MATH3322 - Matrix Computation

Taught by Jianfeng Cai

Notes by Aaron Wang

Contents

1 March 22nd, 2019

1.1 Eigenvalue Decomposition

Definition 1.1. Let $A \in \mathbb{R}^{n\times n}$ be a square matrix. A non-zero vector x is an **eigenvector** of A with $\lambda \in \mathbb{C}$ being the corresponding **eigenvalue** if:

$$Ax = \lambda x.$$

- Even if A is a real matrix, its eigenvalue and eigenvectors can be complex
- The set of eigenvalues of A is called the spectrum of A. The spectral radius $\rho(A)$ is the maximum value $|\lambda|$ over all eigenvalues of A.
- If (λ, x) is an eigenpair of A, then:

$$\begin{aligned} \left(\lambda^2, x\right) &\text{ is a eigenpair of } A^2 \\ (\lambda - \sigma, x) &\text{ is a eigenpair of } A - \sigma I \\ \left(\frac{1}{\lambda - \sigma}, x\right) &\text{ is a eigenpair of } (A - \sigma I)^{-1}. \end{aligned}$$

Proof. Since (λ, x) is an eigenpair of A, $Ax = \lambda x$ Multiplying both sides by A from the left:

$$\begin{aligned} A \cdot Ax = \lambda Ax &\implies A^2 x = \lambda Ax = \lambda \cdot \lambda x = \lambda^2 x. \\ Ax - \sigma x = \lambda x - \sigma x &\implies (A - \sigma I)\, x = (\lambda - \sigma)\, x \\ \implies x = (\lambda - \sigma)(A - \sigma I)^{-1} x &\implies (A - \sigma I)^{-1} x. \end{aligned}$$

□

Definition 1.2. Two matrices A and B are **similar** with each other if there exists a nonsingular matrix T such that

$$B = TAT^{-1}.$$

Theorem 1.3

If A and B are similar, then A and B have the same eigenvalues.

Proof. Since A, B are similar, $B = TAT^{-1}$, which implies $A = T^{-1}BT$. If (λ, x) is an eigenpair of A, then $Ax = \lambda x$, so that

$$T^{-1}BTx = \lambda x \implies B(Tx) = \lambda (Tx).$$

Thus, (λ, Tx) is an eigenpair of B. i.e. any eigenvalue of A is an eigenvalue of B. The reverse is similar. □

Definition 1.4. An **eigenvalue decomposition** of a square matrix $A \in \mathbb{R}^{n\times n}$ is a factorization

$$A = X\Lambda X^{-1},$$

where $X \in \mathbb{C}^{n\times n}$ is non-singular and $\Lambda \in \mathbb{C}^{n\times n}$ is diagonal.

- If $A \in \mathbb{R}^{n\times n}$ admits an eigenvalue decomposition, then

$$AX = X\Lambda.$$

If we rewrite $X = [x_1 x_2 \dots x_n]$ with $x_i \in \mathbb{C}^n$ the i-th column of x, and $\Lambda = \operatorname{diag}(\lambda_1, \lambda_2 \dots, \lambda_n) = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}$ with $\lambda_i \in \mathbb{C}$ being the i-th diagonal of Λ, then

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

$$\implies [Ax_1 Ax_2 \dots Ax_n] = [\lambda_1 x_1 \lambda_2 x_2 \dots \lambda_n x_n].$$

$$\implies Ax_i = \lambda_i x_i, \quad i = 1, 2 \dots, n.$$

In other words (λ_i, x_i), $i = 1, 2, \dots, n$ are eigenpairs of A.

- Since X is nonsingular, x_i are linearly independent. So, x_i are n independent eigenvectors, which span $\mathbb{C}^n$.

- Eigenvalue decomposition implies $X^{-1}AX = \Lambda$, so that we also say A is diagonalizable.

- Eigenvalue decomposition does not always exist, as a square matrix $A \in \mathbb{R}^{n\times n}$ does not always have n independent eigenvectors.

- Though $A \in \mathbb{R}^{n\times n}$ is real, the eigenvalue decomposition may be complex.

