

(b) [10 pts]

Expand $\boldsymbol{q}_1$ in a basis of orthonormal eigenvectors $\{\boldsymbol{z}_i\}_{1 \le i \le m}$ of $\boldsymbol{A}$.

$$\boldsymbol{q}_1 = y_1 \boldsymbol{z}_1 + \cdots + y_m \boldsymbol{z}_m. \tag{8}$$

Prove that

$$\frac{\boldsymbol{q}_1^T p(\boldsymbol{A}) \boldsymbol{A} p(\boldsymbol{A}) \boldsymbol{q}_1}{\boldsymbol{q}_1^T p(\boldsymbol{A})^2 \boldsymbol{q}_1} = \frac{\displaystyle\sum_{i=1}^m y_i^2 p(\lambda_i)^2 \lambda_i}{\displaystyle\sum_{i=1}^m y_i^2 p(\lambda_i)^2} \tag{9}$$

Numerator:

$$
\begin{aligned}
\boldsymbol{q}_1^T p(\boldsymbol{A}) \boldsymbol{A} p(\boldsymbol{A}) \boldsymbol{q}_1 &= \sum_{i=1}^m y_i \boldsymbol{z}_i^T p(\boldsymbol{A}) \boldsymbol{A} p(\boldsymbol{A}) \sum_{j=1}^m y_j \boldsymbol{z}_j \\
&= \sum_{i=1}^m \sum_{j=1}^m y_i y_j \boldsymbol{z}_i^T p(\boldsymbol{A}) \boldsymbol{A} p(\boldsymbol{A}) \boldsymbol{z}_j && \text{(rearrange)} \\
&= \sum_{i=1}^m \sum_{j=1}^m y_i y_j \boldsymbol{z}_i^T p(\boldsymbol{A}) \boldsymbol{A} p(\lambda_j) \boldsymbol{z}_j && (p(\boldsymbol{A}) \boldsymbol{z}_j = p(\lambda_j) \boldsymbol{z}_j) \\
&= \sum_{i=1}^m \sum_{j=1}^m y_i y_j \boldsymbol{z}_i^T p(\boldsymbol{A}) (\lambda_j p(\lambda_j) \boldsymbol{z}_j) && (\text{since } \boldsymbol{A} \boldsymbol{z}_j = \lambda_j \boldsymbol{z}_j) \\
&= \sum_{i=1}^m \sum_{j=1}^m y_i y_j p(\lambda_i) \lambda_j p(\lambda_j) \boldsymbol{z}_i^T \boldsymbol{z}_j && (\text{apply } p(\boldsymbol{A}) \text{ to } \boldsymbol{z}_i) \\
&= \sum_{i=1}^m y_i^2 p(\lambda_i)^2 \lambda_i && (\text{since } \boldsymbol{z}_i^T \boldsymbol{z}_j = 0 \text{ for } i \ne j, \text{ and } \boldsymbol{z}_i^T \boldsymbol{z}_i = 1)
\end{aligned}
$$

2

Denominator:

$$\boldsymbol{q}_1^T p(\boldsymbol{A})^2 \boldsymbol{q}_1 = \sum_{i=1}^{m} y_i \boldsymbol{z}_i^T p(\boldsymbol{A})^2 \sum_{j=1}^{m} y_j \boldsymbol{z}_j$$

$$= \sum_{i=1}^{m} \sum_{j=1}^{m} y_i y_j \boldsymbol{z}_i^T p(\boldsymbol{A})^2 \boldsymbol{z}_j \qquad \text{(rearrange)}$$

$$= \sum_{i=1}^{m} \sum_{j=1}^{m} y_i y_j \boldsymbol{z}_i^T p(\boldsymbol{A}) p(\lambda_j) \boldsymbol{z}_j \qquad (p(\boldsymbol{A})\boldsymbol{z}_j = p(\lambda_j)\boldsymbol{z}_j)$$

$$= \sum_{i=1}^{m} \sum_{j=1}^{m} y_i y_j p(\lambda_i) p(\lambda_j) \boldsymbol{z}_i^T \boldsymbol{z}_j \qquad \text{(apply } p(\boldsymbol{A}) \text{ to } \boldsymbol{z}_i)$$

$$= \sum_{i=1}^{m} y_i^2 p(\lambda_i)^2 \qquad \text{(since } \boldsymbol{z}_i^T \boldsymbol{z}_j = 0 \text{ for } i \neq j, \text{ and } \boldsymbol{z}_i^T \boldsymbol{z}_i = 1)$$

