

Lecture 10: Dimensionality Reduction with Principal Component Analysis

Yi, Yung (이웅)

Mathematics for Machine Learning
<https://yung-web.github.io/home/courses/mathml.html>
KAIST EE

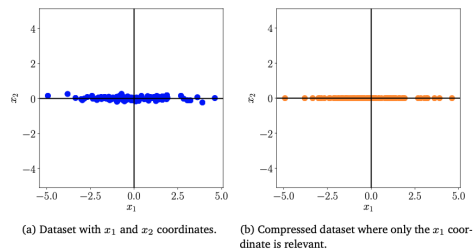
April 2, 2021

Please watch this tutorial video by Luis Serrano on PCA.

<https://www.youtube.com/watch?v=g-Hb26agBFg>

- (1) Problem Setting
- (2) Maximum Variance Perspective
- (3) Projection Perspective
- (4) Eigenvector Computation and Low-Rank Approximations
- (5) PCA in High Dimensions
- (6) Key Steps of PCA in Practice
- (7) Latent Variable Perspective

- (1) **Problem Setting**
- (2) Maximum Variance Perspective
- (3) Projection Perspective
- (4) Eigenvector Computation and Low-Rank Approximations
- (5) PCA in High Dimensions
- (6) Key Steps of PCA in Practice
- (7) Latent Variable Perspective



- High-dimensional data
 - hard to analyze and visualize
 - Often, overcomplete and many dimensions are redundant
- Compact data representation is always preferred just like compression.
- PCA (Principal Component Analysis) is a representative method.

L10(1)

April 2, 2021 5 / 42

- 5 dimensions
 1. Size
 2. Number of rooms
 3. Number of bathrooms
 4. Schools around
 5. Crime rate
- 2 dimensions
 - Size feature
 - Location feature

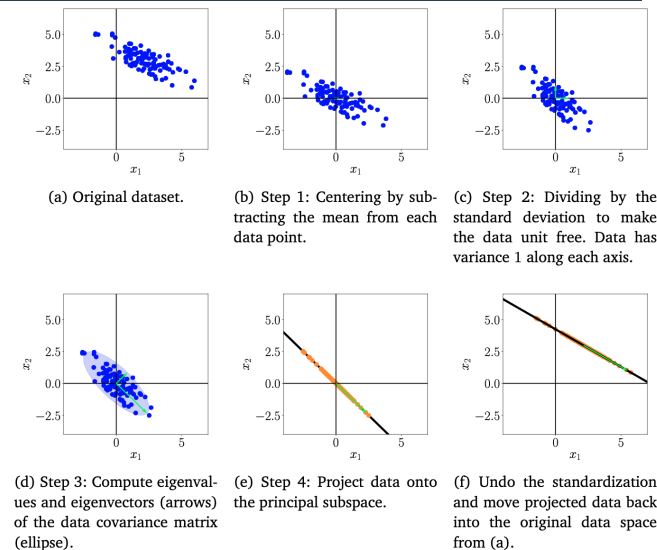
L10(1)

April 2, 2021 6 / 42

- S1. Centering.** Centering the data by subtracting mean
- S2. Standardization.** Divide the data points by the standard deviation for every dimension (original feature) $d = 1, \dots, D$
- S3. Eigenvalue/vector.** Compute the M -largest eigenvalues and the eigenvectors of the data covariance matrix (M is the dimension that needs to be reduced)
- S4. Projection.** Project all data points onto the space defined by the eigenvectors (i.e., principal subspace).
- S5.** Undo standardization and centering.

L10(1)

April 2, 2021 7 / 42



L10(1)

April 2, 2021 8 / 42

- N : number of samples, D : number of measurements (or original features)
- iid dataset $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ whose mean is 0 (well-centered), where each $\mathbf{x}_i \in \mathbb{R}^D$, and its corresponding data matrix

$$\mathbf{X} = (\mathbf{x}_1 \cdots \mathbf{x}_N) = \begin{pmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,N} \\ x_{2,1} & x_{2,2} & \cdots & x_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ x_{D,1} & x_{D,2} & \cdots & x_{D,N} \end{pmatrix} \in \mathbb{R}^{D \times N}$$

- (data) covariance matrix

$$\mathbf{S} = \frac{1}{N} \mathbf{X} \mathbf{X}^T = \frac{1}{N} \sum_{n=1}^N \mathbf{x}_n \mathbf{x}_n^T \in \mathbb{R}^{D \times D}$$

L10(1)

