DDA3020 Machine Learning: Lecture 17 Principal Component Analysis

JIA, Kui
School of Data Science, CUHK-SZ

November 28, 2022

Outline

1. Preliminary
2. Dimensionality Reduction
3. Derivations of Principal Component Analysis
   - Motivation
   - Derivation 1
   - Derivation 2
4. Principal Component Analysis Algorithm
5. Applications

1 Preliminary

2 Dimensionality Reduction

3 Derivations of Principal Component Analysis
- Motivation
- Derivation 1
- Derivation 2

4 Principal Component Analysis Algorithm

5 Applications

Preliminary: Projection onto a subspace

- Given a dataset $\mathcal{D} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)}\}$ with $\mathbf{x}^{(n)} \in \mathbb{R}^D$ and D being the original dimension. And we define the mean as $\boldsymbol{\mu} = \frac{1}{N}\sum_{n=1}^{N} \mathbf{x}^{(n)} \in \mathbb{R}^D$.
- K-dimensional subspace $\mathcal{S}$ is spanned by an orthonormal basis $\{\mathbf{u}_k\}_{k=1}^K$ with $\mathbf{u}_k \in \mathbb{R}^D$.
- $\|\mathbf{u}_k\| = 1, \forall k$; $\mathbf{u}_i^\top \mathbf{u}_j = 0$ if $i \neq j, \forall i, j$.
- Approximate each data point $\mathbf{x} \in \mathbb{R}^D$ as:

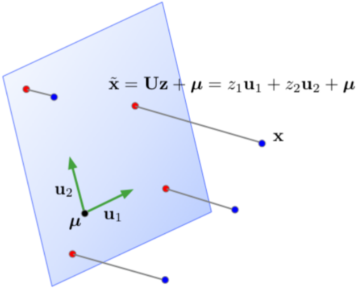
$$\tilde{\mathbf{x}} = \boldsymbol{\mu} + \mathrm{Proj}_{\mathcal{S}}(\mathbf{x} - \boldsymbol{\mu}) = \boldsymbol{\mu} + \sum_{k=1}^{K} z_k \mathbf{u}_k,$$

  where $z_k = \mathbf{u}_k^\top(\mathbf{x} - \boldsymbol{\mu})$ can be seen as the projection length of $\mathbf{x} - \boldsymbol{\mu}$ on the k-th basis $\mathbf{u}_k$.
- Let $\mathbf{U} \in \mathbb{R}^{D \times K}$ be a matrix with columns $\{\mathbf{u}_k\}_{k=1}^K$, then we have

$$\tilde{\mathbf{x}} = \boldsymbol{\mu} + \mathbf{U}\mathbf{z} \in \mathbb{R}^D, \text{ which is called reconstruction of } \mathbf{x} \tag{1}$$

$$\mathbf{z} = \mathbf{U}^\top(\mathbf{x} - \boldsymbol{\mu}) \in \mathbb{R}^K, \text{ which is called representation/code of } \mathbf{x}. \tag{2}$$

Preliminary: Projection onto a subspace



$$\mathbf{z} = \mathbf{U}^\top(\mathbf{x} - \boldsymbol{\mu})$$

- In the above example, the blue point $\mathbf{x} \in \mathbb{R}^3$ is projected onto a 2-dimensional subspace $\mathcal{S}$ spanned by 2 basis vectors $\{\mathbf{u}_1, \mathbf{u}_2\}$. And, the mean vector of all blue points $\boldsymbol{\mu} \in \mathbb{R}^3$ is set as the origin of $\mathcal{S}$.
- Through projection, each blue point $\mathbf{x}$ has a reconstruction $\tilde{\mathbf{x}} \in \mathbb{R}^3$, which locates in $\mathcal{S}$.
- The coordinate value of $\tilde{\mathbf{x}}$ in the new coordinate system $\{\mathbf{u}_1, \mathbf{u}_2\}$ is represented by $\mathbf{z} \in \mathbb{R}^2$.