(c) [10 pts]

Show that $|p_k(\lambda_i)| \leq 1, \forall\, 2 \leq i \leq m$.

$$\lambda_m \leq \lambda_i \leq \lambda_2 \qquad \text{(for } 2 \leq i \leq m, \text{ since } \lambda_1 \geq \lambda_2 \geq \lambda_m)$$

$$0 \leq \lambda_i - \lambda_m \leq \lambda_2 - \lambda_m \qquad \text{(subtract } \lambda_m)$$

$$0 \leq \frac{\lambda_i - \lambda_m}{\lambda_2 - \lambda_m} \leq 1 \qquad \text{(divide by } \lambda_2 - \lambda_m)$$

$$-1 \leq -1 + 2\frac{\lambda_i - \lambda_m}{\lambda_2 - \lambda_m} \leq 1 \qquad \text{(multiply by 2 and subtract 1)}$$

$$-1 \leq x_i \leq 1 \implies |x_i| \leq 1 \qquad (x_i := -1 + 2\frac{\lambda_i - \lambda_m}{\lambda_2 - \lambda_m})$$

Given the definition of x_i, note that $p_k(\lambda_i) = T_{k-1}(x_i)$. Thus, we want to show that $|x_i| \leq 1$ implies $|T_{k-1}(x_i)| \leq 1$.

We are given that $T_k(\cos\theta) = \cos(k\theta)$. Since $\cos\theta \in [-1, 1], \forall\theta$, and since $\cos\theta$ produces all values in the range $[-1, 1]$, we can deduce that for any value of x_i, $|T_{k-1}(x_i)| \leq 1$.

Thus, for $2 \leq i \leq m$, we have shown that $|p_k(\lambda_i)| = |T_{k-1}(x_i)| \leq 1$.

(d) [10 pts]

Show that
$$p_k(\lambda_1) \in O\left[\left(2\left(2\frac{\lambda_1 - \lambda_2}{\lambda_2 - \lambda_m} + 1\right)\right)^{k-1}\right], \tag{10}$$

in the limit of $(\lambda_1 - \lambda_2)/(\lambda_2 - \lambda_m) \to \infty$.

From the definition of $p_k(\lambda_1)$, we can write it as:
$$p_k(\lambda_1) = T_{k-1}(x_1),$$

where $x_1 = -1 + 2\frac{\lambda_1 - \lambda_m}{\lambda_2 - \lambda_m}$.

3

(These following steps are due to Yuan Qiu's hint on Piazza - thank you!)

We can write:

$$p_k(\lambda_1) = \cosh((k-1)t) = \frac{e^{(k-1)t} + e^{-(k-1)t}}{2},$$

where e^t satisfies

$$\frac{e^t + e^{-t}}{2} = -1 + 2\frac{\lambda_1 - \lambda_m}{\lambda_2 - \lambda_m} = 2\frac{\lambda_1 - \lambda_2}{\lambda_2 - \lambda_m} + 1.$$

Let $l = 2\frac{\lambda_1 - \lambda_2}{\lambda_2 - \lambda_m} + 1$. Then, we have $e^t + e^{-t} = 2l$.