April 2, 2021 9 / 42

- Covariance matrix for a random vector $\mathbf{Y} = (Y_1, \dots, Y_D)^T$,

L6(4)

$$\Sigma_{\mathbf{Y}} = \begin{pmatrix} \text{cov}(Y_1, Y_1) & \text{cov}(Y_1, Y_2) & \cdots & \text{cov}(Y_1, Y_D) \\ \vdots & \vdots & \ddots & \vdots \\ \text{cov}(Y_D, Y_1) & \text{cov}(Y_D, Y_2) & \cdots & \text{cov}(Y_D, Y_D) \end{pmatrix}$$

- Data covariance matrix $\mathbf{S} \in \mathbb{R}^{D \times D}$

- Each Y_i has N samples $(x_{i,1} \cdots x_{i,N})$

$$\begin{aligned} S_{ij} = \text{cov}(Y_i, Y_j) &= \frac{1}{N} \sum_{k=1}^N x_{i,k} \cdot x_{j,k} \\ &= \text{average covariance (over samples) btwn features } i \text{ and } j \end{aligned}$$

L10(1)

April 2, 2021 10 / 42

- Low-dimensional compressed representation, also called **code**:

$$\mathbf{z}_n = \mathbf{B}^T \mathbf{x}_n \in \mathbb{R}^M,$$

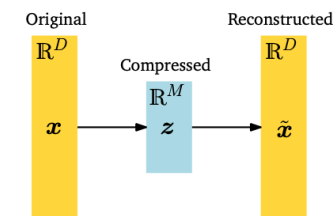
where the projection¹ matrix is $\mathbf{B} := (\mathbf{b}_1, \dots, \mathbf{b}_M) \in \mathbb{R}^{D \times M}$,

- Assume that the columns of \mathbf{B} are orthonormal, i.e., $\mathbf{b}_i^T \mathbf{b}_j = 0$ if $i \neq j$, and $\mathbf{b}_i^T \mathbf{b}_i = 1$ if $i = j$.
- Seek an M -dimensional subspace $U \subset \mathbb{R}^D$, $\dim(U) = M < D$ onto which we project data
- $\tilde{\mathbf{x}}_n \in \mathbb{R}^D$: projected data, \mathbf{z}_n : their coordinates w.r.t. the basis vectors of \mathbf{B} .

¹In L3(8), the coordinate in the projected space becomes $\boldsymbol{\lambda} = (\mathbf{B}^T \mathbf{B})^{-1} \mathbf{B}^T \mathbf{x}$, which is simply $\mathbf{B}^T \mathbf{x}$ for orthonormal bases \mathbf{B} .

L10(1)

April 2, 2021 11 / 42



- Find a suitable matrix \mathbf{B} such that $\mathbf{z} = \mathbf{B}^T \mathbf{x}$ and $\tilde{\mathbf{x}} = \mathbf{B} \mathbf{z}$
- \mathbf{B}^T : encoder, \mathbf{B} : decoder
- **Example.** MNIST dataset
 - handwritten digits, $N = 60,000$ data samples, $D = 28 \times 28 = 784$ pixels

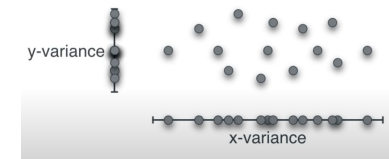


L10(1)

April 2, 2021 12 / 42

- (1) Problem Setting
- (2) **Maximum Variance Perspective**
- (3) Projection Perspective
- (4) Eigenvector Computation and Low-Rank Approximations
- (5) PCA in High Dimensions
- (6) Key Steps of PCA in Practice
- (7) Latent Variable Perspective

- Information content in the data
 - space filling
 - information in the data by looking at how much data is spread out
- PCA
 - a dimensionality reduction algorithm that maximizes the variance in the low-dimensional data representation.



source: Youtube channel by Luis Serrano

- $B = (\mathbf{b}_1 \ \mathbf{b}_2 \ \dots \ \mathbf{b}_M)$, where $\mathbf{b}_i \in \mathbb{R}^D$ and $B \in \mathbb{R}^{D \times M}$
- $B^T = \begin{pmatrix} \mathbf{b}_1^T \\ \vdots \\ \mathbf{b}_M^T \end{pmatrix} \in \mathbb{R}^{M \times D}$, $\mathbf{b}_i^T \in \mathbb{R}^{1 \times D}$, $\mathbf{x}_i \in \mathbb{R}^{D \times 1}$
- $z_n = \begin{pmatrix} z_{1n} \\ \vdots \\ z_{Mn} \end{pmatrix} = B^T \mathbf{x}_n = \begin{pmatrix} \mathbf{b}_1^T \\ \vdots \\ \mathbf{b}_M^T \end{pmatrix} \mathbf{x}_n = \begin{pmatrix} \mathbf{b}_1^T \mathbf{x}_n \\ \vdots \\ \mathbf{b}_M^T \mathbf{x}_n \end{pmatrix}$
- z_{in} : new coordinate (for \mathbf{x}_n) in the projected space by the basis \mathbf{b}_i