Preliminary: Projection onto a subspace

Theorem (Orthogonal theorem)

The vector $\mathbf{x} - \tilde{\mathbf{x}}$ *is orthogonal to the subspace* $\mathcal{S}$, *i.e.,*

$$\mathbf{U}^\top(\mathbf{x} - \tilde{\mathbf{x}}) = \mathbf{0}.$$

Proof:

- Utilizing the definition of $\tilde{\mathbf{x}}$, we have

$$\mathbf{x} - \tilde{\mathbf{x}} = \mathbf{x} - \boldsymbol{\mu} - \mathbf{U}\mathbf{z}$$

- Then, utilizing the definition of $\mathbf{z}$ and the orthonormality of $\mathbf{U}$, we have

$$\mathbf{U}^\top(\mathbf{x} - \tilde{\mathbf{x}}) = \mathbf{U}^\top(\mathbf{x} - \boldsymbol{\mu}) - \mathbf{U}^\top\mathbf{U}\mathbf{z} = \mathbf{z} - \mathbf{z} = \mathbf{0}.$$

1 Preliminary

2 Dimensionality Reduction

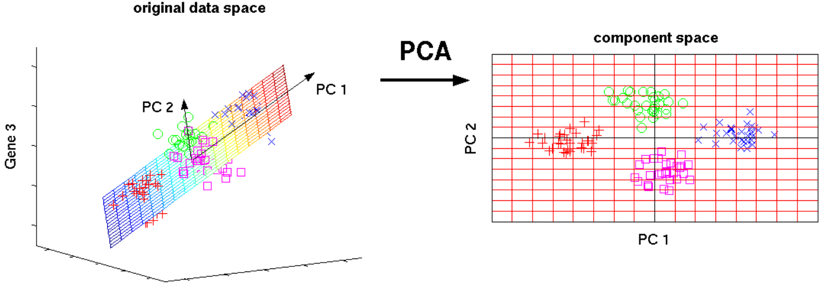
3 Derivations of Principal Component Analysis
- Motivation
- Derivation 1
- Derivation 2

4 Principal Component Analysis Algorithm

5 Applications

Dimensionality Reduction

- Dimensionality reduction aims to find a low-dimensional data vector to represent the original high-dimensional data vector.
- It can be implemented by **unsupervised learning** method or **supervised learning** method. In this lecture, we only introduce one typical unsupervised dimensionality reduction method, called Principal Component Analysis (PCA).
- There are several usages of dimensionality reduction, such as
  - Visualization (as shown below)
  - Alleviate overfitting
  - Reduce the computational cost



Dimensionality Reduction

- The dimensionality of some types of data (*e.g.*, the image) is very high.
- As shown right, these colored images are from ImageNet, and the shape is $224 \times 224 \times 3$. Then, each image can be represented by a $150,528$-dimensional vector.
- If the number of training data is not very large, then the learned model is likely to overfit, leading to poor performance on testing data.
- If we reduce the dimensionality before learning, then the overfitting could be alleviated, and the computational cost in learning will be reduced.

Dimensionality Reduction

Dimensionality reduction:

- Inputs: given a dataset $\mathcal{D} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)}\} \subset \mathbb{R}^D$, with D being the original dimension.
- Goal: find a K-dimensional ($K < D$) subspace $\mathcal{S}$, which consists of K orthonormal basis vectors $\{\mathbf{u}_k\}_{k=1}^K$, and $\mathbf{u}_i^\top \mathbf{u}_j = 0$ for $i \neq j$, while $\mathbf{u}_i^\top \mathbf{u}_i = 1, \forall i$. When projecting all points in $\mathcal{D}$ onto $\mathcal{S}$, it is desired that the structure or property of the original data is well preserved.
- Outputs: the basis vectors $\{\mathbf{u}_k\}_{k=1}^K$, and a new representation $\mathcal{D}' = \{\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(N)}\} \subset \mathbb{R}^K$.

1 Preliminary

2 Dimensionality Reduction

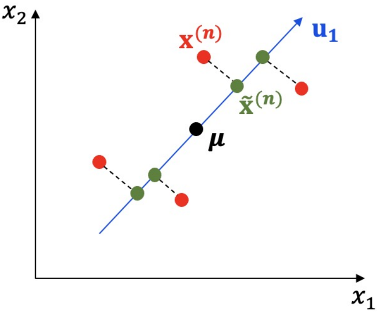
3 Derivations of Principal Component Analysis
- Motivation
- Derivation 1
- Derivation 2

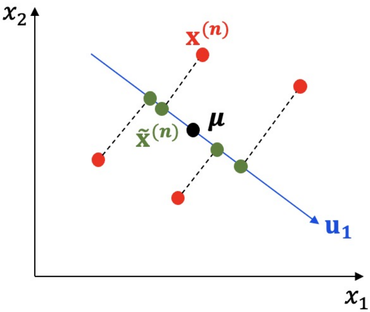
4 Principal Component Analysis Algorithm

