

CS450: Numerical Analysis

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Eigenvalue Problems: Setup

- Given an $n \times n$ matrix A
 - $x \neq 0$ is called an eigenvector of if there exists a λ such that
$$Ax = \lambda x$$
 - In that case, λ is called an eigenvalue
 - An **eigenvector** of a matrix determines a **direction** in which the matrix **expands** or **shrinks** any vector lying in that direction by a scalar multiple, given by the **eigenvalue**
 - For LU and QR, we can obtain exact answers (except rounding).
 - For eigenvalue problems: not possible—**we must perform approximations.**

Recap: Power Method

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

$$\text{err}_k \sim \left(\frac{|\lambda_2|}{|\lambda_1|}\right)^k$$

- Algorithm details

Algorithm 4.1 Power Iteration

x_0 = arbitrary nonzero vector

for $k = 1, 2, \dots$

$x_k = Ax_{k-1} \sim x_k = \frac{x_k}{\|x_k\|_2}$ { generate next vector }

end

- This algorithm finds the eigenvector corresponding to the maximum eigenvalue (a.k.a. the leading eigenvalue)
- More concretely, this algorithm converges to a multiple of x_1

Recap: Rayleigh Quotient Iteration

x_1

- In summary, compute the shift σ using Rayleigh quotient as $\sigma_k = \frac{\mathbf{x}_k^T \mathbf{A} \mathbf{x}_k}{\mathbf{x}_k^T \mathbf{x}_k}$
- Then, apply inverse iteration with that shift: $\mathbf{x}_{k+1} = (\mathbf{A} - \sigma_k \mathbf{I})^{-1} \mathbf{x}_k$
- More concretely

$$\lambda_1 > \lambda_2 > \dots > \lambda_n$$

$$\sigma_k \rightarrow \left(\frac{|\lambda_1 - \sigma_k|}{|\lambda_2 - \sigma_k|} \right)^k$$

Algorithm 4.4 Rayleigh Quotient Iteration

\mathbf{x}_0 = arbitrary nonzero vector

for $k = 1, 2, \dots$

$$\sigma_k = \mathbf{x}_{k-1}^T \mathbf{A} \mathbf{x}_{k-1} / \mathbf{x}_{k-1}^T \mathbf{x}_{k-1}$$

Solve $(\mathbf{A} - \sigma_k \mathbf{I}) \mathbf{y}_k = \mathbf{x}_{k-1}$ for \mathbf{y}_k

$$\mathbf{x}_k = \mathbf{y}_k / \|\mathbf{y}_k\|_\infty$$

end

$$\sigma_k \approx \lambda_1$$

{ compute shift }

{ generate next vector }

{ normalize }

Eigenvalue Decomposition

- If a $n \times n$ matrix A has distinct eigenvectors, it has an eigenvalue decomposition as

$$A = X \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \ddots & \lambda_n \end{bmatrix} X^{-1}$$

$$\underbrace{A = XDX^{-1}}_{\sim} \quad \lambda_1 x_1 x_1^T + \lambda_2 x_2 x_2^T + \cdots + \lambda_n x_n x_n^T$$

where X are the right eigenvectors, X^{-1} are left eigenvectors, and D are eigenvalues

$$AX = [Ax_1, \dots, Ax_n] = XD = [d_{11}x_1, \dots, d_{nn}x_n]$$

$$Ax_1 = \lambda_1 x_1, \quad Ax_2 = \lambda_2 x_2, \quad \dots \quad Ax_n = \lambda_n x_n$$

$$A[x_1, x_2, \dots, x_n] = [x_1, x_2, \dots, x_n] \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \ddots & \lambda_n \end{bmatrix}$$

$$A \quad X \quad X \quad D$$

Similar Matrices



- Definition (similar matrices): matrices A and B are said to be **similar**, if there exist a **nonsingular** matrix S such that $A = SBS^{-1}$
- Theorem: suppose matrices A and B are similar matrices with $A = SBS^{-1}$, and λ is an eigenvalue of A with associated eigenvector x . Then, λ is also an eigenvalue of B with associated eigenvector $S^{-1}x$ (λ, x)
- --> **Similar matrices have same eigenvalues**
- Is the reverse true? ~~✓~~

$$\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \text{ vs } \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

$$\begin{aligned}
 Ax &= \lambda x \\
 S^{-1}SBS^{-1}x &= \lambda x \quad \leftarrow S^{-1} \\
 \Rightarrow B(S^{-1}x) &= \lambda(S^{-1}x)
 \end{aligned}$$

