INTRODUCTION TO PRINCIPAL COMPONENT ANALYSIS (PCA)

INT301 Bio-computation, Week 10, 2025

Preliminary Knowledge
Eigenvalues and Eigenvectors

- If v is a nonzero vector and λ is a number such that

$$\mathbf{Av = \lambda v}$$

then v is said to be an *eigenvector* of A with *eigenvalue* λ.

Example

λ (eigenvalues)

$$\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \times \begin{bmatrix} 1 \\ 1 \end{bmatrix} = 3 \times \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

A

V (eigenvectors)

Preliminary Knowledge Eigenvalues and Eigenvectors

- **Eigenvectors** (for a square $m \times m$ matrix $\mathbf{S}$)

$$\mathbf{S}\mathbf{v} = \lambda\mathbf{v}$$

eigenvector $\mathbf{v} \in \mathbb{R}^m \neq \mathbf{0}$

eigenvalue $\lambda \in \mathbb{R}$

Example

$$\begin{pmatrix} 6 & -2 \\ 4 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{pmatrix} 2 \\ 4 \end{pmatrix} = 2 \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

- How many eigenvalues are there at most?

$$\mathbf{S}\mathbf{v} = \lambda\mathbf{v} \iff (\mathbf{S} - \lambda\mathbf{I})\,\mathbf{v} = \mathbf{0}$$

only has a non-zero solution if $|\mathbf{S} - \lambda\mathbf{I}| = 0$

with **at most m distinct λ values**

Preliminary Knowledge Eigenvalues and Eigenvectors

For symmetric matrices, eigenvectors for distinct eigenvalues are **orthogonal**

$$Sv_{\{1,2\}} = \lambda_{\{1,2\}} v_{\{1,2\}}, \text{ and } \lambda_1 \neq \lambda_2 \Rightarrow v_1 \bullet v_2 = 0$$

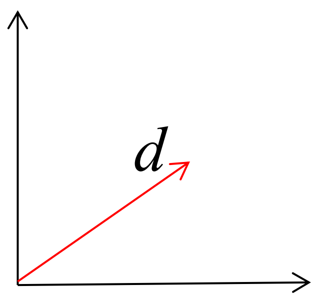
All eigenvalues of a real symmetric matrix are **real**.

半正定矩阵·

All eigenvalues of a positive semidefinite matrix are **non-negative**

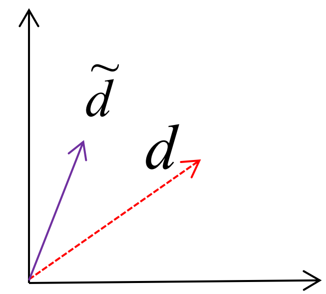
$$\underbrace{\forall w \in \Re^n, w^T S w \geq 0}, \text{ then if } \mathrm{Sv} = \lambda \mathrm{v} \Rightarrow \lambda \geq 0$$

Preliminary Knowledge Eigenvalues and Eigenvectors



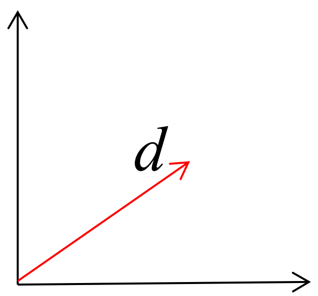
$$S = S^T, \quad Sv_i = \lambda_i v_i, (\lambda_1 = 2, \lambda_2 = 0.5)$$

$$\mathrm{S}\mathrm{d} = \begin{bmatrix} S(1,1), S(1,2) \\ S(2,1), S(2,2) \end{bmatrix} \begin{bmatrix} d(1) \\ d(2) \end{bmatrix} = \begin{bmatrix} S(1,1)d(1) + S(1,2)d(2) \\ S(2,1)d(1) + S(2,2)d(2) \end{bmatrix} = \tilde{d}$$



