Lecture 10: Dimensionality Reduction with Principal Component Analysis

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

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Please watch this tutorial video by Luis Serrano on PCA.
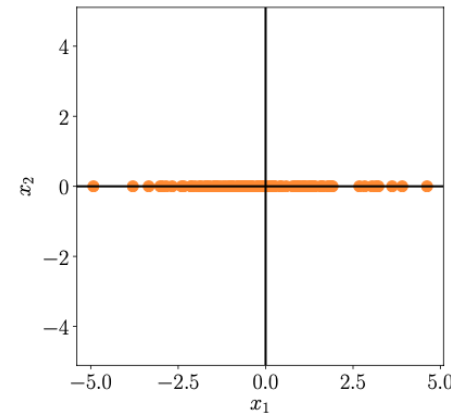
`https://www.youtube.com/watch?v=g-Hb26agBFg`

Roadmap

(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

Roadmap
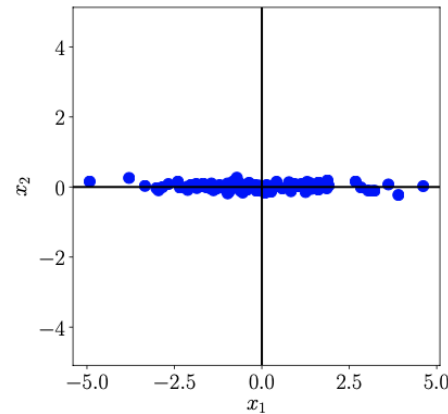
(a) Dataset with x_1 and x_2 coordinates.

(b) Compressed dataset where only the x_1 coordinate is relevant.

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

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

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S1. Centering. Centering the data by subtracting mean

S2. Standardization. Divide the data points by the standard deviation for every dimension (original feature) $d = 1, \ldots, D$

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.
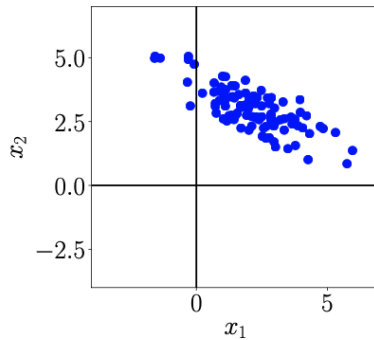
(a) Original dataset.
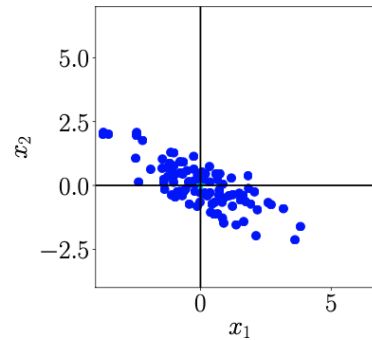
(b) Step 1: Centering by subtracting the mean from each data point.
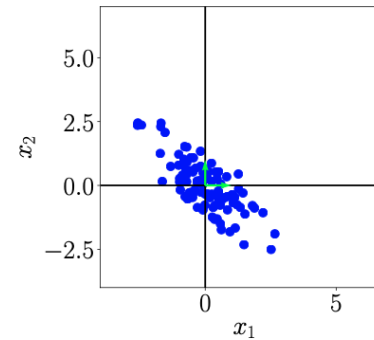
(c) Step 2: Dividing by the standard deviation to make the data unit free. Data has variance 1 along each axis.
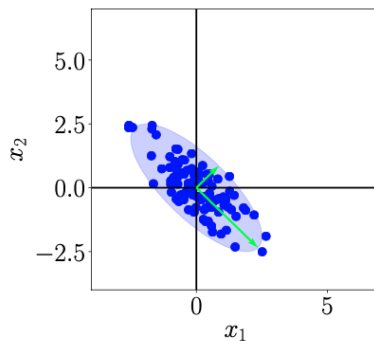
(d) Step 3: Compute eigenvalues and eigenvectors (arrows) of the data covariance matrix (ellipse).

