Lecture 21:

Recap:

QR method to find eigenvalues

Algorithm: (QR algorithm)

Input : $A \in M_{n\times n}(\mathbb{R})$

Step 1: Let $A^{(0)} = A$. Compute QR factorization of $A^{(0)} = Q_0 R_0$.

Let $A^{(1)} = R_0 Q_0$.

Step 2: Assume $A^{(1)}, \dots, A^{(k)}$ are computed. Let $A^{(k)} = Q_k R_k$ be the QR factorization of $A^{(k)}$. Let $A^{(k+1)} = R_k Q_k$.

Observation: 1. QR method gives a sequence of matrices:

$$\{ A^{(0)} = A,\ A^{(1)},\ A^{(2)},\ \ldots,\ A^{(k)}, \ldots \}$$

2. Now, $A^{(1)} = R_0 Q_0 = Q_0^{-1} \underbrace{Q_0 R_0}_{A^{(0)}=A} Q_0 = Q_0^{-1} A Q_0$

$A^{(1)}$ is similar to A (A has the same set of eigenvalues as $A^{(1)}$).

$$\Big(\det(A^{(1)} - \lambda I) = \det(Q_0^{-1} A^{(0)} Q_0 - \lambda I) = \det(Q_0^{-1}(A^{(0)} - \lambda I) Q_0) = \det(A^{(0)} - \lambda I) \Big)$$

Similarly, $A^{(2)} = R_1 Q_1 = Q_1^{-1} \underbrace{Q_1 R_1}_{A^{(1)}} Q_1 \sim A^{(1)}$

$$\therefore \quad A = A^{(0)} \sim A^{(1)} \sim A^{(2)} \cdots \sim A^{(k)} \sim \cdots$$

3. If $A^{(k)}$ converges to an upper triangular matrix, then the diagonal entries of $A^{(k)}$ will converges to all eigenvalues of A.

Idea: To determine ALL eigenvalues using Power's method,

choose n initial guesses: $\left\{ \vec{x}_1^{(0)}, \vec{x}_2^{(0)}, \ldots, \vec{x}_n^{(0)} \right\}$

Let $X^{(0)} = \begin{pmatrix} | & | & & | \\ \vec{x}_1^{(0)} & \vec{x}_2^{(0)} & \cdots & \vec{x}_n^{(0)} \\ | & | & & | \end{pmatrix} \in M_{n\times n}(\mathbb{R})$

Apply power method on $X^{(0)}$:

$$A X^{(0)} = \begin{pmatrix} | & | & & | \\ A\vec{x}_1^{(0)} & A\vec{x}_2^{(0)} & \cdots & A\vec{x}_n^{(0)} \\ | & | & & | \end{pmatrix}$$

$$A^k X^{(0)} = \begin{pmatrix} | & | & & | \\ A^k\vec{x}_1^{(0)} & A^k\vec{x}_2^{(0)} & \cdots & A^k\vec{x}_n^{(0)} \\ | & | & & | \end{pmatrix}$$

$$\begin{array}{ccc} \downarrow k\to\infty & \downarrow k\to\infty & \downarrow k\to\infty \\ \vec{v}_1 & \vec{v}_2 & \vec{v}_n \\ \uparrow & \uparrow & \uparrow \\ \text{first eigenvector} & \text{eigenvector} & \text{eigenvector} \end{array}$$

If $\vec{x}_1^{(0)} = \vec{v}_1$

$\vec{x}_2^{(0)} = \vec{v}_1 + \vec{v}_2$

$\vdots$

$\vec{x}_n^{(0)} = \vec{v}_1 + \vec{v}_2 + \cdots + \vec{v}_n$

then:

$$A^k X^{(0)} \to \begin{pmatrix} | & | & & | \\ k_1\vec{v}_1, & k_2\vec{v}_1 & \cdots, & k_n\vec{v}_1 \\ | & | & & | \end{pmatrix}$$

Relationship between Power method and QR method

Motivation: Consider $A \in M_{n\times n}(\mathbb{R})$ with eigenvalues:

$$|\lambda_1| > |\lambda_2| > |\lambda_3| > \dots > |\lambda_n|$$

Power's method computes ONE eigenvalue (depend on initialijation)

Say $\{\vec{q}_1, \vec{q}_2, \dots, \vec{q}_n\}$ are eigenvectors of $\lambda_1, \lambda_2, \dots, \lambda_n$ respectively.

