PRINCIPLE COMPONENT ANALYSIS AND SINGULAR VALUE DECOMPOSITION

1

吳沛遠 **Pei-Yuan Wu**
Dept. Electrical Engineering
National Taiwan University

2023/10/13

AGENDA

- Linear Algebra Preliminaries
- Spectral theorem for Symmetric matrices
- Principle Component Analyais (PCA)
- Singular Value Decomposition (SVD)

3

LINEAR ALGEBRA PRELIMINARIES

VECTOR SPACE

Vector space $(V, F, +, \cdot)$

- V: A set of objects (called vectors)
- F: Field (e.g., $\mathbb{R}$ or $\mathbb{C}$)
- Addition of vectors $+: V \times V \to V$ (i.e., addition is closed in V)
  - Commutativity: $\boldsymbol{x} + \boldsymbol{y} = \boldsymbol{y} + \boldsymbol{x}$
  - Associativity: $(\boldsymbol{x} + \boldsymbol{y}) + \boldsymbol{z} = \boldsymbol{x} + (\boldsymbol{y} + \boldsymbol{z})$
  - $\exists \mathbf{0} \in V$ such that $\mathbf{0} + \boldsymbol{x} = \boldsymbol{x} + \mathbf{0} = \boldsymbol{x}, \forall \boldsymbol{x} \in V$
    - ✓ Proposition: $\mathbf{0}$ is unique, called the *zero vector*. (Exercise)
  - $\forall \boldsymbol{x} \in V, \exists (-\boldsymbol{x}) \in V$ such that $\boldsymbol{x} + (-\boldsymbol{x}) = \mathbf{0}$
    - ✓ Proposition: $\forall \boldsymbol{x} \in V$, $(-\boldsymbol{x})$ is unique, called the *additive inverse* of $\boldsymbol{x}$. (Exercise)
- Scalar multiplication: $\cdot: F \times V \to V$ (i.e., scalar multiplication is closed in V)
  - Compatibility: $a(b\boldsymbol{x}) = (ab)\boldsymbol{x}, \forall \boldsymbol{x} \in V, a, b \in F$
  - Distributivity: $a(\boldsymbol{x} + \boldsymbol{y}) = a\boldsymbol{x} + a\boldsymbol{y},\ (a + b)\boldsymbol{x} = a\boldsymbol{x} + b\boldsymbol{x}, \forall \boldsymbol{x}, \boldsymbol{y} \in V, a, b \in F$
  - $1\boldsymbol{x} = \boldsymbol{x}$
- Example: Euclidean space $\mathbb{R}^n$.

INNER PRODUCT SPACE

- An ***<u>inner product space</u>*** is a vector space V over the field F ($\mathbb{R}$ or $\mathbb{C}$) together with an inner product

$$\langle \cdot,\cdot \rangle : \mathrm{V} \times \mathrm{V} \rightarrow F$$

  That satisfies the following three axioms for all vectors $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z} \in V$ and all scalars $a \in F$:

  - Conjugate symmetry: $\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \overline{\langle \boldsymbol{y}, \boldsymbol{x} \rangle}$
  - Linearity in the first argument

$$\langle a\boldsymbol{x}, \boldsymbol{y} \rangle = a\langle \boldsymbol{x}, \boldsymbol{y} \rangle$$
$$\langle \boldsymbol{x} + \boldsymbol{y}, \boldsymbol{z} \rangle = \langle \boldsymbol{x}, \boldsymbol{z} \rangle + \langle \boldsymbol{y}, \boldsymbol{z} \rangle$$

  - Positive definiteness

$$\langle \boldsymbol{x}, \boldsymbol{x} \rangle \geq 0$$
$$\langle \boldsymbol{x}, \boldsymbol{x} \rangle = 0 \Leftrightarrow \boldsymbol{x} = 0$$

EUCLIDEAN SPACE

- Euclidean space $\mathbb{R}^n = \left\{ \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} : x_1, \ldots, x_n \in \mathbb{R} \right\}$
- $\mathbb{R}^n$ is a vector space over field $\mathbb{R}$ by defining elementwise addition and scalar multiplication: (Exercise: Prove that vector space axioms hold)
  - Addition: $\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} x_1 + y_1 \\ \vdots \\ x_n + y_n \end{bmatrix}$
  - Scalar multiplication: $\alpha \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} \alpha x_1 \\ \vdots \\ \alpha x_n \end{bmatrix}, \alpha \in \mathbb{R}$
- $\mathbb{R}^n$ is an inner product space by defining inner (dot) product:
  - Inner (dot) product: $\left\langle \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \right\rangle_{\mathbb{R}^n} = x_1 y_1 + \cdots + x_n y_n \in \mathbb{R}$

COMPLEX EUCLIDEAN SPACE

- Complex Euclidean space $\mathbb{C}^n = \left\{ \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} : x_1, \dots, x_n \in \mathbb{C} \right\}$
- $\mathbb{C}^n$ is a vector space over field $\mathbb{C}$ by defining elementwise addition and scalar multiplication: (Exercise: Prove that vector space axioms hold)
  - Addition: $\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} x_1 + y_1 \\ \vdots \\ x_n + y_n \end{bmatrix}$
  - Scalar multiplication: $\alpha \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} \alpha x_1 \\ \vdots \\ \alpha x_n \end{bmatrix}, \alpha \in \mathbb{C}$
- $\mathbb{C}^n$ is an inner product space by defining inner (dot) product:
  - Inner (dot) product: $\left\langle \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \right\rangle_{\mathbb{C}^n} = x_1 \overline{y_1} + \cdots + x_n \overline{y_n} \in \mathbb{C}$

LINEAR MAPPING

- Let V and W be vector spaces over the same field F. A function $T: V \to W$ is said to be a ***linear mapping*** if it preserves the addition and scalar multiplication operations. Namely,

$$T(a\boldsymbol{x} + b\boldsymbol{y}) = aT(\boldsymbol{x}) + bT(\boldsymbol{y}), \forall \boldsymbol{x}, \boldsymbol{y} \in M, a, b \in F$$

