Introduction to Machine Learning

Principal Component Analysis

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Outline

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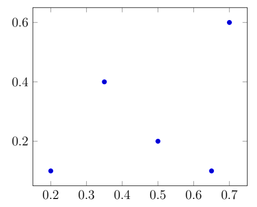
1 Principal Components Analysis

1.1 Introduction to PCA

- Consider the following data points

- *Embed* these points in 1 dimension

- What is the best way?



  - **Along the direction of the maximum variance**
  - Why?

1.2 Principle of Maximal Variance

- Least loss of information

- Best capture the "spread"

- What is the direction of maximal variance?

- Given any direction ($\hat{\mathbf{u}}$), the projection of $\mathbf{x}$ on $\hat{\mathbf{u}}$ is given by:

$$\mathbf{x}_i^\top \hat{\mathbf{u}}$$

- Direction of maximal variance can be obtained by maximizing

$$\begin{aligned}\frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i^\top \hat{\mathbf{u}})^2 &= \frac{1}{N}\sum_{i=1}^{N}\hat{\mathbf{u}}^\top \mathbf{x}_i \mathbf{x}_i^\top \hat{\mathbf{u}} \\ &= \hat{\mathbf{u}}^\top \left(\frac{1}{N}\sum_{i=1}^{N}\mathbf{x}_i\mathbf{x}_i^\top\right)\hat{\mathbf{u}}\end{aligned}$$

Finding Direction of Maximal Variance

- Find:

$$\underset{\hat{\mathbf{u}}:\hat{\mathbf{u}}^\top\hat{\mathbf{u}}=1}{max}\ \hat{\mathbf{u}}^\top \mathbf{S}\hat{\mathbf{u}}$$

  where:

$$\mathbf{S} = \frac{1}{N}\sum_{i=1}^{N}\mathbf{x}_i\mathbf{x}_i^\top$$

- $\mathbf{S}$ is the sample (empirical) covariance matrix of the mean-centered data

The solution to the above constrained optimization problem may be obtained using the Lagrange multipliers method. We maximize the following w.r.t. $\hat{\mathbf{u}}$:

$$(\hat{\mathbf{u}}^\top \mathbf{S}\hat{\mathbf{u}}) - \lambda(\hat{\mathbf{u}}^\top\hat{\mathbf{u}} - 1)$$

to get:

$$\begin{aligned} \frac{d}{d\hat{\mathbf{u}}}(\hat{\mathbf{u}}^\top \mathbf{S}\hat{\mathbf{u}}) - \lambda(\hat{\mathbf{u}}^\top\hat{\mathbf{u}} - 1) &= 0 \\ \mathbf{S}\hat{\mathbf{u}} - \lambda\hat{\mathbf{u}} &= 0 \\ \mathbf{S}\hat{\mathbf{u}} &= \lambda\hat{\mathbf{u}} \end{aligned}$$

Obviously, the solution to the above equation is an eigen vector of the matrix $\mathbf{S}$. But which $\mathbf{S}$? Note that for the optimal solution:

$$\hat{\mathbf{u}}^\top \mathbf{S}\hat{\mathbf{u}} = (\hat{\mathbf{u}}^\top \lambda\hat{\mathbf{u}}) = \lambda$$

Thus we should choose the largest possible λ which means that the first solution is the eigen vector of $\mathbf{S}$ with largest eigen value.

1.3 Defining Principal Components

- First PC: Eigen-vector of the (sample) covariance matrix with largest eigen-value
- Second PC?
- Eigen-vector with next largest value
- Variance of each PC is given by λ_i
- Variance captured by first L PC ($1 \leq L \leq D$)

$$\frac{\sum_{i=1}^{L}\lambda_i}{\sum_{i=1}^{D}\lambda_i} \times 100$$

- What are eigen vectors and values?

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$$

  $\mathbf{v}$ is eigen vector and λ is eigen-value for the **square matrix A**

- Geometric interpretation?

For the second PC we need to optimize the variance with a second constraint that the solution should be orthogonal to the first PC. It is easy to show that this solution will be the PC with second largest eigen value, and so on.

