

CS724: Topics in Algorithms

Spectral Properties of Matrices - 1

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Let $A \in \mathbb{C}^{n \times n}$ be a square matrix.

- An *eigenpair* of A is a pair $(\lambda, \mathbf{x}) \in \mathbb{C} \times (\mathbb{C}^n - \{\mathbf{0}\})$ such that $A\mathbf{x} = \lambda\mathbf{x}$.
- We refer to λ is an *eigenvalue* and to \mathbf{x} is an *eigenvector*.
- The set of eigenvalues of A is the *spectrum* of A and will be denoted by $\text{spec}(A)$.



If (λ, \mathbf{x}) is an eigenpair of A , the linear system $A\mathbf{x} = \lambda\mathbf{x}$ has a non-trivial solution in \mathbf{x} . An equivalent homogeneous system is $(\lambda I_n - A)\mathbf{x} = \mathbf{0}$ and this system has a non-trivial solution only if $\det(\lambda I_n - A) = 0$.

Definition

The *characteristic polynomial* of the matrix A is the polynomial p_A defined by $p_A(\lambda) = \det(\lambda I_n - A)$ for $\lambda \in \mathbb{C}$.

Thus, the eigenvalues of A are the roots of the characteristic polynomial of A .



Lemma

Let $A = (\mathbf{a}_1 \cdots \mathbf{a}_n) \in \mathbb{C}^n$ and let B be the matrix obtained from A by replacing the column \mathbf{a}_j by \mathbf{e}_j . Then, we have

$$\det(B) = \det \left(A \begin{bmatrix} 1 & \cdots & j-1 & j+1 & \cdots & n \\ 1 & \cdots & j-1 & j+1 & \cdots & n \end{bmatrix} \right).$$

If B is obtained from A by replacing the columns $\mathbf{a}_{j_1}, \dots, \mathbf{a}_{j_k}$ by $\mathbf{e}_{j_1}, \dots, \mathbf{e}_{j_k}$ and $\{i_1, \dots, i_p\} = \{1, \dots, n\} - \{j_1, \dots, j_k\}$, then

$$\det(B) = \det \left(A \begin{bmatrix} i_1 & \cdots & i_p \\ i_1 & \cdots & i_p \end{bmatrix} \right). \quad (1)$$

In other words, $\det(B)$ equals a principal p -minor of A .



Theorem

Let $A \in \mathbb{C}^{n \times n}$ be a matrix. Its characteristic polynomial p_A can be written as

$$p_A(\lambda) = \sum_{k=0}^n (-1)^k a_k \lambda^{n-k},$$

where a_k is the sum of the principal minors of order k of A .



Proof

$$p_A(\lambda) = \det(\lambda I_n - A) = (-1)^n \det(A - \lambda I_n)$$

can be written as a sum of 2^n determinants of matrices obtained by replacing each subset of the columns of A by the corresponding subset of columns of $-\lambda I_n$.

If the subset of columns of $-\lambda I_n$ involved are $-\lambda \mathbf{e}_{j_1}, \dots, -\lambda \mathbf{e}_{j_k}$ the result

of the substitution is $(-1)^k \lambda^k \det \left(A \begin{bmatrix} i_1 & \cdots & i_p \\ i_1 & \cdots & i_p \end{bmatrix} \right)$, where

$\{i_1, \dots, i_p\} = \{1, \dots, n\} - \{j_1, \dots, j_k\}$. The total contribution of sets of k columns of $-\lambda I_n$ is $(-1)^k \lambda^k a_{n-k}$. Therefore,

$$p_A(\lambda) = (-1)^n \sum_{k=0}^n (-1)^k \lambda^k a_{n-k}.$$

Replacing k by $n - k$ as the summation index yields

$$p_A(\lambda) = (-1)^n \sum_{k=0}^n (-1)^{n-k} \lambda^{n-k} a_k = \sum_{k=0}^n (-1)^k a_k \lambda^{n-k}.$$



Definition

Two matrices $A, B \in \mathbb{C}^{n \times n}$ are *similar* if there exists an invertible matrix $P \in \mathbb{C}^{n \times n}$ such that $B = PAP^{-1}$. This is denoted by $A \sim B$.

If there exists a unitary matrix U such that $B = UAU^{-1}$, then A is *unitarily similar* to B . This is denoted by $A \sim_u B$.

The matrices A, B are *congruent* if $B = SAS^H$ for some non-singular matrix S . This is denoted by $A \approx B$. If $A, B \in \mathbb{R}^{n \times n}$, we say that they are *t-congruent* if $B = SAS'$ for some invertible matrix S ; this is denoted by $A \approx_t B$.



Similar matrices have the same characteristic polynomial. Indeed, suppose that $B = PAP^{-1}$. We have

$$\begin{aligned} p_B(\lambda) &= \det(\lambda I_n - B) = \det(\lambda I_n - PAP^{-1}) \\ &= \det(\lambda P I_n P^{-1} - PAP^{-1}) = \det(P(\lambda I_n - A)P^{-1}) \\ &= \det(P) \det(\lambda I_n - A) \det(P^{-1}) = \det(\lambda I_n - A) = p_A(\lambda), \end{aligned}$$

because $\det(P) \det(P^{-1}) = 1$. Thus, similar matrices have the same eigenvalues.



Example

Let A be the matrix

$$A = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}.$$

We have

$$p_A = \det(\lambda I_2 - A) = (\lambda - \cos \theta)^2 + \sin^2 \theta = \lambda^2 - 2\lambda \cos \theta + 1.$$

The roots of this polynomial are $\lambda_1 = \cos \theta + i \sin \theta$ and $\lambda_2 = \cos \theta - i \sin \theta$, so they are complex numbers.

We regard A as a complex matrix with real entries. If we were to consider A as a real matrix, we would not be able to find real eigenvalues for A unless θ were equal to 0.



Definition

The *algebraic multiplicity* of the eigenvalue λ of a matrix $A \in \mathbb{C}^{n \times n}$ is the multiplicity of λ as a root of the characteristic polynomial p_A of A .

The algebraic multiplicity of λ is denoted by $\text{algm}(A, \lambda)$. If $\text{algm}(A, \lambda) = 1$ we say that λ is a *simple eigenvalue*.



Example

Let $A \in \mathbb{R}^{2 \times 2}$ be the matrix

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

The characteristic polynomial of A is

$$p_A(\lambda) = \begin{vmatrix} \lambda & 1 \\ -1 & \lambda - 2 \end{vmatrix} = \lambda^2 - 2\lambda + 1.$$

Therefore, A has the eigenvalue 1 with $\text{algm}(A, 1) = 2$.



Theorem

The eigenvalues of Hermitian complex matrices are real numbers.

Proof.