- Example: Let F be a field ($\mathbb{R}$ or $\mathbb{C}$). Each matrix $\mathrm{A} \in F^{m \times n}$ can be considered as a linear mapping $T: F^n \to F^m$ defined as

$$T(\boldsymbol{x}) = A\boldsymbol{x}$$

- Proposition: Let F be a field ($\mathbb{R}$ or $\mathbb{C}$). Each linear mapping $T: F^n \to F^m$ can be represented by a matrix $A \in F^{m \times n}$ such that

$$T(\boldsymbol{x}) = A\boldsymbol{x}, \forall \boldsymbol{x} \in F^n$$

EIGEN-VECTOR AND EIGEN-VALUE

- Let V be vector space over the same field F, $T: V \to V$ be a linear mapping. We call $\boldsymbol{v} \in V$ an ***eigenvector*** of T if $\boldsymbol{v} \neq \mathbf{0}$ and
$$T(\boldsymbol{v}) = \lambda \boldsymbol{v}$$
where $\lambda \in F$. We call λ the ***eigenvalue*** associated with $\boldsymbol{v}$.
- Let F be a field ($\mathbb{R}$ or $\mathbb{C}$). A matrix $A \in F^{n\times n}$ can be viewed as a linear mapping $T: F^n \to F^n$, $T(\boldsymbol{x}) = A\boldsymbol{x}$. Hence we call λ the eigenvalue (of A) associated with eigenvector (of A) $\boldsymbol{v} \in F^n$ if $\boldsymbol{v} \neq \mathbf{0}$ and
$$A\boldsymbol{v} = \lambda \boldsymbol{v}$$
- Exercise: Eigenvector and eigenvalue of
$$A = \begin{bmatrix} -1 & 6 \\ 3 & 2 \end{bmatrix}$$

10

SPECTRAL THEOREM FOR SYMMETRIC MATRICES

In this lecture, we want to prove that

SYMMETRIC MATRIX IS DIAGONALIZABLE

- **Theorem 5:** If $A \in \mathbb{R}^{n\times n}$ is *symmetric*, then there exists diagonal matrix $\Lambda \in \mathbb{R}^{n\times n}$ and *orthogonal* matrix $U \in \mathbb{R}^{n\times n}$ such that $A = U\Lambda U^T$

$$\boldsymbol{U} = [\boldsymbol{v}_1, \boldsymbol{v}_2, \dots, \boldsymbol{v}_n]$$

eigenvectors

$$\boldsymbol{\Lambda} = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & & \vdots \\ \vdots & & \ddots & \vdots \\ & 0 & \cdots & \lambda_n \end{bmatrix}$$

Eigen Values

$$A\boldsymbol{v}_k = \lambda_k \boldsymbol{v}_k$$

Symmetric:

$A = [a_{ij}] \in \mathbb{C}^{n\times n}$ is symmetric if $a_{ij} = a_{ji}$

Orthogonal matrix:

$U = [\boldsymbol{v}_1 \dots \boldsymbol{v}_\mathrm{n}] \in \mathbb{R}^{n\times n}$ is an orthogonal matrix if $\boldsymbol{v}_1, \dots, \boldsymbol{v}_\mathrm{n}$ are orthogonal and have unit length

$$\boldsymbol{v}_\mathrm{k}^T \boldsymbol{v}_\ell = \begin{cases} 1 & \text{if } \mathrm{k} = \ell \\ 0 & \text{if } \mathrm{k} \neq \ell \end{cases}$$

That is, $U^TU = I$, namely, $U^{-1} = U^T$.

We would also want to prove that

HERMITIAN MATRIX IS DIAGONALIZABLE

- **Theorem 4:** If $A \in \mathbb{C}^{n\times n}$ is *Hermitian*, then there exists diagonal matrix $\Lambda \in \mathbb{R}^{n\times n}$ and *unitary* matrix $U \in \mathbb{C}^{n\times n}$ such that $A = U\Lambda U^{\mathrm{H}}$

$$U = [\boldsymbol{v}_1, \boldsymbol{v}_2, \dots, \boldsymbol{v}_n]$$

eigenvectors

$$\Lambda = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & & \\ \vdots & & \ddots & \vdots \\ 0 & & \cdots & \lambda_n \end{bmatrix}$$

Eigen Values

$$A\boldsymbol{v}_k = \lambda_k \boldsymbol{v}_k$$

Conjugate transpose:

The conjugate transpose of $A \in \mathbb{C}^{m\times n}$ *is* denoted as $A^H = \overline{A^T} \in \mathbb{C}^{n\times m}$

Hermitian:

$A = [a_{ij}] \in \mathbb{C}^{n\times n}$ is Hermitian if $a_{ij} = \overline{a_{ji}}$

Unitary Matrix:

$U = [\boldsymbol{v}_1 \dots \boldsymbol{v}_{\mathrm{n}}] \in \mathbb{C}^{n\times n}$ is an unitary matrix if $\boldsymbol{v}_1, \dots, \boldsymbol{v}_{\mathrm{n}}$ are orthogonal and have unit length

$$\boldsymbol{v}_{\mathrm{k}}^H \boldsymbol{v}_\ell = \begin{cases} 1 & \text{if } \mathrm{k} = \ell \\ 0 & \text{if } \mathrm{k} \neq \ell \end{cases}$$

That is, $U^H U = I$

INVARIANT SUBSPACE

- M is called a ***<u>subspace</u>*** of vector space (V, F), if it is closed under vector addition and multiplication. Namely,
$$a\boldsymbol{x} + b\boldsymbol{y} \in M, \forall \boldsymbol{x}, \boldsymbol{y} \in M, a, b \in F$$
- Let V be a vector space, $T: V \to V$ be a linear mapping. M is called an ***<u>invariant subspace</u>*** of T if $T(\boldsymbol{x}) \in M, \forall \boldsymbol{x} \in M$.
- Let F be a field ($\mathbb{R}$ or $\mathbb{C}$). A matrix $A \in F^{m \times n}$ can be viewed as a linear mapping $T: F^n \to F^m, T(\boldsymbol{x}) = A\boldsymbol{x}$. We call M an invariant subspace of A if $A\boldsymbol{x} \in M, \forall \boldsymbol{x} \in M$.