1.2 Characteristic Polynomial

Definition 1.5. The **characteristic polynomial** of $A \in \mathbb{R}^{n\times n}$ denoted P_A is a degree n polynomial defined by

$$P_A(z) = \det(zI - A), \quad \text{where } z \in \mathbb{C}.$$

Let (λ_1, x) be an eigenpair of A. Then $Ax = \lambda x$, which is equivalent to:

$$(\lambda I - A)\, x = 0.$$

Since x is non-zero, $\lambda I - A$ has a non-zero solution. Therefore, $\lambda I - A$ is singular. That is $\det(\lambda I - A) = P_A(\lambda) = 0$. Thus, λ is an eigenvalue of A iff $P_A(\lambda) = 0$, and the corresponding eigenvector x are non-zero solutions of $(\lambda I - A)\, x = 0$.

Example 1.6

$A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$. The characteristic polynomial is:

$$P_A(z) = \det\left(zI - \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}\right) = \det\left(\begin{bmatrix} z & -1 \\ 0 & z \end{bmatrix}\right) = z^2.$$

Therefore, $P_A(\lambda) = \lambda^2 = 0 \implies \lambda_1 = \lambda_2 = 0$ are the eigenvalues of A.

For eigenvectors, solve $(0I - A) = 0$, i.e.

$$\begin{bmatrix} 0 & -1 \\ 0 & 0 \end{bmatrix} x = 0 \implies x = \begin{bmatrix} q \\ 0 \end{bmatrix}.$$

As there is only one independent eigenvector, A is not diagonalizable (i.e. no eigenvalue decomposition.

Example 1.7

$A = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$. The characteristic polynomial is:

$$P_A(z) = \det\left(\begin{bmatrix} z & 1 \\ -1 & z \end{bmatrix}\right) = z^2 + 1.$$

Therefore, $P_A(\lambda) = \lambda^2 + 1 = 0 \implies \lambda_1 = i, \quad \lambda_2 = -i$ are the eigenvalues.
For eigenvector of $\lambda_1 = i$, solve $(iI - A)\, x = 0$, i.e.

$$\begin{bmatrix} i & 1 \\ -1 & i \end{bmatrix} x = 0 \implies x = \alpha \begin{bmatrix} i \\ 1 \end{bmatrix} \quad \alpha \in \mathbb{C}.$$

Therefore, a corresponding eigenvector is $x_i = \begin{bmatrix} i \\ 1 \end{bmatrix}$.
For eigenvector of $\lambda_2 = -i$:

$$\begin{bmatrix} -i & 1 \\ -1 & -i \end{bmatrix} x = 0 \implies x = \beta \begin{bmatrix} i \\ -1 \end{bmatrix} \quad \beta \in \mathbb{C}.$$

The corresponding eigenvector is $x_2 = \begin{bmatrix} i \\ -1 \end{bmatrix}$.

Define $X = \begin{bmatrix} x_1 & x_2 \end{bmatrix} = \begin{bmatrix} i & i \\ 1 & -1 \end{bmatrix}, \Lambda = \begin{bmatrix} \lambda_1 & \\ & \lambda_2 \end{bmatrix} = \begin{bmatrix} i & \\ & -i \end{bmatrix}, X^{-1} = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2}i & -\frac{1}{2} \end{bmatrix}$,
Therefore $A = X\Lambda X^{-1}$

$$\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} i & i \\ 1 & -1 \end{bmatrix} \begin{bmatrix} i & \\ & -i \end{bmatrix} \begin{bmatrix} -\frac{1}{2}i & \frac{1}{2} \\ -\frac{1}{2}i & -\frac{1}{2} \end{bmatrix}.$$

This shows that a real matrix may have a complex eigenvalue decomposition.

Remark 1.8 — However, we don't usually solve the characteristic equation, as polynomial root-finding is not numerically stable in general.

1.3 Special Case: Symmetric Matrix and SPD Matrix

Assume $A \in \mathbb{R}^{n\times n}$ is symmetric. Then

1. The eigenvalues of A are real.

   Proof. Let (λ, x) be an eigenpair of A. Then, $Ax = \lambda x$.
   Multiply both sides by $x^* \equiv \overline{x^T}$ (conjugate transpose) from the left:

   $$x^*Ax = \lambda x^*x \implies \lambda = \frac{x^*Ax}{x^*x}.$$

   - x^*Ax is real because $\overline{x^*Ax} = \overline{(x^*Ax)}^T = \overline{x^TA^T\overline{x}} = x^*Ax$
   - x^*x is also real, because $\overline{x^*x} = \overline{(x^*x)}^T = \overline{x^T\overline{x}} = x^*x$.
   - As such, $\lambda = \frac{x^*Ax}{x^*x}$ is real.