Let $A \in \mathbb{C}^{n \times n}$ be a Hermitian matrix and let λ be an eigenvalue of A . We have $A\mathbf{x} = \lambda\mathbf{x}$ for some $\mathbf{x} \in \mathbb{C}^n - \{\mathbf{0}_n\}$, so $\mathbf{x}^H A^H = \bar{\lambda}\mathbf{x}^H$. Since $A^H = A$, we have

$$\lambda\mathbf{x}^H\mathbf{x} = \mathbf{x}^H A\mathbf{x} = \mathbf{x}^H A^H\mathbf{x} = \bar{\lambda}\mathbf{x}^H\mathbf{x}.$$

Since $\mathbf{x} \neq \mathbf{0}$ implies $\mathbf{x}^H\mathbf{x} \neq 0$, it follows that $\bar{\lambda} = \lambda$. Thus, λ is a real number. □



Corollary

The eigenvalues of symmetric real matrices are real numbers.



Theorem

The eigenvectors of a complex Hermitian matrix corresponding to distinct eigenvalues are orthogonal to each other.

Proof: Let (λ, \mathbf{u}) and (μ, \mathbf{v}) be two eigenpairs of the Hermitian matrix $A \in \mathbb{C}^{n \times n}$, where $\lambda \neq \mu$. Since A is Hermitian, $\lambda, \mu \in \mathbb{R}$. Since $A\mathbf{u} = \lambda\mathbf{u}$ we have $\mathbf{v}^H A \mathbf{u} = \lambda \mathbf{v}^H \mathbf{u}$. The last equality can be written as $(A\mathbf{v})^H \mathbf{u} = \lambda \mathbf{v}^H \mathbf{u}$, or as $\mu \mathbf{v}^H \mathbf{u} = \lambda \mathbf{v}^H \mathbf{u}$. Since $\mu \neq \lambda$, $\mathbf{v}^H \mathbf{u} = 0$, so \mathbf{u} and \mathbf{v} are orthogonal.



Corollary

The eigenvectors of a Hermitian matrix corresponding to distinct eigenvalues form a linearly independent set.



Theorem

(Schur's Triangularization Theorem) *Let $A \in \mathbb{C}^{n \times n}$ be a square matrix. There exists an upper-triangular matrix $T \in \mathbb{C}^{n \times n}$ such that $A \sim_u T$. The diagonal elements of T are the eigenvalues of A ; moreover, each eigenvalue λ of A occurs in the sequence of diagonal elements of T a number of $\text{algm}(A, \lambda)$ times. The columns of U are unit eigenvectors of A .*



Proof

The argument is by induction on n . The base case, $n = 1$, is immediate. Suppose that the statement holds for matrices in $\mathbb{C}^{(n-1) \times (n-1)}$ and let $A \in \mathbb{C}^{n \times n}$. If (λ, \mathbf{x}) is an eigenpair of A with $\|\mathbf{x}\|_2 = 1$, let $H_{\mathbf{v}}$ be a Householder matrix that transforms \mathbf{x} into \mathbf{e}_1 . Since we also have $H_{\mathbf{v}}\mathbf{e}_1 = \mathbf{x}$, \mathbf{x} is the first column of $H_{\mathbf{v}}$ and we can write $H_{\mathbf{v}} = (\mathbf{x} \ K)$, where $K \in \mathbb{C}^{n \times (n-1)}$. Consequently,

$$H_{\mathbf{v}}AH_{\mathbf{v}} = H_{\mathbf{v}}A(\mathbf{x} \ K) = H_{\mathbf{v}}(\lambda\mathbf{x} \ H_{\mathbf{v}}AK) = (\lambda\mathbf{e}_1 \ H_{\mathbf{v}}AK).$$



Proof (cont'd)

Since $H_{\mathbf{v}}$ is Hermitian and $H_{\mathbf{v}} = (\mathbf{x} \ K)$, it follows that

$$H_{\mathbf{v}}^H = \begin{pmatrix} \mathbf{x}^H \\ K^H \end{pmatrix} = H_{\mathbf{v}}.$$

Therefore,

$$H_{\mathbf{v}} A H_{\mathbf{v}} = \begin{pmatrix} \lambda & \mathbf{x}^H A K \\ \mathbf{0}_{n-1} & K^H A K \end{pmatrix}.$$



Proof (cont'd)

Since $K^HAK \in \mathbb{C}^{(n-1) \times (n-1)}$, by the inductive hypothesis, there exists a unitary matrix W and an upper triangular matrix S such that $W^H(K^HAK)W = S$. Note that the matrix

$$U = H_v \begin{pmatrix} 1 & \mathbf{0}'_{n-1} \\ \mathbf{0}_{n-1} & W \end{pmatrix}$$

is unitary and

$$U^H A U = \begin{pmatrix} \lambda & \mathbf{x}^H A K W \\ \mathbf{0}_{n-1} & W^H K^H A K W \end{pmatrix} = \begin{pmatrix} \lambda & \mathbf{x}^H A K W \\ \mathbf{0}_{n-1} & S \end{pmatrix}.$$

The last matrix is clearly upper triangular.



Proof (cont'd)

Since $A \sim_u T$, A and T have the same characteristic polynomials and, therefore, the same eigenvalues, with identical multiplicities.

The factorization of A can be written as $A = UDU^H$ because $U^{-1} = U^H$. Since $AU = UD$, each column \mathbf{u}_i of U is an eigenvector of A that corresponds to the eigenvalue λ_i for $1 \leq i \leq n$.



Corollary

Let $A \in \mathbb{C}^{n \times n}$ and let f be a polynomial. If $\text{spec}(A) = \{\lambda_1, \dots, \lambda_n\}$ (including multiplicities), then $\text{spec}(f(A)) = \{f(\lambda_1), \dots, f(\lambda_n)\}$.

Proof: By Schur's Triangularization Theorem there exists a unitary matrix $U \in \mathbb{C}^{n \times n}$ and an upper-triangular matrix $T \in \mathbb{C}^{n \times n}$ such that $A = UTU^H$ and the diagonal elements of T are the eigenvalues of A , $\lambda_1, \dots, \lambda_n$. Therefore $f(A) = Uf(T)U^H$ and the diagonal elements of $f(T)$ are $f(\lambda_1), \dots, f(\lambda_m)$. Since $f(A) \sim_u f(T)$, we obtain the desired conclusion because two similar matrices have the same eigenvalues with the same algebraic multiplicities.



Definition

A matrix $A \in \mathbb{C}^{n \times n}$ is *diagonalizable* (unitarily diagonalizable) if there exists a diagonal matrix $D = \text{diag}(d_1, \dots, d_n)$ such that $A \sim D$ ($A \sim_u D$).



Theorem

A matrix $A \in \mathbb{C}^{n \times n}$ is diagonalizable if and only if there exists a linearly independent set $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ of n eigenvectors of A .