ADJOINT OPERATOR

- Let H_1, H_2 be inner product spaces, $T: H_1 \to H_2$ be a linear mapping. If a linear mapping $T^*: H_2 \to H_1$ satisfies

$$\langle T\mathbf{x}, \mathbf{y}\rangle_{H_2} = \langle \mathbf{x}, T^*\mathbf{y}\rangle_{H_1}, \forall \mathbf{x} \in H_1, \mathbf{y} \in H_2$$

  Then we call T^* *the* ***adjoint*** of T.

- **Proposition:** T^* is unique (if it does exist) (Exercise)
- **Proposition:** $(T^*)^* = T$

  Proof: $\langle T^*\boldsymbol{y}, \boldsymbol{x}\rangle_{H_1} = \overline{\langle \boldsymbol{x}, T^*\boldsymbol{y}\rangle_{H_1}} = \overline{\langle T\boldsymbol{x}, \boldsymbol{y}\rangle_{H_2}} = \langle \boldsymbol{y}, T\boldsymbol{x}\rangle_{H_2}, \forall \boldsymbol{x} \in H_1, \boldsymbol{y} \in H_2$

- Example: Suppose linear mapping $T: \mathbb{C}^n \to \mathbb{C}^m$ is represented by $A \in \mathbb{C}^{m\times n}$. Since

$$\langle T\boldsymbol{x}, \boldsymbol{y}\rangle = \langle A\boldsymbol{x}, \boldsymbol{y}\rangle = \boldsymbol{y}^H(A\boldsymbol{x}) = (A^H\boldsymbol{y})^H\boldsymbol{x} = \langle \boldsymbol{x}, A^H\boldsymbol{y}\rangle,$$

  therefore T has adjoint $T^*: \mathbb{C}^m \to \mathbb{C}^n$, which is represented by $A^H \in \mathbb{C}^{m\times n}$.

SELF ADJOINT

- Let H be inner product space, $T: H \to H$ be a linear mapping. We call T ***self-adjoint*** if T^* exists and
$$T = T^*$$
- Example: If linear mapping $T: \mathbb{C}^n \to \mathbb{C}^n$ is self-adjoint and represented by $A \in \mathbb{C}^{n \times n}$, then $A = A^H$, i.e., A is Hermitian.
- **Proposition:** If λ is an eigenvalue of self-adjoint mapping T, then $\lambda \in \mathbb{R}$.

Proof: Let $\boldsymbol{x}$ be an eigenvector associated with λ, then
$$\lambda\langle \boldsymbol{x}, \boldsymbol{x}\rangle = \langle T\boldsymbol{x}, \boldsymbol{x}\rangle = \langle \boldsymbol{x}, T^*\boldsymbol{x}\rangle = \langle \boldsymbol{x}, T\boldsymbol{x}\rangle = \bar{\lambda}\langle \boldsymbol{x}, \boldsymbol{x}\rangle$$
Therefore $\lambda = \bar{\lambda}$.

NORMAL OPERATOR

- Let H be inner product space, $T: H \to H$ be a linear mapping. We call T ***normal*** if T^* exists and $TT^* = T^*T$.
- Example: Suppose linear mapping $T: \mathbb{C}^n \to \mathbb{C}^n$ is represented by $A \in \mathbb{C}^{n\times n}$, then T is normal iff $AA^H = A^H A$.
- **Proposition:** If $A \in \mathbb{C}^{n\times n}$ is normal, then

$$\|A\boldsymbol{x} - \lambda\boldsymbol{x}\|^2 = \left\|A^H\boldsymbol{x} - \bar{\lambda}\boldsymbol{x}\right\|^2, \forall \boldsymbol{x} \in \mathbb{C}^n, \lambda \in \mathbb{C}$$

Proof:

$\|A\boldsymbol{x} - \lambda\boldsymbol{x}\|^2 = \boldsymbol{x}^H\left(A^H A - \lambda A^H - \bar{\lambda}A + |\lambda|^2 I\right)\boldsymbol{x} = \boldsymbol{x}^H\left(AA^H - \bar{\lambda}A - \lambda A^H + |\lambda|^2 I\right)\boldsymbol{x} = \left\|A^H\boldsymbol{x} - \bar{\lambda}\boldsymbol{x}\right\|^2$

- **Proposition:** Let $A = U\Lambda U^{\mathrm{H}}$ for which $\Lambda \in \mathbb{C}^{n\times n}$ is diagonal and $U \in \mathbb{C}^{n\times n}$ is unitary, then A is normal

Proof: $AA^H = U\Lambda\Lambda^H U^H = U\Lambda^H\Lambda U^H = A^H A$

NORMAL MATRIX IS DIAGONALIZABLE

- **Lemma 1:** If $\boldsymbol{v}_1, \boldsymbol{v}_2, \dots, \boldsymbol{v}_{\mathrm{k}}$ are eigenvectors of a linear mapping T on inner product space H, then $M_k = \{\boldsymbol{x} \in H | \langle \boldsymbol{x}, \boldsymbol{v}_i \rangle = 0, \forall i = 1,2, \dots, k\}$ is an invariant subspace of T^*.