- **Goal:** Find the orthonormal bases $B = (\mathbf{b}_1 \ \mathbf{b}_2 \ \dots \ \mathbf{b}_M)$ that maximizes the variance.
- **Result:** For the M -largest eigenvalues $\lambda_1, \dots, \lambda_M$ of the data covariance matrix S , their corresponding M eigenvectors become $\mathbf{b}_1, \dots, \mathbf{b}_M$
- **Question.** Why data covariance matrix? Why eigenvectors ordered by their eigenvalues?
- Strategy: Induction
 - Step 1.** We seek a single vector \mathbf{b}_1 that maximizes the variance of the projected data, assuming that we project the data onto an 1D line. We show that \mathbf{b}_1 is the **eigenvector of the largest eigenvalue**.
 - Step k.** Suppose that we found $\mathbf{b}_1, \dots, \mathbf{b}_{k-1}$ for the variance maximization. Then, we seek \mathbf{b}_k that maximizes the variance of the projected data onto k -D plain with the constraint that \mathbf{b}_k is orthogonal to $\mathbf{b}_1, \dots, \mathbf{b}_{k-1}$. We prove that \mathbf{b}_k is the **eigenvector of the k -th largest eigenvalue**.

Step 1: Finding \mathbf{b}_1 (1)

- Variance (over N sample data) of the first coordinate z_1 of $\mathbf{z} \in \mathbb{R}^M$, so that

$$V_1 := \text{var}[z_1] = \frac{1}{N} \sum_{n=1}^N z_{1n}^2, \quad z_{1n} = \mathbf{b}_1^T \mathbf{x}_n$$

where z_{1n} (z_{in}) is the first (i -th) coordinate of the low-dimensional representation \mathbf{z}_n of \mathbf{x}_n

$$V_1 = \frac{1}{N} \sum_{n=1}^N (\mathbf{b}_1^T \mathbf{x}_n)^2 = \frac{1}{N} \sum_{n=1}^N \mathbf{b}_1^T \mathbf{x}_n \mathbf{x}_n^T \mathbf{b}_1 = \mathbf{b}_1^T \left(\frac{1}{N} \sum_{n=1}^N \mathbf{x}_n \mathbf{x}_n^T \right) \mathbf{b}_1 = \mathbf{b}_1^T \mathbf{S} \mathbf{b}_1$$

- Find \mathbf{b}_1 that maximizes V_1 .

$$\max_{\mathbf{b}_1} \mathbf{b}_1^T \mathbf{S} \mathbf{b}_1, \quad \text{subject to} \quad \|\mathbf{b}_1\|^2 = 1$$

Step 1: Finding \mathbf{b}_1 (2)

- Optimization problem

$$\max_{\mathbf{b}_1} \mathbf{b}_1^T \mathbf{S} \mathbf{b}_1, \quad \text{subject to} \quad \|\mathbf{b}_1\|^2 = 1$$

- Using the Lagrange multiplier method, we get:

L7(2), L7(4)

$$\mathbf{S} \mathbf{b}_1 = \lambda_1 \mathbf{b}_1, \quad \mathbf{b}_1^T \mathbf{b}_1 = 1 \implies \lambda_1: \text{eigenvalue}, \mathbf{b}_1: \text{eigenvector of } \mathbf{S}$$

- Then, $V_1 = \mathbf{b}_1^T \mathbf{S} \mathbf{b}_1 = \lambda_1 \mathbf{b}_1^T \mathbf{b}_1 = \lambda_1$ (the variance V_1 is the eigenvalue of \mathbf{S})
- To maximize the variance, we take the largest eigenvalue, and the corresponding eigenvector is called the (first) principal component.