Similar Matrices (Cont'd)

- Are the following matrices similar to each other?

$$A = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$$

$$B = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} A \quad \Rightarrow \quad B \not\sim SAS^{-1}$$

Similar Matrices (Cont'd)

$$A = X D X^{-1}$$

- Theorem: an $n \times n$ matrix A is similar to a **diagonal** matrix D if and only if A has n linearly independent eigenvectors

► Theorem (Schur): let A be an arbitrary $n \times n$ matrix. A nonsingular matrix U exists with the property that



$$T = U^{-1} A U$$

where T is an **upper triangular matrix** whose diagonal entries consist of the eigenvalues of A

Symmetric Matrices



- Theorem: an $n \times n$ matrix A is **symmetric** if and only if there exists a diagonal matrix D and an orthogonal matrix Q with $A = QDQ^T$
- Theorem: let A be a **symmetric** $n \times n$ matrix. There exists n eigenvectors of A that form an orthonormal set, and the eigenvalues of A are real.

Sensitivity

- Recall condition number
 - The condition number is a **property of the problem**, measuring its sensitivity to perturbations in input
 - How much a small change in the input leads to changes in the output
- Investigate the condition number/sensitivity of an eigenvalue problem
- Setting: Suppose \underline{A} is nonsingular. Suppose that $X^{-1}AX = \underline{D}$. For a certain perturbation in the input, i.e., $A \rightarrow \underline{A} + \tilde{E}$, how much would it affect the eigenvalues $\underline{\lambda}$?

$$\underline{\lambda}_1, \dots, \underline{\lambda}_n \xrightarrow{\tilde{E} \in \mathbb{R}^{n \times n}} \tilde{\lambda}_1, \tilde{\lambda}_2, \dots, \tilde{\lambda}_n$$
$$|\tilde{\lambda}_n - \underline{\lambda}_n|$$

Sensitivity (Cont'd)

- Suppose A is not defective. Suppose that $\boxed{X^{-1}AX = D}$. For a certain perturbation in the input, i.e., $A \rightarrow A + E$, how much would it affect the eigenvalues D ? ① ✓
- Recall: in linear system or linear least square, the sensitivity depends on A , would it be similar case here?
- Note that $\underbrace{X^{-1}(A+E)X}_{\text{---}} = \underbrace{D+F}_{\text{---}}$
 - $\underbrace{A+E}_{\text{---}}$ and $\underbrace{D+F}_{\text{---}}$ have the same eigenvalues ?
 - $D+F$ is not necessarily diagonal

$$\begin{aligned}
 \underline{Ax = y} &\rightarrow R(A) \\
 X^{-1}(A+E)X &= X^{-1}AE + X^{-1}EX \\
 &= D + \underbrace{X^{-1}EX}_{=F}
 \end{aligned}$$

Sensitivity (Cont'd)

$$(\mu I - D)^{-1} = \begin{bmatrix} \nu & \nu \\ \nu & \mu \end{bmatrix} - \begin{bmatrix} \lambda_1 & \lambda_2 \\ \lambda_2 & \lambda_1 \end{bmatrix}^{-1} = \frac{1}{(\mu - \lambda_1)} \begin{bmatrix} \mu - \lambda_1 & 0 \\ 0 & \mu - \lambda_2 \end{bmatrix} = \frac{1}{(\mu - \lambda_1)} (\mu I - D)^{-1}$$

- Suppose v is an eigen vector of the perturbed matrix $A + E$ with an eigenvalue μ , satisfying $(D + F)v = \mu v$, it gives $Fv = \mu D - DV = (\mu I - D)v$

$$Fv = (\mu I - D)v \Rightarrow (\mu I - D)^{-1}Fv = v \quad (\text{when is it invertible?})$$

$$\begin{aligned} & \left\| \begin{bmatrix} \frac{1}{\lambda_1 - \mu} & \frac{1}{\lambda_2 - \mu} \\ \vdots & \vdots \\ \frac{1}{\lambda_n - \mu} \end{bmatrix} \right\| \Rightarrow \|v\| \leq \|(\mu I - D)^{-1}\| \cdot \|F\| \cdot \|v\| \\ & \Rightarrow \|(\mu I - D)^{-1}\|^{-1} \leq \|F\| \end{aligned}$$

$$\begin{aligned} & X^{-1}EX \\ & \| \leq \|(\mu I - D)^{-1}\| \cdot \|F\| \end{aligned}$$

