SOON CHUN HYANG UNIVERSITY

PCA(Principal Component Analysis)

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개요

1. 주성분 분석 개요

2. 주성분 분석 수리적 배경

3. 주성분 분석 알고리즘

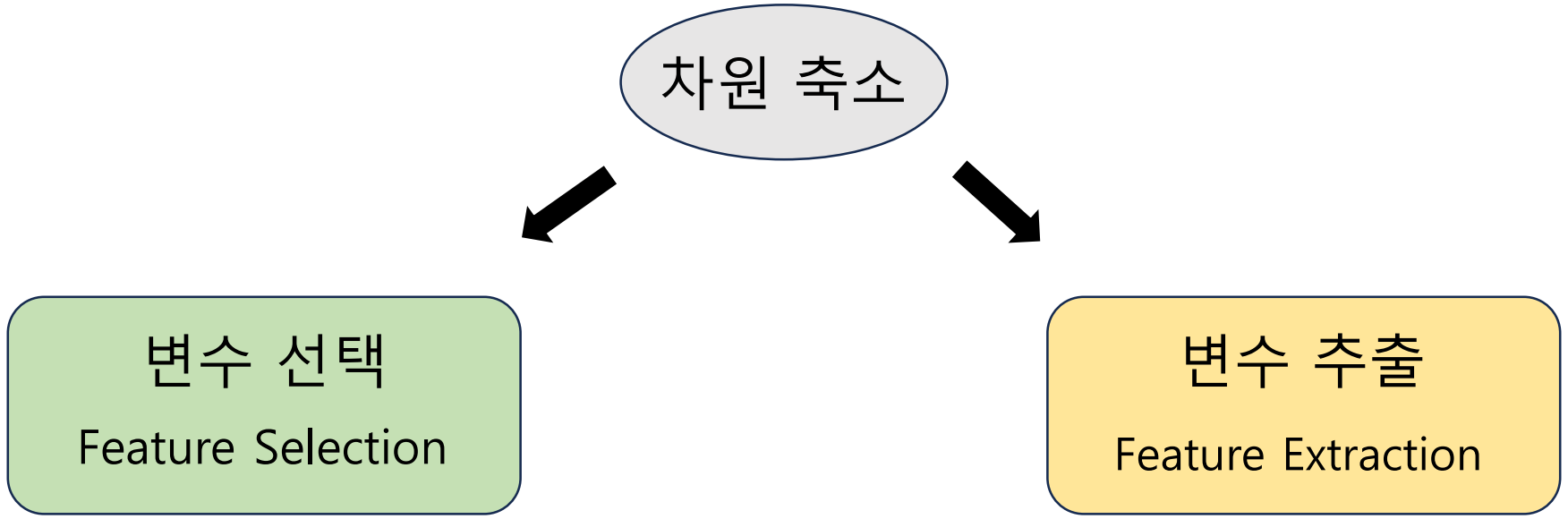
4. 주성분 분석 예제

주성분 분석 개요 – 고차원 데이터

변수 / 관측치	X_1	…	X_i	…	X_p
N_1	X_{11}	…	X_{1i}	…	X_{1p}
…	…	…	…	…	…
N_i	X_{i1}	…	X_{ii}	…	X_{ip}
…	…	…	…	…	…
N_n	X_{n1}	…	X_{ni}	…	X_{np}

- 3차원 이상의 데이터 → 시각적 표현 한계
- 차원이 클수록 계산복잡도 ↑, 모델링 비효율적
- 따라서 중요한 변수들로 차원을 줄일 필요가 있음

주성분 분석 개요



장점: 선택한 변수들의 해석이 용이함

단점: 변수간 상관관계 고려가 어려움

장점: 변수간 상관관계 고려함

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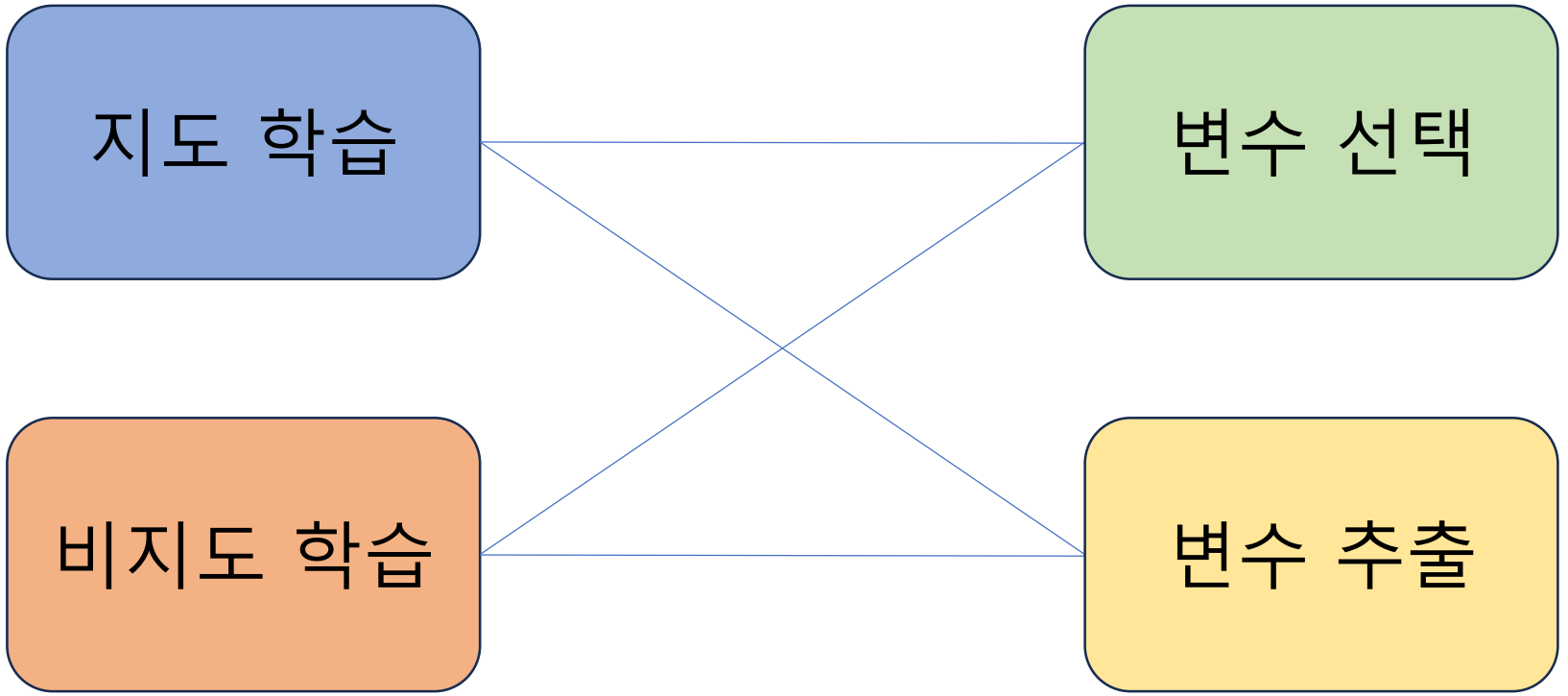

주성분 분석 개요

Supervised feature selection: Information Gain, Stepwise regression, LASSO, Genetic algorithm

Supervised feature extraction: Partial least squares (PLS)

Unsupervised feature selection: PCA loading

Unsupervised feature extraction: Principal component analysis (PCA), Wavelets transforms, Autoencoder

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주성분 분석 개요

PCA의 개념: 고차원 데이터를 효과적으로 분석하기 위한 대표적 분석 기법

목적) 차원 축소, 군집화, 시각화, 압축 등

PCA는 n개 관측치, p개 변수로 구성된 데이터를 상관관계가 없는 k개의 변수로 구성된 데이터로 요약하는 방식으로, 이 때 요약된 변수는 기존 변수의 선형 조합으로 생성됨

