THE CHINESE UNIVERSITY OF HONG KONG
Department of Mathematics
MATH3310 2024-2025
Assignment 5
Due Date: December 7 before 11:59 PM

1. Below are the simultaneous iteration method with shift and the QR iteration method with shift.

> **Shifted Simultaneous Iteration**
>
> Let $Q^{(0)} = I$
> For $k = 0, 1, 2, \ldots$
>
> - Choose shift s_k
> - $Y = (A - s_k I)\bar{Q}^{(k)}$
> - QR factorization of Y: $Y = \bar{Q}^{(k+1)} R^{(k+1)}$
>
> Denote $\bar{R}^{(k)} = R^{(k)} R^{(k-1)} \cdots R^{(1)}$

> **Shifted QR Iteration**
>
> Let $A^{(0)} = A$
> For $k = 0, 1, 2, \ldots$
>
> - Choose shift s_k
> - $Q_{QR}^{(k+1)} R_{QR}^{(k+1)} = A^{(k)} - s_k I$
> - $A^{(k+1)} = R_{QR}^{(k+1)} Q_{QR}^{(k+1)} + s_k I$
>
> Denote $\bar{Q}_{QR}^{(k)} = Q_{QR}^{(1)} Q_{QR}^{(2)} \cdots Q_{QR}^{(k)}, \bar{R}_{QR}^{(k)} = R_{QR}^{(k)} R_{QR}^{(k-1)} \cdots R_{QR}^{(1)}$

(a) According to the definition of shifted QR iteration, directly prove $A^{(k+1)} = \left(Q_{QR}^{(k+1)}\right)^T A^{(k)} Q_{QR}^{(k+1)}$ and $A^{(k)} = \left(\bar{Q}_{QR}^{(k)}\right)^T A \bar{Q}_{QR}^{(k)}$.

(b) To prove the following properties, you may need mathematical induction.

i. $(A - s_k I)(A - s_{k-1} I) \cdots (A - s_0 I) = \bar{Q}^{(k+1)} \bar{R}^{(k+1)}$

ii. $(A - s_k I)(A - s_{k-1} I) \cdots (A - s_0 I) = \bar{Q}_{QR}^{(k+1)} \bar{R}_{QR}^{(k+1)}$

(Hint: using the conclusion in (a), show $A - s_k I = \bar{Q}_{QR}^{(k+1)} \left(A^{(k+1)} - s_k I\right) \left(\bar{Q}_{QR}^{(k+1)}\right)^T$)

iii. $\bar{Q}^{(k+1)} = \bar{Q}_{QR}^{(k+1)}$ and $\bar{R}^{(k+1)} = \bar{R}_{QR}^{(k+1)}$

2. Suppose A is real symmetric positive definite, and let the nonzero $\boldsymbol{p}_i$'s be $A-$**orthogonal**, that is. $\boldsymbol{p}_i^T A \boldsymbol{p}_j = 0$ if $i \neq j$. let $\boldsymbol{x}_k = \boldsymbol{x}_0 + \sum_{\mathbf{j=0}}^{\mathbf{k\text{-}1}} \alpha_j \boldsymbol{p}_j$, and $f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T A \boldsymbol{x} - \boldsymbol{b}^T \boldsymbol{x}$

(a) show that $\boldsymbol{p}_i$'s are linearly independent.

(b) Given a fixed integer k, show that if $\boldsymbol{x}_k$ was chosen to minimize the $f(\boldsymbol{x}), \forall \boldsymbol{x} \in \boldsymbol{x}_0 + \operatorname{span}\{\boldsymbol{p}_0, \ldots, \boldsymbol{p}_{k-1}\}$, then determining the α_k such that $\boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k$ minimizing $f(\boldsymbol{x})$ is the same as choosing $\boldsymbol{x}_{k+1}$ to minimize $f(\boldsymbol{x}), \forall \boldsymbol{x} \in \boldsymbol{x}_0 + \operatorname{span}\{\boldsymbol{p}_0, \ldots, \boldsymbol{p}_{k-1}, \boldsymbol{p}_k\}$. Moreover, what are the values of $\alpha_0, \ldots, \alpha_{k-1}$ such that $\boldsymbol{x}_k = \underset{\alpha_0, \alpha_1, \ldots, \alpha_{k-1}}{\operatorname{argmin}} f(\boldsymbol{x}_0 + \sum_{\mathbf{j=0}}^{\mathbf{k\text{-}1}} \alpha_j \boldsymbol{p}_j)$?