5 Applications

1. Preliminary
2. Dimensionality Reduction
3. Derivations of Principal Component Analysis
   - Motivation
   - Derivation 1
   - Derivation 2
4. Principal Component Analysis Algorithm
5. Applications

Motivation





- In the above example, there is a 2-dimensional data set $\mathcal{D} = \{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(N)}\}$, where $\mathbf{x}^{(n)} \in \mathbb{R}^2$.
- We aim to find a one-dimensional sub-space $\mathcal{S} = \{\mathbf{u}_1\} \in \mathbb{R}^2$, such that when projecting each point $\mathbf{x}^{(n)}$ onto this subspace, we obtain the corresponding reconstruction $\tilde{\mathbf{x}}^{(n)}$ and the representation z.
- According to your intuition, which subspace is better, **left** or **right**?

1. Preliminary
2. Dimensionality Reduction
3. Derivations of Principal Component Analysis
   - Motivation
   - Derivation 1
   - Derivation 2
4. Principal Component Analysis Algorithm
5. Applications

Derivation 1: maximal variance

Principal Component Analysis:

- Given a dataset $\mathcal{D} = \{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(N)}\} \in \mathbb{R}^D$, we want to find a K-dimensional ($K < D$) subspace $\mathcal{S}$, which consists of K orthonormal basis vectors $\{\mathbf{u}_k\}_{k=1}^K$, such that the variance of the reconstructions $\tilde{\mathcal{D}} = \{\tilde{\mathbf{x}}^{(1)}, \ldots, \tilde{\mathbf{x}}^{(N)}\}$ is maximal, *i.e.*,

$$\max_{\mathbf{U}, \mathbf{U}^\top \mathbf{U} = \mathbf{I}} \frac{1}{N} \sum_{n=1}^N \|\tilde{\mathbf{x}}^{(n)} - \tilde{\boldsymbol{\mu}}\|^2, \tag{3}$$

where $\tilde{\boldsymbol{\mu}} = \frac{1}{N} \sum_{n=1}^N \tilde{\mathbf{x}}^{(n)}$ denotes the mean of the reconstructions.

- Utilizing the definitions of $\tilde{\mathbf{x}}^{(n)}$ (Eq. 1) and $\mathbf{z}^{(n)}$ (Eq. 2), it is easy to prove

$$\begin{aligned} \tilde{\boldsymbol{\mu}} &= \frac{1}{N} \sum_{n=1}^N \tilde{\mathbf{x}}^{(n)} = \boldsymbol{\mu} + \mathbf{U}\left(\frac{1}{N} \sum_{n=1}^N \mathbf{z}^{(n)}\right) \\ &= \boldsymbol{\mu} + \frac{1}{N} \mathbf{U}\mathbf{U}^\top \sum_{n=1}^N (\mathbf{x}^{(n)} - \boldsymbol{\mu}) = \boldsymbol{\mu} \end{aligned} \tag{4}$$

- Substitute it into (3), we have

$$\max_{\mathbf{U}, \mathbf{U}^\top \mathbf{U} = \mathbf{I}} \frac{1}{N} \sum_{n=1}^N \|\tilde{\mathbf{x}}^{(n)} - \boldsymbol{\mu}\|^2, \tag{5}$$

Derivation 1: maximal variance

Principal Component Analysis:

- Utilizing the definition $\tilde{\mathbf{x}} = \boldsymbol{\mu} + \mathbf{U}\mathbf{z}$, the above problem can be reformulated to

$$\max_{\mathbf{U}, \mathbf{U}^\top \mathbf{U} = \mathbf{I}} \frac{1}{N} \sum_{n=1}^{N} \|\mathbf{U}\mathbf{z}^{(n)}\|^2 \equiv \max_{\mathbf{U}, \mathbf{U}^\top \mathbf{U} = \mathbf{I}} \frac{1}{N} \sum_{n=1}^{N} \|\mathbf{z}^{(n)}\|^2. \tag{6}$$

