

MACHINE INTELLIGENCE

UNIT - 4

Dimensionality Reduction

feedback/corrections: vibha@pesu.pes.edu

VIBHA MASTI

Q: Comment on the usefulness of the following feature vectors

Set 1

| | | | | | | |
|-----------|---|----|----|----|----|---|
| Feature 1 | 5 | 17 | 13 | 29 | 72 | 7 |
|-----------|---|----|----|----|----|---|

| | | | | | | |
|-----------|-----|-----|-----|------|------|------|
| Feature 2 | 0.9 | 1.1 | 1.0 | 0.95 | 1.05 | 0.91 |
|-----------|-----|-----|-----|------|------|------|

Retain feature 1

Set 2

| | | | | | | |
|-----------|---|----|----|----|----|---|
| Feature 1 | 5 | 17 | 13 | 29 | 72 | 7 |
|-----------|---|----|----|----|----|---|

| | | | | | | |
|-----------|-----|----|----|-----|------|------|
| Feature 2 | 1.9 | 35 | 65 | 3.8 | 11.8 | 45.8 |
|-----------|-----|----|----|-----|------|------|

Retain both

Set 3

| | | | | | | |
|-----------|---|----|----|----|----|----|
| Feature 1 | 5 | 20 | 30 | 10 | 45 | 71 |
|-----------|---|----|----|----|----|----|

| | | | | | | |
|-----------|-----|----|----|-----|----|------|
| Feature 2 | 5.5 | 19 | 28 | 9.5 | 44 | 70.5 |
|-----------|-----|----|----|-----|----|------|

Transform by 45°

$$\theta = \pi/4 \quad \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} 30 \\ 28 \end{bmatrix} = \begin{bmatrix} 41 \\ -1.4 \end{bmatrix}$$

| | | | | | | |
|------------|------|------|------|------|------|------|
| Feature 1' | 7.4 | 27.5 | 41 | 13.6 | 63 | 100 |
| Feature 2' | 0.35 | 0.7 | -1.4 | 0.35 | 0.70 | 0.35 |

Retain Feature 1'

Assumptions

1. Features with high variance are useful
2. Only one feature from set of highly correlated features is useful

COVARIANCE MATRIX

$$\hat{\Sigma} = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})(x_i - \bar{x})^T$$

Covariance Matrix with Mean Centered Data

- Unbiased estimate

$$C_X = \frac{1}{n-1} X X^T$$

Principle Component Analysis

| | | | | | | | |
|-------------|------|------|-----|------|------|------|-------------|
| Feature 1': | 7.4 | 27.5 | 41 | 13.6 | 63 | 100 | Mean = 42 |
| Feature 2': | 0.35 | 0.7 | 1.4 | 0.35 | 0.70 | 0.35 | Mean = 0.64 |

Mean-Centered Data:

| | | | | | | |
|-------------|-------|-------|------|-------|------|-------|
| Feature 1': | -34.6 | -14.5 | -1.0 | -28.4 | 21 | 58 |
| Feature 2': | -0.29 | 0.06 | 0.76 | -0.29 | 0.06 | -0.29 |

Covariance Matrix

$$\begin{bmatrix} 1204 & 0.216 \\ 0.216 & 0.167 \end{bmatrix}$$

- Desirable covariance matrix:
off diagonal entries ≈ 0 & sorted by mag

→ $\begin{bmatrix} 1204 & 0.216 \\ 0.216 & 0.167 \end{bmatrix}$ good cov matrix

- Change coordinate axis to make cov matrix better
- Transform X (original feature space) such that new covariance matrix is desirable

$$Y = P X$$

\uparrow new feature space \uparrow transformation matrix

- Rows of P are called principle components

$$C_y = \frac{1}{n-1} Y Y^T$$

$$= \frac{1}{n-1} (PX) (PX)^T$$

$$= \frac{1}{n-1} (PX) X^T P^T$$

$$= \frac{1}{n-1} P (X X^T) P^T$$

original cov matrix

Let $X X^T = E D E^T$ (diagonalisation of square symmetric matrix)

eigenvectors of $X X^T$

$$C_y = \frac{1}{n-1} P E D E^T P^T$$

let us take $P = E^T$

$$C_y = \frac{1}{n-1} (E^T E) D (E^T E)$$

identity matrix (orthonormal)