   □

2. Eigenvectors corresponding to distinct eigenvalues are orthogonal.

3. A is always diagonalizable, and the eigenvalue decomposition has a special form

   $$A = Q\Lambda Q^T$$

   where $Q \in \mathbb{R}^{n\times n}$ is orthonormal and $\Lambda \in \mathbb{R}^{n\times n}$ is diagonal.

4. If A is SPD, then all eigenvalues are positive.

5. If A is SPSD, then all eigenvalues are non-negative.

   Proof. Let (λ, x) a be an eigenpair of A. then $Ax = \lambda x$, and λ, x are real. So

   $$x^TAx = \lambda x^Tx \implies \lambda = \frac{x^TAx}{x^Tx} > 0.$$

   if A is SPD. If A is SPSD, then $\lambda = \frac{x^TAx}{x^Tx} \geq 0$, since $x^TAx \geq 0$. □

2 March 27th, 2019

2.1 Computation of Eigenvalue Decomposition

For simplicity, we assume that $A \in \mathbb{R}^{n\times n}$ is symmetric, so that all eigenvalues/eigenvectors are real. Let λ_i $i = 1, 2 \ldots, n$ be the eigenvalues of A, which are sorted in magnitude, i.e.

$$|\lambda_1| \geq |\lambda_2| \geq \ldots \geq |\lambda_n|.$$

The corresponding eigenvectors are denoted by q_i. We have

$$Q = \begin{bmatrix} q_1 & q_2 & \ldots & q_n \end{bmatrix} \in \mathbb{R}^{n\times n}$$

satisfying $Q^TQ = Q^T = I$.

Definition 2.1. Let $A \in \mathbb{R}^{n\times n}$ be symmetric. For a given vector $x \in \mathbb{R}^n$, the **Rayleigh Quotient** is defined by

$$r(x) = \frac{x^T A x}{x^T x}.$$

If x is an eigenvector,

$$r(x) = \frac{x^T A x}{x^T x} = \frac{\lambda x^T x}{x^T x} = \lambda,$$

i.e. $r(x)$ is an eigenvalue.

The eigenvalues are critical points of $r(x)$, with $\nabla r(x) = 0$. It can be proven that

$$\min_i \lambda_i = \min_{x\neq 0} r(x).$$

Remark 2.2 — This can be extended to non-symmetric matrices/ matrices or eigenvalues that are complex.

2.2 Power Iteration

Purpose: Find λ_1 and its associated eigenvector x_1, with $\|x_1\|_2 = 1$.

Algorithm 2.3 1. Choose $y^{(0)} \in R^n$ s.t. $\|y^{(0)}\|_2 = 1$.

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

$$z^{(k)} = Ay^{(k-1)}$$

$$y^{(k)} = \frac{z^{(k)}}{\|z^{(k)}\|_2}$$

$$\mu^{(k)} = \frac{\left(y^{(k)}\right)^T Ay^{(k)}}{\left(y^{(k)}\right)^T y^{(k)}} = \left(y^{(k)}\right)^T Ay^{(k)}.$$

Remark 2.4 — $y^{(k)}$ is an approximation to $\pm x_1$, $\mu^{(k)}$ is an approximation to λ_1.

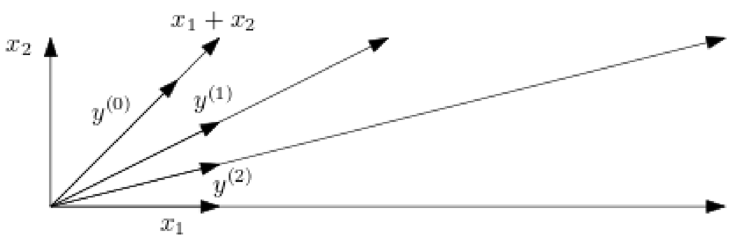

Figure 1

- Assume $(2, x_1)$, $(1, x_2)$ are two eigenpairs of $A \in \mathbb{R}^{2\times 2}$ (so that $x_1 \perp x_2$).
- Assume $y^{(0)} = \frac{1}{\sqrt{2}}(x_1 + x_2)$

- $k = 1$:

$$z^{(1)} = Ay^{(0)} = A\left(\frac{1}{\sqrt{2}}(x_1 + x_2)\right) = \frac{1}{\sqrt{2}}(Ax_1 + Ax_2) = \frac{1}{\sqrt{2}}(2x_1 + x_2).$$

$$y^{(1)} = \frac{1}{\sqrt{5}}(2x_1 + x_2).$$

Note that $y^{(k)}$ approaches x_1 more than x_2.