Proof: For $\mathrm{x} \in \mathrm{M}_{\mathrm{k}}$, holds

$$\langle T^* \boldsymbol{x}, \boldsymbol{v}_i \rangle = \langle \boldsymbol{x}, T \boldsymbol{v}_i \rangle = \overline{\lambda_i} \langle \boldsymbol{x}, \boldsymbol{v}_i \rangle = 0, \forall \boldsymbol{x} \in M_k, i = 1,2, \dots, k$$

NORMAL MATRIX IS DIAGONALIZABLE

- **Lemma 2:** If M is a non-trivial invariant subspace of linear mapping $T: \mathbb{C}^n \to \mathbb{C}^n$, then there exists $\lambda \in \mathbb{C}$, $\boldsymbol{v} \in M$, $\boldsymbol{v} \neq \mathbf{0}$ such that $T\boldsymbol{v} = \lambda\boldsymbol{v}$

Proof: Take $\mathrm{A} \in \mathbb{C}^{n\times n}$ which represents T. Take $\mathrm{U} \in \mathbb{C}^{n\times m}$ whose columns $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_m$ form an orthonormal basis of M. Define $\psi: \mathbb{C}^m \to M$ as

$$\psi\left(\begin{bmatrix} c_1 \\ \vdots \\ c_m \end{bmatrix}\right) = \sum_{i=1}^{m} c_i \boldsymbol{u}_i$$

Then ψ is a one-to-one onto linear mapping. Consider linear mapping $\psi^{-1} \circ T \circ \psi: \mathbb{C}^m \to \mathbb{C}^m$ which can be represented by $U^H A U \in \mathbb{C}^{m\times m}$, it is evident that there exists some $\lambda \in \mathbb{C}$, $\boldsymbol{c} \in \mathbb{C}^m$, $\mathbf{c} \neq \mathbf{0}$ such that $U^H A U\boldsymbol{c} = \lambda\boldsymbol{c}$. (Hint: Take λ sastisfying $\det(U^H A U - \lambda I) = 0$ and nonzero vector $\boldsymbol{c} \in Null(U^H A U - \lambda I)$). Note that

$$\psi^{-1} \circ T \circ \psi(\boldsymbol{c}) = U^H A U\boldsymbol{c} = \lambda\boldsymbol{c} \Rightarrow T\big(\psi(\boldsymbol{c})\big) = \psi(\lambda\boldsymbol{c}) = \lambda\psi(\boldsymbol{c})$$

Therefore $\boldsymbol{v} = \psi(\boldsymbol{c}) \in M$ is a nonzero vector satisfying $T\boldsymbol{v} = \lambda\boldsymbol{v}$. Q.E.D.

NORMAL MATRIX IS DIAGONALIZABLE

- **Theorem 3:** If $A \in \mathbb{C}^{n\times n}$ is normal, then there exists diagonal matrix $\Lambda \in \mathbb{C}^{n\times n}$ and unitary matrix $U \in \mathbb{C}^{n\times n}$ such that $A = U\Lambda U^H$.

Proof: We will construct pairwise-orthogonal eigenvectors $\boldsymbol{v}_1, \dots, \boldsymbol{v}_\mathrm{n}$ with associating eigenvalues $\lambda_1, \dots, \lambda_\mathrm{n}$ of A as follows:

For $k = 1,2, \dots, n$, suppose $\boldsymbol{v}_1, \dots, \boldsymbol{v}_{\mathrm{k}-1}$ are pairwise-orthogonal eigenvectors of A. By Lemma 1,

$$M_{k-1} = \{\boldsymbol{x} \in \mathbb{C}^n | \langle \boldsymbol{x}, \boldsymbol{v}_i \rangle = 0, \forall i = 1, \dots, k-1\}$$

is a non-trivial invariant subspace of A. Therefore, by Lemma 2, there exists $\lambda_\mathrm{k} \in \mathbb{C}$, $\boldsymbol{v}_\mathrm{k} \in M_{k-1}$, $\boldsymbol{v}_\mathrm{k} \neq \mathbf{0}$ such that $A^H \boldsymbol{v}_\mathrm{k} = \overline{\lambda_\mathrm{k}} \boldsymbol{v}_\mathrm{k}$, which implies $A\boldsymbol{v}_\mathrm{k} = \lambda_\mathrm{k} \boldsymbol{v}_\mathrm{k}$. In other words, $\boldsymbol{v}_\mathrm{k}$ is an eigenvector of A with associating eigenvalue λ_k which is orthogonal to $\boldsymbol{v}_1, \dots, \boldsymbol{v}_{\mathrm{k}-1}$. Hence $\boldsymbol{v}_1, \dots, \boldsymbol{v}_\mathrm{k}$ are pairwise-orthogonal eigenvectors of A.

The above procedure thus constructs pairwise-orthogonal eigenvectors $\boldsymbol{v}_1, \dots, \boldsymbol{v}_\mathrm{n}$ with associating eigenvalues $\lambda_1, \dots, \lambda_\mathrm{n}$ of A.

NORMAL MATRIX IS DIAGONALIZABLE

- **Theorem 3:** If $A \in \mathbb{C}^{n\times n}$ is normal, then there exists diagonal matrix $\Lambda \in \mathbb{C}^{n\times n}$ and unitary matrix $U \in \mathbb{C}^{n\times n}$ such that $A = U\Lambda U^H$.

Proof: (cont'd) We have shown the existence of pairwise-orthogonal eigenvectors $\boldsymbol{v}_1, \dots, \boldsymbol{v}_\mathrm{n}$, normalized to unit length $\|\boldsymbol{v}_i\| = 1$, with associating eigenvalues $\lambda_1, \dots, \lambda_\mathrm{n}$. Set $U = [\boldsymbol{v}_1 \dots \boldsymbol{v}_\mathrm{n}] \in \mathbb{C}^{n\times n}$, then $U^\mathrm{H} U = I$, i.e., U is unitary. Since for every $\boldsymbol{c} \in \mathbb{C}^n$, one has

$$AU\boldsymbol{c} = A\sum_{i=1}^{m} c_i\boldsymbol{v}_i = \sum_{i=1}^{m} c_i A\boldsymbol{v}_i = \sum_{i=1}^{m} c_i\lambda_i\boldsymbol{v}_i = U\Lambda\boldsymbol{c}$$

Where $\Lambda = diag(c_1, \dots, c_n)$. Therefore $AU = U\Lambda$ which implies $A = U\Lambda U^{-1} = U\Lambda U^H$.
Q.E.D.