- Substitute in the definition $\mathbf{z} = \mathbf{U}^\top(\mathbf{x} - \boldsymbol{\mu})$, we have

$$\max_{\mathbf{U}, \mathbf{U}^\top \mathbf{U} = \mathbf{I}} \frac{1}{N} \sum_{n=1}^{N} \|\mathbf{U}^\top(\mathbf{x} - \boldsymbol{\mu})\|^2 \tag{7}$$

$$\equiv \max_{\mathbf{U}, \mathbf{U}^\top \mathbf{U} = \mathbf{I}} \frac{1}{N} \sum_{n=1}^{N} \mathrm{Trace}\big(\mathbf{U}^\top(\mathbf{x}^{(n)} - \boldsymbol{\mu})(\mathbf{x}^{(n)} - \boldsymbol{\mu})^\top \mathbf{U}\big). \tag{8}$$

1. Preliminary
2. Dimensionality Reduction
3. Derivations of Principal Component Analysis
   - Motivation
   - Derivation 1
   - Derivation 2
4. Principal Component Analysis Algorithm
5. Applications

Principal Component Analysis:

- Given a dataset $\mathcal{D} = \{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(N)}\} \in \mathbb{R}^D$, we want to find a K-dimensional ($K < D$) subspace $\mathcal{S}$, which consists of K orthonormal basis vectors $\{\mathbf{u}_k\}_{k=1}^K$, such that the reconstruction loss between $\mathbf{x}$ and $\tilde{\mathbf{x}}$ is minimized, *i.e.*,

$$\min_{\mathbf{U}, \mathbf{U}^\top \mathbf{U} = \mathbf{I}} \frac{1}{N} \sum_{n=1}^{N} \|\mathbf{x}^{(n)} - \tilde{\mathbf{x}}^{(n)}\|^2. \tag{9}$$

Two derivations are equivalent

Theorem

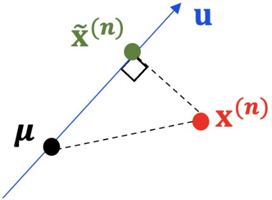
Problem (5) and Problem (9) are equivalent, i.e.,

$$\max_{\mathbf{U},\mathbf{U}^\top\mathbf{U}=\mathbf{I}} \frac{1}{N}\sum_{n=1}^{N} \|\tilde{\mathbf{x}}^{(n)} - \boldsymbol{\mu}\|^2 \equiv \min_{\mathbf{U},\mathbf{U}^\top\mathbf{U}=\mathbf{I}} \frac{1}{N}\sum_{n=1}^{N} \|\mathbf{x}^{(n)} - \tilde{\mathbf{x}}^{(n)}\|^2. \quad (10)$$

Proof: By the Pythagorean Theorem, we have

$$\underbrace{\frac{1}{N}\sum_{n=1}^{N} ||\tilde{\mathbf{x}}^{(n)} - \boldsymbol{\mu}||^2}_{\text{projected variance}} + \underbrace{\frac{1}{N}\sum_{n=1}^{N} ||\mathbf{x}^{(n)} - \tilde{\mathbf{x}}^{(n)}||^2}_{\text{reconstruction error}}$$

$$= \underbrace{\frac{1}{N}\sum_{n=1}^{N} ||\mathbf{x}^{(n)} - \boldsymbol{\mu}||^2}_{\text{constant}}$$



1 Preliminary

2 Dimensionality Reduction

3 Derivations of Principal Component Analysis
- Motivation
- Derivation 1
- Derivation 2

4 Principal Component Analysis Algorithm

5 Applications

PCA algorithm

- Until now, we have known that PCA aims to solve the following optimization problem,

$$\max_{\mathbf{U},\mathbf{U}^\top\mathbf{U}=\mathbf{I}} \frac{1}{N}\sum_{n=1}^{N} \mathrm{Trace}\big(\mathbf{U}^\top(\mathbf{x}^{(n)}-\boldsymbol{\mu})(\mathbf{x}^{(n)}-\boldsymbol{\mu})^\top\mathbf{U}\big). \tag{11}$$

- We define the empirical covariance matrix, as follows:

$$\boldsymbol{\Sigma} = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}^{(n)}-\boldsymbol{\mu})(\mathbf{x}^{(n)}-\boldsymbol{\mu})^\top. \tag{12}$$

- Then, the above optimization can be reformulated as follows:

$$\max_{\mathbf{U}} \ \mathrm{Trace}\big(\mathbf{U}^\top\boldsymbol{\Sigma}\mathbf{U}\big) = \sum_{k=1}^{K}\mathbf{u}_k^\top\boldsymbol{\Sigma}\mathbf{u}_k, \ \text{s.t. } \mathbf{U}^\top\mathbf{U}=\mathbf{I}. \tag{13}$$