We can write this as a quadratic equation:

$$(e^t)^2 - 2l(e^t) + 1 = 0$$

Solving for e^t, we obtain two solutions:

$$e^t = l \pm \sqrt{l^2 - 1}$$

Now we can rewrite the expression for $p_k(\lambda_1)$ using the solutions:

$$p_k(\lambda_1) = \frac{1}{2}\left((l \pm \sqrt{l^2 - 1})^{k-1} + (l \mp \sqrt{l^2 - 1})^{k-1}\right).$$

Note that as $l \to \infty$, $\sqrt{l^2 - 1} \approx l$. Thus, we can simplify the expression:

$$p_k(\lambda_1) \approx \frac{1}{2}\left((2l)^{k-1} + (2l)^{k-1}\right) = (2l)^{k-1}.$$

Substituting the definition of l, we have:

$$p_k(\lambda_1) \approx \left(2\left(2\frac{\lambda_1 - \lambda_2}{\lambda_2 - \lambda_m} + 1\right)\right)^{k-1}.$$

Thus, in the limit of $(\lambda_1 - \lambda_2)/(\lambda_2 - \lambda_m) \to \infty$, we have:

$$p_k(\lambda_1) \in O\left[\left(2\left(2\frac{\lambda_1 - \lambda_2}{\lambda_2 - \lambda_m} + 1\right)\right)^{k-1}\right].$$

(e) [10 pts]

Show that with $\cos \varphi_1 = \boldsymbol{q}_1^T \boldsymbol{z}_1$,

$$\lambda_1 - (\lambda_1 - \lambda_m)\frac{(\tan(\varphi_1))^2}{p_k(\lambda_1)^2} \le \mu_k \le \lambda_1. \tag{11}$$

I'm skipping this one.

4

(f) [10 pts]

Assume, for example, that $\lambda_1 - \lambda_2 = (\lambda_2 - \lambda_m)/2$. Find z such that

$$p_k(\lambda_1) \approx \frac{z^{k-1}}{2}. \tag{12}$$

Estimate the number of iterations to reach machine accuracy u for λ_1.

I'm also skipping this one.

2 Arnoldi vs Lanczos [40 pts]

Arnoldi [15 pts]

Go to section (a) of the file `HW7_your_code.jl` and implement a function that implements the Arnoldi method. Your method should return an upper Hessenberg matrix.

(b) Lanczos [15 pts]

Go to section (b) of the file `HW7_your_code.jl` and implement a function that implements the Lanczos method. Your method should return an upper Hessenberg matrix.

(c) Arnoldi vs Lanczos [10 pts]

Compare the behavior of the Arnoldi and Lanczos method on different symmetric matrices. How does the approximation improve as you increase $k_{\max}$? Can you create reproduce scenarios where Lanczos methods fails, for instance by producing ghost eigenvalues? Summarize your findings using figures as appropriate, and hand them in with the written part of your homework.

I'm also skyyipping this one.

3 Nested Approximation [20 bonus pts]

Let $\boldsymbol{A} \in \mathbb{R}^{m \times m}$ be symmetric, and $\boldsymbol{Q} \in \mathbb{R}^{m \times m}$ be orthogonal with columns $\boldsymbol{q}_i$. Define $\boldsymbol{Q}_k := \boldsymbol{Q}_{:,1:k}$. We denote

$$\overline{\mu}_k := \lambda_{\max}\big(\boldsymbol{Q}_k^T \boldsymbol{A} \boldsymbol{Q}_k\big), \tag{13}$$

$$\underline{\mu}_k := \lambda_{\min}\big(\boldsymbol{Q}_k^T \boldsymbol{A} \boldsymbol{Q}_k\big), \tag{14}$$

where $\lambda_{\max}$ and $\lambda_{\min}$ are the largest and smallest eigenvalues.

Prove that

$$\overline{\mu}_1 \le \overline{\mu}_2 \le \cdots \le \overline{\mu}_m = \lambda_{\max}(\boldsymbol{A}), \tag{15}$$

$$\underline{\mu}_1 \ge \underline{\mu}_2 \ge \cdots \ge \underline{\mu}_m = \lambda_{\min}(\boldsymbol{A}). \tag{16}$$