Proof

Let $A \in \mathbb{C}^{n \times n}$ such that there exists a set $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ of n eigenvectors of A that is linearly independent and let P be the matrix $(\mathbf{v}_1 \ \mathbf{v}_2 \ \dots \ \mathbf{v}_n)$ that is clearly invertible. We have:

$$\begin{aligned} P^{-1}AP &= P^{-1}(A\mathbf{v}_1 \ A\mathbf{v}_2 \ \dots \ A\mathbf{v}_n) = P^{-1}(\lambda_1\mathbf{v}_1 \ \lambda_2\mathbf{v}_2 \ \dots \ \lambda_n\mathbf{v}_n) \\ &= P^{-1}P \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & \lambda_n \end{pmatrix} = \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & \lambda_n \end{pmatrix}. \end{aligned}$$



Proof (cont'd)

Therefore, we have $A = PDP^{-1}$, where

$$D = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix},$$

so $A \sim D$.

Conversely, suppose that A is diagonalizable, so $AP = PD$, where D is a diagonal matrix and P is an invertible matrix, and let $\mathbf{v}_1, \dots, \mathbf{v}_n$ be the columns of the matrix P . We have $A\mathbf{v}_i = d_{ii}\mathbf{v}_i$ for $1 \leq i \leq n$, so each \mathbf{v}_i is an eigenvector of A . Since P is invertible, its columns are linear independent.



Corollary

If $A \in \mathbb{C}^{n \times n}$ is diagonalizable then the columns of any matrix P such that $D = P^{-1}AP$ is a diagonal matrix are eigenvectors of A . Furthermore, the diagonal entries of D are the eigenvalues that correspond to the columns of P .



Corollary

A matrix $A \in \mathbb{C}^{n \times n}$ is unitarily diagonalizable if and only if there exists a set $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ of n orthonormal eigenvectors of A .



Theorem

Let A be a Hermitian matrix, $\lambda_1 \geq \dots \geq \lambda_n$ be its eigenvalues having the orthonormal eigenvectors $\mathbf{u}_1, \dots, \mathbf{u}_n$, respectively.

Define the subspace $M = \langle \mathbf{u}_p, \dots, \mathbf{u}_q \rangle$, where $1 \leq p \leq q \leq n$. If $\mathbf{x} \in M$ and $\|\mathbf{x}\|_2 = 1$, we have $\lambda_q \leq \mathbf{x}^H A \mathbf{x} \leq \lambda_p$.



Proof

If \mathbf{x} is a unit vector in M , then $\mathbf{x} = a_p \mathbf{u}_p + \cdots + a_q \mathbf{u}_q$, so $\mathbf{x}^H \mathbf{u}_i = \overline{a_i}$ for $p \leq i \leq q$. Since $\|\mathbf{x}\|_2 = 1$, we have $|a_p|^2 + \cdots + |a_q|^2 = 1$. This allows us to write:

$$\begin{aligned} \mathbf{x}^H A \mathbf{x} &= \mathbf{x}^H (a_p A \mathbf{u}_p + \cdots + a_q A \mathbf{u}_q) \\ &= \mathbf{x}^H (a_p \lambda_p \mathbf{u}_p + \cdots + a_q \lambda_q \mathbf{u}_q) \\ &= \mathbf{x}^H (|a_p|^2 \lambda_p + \cdots + |a_q|^2 \lambda_q). \end{aligned}$$

Since $|a_p|^2 + \cdots + |a_q|^2 = 1$, the desired inequalities follow immediately.



Corollary

Let A be a Hermitian matrix, $\lambda_1 \geq \dots \geq \lambda_n$ be its eigenvalues having the orthonormal eigenvectors $\mathbf{u}_1, \dots, \mathbf{u}_n$, respectively. The following statements hold for a unit vector \mathbf{x} :

- if $\mathbf{x} \in \langle \mathbf{u}_1, \dots, \mathbf{u}_i \rangle$, then $\mathbf{x}^H A \mathbf{x} \geq \lambda_i$;
- if $\mathbf{x} \in \langle \mathbf{u}_1, \dots, \mathbf{u}_{i-1} \rangle^\perp$, then $\mathbf{x}^H A \mathbf{x} \leq \lambda_i$.



Theorem

(Rayleigh-Ritz Theorem) *Let A be a Hermitian matrix and let $(\lambda_1, \mathbf{u}_1), \dots, (\lambda_n, \mathbf{u}_n)$ be the eigenpairs of A , where $\lambda_1 \geq \dots \geq \lambda_n$. If \mathbf{x} is a unit vector, we have $\lambda_n \leq \mathbf{x}^H A \mathbf{x} \leq \lambda_1$.*

Proof.

This statement follows by observing that the subspace generated by $\mathbf{u}_1, \dots, \mathbf{u}_n$ is the entire space \mathbb{C}^n . □



The Courant-Fisher Theorem

Let \mathcal{S}_p^n be the collection of p -dimensional subspaces of \mathbb{C}^n . Note that $\mathcal{S}_0^n = \{\{\mathbf{0}_n\}\}$ and $\mathcal{S}_n^n = \{\mathbb{C}^n\}$.

Theorem

Let $A \in \mathbb{C}^{n \times n}$ be a Hermitian matrix having the eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$. We have

$$\begin{aligned}\lambda_k &= \max_{U \in \mathcal{S}_k^n} \min\{\mathbf{x}^H A \mathbf{x} \mid \mathbf{x} \in U \text{ and } \|\mathbf{x}\|_2 = 1\} \\ &= \min_{U \in \mathcal{S}_{n-k+1}^n} \max\{\mathbf{x}^H A \mathbf{x} \mid \mathbf{x} \in U \text{ and } \|\mathbf{x}\|_2 = 1\}.\end{aligned}$$



Proof

Let $A = V^H \text{diag}(\lambda_1, \dots, \lambda_n) V$ be the factorization of A , where $V = (\mathbf{u}_1 \cdots \mathbf{u}_n)$ is a unitary matrix.

If

$$U = \langle \mathbf{u}_1, \dots, \mathbf{u}_k \rangle \in \mathcal{S}_k^n \text{ and } W = \langle \mathbf{u}_k, \dots, \mathbf{u}_n \rangle \in \mathcal{S}_{n-k+1}^n,$$

then there is a non-zero vector $\mathbf{x} \in U \cap W$ because $\dim(U) + \dim(W) = n + 1$; we can assume that $\|\mathbf{x}\|_2 = 1$.