(e) Step 4: Project data onto the principal subspace.
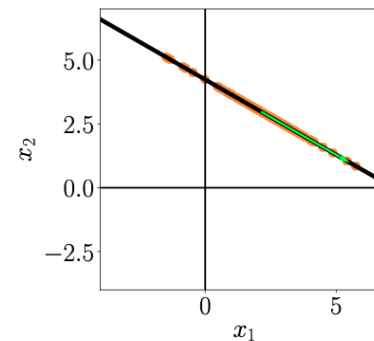
(f) Undo the standardization and move projected data back into the original data space from (a).

- N: number of samples, D: number of measurements (or original features)
- iid dataset $\mathcal{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ whose mean is 0 (well-centered), where each $\boldsymbol{x}_i \in \mathbb{R}^D$, and its corresponding data matrix
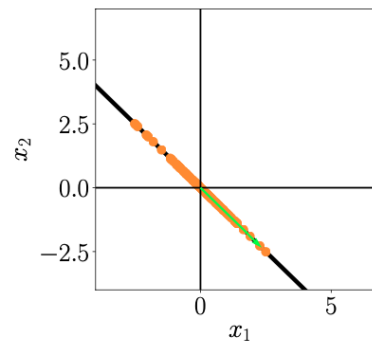
$$\boldsymbol{X} = \begin{pmatrix} \boldsymbol{x}_1 & \cdots & \boldsymbol{x}_N \end{pmatrix} = \begin{pmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,N} \\ x_{2,1} & x_{2,2} & \cdots & x_{2,N} \\ & & \vdots & \\ x_{D,1} & x_{D,2} & \cdots & x_{D,N} \end{pmatrix} \in \mathbb{R}^{D \times N}$$

- (data) covariance matrix

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

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- Covaiance matrix for a random vector $\boldsymbol{Y} = (Y_1, \ldots, Y_D)^\mathsf{T}$, L6(4)

$$\boldsymbol{\Sigma_Y} = \begin{pmatrix} \mathrm{cov}(Y_1, Y_1) & \mathrm{cov}(Y_1, Y_2) & \cdots \mathrm{cov}(Y_1, Y_D) \\ \vdots & \vdots & \vdots \\ \mathrm{cov}(Y_D, Y_1) & \mathrm{cov}(Y_n, Y_2) & \cdots \mathrm{cov}(Y_D, Y_D) \end{pmatrix}$$

- Data convariance matrix $\boldsymbol{S} \in \mathbb{R}^{D \times D}$
  - Each Y_i has N samples $\begin{pmatrix} x_{i,1} & \cdots & x_{i,N} \end{pmatrix}$

$$\boldsymbol{S}_{ij} = \mathrm{cov}(Y_i, Y_j) = \frac{1}{N} \sum_{k=1}^{N} x_{i,k} \cdot x_{j,k}$$
$$= \text{average covariance (over samples) btwn feastures } i \text{ and } j$$

- Low-dimensional compressed representation, also called code:

$$z_n = B^\mathsf{T} x_n \in \mathbb{R}^M,$$

where the projection[1] matrix is $B := (b_1, \ldots, b_M) \in \mathbb{R}^{D \times M}$,

- Assume that the columns of B are orthonormal, i.e., $b_i^\mathsf{T} b_j = 0$ if $i \neq j$, and $b_i^\mathsf{T} b_i = 1$ if $i = j$.

- Seek an M-dimensional subspace $U \subset \mathbb{R}^D$, $\dim(U) = M < D$ onto which we project data

- $\tilde{x}_n \in \mathbb{R}^D$: projected data, z_n: their coordinates w.r.t. the basis vectors of B.