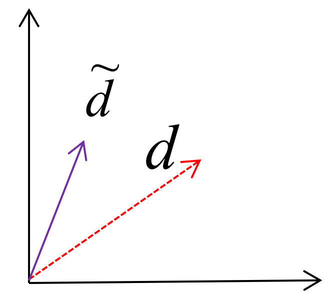
v_1

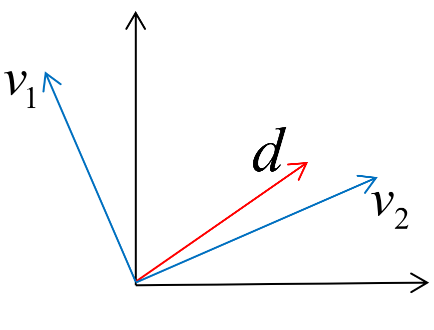
Preliminary Knowledge
Eigenvalues and Eigenvectors

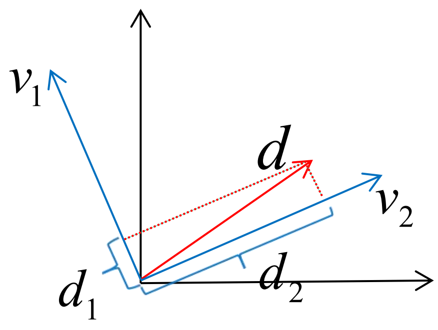


$$S = S^T,\quad Sv_i = \lambda_i v_i, (\lambda_1 = 2, \lambda_2 = 0.5)$$

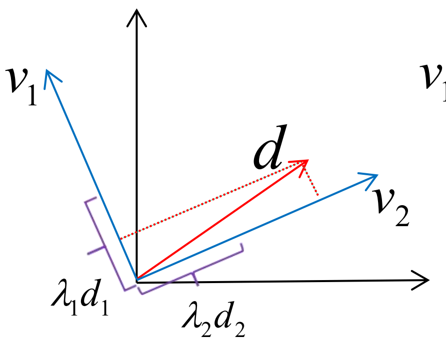
$$Sd = \begin{bmatrix} S(1,1), S(1,2) \\ S(2,1), S(2,2) \end{bmatrix} \begin{bmatrix} d(1) \\ d(2) \end{bmatrix} = \begin{bmatrix} S(1,1)d(1) + S(1,2)d(2) \\ S(2,1)d(1) + S(2,2)d(2) \end{bmatrix} = \tilde{d}$$



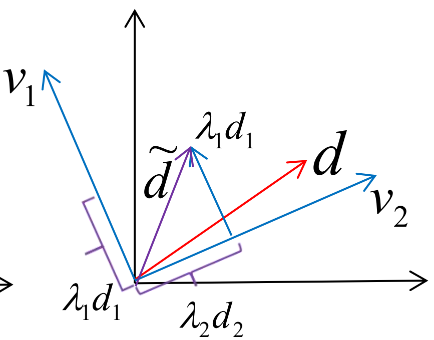




Projection on the eigenvectors



Scaling with eigenvalues



Vector addition

Preliminary Knowledge Eigenvalues and Eigenvectors

- Let $$S = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$ ← Real, symmetric.
- Then $$S - \lambda I = \begin{bmatrix} 2-\lambda & 1 \\ 1 & 2-\lambda \end{bmatrix} \Rightarrow (2-\lambda)^2 - 1 = 0.$$
- The eigenvalues are 1 and 3 (nonnegative, real).
- The eigenvectors are orthogonal (and real):

$$\begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Substitute these values and solve for eigenvectors

Diagonal Decomposition 对角分解

- Let $\mathbf{S} \in \mathbb{R}^{m \times m}$ be a **square** matrix with ***m*** **linearly independent eigenvectors**
- **Theorem**: Exists an **eigen decomposition** 特征分解

$$\mathbf{S} = \mathbf{U}\underbrace{\mathbf{\Lambda}}_{\text{diagonal}}\mathbf{U}^{-1}$$

  - (matrix diagonalization theorem)

Unique for distinct eigen-values

- Columns of **U** are **eigenvectors** of $\mathbf{S}$
- Diagonal elements of $\mathbf{\Lambda}$ are **eigenvalues** of $\mathbf{S}$

$$\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \ldots, \lambda_m), \quad \lambda_i \geq \lambda_{i+1}$$