$$C_y = \frac{1}{n-1} D \rightarrow \text{diagonal cov matrix}$$

Q: x y Reduce to 1 feature

4 11
8 4
13 5
7 14

Mean-centric

$$\bar{x} = 8$$

$$\bar{y} = 8.5$$

$$\begin{array}{cc} x' & y' \\ -4 & 2.5 \\ 0 & -4.5 \\ 5 & -3.5 \\ -1 & 5.5 \end{array}$$

$$\Sigma = \frac{1}{4-1} \begin{bmatrix} -4 & 0 & 5 & -1 \\ 2.5 & -4.5 & -3.5 & 5.5 \end{bmatrix} \begin{bmatrix} -4 & 2.5 \\ 0 & -4.5 \\ 5 & -3.5 \\ -1 & 5.5 \end{bmatrix}$$

$$\Sigma = \frac{1}{3} \begin{bmatrix} 42 & -33 \\ -33 & 69 \end{bmatrix} = \begin{bmatrix} 14 & -11 \\ -11 & 23 \end{bmatrix}$$

$$|\Sigma - \lambda I| = 0$$

$$\begin{vmatrix} 14 - \lambda & -11 \\ -11 & 23 - \lambda \end{vmatrix} = (\lambda - 23)(\lambda - 14) - 121$$
$$= \lambda^2 - 37\lambda + 201 = 0$$

$$\lambda_1 = \frac{37 + \sqrt{565}}{2}$$

$$\approx 30.39$$

$$\lambda_2 = \frac{37 - \sqrt{565}}{2}$$

$$\approx 6.62$$

Eigenvectors

$$(\Sigma - \lambda I) v = 0$$

$$\begin{bmatrix} 14 - \lambda & -11 \\ -11 & 23 - \lambda \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$(14 - \lambda) v_1 - 11 v_2 = 0 \longrightarrow (1)$$

$$-11 v_1 + (23 - \lambda) v_2 = 0 \longrightarrow (2)$$

$$(1) \quad (14 - \lambda) v_1 = 11 v_2$$

$$\frac{v_1}{v_2} = \frac{11}{14 - \lambda} = 1$$

$$v_1 = 11$$

$$v_2 = 14 - \lambda$$

$$(a) \text{ for } \lambda = \frac{37 + \sqrt{565}}{2}$$

$$v_1 = 11$$

$$v_2 = - \left(\frac{9 + \sqrt{565}}{2} \right)$$

$$= -16.38$$

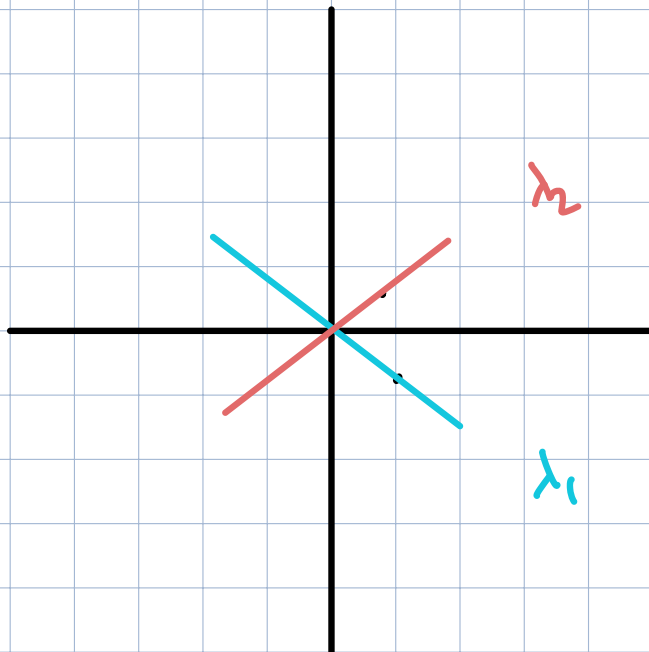
$$\text{normalised : } \|v\| = 19.73$$

$$v_1 = \begin{bmatrix} 0.557 \\ -0.830 \end{bmatrix}$$

New data

$$\begin{bmatrix} 0.557 & -0.830 \end{bmatrix} \begin{bmatrix} -4 & 0 & 5 & -1 \\ 2.5 & -4.5 & -3.5 & 5.5 \end{bmatrix}$$

