# CZ4041/CE4041: Machine Learning

## Week 12: Dimensionality Reduction

# Question 1

- A dataset of five 4-dimensional instances is given in Table 1. Suppose an SVD is performed on the data matrix **X** (5-by-4) via $\mathbf{X} = \mathbf{V}\mathbf{D}\mathbf{U}^{\top}$. The matrices **V**, **D**, and **U** are shown in Tables 2-4, respectively. Use principal component analysis to project the 5 data points in Table 1 to 2-dimensional space.

$\mathbf{X}$

| $X_1$ | $X_2$ | $X_3$ | $X_4$ |
|---|---|---|---|
| 2 | 4 | 1 | 3 |
| 1 | 2 | 3 | 5 |
| −2 | −4 | −4 | −1 |
| 0 | −1 | −2 | −6 |
| −1 | −1 | 2 | −1 |

Step 1: Center the data points s.t. the mean is **0**

$\hat{\boldsymbol{\mu}}$

| $X_1$ | $X_2$ | $X_3$ | $X_4$ |
|---|---|---|---|
| 0 | 0 | 0 | 0 |

Already centered

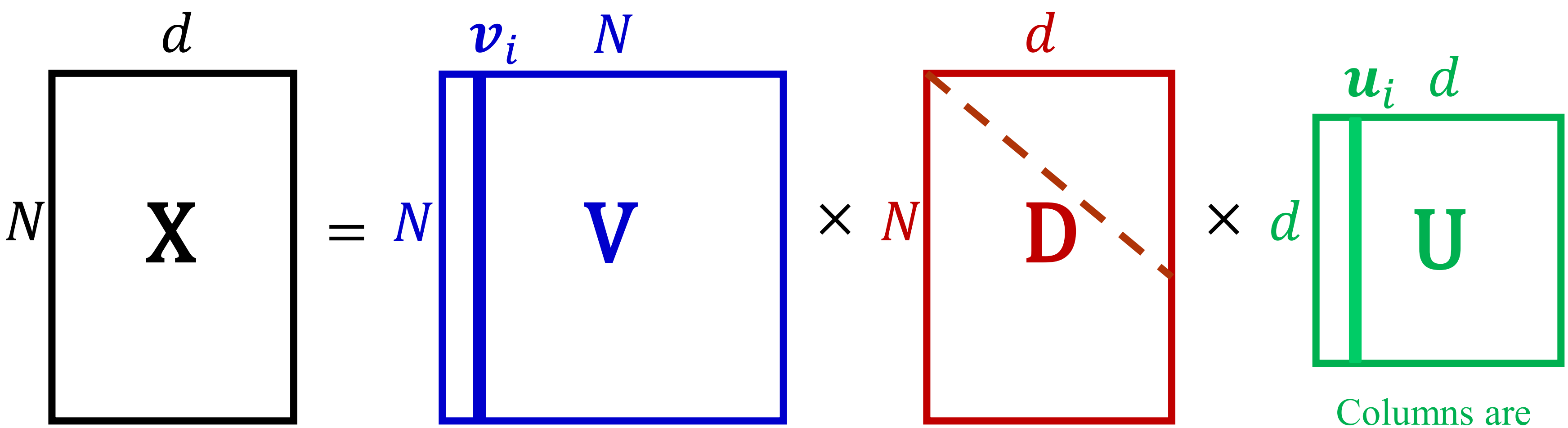
# PCA

- Step 1: Center the data points s.t. the mean is $\mathbf{0}$
- Step 2: Compute sample covariance matrix $\widetilde{\boldsymbol{\Sigma}}$
- Step 3: Compute eigenvectors of $\widetilde{\boldsymbol{\Sigma}}$, $\{\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_d\}$, which are sorted based on their eigenvalues in non-increasing order, i.e., $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d$
- Step 4: Select the first $k$ eigenvectors to construct principal components
- Step 5: Project the data instances to k-dimensional space

# Singular Value Decomposition (SVD)

- The SVD of $\mathbf{X}$ ($N$-by-$d$) has the following form

$$\mathbf{X} = \mathbf{V}\mathbf{D}\mathbf{U}^T$$




Columns are orthonormal to each other

$$\mathrm{V}^T\mathrm{V} = \mathrm{I}_N$$

Supporse $d < N$. All elements are zero expect for the first $d$-by-$d$ submatrix diagonal being $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d \geq 0$

Columns are orthonormal to each other

$$\mathrm{U}^T\mathrm{U} = \mathrm{I}_d$$

# U = the Eigenvectors

$$\tilde{\boldsymbol{\Sigma}} = \frac{1}{5-1}\mathbf{X}^T\mathbf{X} = \frac{1}{4}(\mathrm{VDU}^T)^T\mathbf{VDU}^T$$

$$= \frac{1}{4}\mathbf{UD}^T\underbrace{\boxed{\mathbf{V}^T\mathbf{V}}}_{\mathbf{I}}\mathbf{DU}^T$$

$$\tilde{\mathbf{D}} = \frac{1}{4}\mathbf{D}^T\mathbf{D} \qquad = \mathbf{U}\tilde{\mathbf{D}}\mathbf{U}^T$$