Step k : Finding \mathbf{b}_k (1)

- Finding k -th principal component: Solving the following optimization problem

$$\max_{\mathbf{b}} \mathbf{b}^T \mathbf{S} \mathbf{b}, \quad \text{subject to} \quad \mathbf{b}^T \mathbf{b} = 1 \text{ and } \mathbf{b}^T \mathbf{b}_i = 0, \quad i = 1, \dots, k-1$$

- Claim.** The solution of the above is the eigenvector of \mathbf{S} corresponding to its k -th largest eigenvalue.
- Proof.** By induction hypothesis, $\mathbf{b}_1, \dots, \mathbf{b}_k$ are the orthonormal eigenvectors of \mathbf{S} . Denote the i -th largest eigenvalue of \mathbf{S} by λ_i , where note that $\mathbf{S} \mathbf{b}_i = \lambda_i \mathbf{b}_i$. The lagrangian of the objective function is:

$$\mathcal{L}(\mathbf{b}) = \mathbf{b}^T \mathbf{S} \mathbf{b} - \lambda(\mathbf{b}^T \mathbf{b} - 1) + \sum_{i=1}^k \eta_i \mathbf{b}^T \mathbf{b}_i$$

Step k : Finding \mathbf{b}_k (2)

- Letting the solution be denoted by \mathbf{b}_{k+1} , the first-order necessary condition for optimality is:

$$\nabla \mathcal{L}(\mathbf{b}_{k+1}) = 2\mathbf{S} \mathbf{b}_{k+1} - 2\lambda \mathbf{b}_{k+1} + \sum_{i=1}^k \eta_i \mathbf{b}_i = 0 \quad (*)$$

- Now, for any $j \in \{1, \dots, k\}$,

$$\begin{aligned} 0 &= \mathbf{b}_j^T \nabla \mathcal{L}(\mathbf{b}_{k+1}) = 2\mathbf{b}_j^T \mathbf{S} \mathbf{b}_{k+1} - 2\lambda \mathbf{b}_j^T \mathbf{b}_{k+1} + \sum_{i=1}^k \eta_i \mathbf{b}_j^T \mathbf{b}_i = 2(\mathbf{S} \mathbf{b}_j)^T \mathbf{b}_{k+1} + \eta_j \\ &= 2(\lambda \mathbf{b}_j)^T \mathbf{b}_{k+1} + \eta_j = 2\lambda \mathbf{b}_j^T \mathbf{b}_{k+1} + \eta_j = \eta_j \end{aligned}$$

- From $\eta_j = 0$ and $(*)$, $\mathbf{S} \mathbf{b}_{k+1} = \lambda \mathbf{b}_{k+1} \implies \lambda$ is an eigenvalue and its corresponding eigenvector is \mathbf{b}_{k+1} .
- Note that the objective function is λ , because $\mathbf{b}^T \mathbf{S} \mathbf{b} = \lambda \mathbf{b}^T \mathbf{b}$.

- **Question.** How can we choose the largest λ with the constraint that $\mathbf{b}_{k+1} \perp (\mathbf{b}_1, \dots, \mathbf{b}_k)$?
- Clearly, if \mathbf{b}_{k+1} is equal to any of these eigenvectors (up to sign), the constraint will be violated, so, to maximize λ , \mathbf{b}_{k+1} should be a unit eigenvector of \mathbf{S} corresponding to $(k+1)$ -th largest eigenvalue.
- By spectral theorem, we can choose this vector in such a way that it is orthogonal to $\mathbf{b}_1, \dots, \mathbf{b}_k$.

L4(4)

- (1) Problem Setting
- (2) Maximum Variance Perspective
- (3) **Projection Perspective**
- (4) Eigenvector Computation and Low-Rank Approximations
- (5) PCA in High Dimensions
- (6) Key Steps of PCA in Practice
- (7) Latent Variable Perspective

- An ordered orthonormal basis (ONB) $\mathbf{B} = (\mathbf{b}_1, \dots, \mathbf{b}_D)$
- $\mathbf{B} = (\mathbf{b}_1 \ \mathbf{b}_2 \ \dots \ \mathbf{b}_M)$, where $\mathbf{b}_i \in \mathbb{R}^D$ and $\mathbf{B} \in \mathbb{R}^{D \times M}$
- Encoding: $\mathbf{z}_n = \phi(\mathbf{x}_n)$ for some mapping $\phi(\cdot)$
- Decoding: $\tilde{\mathbf{x}}_n := \mathbf{B}\mathbf{z}_n = \sum_{m=1}^M z_{mn} \mathbf{b}_m$
- Goal: find the best linear projection of $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ onto a lower-dimensional subspace U (also, called **principal subspace**) of \mathbb{R}^D with $\dim(U) = M$.
- Formally, minimize the following **reconstruction error**

$$J_M := \frac{1}{N} \sum_{n=1}^N \|\mathbf{x}_n - \tilde{\mathbf{x}}_n\|^2,$$

where the variables are $(\mathbf{z}_n : n = 1, \dots, N)$ and $(\mathbf{b}_1, \dots, \mathbf{b}_M)$