We have $\lambda_k \geq \mathbf{x}^H A \mathbf{x}$, and, therefore, for any $U \in \mathcal{S}_k^n$, $\lambda_k \geq \min\{\mathbf{x}^H A \mathbf{x} \mid \mathbf{x} \in U \text{ and } \|\mathbf{x}\|_2 = 1\}$. This implies

$$\lambda_k \geq \max_{U \in \mathcal{S}_k^n} \min\{\mathbf{x}^H A \mathbf{x} \mid \mathbf{x} \in U \text{ and } \|\mathbf{x}\|_2 = 1\}.$$



Proof (cont'd)

For a unit vector $\mathbf{x} \in \langle \mathbf{u}_1, \dots, \mathbf{u}_k \rangle \in \mathcal{S}_k^n$ we have $\mathbf{x}^H A \mathbf{x} \geq \lambda_k$ and $\mathbf{u}_k^H A \mathbf{u}_k = \lambda_k$. Therefore, for $U = \langle \mathbf{u}_1, \dots, \mathbf{u}_k \rangle \in \mathcal{S}_k^n$ we have $\min\{\mathbf{x}^H A \mathbf{x} \mid \mathbf{x} \in U, \|\mathbf{x}\|_2 = 1\} \geq \lambda_k$, so $\max_{U \in \mathcal{S}_k^n} \min\{\mathbf{x}^H A \mathbf{x} \mid \mathbf{x} \in U, \|\mathbf{x}\|_2 = 1\} \geq \lambda_k$. The inequalities proved above yield

$$\lambda_k = \max_{U \in \mathcal{S}_k^n} \min\{\mathbf{x}^H A \mathbf{x} \mid \mathbf{x} \in U \text{ and } \|\mathbf{x}\|_2 = 1\}.$$



Proof (cont'd)

For the second equality, let $U \in \mathcal{S}_{n-k+1}^n$. If $W = \langle \mathbf{u}_1, \dots, \mathbf{u}_k \rangle$, there is a non-zero unit vector $\mathbf{x} \in U \cap W$ because $\dim(U) + \dim(W) \geq n + 1$. We have $\mathbf{x}^H A \mathbf{x} \leq \lambda_k$. Therefore, for any $U \in \mathcal{S}_{n-k+1}^n$,

$$\lambda_k \geq \max\{\mathbf{x}^H A \mathbf{x} \mid \mathbf{x} \in U \text{ and } \|\mathbf{x}\|_2 = 1\}.$$

This implies

$$\lambda_k \geq \min_{U \in \mathcal{S}_{n-k+1}^n} \max\{\mathbf{x}^H A \mathbf{x} \mid \mathbf{x} \in U \text{ and } \|\mathbf{x}\|_2 = 1\}.$$


Proof (cont'd)

For a unit vector $\mathbf{x} \in \langle \mathbf{u}_k, \dots, \mathbf{u}_n \rangle \in \mathcal{S}_{n-k+1}^n$ we have $\lambda_k \leq \mathbf{x}^H A \mathbf{x}$ and $\lambda_k = \mathbf{u}_k^H A \mathbf{u}_k$. Thus, $\lambda_k \leq \max\{\mathbf{x}^H A \mathbf{x} \mid \mathbf{x} \in U \text{ and } \|\mathbf{x}\|_2 = 1\}$. Consequently, $\lambda_k \leq \min_{U \in \mathcal{S}_{n-k+1}^n} \max\{\mathbf{x}^H A \mathbf{x} \mid \mathbf{x} \in U \text{ and } \|\mathbf{x}\|_2 = 1\}$, which completes the proof of the second equality of the theorem.



An equivalent formulation of Courant-Fisher Theorem is given next.

Theorem

Let $A \in \mathbb{C}^{n \times n}$ be a Hermitian matrix having the eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$. We have

$$\begin{aligned}\lambda_k &= \max_{\mathbf{w}_1, \dots, \mathbf{w}_{n-k}} \min \{ \mathbf{x}^H A \mathbf{x} \mid \mathbf{x} \perp \mathbf{w}_1, \dots, \mathbf{x} \perp \mathbf{w}_{n-k} \text{ and } \|\mathbf{x}\|_2 = 1 \} \\ &= \min_{\mathbf{w}_1, \dots, \mathbf{w}_{k-1}} \max \{ \mathbf{x}^H A \mathbf{x} \mid \mathbf{x} \perp \mathbf{w}_1, \dots, \mathbf{x} \perp \mathbf{w}_{k-1} \text{ and } \|\mathbf{x}\|_2 = 1 \}.\end{aligned}$$

Proof: The equalities of the Theorem follow from the Courant-Fisher theorem taking into account that if $U \in \mathcal{S}_k^n$, then $U^\perp = \langle \mathbf{w}_1, \dots, \mathbf{w}_{n-k} \rangle$ for some vectors $\mathbf{w}_1, \dots, \mathbf{w}_{n-k}$, and if $U \in \mathcal{S}_{n-k+1}^n$, then $U = \langle \mathbf{w}_1, \dots, \mathbf{w}_{k-1} \rangle$ for some vectors $\mathbf{w}_1, \dots, \mathbf{w}_{k-1}$ in \mathbb{C}^n .



Ky Fan's Theorem

Theorem

Let $A \in \mathbb{C}^{n \times n}$ be a Hermitian matrix such that $\text{spec}(A) = \{\lambda_1, \dots, \lambda_n\}$, where $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. Also, let $V \in \mathbb{C}^{n \times n}$ be a matrix, $V = (\mathbf{v}_1, \dots, \mathbf{v}_n)$ whose set of columns constitutes an orthonormal set of eigenvectors of A . For every $q \in \mathbb{N}$ such that $1 \leq q \leq n$, the sums

$$\sum_{i=1}^q \lambda_i = \lambda_1 + \dots + \lambda_q$$

and

$$\sum_{i=1}^q \lambda_{n+1-i} = \lambda_n + \lambda_{n-1} + \dots + \lambda_{n-(q-1)}$$

are the maximum and minimum of $\sum_{j=1}^q \mathbf{x}_j^H A \mathbf{x}_j$, respectively, where $\{\mathbf{x}_1, \dots, \mathbf{x}_q\}$ is an orthonormal set of vectors in \mathbb{C}^n . The maximum (minimum) is achieved when $\mathbf{x}_1, \dots, \mathbf{x}_q$ are the first (last) columns of V .

Proof

Let $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ be an orthonormal set of eigenvectors of A and let $\mathbf{x}_i = \sum_{k=1}^n b_{ki} \mathbf{v}_k$ be the expression of \mathbf{x}_i using the columns of V as a basis for $1 \leq i \leq n$. Since each \mathbf{x}_i is a unit vector we have

$$\|\mathbf{x}_i\|^2 = \mathbf{x}_i^H \mathbf{x}_i = \sum_{k=1}^n |b_{ki}|^2 = 1$$

for $1 \leq i \leq n$. Also, note that

$$\mathbf{x}_i^H \mathbf{v}_r = \left(\sum_{k=1}^n \overline{b_{ki}} \mathbf{v}_k^H \right) \mathbf{v}_r = \overline{b_{ri}},$$

due to the orthonormality of the set of columns of V .