Diagonal Decomposition

Write ***U*** with the eigenvectors as columns: $U = \begin{bmatrix} v_1 & \dots & v_m \end{bmatrix}$

Then, ***SU*** can be written

$$SU = S\begin{bmatrix} v_1 & \dots & v_m \end{bmatrix} = \begin{bmatrix} \lambda_1 v_1 & \dots & \lambda_m v_m \end{bmatrix} = \begin{bmatrix} v_1 & \dots & v_m \end{bmatrix}\begin{bmatrix} \lambda_1 & & \\ & \dots & \\ & & \lambda_m \end{bmatrix}$$

Thus ***SU=UΛ***, or ***U⁻¹SU=Λ***

Therefore ***S=UΛU⁻¹***

Diagonal Decomposition

Recall $S = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}; \lambda_1 = 1, \lambda_2 = 3.$

The eigenvectors $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ and $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ form $U = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$

Inverting U, we have

$$U^{-1} = \begin{bmatrix} 1/2 & -1/2 \\ 1/2 & 1/2 \end{bmatrix}$$

Recall $UU^{-1} = 1.$

Then, ***S=UΛU⁻¹ =*** $\begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} 1/2 & -1/2 \\ 1/2 & 1/2 \end{bmatrix}$

Diagonal Decomposition

Let's divide $\boldsymbol{U}$ (and multiply $\boldsymbol{U}^{-1}$) by $\sqrt{2}$ 单位向量

Then, $\boldsymbol{S} = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$

$\boldsymbol{Q}$ $\qquad$ Λ $\qquad$ $(\boldsymbol{Q}^{-1} = \boldsymbol{Q}^T)$

Symmetric Diagonal Decomposition

- **Theorem**: If $\mathrm{S} \in \mathbb{R}^{m \times m}$ is a **symmetric** matrix, there exists an **eigen decomposition**, where ***Q*** is **orthogonal:**

$$S = Q\Lambda Q^T$$

  - $Q^{-1} = Q^T$
  - Columns of ***Q*** are normalized eigenvectors
  - Columns are orthogonal.
  - (everything is real)

奇异值分解

Singular Value Decomposition

For an $m \times n$ matrix **A** of rank r, there exists a factorization (Singular Value Decomposition = **SVD**) as follows:

$$\underset{m\times n}{A} = \underbrace{U}_{m\times m}\ \underbrace{\Sigma}_{m\times n,\ \text{nonnegative real}}\ \underbrace{V^T}_{n\times n}$$

The columns of ***U*** are orthogonal eigenvectors of ***AA^T***.

The columns of ***V*** are orthogonal eigenvectors of ***A^TA***.

Eigenvalues $\lambda_1 \dots \lambda_r$ of ***AA^T*** are the eigenvalues of ***A^TA***.

$$\sigma_i = \sqrt{\lambda_i}$$

$$\Sigma = diag(\sigma_1 \dots \sigma_r)$$

Singular values

Singular Value Decomposition

- Illustration of SVD dimensions and

$$\underbrace{\begin{bmatrix} * & * & * \\ * & * & * \\ * & * & * \\ * & * & * \\ * & * & * \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} \bullet & & \\ & \bullet & \\ & & \bullet \\ & & \\ & & \end{bmatrix}}_{\Sigma} \underbrace{\begin{bmatrix} \star & \star & \star \\ \star & \star & \star \\ \star & \star & \star \end{bmatrix}}_{V^T}$$

$$\underbrace{\begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} \star & \star & \star \\ \star & \star & \star \\ \star & \star & \star \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} \bullet & & & & \\ & \bullet & & & \\ & & \bullet & & \end{bmatrix}}_{\Sigma} \underbrace{\begin{bmatrix} \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star \end{bmatrix}}_{V^T}$$