That is, a normal matrix A can always be written as $A = U\Lambda U^H$, where U is an unitary matrix of eigenvectors, and Λ is a diagonal matrix of the associated eigenvalues.

HERMITIAN MATRIX IS DIAGONALIZABLE

Since every Hermitian matrix is normal (so is diagonizable) and self-adjoint (so eigenvalues are real), one immediately obtains Theorem 4, as restated below:

- **Theorem 4:** If $A \in \mathbb{C}^{n \times n}$ is *Hermitian*, then there exists diagonal matrix $\Lambda \in \mathbb{R}^{n \times n}$ and *unitary* matrix $U \in \mathbb{C}^{n \times n}$ such that $A = U \Lambda U^{\mathrm{H}}$.

REAL SYMMETRIC MATRIX IS DIAGONALIZABLE WITH REAL EIGENVECTORS

- **Lemma 3:** If M is a non-trivial invariant subspace of self-adjoint operator $T: \mathbb{R}^n \to \mathbb{R}^n$, then there exists $\lambda \in \mathbb{R}, \boldsymbol{v} \in M, \boldsymbol{v} \neq \boldsymbol{0}$ such that $T\boldsymbol{v} = \lambda\boldsymbol{v}$

Proof: Take symmetric matrix $\mathrm{A} \in \mathbb{R}^{n\times n}$ which represents T. Take $\mathrm{U} \in \mathbb{R}^{n\times m}$ whose columns $\boldsymbol{u}_1, \dots, \boldsymbol{u}_m$ form an orthonormal basis of M. Define $\psi: \mathbb{R}^m \to M$ as

$$\psi\left(\begin{bmatrix} c_1 \\ \vdots \\ c_m \end{bmatrix}\right) = \sum_{i=1}^{m} c_i \boldsymbol{u}_i$$

Then ψ is a one-to-one onto linear mapping. Consider linear mapping $\psi^{-1} \circ T \circ \psi: \mathbb{R}^m \to \mathbb{R}^m$ which can be represented by $U^T AU \in \mathbb{R}^{m\times m}$. Note that $U^T AU$ is self-adjoint, so it has eigenvalue $\lambda \in \mathbb{R}$ and there is non-zero $\boldsymbol{c} \in \mathbb{R}^m$ for which $U^T AU\boldsymbol{c} = \lambda\boldsymbol{c}$. Note that

$$\psi^{-1} \circ T \circ \psi(\boldsymbol{c}) = U^T AU\boldsymbol{c} = \lambda\boldsymbol{c} \Rightarrow T\big(\psi(\boldsymbol{c})\big) = \psi(\lambda\boldsymbol{c}) = \lambda\psi(\boldsymbol{c})$$

Therefore $\boldsymbol{v} = \psi(\boldsymbol{c}) \in M$ is a nonzero vector satisfying $T\boldsymbol{v} = \lambda\boldsymbol{v}$. Q.E.D.

REAL SYMMETRIC MATRIX IS DIAGONALIZABLE WITH REAL EIGENVECTORS

- **Theorem 5:** If $A \in \mathbb{R}^{n\times n}$ is symmetric, then there exists diagonal matrix $\Lambda \in \mathbb{R}^{n\times n}$ and orthogonal matrix $U \in \mathbb{R}^{n\times n}$ such that $A = U\Lambda U^T$.

Proof: We will construct pairwise-orthogonal eigenvectors $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_\mathrm{n}$ with associating eigenvalues $\lambda_1, \ldots, \lambda_\mathrm{n}$ of A as follows:

For $k = 1,2, \ldots, n$, suppose $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{\mathrm{k}-1}$ are pairwise-orthogonal eigenvectors of A. By Lemma 1,

$$M_{k-1} = \{\mathbf{x} \in \mathbb{R}^n | \langle \mathbf{x}, \boldsymbol{v}_\mathrm{i} \rangle = 0, \forall \mathrm{i} = 1, \ldots, \mathrm{k} - 1\}$$

is a non-trivial invariant subspace of $A^T = A$. Therefore, by Lemma 3, there exists $\lambda \in \mathbb{R}$, $\boldsymbol{v}_\mathrm{k} \in M_{k-1}$, $\boldsymbol{v}_\mathrm{k} \neq \mathbf{0}$ such that $\mathrm{A}\boldsymbol{v}_\mathrm{k} = \lambda_\mathrm{k}\boldsymbol{v}_\mathrm{k}$. In other words, $\boldsymbol{v}_\mathrm{k}$ is an eigenvector of A with associating eigenvalue λ_k which is orthogonal to $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{\mathrm{k}-1}$. Hence $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_\mathrm{k}$ are pairwise-orthogonal eigenvectors of A.

The above procedure thus constructs pairwise-orthogonal eigenvectors $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_\mathrm{n}$ with associating eigenvalues $\lambda_1, \ldots, \lambda_\mathrm{n}$ of A.

REAL SYMMETRIC MATRIX IS DIAGONALIZABLE WITH REAL EIGENVECTORS

- **Theorem 5:** If $A \in \mathbb{R}^{n\times n}$ is symmetric, then there exists diagonal matrix $\Lambda \in \mathbb{R}^{n\times n}$ and orthogonal matrix $U \in \mathbb{R}^{n\times n}$ such that $A = U\Lambda U^T$.