PCA algorithm

- The Lagrangian function is formulated as follows:

$$L(\mathbf{U}, \mathbf{\Lambda}_K) = \text{Trace}\big(\mathbf{U}^\top \mathbf{\Sigma} \mathbf{U}\big) + \text{Trace}\big(\mathbf{\Lambda}_K^\top (\mathbf{I} - \mathbf{U}^\top \mathbf{U})\big), \tag{14}$$

  where $\mathbf{\Lambda}_K = \text{diag}([\hat{\lambda}_1, \ldots, \hat{\lambda}_K]) \in \mathbb{R}^{K \times K}$.
- Then, its optimal solution should satisfy

$$\frac{\partial L(\mathbf{U}, \mathbf{\Lambda}_K)}{\partial \mathbf{U}} = 2\mathbf{\Sigma}\mathbf{U} - 2\mathbf{U}\mathbf{\Lambda}_K = \mathbf{0} \tag{15}$$

$$\Rightarrow \ \mathbf{\Sigma}\mathbf{u}_k = \hat{\lambda}_k \mathbf{u}_k, \ k = 1, \ldots, K. \tag{16}$$

- It implies that the optimal primal solution $\mathbf{u}_k$ and the corresponding dual optimal solution $\hat{\lambda}_k$ are one of the eigenvectors and one of the eigenvalues of $\mathbf{\Sigma}$, which also satisfy the constraint $\mathbf{U}^\top \mathbf{U} = \mathbf{I}$.

For matrix derivative, please refer to wikipedia:
https://en.wikipedia.org/wiki/Matrix_calculus

PCA algorithm

- Utilizing SVD decomposition, we have

$$\mathbf{\Sigma} = \mathbf{Q}\mathbf{\Lambda}_D\mathbf{Q}^\top = \sum\nolimits_{i=1}^{D} \lambda_i \mathbf{q}_i \mathbf{q}_i^\top,$$

  where $\mathbf{Q} = [\mathbf{q}_1, \ldots, \mathbf{q}_D] \in \mathbb{R}^{D \times D}$ with $\mathbf{q}_i$ being the eigenvector corresponding to the i-th largest eigenvalue λ_i, and $\mathbf{\Lambda}_D = \mathrm{diag}([\lambda_1, \ldots, \lambda_D])$ with $\lambda_1 \geq \ldots \geq \lambda_D$.

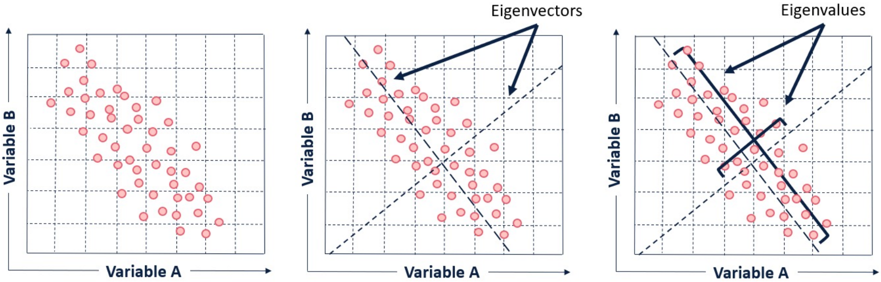
- Substitute into the objective function, we have

$$\sum\nolimits_{k=1}^{K} \mathbf{u}_k^\top \mathbf{\Sigma} \mathbf{u}_k = \sum\nolimits_{k=1}^{K} \sum\nolimits_{i=1}^{D} \lambda_i (\mathbf{u}_k^\top \mathbf{q}_i) \cdot (\mathbf{q}_i^\top \mathbf{u}_k) = \sum\nolimits_{t \in T} \lambda_t,$$

  where we utilize the property of eigenvectors (unit and orthogonal to each other), and $T \subset \{1, \ldots, D\}$ with $|T| = K$ denotes the index subset of K picked eigenvalues.