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[1]In L3(8), the coordinate in the projected space becomes $\lambda = (B^\mathsf{T} B)^{-1} B^\mathsf{T} x$, which is simply $B^\mathsf{T} x$ for orthonormal bases B.
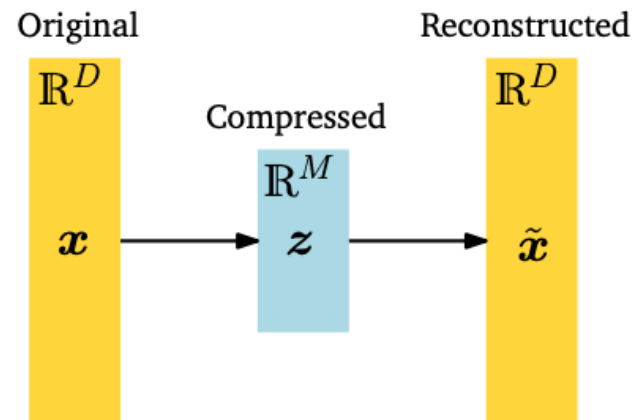
- Find a suitable matrix B such that $\boldsymbol{z} = \boldsymbol{B}^{\mathsf{T}}\boldsymbol{x}$ and $\tilde{\boldsymbol{x}} = \boldsymbol{B}\boldsymbol{z}$

- $\boldsymbol{B}^{\mathsf{T}}$: encoder, $\boldsymbol{B}$: decoder

- Example. MNIST dataset
  - ◦ handwritten digits, $N = 60,000$ data samples, $D = 28 \times 28 = 784$ pixels

Roadmap

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(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 dimensinoality reduction algorithm that maximizes the variance in the low-dimensional data representation.
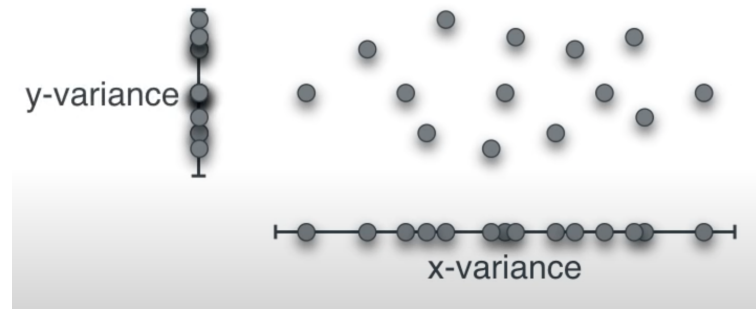
source: Youtube channel by Luis Serrano

- $\boldsymbol{B} = \begin{pmatrix} \boldsymbol{b}_1 & \boldsymbol{b}_2 & \ldots & \boldsymbol{b}_M \end{pmatrix}$, where $\boldsymbol{b}_i \in \mathbb{R}^D$ and $\boldsymbol{B} \in \mathbb{R}^{D \times M}$

- $\boldsymbol{B}^\mathsf{T} = \begin{pmatrix} \boldsymbol{b}_1^\mathsf{T} \\ \vdots \\ \boldsymbol{b}_M^\mathsf{T} \end{pmatrix} \in \mathbb{R}^{M \times D}$, $\boldsymbol{b}_i^\mathsf{T} \in \mathbb{R}^{1 \times D}$, $\boldsymbol{x}_i \in \mathbb{R}^{D \times 1}$

- $\boldsymbol{z}_n = \begin{pmatrix} z_{1n} \\ \vdots \\ z_{Mn} \end{pmatrix} = \boldsymbol{B}^\mathsf{T} \boldsymbol{x}_n = \begin{pmatrix} \boldsymbol{b}_1^\mathsf{T} \\ \vdots \\ \boldsymbol{b}_M^\mathsf{T} \end{pmatrix} \boldsymbol{x}_n = \begin{pmatrix} \boldsymbol{b}_1^\mathsf{T} \boldsymbol{x}_n \\ \vdots \\ \boldsymbol{b}_M^\mathsf{T} \boldsymbol{x}_n \end{pmatrix}$

- z_{in}: new coordinate (for $\boldsymbol{x}_n$) in the projected space by the basis $\boldsymbol{b}_i$

- Goal: Find the orthonormal bases $\boldsymbol{B} = \begin{pmatrix} \boldsymbol{b}_1 & \boldsymbol{b}_2 & \ldots & \boldsymbol{b}_M \end{pmatrix}$ that maximizes the variance.