Proof: (cont'd): We have shown the existence of pairwise-orthogonal eigenvectors $\boldsymbol{v}_1, \dots, \boldsymbol{v}_{\mathrm{n}}$, normalized to unit length $\|\boldsymbol{v}_i\| = 1$, with associating eigenvalues $\lambda_1, \dots, \lambda_{\mathrm{n}}$. Set $U = [\boldsymbol{v}_1 \dots \boldsymbol{v}_{\mathrm{n}}] \in \mathbb{R}^{n\times n}$, then $U^T U = I$, i.e., U is orthogonal. Since for every $\boldsymbol{c} \in \mathbb{R}^n$, one has

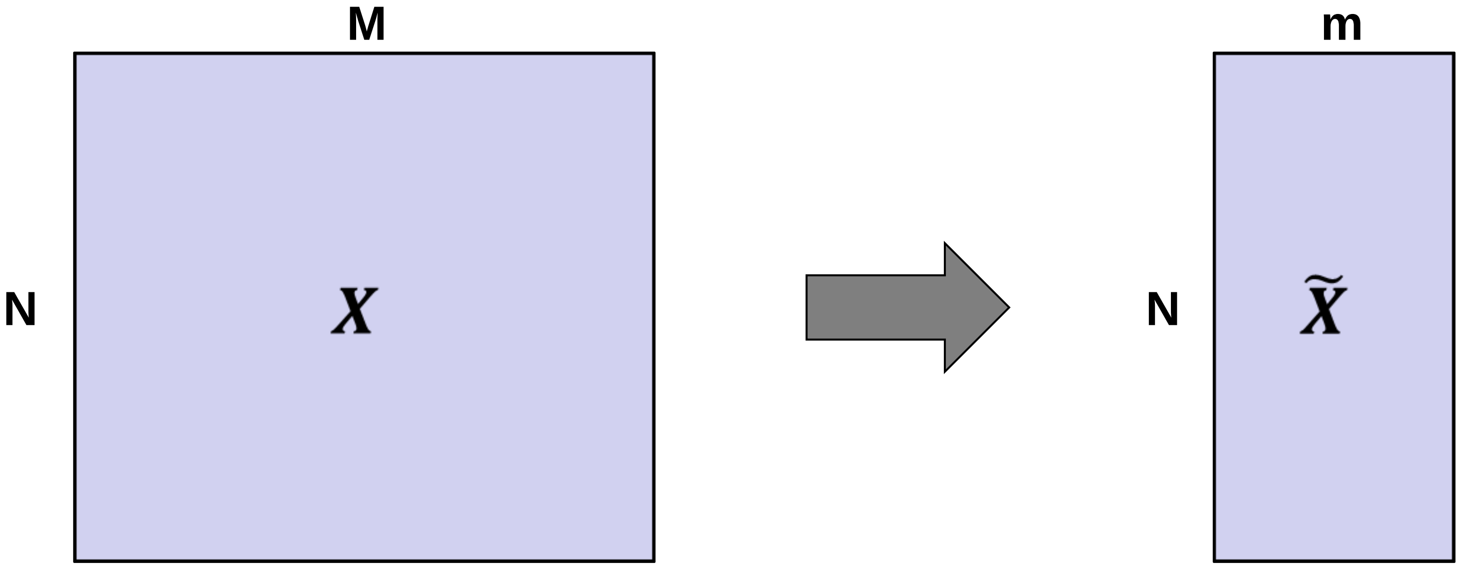
$$AU\boldsymbol{c} = A\sum_{i=1}^{m} c_i\boldsymbol{v}_i = \sum_{i=1}^{m} c_i A\boldsymbol{v}_i = \sum_{i=1}^{m} c_i\lambda_i\boldsymbol{v}_i = U\Lambda\boldsymbol{c}$$

Where $\Lambda = diag(c_1, \dots, c_n)$. Therefore $AU = U\Lambda$ which implies $A = U\Lambda U^{-1} = U\Lambda U^T$.
Q.E.D.

PRINCIPLE COMPONENT ANALYAIS (PCA)