Step 1. We optimize the coordinate \mathbf{z}_n in the space U for a given ONB $(\mathbf{b}_1, \dots, \mathbf{b}_M)$

Step 2. Then, we find the optimal ONB, knowing the optimal \mathbf{z}_n in **Step 1**.

- Intuition: Orthogonal projection

L3(8)

$$\text{Result : } \tilde{\mathbf{x}}_n = \mathbf{B}(\mathbf{B}^\top \mathbf{B})^{-1} \mathbf{B}^\top \mathbf{x}_n = \mathbf{B} \mathbf{B}^\top \mathbf{x}_n = \mathbf{B} \mathbf{z}_n, \mathbf{z}_n = \mathbf{B}^\top \mathbf{x}_n$$

- Proof.** Assume an ONB $(\mathbf{b}_1, \dots, \mathbf{b}_M)$. Noting that J_M is a function of $\tilde{\mathbf{x}}_n$ and $\tilde{\mathbf{x}}_n$ is a function of \mathbf{z}_n ,

$$\frac{\partial J_M}{\partial \mathbf{z}_{in}} = \frac{\partial J_M}{\partial \tilde{\mathbf{x}}_n} \frac{\partial \tilde{\mathbf{x}}_n}{\partial \mathbf{z}_{in}}, \quad \frac{\partial J_M}{\partial \tilde{\mathbf{x}}_n} = -\frac{2}{N} (\mathbf{x}_n - \tilde{\mathbf{x}}_n)^\top, \quad \frac{\partial \tilde{\mathbf{x}}_n}{\partial \mathbf{z}_{in}} = \frac{\partial}{\partial \mathbf{z}_{in}} \left(\sum_{m=1}^M z_{mn} \mathbf{b}_m \right) = \mathbf{b}_i$$

$$\begin{aligned} \frac{\partial J_M}{\partial \mathbf{z}_{in}} &= -\frac{2}{N} (\mathbf{x}_n - \tilde{\mathbf{x}}_n)^\top \mathbf{b}_i = -\frac{2}{N} \left(\mathbf{x}_n - \sum_{m=1}^M z_{mn} \mathbf{b}_m \right)^\top \mathbf{b}_i \stackrel{\text{ONB}}{=} -\frac{2}{N} (\mathbf{x}_n^\top \mathbf{b}_i - z_{in} \mathbf{b}_i^\top \mathbf{b}_i) \\ &= -\frac{2}{N} (\mathbf{x}_n^\top \mathbf{b}_i - z_{in}) \end{aligned}$$

- $z_{in} = \mathbf{x}_n^\top \mathbf{b}_i = \mathbf{b}_i^\top \mathbf{x}_n$ for $i = 1, \dots, M$ and $n = 1, \dots, N$ (ortho. proj. onto 1D L3(8))

L10(3)

April 2, 2021 25 / 42

- The difference: $\mathbf{x}_n - \tilde{\mathbf{x}}_n = \left(\sum_{j=M+1}^D \mathbf{b}_j \mathbf{b}_j^\top \right) \mathbf{x}_n = \sum_{j=M+1}^D (\mathbf{x}_n^\top \mathbf{b}_j) \mathbf{b}_j$

$$\tilde{\mathbf{x}}_n = \sum_{m=1}^M z_{mn} \mathbf{b}_m \stackrel{\text{Step 1}}{=} \sum_{m=1}^M (\mathbf{x}_n^\top \mathbf{b}_m) \mathbf{b}_m = \sum_{m=1}^M \mathbf{b}_m (\mathbf{b}_m^\top \mathbf{x}_n) = \left(\sum_{m=1}^M \mathbf{b}_m \mathbf{b}_m^\top \right) \mathbf{x}_n$$

$$\mathbf{x}_n = \sum_{d=1}^D z_{dn} \mathbf{b}_d = \left(\sum_{m=1}^M \mathbf{b}_m \mathbf{b}_m^\top \right) \mathbf{x}_n + \left(\sum_{j=M+1}^D \mathbf{b}_j \mathbf{b}_j^\top \right) \mathbf{x}_n$$