- Result: For the M-largest eigenvalues $\lambda_1, \ldots, \lambda_M$ of the data covariance matrix $\boldsymbol{S}$, their corresponding M eigenvectors become $\boldsymbol{b}_1, \ldots, \boldsymbol{b}_M$

- Question. Why data covariance matrix? Why eigenvectors ordered by their eigenvalues?

- Strategy: Induction

  Step 1. We seek a single vector $\boldsymbol{b}_1$ that maximizes the variance of the projected data, assuming that we project the data onto an 1D line. We show that $\boldsymbol{b}_1$ is the eigenvector of the largest eigenvalue.

  Step k. Suppose that we found $\boldsymbol{b}_1, \ldots, \boldsymbol{b}_{k-1}$ for the variance maximization. Then, we seek $\boldsymbol{b}_k$ that maximizes the variance of the projected data onto k-D plain with the constraint that $\boldsymbol{b}_k$ is orthogonal to $\boldsymbol{b}_1, \ldots, \boldsymbol{b}_{k-1}$. We prove that $\boldsymbol{b}_k$ is the eigenvector of the k-th largest eigenvalue.

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

$$V_1 := \text{var}[z_1] = \frac{1}{N} \sum_{n=1}^{N} z_{1n}^2, \quad z_{1n} = b_1^\mathsf{T} x_n$$

where z_{1n} (z_{in}) is the first (i-th) coordinate of the low-dimensional representation z_n of x_n

$$V_1 = \frac{1}{N} \sum_{n=1}^{N} (b_1^\mathsf{T} x_n)^2 = \frac{1}{N} \sum_{n=1}^{N} b_1^\mathsf{T} x_n x_n^\mathsf{T} b_1 = b_1^\mathsf{T} \left(\frac{1}{N} \sum_{n=1}^{N} x_n x_n^\mathsf{T} \right) b_1 = b_1^\mathsf{T} S b_1$$

- Find b_1 that maximizes V_1.

$$\max_{b_1} b_1^\mathsf{T} S b_1, \quad \text{subject to} \quad \|b_1\|^2 = 1$$

- Optimization problem

$$\max_{b_1} b_1^\mathsf{T} S b_1, \quad \text{subject to} \quad \|b_1\|^2 = 1$$

- Using the Lagrange multiplier method, we get: L7(2), L7(4)

$$S b_1 = \lambda_1 b_1, \quad b_1^\mathsf{T} b_1 = 1 \implies \lambda_1: \text{eigenvalue}, \ b_1: \text{eigenvector of } S$$

- Then, $V_1 = b_1^\mathsf{T} S b_1 = \lambda_1 b_1^\mathsf{T} b_1 = \lambda_1$ (the variance V_1 is the eigenvalue of S)

- To maximize the variance, we take the largest eigenvalue, and the corresponding eigenvector is called the (first) principal component.

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

$$\max_{\boldsymbol{b}} \boldsymbol{b}^\mathsf{T} \boldsymbol{S} \boldsymbol{b}, \quad \text{subject to} \quad \boldsymbol{b}^\mathsf{T} \boldsymbol{b} = 1 \text{ and } \boldsymbol{b}^\mathsf{T} \boldsymbol{b}_i, \ i = 1, \ldots, k-1$$

- Claim. The solution of the above is the eigenvector of $\boldsymbol{S}$ corresponding to its k-th largest eigenvalue.