$\vdots$

- $k + 1$:

$$z^{(k+1)} = Ay^{(k)} = A\left(\frac{1}{\sqrt{2^{2k}+1}}\left(2^k x_1 + x_2\right)\right) = \frac{1}{\sqrt{2^{2k}+1}}\left(2^{k+1}x_1 + x_2\right).$$

If the component of x_1 is non-zero, then it will converge to x_1, i.e. as long as $y^{(0)}$ is not a multiple of x_2, it will converge to x_1.

Claim 2.5. Power iteration may not be convergent:

Example 2.6

Assume $(1, x_1)$, $(-1, x_2)$ are two eigenpairs of $A \in \mathbb{R}^{2\times 2}$. Assume $y^{(0)} = \frac{1}{\sqrt{2}}(x_1 + x_2)$.

$$k = 1 : z^{(1)} = Ay^{(0)} = \frac{1}{\sqrt{2}}\left(x_1 - x_2\right).$$

$$y^{(1)} = \frac{1}{\sqrt{2}}(x_1 - x_2).$$

$$k = 2 : z^{(2)} = \frac{1}{\sqrt{2}}\left(x_1 + x_2\right)$$

$$y^{(2)} = \frac{1}{\sqrt{2}}\left(x_1 + x_2\right).$$

which just repeats itself.

Remark 2.7 — Try with $(-2, x_1)$, $(1, x_2)$. Does not converge, but we can get the direction of x_1 since both x_1 and $-x_1$ are eigenvectors.

Remark 2.8 — Power iteration may not converge to (λ_1, x_1), e.g. $y^{(0)} = x_2$. This is because there is no x_1 component.

2.3 Analysis of Power Iteration

We will show $|\langle y^{(k)}, x\rangle| \to 1$. It is the same as $1 - \langle y^{(k)}, x_1\rangle^2 \to 0,\ k \to \infty$

Theorem 2.9

Assume $A \in \mathbb{R}^{n\times n}$ is symmetric and $|\lambda_1| > |\lambda_2|$ (otherwise they might be amplified at the same rate).

If $\langle y^{(0)}, x_1\rangle \neq 0$, then $\exists C_0 > 0$ depending on $y^{(0)}$ only such that

$$\left(1 - \langle y^{(k)}, x_1\rangle^2\right)^{\frac{1}{2}} \leq C_0 \left|\frac{\lambda_2}{\lambda_1}\right|^k \to 0, \text{ as } k \to \infty.$$

Consequently,

- $\min\{\|y^{(k)} - x_1\|_2, \|y^{(k)} + x_1\|_2\} \leq \sqrt{2}C_o \left|\frac{\lambda_2}{\lambda_1}\right|^k$, i.e. $y^{(k)} \to \pm x_1$
- $|\mu^{(k)} - \lambda_1| \leq 2\sqrt{2}C_o \left|\frac{\lambda_2}{\lambda_1}\right|^k \to 0$

Proof. Note that

$$y^{(k)} = \frac{A^k y^{(0)}}{\|A^k y^{(0)}\|_2}.$$

Let $A = X\Lambda X^T$ be the eigenvalue decomposition of A. Then

$$A^k = X\Lambda X^T X\Lambda X^T \ldots X\lambda X^T = X\Lambda^k X^T.$$

So

$$A^k y^{(0)} = X\Lambda^k X^T y^{(0)} = X\Lambda^k v$$

$$A^k y^{(0)} = \begin{bmatrix} x_1 & x_2 & \ldots & x_n \end{bmatrix} \begin{bmatrix} \lambda_1^k v_1 \\ \vdots \\ \lambda_n^k v_n \end{bmatrix} = \sum_{i=1}^n \lambda_i^k v_i x_i, \ v_i \in \mathbb{R}, \ x_i \in \mathbb{R}^n.$$