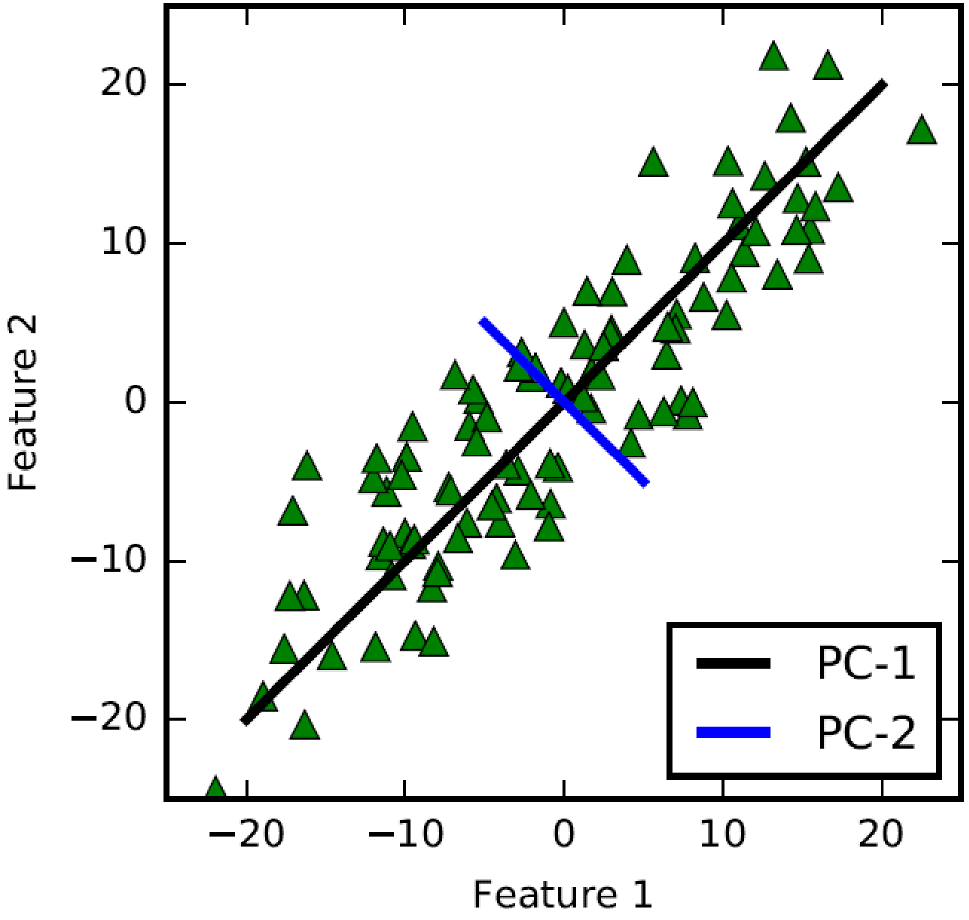
DIMENSIONALITY REDUCTION

- Mapping the original high-dimensional data onto a lower-dimensional subspace.
- Pros for dimensionality reduction
  - Clarity of representation, ease of understanding (e.g., visualization in 2D or 3D)
  - Data compression, computational cost reduction.
  - Noise reduction, prevention of overfitting
- Cons for dimensionality reduction
  - oversimplification: loss of important or relevant information



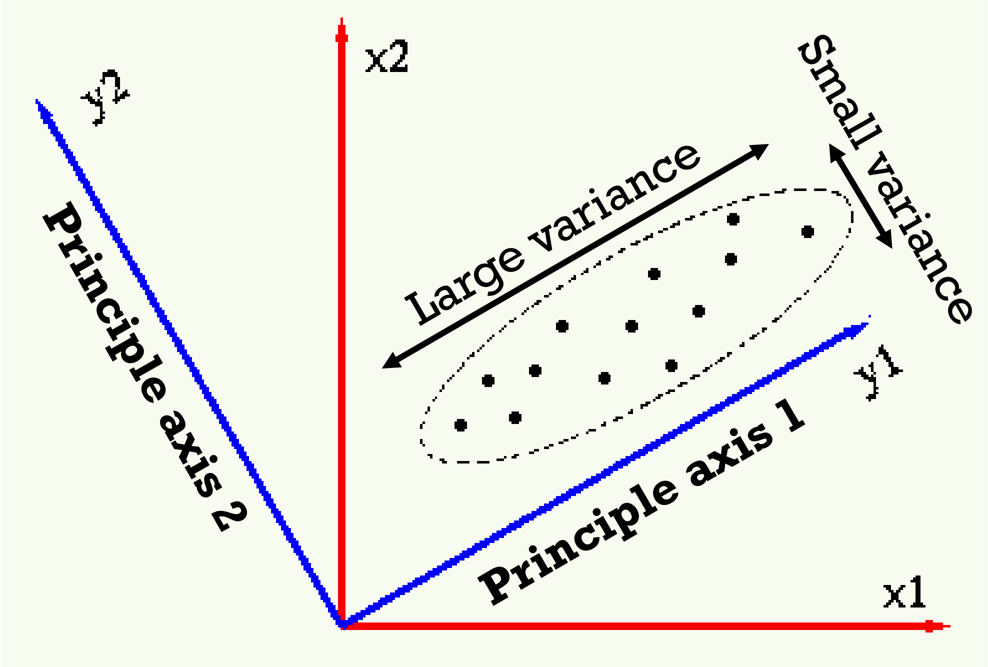
PRINCIPAL COMPONENT ANALYSIS (PCA)

- PCA's target: finding the best lower dimensional sub-space that conveys most of the variance in the original data
- Example: If we were to compress 2-D data to 1-D subspace, then PCA prefers projecting to the ***black*** line, since it preserves more variance comparing to ***blue*** line.



PRINCIPLE AXES

- Objective of PCA: Given data in $\mathbb{R}^M$, want to *rigidly rotate* the axes to new positions (principle axes) with the following properties:
  - ➢ *Ordered such that principle axis 1 has the highest variance, axis 2 has the next highest variance, …, and axis M has the lowest variance.*
  - ➢ *Covariance among each pair of the principal axes is zero.*
- The k'th ***principle component*** is the projection to the k'th principle axis.
- Keep the first $m < M$ principle components for dimensionality reduction.



PRINCIPLE COMPONENT COMPUTATION

- Given N data $\boldsymbol{x}_1, \dots, \boldsymbol{x}_N \in \mathbb{R}^M$, PCA first compute the covariance matrix for the data
$$\boldsymbol{\Sigma} = \frac{1}{N}\sum_{i=1}^{N}(\boldsymbol{x}_i - \boldsymbol{\mu})(\boldsymbol{x}_i - \boldsymbol{\mu})^T = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^T$$
where $\boldsymbol{\mu} \in \mathbb{R}^M$ is the data mean.
- Since $\boldsymbol{\Sigma}$ is symmetric, $\boldsymbol{\Sigma}$ can be written as $\boldsymbol{\Sigma} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^T$, where $\boldsymbol{U} = [\boldsymbol{v}_1 \dots \boldsymbol{v}_{\mathrm{n}}]$ is unitary matrix of eigenvectors (of $\boldsymbol{\Sigma}$), $\boldsymbol{\Lambda} = diag(\lambda_1, \dots, \lambda_M)$ is diagonal matrix of the associated eigenvalues arranged in non-ascending order $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_M \geq 0$. (Note that all eigenvalues are non-negative real scalars since $\boldsymbol{\Sigma}$ is ***semi-positive definite***.)
- For data $\boldsymbol{x} \in \mathbb{R}^M$, compute its 1st principle component as $\boldsymbol{v}_1^T\boldsymbol{x}$, 2nd principle component as $\boldsymbol{v}_2^T\boldsymbol{x}$,…, M'th principle component as $\boldsymbol{v}_M^T\boldsymbol{x}$

Positive definite:
$A \in \mathbb{R}^{n\times n}$ is semi-positive definite if $\boldsymbol{x}^T A\boldsymbol{x} \geq 0$ for all $\boldsymbol{x} \in \mathbb{R}^n$. If the equality holds only when $\boldsymbol{x} = \boldsymbol{0}$, then A is positive definite.

