CONTENTS MATH3322 Notes

MATH3322 - Matrix Computation

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Contents

| 1 | March 22nd, 2019 | | 2 |
|-------|------------------|-----------------------------------------------|----------|
| | 1.1 | Eigenvalue Decomposition | 2 |
| | 1.2 | Characteristic Polynomial | 3 |
| | 1.3 | Special Case: Symmetric Matrix and SPD Matrix | 5 |
| 2 | March 27th, 2019 | | |
| | 2.1 | Computation of Eigenvalue Decomposition | 5 |
| | 2.2 | Power Iteration | 6 |
| | 2.3 | Analysis of Power Iteration | 7 |
| 3 | March 29th, 2019 | | 10 |
| | 3.1 | Inverse Power Iteration | 10 |
| | 3.2 | Shifted Inverse Power Iteration | 11 |
| Index | | | 12 |

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:

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

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

$$A \cdot A = \lambda Ax \implies A^2 x = \lambda Ax = \lambda \cdot \lambda x = \lambda^2 x.$$

$$Ax - \sigma x = \lambda x - \sigma x \implies (A - \sigma I) x = (\lambda - \sigma) x$$

$$\implies x = (\lambda - \sigma) (A - \sigma I)^{-1} x \implies (A - \sigma I)^{-1} x.$$

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

$$A[x_1x_2...x_n] = [x_1x_2...x_n] \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}.$$

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

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

In other words (λ_i, x_i) , i = 1, 2, ..., 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 $X^{-1}\Lambda X \Lambda$, 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

$$P_A(z) = \det(zI - A)$$
, 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, $P_A(\lambda) = \lambda^2 + 1 = 0 \implies \lambda_1 = i$, $\lambda_2 = -i$ 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 $x^* \equiv \overline{x^*}$ (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

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

if A is SPD. If A is SPSD, then $\lambda = \frac{x^T A x}{x^T x} \ge 0$, since $x^T A x \ge 0$.

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, ..., 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

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

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

2.2 Power Iteration MATH3322 Notes

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,

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

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

2. for k = 1, 2, ..., n

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

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

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

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

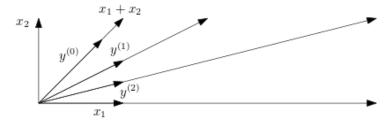


Figure 1

- 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 . :

• k+1:

$$z^{(k+1)} = Ay^{(k)} = A\left(\frac{1}{\sqrt{2^{2k}+1}}\left(2^kx_1 + x_2\right)\right) = \frac{1}{\sqrt{2^{2k}+1}}\left(2^{k+1}x_1 + x_2\right).$$

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 $y^{(0)} = \frac{1}{\sqrt{2}}(x_1 + x_2)$.

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

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

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

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

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

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

Consequently,

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

•
$$|\mu^{(k)} - \lambda_1| \le 2\sqrt{2}C_o \left|\frac{\lambda_2}{\lambda_1}\right|^k \to 0$$

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

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

So

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

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

Because x_i are othronormal,

$$||A^k y^{(0)}||_2^2 = \sum_{i=1}^n \lambda_i^{2k} v_1^2 = \sum_{i=1}^n |\lambda_i|^{2k} |v_i|^2 = |\lambda_1|^{2k} |v_1|^2 (1 + \dots) \ge (|\lambda_1|^k |v_1|)^2$$

and

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

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

Thus

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

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

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

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

So

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

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

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

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 convergence 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.

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

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

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.

March 29th, 2019 MATH3322 Notes

3 March 29th, 2019

3.1 Inverse Power Iteration

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

 $\frac{1}{|\lambda_1|} \le \frac{1}{|\lambda_2|} \le \dots \le \frac{1}{|\lambda_n|}.$

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 $k = 1, 2, \dots$

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

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.

3.2 Shifted Inverse Power Iteration

Index

characteristic polynomial, 3 eigenvalue decomposition, 2 power iteration, 6 Rayleigh quotient, 6 similar matrices, 2