Singular Value Decomposition

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

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

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

$\det |M - \lambda I| = 0$

Thus *m*=3, *n*=2. Its SVD is

$$\begin{bmatrix} 0 & 2/\sqrt{6} & 1/\sqrt{3} \\ 1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ 1/\sqrt{2} & 1/\sqrt{6} & -1/\sqrt{3} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \sqrt{3} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{bmatrix}$$

Dimensionality Reduction

- One approach to deal with high dimensional data is by reducing their dimensionality.
- Project high dimensional data onto a lower dimensional subspace using linear or non-linear transformations.

$$\mathrm{x} = \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_N \end{bmatrix} \xrightarrow{\textbf{Reduce dimensionality}} \mathrm{y} = \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_k \end{bmatrix} \quad \text{(K<<N)}$$

- Linear transformations are simple to compute

$$Y = U \quad X \qquad (b_i = u_i^t a_i)$$

Dimensionality Reduction

- **Find a basis in a low dimensional sub-space:**
  - Approximate vectors by projecting them in a low dimensional <u>sub-space</u>:

    (1) Original space representation:

$$\begin{bmatrix} a_1 \\ a_2 \\ \dots \\ a_N \end{bmatrix}$$

$$x = a_1 v_1 + a_2 v_2 + \dots + a_N v_N$$

where $v_1, v_2, \dots, v_n$ is a base in the original N-dimensional space

    (2) Lower-dimensional <u>sub-space</u> representation:

$$\begin{bmatrix} b_1 \\ b_2 \\ \dots \\ b_k \end{bmatrix}$$

$$\hat{x} = b_1 u_1 + b_2 u_2 + \dots + b_K u_K$$

where $u_1, u_2, \dots, u_K$ is a base in the K-dimensional sub-space $(K<N)$

Dimensionality Reduction

- If K=N, then $\hat{x} = x$
- Example (K=N):

$$v_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, v_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, v_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \quad \text{(standard basis)}$$

$$x_v = \begin{bmatrix} 3 \\ 3 \\ 3 \end{bmatrix} = 3v_1 + 3v_2 + 3v_3$$

$$u_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, u_2 = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, u_3 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \quad \text{(some other basis)}$$

$$x_u = \begin{bmatrix} 3 \\ 3 \\ 3 \end{bmatrix} = 0u_1 + 0u_2 + 3u_3$$

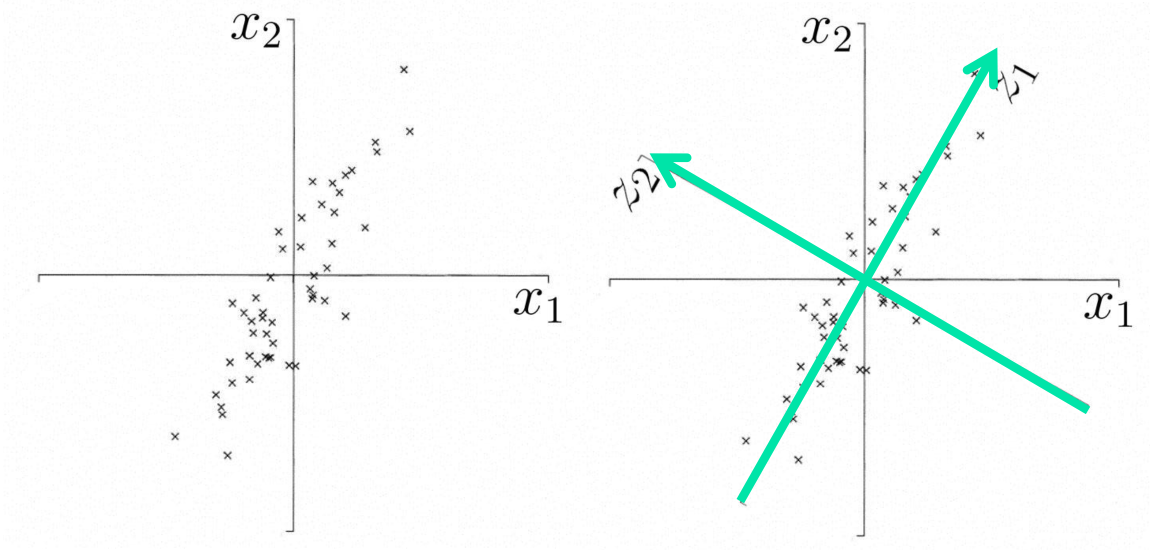
Principal Component Analysis (PCA)

- Each dimensionality reduction technique finds an *appropriate transformation* by satisfying certain criteria (e.g., *information loss, data discrimination*, etc.)