Because x_i are othronormal,

$$\|A^k y^{(0)}\|_2^2 = \sum_{i=1}^n \lambda_i^{2k} v_1^2 = \sum_{i=1}^n |\lambda_i|^{2k} |v_i|^2 = |\lambda_1|^{2k}|v_1|^2\,(1 + \ldots) \geq \left(|\lambda_1|^k |v_1|\right)^2$$

and

$$\langle y^{(k)}, x_1\rangle^2 = \frac{1}{\|A^k y^{(0)}\|_2^2}\langle A^k y^{(0)}, x_1\rangle^2 = \frac{1}{\|A^k y^{(0)}\|_2^2}\langle \sum_{i=1}^n \lambda_i^k v_i x_i, x_1\rangle^2 = \frac{1}{\|A^k y^{(0)}\|_2^2}\left(\lambda_1^k v_1\right)^2.$$

$$\leq \left|\frac{\lambda_2}{\lambda_1}^{2k}\right| \left(\left|\frac{v_2}{v_1}\right|^2 + \left|\frac{v_3}{v_1}\right|^2 + \left|\frac{v_4}{v_1}\right|^2 + \ldots + \left|\frac{v_n}{v_1}\right|^2\right) = C_0^2 \left|\frac{\lambda_2}{\lambda_1}^k\right|.$$

Thus

$$\sqrt{1 - \langle y^{(k)}, x_1\rangle^2} \leq C_0 \left|\frac{\lambda_2}{\lambda_1}^k\right|.$$

Because $C_0 < +\infty$, as $v_1 = \angle x_1, y^{(0)} \neq 0$ by assumption,

$$\sqrt{1 - \langle y^{(k)}, x_1\rangle^2} \leq C_0 \left|\frac{\lambda_2}{\lambda_1}^k\right| \to 0, \text{ as } k \to \infty.$$

$$\langle y^{(k)}, x_1\rangle^2 \geq 1 - C_0^2 \left|\frac{\lambda_2}{\lambda_1}\right|^{2k} \implies \langle y^{(k)}, x_1\rangle^2 \leq \|y^{(k)}\|_2^2 \|x_1\|_2^2 = 1.$$

So

$$1 - C_0^2 \left|\frac{\lambda_2}{\lambda_1}\right|^{2k} \leq 1.$$

If $\langle y^{(k)}, x_1\rangle \geq 0$, then

$$\|y^{(k)} - x_1\|_2 = \sqrt{\|y^{(k)}\|_2^2 + \|x_1\|_2^2 - 2\langle y^{(k)}, x_1\rangle} = \sqrt{2 - 2\langle y^{(k)}, x_1\rangle} \leq \left(2 - 2\sqrt{1 - C_0^2 \left|\frac{\lambda_2}{\lambda_1}\right|^{2k}}\right)^{\frac{1}{2}}.$$

I give up will do this later □

Remark 2.10 —

1. $\langle y^{(k)}, x_1\rangle = \cos\theta$. Genearlly,

$$\cos\angle(x, y) = \frac{\langle x, y\rangle}{\|x\|_2 \|y\|_2}.$$

2. The convergenec rate depends on $\left|\frac{\lambda_2}{\lambda_1}\right| < 1$, the smaller $\left|\frac{\lambda_2}{\lambda_1}\right|$, the faster the convergence. When $|\lambda_1| = |\lambda_2|$, the power iteration may not converge.

3. When $\langle y^{(0)}, x_1\rangle = 0$, then $C_0 = +\infty$, so y will not converge to λ_1.

4. In power iteration, only one matrix-product and several vector operations are used, the ocst per step is $O(n^2)$. If we want an approximate eigenvalue/eigenvector of error ϵ, we need to choose k, s.t.

$$C\left|\frac{\lambda_2}{\lambda_1}\right|^{\frac{k}{2}} \leq \epsilon \implies \left|\frac{\lambda_1}{\lambda_2}\right|^{\frac{k}{2}} \geq \frac{c}{\epsilon}.$$

$$\frac{k}{2}\log\left|\frac{\lambda_1}{\lambda_2}\right| \geq \log\left(\frac{c}{\epsilon}\right) \implies k \geq \frac{\log\left(\frac{c}{\epsilon}\right)}{\log\left(\left|\frac{\lambda_1}{\lambda_2}\right|\right)} \sim O\left(\log\left(\frac{1}{\epsilon}\right)\right).$$

Then the total computational cost is

$$O\left(\log\left(\frac{1}{\epsilon}\right) \cdot n^2\right).$$

5. Only the matrix-cector product involving A is needed. This means that A is not needed explicitly, only the subroutine to compute Ax is sufficient.