$$= \begin{bmatrix} -4.303 & 3.735 & 5.69 & -5.122 \end{bmatrix}$$



$$\text{C67 for } \lambda = \frac{37 - \sqrt{565}}{2}$$

$$\begin{aligned} v_1 &= 11 & v_2 &= 14 - \lambda \\ & & &= \frac{-9 + \sqrt{565}}{2} \\ & & &\approx 7.39 \end{aligned}$$

$$\text{normalised : } \|v\| = 13.25$$

$$v_2 = \begin{bmatrix} 0.83 \\ 0.53 \end{bmatrix}$$

New data

$$\begin{bmatrix} 0.83 & 0.53 \end{bmatrix} \begin{bmatrix} -4 & 0 & 5 & -1 \\ 2.5 & -4.5 & -3.5 & 5.5 \end{bmatrix}$$

$$= \begin{bmatrix} -1.93 & -2.5 & 2.2 & 2.24 \end{bmatrix}$$

Non-parametric method

Q: PCA

| x | y | $x - \bar{x}$ | $y - \bar{y}$ |
|-----|-----|---------------|---------------|
| 2.5 | 2.4 | 0.69 | 0.49 |
| 0.5 | 0.7 | -1.31 | -1.21 |
| 2.2 | 2.9 | 0.39 | 0.99 |
| 1.9 | 2.2 | 0.09 | 0.29 |
| 3.1 | 3.0 | 1.29 | 1.09 |
| 2.3 | 2.7 | 0.49 | 0.79 |
| 2 | 1.6 | 0.19 | -0.31 |
| 1 | 1.1 | -0.81 | -0.81 |
| 1.5 | 1.6 | -0.31 | -0.31 |
| 1.1 | 0.9 | -0.71 | -1.01 |

$$\bar{x} = 1.81 \quad \bar{y} = 1.91$$

$$\Sigma = \begin{bmatrix} 0.616 & 0.615 \\ 0.615 & 0.716 \end{bmatrix}$$

Eigenvalues

$$\lambda_1 = 1.28303$$

$$\lambda_2 = 0.04897$$

$$V_1 = (0.922, 1)$$

$$V_2 = (-1.085, 1)$$

Normalising

$$\|v_1\| = 1.3602$$

$$v_1 = \begin{bmatrix} 0.678 \\ 0.735 \end{bmatrix}$$

$$\|v_2\| = 1.4755$$

$$v_2 = \begin{bmatrix} -0.7353 \\ 0.6777 \end{bmatrix}$$

Singular Value Decomposition

- If $A_{n \times n}$ is a square matrix,

$$(A_{n \times n} - \lambda I) V_{n \times 1} = 0$$

or $A_{n \times n} V_{n \times 1} = \lambda V_{n \times 1}$

\swarrow eigen value \searrow eigen vector

- For rectangular matrix $A_{m \times n}$

$$A_{m \times n} V_{n \times 1} = \text{some scalar } U_{m \times 1}$$

- we will need to find two vectors & a scalar
- For $A_{m \times n}$, $(A^T A)_{n \times n}$ and $(A A^T)_{m \times m}$ are square symmetric matrices
- Decompose using Eigenvalue decomposition
 - Let $\lambda_1, \lambda_2, \dots, \lambda_r$ be eigenvalues and (sorted in desc)
 v_1, v_2, \dots, v_r be the corresponding eigenvectors

$$(A^T A) v_i = \lambda_i v_i$$

Premultiply with A (associative)

$$(A A^T) A v_i = \lambda_i v_i$$

Divide by $\|A v_i\|$

$$(A A^T) u_i = \lambda u_i$$

$$\text{where } u_i = \frac{A v_i}{\|A v_i\|}$$

To Summarise

- $A^T A$ is $n \times n$

$$(A^T A) v_i = \lambda_i v_i$$

- $A A^T$ is $m \times m$

$$(A A^T) u_i = \lambda_i u_i$$

$$u_i = \frac{A v_i}{\|A v_i\|}$$

- $\|A v_i\|^2 = \lambda_i$

$$(A^T A) v_i = \lambda_i v_i$$

$$v_i^T (A^T A) v_i = v_i^T \lambda_i v_i$$

$$(A v_i)^T (A v_i) = \lambda_i v_i^T v_i$$

$$\|A v_i\|^2 = \lambda_i$$

$$\|A v_i\| = \sqrt{\lambda_i} = \sigma_i$$

$$\cdot \quad u_i = \frac{A v_i}{\|A v_i\|} = \frac{A v_i}{\sigma_i}$$

$$\cdot \quad A v_i = u_i \sigma_i \rightarrow \text{singular value of } A = \sqrt{\lambda_i}$$