- The projection of the data point onto the orthogonal complement of the principal subspace L3(6)

L10(3)

April 2, 2021 26 / 42

$$\begin{aligned} J_M &= \frac{1}{N} \sum_{n=1}^N \|\mathbf{x}_n - \tilde{\mathbf{x}}_n\|^2 = \frac{1}{N} \sum_{n=1}^N \left\| \sum_{j=M+1}^D (\mathbf{b}_j^\top \mathbf{x}_n) \mathbf{b}_j \right\|^2 = \frac{1}{N} \sum_{n=1}^N \sum_{j=M+1}^D (\mathbf{b}_j^\top \mathbf{x}_n)^2 \\ &= \frac{1}{N} \sum_{n=1}^N \sum_{j=M+1}^D \mathbf{b}_j^\top \mathbf{x}_n \mathbf{x}_n^\top \mathbf{b}_j = \sum_{j=M+1}^D \mathbf{b}_j^\top \left(\frac{1}{N} \sum_{n=1}^N \mathbf{x}_n \mathbf{x}_n^\top \right) \mathbf{b}_j = \sum_{j=M+1}^D \mathbf{b}_j^\top \mathbf{S} \mathbf{b}_j \end{aligned}$$

- minimizing the squared reconstruction error = minimizing the variance when projected onto the orthogonal complement of the principal subspace = maximizing the variance of the projection in the principal subspace

- $J_M = \sum_{j=M+1}^D \lambda_j$ (because of the projection). To minimize this error, we need to choose the smallest $D - M$ eigenvalues, which means that we need to choose the M largest eigenvalues and take their corresponding eigenvectors for projection.

L10(3)

April 2, 2021 27 / 42

- (1) Problem Setting
- (2) Maximum Variance Perspective
- (3) Projection Perspective
- (4) Eigenvector Computation and Low-Rank Approximations
- (5) PCA in High Dimensions
- (6) Key Steps of PCA in Practice
- (7) Latent Variable Perspective

L10(4)

April 2, 2021 28 / 42

- Approach 1: **EVD** L4(4)
 - Perform an eigendecomposition and compute the eigenvalues and eigenvectors of the symmetric matrix \mathbf{S} directly.
- Approach 2: **SVD** L4(5)
 - SVD of the data matrix \mathbf{X} : $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$ ($[D \times N] = [D \times D] \cdot [D \times N] \cdot [N \times N]$)
 - \mathbf{U} and \mathbf{V}^T : orthogonal matrices, $\mathbf{\Sigma}$: only nonzero entries are the singular values $\sigma_{ii} \geq 0$.
$$\mathbf{S} = \frac{1}{N} \mathbf{X}\mathbf{X}^T = \frac{1}{N} \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T \mathbf{V}\mathbf{\Sigma}^T \mathbf{U}^T \stackrel{(\mathbf{V}^T = \mathbf{V}^{-1})}{=} \frac{1}{N} \mathbf{U}\mathbf{\Sigma}\mathbf{\Sigma}^T \mathbf{U}^T$$
 - The columns of \mathbf{U} are the eigenvectors of $\mathbf{X}\mathbf{X}^T$ (thus \mathbf{S})
 - The eigenvalues λ_d of \mathbf{S} are related to the singular values of \mathbf{X} : $\lambda_d = \frac{\sigma_d^2}{N}$

L10(4)

April 2, 2021 29 / 42

- In SVD, \mathbf{U} corresponds to the projection matrix \mathbf{B} , so that we maximize the variance of the projected data or minimize the average squared reconstruction error.

- Consider the best rank- M approximation

$$\tilde{\mathbf{X}}_M := \arg \min_{\text{rk}(\mathbf{A})=M} \|\mathbf{X} - \mathbf{A}\|_2$$

- From Eckart-Young Theorem, by truncating the SVD at the top- M singular value, we obtain the reconstructed data matrix $\tilde{\mathbf{X}}_M$ as: L4(5), L4(6)

$$\tilde{\mathbf{X}}_M = \underbrace{\mathbf{U}_M}_{D \times M} \underbrace{\mathbf{\Sigma}_M}_{M \times M} \underbrace{\mathbf{V}_M^T}_{M \times N} \iff \tilde{\mathbf{X}}_M = \sum_{i=1}^M \sigma_i \mathbf{u}_i \mathbf{v}_i^T,$$

where σ_i is the i -th singular value.