# U = the Eigenvectors

The matrix **D** (5-by-4) obtained by SVD ($\mathbf{X} = \mathbf{V}\mathbf{D}\mathbf{U}^\top$)

| | | | |
|---|---|---|---|
| 10.9040 | 0 | 0 | 0 |
| 0 | 4.8385 | 0 | 0 |
| 0 | 0 | 3.3973 | 0 |
| 0 | 0 | 0 | 0.3867 |
| 0 | 0 | 0 | 0 |

$$\widetilde{\boldsymbol{\Sigma}} = \frac{1}{5-1}\mathbf{X}^T\mathbf{X} = \frac{1}{4}(\mathbf{V}\mathbf{D}\mathbf{U}^T)^T\mathbf{V}\mathbf{D}\mathbf{U}^T$$

$$= \frac{1}{4}\mathbf{U}\mathbf{D}^T\underbrace{\boxed{\mathbf{V}^T\mathbf{V}}}_{\mathbf{I}}\mathbf{D}\mathbf{U}^T$$

$$\widetilde{\mathbf{D}} = \frac{1}{4}\mathbf{D}^T\mathbf{D} \qquad = \mathbf{U}\widetilde{\mathbf{D}}\mathbf{U}^T$$

$$\widetilde{\boldsymbol{\Sigma}}\mathbf{U} = \mathbf{U}\widetilde{\mathbf{D}}$$

$\mathbf{U}^T\mathbf{U}=\mathbf{I}$

$\widetilde{\mathbf{D}}$

$\frac{1}{4}\times$

| | | | |
|---|---|---|---|
| $10.90^2$ | 0 | 0 | 0 |
| 0 | $4.84^2$ | 0 | 0 |
| 0 | 0 | $3.40^2$ | 0 |
| 0 | 0 | 0 | $0.39^2$ |

$$\widetilde{\boldsymbol{\Sigma}}\boldsymbol{u}_i = \widetilde{\mathbf{D}}_{ii}\boldsymbol{u}_i$$

# Question 1 (cont.)

$$A = U^T \begin{bmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \lambda_D \end{bmatrix} U$$

$$A = \begin{bmatrix} u_1 & u_2 & \cdots & u_D \end{bmatrix} \begin{bmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \lambda_D \end{bmatrix} \begin{bmatrix} u_1^T \\ u_2^T \\ \vdots \\ u_D^T \end{bmatrix}$$

# Question 1 (cont.)

$$A = [u_1 \quad u_2 \quad \dots \quad u_D] \begin{bmatrix} \lambda_1 u_1^T \\ \lambda_2 u_2^T \\ \vdots \\ \lambda_D u_D^T \end{bmatrix}$$

$$A = \lambda_1 u_1 u_1^T + \lambda_2 u_2 u_2^T + \cdots + \lambda_D u_D u_D^T$$

$$\alpha A = \alpha\lambda_1 u_1 u_1^T + \alpha\lambda_1 u_2 u_2^T + \cdots + \alpha\lambda_D u_D u_D^T$$

# Question 1 (cont.)

$$\alpha A = \alpha\lambda_1 x_1 x_1^T + \alpha\lambda_1 x_2 x_2^T + \cdots + \alpha\lambda_D x_D x_D^T$$

$$\alpha A = U^T \begin{bmatrix} \alpha\lambda_1 & 0 & 0 & 0 \\ 0 & \alpha\lambda_2 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \alpha\lambda_D \end{bmatrix} U$$

# Question 1 (cont.)

- Step 2: Compute sample covariance matrix $\widetilde{\boldsymbol{\Sigma}}$
- Step 3: Compute eigenvectors of $\widetilde{\boldsymbol{\Sigma}}$, $\{\boldsymbol{u}_1, \boldsymbol{u}_2, \dots, \boldsymbol{u}_d\}$, which are sorted based on their eigenvalues in non-increasing order, i.e., $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d$

$\Downarrow$

- Perform SVD on the centered data matrix **X** (5-by-4) to obtain

  $\mathbf{X} = \mathbf{VDU}^\top$ (already done in this question)

# Question 1 (cont.)

- Step 4: Select the first $k$ eigenvectors to construct principal components

- Select the first 2 eigenvectors of $\widetilde{\boldsymbol{\Sigma}}$, i.e, the first two column vectors of the matrix **U** to construct the principle component matrix $\mathbf{U_2} = [\boldsymbol{u}_1, \boldsymbol{u}_2]$

$\mathbf{U_2}$

**U**

| | | | |
|---|---|---|---|
| −0.2224 | 0.3430 | −0.3302 | −0.8508 |
| −0.4880 | 0.5756 | −0.4046 | 0.5166 |
| −0.4479 | 0.2924 | 0.8400 | −0.0911 |
| −0.7154 | −0.6823 | −0.1473 | −0.00309 |

# Question 1 (cont.)

- Step 5: Project the instances to k-dimensional space

- Compute $\mathbf{XU_2}$

$$\underbrace{\begin{bmatrix} 2 & 4 & 1 & 3 \\ 1 & 2 & 3 & 5 \\ -2 & -4 & -4 & -1 \\ 0 & -1 & -2 & -6 \\ -1 & -1 & 2 & -1 \end{bmatrix}}_{\mathbf{X}} \times \underbrace{\begin{bmatrix} -0.2224 & 0.3430 \\ -0.4880 & 0.5756 \\ -0.4479 & 0.2924 \\ -0.7154 & -0.6823 \end{bmatrix}}_{\mathbf{U_2}} = \underbrace{\begin{bmatrix} -4.9908 & 1.2338 \\ -6.1191 & -1.0402 \\ 4.9038 & -3.4759 \\ 5.6762 & 2.9335 \\ 0.5399 & 0.3486 \end{bmatrix}}_{\mathbf{Z}}$$

# Thank you!