3 March 29th, 2019

3.1 Inverse Power Iteration

If λ_i, $i \in 1, \ldots, n$ with $|\lambda_1| \geq |\lambda_2| \geq \ldots \geq |\lambda_n|$ are eigenvalues of A, then $\frac{1}{\lambda_i}$ are eigenvalues of A^{-1} and

$$\frac{1}{|\lambda_1|} \leq \frac{1}{|\lambda_2|} \leq \ldots \leq \frac{1}{|\lambda_n|}.$$

Therefore, we can apply power iteration to A^{-1} to get λ_n and hence x_n. This is called the inverse power iteration.

Algorithm 3.1 1. Choose $y^{(0)} \in \mathbb{R}^n$ s.t. $\|y^{(0)}\|_2 = 1$

2. for $k = 1, 2, \ldots$

$$z^{(k)} = A^{-1} y^{(k-1)}$$
$$y^{(k)} = \frac{z^{(k)}}{\|z^{(k)}\|_2}$$
$$\mu^{(k)} = \left(y^{(k)}\right)^T A y^{(k)}.$$

Remark 3.2 — 1. From the convergence of power iteration, if:

- $\langle y^{(0)}, x_n \rangle \neq 0$
- $\frac{1}{|\lambda_n|} > \frac{1}{|\lambda_{n-1}|}$ (i.e. $|\lambda_n| < |\lambda_{n-1}|$)
- A^{-1} is symmetric (always true because A is symmetric.

then the limit of the iteration is:

$$y^{(k)} \to \pm x_n, \quad \mu^{(k)} \to \lambda_n,$$

with a rate $\left(\frac{|\lambda_n|}{|\lambda_{n-1}|}\right)^{\frac{k}{2}}$

2. We need to solve $Az^{(k)} = y^{(k-1)}$ in each iteration, which can be done by Gaussian Elimination. But we only need to compute $A = LU$ before the iteration and then, in each iteration, we obtain:

$$z^{(k)} = U^{-1} L^{-1} y^{(k-1)},$$

which is just a forward and backward substitution.

- Thus the total computational cost is:

$$O(n^3) + O\left(n^2 \cdot \log\left(\frac{1}{\epsilon}\right)\right)$$

for an ϵ-solution, ($O(n^3)$ for the LU decomposition)

3. If $|\lambda_n|$ is very close to 0, then, A is very close to singular, meaning that the solution of $Az^{(k)} = y^{(k-1)}$ may have a large error. However, we can still get a very accurate solution.

4 April 3rd, 2019

4.1 Shifted Inverse Power Iteration Part 2

Let λ_i, $i = 1, 2, \ldots, n$ with $|\lambda_1| \leq |\lambda_2| \leq \ldots \leq |\lambda_n|$ be eigenvalues of A. Note that $(\lambda_i - \mu)^{-1}$ are eigenvalues of $(A - \mu I)^{-1}$.

Thus we can apply the power iteration to $(A - \mu I)^{-1}$:

Algorithm 4.1

Choose $y^{(0)} \in \mathbb{R}^n$ s.t. $\|y^{(0)}\|_2 = 1$

For $k = 1, 2, \ldots$

- $z^{(k)} = (A - \mu I)^{-1} y^{(k-1)}$ (Done by solving $(A - \mu I) z^{(k)} = y^{(k-1)}$.
- $y^{(k)} = \frac{z^{(k)}}{\|z^{(k)}\|_2}$.
- $\mu^{(k)} = (y^{(k)})^T A y^{(k)}$ (the Rayleigh Quotient of A)

1. This iteration is the "shifted inverse power iteration"
2. To make the iteration converge to (λ_j, x_j), the following has to be satisfied:
   (a) μ is chosen s.t. $\frac{1}{|\lambda_j - \mu|}$ is the largest among $\frac{1}{|\lambda_i - \mu|}$