(c) Denote $\mathcal{K}_{m+1}(A; r_0) = \operatorname{span}\left\{r_0, Ar_0, A^2 r_0, \ldots, A^m r_0\right\}$, and here is an equivalent statement of conjugate gradient method.

Conjugate gradient method for solving $Ax = b$ (not optimized)

Let $\mathbf{x}_0$ be the initial vector and $\mathbf{r}_0 = A\mathbf{x}_0 - \mathbf{b}, \mathbf{p}_0 = -\mathbf{r}_0$.
For $k = 0, 1, \ldots,$

$$\begin{aligned} \alpha_k &= -\frac{\mathbf{p}_k^T \mathbf{r}_k}{\mathbf{p}_k^T A \mathbf{p}_k} \\ \mathbf{x}_{k+1} &= \mathbf{x}_k + \alpha_k \mathbf{p}_k \\ \mathbf{r}_{k+1} &= A\mathbf{x}_{k+1} - \mathbf{b} \\ \beta_k &= -\frac{\mathbf{r}_{k+1}^T A \mathbf{p}_k}{\mathbf{p}_k^T A \mathbf{p}_k} \\ \mathbf{p}_{k+1} &= -\mathbf{r}_{k+1} - \beta_k \mathbf{p}_k. \end{aligned}$$

in the class, we have proven the following several properties by induction.

i. for $k = 0, 1, \ldots, n$,

$$\text{span}\{\mathbf{r}_0, \mathbf{r}_1, \ldots, \mathbf{r}_k\} = \text{span}\{\mathbf{p}_0, \mathbf{p}_1, \ldots, \mathbf{p}_k\} = \mathcal{K}_{k+1}(A; \boldsymbol{r}_0)$$

ii. for $1 \leq i, j \leq n$ and $i \neq j$,

$$\mathbf{r}_i^T \mathbf{r}_j = 0 \quad \text{and} \quad \mathbf{p}_i^T A \mathbf{p}_j = 0$$

Using these properties and conclusion in (b), prove that

$$\boldsymbol{x}_k = \underset{\boldsymbol{x} \in \boldsymbol{x}_0 + \mathcal{K}_k(A; \boldsymbol{r}_0)}{\text{argmin}} f(\boldsymbol{x})$$

3. Suppose A is a real symmetric matrix and $A = QDQ^T$ where $Q^TQ = I$ and $D = \text{diag}(\lambda_1, \ldots, \lambda_n)$. Assume

$$|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_k| > |\lambda_{k+1}| \geq \cdots \geq |\lambda_n|.$$

Let E_k denote the subspace spanned by the first k columns of Q, equivalently, subspace spanned by eigenvectors associated with $\lambda_1, \lambda_2, \ldots, \lambda_k$, and let $\cos\angle(\boldsymbol{x}^{(0)}, E_k) \neq 0$ We define

$$\begin{aligned} \cos\angle(\boldsymbol{x}, E_k) &:= \max\{\cos\angle(\boldsymbol{x}, \boldsymbol{y}) : \boldsymbol{y} \in E_k \backslash \{0\}\}, \\ \sin\angle(\boldsymbol{x}, E_k) &:= \min\{\sin\angle(\boldsymbol{x}, \boldsymbol{y}) : \boldsymbol{y} \in E_k \backslash \{0\}\}, \\ \tan\angle(\boldsymbol{x}, E_k) &:= \frac{\sin\angle(\boldsymbol{x}, E_k)}{\cos\angle(\boldsymbol{x}, E_k)}. \end{aligned}$$

Let $\boldsymbol{x}^{(m)} = A^m \boldsymbol{x}^{(0)} = A\boldsymbol{x}^{(m-1)}$,

(a) Suppose $\boldsymbol{x}^{(0)} = \sum_{i=1}^{n} a_i \vec{q}_i$, where $\vec{q}_i$ is the eigenvector associated with λ_i, show that

$$\tan^2\angle(\boldsymbol{x}^{(m+1)}, E_k) = \frac{\sum_{i=k+1}^{n} (a_i)^2 |\lambda_i|^{2(m+1)}}{\sum_{i=1}^{k} (a_i)^2 |\lambda_i|^{2(m+1)}}$$

(b) prove that

$$\tan\angle(x^{(m+1)}, E_k) \leq \frac{|\lambda_{k+1}|}{|\lambda_k|} \tan\angle(x^{(m)}, E_k)$$