Proof (cont'd)

We have

$$\begin{aligned}\mathbf{x}_i^H A \mathbf{x}_i &= \mathbf{x}_i^H A \sum_{k=1}^n b_{ki} \mathbf{v}_k = \sum_{k=1}^n b_{ki} \mathbf{x}_i^H A \mathbf{v}_k \\&= \sum_{k=1}^n b_{ki} \mathbf{x}_i^H \lambda_k \mathbf{v}_k = \sum_{k=1}^n \lambda_k b_{ki} \overline{b_{ki}} = \sum_{k=1}^n |b_{ki}|^2 \lambda_k \\&= \lambda_q \sum_{k=1}^n |b_{ki}|^2 + \sum_{k=1}^q (\lambda_k - \lambda_q) |b_{ki}|^2 + \sum_{k=q+1}^n (\lambda_k - \lambda_q) |b_{ki}|^2 \\&\leq \lambda_q + \sum_{k=1}^q (\lambda_k - \lambda_q) |b_{ki}|^2.\end{aligned}$$

The last inequality implies

$$\sum_{i=1}^q \mathbf{x}_i^H A \mathbf{x}_i \leq q \lambda_q + \sum_{i=1}^q \sum_{k=1}^q (\lambda_k - \lambda_q) |b_{ki}|^2.$$



Proof (cont'd)

Therefore,

$$\sum_{i=1}^q \lambda_i - \sum_{i=1}^q \mathbf{x}_i^H \mathbf{A} \mathbf{x}_i \geq \sum_{i=1}^q (\lambda_i - \lambda_q) \left(1 - \sum_{k=1}^q |b_{ki}|^2 \right). \quad (2)$$

We have $\sum_{k=1}^q |b_{ik}|^2 \leq \|\mathbf{x}_i\|^2 = 1$, so

$$\sum_{i=1}^q (\lambda_i - \lambda_q) \left(1 - \sum_{k=1}^q |b_{ki}|^2 \right) \geq 0.$$

The left member of Inequality 2 becomes 0 when $\mathbf{x}_i = \mathbf{v}_i$, so

$\sum_{i=1}^q \mathbf{x}_i^H \mathbf{A} \mathbf{x}_i \leq \sum_{i=1}^q \lambda_i$. The maximum of $\sum_{i=1}^q \mathbf{x}_i^H \mathbf{A} \mathbf{x}_i$ is obtained when $\mathbf{x}_i = \mathbf{v}_i$ for $1 \leq i \leq q$, that is, when X consists of the first q columns of V . The argument for the minimum is similar.



Theorem

Let $A \in \mathbb{C}^{n \times n}$ be a Hermitian matrix. If A is positive semidefinite, then all its eigenvalues are non-negative; if A is positive definite then its eigenvalues are positive.

Proof.

Since A is Hermitian all its eigenvalues are real numbers. Suppose that A is positive semidefinite, that is, $\mathbf{x}^H A \mathbf{x} \geq 0$ for $\mathbf{x} \in \mathbb{C}^n$. If $\lambda \in \text{spec}(A)$, then $A\mathbf{v} = \lambda\mathbf{v}$ for some eigenvector $\mathbf{v} \neq \mathbf{0}$. The positive semi-definiteness of A implies $\mathbf{v}^H A \mathbf{v} = \lambda \mathbf{v}^H \mathbf{v} = \lambda \|\mathbf{v}\|_2^2 \geq 0$, which implies $\lambda \geq 0$. It is easy to see that if A is positive definite, then $\lambda > 0$. □



Theorem

Let $A \in \mathbb{C}^{n \times n}$ be a Hermitian matrix. If A is positive semidefinite, then all its principal minors are non-negative real numbers. If A is positive definite then all its principal minors are positive real numbers.

Proof.

Since A is positive semidefinite, every sub-matrix $A \begin{bmatrix} i_1 & \cdots & i_k \\ i_1 & \cdots & i_k \end{bmatrix}$ is a Hermitian positive semidefinite matrix by Theorem ??, so every principal minor is a non-negative real number. The second part of the theorem is proven similarly. □



Corollary

Let $A \in \mathbb{C}^{n \times n}$ be a Hermitian matrix. The following statements are equivalent.

- *A is positive semidefinite;*
- *all eigenvalues of A are non-negative numbers;*
- *there exists a Hermitian matrix $C \in \mathbb{C}^{n \times n}$ such that $C^2 = A$;*
- *A is the Gram matrix of a sequence of vectors, that is, $A = B^H B$ for some $B \in \mathbb{C}^{n \times n}$.*



Definition

Let $A \in \mathbb{C}^{m \times n}$ be a matrix. A *singular triplet* of A is a triplet $(\sigma, \mathbf{u}, \mathbf{v})$ such that $\sigma \in \mathbb{R}_{>0}$, $\mathbf{u} \in \mathbb{C}^n$, $\mathbf{v} \in \mathbb{C}^m$, $A\mathbf{u} = \sigma\mathbf{v}$ and $A^H\mathbf{v} = \sigma\mathbf{u}$.

The number σ is a *singular value* of A , \mathbf{u} is a *left singular vector* and \mathbf{v} is a *right singular vector*.



For a singular triplet $(\sigma, \mathbf{u}, \mathbf{v})$ of A we have

$$A^H A \mathbf{u} = \sigma A^H \mathbf{v} = \sigma^2 \mathbf{u} \text{ and } A A^H \mathbf{v} = \sigma A \mathbf{u} = \sigma^2 \mathbf{v}.$$

Therefore, σ^2 is both an eigenvalue of AA^H and an eigenvalue of $A^H A$.



Example

Let A be the real matrix

$$A = \begin{pmatrix} \cos \alpha & \sin \alpha \\ \cos \beta & \sin \beta \end{pmatrix}.$$

We have $\det(A) = \sin(\beta - \alpha)$, so the eigenvalues of $A'A$ are the roots of the equation $\lambda^2 - 2\lambda + \sin^2(\beta - \alpha) = 0$, that is, $\lambda_1 = 1 + \cos(\beta - \alpha)$ and $\lambda_2 = 1 - \cos(\beta - \alpha)$. Therefore, the singular values of A are $\sigma_1 = \sqrt{2} \left| \cos \frac{\beta - \alpha}{2} \right|$ and $\sigma_2 = \sqrt{2} \left| \sin \frac{\beta - \alpha}{2} \right|$.

It is easy to see that a unit left singular vector that corresponds to the eigenvalue $1 + \cos(\beta - \alpha)$ is

$$\mathbf{u} = \begin{pmatrix} \cos \frac{\alpha + \beta}{2} \\ \sin \frac{\alpha + \beta}{2} \end{pmatrix},$$

which corresponds to the average direction of the rows of A .

- The eigenvalues of a positive semi-definite matrix are non-negative numbers. Since both AA^H and A^HA are positive semi-definite matrices for $A \in \mathbb{C}^{m \times n}$, the spectra of these matrices consist of non-negative numbers $\lambda_1, \dots, \lambda_n$.
- AA^H and A^HA have the same rank r and therefore, the same number r of non-zero eigenvalues $\lambda_1, \dots, \lambda_r$.
- The singular values of A have the form $\sqrt{\lambda_1} \geq \dots \geq \sqrt{\lambda_r}$.

Notation: $\sigma_i = \sqrt{\lambda_i}$ for $1 \leq i \leq r$ and will assume that $\sigma_1 \geq \dots \geq \sigma_r > 0$.