PRINCIPLE COMPONENTS ARE UNCORRELATED

- The covariance of the k'th and ℓ'th principle components of data $\boldsymbol{x}_1, \dots, \boldsymbol{x}_N$ is

$$\frac{1}{N}\sum_{i=1}^{N}\left[\boldsymbol{v}_k^T(\boldsymbol{x}_i-\boldsymbol{\mu})\right]\left[\boldsymbol{v}_\ell^T(\boldsymbol{x}_i-\boldsymbol{\mu})\right] = \frac{1}{N}\sum_{i=1}^{N}\boldsymbol{v}_k^T(\boldsymbol{x}_i-\boldsymbol{\mu})(\boldsymbol{x}_i-\boldsymbol{\mu})^T\boldsymbol{v}_\ell$$

$$= \boldsymbol{v}_k^T\boldsymbol{\Sigma}\boldsymbol{v}_\ell = \boldsymbol{v}_k^T\boldsymbol{U\Lambda U}^T\boldsymbol{v}_\ell = \boldsymbol{e}_k^T\boldsymbol{\Lambda}\boldsymbol{e}_\ell = \begin{cases}\lambda_k & \text{if k} = \ell \\ 0 & \text{if k} \neq \ell\end{cases}$$

Therefore

- The variance of the k'th principle components is λ_k.

  ⇒ *principle axis 1 has the highest variance, axis 2 has the next highest variance, …, and axis M has the lowest variance.*

- The covariance of different principle components is zero.
- ⇒ *Covariance among each pair of the principal axes is zero.*

31

SINGULAR VALUE DECOMPOSITION (SVD)

THEOREM OF SVD

- **Theorem:** Suppose $A \in \mathbb{R}^{m\times n}$, then there exists a factorization, called ***singular value decomposition*** of A, of the form

$$A = U\Sigma V^T$$

where $U \in \mathbb{R}^{m\times m}$ and $\mathrm{V} \in \mathbb{R}^{n\times n}$ are orthogonal matrices, $\Sigma \in \mathbb{R}^{m\times n}$ is a diagonal matrix with non-negative numbers on the diagonal.

Proof: Since $A^T A \in \mathbb{R}^{n\times n}$ is symmetric and semi-positive definite, it can be factorized in the form

$$A^T A = V\Lambda V^T$$

where $\mathrm{V} = [\boldsymbol{v}_1, \dots, \boldsymbol{v}_n] \in \mathbb{R}^{n\times n}$ is orthogonal matrix, $\Lambda = diag(\lambda_1, \dots, \lambda_n) \in \mathbb{R}^{n\times n}$ is a diagonal matrix of eigenvalues arranged in non-ascending order

$$\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n \ge 0$$

THEOREM OF SVD

<u>*Proof (cont'd):*</u> Let $p = \max\{i: \lambda_i > 0\}$ be the rank of A. Define $\boldsymbol{u}_i = \frac{A\boldsymbol{v}_i}{\sqrt{\lambda_i}} \in \mathbb{R}^m$ for $i = 1, \dots, p$. Then

$$\langle \boldsymbol{u}_i, \boldsymbol{u}_j \rangle = \langle \frac{A\boldsymbol{v}_i}{\sqrt{\lambda_i}}, \frac{A\boldsymbol{v}_j}{\sqrt{\lambda_j}} \rangle = \frac{\langle \boldsymbol{v}_i, A^T A\boldsymbol{v}_j \rangle}{\sqrt{\lambda_i}\sqrt{\lambda_j}} = \frac{\sqrt{\lambda_j}}{\sqrt{\lambda_i}} \langle \boldsymbol{v}_i, \boldsymbol{v}_j \rangle = \delta_{ij} = \begin{cases} 1, \text{if i} = \text{j} \\ 0, \text{if i} \neq \text{j} \end{cases}$$

That is, $\boldsymbol{u}_1, \dots, \boldsymbol{u}_p$ are pairwise orthogonal unit vectors in $\mathbb{R}^m$. By Gram-Schmidt process we can construct $\boldsymbol{u}_{p+1}, \dots, \boldsymbol{u}_m \in \mathbb{R}^m$(if $p < m$) such that $\boldsymbol{u}_1, \dots, \boldsymbol{u}_m$ are pairwise orthogonal unit vectors. This gives orthogonal matrix $\mathrm{U} = [\boldsymbol{u}_1, \dots, \boldsymbol{u}_m] \in \mathbb{R}^{m \times m}$.

We have the following claim:

Claim: $\boldsymbol{u}_i^T A\boldsymbol{v}_j = \sqrt{\lambda_j}\delta_{ij}$ for $i = 1, \dots, m$, j $= 1, \dots, n$

<u>*Proof:*</u> If j $\leq p$, then $A\boldsymbol{v}_j = \sqrt{\lambda_j}\boldsymbol{u}_j$, therefore $\boldsymbol{u}_i^T A\boldsymbol{v}_j = \sqrt{\lambda_j}\boldsymbol{u}_i^T\boldsymbol{u}_j = \sqrt{\lambda_j}\delta_{ij}$.

If j $> p$, since $\boldsymbol{v}_j$ is an eigenvector of $A^T A$ with associating eigenvalue $\lambda_j = 0$, therefore

$$(A\boldsymbol{v}_j)^T (A\boldsymbol{v}_j) = \boldsymbol{v}_j^T A^T A\boldsymbol{v}_j = \boldsymbol{v}_j^T \lambda_j \boldsymbol{v}_j = 0$$

Hence $A\boldsymbol{v}_j = \mathbf{0}$ and $\boldsymbol{u}_i^T A\boldsymbol{v}_j = 0 = \sqrt{\lambda_j}\delta_{ij}$. **Q.E.D.**

Therefore $\Sigma = U^T AV = diag(\sqrt{\lambda_1}, \dots, \sqrt{\lambda_p}, 0, \dots 0) \in \mathbb{R}^{m \times n}$ is a diagonal matrix.

Therefore $A = U\Sigma V^T$. ***Q.E.D.***