Assume A is symmetric.

Properties of $\{\vec{q}_j\}_{j=1}^n$

$$A = \quad = \lambda_j \vec{q}_j$$

$$\underset{\lambda_i \vec{q}_i}{\overset{\shortparallel}{A\vec{q}_i}} \cdot \vec{q}_j = (A\vec{q}_i)^T \vec{q}_j = q_i^T \underset{}{A^T} \vec{q}_j$$

$$\Leftrightarrow \quad \lambda_i \vec{q}_i \cdot \vec{q}_j = \lambda_j \vec{q}_i \cdot \vec{q}_j \Leftrightarrow \overset{\neq 0}{(\lambda_i - \lambda_j)} \vec{q}_i \cdot \vec{q}_j = 0$$

$$\Rightarrow \vec{q}_i \cdot \vec{q}_j = 0 \text{ for } i \neq j$$

$\therefore \{\vec{q}_j\}_{j=1}^n$ is orthogonal

WLOG, assume $\{\vec{q}_j\}_{j=1}^n$ are o.n.

In general, if we choose $\vec{x}^{(0)} = c_i \vec{q}_i + c_{i+1} \vec{q}_{i+1} + \dots + c_n \vec{q}_n$ $(c_i \neq 0)$

then the power method converges to : $|\lambda_i|$.

To determine ALL eigenvalues, choose n initial guesses:

$$\{\vec{x}_1^{(0)}, \vec{x}_2^{(0)}, \dots, \vec{x}_n^{(0)}\} \to X^{(0)} = \begin{pmatrix} | & | & & | \\ \vec{x}_1^{(0)} & \vec{x}_2^{(0)} & \dots & \vec{x}_n^{(0)} \\ | & | & & | \end{pmatrix} \in M_{n\times n}(\mathbb{R})$$

Goal: Apply Power's method on $X^{(0)}$.

Let $V^{(k)} = A^k X^{(0)}$

We hope that $V^{(k)} \to \begin{pmatrix} | & | & & | \\ k_1 \vec{q}_1 & k_2 \vec{q}_2 & \dots & k_n \vec{q}_n \\ | & | & & | \end{pmatrix}$ for

some constants $k_1, k_2, \dots, k_n$

<u>Strategy:</u> Make sure that $A^k X^{(0)}$ (after some normalization is orthogonal)

<u>How?</u> QR factorization.

Consider an initial guess $X^{(0)}$ (usually I_n)

Take the "orthogonal part" of $X^{(0)}$:

$$X^{(0)} = \bar{Q}^{(0)} R^{(0)} \quad \text{(QR factorization)}$$

Apply the Power's method on $\bar{Q}^{(0)}$ to get:

$$W = A \bar{Q}^{(0)}$$

Repeat: take "orthogonal part" of W:

$$W = \bar{Q}^{(1)} R^{(1)}$$

Apply Power's method on $\bar{Q}^{(1)}$ to get

$$W = A \bar{Q}^{(1)} \qquad \text{etc} \ldots$$

Algorithm: (Simultaneous Iteration) (*)

Input: Initial matrix $X^{(0)} = \begin{pmatrix} | & & | \\ \vec{x}_1^{(0)} & \cdots & \vec{x}_n^{(0)} \\ | & & | \end{pmatrix} \in M_{n \times n}(\mathbb{R})$.

Output: $\overline{Q}^{(k)} \to \begin{pmatrix} | & | & & | \\ \vec{q}_1 & \vec{q}_2 & \cdots & \vec{q}_n \\ | & | & & | \end{pmatrix}$

Step 1: Obtain QR factorization of $X^{(0)} = \overline{Q}^{(0)} R^{(0)}$

Step 2: For $k = 1, 2, \ldots$, let $W = A\overline{Q}^{(k-1)}$

Obtain QR factorization of $W = \overline{Q}^{(k)} R^{(k)}$

Let $A^{(k)} = \overline{Q}^{(k)T} A \overline{Q}^{(k)}$.