Theorem

Let $A \in \mathbb{C}^{n \times n}$ be a matrix having the singular values $\sigma_1 \geq \dots \geq \sigma_n$. If λ is an eigenvalue value of A , then $\sigma_n \leq |\lambda| \leq \sigma_1$.

Proof.

Let \mathbf{u} be an unit eigenvector for the eigenvalue λ . Since $A\mathbf{u} = \lambda\mathbf{u}$ it follows that $(A^H A \mathbf{u}, \mathbf{u}) = (A\mathbf{u}, A\mathbf{u}) = \bar{\lambda}\lambda(\mathbf{u}, \mathbf{u}) = \bar{\lambda}\lambda = |\lambda|^2$. The matrix $A^H A$ is Hermitian and its largest and smallest eigenvalues are σ_1^2 and σ_n^2 , respectively. Thus, $\sigma_n \leq |\lambda| \leq \sigma_1$. □



The SVD Theorem

Theorem

If $A \in \mathbb{C}^{m \times n}$ is a matrix and $\text{rank}(A) = r$, then A can be factored as $A = UDV^H$, where $U \in \mathbb{C}^{m \times m}$ and $V \in \mathbb{C}^{n \times n}$ are unitary matrices, and $D = \text{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0) \in \mathbb{R}^{m \times n}$, where $\sigma_1 \geq \dots \geq \sigma_r$ are real positive numbers.



Proof

The square matrix $A^H A \in \mathbb{C}^{n \times n}$ has the same rank r as the matrix A and is positive semidefinite. Therefore, there are r positive eigenvalues of this matrix, denoted by $\sigma_1^2, \dots, \sigma_r^2$, where $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$. Let $\mathbf{v}_1, \dots, \mathbf{v}_r$ be the corresponding pairwise orthogonal unit eigenvectors in \mathbb{C}^n .

We have $A^H A \mathbf{v}_i = \sigma_i^2 \mathbf{v}_i$ for $1 \leq i \leq r$. Define $V = (\mathbf{v}_1 \ \dots \ \mathbf{v}_r \ \mathbf{v}_{r+1} \ \dots \ \mathbf{v}_n)$ by completing the set $\{\mathbf{v}_1, \dots, \mathbf{v}_r\}$ to an orthogonal basis

$$\{\mathbf{v}_1, \dots, \mathbf{v}_r, \mathbf{v}_{r+1}, \dots, \mathbf{v}_n\}$$

for \mathbb{C}^n . If $V_1 = (\mathbf{v}_1 \ \dots \ \mathbf{v}_r)$ and $V_2 = (\mathbf{v}_{r+1} \ \dots \ \mathbf{v}_n)$, we can write $V = (V_1 \ V_2)$.



Proof (cont'd)

The equalities involving the eigenvectors can now be written as $A^H AV_1 = V_1 E^2$, where $E = \text{diag}(\sigma_1, \dots, \sigma_r)$.

Define $U_1 = AV_1 E^{-1} \in \mathbb{C}^{m \times r}$. We have $U_1^H = E^{-1} V_1^H A^H$, so

$$U_1^H U_1 = E^{-1} V_1^H A^H AV_1 E^{-1} = E^{-1} V_1^H V_1 E^2 E^{-1} = I_r,$$

which shows that the columns of U_1 are pairwise orthogonal unit vectors. Consequently, $U_1^H AV_1 E^{-1} = I_r$, so $U_1^H AV_1 = E$.



Proof (cont'd)

If $U_1 = (\mathbf{u}_1 \cdots, \mathbf{u}_r)$, let $U_2 = (\mathbf{u}_{r+1}, \dots, \mathbf{u}_m)$ be the matrix whose columns constitute the extension of the set $\{\mathbf{u}_1 \cdots, \mathbf{u}_r\}$ to an orthogonal basis of \mathbb{C}^m .

Define $U \in \mathbb{C}^{m \times m}$ as $U = (U_1 \ U_2)$. Note that

$$\begin{aligned} U^H A V &= \begin{pmatrix} U_1^H \\ U_2^H \end{pmatrix} A (V_1 \ V_2) = \begin{pmatrix} U_1^H A V_1 & U_1^H A V_2 \\ U_2^H A V_1 & U_2^H A V_2 \end{pmatrix} \\ &= \begin{pmatrix} U_1^H A V_1 & U_1^H A V_2 \\ U_2^H A V_1 & U_2^H A V_2 \end{pmatrix} = \begin{pmatrix} U_1^H A V_1 & O \\ O & O \end{pmatrix} = \begin{pmatrix} E & O \\ O & O \end{pmatrix}, \end{aligned}$$

which is the desired decomposition.



Corollary

Let $A \in \mathbb{C}^{m \times n}$ be a matrix such that $\text{rank}(A) = r$. If $\sigma_1 \geq \dots \geq \sigma_r$ are non-zero singular values, then

$$A = \sigma_1 \mathbf{u}_1 \mathbf{v}_1^H + \dots + \sigma_r \mathbf{u}_r \mathbf{v}_r^H, \quad (3)$$

where $(\sigma_i, \mathbf{u}_i, \mathbf{v}_i)$ are singular triplets of A for $1 \leq i \leq r$.



The value of a unitarily invariant norm of a matrix depends only on its singular values.

Corollary

Let $A \in \mathbb{C}^{m \times n}$ be a matrix and let $A = UDV^H$ be the singular value decomposition of A . If $\|\cdot\|$ is a unitarily invariant norm, then

$$\|A\| = \|D\| = \|diag(\sigma_1, \dots, \sigma_r, 0, \dots, 0)\|.$$

Proof.

This statement follows because the matrices $U \in \mathbb{C}^{m \times m}$ and $V \in \mathbb{C}^{n \times n}$ are unitary. \square



$\|\cdot\|_2$ and $\|\cdot\|_F$ are unitarily invariant. Therefore, the Frobenius norm can be written as

$$\|A\|_F = \sqrt{\sum_{i=1}^r \sigma_i^2}.$$

and $\|A\|_2 = \sigma_1$.



Theorem

Let A and B be two matrices in $\mathbb{C}^{m \times n}$. If $A \sim_u B$, then they have the same singular values.

Proof.

Suppose that $A \sim_u B$, that is, $A = W_1^H B W_2$ for some unitary matrices W_1 and W_2 . If A has the SVD $A = U^H \text{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0) V$, then

$$B = W_1 A W_2^H = (W_1 U^H) \text{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0) (V W_2^H).$$

Since $W_1 U^H$ and $V W_2^H$ are both unitary matrices, it follows that the singular values of B are the same as the singular values of A . □



Let $\mathbf{v} \in \mathbb{C}^n$ be an eigenvector of the matrix $A^H A$ that corresponds to a non-zero, positive eigenvalue σ^2 , that is, $A^H A \mathbf{v} = \sigma^2 \mathbf{v}$. Define $\mathbf{u} = \frac{1}{\sigma} A \mathbf{v}$. We have $A \mathbf{v} = \sigma \mathbf{u}$. Also,

$$A^H \mathbf{u} = A^H \left(\frac{1}{\sigma} A \mathbf{v} \right) = \sigma \mathbf{v}.$$

This implies $AA^H \mathbf{u} = \sigma^2 \mathbf{u}$, so \mathbf{u} is an eigenvector of AA^H that corresponds to the same eigenvalue σ^2 .