- Let λ_k be the entry in D that is closest to μ , then

$$|\lambda_k - \mu| = \|(\mu I - D)^{-1}\|^{-1} \leq \|F\| = \|X^{-1}EX\| \leq \|X^{-1}\| \|E\| \|X\| = \kappa(X) \|E\|$$

$$\max_m \frac{1}{|\lambda_i - \mu|}$$

Sensitivity (Cont'd)

$$\begin{matrix} A_{k+1} \\ \downarrow \\ \kappa(A) \end{matrix}$$

- Let λ_k be the entry in D that is closest to μ , then

$$|\lambda_k - \mu| \leq \underbrace{\kappa(X)}_{\text{condition number}} \underbrace{\|E\|}_{\text{perturbation}} \quad [x_1 \ x_2 \ \dots \ x_n]$$

- The conditioning depends on the eigenvectors

- The solutions are **sensitive** to input perturbations if the eigenvectors are nearly **linearly dependent**
- If X is **orthogonal** (e.g., for symmetric matrix A), then eigenvalues are always **well-conditioned**
- This bound is in terms of all eigenvalues, so may **overestimate** for each individual eigenvalue

Rethinking Power Method

- All power iteration methods compute **one eigenvalue** at a time.
- What if I want multiple (or, all the) eigenvalues?
- One approach is via deflation (how to do it?), but it is not widely used in practice (why?)
- Can I make this process “faster” by obtaining several (or all of the) eigenvalues/eigenvectors simultaneously?

$$A - \lambda_1 x_1 x_1^T - \lambda_2 x_2 x_2^T$$

QR Method

Goal: get eigenvectors
 x_1, x_2, \dots, x_n from A
 $\lambda_1, \lambda_2, \dots, \lambda_n$

- Given an $n \times n$ matrix \underline{A} , do the following

- Set $\underline{X}_0 = A$
- For $k = 1, 2, \dots$ perform QR factorization as follows

$$Q_k R_k = X_{k-1}$$

- Update X_k as

$$X_k = R_k Q_k$$

- Repeat until converge

Step 1: $Q_1 R_1 = X_0 = A$

$$X_1 = R_1 Q_1$$

Step 2: $Q_2 R_2 = X_1$

$$X_2 = R_2 Q_2$$

⋮

Recall: QR Factorization

- For a rectangular matrix $\mathbf{A} \in R^{m \times n}$ with $m \geq n$. The QR factorization to this matrix can be written as

$$\mathbf{H}_n \cdots \mathbf{H}_1 \mathbf{A} = \begin{bmatrix} \mathbf{R} \\ \mathbf{O} \end{bmatrix}$$

- The product of successive Householder transformations $\mathbf{H}_n \cdots \mathbf{H}_1$ is itself an orthogonal matrix. Thus, if we take $\mathbf{Q}^T = \mathbf{H}_n \cdots \mathbf{H}_1$, or equivalently, $\mathbf{Q} = \mathbf{H}_1 \cdots \mathbf{H}_n$, then

$$\mathbf{A} = \mathbf{Q} \begin{bmatrix} \mathbf{R} \\ \mathbf{O} \end{bmatrix}$$

Illustrative Example

$$A = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$$

```
% Define your matrix
A = [2, -1, 0; -1, 2, -1; 0, -1, 2];

% Set convergence tolerance and maximum iterations
tolerance = 1e-8;
max_iterations = 1000;

% Initialize variables
n = size(A, 1);
Q = eye(n);
iterations = 0;

while iterations < max_iterations
    [Q, R] = qr(A); →
    A = R * Q;
    iterations = iterations + 1;
    if norm(tril(A,-1), 'fro') < tolerance
        break;
    end

    fprintf('Intermediate evaluation of eigenvalues:\n')
    disp(diag(A));

    fprintf('\nIntermediate evaluation of eigenvectors:\n');
    disp(Q);

end
```

① Intermediate evaluation of eigenvalues:
 2.8000
 2.3429
 0.8571

Intermediate evaluation of eigenvectors:
 -0.8944 -0.3586 0.2673
 0.4472 -0.7171 0.5345
 0 0.5976 0.8018