- Proof. By induction hypothesis, $\boldsymbol{b}_1, \ldots, \boldsymbol{b}_k$ are the orthonormal eigenvectors of $\boldsymbol{S}$. Denote the i-th largest eigenvalue of $\boldsymbol{S}$ by λ_i, where note that $\boldsymbol{S}\boldsymbol{b}_i = \lambda_i \boldsymbol{b}_i$.
  The lagrangian of the objective function is:

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

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

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

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

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

$$= 2(\lambda\boldsymbol{b}_j)^\mathsf{T}\boldsymbol{b}_{k+1} + \eta_j = 2\lambda\boldsymbol{b}_j^\mathsf{T}\boldsymbol{b}_{k+1} + \eta_j = \eta_j$$

- From $\eta_j = 0$ and $(*)$, $\boldsymbol{S}\boldsymbol{b}_{k+1} = \lambda\boldsymbol{b}_{k+1}$. $\implies$ λ is an eigenvalue and its corresponding eigenvector is $\boldsymbol{b}_{k+1}$.

- Note that the objective function is λ, because $\boldsymbol{b}^\mathsf{T}\boldsymbol{S}\boldsymbol{b} = \lambda\boldsymbol{b}^\mathsf{T}\boldsymbol{b}$.

- Question. How can we choose the largest λ with the constraint that $\boldsymbol{b}_{k+1} \perp (\boldsymbol{b}_1, \ldots \boldsymbol{b}_k)$?

- Clearly, if $\boldsymbol{b}_{k+1}$ is equal to any of these eigenvectors (up to sign), the constraint will be violated, so, to maximize λ, $\boldsymbol{b}_{k+1}$ should be a unit eigenvector of $\boldsymbol{S}$ corresponding to $(k+1)$-th largest eigenvalue.

- By spectral theorem, we can choose this vector in such a way that it is orthogonal to $\boldsymbol{b}_1, \ldots, \boldsymbol{b}_k$. L4(4)

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- An ordered orthonormal bais (ONB) $B = (\boldsymbol{b}_1, \ldots, \boldsymbol{b}_D)$

- $\boldsymbol{B} = \begin{pmatrix} \boldsymbol{b}_1 & \boldsymbol{b}_2 & \ldots & \boldsymbol{b}_M \end{pmatrix}$, where $\boldsymbol{b}_i \in \mathbb{R}^D$ and $\boldsymbol{B} \in \mathbb{R}^{D \times M}$

- Encoding: $\boldsymbol{z}_n = \phi(\boldsymbol{x}_n)$ for some mapping $\phi(\cdot)$

- Decoding: $\tilde{\boldsymbol{x}}_n := \boldsymbol{B}\boldsymbol{z}_n = \sum_{m=1}^{M} z_{mn}\boldsymbol{b}_m$

- Goal: find the best linear projection of $\mathcal{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ onto a lower-dimensional subspace U (also, called principal subspace) of $\mathbb{R}^D$ with $\dim(U) = M$.

- Formally, minimize the following reconstruction error

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

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

Step 1. We optimize the coordinate z_n in the space U for a given ONB $(b_1, \ldots, b_M)$

Step 2. Then, we find the optimal ONB, knowing the optimal z_n in **Step 1.**

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- Intuition: Orthogonal projection   L3(8)

$$Result : \tilde{x}_n = B(B^\top B)^{-1} B^\top x_n = BB^\top x_n = Bz_n, z_n = B^\top x_n$$

- Proof. Assume an ONB $(b_1, \ldots, b_M)$. Noting that J_M is a function of $\tilde{x}_n$ and $\tilde{x}_n$ is a function of z_n,

$$\frac{\partial J_M}{\partial z_{in}} = \frac{\partial J_M}{\partial \tilde{x}_n} \frac{\partial \tilde{x}_n}{\partial z_{in}}, \quad \frac{\partial J_M}{\partial \tilde{x}_n} = -\frac{2}{N}(x_n - \tilde{x}_n)^\top, \quad \frac{\partial \tilde{x}_n}{\partial z_{in}} = \frac{\partial}{\partial z_{in}}\left(\sum_{m=1}^{M} z_{mn} b_m\right) = b_i$$

$$\frac{\partial J_M}{\partial z_{in}} = -\frac{2}{N}(x_n - \tilde{x}_n)^\top b_i = -\frac{2}{N}\left(x_n - \sum_{m=1}^{M} z_{mn} b_m\right)^\top b_i \overset{\text{ONB}}{=} -\frac{2}{N}(x_n^\top b_i - z_{in} b_i^\top b_i)$$

$$= -\frac{2}{N}(x_n^\top b_i - z_{in})$$

- $z_{in} = x_n^\top b_i = b_i^\top x_n$ for $i = 1, \ldots, M$ and $n = 1, \ldots, N$ (ortho. proj. onto 1D L3(8))