원래 데이터의 분산을 최대한 보존하는 새로운 축을 찾고, 그 축에 데이터를 사영 시키는 기법

주요 목적은 데이터 차원 축소 (n by p → n by k, where k << p)와 데이터 시각화 및 해석

전체 분석 과정 중 주로 초기에 사용됨 (변수 많을 때)

주성분 분석 개요

	X_1	X_2	…	X_{p-1}	X_p
1					
2					
…					
N-1					
N					

	Z_1	Z_2
1		
2		
…		
N-1		
N		

	Z_1	Z_2	Z_3
1			
2			
…			
N-1			
N			

Z_1, Z_2, , Z_3은 기존 변수인 X_1, X_2,…, X_p의 선형 조합으로 새롭게 생성된 변수

주성분 분석 개요

Z is linear combination (선형 결합) of the original all p variables in X

$$
\begin{aligned}
Z_1 &= \alpha_1^T X = \alpha_{11}X_1 + \alpha_{12}X_2 + \cdots + \alpha_{1p}X_p \\
Z_2 &= \alpha_2^T X = \alpha_{21}X_1 + \alpha_{22}X_2 + \cdots + \alpha_{2p}X_p \\
&\vdots \qquad\qquad\qquad\qquad \vdots \\
Z_p &= \alpha_p^T X = \alpha_{p1}X_1 + \alpha_{p2}X_2 + \cdots + \alpha_{1p}X_p
\end{aligned}
$$

$\boldsymbol{X_1}$, $\boldsymbol{X_2}$,⋯, $\boldsymbol{X_p}$: 원래 변수 (Original Variable)

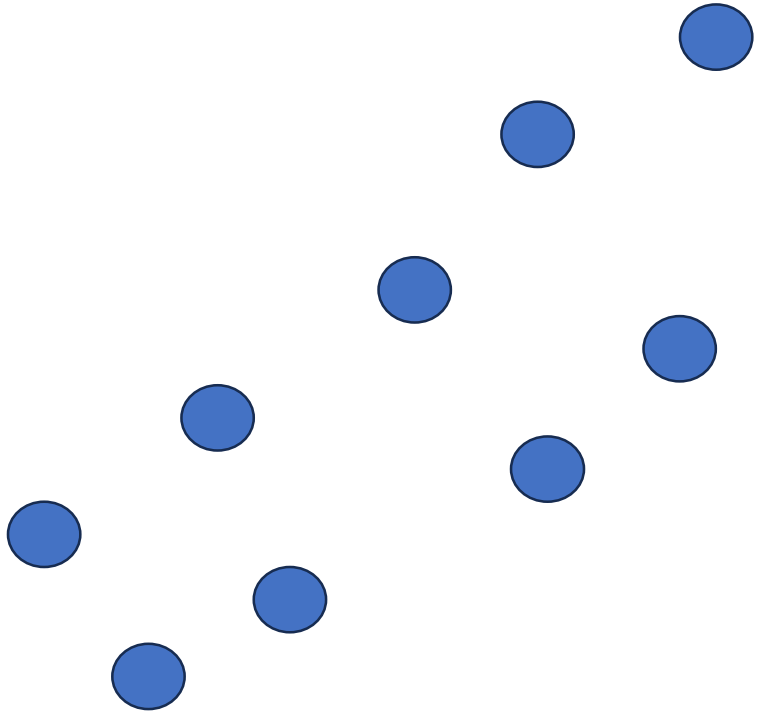
$\alpha_i = [\alpha_{i1}, \alpha_{i2},\cdots,\alpha_{ip}]$: i번째 기저(basis) 또는 계수 (Loading)

$\boldsymbol{Z_1}$, $\boldsymbol{Z_2}$,⋯, $\boldsymbol{Z_p}$: 각 기저로 사영 변환 후 변수 (주성분, Score)

주성분 분석 개요

Find the new axis that

maximizes the variance of data



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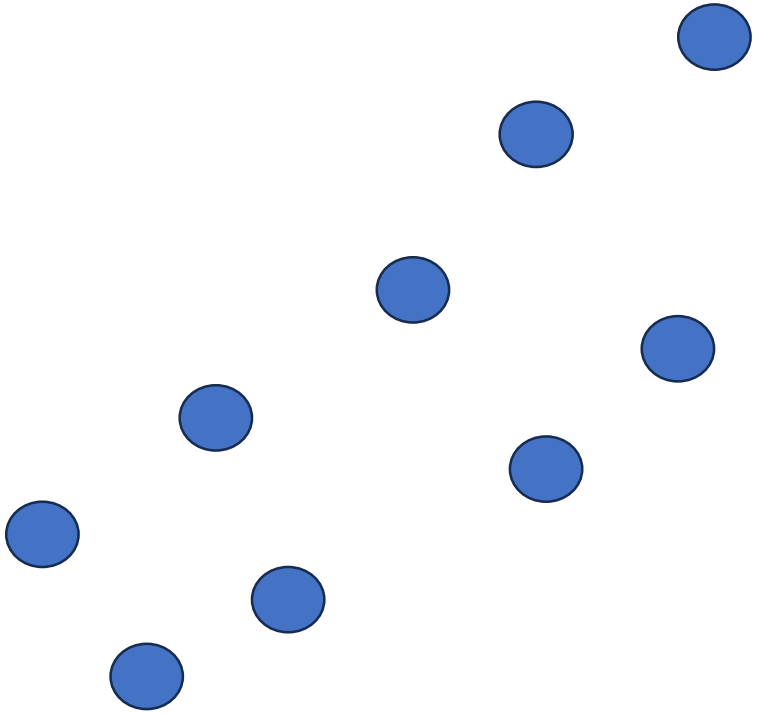

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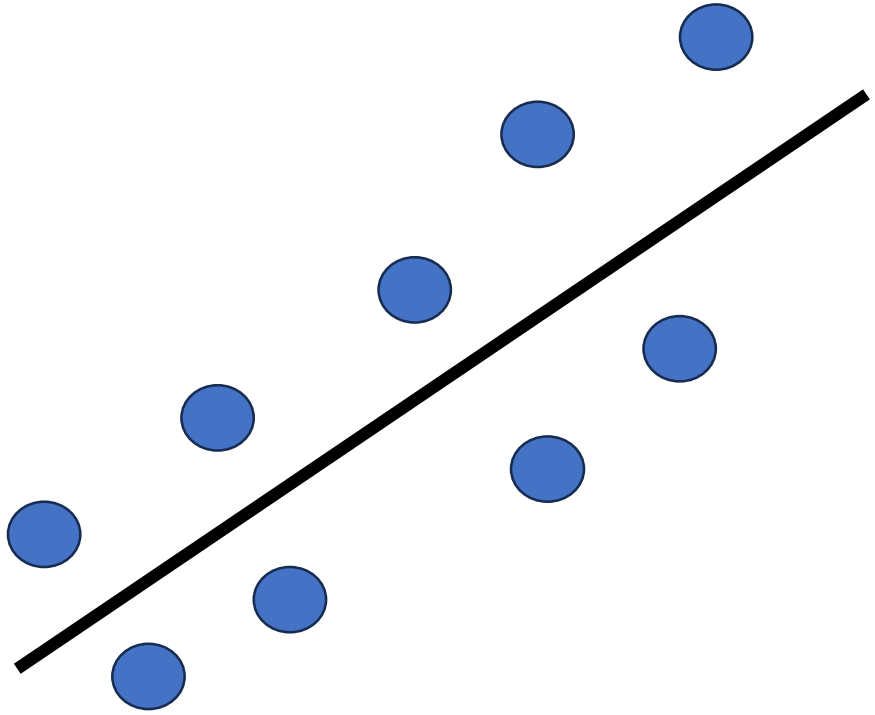