② Intermediate evaluation of eigenvalues:
 3.1429
 2.2484
 0.6087

Intermediate evaluation of eigenvectors:
 -0.9661 -0.2467 -0.0761
 0.2582 -0.9231 -0.2849
 0 -0.2949 0.9555

③ Intermediate evaluation of eigenvalues:
 3.3084
 2.1039
 0.5876

Intermediate evaluation of eigenvectors:
 -0.9845 -0.1745 0.0155
 0.1752 -0.9807 0.0871
 0 0.0884 0.9961

④ Intermediate evaluation of eigenvalues:
 3.3761
 2.0380
 0.5859

Intermediate evaluation of eigenvectors:
 -0.9937 -0.1118 -0.0028
 0.1118 -0.9934 -0.0253
 0 -0.0255 0.9997

⑤ Intermediate evaluation of eigenvalues:
 3.4096
 2.0046
 0.5858

Intermediate evaluation of eigenvectors:
 -0.9992 -0.0401 -0.0001
 0.0401 -0.9992 -0.0022
 0 -0.0022 1.0000

Intermediate evaluation of eigenvalues:
 3.4126
 2.0016
 0.5858

Intermediate evaluation of eigenvectors:
 -0.9997 -0.0236 0.0000
 0.0236 -0.9997 0.0006
 0 0.0006 1.0000

Intermediate evaluation of eigenvalues:
 3.4137
 2.0005
 0.5858

Intermediate evaluation of eigenvectors:
 -0.9999 -0.0139 -0.0000
 0.0139 -0.9999 -0.0002
 0 -0.0002 1.0000

Intermediate evaluation of eigenvalues:
 3.4140
 2.0002
 0.5858

Intermediate evaluation of eigenvectors:
 -1.0000 -0.0081 0.0000
 0.0081 -1.0000 0.0001
 0 0.0001 1.0000

QR Method (Cont'd)

- Given an $n \times n$ matrix A , do the following
 - Set $X_0 = A$
 - For $k = 1, 2, \dots$ perform QR factorization as follows

$$Q_k R_k = \underline{X_{k-1}}$$

- Update X_k as
 - Repeat until converge
-
- What is going on?
 - What is the relationship between X_k and X_{k-1} ?

$$\begin{aligned} X_k &= \underbrace{R_k Q_k}_{\uparrow \text{ similar}} = Q_k^T Q_k R_k Q_k = Q_k^T (Q_k R_k) Q_k \\ &= \underbrace{Q_k^T X_{k-1} Q_k}_{\rightarrow} \\ &= Q_k^T Q_{k-1}^T X_{k-2} Q_{k-1} Q_k \\ &= \dots = \\ &\quad \dots Q_1^T Q_{k-1}^T \dots Q_2^T A Q_{k-1} Q_1 \\ &\quad \dots Q_k \end{aligned}$$

QR Method (Cont'd)

- What is the relationship between X_k and X_{k-1} ?

$$X_k = R_k Q_k = Q_k^T Q_k R_k Q_k = Q_k^T X_{k-1} Q_k$$

- X_k and X_{k-1} are **similar** to each other

- What is the relationship between X_k and A ?

$$X_k = Q_k^T X_{k-1} Q_k = Q_k^T Q_{k-1}^T X_{k-2} Q_{k-1} Q_k = Q_k^T Q_{k-1}^T \dots Q_1^T A Q_1 \dots Q_{k-1} Q_k$$

- X_k and A are **similar** to each other ($X_k = \tilde{Q}_k^T A \tilde{Q}_k$, where $\tilde{Q}_k = Q_1 \dots Q_{k-1} Q_k$)

QR Method (Cont'd)

- Theorem: Suppose the eigenvalues of matrix \underline{A} satisfies $|\lambda_1| > |\lambda_2| > \dots > |\lambda_n| > 0$. Let \underline{Y} be a matrix such that the i -th row \underline{y}_i^T of \underline{Y} satisfies $\underline{y}_i^T \underline{A} = \underline{\lambda_i} \underline{y}_i^T$. If \underline{Y} has an LU factorization, then the entries under the diagonal of the matrix $\underline{X}_k = [\underline{x}_{ij}^{(k)}]$ produced by the QR method tend to zero as $k \rightarrow \infty$. At the same time,

$$\underline{x}_{ii}^{(k)} \rightarrow \underline{\lambda_i}$$

for $i = 1, 2, \dots, n$.