- The goal of PCA is to reduce the dimensionality of the data while ***retaining as much as possible of the variation present in the dataset***.

Principal Component Analysis (PCA)

- **Motivation**
  - Find bases which has high variance in data
  - Encode data with small number of bases with low MSE



- First PC is direction of maximum variance
- Subsequent PCs are orthogonal to 1st PC and describe maximum

Principal Component Analysis (PCA)

Assume that $E[\mathbf{x}] = \mathbf{0}$ $\quad a = \mathbf{x}^T\mathbf{q} = \mathbf{q}^T\mathbf{x}$ $\quad \|\mathbf{q}\| = (\mathbf{q}^T\mathbf{q})^{1/2} = 1$

$$\Rightarrow \sigma^2 = E[a^2] - E[a]^2 = E[a^2]$$
$$= E[(\mathbf{q}^T\mathbf{x})(\mathbf{x}^T\mathbf{q})] = \mathbf{q}^T E[\mathbf{x}\mathbf{x}^T]\mathbf{q} = \mathbf{q}^T\mathbf{R}\mathbf{q}$$

Find q's maximizing variance!!

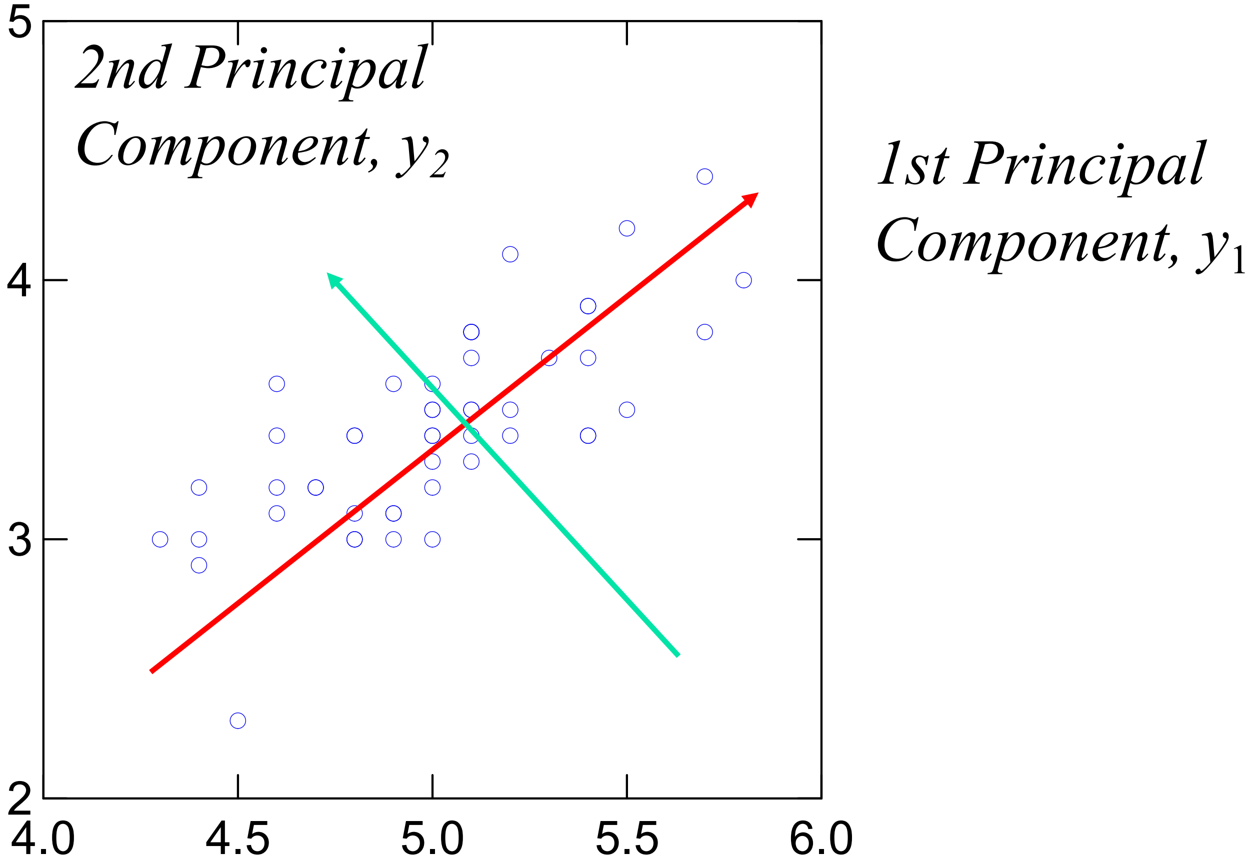
It can be shown that variance is maximized when q is the principal component of R.