L10(4)

April 2, 2021 30 / 42

- (1) Problem Setting
- (2) Maximum Variance Perspective
- (3) Projection Perspective
- (4) Eigenvector Computation and Low-Rank Approximations
- (5) **PCA in High Dimensions**
- (6) **Key Steps of PCA in Practice**
- (7) Latent Variable Perspective

L10(4)

April 2, 2021 31 / 42

- In some practical cases, $\mathbf{S} = \frac{1}{N} \mathbf{X}\mathbf{X}^T \in \mathbb{R}^{D \times D}$, where D is pretty high.
 - **Example.** 100 × 100 pixel image: $D = 10,000$.
- What if $N \ll D$?
 - With no duplicate data, $\text{rk}(\mathbf{S}) = N$, and $D - N + 1$ eigenvalues are 0! \implies no need to maintain $D \times D$ data covariance matrix.

- In PCA, $\mathbf{S}\mathbf{b}_m = \lambda_m \mathbf{b}_m$, $m = 1, \dots, M$.

$$\mathbf{S}\mathbf{b}_m = \frac{1}{N} \mathbf{X}\mathbf{X}^T \mathbf{b}_m = \lambda_m \mathbf{b}_m \implies \frac{1}{N} \underbrace{\mathbf{X}^T \mathbf{X}}_{N \times N} \underbrace{\mathbf{X}^T \mathbf{b}_m}_{:= \mathbf{c}_m} = \lambda_m \mathbf{X}^T \mathbf{b}_m \iff \frac{1}{N} \mathbf{X}^T \mathbf{X} \mathbf{c}_m = \lambda_m \mathbf{c}_m$$

- λ_m is an eigenvalue of $\frac{1}{N} \mathbf{X}^T \mathbf{X}$ with its associated eigenvector $\mathbf{c}_m = \mathbf{X}^T \mathbf{b}_m$
- $\frac{1}{N} \mathbf{X}^T \mathbf{X} \in \mathbb{R}^{N \times N}$, so much easier to compute the eigenvectors
- To recover the eigenvector of \mathbf{S} , by left-multiplying \mathbf{X} , we get $\frac{1}{N} \mathbf{X}\mathbf{X}^T \mathbf{X} \mathbf{c}_m = \lambda_m \mathbf{X} \mathbf{c}_m$

L10(4)

April 2, 2021 32 / 42

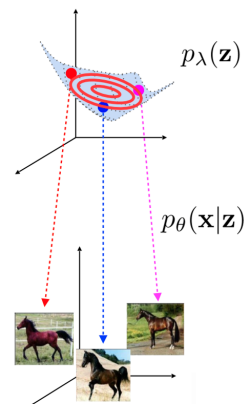
- S1. Centering.** Centering the data by subtracting mean
- S2. Standardization.** Divide the data points by the standard deviation for every dimension (original feature) $d = 1, \dots, D$
- S3. Eigenvalue/vector.** Compute the M -largest eigenvalues and the eigenvectors of the data covariance matrix (M is the dimension that needs to be reduced)
- S4. Projection.** Project all data points onto the space defined by the eigenvectors (i.e., principal subspace).
- S5.** Undo standardization and centering.

- (1) Problem Setting
- (2) Maximum Variance Perspective
- (3) Projection Perspective
- (4) Eigenvector Computation and Low-Rank Approximations
- (5) PCA in High Dimensions
- (6) Key Steps of PCA in Practice
- (7) Latent Variable Perspective

- Generative process
 - $\mathbf{z} \sim p(\mathbf{z})$
 - $\mathbf{x} \sim p(\mathbf{x}|\mathbf{z})$

$$p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$

$$= \int p(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z}$$



Source: <https://dlvu.github.io/slides/dlvu.lecture06.pdf>

- $p(\mathbf{z}) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
- A linear relationship between \mathbf{z} and \mathbf{x} : For Gaussian observation noise $\epsilon \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$ and affine mapping defined by $\mathbf{B} \in \mathbb{R}^{D \times M}$ and $\boldsymbol{\mu} \in \mathbb{R}^D$,

$$\mathbf{x} = \mathbf{B}\mathbf{z} + \boldsymbol{\mu} + \epsilon \in \mathbb{R}^D$$
- Conditional distribution for the links between latent and observed variables

$$p(\mathbf{x}|\mathbf{z}, \mathbf{B}, \boldsymbol{\mu}, \sigma^2) = \mathcal{N}(\mathbf{x}|\mathbf{B}\mathbf{z} + \boldsymbol{\mu}, \sigma^2 \mathbf{I})$$
- Data point generation: **ancestral sampling**
 - First, sample \mathbf{z}_n from $p(\mathbf{z})$
 - Then, use \mathbf{z}_n to generate a sample $\mathbf{x}_n \sim p(\mathbf{x}|\mathbf{z}_n, \mathbf{B}, \boldsymbol{\mu}, \sigma^2)$