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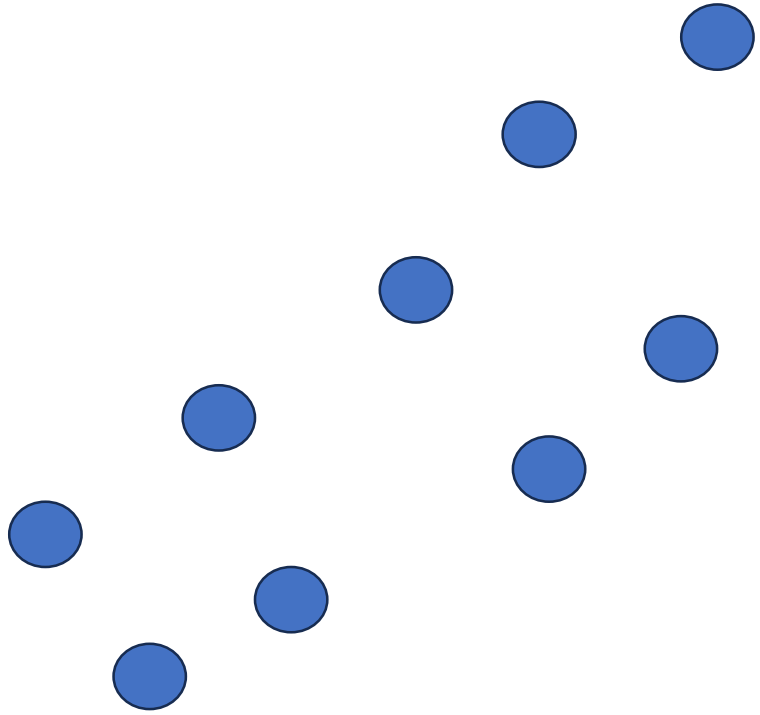

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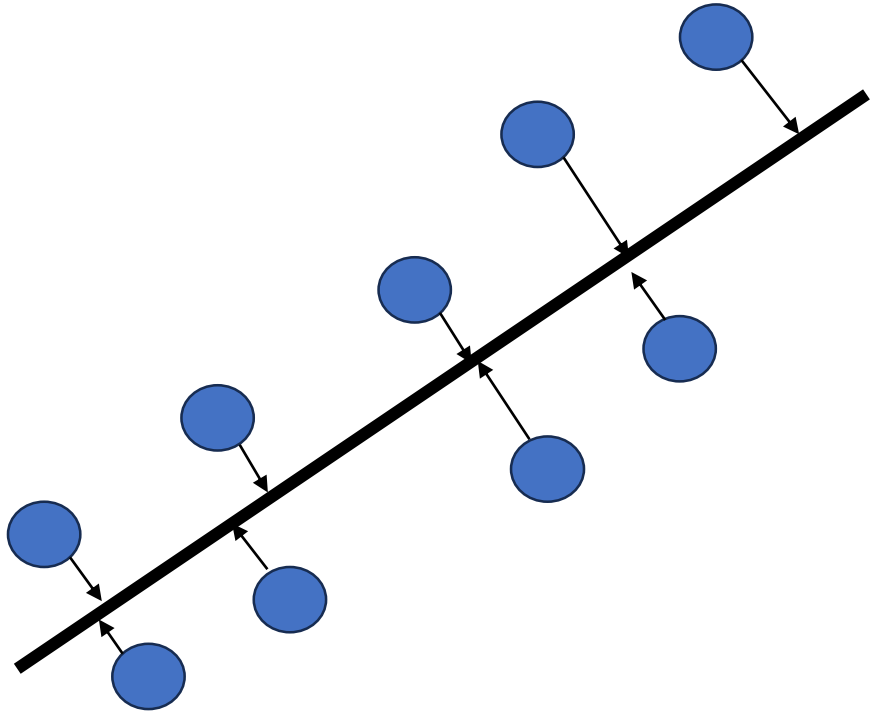

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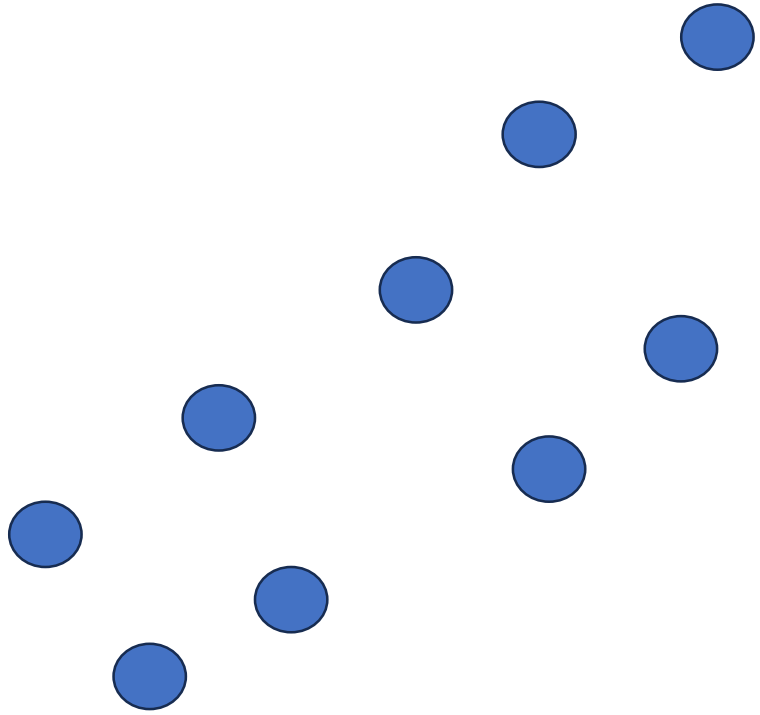

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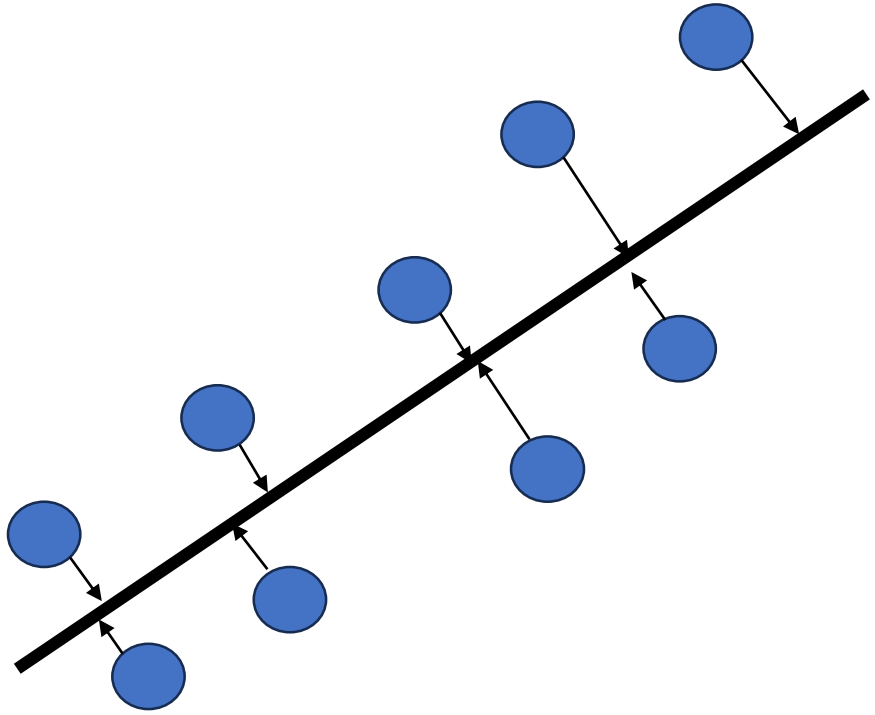