Principal component q can be obtained by **eigenvector decomposition**:

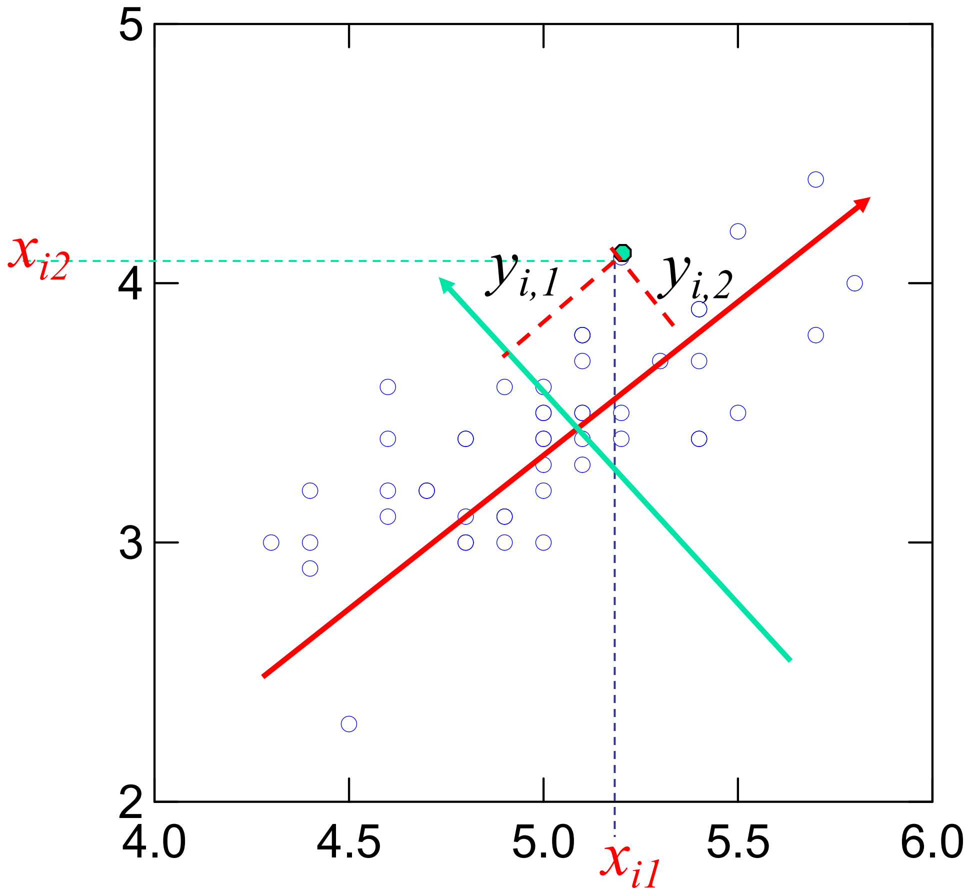
$$\mathbf{R} = \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^T, \quad \mathbf{Q} = [\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_j, \ldots, \mathbf{q}_m], \boldsymbol{\Lambda} = diag[\lambda_1, \lambda_2, \ldots, \lambda_j, \ldots, \lambda_m]$$

$$\Leftrightarrow \mathbf{R}\mathbf{q}_j = \lambda_j\mathbf{q}_j \quad j = 1, 2, \ldots, m \quad \Rightarrow \quad \mathbf{R}\mathbf{q} = \lambda\mathbf{q}$$

