Introduction to Machine Learning

Principal Component Analysis

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Outline

What have we seen so far?

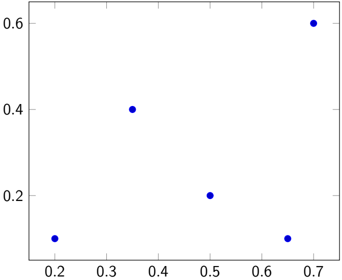
- Factor Analysis Models
  - **Assumption**: $\mathbf{x}_i$ is a multivariate Gaussian random variable
  - Mean is a function of $\mathbf{z}_i$
  - Covariance matrix is fixed

$$p(\mathbf{x}_i|\mathbf{z}_i, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{W}\mathbf{z}_i + \boldsymbol{\mu}, \boldsymbol{\Psi})$$

  - $\mathbf{W}$ is a $D \times L$ matrix (loading matrix)
  - $\boldsymbol{\Psi}$ is a $D \times D$ diagonal covariance matrix
- Extensions:
  - *Independent Component Analysis*.
  - If $\boldsymbol{\Psi} = \sigma^2\mathbf{I}$ and $\mathbf{W}$ is orthonormal $\Rightarrow$ FA is equivalent to **Probabilistic Principal Components Analysis** (PPCA)
  - If $\sigma^2 \rightarrow 0$, FA is equivalent to PCA

Introduction to PCA

- Consider the following data points



Introduction to PCA

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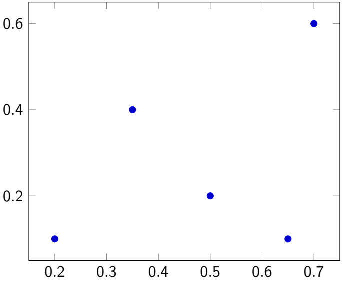

- *Embed* these points in 1 dimension
- What is the best way?
  - **Along the direction of the maximum variance**
  - Why?

Why Maximal Variance?

- Least loss of information
- Best capture the "spread"

Why 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

Defining Principal Components

- First PC: Eigen-vector of the (sample) covariance matrix with largest eigen-value
- Second PC?

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?

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

PCA Algorithm

1. *Center* $\mathbf{X}$
$$\mathbf{X} = \mathbf{X} - \hat{\mu}$$
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 $\mathbf{x}_i$

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 (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 $z_i = \mathbf{W}^\top \mathbf{x}_i$

Using PCA for Face Recognition

EigenFaces [?]

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

Probabilistic PCA

- Recall the **Factor Analysis** model

$$p(\mathbf{x}_i|\mathbf{z}_i, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{W}\mathbf{z}_i + \boldsymbol{\mu}, \boldsymbol{\Psi})$$

- For PPCA, $\boldsymbol{\Psi} = \sigma^2\mathbf{I}$
- Covariance for each observation $\mathbf{x}$ is given by:

$$\mathbf{W}\mathbf{W}^\top + \sigma^2\mathbf{I}$$

- If we maximize the log-likelihood of a data set $\mathbf{X}$, the MLE for $\mathbf{W}$ is:

$$\hat{W} = \mathbf{V}(\boldsymbol{\Lambda} - \sigma^2\mathbf{I})^{\frac{1}{2}}$$

- $\mathbf{V}$ - first L eigenvectors of $\mathbf{S} = \frac{1}{N}\mathbf{X}^\top\mathbf{X}$
- $\boldsymbol{\Lambda}$ - diagonal matrix with first L eigen values

EM for PCA

- PPCA formulation allows for EM based learning of parameters
- $\mathbf{Z}$ is a matrix containing N latent random variables

Benefits of EM

- EM can be faster
- Can be implemented in an online fashion
- Can handle missing data

References