1.4 Dimensionality Reduction Using PCA

- Consider first L eigen values and eigen vectors
- Let $\mathbf{W}$ denote the $D\times L$ matrix with first L eigen vectors in the columns (sorted by λ's)
- PC score matrix

$$\mathbf{Z} = \mathbf{X}\mathbf{W}$$

- Each input vector $(D \times 1)$ is replaced by a shorter $L \times 1$ vector

1.5 PCA Algorithm

1. *Center* $\mathbf{X}$

$$\mathbf{X} = \mathbf{X} - \hat{\boldsymbol{\mu}}$$

2. Compute sample covariance matrix:

$$\mathbf{S} = \frac{1}{N-1}\mathbf{X}^\top\mathbf{X}$$

3. Find eigen vectors and eigen values for $\mathbf{S}$
4. $\mathbf{W}$ consists of first L eigen vectors as columns
   - Ordered by decreasing eigen-values
   - $\mathbf{W}$ is $D \times L$
5. Let $\mathbf{Z} = \mathbf{X}\mathbf{W}$
6. Each row in $\mathbf{Z}$ (or $\mathbf{z}_i^\top$) is the lower dimensional embedding of $\mathbf{x}_i$

1.6 Recovering Original Data

- Using $\mathbf{W}$ and $\mathbf{z}_i$

$$\hat{\mathbf{x}}_i = \mathbf{W}\mathbf{z}_i$$

- **Average Reconstruction Error**

$$J(\mathbf{W}, \mathbf{Z}) = \frac{1}{N}\sum_{i=1}^{N} \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|^2$$

Theorem 1 (Classical PCA Theorem)**.** *Among all possible orthonormal sets of L basis vectors, PCA gives the solution which has the minimum reconstruction error.*

- Optimal "embedding" in L dimensional space is given by $z_i = \mathbf{W}^\top \mathbf{x}_i$

1.7 Eigen Faces

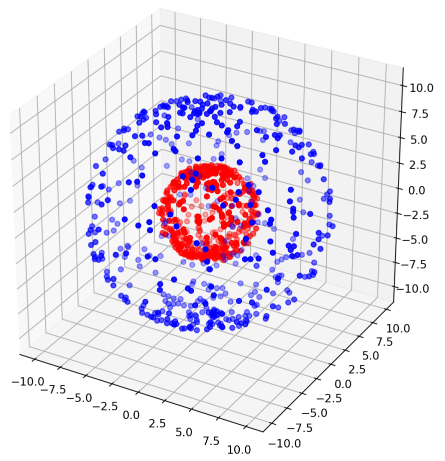
EigenFaces [2]

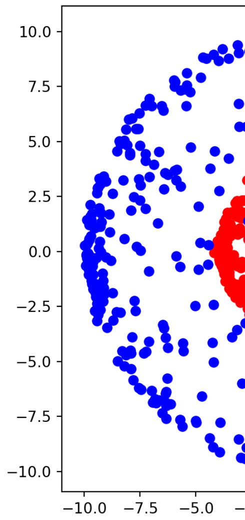
- **Input:** A set of images (of faces)
- **Task:** Identify if a new image is a face or not.

2 Kernel PCA

Issues with PCA

- A linear transformation of the data
- Might not work everytime





Kernel PCA - Applying the kernel trick [1]

- Assume a non-linear transformation of input:

$$\mathbf{x_i} \Rightarrow \Phi(\mathbf{x_i}),\ \ \Phi(\mathbf{x_i}) \in \mathbb{R}^M$$

- We will assume that the new data is mean centered:

$$\frac{1}{N}\sum_{i=1}^{N} \Phi(\mathbf{x_i}) = 0$$

Of course, if it is not centered, then we can mean-center it first.

- The covariance matrix of the projected data, $\mathbf{C}$:

$$\mathbf{C} = \frac{1}{N}\sum_{i=1}^{N}\Phi(\mathbf{x_i})\Phi(\mathbf{x_i})^\top$$

- The eigen vectors and eigen values of $\mathbf{C}$ are given by:

$$\mathbf{C}\mathbf{v}_k = \lambda_k\mathbf{v}_k$$

where $k = 1, 2, \ldots, M$

- Substituting the expression for $\mathbf{C}$:

$$\frac{1}{N}\sum_{i=1}^{N}\Phi(\mathbf{x_i})\Phi(\mathbf{x_i})^\top\mathbf{v}_k = \lambda_k\mathbf{v}_k$$

- Rearranging and assuming $a_{ki} = \frac{\Phi(\mathbf{x_i})^\top\mathbf{v}_k}{N\lambda_k}$

$$\mathbf{v}_k = \sum_{i=1}^{N}a_{ki}\Phi(\mathbf{x_i})$$

a_{ki} will be a scalar value which is a scalar multiple of the dot product between the projection of the i^{th} data point and the k^{th} eigen vector.

- Substituting this back in the above equation

$$\frac{1}{N}\sum_{i=1}^{N}\Phi(\mathbf{x_i})\Phi(\mathbf{x_i})^\top\sum_{j=1}^{N}a_{kj}\Phi(\mathbf{x_j}) = \lambda_k\sum_{i=1}^{N}a_{ki}\Phi(\mathbf{x_i})$$

Note the subscript j in the second summation on the left hand side.