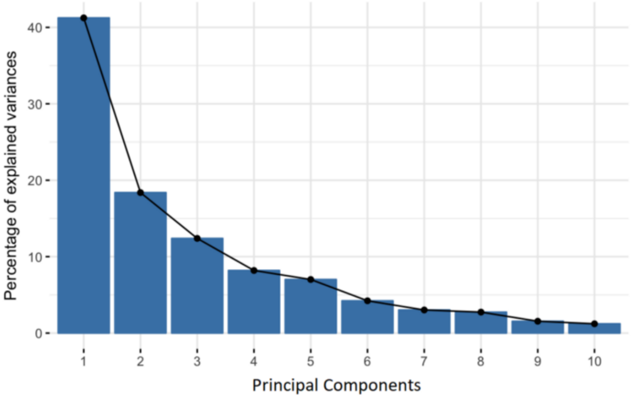
- It is obvious that we should pick the top-K eigenvalues. Correspondingly, the first K columns of $\mathbf{Q}$ should be used as the optimal solution to $\mathbf{U}$.

PCA algorithm



- One eigenvector corresponds to one of the basis vectors of the subspace obtained by PCA.
- One eigenvalue correspond to the variance of the projected points on one basis vector (*i.e.*, eigenvector). Larger eigenvalue indicates more information about the original data.

PCA algorithm



- The variance/information of top-K eigenvectors (*i.e.*, top-K principal components) often takes a large percentage of the whole variance/information.
- Abandon the remaining components will not lost too much information of the data.

PCA algorithm

The above derivation of the optimal solution is summarized as the following steps:

- Step 1: Calculate the empirical covariance matrix $\boldsymbol{\Sigma} = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}^{(n)} - \boldsymbol{\mu})(\mathbf{x}^{(n)} - \boldsymbol{\mu})^\top$
- Step 2: Do SVD decomposition of $\boldsymbol{\Sigma}$ to obtain its D eigenvalues $\{\lambda_i\}_{i=1}^{D}$ and eigenvectors $\{\mathbf{q}_i\}_{i=1}^{D}$, and rank them from large to small according to the eigenvalues.
- Step 3: Pick the top-K eigenvectors to form the matrix $\mathbf{U} = [\mathbf{q}_1, \ldots, \mathbf{q}_K] \in \mathbb{R}^{D\times K}$
- Step 4: The new representation of $\mathbf{x}^{(n)}$ is $\mathbf{U}^\top(\mathbf{x}^{(n)} - \boldsymbol{\mu})$.

Examples

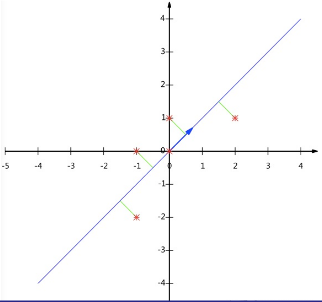
- Suppose that we have a set of 5 points in 2-dimensional space

$$X = \begin{pmatrix} -1 & -1 & 0 & 2 & 0 \\ -2 & 0 & 0 & 1 & 1 \end{pmatrix},$$

of which the mean column vector is $\boldsymbol{\mu} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$.

- We calculate its covariance matrix as

$$\boldsymbol{\Sigma} = \frac{1}{5} X X^\top = \frac{1}{5} \begin{pmatrix} 6 & 4 \\ 4 & 6 \end{pmatrix}.$$



Examples

- SVD decomposition: we obtain

$$\mathbf{q}_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix},\ \mathbf{q}_2 = \begin{bmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix},\ \lambda_1 = 2,\ \lambda_2 = \frac{2}{5}.$$

- Thus, we set $\mathbf{U} = \mathbf{q}_1$
- The new representation is $\mathbf{U}^\top X = \begin{pmatrix} \frac{-3}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 & \frac{3}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix}$.

Reference:
Demo with code: https://zhuanlan.zhihu.com/p/37777074

Decorrelation of the new representation

- Interesting property: the dimensions of $\mathbf{z}$ are decorrelated. For now, let Cov denote the empirical covariance.

$$
\begin{aligned}
\mathrm{Cov}(\mathbf{z}) &= \mathrm{Cov}(\mathbf{U}^T(\mathbf{x} - \boldsymbol{\mu})) \\
&= \mathbf{U}^T \mathrm{Cov}(\mathbf{x}) \mathbf{U} \\
&= \mathbf{U}^T \boldsymbol{\Sigma} \mathbf{U} \\
&= \mathbf{U}^T \mathbf{Q} \boldsymbol{\Lambda} \mathbf{Q}^T \mathbf{U} \\
&= \begin{pmatrix} \mathbf{I} & 0 \end{pmatrix} \boldsymbol{\Lambda} \begin{pmatrix} \mathbf{I} \\ 0 \end{pmatrix} && \text{by orthogonality} \\
&= \text{top left } K \times K \text{ block of } \boldsymbol{\Lambda}
\end{aligned}
$$

- If the covariance matrix is diagonal, this means the features are uncorrelated.