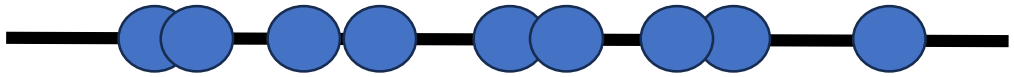

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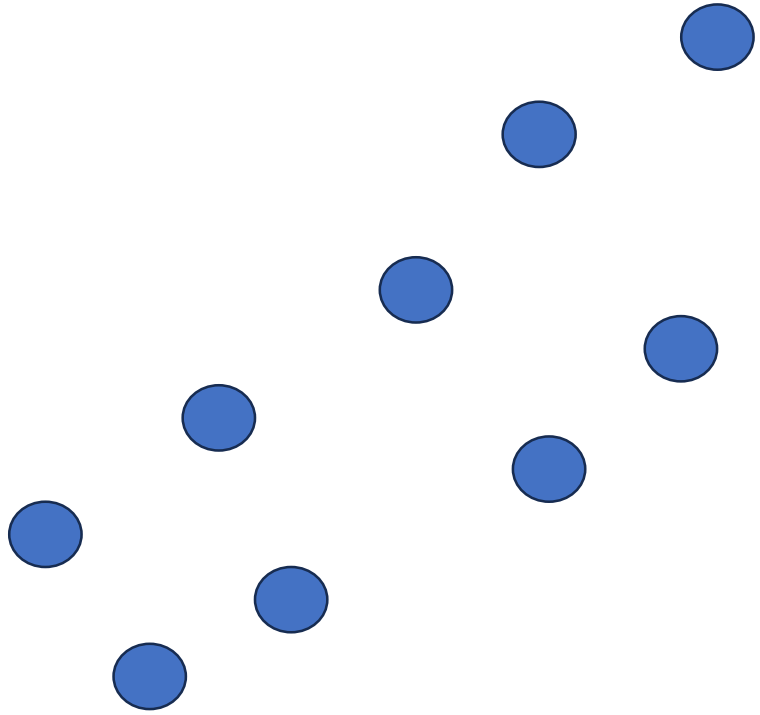

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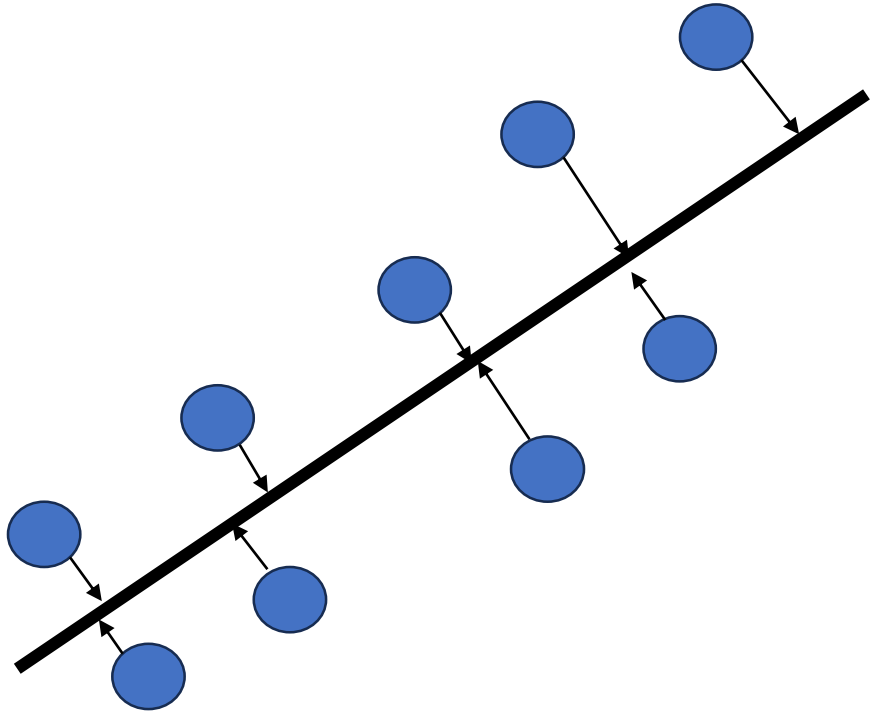

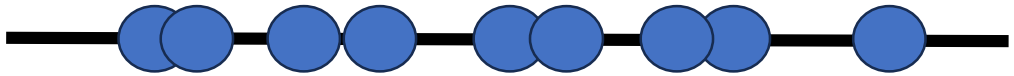

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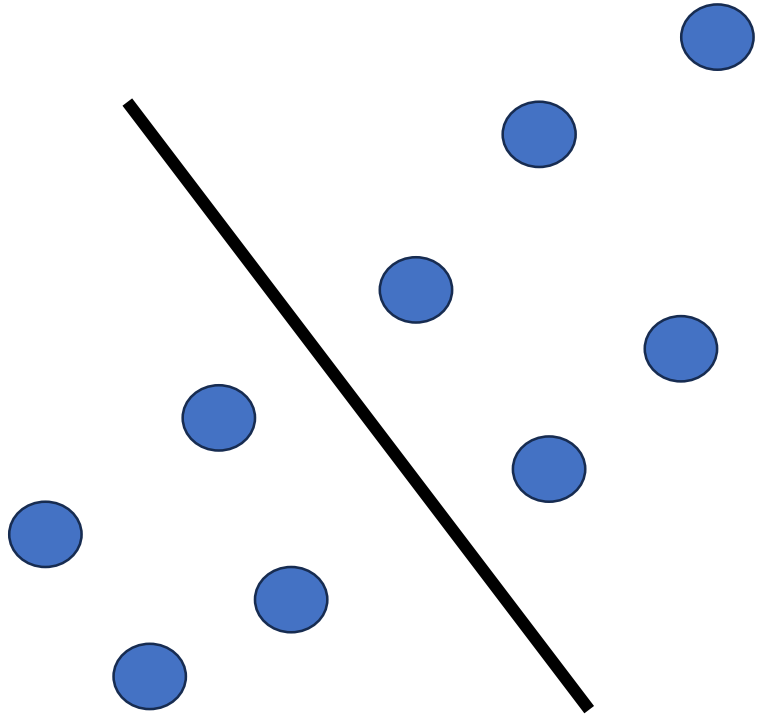

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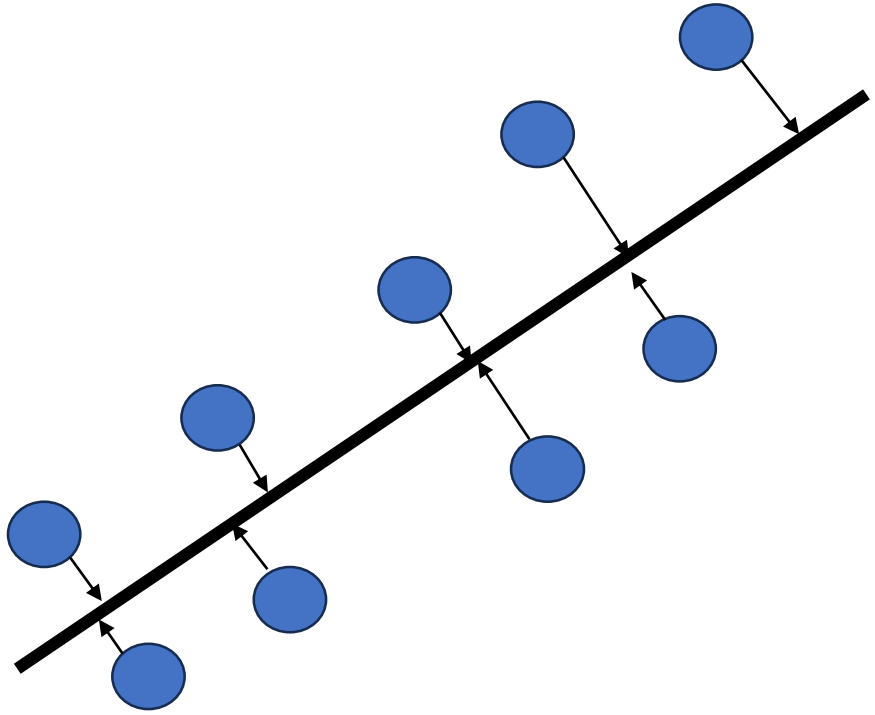