- Now multiplying both sides with $\Phi(\mathbf{x_l})^\top$:

$$\frac{1}{N}\Phi(\mathbf{x_l})^\top\sum_{i=1}^{N}\Phi(\mathbf{x_i})\Phi(\mathbf{x_i})^\top\sum_{j=1}^{N}a_{kj}\Phi(\mathbf{x_j}) = \lambda_k\Phi(\mathbf{x_l})^\top\sum_{i=1}^{N}a_{ki}\Phi(\mathbf{x_i})$$

which is the same as:

$$\sum_{i=1}^{N}\underbrace{\Phi(\mathbf{x_l})^\top\Phi(\mathbf{x_i})}\sum_{j=1}^{N}a_{kj}\,\underbrace{\Phi(\mathbf{x_i})^\top\Phi(\mathbf{x_j})} = N\lambda_k\sum_{i=1}^{N}\underbrace{a_{ki}\Phi(\mathbf{x_l})^\top\Phi(\mathbf{x_i})}$$

- Let $k()$ be a function, such that: $k(\mathbf{x_i}, \mathbf{x_j}) = \Phi(\mathbf{x_i})^\top\Phi(\mathbf{x_j})$
- The above expression can be written as:

$$\sum_{i=1}^{N}k(\mathbf{x_l}, \mathbf{x_i})\sum_{j=1}^{N}a_{kj}k(\mathbf{x_i}, \mathbf{x_j}) = N\lambda_k\sum_{i=1}^{N}k(\mathbf{x_l}, \mathbf{x_i})$$

- Consider the $N \times 1$ vector, $\mathbf{a}_k$ amd $N \times N$ matrix, $\mathbf{K}$, such that

$$\mathbf{a}_k = \begin{bmatrix} a_{k1} \\ a_{k2} \\ \vdots \\ a_{kN} \end{bmatrix}$$

and,

$$\mathbf{K}[i][j] = k(\mathbf{x_i}, \mathbf{x_j})$$

- The above expression can be written, using matrix notation, as:

$$\mathbf{K}^2\mathbf{a}_k = \lambda_k N\mathbf{K}\mathbf{a}_k$$

- To solve for $\mathbf{a}_k$, we can solve the following:

$$\mathbf{K}\mathbf{a}_k = \lambda_k N\mathbf{a}_k$$

This can be obtained by calculating the eigenvectors of the kernel matrix $\mathbf{K}$

Projecting data using Kernel PCA

- For a new data instance, $\mathbf{x}^*$, the k^{th} entry of the corresponding $\mathbf{z}^*$ will be:

$$\begin{aligned} z_k^* &= \Phi(\mathbf{x}^*)^\top\mathbf{v}_k \\ &= \Phi(\mathbf{x}^*)^\top\sum_{i=1}^{N}a_{ki}\Phi(\mathbf{x_i}) \\ &= \sum_{i=1}^{N}a_{ki}\Phi(\mathbf{x}^*)^\top\Phi(\mathbf{x_i}) \\ &= \sum_{i=1}^{N}a_{ki}k(\mathbf{x}^*, \mathbf{x}_i) \end{aligned}$$

Centering the projected data

- How do we ensure that the projected new features have a zero mean, without doing the actual projection?
- Use the **Gram matrix**:

$$\tilde{\mathbf{K}} = \mathbf{K} - \mathbf{1}_N\mathbf{K} - \mathbf{K}\mathbf{1}_N + \mathbf{1}_N\mathbf{K}\mathbf{1}_N$$

  where $\mathbf{1}_N$ is a $N \times N$ matrix with all entries equal to $\frac{1}{N}$

Kernel PCA Algorithm

1. Given the data set $\mathbf{X}$ and a kernel function $k()$, construct the kernel matrix $\mathbf{K}$
2. Compute the Gram matrix $\tilde{\mathbf{K}}$
3. Find eigen-vectors of $\tilde{\mathbf{K}}$
4. Use top M eigen-vectors to project a new data instance, $\mathbf{x}^*$ to the corresponding $\mathbf{z}^*$

Kernel PCA - Final Thoughts

- Very sensitive to the kernel chocie and kernel parameters
- Slow ($O(N^3)$)
- Recovering original data is not straightforward as linear PCA

References

References

[1] B. Schölkopf, A. J. Smola, and K.-R. Müller. *Kernel Principal Component Analysis*, page 327–352. MIT Press, Cambridge, MA, USA, 1999.

[2] M. Turk and A. Pentland. Face recognition using eigenfaces. In *Computer Vision and Pattern Recognition, 1991. Proceedings CVPR '91., IEEE Computer Society Conference on*, pages 586–591, Jun 1991.