Step 3: Keep iteration going.

Remark: To ensure the uniqueness of QR factorization, R is restricted to have positive diagonal entries.

Recap: QR method can be written as :

Input: $A \in M_{n\times n}(\mathbb{R})$

Output: $Q^{(k)}$, $A^{(k)}$

Step 1: Let $A^{(0)}_{QR} = A$

Step 2: For $k = 1, 2, \ldots$, obtain QR factorizatin of

$$A^{(k-1)}_{QR} = Q^{(k)}_{QR} R^{(k)}_{QR}$$

Let $A^{(k)}_{QR} = R^{(k)}_{QR} Q^{(k)}_{QR}$

Algorithm: (Simultaneous Iteration) (*)

Input: Initial matrix $X^{(0)} = (\vec{x}_1^{(0)}\ \vec{x}_2^{(0)}\ \cdots\ \vec{x}_n^{(0)}) \in M_{n\times n}(\mathbb{R})$ $= I_n$

Output: $\bar{Q}^{(k)} \to (\vec{q}_1\ \vec{q}_2\ \cdots\ \vec{q}_n)$

Step 1: Obtain QR factorization of $X^{(0)} = \bar{Q}^{(0)} R^{(0)}$.

Step 2: For $k = 1, 2, \dots$, let $W = A\bar{Q}^{(k-1)}$ (Power's method on $\bar{Q}^{(k-1)}$)

Obtain QR factorization of $W = \bar{Q}^{(k)} R^{(k)}$.

Step 3: Keep iteration going!

Let $\bar{R}^{(k)} = R^{(k)} R^{(k-1)} \cdots R^{(1)}$

$A^{(k)} = \bar{Q}^{(k)T} A \bar{Q}^{(k)}$.

Going to show:

$$A_{QR}^{(k)} = A^{(k)}$$

Recall: QR method can be written as: (**)

Input: $A \in M_{n\times n}(\mathbb{R})$

Output: $Q^{(k)}$

Step 1: Let $A_{QR}^{(0)} = A$.

Step 2: For $k = 1, 2, \dots$, obtain QR factorization of:

$A_{QR}^{(k-1)} = Q_{QR}^{(k)} R_{QR}^{(k)}$

Let $A_{QR}^{(k)} = R_{QR}^{(k)} Q_{QR}^{(k)}$

Let $\bar{Q}_{QR}^{(k)} = Q_{QR}^{(1)} Q_{QR}^{(2)} \cdots Q_{QR}^{(k)}$ and $\bar{R}_{QR}^{(k)} = R_{QR}^{(k)} R_{QR}^{(k-1)} \cdots R_{QR}^{(1)}$

Theorem:

1. $A_{QR}^{(k)} = A^{(k)}$
2. $\overline{Q}_{QR}^{(k)} = \overline{Q}^{(k)}$
3. $\overline{R}_{QR}^{(k)} = \overline{R}^{(k)}$
4. $\underset{\underbrace{A \cdot A \cdot A \cdot \dots A}_{k}}{\overset{\shortparallel}{A^k}} = \overline{Q}^{(k)} \overline{R}^{(k)} = \overline{Q}_{QR}^{(k)} \overline{R}_{QR}^{(k)}$
5. $A^{(k)} = \left(\overline{Q}^{(k)}\right)^T A \, \overline{Q}^{(k)} = \left(\overline{Q}_{QR}^{(k)}\right)^T A \, \overline{Q}_{QR}^{(k)}$

Remark: QR method and Power's method (Simultaneous iteration) produces the SAME sequences of matrices

They are equivalent.

Proof: We use mathematical induction on k.