Conversely, if $\mathbf{u} \in \mathbb{C}^m$ is an eigenvector of the matrix AA^H that corresponds to a non-zero, positive eigenvalue σ^2 , we have $AA^H \mathbf{u} = \sigma^2 \mathbf{u}$. Thus, if $\mathbf{v} = \frac{1}{\sigma} A \mathbf{u}$ we have $A \mathbf{v} = \sigma \mathbf{u}$ and \mathbf{v} is an eigenvector of $A^H A$ for the eigenvalue σ^2 .



The Courant-Fisher Theorem allows the formulation of a similar result for singular values.

Theorem

Let $A \in \mathbb{C}^{m \times n}$ be a matrix such that $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r$ is the non-increasing sequence of singular values of A . For $1 \leq k \leq r$ we have

$$\sigma_k = \min_{\dim(S)=n-k+1} \max\{\|Ax\|_2 \mid x \in S \text{ and } \|x\|_2 = 1\}$$

$$\sigma_k = \max_{\dim(T)=k} \min\{\|Ax\|_2 \mid x \in T \text{ and } \|x\|_2 = 1\},$$

where S and T range over subspaces of \mathbb{C}^n .



Proof

We give the argument only for the second equality of the theorem; the first can be shown in a similar manner.

We saw that σ_k equals the square root of k^{th} largest absolute value of the eigenvalue $|\lambda_k|$ of the matrix $A^H A$. By Courant-Fisher Theorem, we have

$$\begin{aligned}\lambda_k &= \max_{\dim(T)=k} \min_{\mathbf{x}} \{ \mathbf{x}^H A^H A \mathbf{x} \mid \mathbf{x} \in T \text{ and } \|\mathbf{x}\|_2 = 1 \} \\ &= \max_{\dim(T)=k} \min_{\mathbf{x}} \{ \|\mathbf{Ax}\|_2^2 \mid \mathbf{x} \in T \text{ and } \|\mathbf{x}\|_2 = 1 \},\end{aligned}$$

which implies the second equality of the theorem.



Corollary

The smallest singular value of a matrix $A \in \mathbb{C}^{m \times n}$ equals

$$\min\{\|Ax\|_2 \mid x \in \mathbb{C}^n \text{ and } \|x\|_2 = 1\}.$$

The largest singular value of a matrix $A \in \mathbb{C}^{m \times n}$ equals

$$\max\{\|Ax\|_2 \mid x \in \mathbb{C}^n \text{ and } \|x\|_2 = 1\}.$$



The SVD allows us to find the best approximation of a matrix by a matrices of limited rank.

Lemma

Let $A = \sigma_1 \mathbf{u}_1 \mathbf{v}_1^H + \cdots + \sigma_r \mathbf{u}_r \mathbf{v}_r^H$ be the SVD of a matrix $A \in \mathbb{R}^{m \times n}$, where $\sigma_1 \geq \cdots \geq \sigma_r > 0$. For every k , $1 \leq k \leq r$ the matrix $B(k) = \sum_{i=1}^k \sigma_i \mathbf{u}_i \mathbf{v}_i^H$ has rank k .

Proof.

The null space of the matrix $B(k)$ consists of those vectors \mathbf{x} such that $B(k)\mathbf{x} = \sum_{i=1}^k \sigma_i \mathbf{u}_i \mathbf{v}_i^H \mathbf{x} = \mathbf{0}$. The linear independence of the vectors \mathbf{u}_i and the fact that $\sigma_i > 0$ for $1 \leq i \leq r$ implies the equalities $\mathbf{v}_i^H \mathbf{x} = 0$ for $1 \leq i \leq k$. Thus, $\mathbf{x} \in \langle \mathbf{v}_1, \dots, \mathbf{v}_k \rangle^\perp$ and, since $\mathbf{v}_1, \dots, \mathbf{v}_k$ are linearly independent it follows that $\dim(\text{NullSp}(B(k))) = n - k$, which implies $\text{rank}(B(k)) = k$ for $1 \leq k \leq r$. □



Theorem

(Eckhart-Young Theorem) Let $A \in \mathbb{C}^{m \times n}$ be a matrix whose sequence of non-zero singular values is $(\sigma_1, \dots, \sigma_r)$. Assume that $\sigma_1 \geq \dots \geq \sigma_r > 0$ and that A can be written as

$$A = \sigma_1 \mathbf{u}_1 \mathbf{v}_1^H + \dots + \sigma_r \mathbf{u}_r \mathbf{v}_r^H.$$

Let $B(k) \in \mathbb{C}^{m \times n}$ be the matrix defined by

$$B(k) = \sum_{i=1}^k \sigma_i \mathbf{u}_i \mathbf{v}_i^H.$$

If $r_k = \inf\{\|A - X\|_2 \mid X \in \mathbb{C}^{m \times n} \text{ and } \text{rank}(X) \leq k\}$, then

$$\|A - B(k)\|_2 = r_k = \sigma_{k+1},$$

for $1 \leq k \leq r$, where $\sigma_{r+1} = 0$ and $B(k)$ is the best approximation of A among the matrices of rank no larger than k in the sense of the norm $\|\cdot\|_2$.

Proof

Observe that

$$A - B(k) = \sum_{i=k+1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^H,$$

and the largest singular value of the matrix $\sum_{i=k+1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^H$ is σ_{k+1} . Since σ_{k+1} is the largest singular value of $A - B(k)$ we have

$\|A - B(k)\|_2 = \sigma_{k+1}$ for $1 \leq k \leq r$.



Proof (cont'd)

We prove now that for every matrix $X \in \mathbb{C}^{m \times n}$ such that $\text{rank}(X) \leq k$, we have $\|A - X\|_2 \geq \sigma_{k+1}$.

Since $\dim(\text{NullSp}(X)) = n - \text{rank}(X)$, it follows that $\dim(\text{NullSp}(X)) \geq n - k$. If T is the subspace of \mathbb{R}^n spanned by $\mathbf{v}_1, \dots, \mathbf{v}_{k+1}$, we have $\dim(T) = k + 1$. Since $\dim(\text{NullSp}(X)) + \dim(T) > n$, the intersection of these subspaces contains a unit non-zero vector \mathbf{x} .

We have $\mathbf{x} = a_1\mathbf{v}_1 + \dots + a_k\mathbf{v}_k + a_{k+1}\mathbf{v}_{k+1}$ because $\mathbf{x} \in T$. The orthogonality of $\mathbf{v}_1, \dots, \mathbf{v}_k, \mathbf{v}_{k+1}$ implies $\|\mathbf{x}\|_2^2 = \sum_{i=1}^{k+1} |a_i|^2 = 1$.