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

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

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

- The projection of the data point onto the orthogonal complement of the principal subspace $\boxed{\text{L3(6)}}$

$$J_M = \frac{1}{N} \sum_{n=1}^{N} \|\boldsymbol{x}_n - \tilde{\boldsymbol{x}}_n\|^2 = \frac{1}{N} \sum_{n=1}^{N} \left\| \sum_{j=M+1}^{D} (\boldsymbol{b}_j^\mathsf{T} \boldsymbol{x}_n) \boldsymbol{b}_j \right\|^2 = \frac{1}{N} \sum_{n=1}^{N} \sum_{j=M+1}^{D} (\boldsymbol{b}_j^\mathsf{T} \boldsymbol{x}_n)^2$$

$$= \frac{1}{N} \sum_{n=1}^{N} \sum_{j=M+1}^{D} \boldsymbol{b}_j^\mathsf{T} \boldsymbol{x}_n \boldsymbol{x}_n^\mathsf{T} \boldsymbol{b}_j = \sum_{j=M+1}^{D} \boldsymbol{b}_j^\mathsf{T} \left(\frac{1}{N} \sum_{n=1}^{N} \boldsymbol{x}_n \boldsymbol{x}_n^\mathsf{T} \right) \boldsymbol{b}_j = \sum_{j=M+1}^{D} \boldsymbol{b}_j^\mathsf{T} \boldsymbol{S} \boldsymbol{b}_j$$

- 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.

Roadmap

- Approach 1: EVD <mark>L4(4)</mark>
  - Perform an eigendecomposition and compute the eigenvalues and eigenvectors of the symmetric matrix $\boldsymbol{S}$ directly.

- Approach 2: SVD <mark>L4(5)</mark>
  - SVD of the data matrix $\boldsymbol{X}$: $\boldsymbol{X} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\mathsf{T}}$ ($[D \times N] = [D \times D] \cdot [D \times N] \cdot [N \times N]$)

  - $\boldsymbol{U}$ and $\boldsymbol{V}^{\mathsf{T}}$: orthogonal matrices, $\boldsymbol{\Sigma}$: only nonzero entries are the singular values $\sigma_{ii} \geq 0$.

$$\boldsymbol{S} = \frac{1}{N}\boldsymbol{X}\boldsymbol{X}^{\mathsf{T}} = \frac{1}{N}\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\mathsf{T}}\boldsymbol{V}\boldsymbol{\Sigma}^{\mathsf{T}}\boldsymbol{U}^{\mathsf{T}} \overset{(\boldsymbol{V}^{\mathsf{T}}=\boldsymbol{V}^{-1})}{=} \frac{1}{N}\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{\Sigma}^{\mathsf{T}}\boldsymbol{U}^{\mathsf{T}}$$

  - The columns of $\boldsymbol{U}$ are the eigenvectors of $\boldsymbol{X}\boldsymbol{X}^{\mathsf{T}}$ (thus $\boldsymbol{S}$)

  - The eigenvalues λ_d of $\boldsymbol{S}$ are related to the singular values of $\boldsymbol{X}$: $\lambda_d = \dfrac{\sigma_d^2}{N}$

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

- Consider the best rank-M approximation

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

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

$$\tilde{\boldsymbol{X}}_M = \overbrace{\boldsymbol{U}_M}^{D \times M} \overbrace{\Sigma_M}^{M \times M} \overbrace{\boldsymbol{V}_M^{\mathsf{T}}}^{M \times N} \iff \tilde{\boldsymbol{X}}_M = \sum_{i=1}^{M} \sigma_i \boldsymbol{u}_i \boldsymbol{v}_i^{\mathsf{T}},$$

where σ_i is the i-th singular value.