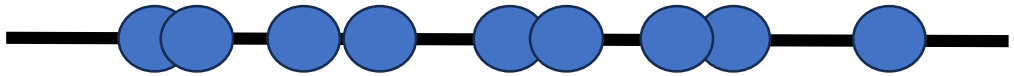

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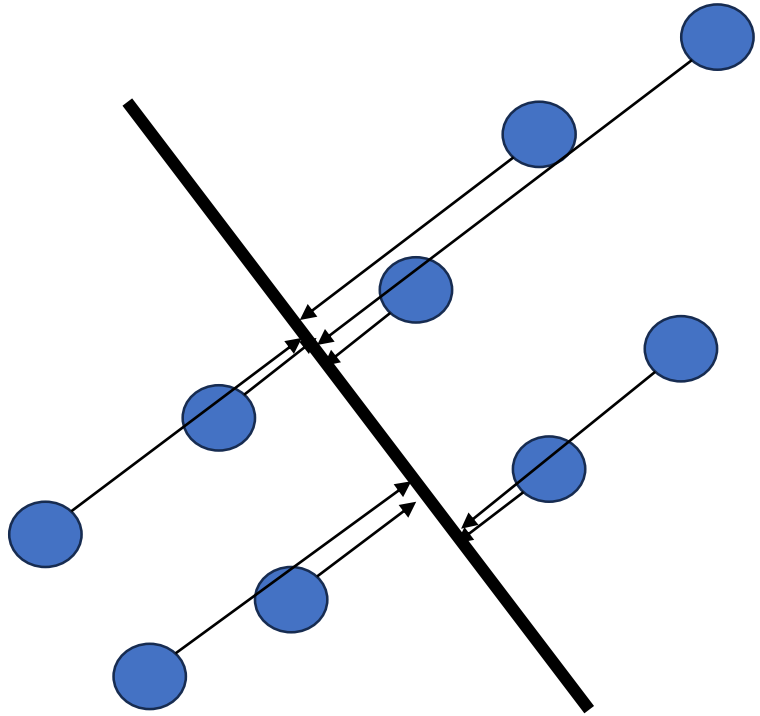

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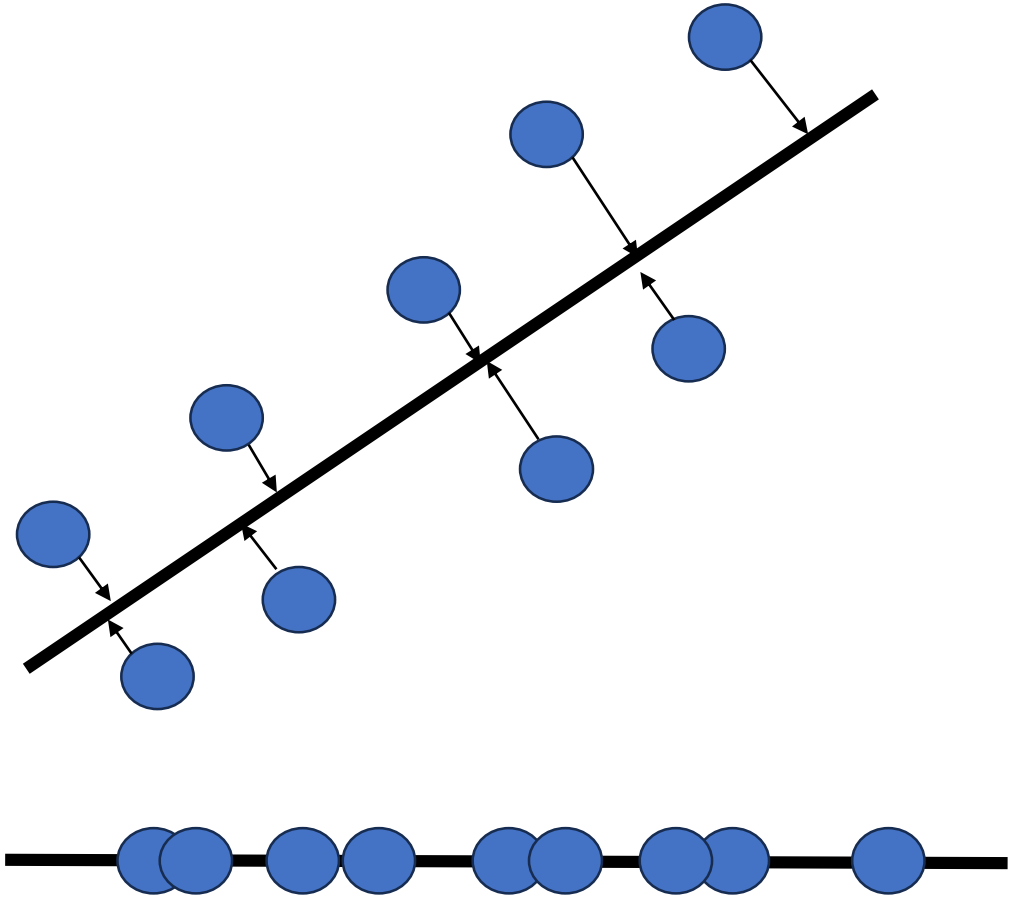

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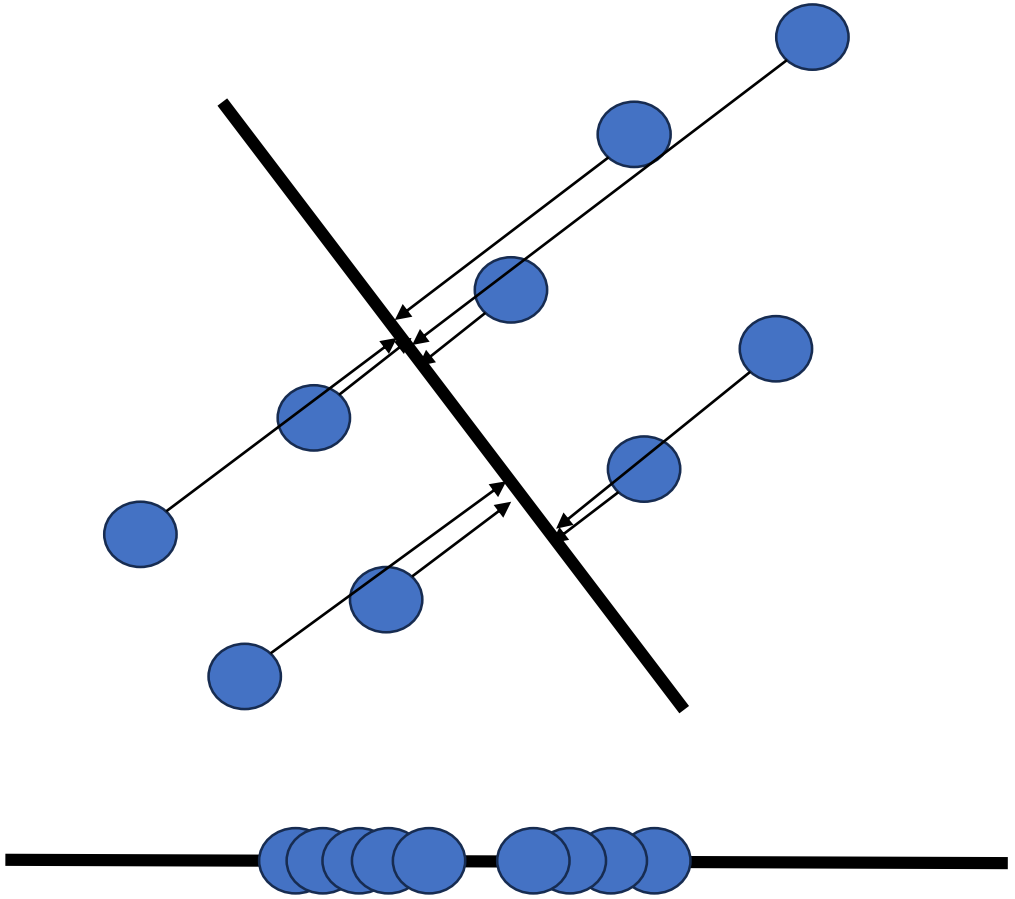