Recap of PCA

- Dimensionality reduction aims to find a low-dimensional representation of the data.
- PCA projects the data onto a subspace which maximizes the projected variance, or equivalently, minimizes the reconstruction error.
- The optimal subspace is given by the top eigenvectors of the empirical covariance matrix.
- PCA gives a set of decorrelated features.

1. Preliminary
2. Dimensionality Reduction
3. Derivations of Principal Component Analysis
   - Motivation
   - Derivation 1
   - Derivation 2
4. Principal Component Analysis Algorithm
5. Applications

Applying PCA to faces

- Consider running PCA on 2429 19×19 grayscale facial images (CBCL data), and each image is represented by a 361-dimensional column vector

- After running PCA, we can obtain several eigenfaces. With only top-3 eigenfaces, we achieve 79% accuracy on face/non-face discrimination on test data.
- We visualize the first 60 eigenvectors to the original shape, as follows:

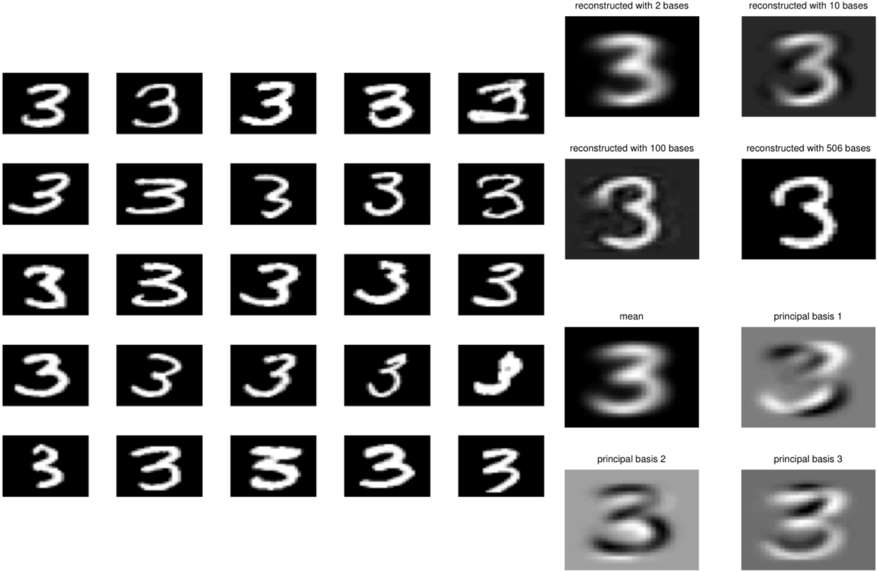
Reference:

- Wikipedia: https://en.wikipedia.org/wiki/Eigenface
- Demo with code: https://scikit-learn.org/stable/auto_examples/applications/plot_face_recognition.html

Applying PCA to faces: Learned basis

Principal components of face images ("eigenfaces")

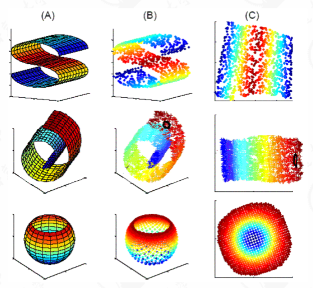
Applying PCA to digits



Further readings

Note that PCA is an orthogonal linear transformation method, thus it cannot handle non-linear data. There are some interesting variants of PCA, such as

- Kernel PCA: see Chapter 12.3 of Bishop's book (Link)
- Probabilistic PCA: see Chapter 12.2 of Bishop's book
- Nonlinear PCA: see http://www.nlpca.org/
- Robust PCA: see https://en.wikipedia.org/wiki/Robust_principal_component_analysis



CTE

Please take 5 mins to finish CTE, thanks.
Link: https://octe.cuhk.edu.cn/a/login

DDA3020-2022Atumn/figs/CTE-DDA3020.png