Since $\mathbf{x} \in \text{NullSp}(X)$, we have $X\mathbf{x} = \mathbf{0}$, so

$$(A - X)\mathbf{x} = A\mathbf{x} = \sum_{i=1}^{k+1} a_i A\mathbf{v}_i = \sum_{i=1}^{k+1} a_i \sigma_i \mathbf{u}_i.$$

Thus, we have

$$\|(A - X)\mathbf{x}\|_2^2 = \sum_{i=1}^{k+1} |\sigma_i a_i|^2 \geq \sigma_{k+1}^2 \sum_{i=1}^{k+1} |a_i|^2 = \sigma_{k+1}^2,$$

because $\mathbf{u}_1, \dots, \mathbf{u}_k$ are also orthonormal. This implies

$$\|A - X\|_2 \geq \sigma_{k+1} = \|A - B(k)\|_2.$$



It is interesting to observe that the matrix $B(k)$ provides an optimal approximation of A not only with respect to $\|\cdot\|_2$ but also relative to the Frobenius norm.

Theorem

$B(k)$ is the best approximation of A among matrices of rank no larger than k in the sense of the Frobenius norm.



Proof

Note that $\|A - B(k)\|_F^2 = \|A\|_F^2 - \sum_{i=1}^k \sigma_i^2$. Let X be a matrix of rank k , which can be written as $X = \sum_{i=1}^k \mathbf{x}_i \mathbf{y}_i^H$. Without loss of generality we may assume that the vectors $\mathbf{x}_1, \dots, \mathbf{x}_k$ are orthonormal. If this is not the case, we can use the Gram-Schmidt algorithm to express them as linear combinations of orthonormal vectors, replace these expressions in $\sum_{i=1}^k \mathbf{x}_i \mathbf{y}_i^H$ and rearrange the terms. Now, the Frobenius norm of $A - X$ can be written as

$$\begin{aligned}\|A - X\|_F^2 &= \text{trace} \left(\left(A - \sum_{i=1}^k \mathbf{x}_i \mathbf{y}_i^H \right)^H \left(A - \sum_{i=1}^k \mathbf{x}_i \mathbf{y}_i^H \right) \right) \\ &= \text{trace} \left(A^H A + \sum_{i=1}^k (\mathbf{y}_i - A^H \mathbf{x}_i)(\mathbf{y}_i - A^H \mathbf{x}_i)^H - \sum_{i=1}^k A^H \mathbf{x}_i \mathbf{x}_i^H A \right)\end{aligned}$$



Taking into account that $\sum_{i=1}^k (\mathbf{y}_i - A^H \mathbf{x}_i)(\mathbf{y}_i - A^H \mathbf{x}_i)^H$ is a real non-negative number and that $\sum_{i=1}^k A^H \mathbf{x}_i \mathbf{x}_i^H A = \|A \mathbf{x}_i\|_F^2$ we have

$$\|A - X\|_F^2 \geq \text{trace} \left(A^H A - \sum_{i=1}^k A^H \mathbf{x}_i \mathbf{x}_i^H A \right) = \|A\|_F^2 - \text{trace} \left(\sum_{i=1}^k A^H \mathbf{x}_i \mathbf{x}_i^H A \right)$$

Let $A = U \text{diag}(\sigma_1, \dots, \sigma_n) V^H$ be the singular value decomposition of A . If $V = (V_1 \ V_2)$, where V_1 has k columns $\mathbf{v}_1, \dots, \mathbf{v}_k$, $D_1 = \text{diag}(\sigma_1, \dots, \sigma_k)$ and $D_2 = \text{diag}(\sigma_{k+1}, \dots, \sigma_n)$, then

$$\begin{aligned} A^H A &= V D^H U^H U D V^H = (V_1 \ V_2) \begin{pmatrix} D_1^2 & O \\ O & D_2^2 \end{pmatrix} \begin{pmatrix} V_1^H \\ V_2^H \end{pmatrix} \\ &= V_1 D_1^2 V_1^H + V_2 D_2^2 V_2^H. \end{aligned}$$

and $A^H A = V D^2 V^H$.



Proof (cont'd)

These equalities allow us to write:

$$\begin{aligned}\|A\mathbf{x}_i\|_F^2 &= \text{trace}(\mathbf{x}_i^H A^H A \mathbf{x}_i) \\ &= \text{trace}(\mathbf{x}_i^H V_1 D_1^2 V_1^H \mathbf{x}_i + \mathbf{x}_i^H V_2 D_2^2 V_2^H \mathbf{x}_i) \\ &= \|D_1 V_1^H \mathbf{x}_i\|_F^2 + \|D_2 V_2^H \mathbf{x}_i\|_F^2 \\ &= \sigma_k^2 + (\|D_1 V_1^H \mathbf{x}_i\|_F^2 - \sigma_k^2 \|V_1^H \mathbf{x}_i\|_F^2) \\ &\quad - (\sigma_k^2 \|V_2^H \mathbf{x}_i\|_F^2 - \|D_2 V_2^H \mathbf{x}_i\|_F^2) - \sigma_k^2(1 - \|V^H \mathbf{x}_i\|_F^2).\end{aligned}$$

Since $\|V^H \mathbf{x}_i\|_F^2 = 1$ (because \mathbf{x}_i is a unit vector and V is a unitary matrix) and $\sigma_k^2 \|V_2^H \mathbf{x}_i\|_F^2 - \|D_2 V_2^H \mathbf{x}_i\|_F^2 \geq 0$, it follows that

$$\|A\mathbf{x}_i\|_F^2 \leq \sigma_k^2 + (\|D_1 V_1^H \mathbf{x}_i\|_F^2 - \sigma_k^2 \|V_1^H \mathbf{x}_i\|_F^2).$$



Proof (cont'd)

Consequently,

$$\begin{aligned}\sum_{i=1}^k \|A\mathbf{x}_i\|_F^2 &\leq k\sigma_k^2 + \sum_{i=1}^k (\|D_1 V_1^H \mathbf{x}_i\|_F^2 - \sigma_k^2 \|V_1^H \mathbf{x}_i\|_F^2) \\&= k\sigma_k^2 + \sum_{i=1}^k \sum_{j=1}^k (\sigma_j^2 - \sigma_k^2) |\mathbf{v}_j^H \mathbf{x}_i|^2 \\&= \sum_{j=1}^k \left(\sigma_k^2 + (\sigma_j^2 - \sigma_k^2) \sum_{i=1}^k |\mathbf{v}_j^H \mathbf{x}_i|^2 \right) \\&\leq \sum_{j=1}^k (\sigma_k^2 + (\sigma_j^2 - \sigma_k^2)) = \sum_{j=1}^k \sigma_j^2,\end{aligned}$$

which concludes the argument.