주성분 분석 수리적 배경

변수 / 관측치	X_1	⋯	X_i	⋯	X_p
N_1	X_{11}	⋯	X_{1i}	⋯	X_{1p}
⋯	⋯	⋯	⋯	⋯	⋯
N_i	X_{i1}	⋯	X_{ii}	⋯	X_{ip}
⋯	⋯	⋯	⋯	⋯	⋯
N_n	X_{n1}	⋯	X_{ni}	⋯	X_{np}

$$\overline{X} = \begin{bmatrix} \overline{X}_1 \\ \overline{X}_2 \\ \cdots \\ \overline{X}_p \end{bmatrix}$$

Mean vector

$$C_n = \begin{bmatrix} S_{11} & \cdots & S_{1p} \\ \vdots & \ddots & \vdots \\ S_{p1} & \cdots & S_{pp} \end{bmatrix}$$

Covariance Matrix

$$R = \begin{bmatrix} 1 & r_{12} & \cdots & r_{1p} \\ r_{21} & 1 & \cdots & r_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ r_{p1} & r_{p2} & \cdots & 1 \end{bmatrix}$$

Correlation Matrix

주성분 분석 수리적 배경

- 공분산 (Covariance)의 성질
  - X를 p개의 변수와 n개의 개체로 구성된 n by p 행렬로 정의할 때 X의 공분산 행렬은 다음과 같음

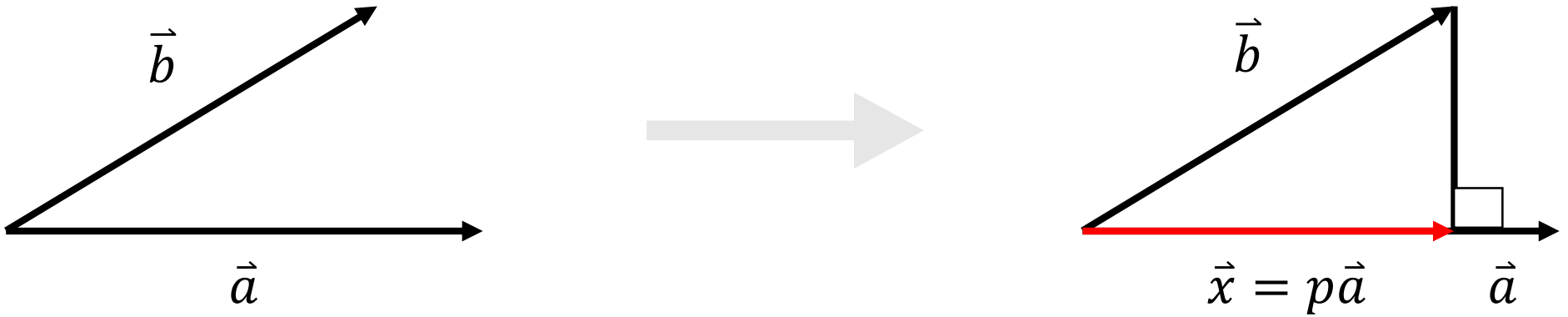
$$Cov(X) = \frac{1}{n}(X - \bar{X})\,(X - \bar{X})^T$$

  - 공분산 행렬의 대각 성분은 각 변수의 분산과 같으며, 비대각행렬은 대응하는 두 변수의 공분산과 같음

  - 데이터의 총분산은 공분산행렬의 대각성분들의 합으로 표현됨

주성분 분석 수리적 배경

- 사영 (Projection)
  - 한 벡터 $\vec{b}$를 다른 벡터 $\vec{a}$에 사영시킨다는 것은 벡터 $\vec{b}$로부터 벡터 $\vec{a}$에 수직인 점까지의 길이를 가지며 벡터 $\vec{a}$와 같은 방향을 갖는 벡터를 찾는다는 것을 의미



$$(\vec{b} - p\vec{a})^T\vec{a} = 0 \Rightarrow \vec{b}^T\vec{a} - p\vec{a}^T\vec{a} = 0 \Rightarrow p = \frac{\vec{b}^T\vec{a}}{\vec{a}^T\vec{a}}$$

$$\vec{x} = p\vec{a} = \frac{\vec{b}^T\vec{a}}{\vec{a}^T\vec{a}}\vec{a}$$

If $\vec{a}$ is unit vector

$$\mathrm{p} = \vec{b}^T\vec{a} \Rightarrow \vec{x} = p\vec{a}(\vec{b}^T\vec{a})\vec{a}$$

주성분 분석 수리적 배경

- 고유값(eigenvalue) 및 고유벡터(eigenvector)
  - 어떤 행렬 A에 대해 상수 λ와 벡터 x가 다음 식을 만족할 때,

    λ와 x를 각각 행렬 A의 고유값, 고유벡터라고 함

$$Ax = \lambda x \rightarrow (A - \lambda I)x = 0$$

  - 벡터에 행렬을 곱한다는 것은 해당 벡터를 선형변환(linear transformation)

    한다는 의미 → 고유벡터는 이 변환에 의해 방향이 변하지 않는 벡터를 의미

주성분 분석 알고리즘 – 주성분 추출

- Assume that we have the centered data (i.e., $\bar{X}_i = 0,\ \mathrm{i} = 1,\cdots,\mathrm{p}$)
- Let X be an p-dimensional random vector with the covariance matrix Σ
- Let α be an p-dimensional vector of length one (i.e., $\alpha^T\alpha = 1$)
- Let $\mathrm{Z} = \alpha^T\mathrm{X}$ be the projection of X onto the direction α

The main purpose in PCA is

to find α that produces the largest variance of Z

$$Max\ Var(Z) = Var(\alpha^T X) = \alpha^T \mathrm{Var(x)}\alpha = \alpha^T \Sigma \alpha$$
$$s.t. \|\alpha\| = \alpha^T\alpha = 1$$

주성분 분석 알고리즘 – 주성분 추출

$$\Sigma = E\Lambda E^T$$

$$Max\ \alpha^T \Sigma \alpha = \alpha^T E \Lambda E^T \alpha$$

$$s.t. \|\alpha\| = 1$$

eigenvalues and eigenvector of Σ

$$[E \wedge V] = svd(\Sigma)$$

$$\lambda_1 \geq \cdots \lambda_p \geq 0$$

$$e_1, \cdots, e_p$$

$$\Lambda = diag(\lambda_1, \cdots, \lambda_p)$$

$$Max\ \beta^T \Lambda\, \beta\ where\ \beta = E^T \alpha$$

$$s.t. \|\beta\| = 1$$

$$Max\ \lambda_1 {\beta_1}^2 + \lambda_2 {\beta_2}^2 + \cdots + \lambda_p {\beta_p}^2$$

$$s.t.\ {\beta_1}^2 + {\beta_2}^2 + \cdots + {\beta_p}^2 = 1$$

$$\lambda_1 > \lambda_2 > \cdots > \lambda_p$$

Thus, the optimal value is λ_1 and $\alpha = e_1$

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$$\begin{bmatrix} \lambda_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \lambda_2 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \lambda_p \end{bmatrix}$$