Principal Component Analysis (PCA)



Principal Component Analysis (PCA)



Principal Component Analysis (PCA)

- Advantage
  - Reduce the dimension of the original data
    - reduce time consumption in the training process, and improve efficiency
  - Discard some information of the original data
    - if this information is noise

丢弃

Principal Component Analysis (PCA)

- Limitation
  - Discard some information of the original data
    - if the discarded information is important, it is not appropriate to apply PCA
  - The meaning of the principal component
    - PC or basis may not be interpretable
  - Linear model of PCA
    - not suitable for nonlinear problem
  - Assume first PC has higher importance

$v^T A v = v^T \lambda v$

Case study: Eigenface

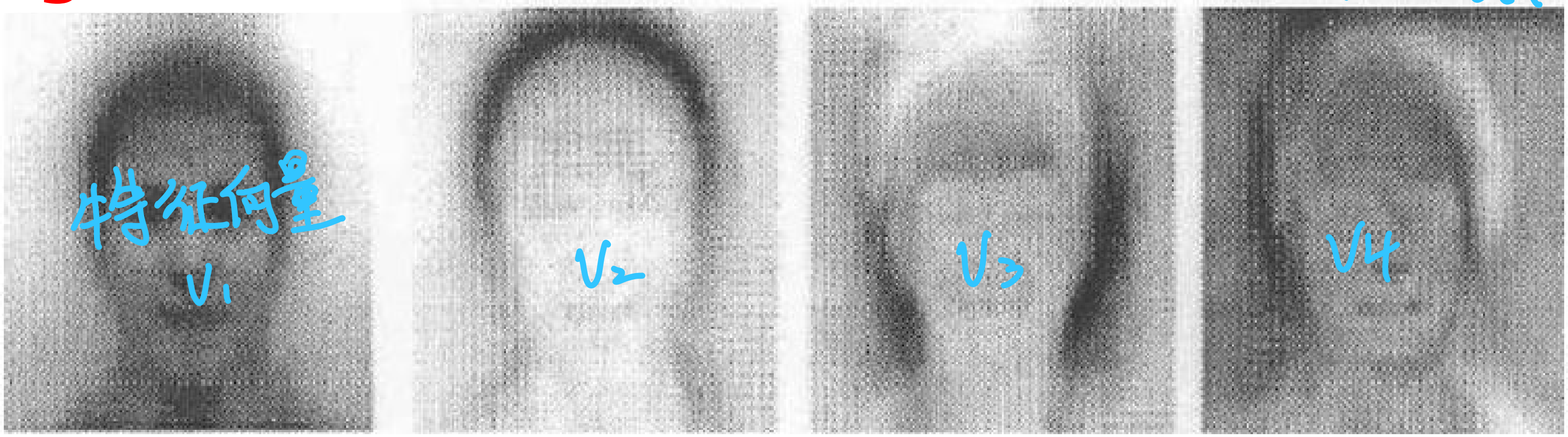
Face image: high-dimensional vector

face image = linear combination of eigenvectors

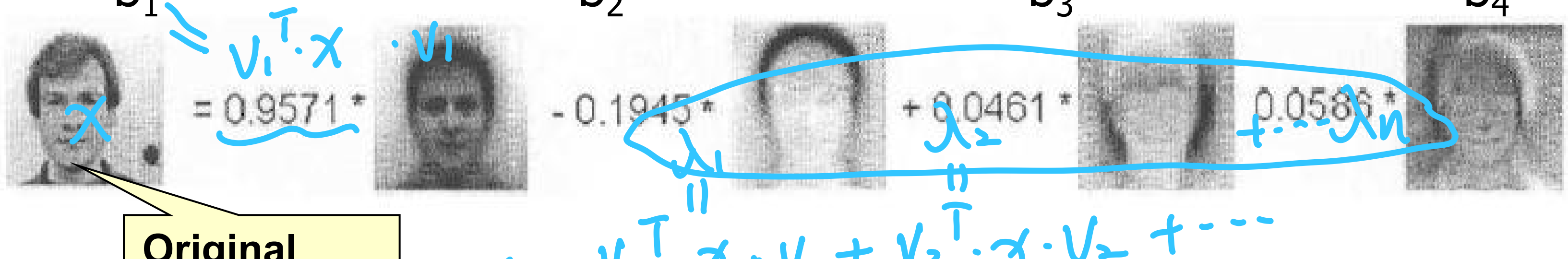
The eigenvectors can be viewed as images.

$\Rightarrow \frac{\lambda_1 + \lambda_2 + \cdots \lambda_4}{x = \lambda_1 + \cdots \lambda_n} = \text{ratio}$

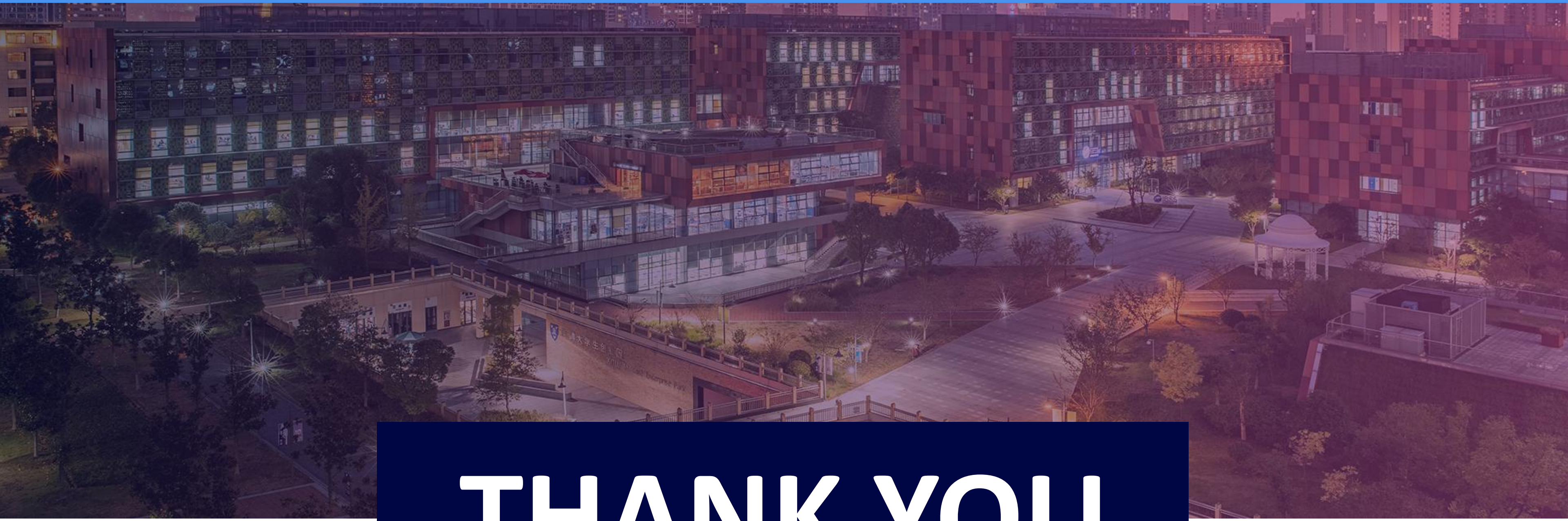
Eigenfaces:



b_1 b_2 b_3 b_4



$x = v_1^T \cdot x \cdot v_1 + v_2^T \cdot x \cdot v_2 + \cdots$



THANK YOU

VISIT US

WWW.XJTLU.EDU.CN

FOLLOW US

@XJTLU

Xi'an Jiaotong-Liverpool University
西交利物浦大学