\swarrow $n \times 1$ unit vector \searrow $m \times 1$ unit vector

$$\cdot \quad A V = U \Sigma$$

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

Optionally:

- Extend $\{U_1, U_2, \dots, U_r\}$ by adding $(m-r)$ zero vectors of size $m \times 1$ to get an $m \times m$ matrix U
- Extend V s similarly by adding $(n-r)$ zero vectors of size $n \times 1$ to get an $n \times n$ matrix V

Not Done in Practice - reduced SVD

SVD and PCA

- Let $Y = \frac{1}{\sqrt{n-1}} X^T$ (mean centered)

$$Y^T Y = C_X$$

- Columns of SVD of $Y^T Y$ are V
- SVD of X^T as $U \Sigma V^T$
- Columns of V are principle components of X
- No need to explicitly calc cov $X^T X$

Q: $A = \begin{bmatrix} 4 & 4 \\ -3 & 3 \end{bmatrix}$ (not sym) . Do SVD.

$$A^T A = \begin{bmatrix} 4 & -3 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} 4 & 4 \\ -3 & 3 \end{bmatrix} = \begin{bmatrix} 25 & 7 \\ 7 & 25 \end{bmatrix} = Y$$

Find eigenvalues & eigenvectors

$$\begin{vmatrix} 25-\lambda & 7 \\ 7 & 25-\lambda \end{vmatrix} = 0$$

$$(\lambda - 25)^2 - 49 = 0$$

$$\lambda^2 - 50\lambda + 576 = 0$$

$$\lambda_1 = 32 \quad \lambda_2 = 18$$

$$(i) \quad (A - \lambda_1 I) v_1 = 0$$

$$\begin{bmatrix} -7 & 7 \\ 7 & -7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$-7x_1 + 7x_2 = 0$$

$$\frac{x_1}{x_2} = 1 \Rightarrow x_1 = \frac{1}{\sqrt{2}}, \quad x_2 = \frac{1}{\sqrt{2}}$$

$$v_1 = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

$$(ii) (A - \lambda_2 I) v_2 = 0$$

$$\begin{bmatrix} 7 & 7 \\ 7 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$7x_1 + 7x_2 = 0 \Rightarrow -7x_1 = 7x_2$$

$$\frac{x_1}{x_2} = -1 \Rightarrow v_2 = \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

Find Σ

$$\Sigma = \begin{bmatrix} \sqrt{32} & 0 \\ 0 & \sqrt{18} \end{bmatrix} \quad V = \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

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

$$u_i = \frac{A v_i}{\|A v_i\|} = \frac{A v_i}{\sigma_i}$$

$$u_1 = \frac{\begin{bmatrix} 4 & 4 \\ -3 & 3 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}}{\sqrt{32}} = \frac{\begin{bmatrix} 4\sqrt{2} \\ 0 \end{bmatrix}}{4\sqrt{2}} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$u_2 = \frac{\begin{bmatrix} 4 & 4 \\ -3 & 3 \end{bmatrix} \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}}{\sqrt{18}} = \frac{\begin{bmatrix} 0 \\ 3\sqrt{2} \end{bmatrix}}{3\sqrt{2}} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 4\sqrt{2} & 0 \\ 0 & 3\sqrt{2} \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

$\uparrow \quad \uparrow$
 attributes

Q: $A = \begin{bmatrix} 1 & -1 \\ -2 & 2 \\ 2 & -2 \end{bmatrix}$ (tall)

$$A^T A = \begin{bmatrix} 1 & -2 & 2 \\ -1 & 2 & -2 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ -2 & 2 \\ 2 & -2 \end{bmatrix}$$

$$= \begin{bmatrix} 9 & -9 \\ -9 & 9 \end{bmatrix}$$

in eigenvalues

$$\begin{vmatrix} 9-\lambda & -9 \\ -9 & 9-\lambda \end{vmatrix} = 0$$

$$(\lambda - 9)^2 - 81 = 0$$

$$\lambda^2 - 18\lambda = 0$$

$$\lambda_1 = 18$$

$$\lambda_2 = 0$$

$$E = \begin{bmatrix} \sqrt{18} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