QR Iteration: Incorporating a Shift

- How can we accelerate the convergence of QR iteration by using shifts?
- Recall: any variant of power iteration has the convergence rate depending on the ratio of magnitudes of successive eigenvalues
- Similar to Rayleigh quotient iteration, introduce a shift operation to QR

Algorithm 4.8 QR Iteration with Shifts

$$\mathbf{A}_0 = \mathbf{A}$$

for $k = 1, 2, \dots$

 Choose shift σ_k

 Compute QR factorization

{ normalize }

$$\mathbf{Q}_k \mathbf{R}_k = \mathbf{A}_{k-1} - \sigma_k \mathbf{I}$$

$$\mathbf{A}_k = \mathbf{R}_k \mathbf{Q}_k + \sigma_k \mathbf{I}$$

{ generate next matrix }

end

QR Iteration: Incorporating a Shift (Cont'd)

Algorithm 4.8 QR Iteration with Shifts

```
 $A_0 = A$ 
for  $k = 1, 2, \dots$ 
    Choose shift  $\sigma_k$ 
    Compute QR factorization { normalize }
     $Q_k R_k = A_{k-1} - \sigma_k I$ 
     $A_k = R_k Q_k + \sigma_k I$  { generate next matrix }
end
```

- Why it works? – notice that $A_k \sim A_{k-1}$
 - Calculate $R_k Q_k = Q_k^T (A_{k-1} - \sigma_k I) Q_k$
 - Compute $A_k = R_k Q_k + \sigma_k I = Q_k^T A_{k-1} Q_k - Q_k^T \sigma_k I Q_k + \sigma_k I = Q_k^T A_{k-1} Q_k$
- Such a shifting operation does not change anything

QR Iteration: Incorporating a Shift (Cont'd)

Algorithm 4.8 QR Iteration with Shifts

```
 $A_0 = A$ 
for  $k = 1, 2, \dots$ 
    Choose shift  $\sigma_k$ 
    Compute QR factorization { normalize }
     $Q_k R_k = A_{k-1} - \sigma_k I$ 
     $A_k = R_k Q_k + \sigma_k I$  { generate next matrix }
end
```

- Why it works?
- QR iteration on A is also performing inverse iteration on A_k at each step
- Therefore, $A_k - \sigma_k I$ can accelerate using similar argument before
- Which σ_k to choose? The left most.

Example (2)

- Apply QR iteration to the following matrix

$$A = \begin{bmatrix} 2.9766 & 0.3945 & 0.4198 & 1.1159 \\ 0.3945 & 2.7328 & -0.3097 & 0.1129 \\ 0.4198 & -0.3097 & 2.5675 & 0.6079 \\ 1.1159 & 0.1129 & 0.6079 & 1.7231 \end{bmatrix}$$

- This matrix has eigenvalues $\lambda_1 = 4, \lambda_2 = 3, \lambda_3 = 2, \lambda_4 = 1$, use $\sigma_1 = 1.7231$ as the shift for the first iteration

$$A_1 = \begin{bmatrix} 3.8816 & -0.0178 & 0.2355 & 0.5065 \\ -0.0178 & 2.9528 & -0.2134 & -0.1602 \\ 0.2355 & -0.2134 & 2.0404 & -0.0951 \\ 0.5065 & -0.1602 & -0.0951 & 1.1253 \end{bmatrix}$$

Example (2)

- Next shift factor is $\sigma_2 = 1.1253$, giving the following

$$\mathbf{A}_2 = \begin{bmatrix} 3.9946 & -0.0606 & 0.0499 & 0.0233 \\ -0.0606 & 2.9964 & -0.0882 & -0.0103 \\ 0.0499 & -0.0882 & 2.0081 & -0.0252 \\ 0.0233 & -0.0103 & -0.0252 & 1.0009 \end{bmatrix}$$

- Finally, use $\sigma_3 = 1.0009$ and we have

$$\mathbf{A}_3 = \begin{bmatrix} 3.9980 & -0.0426 & 0.0165 & 0.0000 \\ -0.0426 & 3.0000 & -0.0433 & 0.0000 \\ 0.0165 & -0.0433 & 2.0020 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 1.0000 \end{bmatrix}$$

Learning Objectives

- Variants of power methods
- Simultaneous iterations
- QR iteration
- QR iteration with a shift