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$$\vdots$$
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$$s.t.\ {\beta_1}^2 + {\beta_2}^2 + \cdots + {\beta_p}^2 = 1$$

$$\lambda_1 > \lambda_2 > \cdots > \lambda_p$$

$$\beta_1 = 1,\ \beta_2 = 0,\ \vdots,\ \beta_p = 0 \qquad \alpha = E\beta$$

$$\begin{bmatrix} \lambda_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \lambda_2 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \lambda_p \end{bmatrix}$$

Thus, the optimal value is $\boldsymbol{\lambda_1}$ and $\boldsymbol{\alpha = e_1}$

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$$e_1, \cdots, e_p$$

$$\Lambda = diag(\lambda_1, \cdots, \lambda_p)$$

$$Max\ \beta^T \Lambda\, \beta\ where\ \beta = E^T \alpha$$

$$s.t. \|\beta\| = 1$$

$$Max\ \lambda_1 {\beta_1}^2 + \lambda_2 {\beta_2}^2 + \cdots + \lambda_p {\beta_p}^2$$

$$s.t.\ {\beta_1}^2 + {\beta_2}^2 + \cdots + {\beta_p}^2 = 1$$

$$\lambda_1 > \lambda_2 > \cdots > \lambda_p$$

$$\beta_1 = 1,\ \beta_2 = 0,\ \cdots,\ \beta_p = 0$$

$$\alpha = E\beta = [e_1 \quad \cdots \quad e_p] \begin{bmatrix} \beta_1 \\ \cdots \\ \beta_p \end{bmatrix} \begin{bmatrix} \lambda_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \lambda_2 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \lambda_p \end{bmatrix}$$

Thus, the optimal value is $\boldsymbol{\lambda_1}$ and $\boldsymbol{\alpha = e_1}$

주성분 분석 예제

$\mathbf{X} =$

X_1	X_2	X_3
0.2	5.6	3.56
0.45	5.89	2.4
0.33	6.37	1.95
0.54	7.9	1.32
0.77	7.87	0.98

$\mathbf{X} =$

X_1	X_2	X_3
-1.1930	-1.0300	1.5012
-0.0370	-0.7647	0.3540
-0.5919	-0.3257	-0.0910
0.3792	1.0739	-0.7140
1.4427	1.0464	-1.0502

normalize X to

$\mathrm{E}(X_i) = 0$

$\mathrm{Var}(X_i) = 1$

주성분 분석 예제

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normalize X to

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$\mathrm{Covariance}(X) =$

0.0468	0.1990	-0.1993
0.1990	1.1951	-1.0096
-0.1993	-1.0096	1.0225

$\mathrm{Correlation}(X) =$

1	0.8417	-0.8840
0.8417	1	-0.9133
-0.8840	-0.9133	1

주성분 분석 예제

The eigenvalue-eigenvector pairs on the correlation matrix, Σ

$$[E \wedge V] = svd(\Sigma)$$

$$\lambda_1 = 0.0786, \qquad {e_1}^T = [0.2590 \quad 0.5502 \quad 0.7938]$$

$$\lambda_2 = 0.1618, \qquad {e_2}^T = [0.7798 \quad -0.6041 \quad 0.1643]$$

$$\lambda_3 = 2.7596, \qquad {e_3}^T = [0.5699 \quad 0.5765 \quad -0.5855]$$

주성분 분석 예제

$\lambda_1 = 0.0786,\ {e_1}^T = [0.2590 \quad 0.5502 \quad 0.7938]$

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$\lambda_3 > \lambda_2 > \lambda_1$

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0.3792	1.0739	-0.7140
1.4427	1.0464	-1.0502

normalize X to

$\mathrm{E}(X_i) = 0$

$\mathrm{Var}(X_i) = 1$

$\lambda_3 > \lambda_2 > \lambda_1$

$$Z_1 = {e_3}^T X = 0.5699 \cdot X_1 + 0.5765 \cdot X_2 - 0.5855 \cdot X_3 = 0.5699 \cdot \begin{bmatrix} -1.1930 \\ -0.0370 \\ -0.5919 \\ 0.3792 \\ 1.4427 \end{bmatrix} + 0.5765 \cdot \begin{bmatrix} -1.0300 \\ -0.7647 \\ -0.3257 \\ 1.0739 \\ 1.0464 \end{bmatrix} - 0.5855 \cdot \begin{bmatrix} 1.5012 \\ 0.3540 \\ -0.0910 \\ -0.7140 \\ -1.0502 \end{bmatrix} = \begin{bmatrix} -2.1527 \\ -0.6692 \\ -0.4718 \\ 1.2533 \\ 2.0404 \end{bmatrix}$$

주성분 분석 예제

$$\lambda_1 = 0.0786,\ e_1{}^T = [0.2590 \quad 0.5502 \quad 0.7938]$$
$$\lambda_2 = 0.1618,\ e_2{}^T = [0.7798 \quad -0.6041 \quad 0.1643]$$
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$$\lambda_3 > \lambda_2 > \lambda_1$$

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1.4427	1.0464	-1.0502

normalize X to

$\mathrm{E}(X_i) = 0$

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$$Z_1 = e_3{}^T X = 0.5699 \cdot X_1 + 0.5765 \cdot X_2 - 0.5855 \cdot X_3 = 0.5699 \cdot \begin{bmatrix} -1.1930 \\ -0.0370 \\ -0.5919 \\ 0.3792 \\ 1.4427 \end{bmatrix} + 0.5765 \cdot \begin{bmatrix} -1.0300 \\ -0.7647 \\ -0.3257 \\ 1.0739 \\ 1.0464 \end{bmatrix} - 0.5855 \cdot \begin{bmatrix} 1.5012 \\ 0.3540 \\ -0.0910 \\ -0.7140 \\ -1.0502 \end{bmatrix} = \begin{bmatrix} -2.1527 \\ -0.6692 \\ -0.4718 \\ 1.2533 \\ 2.0404 \end{bmatrix}$$

$$Z_2 = e_2{}^T X = \begin{bmatrix} -0.0615 \\ 0.4912 \\ -0.2798 \\ -0.4703 \\ 0.3204 \end{bmatrix} \qquad Z_3 = e_1{}^T X = \begin{bmatrix} 0.3160 \\ -0.1493 \\ -0.4047 \\ 0.1223 \\ 0.1157 \end{bmatrix}$$

주성분 분석 예제

$$\lambda_1 = 0.0786,\ {e_1}^T = [0.2590 \quad 0.5502 \quad 0.7938]$$
$$\lambda_2 = 0.1618,\ {e_2}^T = [0.7798 \quad -0.6041 \quad 0.1643]$$
$$\lambda_3 = 2.7596,\ {e_3}^T = [0.5699 \quad 0.5765 \quad -0.5855]$$

$$\lambda_3 > \lambda_2 > \lambda_1$$

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-1.1930	-1.0300	1.5012
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-0.5919	-0.3257	-0.0910
0.3792	1.0739	-0.7140
1.4427	1.0464	-1.0502

normalize X to

$\mathrm{E}(X_i) = 0$

$\mathrm{Var}(X_i) = 1$

$$Z_1 = {e_3}^T X = 0.5699 \cdot X_1 + 0.5765 \cdot X_2 - 0.5855 \cdot X_3 = 0.5699 \cdot \begin{bmatrix} -1.1930 \\ -0.0370 \\ -0.5919 \\ 0.3792 \\ 1.4427 \end{bmatrix} + 0.5765 \cdot \begin{bmatrix} -1.0300 \\ -0.7647 \\ -0.3257 \\ 1.0739 \\ 1.0464 \end{bmatrix} - 0.5855 \cdot \begin{bmatrix} 1.5012 \\ 0.3540 \\ -0.0910 \\ -0.7140 \\ -1.0502 \end{bmatrix} = \begin{bmatrix} -2.1527 \\ -0.6692 \\ -0.4718 \\ 1.2533 \\ 2.0404 \end{bmatrix}$$