- Probabilistic model: joint distribution

$$p(\mathbf{x}, \mathbf{z} | \mathbf{B}, \boldsymbol{\mu}, \sigma^2) = p(\mathbf{x} | \mathbf{z}, \mathbf{B}, \boldsymbol{\mu}, \sigma^2) p(\mathbf{z})$$

- Likelihood

$$p(\mathbf{x} | \mathbf{B}, \boldsymbol{\mu}, \sigma^2) = \int p(\mathbf{x} | \mathbf{z}, \mathbf{B}, \boldsymbol{\mu}, \sigma^2) p(\mathbf{z}) d\mathbf{z} = \int \mathcal{N}(\mathbf{x} | \mathbf{B}\mathbf{z} + \boldsymbol{\mu}, \sigma^2 \mathbf{I}) \mathcal{N}(\mathbf{z} | \mathbf{0}, \mathbf{I}) d\mathbf{z} \\ = \mathcal{N}(\boldsymbol{\mu}, \mathbf{B}\mathbf{B}^T + \sigma^2 \mathbf{I})$$

- Using the property of marginal and conditional Gaussians

L6(5)

L10(7)

April 2, 2021 37 / 42

- The joint Gaussian distribution $p(\mathbf{x}, \mathbf{z} | \mathbf{B}, \boldsymbol{\mu}, \sigma^2)$ leads us to the posterior distribution

$$p(\mathbf{z} | \mathbf{x}) = \mathcal{N}(\mathbf{z} | \mathbf{m}, \mathbf{C}), \text{ where}$$

$$\mathbf{m} = \mathbf{B}^T (\mathbf{B}\mathbf{B}^T + \sigma^2 \mathbf{I})^{-1} (\mathbf{x} - \boldsymbol{\mu}), \quad \mathbf{C} = \mathbf{I} - \mathbf{B}^T (\mathbf{B}\mathbf{B}^T + \sigma^2 \mathbf{I})^{-1} \mathbf{B}$$

L10(7)

April 2, 2021 38 / 42

Learning Probabilistic PCA: MLE

PCA as Linear Auto-Encoder

- For data samples $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_N)$, we are able to compute the likelihood as:

$$\log p(\mathbf{X} | \mathbf{B}, \boldsymbol{\mu}, \sigma^2) = \sum_{n=1}^N \log p(\mathbf{x}_n | \mathbf{B}, \boldsymbol{\mu}, \sigma^2)$$

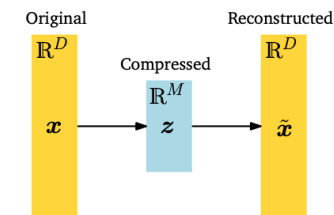
$$\boldsymbol{\mu}_{\text{ML}} = \frac{1}{N} \sum_{n=1}^N \mathbf{x}_n, \quad \mathbf{B}_{\text{ML}} = \mathbf{U}(\boldsymbol{\Lambda} - \sigma^2 \mathbf{I})^{1/2} \mathbf{R}, \quad \sigma_{\text{ML}}^2 = \frac{1}{D-M} \sum_{j=M+1}^D \lambda_j, \text{ where}$$

- \mathbf{U} is a $D \times M$ matrix whose columns are eigenvectors of \mathbf{S}
- $\boldsymbol{\Lambda}$ is a $M \times M$ diagonal matrix whose elements are eigenvalues of \mathbf{S}
- \mathbf{R} is an arbitrary orthogonal matrix (i.e., rotation)

- In the noise-free limit where $\sigma \rightarrow 0$, PPCA and PCA provide the identical solution.

L10(7)

April 2, 2021 39 / 42



- **Non-linear auto-encoder**: we replace the linear mapping of PCA with a non-linear mapping. An example is a deep auto-encoder with deep neural networks.
- **(Fully) Bayesian PCA**: place a prior on the model parameters and integrate them out, rather than having a point estimate.
- **Factor analysis**: allow each observation dimension d to have a different variance σ_d^2

L10(7)

April 2, 2021 40 / 42

1)

Questions?