When $k = 1$. Consider $(*)$

$$A^{(1)} = \bar{Q}^{(1)T} A \bar{Q}^{(1)} = \bar{Q}^{(1)T} W \bar{Q}^{(1)}$$

QR factorization of $A = W$

$$= \bar{Q}^{(1)T} \bar{Q}^{(1)} R^{(1)} \bar{Q}^{(1)}$$

QR factorization of A

$$= R^{(1)} \bar{Q}^{(1)} = R^{(1)}_{QR} Q^{(1)}_{QR} = A^{(1)}_{QR}$$

Now, $\bar{Q}^{(1)}$ is obtained by QR factorization of $W = A$

$R^{(1)}$ " " " " " " "

$\therefore \quad \bar{Q}^{(1)} = Q^{(1)}_{QR} = \bar{Q}^{(1)}_{QR}$ (Here, we assume the diagonal entries of R are positive)

$\bar{R}^{(1)} = R^{(1)} = R^{(1)}_{QR} = \bar{R}^{(1)}_{QR}$

It is easy to see that (4) and (5) are true for $k = 1$.

$\therefore$ the statement is true for $k = 1$.

Suppose now that the statement is true for $k-1$.

For k, consider $(*)$

$$A^k = A A^{k-1} = \underbrace{A \bar{Q}^{(k-1)}} \bar{R}^{(k-1)}$$

$$= W \bar{R}^{(k-1)} = \bar{Q}^{(k)} R^{(k)} \bar{R}^{(k-1)} = \bar{Q}^{(k)} \bar{R}^{(k)}$$

QR factorization of A^k

Now, consider $(**)$:

$$A^k = A A^{k-1} = A \bar{Q}^{(k-1)}_{QR} \bar{R}^{(k-1)}_{QR} = A\left(Q^{(1)}_{QR} Q^{(2)}_{QR} \cdots Q^{(k-1)}_{QR} R^{(k-1)}_{QR} R^{(k-2)}_{QR} \cdots R^{(1)}_{QR}\right)$$

$$= Q^{(1)}_{QR} \underbrace{R^{(1)}_{QR} Q^{(1)}_{QR}} Q^{(2)}_{QR} \cdots Q^{(k-1)}_{QR} R^{(k-1)}_{QR} R^{(k-2)}_{QR} \cdots R^{(1)}_{QR}$$

$$A^{(1)}_{QR} = Q^{(2)}_{QR} R^{(2)}_{QR}$$

$$= Q^{(1)}_{QR} Q^{(2)}_{QR} \underbrace{R^{(2)}_{QR} Q^{(2)}_{QR}} \cdots Q^{(k-1)}_{QR} R^{(k-1)}_{QR} \cdots R^{(1)}_{QR}$$

$$A^{(2)}_{QR} = Q^{(3)}_{QR} R^{(3)}_{QR}$$

$$= \vdots$$

$$= Q^{(1)}_{QR} Q^{(2)}_{QR} \cdots Q^{(k)}_{QR} R^{(k)}_{QR} \cdots R^{(1)}_{QR} = \bar{Q}^{(k)}_{QR} \bar{R}^{(k)}_{QR}$$

$\therefore$ $\{ \bar{Q}_{QR}^{(k)}, \bar{R}_{QR}^{(k)} \}$ and $\{ \bar{Q}^{(k)}, \bar{R}^{(k)} \}$ are both QR factorization of A^k.

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

Now, $A_{QR}^{(k)} = R_{QR}^{(k)} Q_{QR}^{(k)} = \overbrace{Q_{QR}^{(k)T} Q_{QR}^{(k)}}^{I} R_{QR}^{(k)} Q_{QR}^{(k)}$

$$A_{QR}^{(k-1)} = \bar{Q}_{QR}^{(k-1)T} A \bar{Q}_{QR}^{(k-1)}$$

$$= \underbrace{Q_{QR}^{(k)T} \bar{Q}_{QR}^{(k-1)T}}_{\bar{Q}_{QR}^{(k)T}} A \underbrace{\bar{Q}_{QR}^{(k-1)} Q_{QR}^{(k)}}_{\bar{Q}_{QR}^{(k)}}$$

$$= \bar{Q}_{QR}^{(k)T} A \bar{Q}_{QR}^{(k)}$$

$$= \bar{Q}^{(k)T} A \bar{Q}^{(k)} = A^{(k)}$$

$\therefore$ (1), (2), (3), (4) and (5) are true for $n=k$.

By M.I, the statement is true for all k.