(ii) eigenvectors (v)

$$\begin{bmatrix} 9-18 & -9 \\ -9 & 9-18 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 9 & -9 \\ -9 & 9 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$9x_1 - 9x_2 = 0$$

$$x_1 = x_2 = 1$$

normalised

$$v_1 = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

$$v_2: \begin{bmatrix} 9 & -9 \\ -9 & 9 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 6 \\ 0 \end{bmatrix}$$

$$v_2 = \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

(iii) solve for v

$$v_1 = \frac{A v_1}{\sigma_1} = \frac{\begin{bmatrix} 1 & -1 \\ -2 & 2 \\ 2 & -2 \end{bmatrix} \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}}{\sqrt{18}}$$

$$v_1 = \frac{\begin{bmatrix} -\sqrt{2} \\ 2\sqrt{2} \\ -2\sqrt{2} \end{bmatrix}}{3\sqrt{2}} = \begin{bmatrix} -1/3 \\ 2/3 \\ -2/3 \end{bmatrix}$$

Find u_2 & u_3 from orthogonality

$$\begin{bmatrix} -1/3 & 2/3 & -2/3 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = [0]$$

row space & null space

y & z are independent

$$-\frac{1}{3}x + \frac{2}{3}y - \frac{2}{3}z = 0$$

$$x = 2y - 2z$$

$$\therefore NS = \begin{bmatrix} 2y - 2z \\ y \\ z \end{bmatrix} = \left\{ y \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix} + z \begin{bmatrix} -2 \\ 0 \\ 1 \end{bmatrix} \right\}$$

$$\therefore u_2 = \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix} \quad u_3 = \begin{bmatrix} -2 \\ 0 \\ 1 \end{bmatrix}$$

Gram-Schmidt process:

$$q_1 = \frac{(2 \ 1 \ 0)}{\sqrt{5}} = \begin{bmatrix} 2/\sqrt{5} \\ 1/\sqrt{5} \\ 0 \end{bmatrix}$$

$$B = \begin{bmatrix} -2 \\ 0 \\ 1 \end{bmatrix} - q_1^T \begin{bmatrix} -2 \\ 0 \\ 1 \end{bmatrix} q_1$$

$$B = \begin{bmatrix} -2 \\ 0 \\ 1 \end{bmatrix} - [2/\sqrt{5} \ 1/\sqrt{5} \ 0] \begin{bmatrix} -2 \\ 0 \\ 1 \end{bmatrix} \begin{bmatrix} 2/\sqrt{5} \\ 1/\sqrt{5} \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} -2 \\ 0 \\ 1 \end{bmatrix} + 4/\sqrt{5} \begin{bmatrix} 2/\sqrt{5} \\ 1/\sqrt{5} \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} -2 \\ 0 \\ 1 \end{bmatrix} + \begin{bmatrix} 8/5 \\ 4/5 \\ 0 \end{bmatrix} = \begin{bmatrix} -2/5 \\ 4/5 \\ 1 \end{bmatrix}$$

$$q_2 = \frac{\begin{bmatrix} -2/5 \\ 4/5 \\ 1 \end{bmatrix}}{\frac{3\sqrt{5}}{5}} = \frac{\begin{bmatrix} -2 \\ 4 \\ 5 \end{bmatrix}}{3\sqrt{5}} = \begin{bmatrix} -2/(3\sqrt{5}) \\ 4/(3\sqrt{5}) \\ 5/(3\sqrt{5}) \end{bmatrix}$$

$$q_2 = \begin{bmatrix} -2/\sqrt{45} \\ 4/\sqrt{45} \\ 5/\sqrt{45} \end{bmatrix}$$

$$U = \begin{bmatrix} -1/3 & 2/\sqrt{5} & -2/\sqrt{45} \\ 2/3 & 1/\sqrt{5} & 4/\sqrt{45} \\ -2/3 & 0 & 5/\sqrt{45} \end{bmatrix}$$

$$\Sigma = \begin{bmatrix} \sqrt{18} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$$V = \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \quad V^T = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$