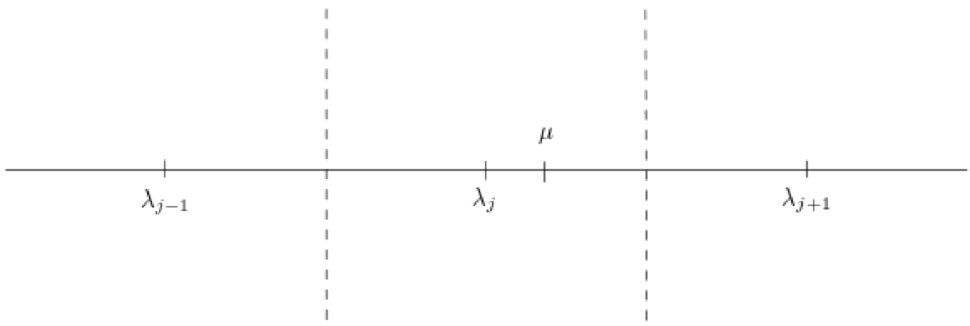

Figure 2: Choosing μ to guarantee convergence

   (b) $\langle y^{(0)}, x_j \rangle \neq 0$. (or else it will converge to another eigenvector.
   (c) The convergence rate depends on:

$$\frac{\frac{1}{|\lambda_j' - \mu|}}{\frac{1}{|\lambda_j - \mu|}} = \frac{|\lambda_j - \mu|}{|\lambda_j' - \mu}$$

, where $\frac{1}{|\lambda_j' - \mu|}$ is the second largest among $\frac{1}{|\lambda_i - \mu|}$ and

$$|\lambda_j - \mu| < |\lambda_j' - \mu|.$$

(d) For an ϵ- precision solution, the computational complexity is

$$O(n^3) + O\left(\log\frac{1}{\epsilon}\cdot n^2\right),$$

since we only compute the LU decomposition of $(A - \mu I)$ once.

To accelerate the shifted power iteration, we can also use an adaptive shift (if we shift μ to be closer to the target eigenpair, it will converge faster).

Algorithm 4.2 (Rayleigh Quotient Iteration)
Choose $y^{(0)} \in \mathbb{R}^n$ s.t. $\|y^{(0)}\|_2 = 1$
$\mu^{(0)} = (y^{(0)})^T A y^{(0)}$
For $k = 1, 2, \ldots$

- $z^{(k)} = (A - \mu^{(k-1)} I)^{-1} y^{(k-1)}$ (Done by solving $(A - \mu I) z^{(k)} = y^{(k-1)}$.
- $y^{(k)} = \frac{z^{(k)}}{\|z^{(k)}\|_2}$.
- $\mu^{(k)} = (y^{(k)})^T A y^{(k)}$ (the Rayleigh Quotient of A)

i.e. we choose μ to be close to the desired eigenvalue.

- This converges to some eigenpair (λ_i, x_i) such that λ_i is close to $\mu^{(0)}$.
- This Rayleigh Quotient iteration converges very fast (cubic).
- However since $(A - \mu^{(k-1)} I)$ is changing, we have to calcualte the LU decomposition each time.
- However, this will only converge to one eivenpair.

4.2 Simultaneous Iteration

To compute r eigenpairs:

Algorithm 4.3
Choose $Y^{(0)} \in R^{n\times r}$ s.t. $(Y^{(0)})^T (Y^{(0)}) = I$
For $k = 1, 2, \ldots$

- $Z^{(k)} = AY^{(k-1}$
- Set $Y^{(k)}$ to be the Q matrix in the QR decomposition of $Z^{(k)}$.
- $\mu_i^{(k)} = (y_i^{(k)})^T A y_i^{(k)}$, where $y_i^{(k)}$ is the i-th column of $Y^{(k)}$

Under some assumption, we have:

$$\|y_i^{(k)} - \pm x\| \le C\rho^k, i = 1, \ldots, r,$$

where $\rho = \max\limits_{i=1,\ldots,r} \frac{|\lambda_i+1}{\lambda_i} < 1$ and $|\mu_i^{(k)} - \lambda_i| \le C\rho^k$

4.3 QR algorithm for Eigenvalue Decomposition

We set $r = n$ in the simultaneous power iteration

$$Z^{(k)} = AY^{(k-1)}$$
$$Y^{(k)}R^{(k)} = Z^{(k)},$$

i.e. let $Z^{(k)} = Y^{(k)}R^{(k)}$ be the QR decomposition of $Z^{(k)}$. Eliminating $Z^{(k)}$, we have

$$Y^{(k)}R^{(k)} = AY^{(k-1)} \iff (Y^{(k)})^T AY^{(k-1)} = R,$$

because $(Y^{(k)})^T Y^{(k)} = Y^{(k)}(Y^{(k)})^T = I$.