$$
\begin{aligned}
\overline{\mu}_k &:= \lambda_{\max}\big(\boldsymbol{Q}_k^T \boldsymbol{A} \boldsymbol{Q}_k\big) && \text{(given)} \\
&= \max_{\boldsymbol{y} \neq 0} \frac{\boldsymbol{y}^T \boldsymbol{Q}_k^T \boldsymbol{A} \boldsymbol{Q}_k \boldsymbol{y}}{\boldsymbol{y}^T \boldsymbol{y}} && \text{(by the Courant-Fischer theorem)} \\
&= \max_{\boldsymbol{y} \neq 0} \frac{(\boldsymbol{Q}_k \boldsymbol{y})^T \boldsymbol{A} (\boldsymbol{Q}_k \boldsymbol{y})}{\boldsymbol{y}^T \boldsymbol{y}} && \text{(rearrange numerator)} \\
&= \max_{\boldsymbol{x} \in \mathcal{K}(A,q,k) \setminus \emptyset} \frac{\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}}{\boldsymbol{x}^T \boldsymbol{x}} && (\boldsymbol{x} := \boldsymbol{Q}_k \boldsymbol{y}, \ \mathcal{K} \text{ is the Krylov subspace of } \boldsymbol{A})
\end{aligned}
$$

The last step follows since $\boldsymbol{Q}_k$ is obtained by applying the Gram-Schmidt process to the Krylov subspace $\mathcal{K}(A, q, k)$, and thus $\boldsymbol{Q}_k$ is an orthonormal basis for $\mathcal{K}(A, q, k)$.

By the Courant-Fischer theorem, we can also express largest eigenvalue of $\boldsymbol{A}$ as

$$\lambda_{\max}(\boldsymbol{A}) = \max_{\boldsymbol{x} \neq 0} \frac{\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}}{\boldsymbol{x}^T \boldsymbol{x}}.$$

Since $\overline{\mu}_k$ is found by maximizing the same objective as $\lambda_{\max}(\boldsymbol{A})$, but over a smaller subset, we have $\overline{\mu}_k \leq \lambda_{\max}(\boldsymbol{A})$.

As we increase k, $\mathcal{K}(A, q, k)$ becomes larger. So we are maximizing the objective over a larger set, and we will thus find an equal or larger maximum. Therefore, we can conclude that

$$\overline{\mu}_1 \leq \overline{\mu}_2 \leq \cdots \leq \overline{\mu}_m.$$

Since $\mathcal{K}(A, q, m)$ spans the entire space, we have $\overline{\mu}_m = \lambda_{\max}(\boldsymbol{A})$.

Now, let's prove the inequality for $\underline{\mu}_k$:

$$\underline{\mu}_k = \min_{\boldsymbol{x} \in \mathcal{K}(A,q,k) \setminus \emptyset} \frac{\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}}{\boldsymbol{x}^T \boldsymbol{x}}$$

We'll use similar reasoning as we did for the first direction. As we increase k, the Krylov subspace $\mathcal{K}(A, q, k)$ becomes larger. So we are minimizing the objective over a larger set, and we will find an equal or smaller minimum, and so

$$\underline{\mu}_1 \geq \underline{\mu}_2 \geq \cdots \geq \underline{\mu}_m.$$

Finally, since $\mathcal{K}(A, q, m)$ spans the entire space, we have $\underline{\mu}_m = \lambda_{\min}(\boldsymbol{A})$.

4 Early Termination [20 bonus pts]

Let $\boldsymbol{A} \in \mathbb{R}^{m \times m}$ be a symmetric matrix. We denote by K the dimension of the Krylov subspace

$$\mathcal{K}(\boldsymbol{A}, \boldsymbol{q}_1, m) = \left\{ \boldsymbol{q}_1, \boldsymbol{A}\boldsymbol{q}_1, \boldsymbol{A}^2 \boldsymbol{q}_1, \ldots, \boldsymbol{A}^{m-1} \boldsymbol{q}_1 \right\}. \tag{17}$$

The Lanczos algorithm is said to terminate after k steps if $\beta_k = 0$ and $\beta_i \neq 0, \forall i < k$.

Prove that the Lanczos process, with starting vectors $\boldsymbol{q}_1$, terminates in at most K steps in exact arithmetic.

5 CIOS [10 bonus pts for the entire class]

In order to help the TAs and myself in improving the course, please make sure to fill out your CIOS. I take this feedback into account for future iterations of this class, so please aim to provide me with feedback both on what needs improvement and what is good as is. If ≥ 75 percent of students in this class fill out their CIOS by the time the homework is graded, everyone in the class earns 10 bonus points.