

Today: PCA

- Symmetric Matrices.
- Spectral Thm.

Admin

- Midterm, March 12. Keep 5-9pm free.
- Enrollment.
- Discussion Sections.

①

Principal Component Analysis.

- High-dimensional data
- "Dimensionality reduction"
p-dimensional data

"Maximize" the variance of the data.

$$\max_{\|\vec{w}\|=1} \vec{w}^T C \cdot \vec{w}$$

$\vec{x}_1, \vec{x}_2, \dots, \vec{x}_n \in \mathbb{R}^p$ (zero-mean)

Uncover underlying lower-dimensional structure.

$(x, y) \rightarrow (x, y, z)$

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} \\ \\ \end{bmatrix}$$

Goal: Project our data into lower-dimension and recover low-dim. structure.

Project: $\vec{w} \in \mathbb{R}^p$ s.t. the projected vectors are as close to the original vectors as possible.

$$\|\vec{w}\|_2^2 = 1.$$

$\vec{x}_1, \vec{x}_2, \dots, \vec{x}_n$: Projections: $\langle \vec{x}_i, \vec{w} \rangle \cdot \vec{w}$

Error: $\|\vec{x}_i - \langle \vec{w}, \vec{x}_i \rangle \vec{w}\|^2 = e_i^2$ on \vec{x}_i

Average proj. error: $\frac{1}{n} \sum_{i=1}^n e_i^2 = \text{MSE}(\vec{w})$

Zero-mean

What is the mean of the projection?

$$\begin{aligned} \frac{1}{n} \sum_{i=1}^n \langle \vec{x}_i, \vec{w} \rangle \vec{w} &= \left(\frac{1}{n} \sum_{i=1}^n \vec{x}_i^T \vec{w} \right) \vec{w} \\ &= \left(\underbrace{\left(\frac{1}{n} \sum \vec{x}_i^T \right)}_0 \vec{w} \right) \vec{w} \\ &= 0 \end{aligned}$$

$$\begin{aligned} \underbrace{\|\vec{x}_i - \langle \vec{w}, \vec{x}_i \rangle \vec{w}\|}_{\vec{u}_i}^2 &= (\vec{u}_i^T \cdot \vec{u}_i) \\ &= (\vec{x}_i - \langle \vec{w}, \vec{x}_i \rangle \vec{w})^T (\vec{x}_i - \langle \vec{w}, \vec{x}_i \rangle \vec{w}) \\ &= \|\vec{x}_i\|^2 - 2\langle \vec{w}, \vec{x}_i \rangle \cdot \langle \vec{w}, \vec{x}_i \rangle + \langle \vec{w}, \vec{x}_i \rangle^2 \cdot \|\vec{w}\|^2 \\ &= \|\vec{x}_i\|^2 - \langle \vec{w}, \vec{x}_i \rangle^2 \end{aligned}$$

$$MSE(\vec{w}) = \frac{1}{n} \sum \|\vec{x}_i\|^2 - \frac{1}{n} \sum \langle \vec{w}, \vec{x}_i \rangle^2$$

$$E[X^2] = E[X]^2 + \text{Var}(X)$$

Goal: Maximize: $\frac{1}{n} \sum \langle \vec{w}, \vec{x}_i \rangle^2$

$$= \left(\frac{1}{n} \sum \langle \vec{x}_i, \vec{w} \rangle \right)^2 + \text{Var}(\langle \vec{w}, \vec{x}_i \rangle)$$

Data is zero mean.

$$\frac{1}{n} \sum \langle \vec{w}, \vec{x}_i \rangle^2 = \frac{1}{n} \|X \cdot \vec{w}\|^2$$

$$X = \begin{bmatrix} \vec{x}_1^T \\ \vec{x}_2^T \\ \vdots \\ \vec{x}_n^T \end{bmatrix} \quad \vec{w} = \begin{bmatrix} \\ \\ \dots \\ \end{bmatrix}$$

$n \times p$

$$\begin{aligned} &= \frac{1}{n} (X \vec{w})^T (X \vec{w}) \\ &= \frac{1}{n} \vec{w}^T X^T X \vec{w} \\ &= \vec{w}^T \cdot \underbrace{\left(\frac{X^T X}{n} \right)}_C \cdot \vec{w} \end{aligned}$$

maximize $\vec{w}^T \cdot C \cdot \vec{w}$
 $\|\vec{w}\|_2^2 = 1$

where C is the Covariance matrix of your data.

$$C = \begin{bmatrix} \sum x_{i1}^2 & \sum x_{i1} x_{i2} \\ \sum x_{i1} x_{i2} & \sum x_{i2}^2 \\ & \dots \\ & & \sum x_{ip}^2 \end{bmatrix}$$

Symmetric matrices

(5)

• Matrix $A \in S^n$ if $A^T = A$.

$$A \in \mathbb{R}^{n \times n} \quad A_{ij} = A_{ji} \quad \forall i, j, 1 \leq i, j \leq n.$$

e.g. Graph Laplacian

Diagonalization of Matrices

Condition for diagonalization:

"Algebraic" multiplicity = "Geometric" multiplicity.
 $\dim(N(A - \lambda I))$

$$\det(A - \lambda I) \rightarrow \# \text{ of roots} = \lambda.$$

$$\text{eg. } A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} y \\ 0 \end{bmatrix}$$

$$N(A) = \dim 1.$$

$$\text{eg. } \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$$

⑥
Properties of Symmetric Matrices. (C.E.G: Thm 4.1)

- $A \in \mathbb{R}^{n \times n}$, S^n is a symmetric matrix.
- $\lambda_1, \lambda_2, \dots, \lambda_k$ are all eigenvalues.
- $\mu_1, \mu_2, \dots, \mu_k$ are algebraic multiplicities.
- $\phi_i = N(A - \lambda_i I)$.

- Then:
- ① $\lambda_i \in \mathbb{R}$
 - ② $\phi_i \perp \phi_j$
 - ③ $\dim(\phi_i) = \mu_i$

"Spectral" Thm.

$$A = U \Lambda U^T$$

U : orthonormal matrix.

Λ : diagonal.

Proof of ③:

Lemma: (λ, \vec{u}) eigenpair for A . Then, there exists an orthonormal U such that.

$$U^T A U = \begin{bmatrix} \lambda & 0 \\ 0 & \boxed{B} \end{bmatrix}$$

$B \in S^{n-1}$

Proof: $U = \begin{bmatrix} \vec{u} \\ U_1 \end{bmatrix}$

Gram-Schmidt.

$$U^T A U = \begin{bmatrix} \vec{u}^T \\ \hline \end{bmatrix} \begin{bmatrix} A \end{bmatrix} \begin{bmatrix} \vec{u} & U_1 \end{bmatrix}$$

$$= \begin{bmatrix} \vec{u}^T \\ \hline U_1^T \end{bmatrix} \begin{bmatrix} \lambda \vec{u} & AU_1 \end{bmatrix}$$

$$= \begin{bmatrix} \lambda & 0 & \dots & 0 \\ \hline 0 & & & \\ \vdots & & U_1^T A U_1 & \\ 0 & & & \end{bmatrix}$$

$$B = U_1^T A U_1$$

$$B^T = B.$$

$\therefore B$ is symmetric. \square

Proceed by Induction.