Let $A^{(k)} = (Y^{(k)})^T AY^{(k)}$, then

$$A^{(k-1)} = (Y^{(k-1)})^T AY^{(k-1)} = (Y^{(k-1)})^T Y^{(k)}R^{(k)}.$$

Since $(Y^{(k-1)})^T Y^{(k)}$ is orthogonal and $R^{(k)}$ is upper triangular, $A^{(k)}$ is just an orthogonal square matrix. Note that

$$A^{(k)} = (Y^{(k)})^T AY^{(k)} = (Y^{(k)})^T AY^{(k-1)}(Y^{(k-1)})^T Y^{(k)} = R^{(k)}(Y^{(k-1)})^T Y^{(k)}.$$

This means that after getting the QR decomposition of $A^{(k-1)}$, we swap the two matrices to get $A^{(k)}$.

Algorithm 4.4 (QR Algorithm)
Choose initial guess $A^{(0)} = (Q^{(0)})^T \forall Q^{(0)}$, e.g. $Q^{(0)} = I \implies A^{(0)} = A$.
For $k = 1, 2, \ldots$

- Compute the QR decomposition: $A^{(k-1)} = Q^{(k)}R^{(k)}$.
- Set $A^{(k)} = R^{(k)}Q^{(k)}$.

Remark 4.5 —

1. Note that $A^{(k)} = R^{(k)}Q^{(k)} = (Q^{(k)})^T A^{(k-1)}Q^{(k)}$. By induction

$$A^{(k)} = (Q^{(k)})^T \cdots (Q^{(1)})^T (A^{(0)})^T AQ^{(0)}Q^{(1)} \cdots Q^{(k)} \implies A^{(k)} \text{ is similar to } A$$

as $Q^{(0)}Q^{(1)} \cdots$ is an orthogonal matrix.

2. Since $Y^{(k)}$ is <u>expected</u> to converge to the eigenvectors of A,

$$A^{(k)} = (Y^{(k)})^T AY^{(k)} \text{ is expected to converge to } \Lambda = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}.$$

It can be proven that if the eigenvalues of A are well separated, then $A^{(k)} \to \Lambda$ and $Q^{(0)} \cdots Q^{(k)}$ converges to the eigenvectors of A.

3. Since QR decomposition and matrix-matrix product costs $O(n^3)$, the total computational cost is

$$O(kn^3), \text{ where } k \text{ is the number of iteration needed.}$$

> Note that if k iterations is done (or if $k \sim O(n)$), then it will be $O(n^4)$, which is expensive.

Note that even though the QR decomposition is not unique, it will still work since the QR have similar properties/structure.

4.4 Practical Implementation of QR Algorithm

The idea is to choose $Q^{(0)}$ such that $A^{(0)}$ is "well structured". This will allow QR decomposition to be done in $O(n^2)$. For our purpose, this "structure" is to be tridiagonal.

Thus this implementation has two phases:

1. Find $Q^{(0)}$ such that $A^{(0)} = (Q^{(0)})^T A Q^{(0)}$ is tridiagonal.
2. QR decomposition of tridiagonal matrices is done in $O(n^2)$ and so that $A^{(k)}$ preserves the tridiagonal structure.

Algorithm 4.6 (Phase 1)
We will use the Householder transformation.

1. Let P_1 be the Householder transform s.t.

$$P_1 = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & H_1 & \\ 0 & & & \end{bmatrix} : \begin{bmatrix} \times & \times & \cdots & \times \\ \times & \times & \cdots & \times \\ \vdots & \vdots & \ddots & \\ \times & \times & & \times \end{bmatrix} \to \begin{bmatrix} \Delta & \Delta & \cdots & \Delta \\ \times & \times & \cdots & \times \\ 0 & & & \\ \vdots & \vdots & \ddots & \\ 0 & \times & & \times \end{bmatrix}.$$

Then $P_1 A P_1^T$

Index