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$$\therefore Z = \begin{bmatrix} -2.1527 & -0.0615 & 0.3160 \\ -0.6692 & 0.4912 & -0.1493 \\ -0.4718 & -0.2798 & -0.4047 \\ 1.2533 & -0.4703 & 0.1223 \\ 2.0404 & 0.3204 & 0.1157 \end{bmatrix}$$

주성분 분석 예제

$$Z = \begin{bmatrix} -2.1527 & -0.0615 & 0.3160 \\ -0.6692 & 0.4912 & -0.1493 \\ -0.4718 & -0.2798 & -0.4047 \\ 1.2533 & -0.4703 & 0.1223 \\ 2.0404 & 0.3204 & 0.1157 \end{bmatrix}$$

$$Cov(Z) = \begin{bmatrix} 2.7596 & 0 & 0 \\ 0 & 0.1618 & 0 \\ 0 & 0 & 0.0786 \end{bmatrix}$$

주성분 (Z)들은 서로 독립

주성분 분석 예제

$\mathbf{X} =$

X_1	X_2	X_3
-1.1930	-1.0300	1.5012
-0.0370	-0.7647	0.3540
-0.5919	-0.3257	-0.0910
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1.4427	1.0464	-1.0502

$\mathbf{Z} =$

Z_1	Z_2	Z_3
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2.0404	0.3204	0.1157

주성분 몇 개 사용?

주성분 분석 예제

Eigenvalues of the covariance matrix $(\lambda_1, \lambda_2, \lambda_3)$

= Variance of each principal component (각 주성분의 분산)

Covariance matrix of principal components

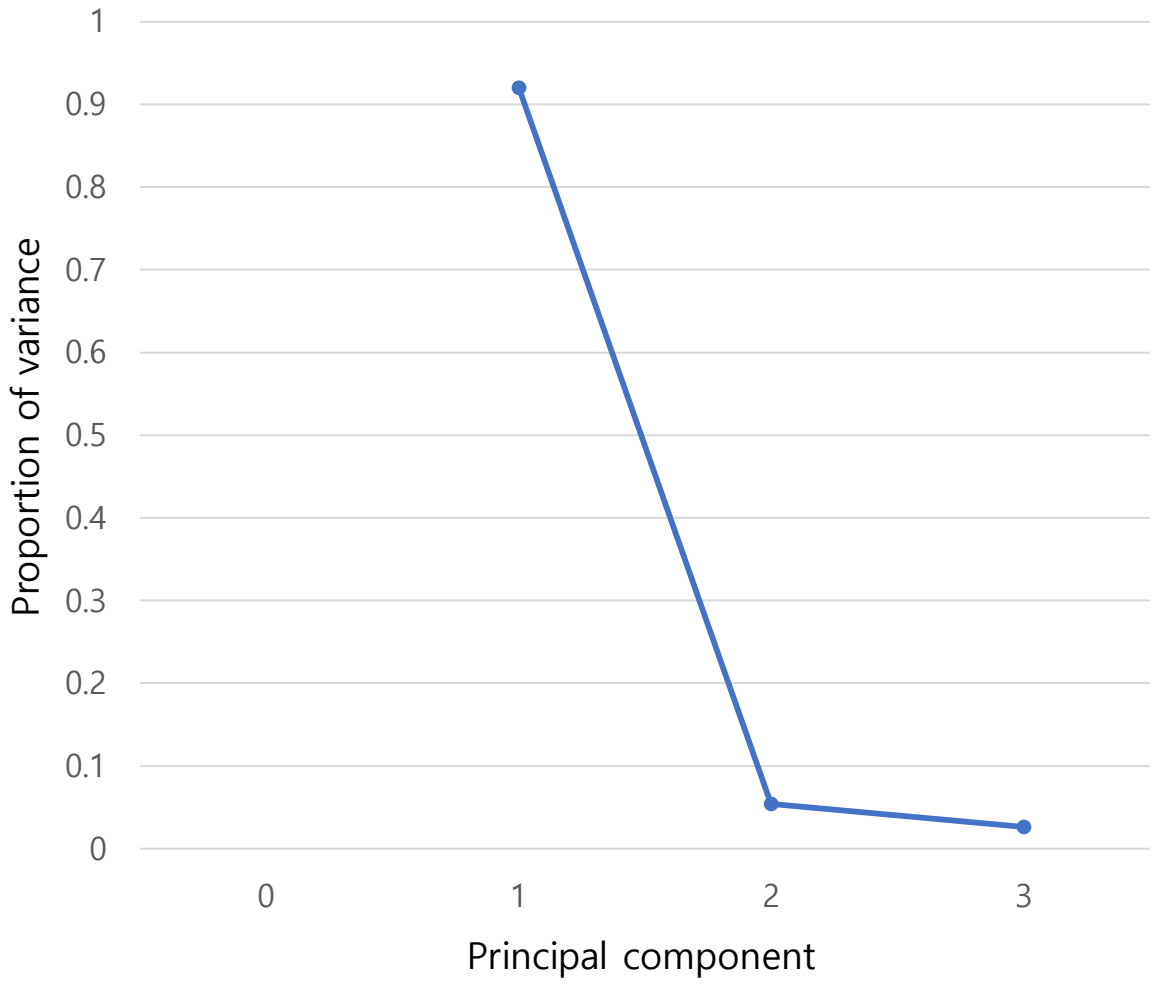
$$Cov(Z) = \begin{bmatrix} 2.7596 & 0 & 0 \\ 0 & 0.1618 & 0 \\ 0 & 0 & 0.0786 \end{bmatrix}$$

$$Var(Z_1) = 2.7596 = \lambda_3 \text{ (Largest eigenvalue)}$$
$$Var(Z_2) = 0.1618 = \lambda_2$$
$$Var(Z_3) = 0.0786 = \lambda_1$$

Proportion of total population Variance due to the 1st Principal component

$$= \frac{\lambda_3}{\lambda_1 + \lambda_2 + \lambda_3} = \frac{2.7596}{0.0786 + 0.1618 + 2.7596} = 0.920$$

주성분 분석 예제



선택방식 1: 고유값 감소율이 유의미하게 낮아지는 Elbow Point에 해당하는 주성분 수를 선택

선택방식 2: 일정 수준 이상의 분산비를 보존하는 최소의 주성분을 선택 (70% 이상)

주성분 분석 알고리즘 요약

Step 1. 데이터 정규화 **(mean centering)**

Step 2. 기존 변수의 **covariance (correlation) matrix** 계산

Step 3. **Covariance (correlation) matrix**로부터 **eigenvalue** 및 이에 해당되는 **eigenvector**를 계산

Step 4. **eigenvalue** 및 해당되는 **eigenvectors**를 순서대로 나열

$$\lambda(1) > \lambda(2) > \lambda(3) > \lambda(4) > \lambda(5)$$

$$\mathrm{e}(1) > e(2) > e(3) > e(4) > e(5), \quad e(i), \quad i = 1, \cdots, 5 \; is \; a \; vector$$

Step 5. 정렬된 **eigenvector**를 토대로 기존 변수를 변환

$$Z_1 = e(1)X = e_{11} \cdot X_1 + e_{12} \cdot X_2 + \cdots + e_{15} \cdot X_5$$
$$Z_2 = e(2)X = e_{21} \cdot X_1 + e_{22} \cdot X_2 + \cdots + e_{25} \cdot X_5$$
$$\cdots \qquad = \qquad \cdots$$
$$Z_5 = e(5)X = e_{51} \cdot X_1 + e_{52} \cdot X_2 + \cdots + e_{55} \cdot X_5$$

Thank you