Roadmap

- In some practical cases, $S = \frac{1}{N}XX^\top \in \mathbb{R}^{D \times D}$, where D is pretty high.
  - Example. 100×100 pixel image: $D = 10,000$.
- What if $N << D$?
  - With no duplicate data, $\text{rk}(S) = N$, and $D - N + 1$ eigenvalues are 0! $\implies$ no need to maintain $D \times D$ data covariance matrix.
- In PCA, $Sb_m = \lambda_m b_m$, $m = 1, \ldots, M$.

$$Sb_m = \frac{1}{N}XX^\top b_m = \lambda_m b_m \implies \frac{1}{N}\underbrace{X^\top X}_{N \times N}\underbrace{X^\top b_m}_{:= c_m} = \lambda_m X^\top b_m \iff \frac{1}{N}X^\top X c_m = \lambda_m c_m$$

- λ_m is an eigenvalue of $\frac{1}{N}X^\top X$ with its associated eigenvector $c_m = X^\top b_m$
- $\frac{1}{N}X^\top X \in \mathbb{R}^{N \times N}$, so much easier to compute the eigenstuff
- To recover the eigenvector of S, by left-multiplying X, we get
  $\frac{1}{N}XX^\top X c_m = \lambda_m X c_m$

S1. Centering. Centering the data by subtracting mean

S2. Standardization. Divide the data points by the standard deviation for every dimension (original feature) $d = 1, \ldots, D$

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.

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Please go back to L8(4) for the background on generative models via latent variable models (LVMs).

- $p(\boldsymbol{z}) = \mathcal{N}(0, \boldsymbol{I})$

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

$$\boldsymbol{x} = \boldsymbol{B}\boldsymbol{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon} \in \mathbb{R}^D$$

- Conditional distribution for the links between latent and observed variables

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

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

- Probabilistic model: joint distribution

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

- Likelihood

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

  ◦ Using the property of marginal and conditional Gaussians <mark>L6(5)</mark>

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

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

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

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

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

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

- $\boldsymbol{U}$ is a $D \times M$ matrix whose columns are eigenvectors of $\boldsymbol{S}$

- $\boldsymbol{\Lambda}$ is a $M \times M$ diagonal matrix whose elements are eigenvalues of $\boldsymbol{S}$

- $\boldsymbol{R}$ is an arbitrary orthogonal matrix (i.e., rotation)

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

KAIST EE

Original Reconstructed

$\mathbb{R}^D$ $\mathbb{R}^D$

Compressed

$\mathbb{R}^M$

$\boldsymbol{x}$ $\boldsymbol{z}$ $\tilde{\boldsymbol{x}}$
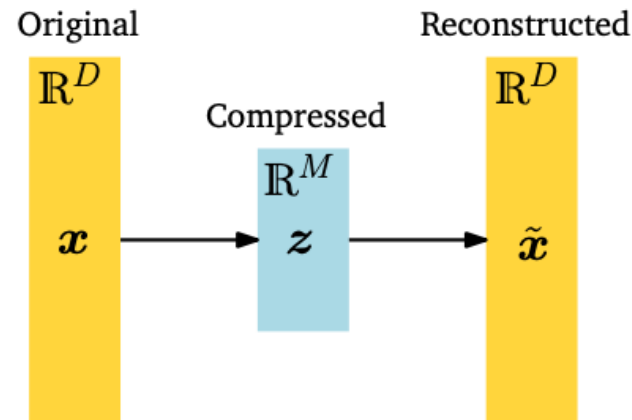
- Non-linear auto-encoder: we replace the linear mapping of PCA with a non-linear mapping. An example is a deep auto-encoder with deep neutral networks.

- (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

Questions?

1)