Principal Component Analysis (PCA)

Machine Learning (CSCI 5770G)

Faisal Z. Qureshi

http://vclab.science.ontariotechu.ca

Principal Component Analysis

- PCA takes advantage of correlations in data dimensions to produce the best possible lower dimensional representations (according to the reconstruction error)
- PCA should not be used for discovering patterns
- PCA should not be used for making predictions
- PCA should be used for dimensionality reduction

PCA (1)

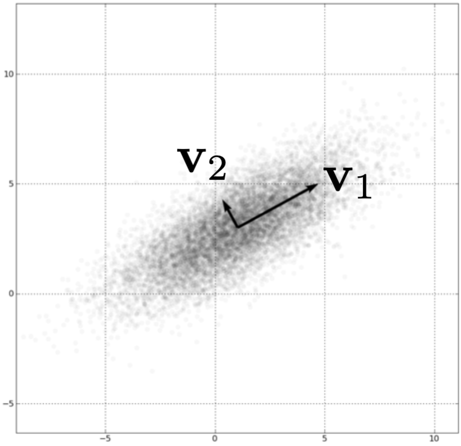
- Given n d-dimensional data points: $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \mathbf{x}^{(3)}, \cdots, \mathbf{x}^{(n)}$
- Compute $\mathbf{z}^{(i)} = \mathbf{x}^{(i)} - \mu$, where $\mu = \frac{1}{n} \sum_i \mathbf{x}^{(i)}$
- Generate matrix $\mathbf{Z} \in \mathbb{R}^{d \times n}$

$$\begin{bmatrix} \vdots & \vdots & \vdots & & \vdots \\ \mathbf{z}^{(1)} & \mathbf{z}^{(2)} & \mathbf{z}^{(3)} & \cdots & \mathbf{z}_n \\ \vdots & \vdots & \vdots & & \vdots \end{bmatrix}$$

- Compute $\mathbf{Z}\mathbf{Z}^T \in \mathbb{R}^{d \times d}$

PCA (2)

- Compute eigenvectors $\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \mathbf{v}^{(3)}, \cdots, \mathbf{v}^{(d)}$, where $\mathbf{v}^{(i)} \in \mathbb{R}^d$ and eigenvalues $\lambda^{(1)} \geq \lambda^{(2)} \geq \lambda^{(3)} \geq \cdots \geq \lambda^{(d)}$ of $\mathbf{Z}\mathbf{Z}^T$.



PCA (3)

- Construct a project matrix consisting of the eigenvectors corresponding to top k eigenvectors, where $k \ll n$

$$\mathbf{P} = \begin{bmatrix} \vdots & \vdots & \vdots & & \vdots \\ \mathbf{v}^{(1)} & \mathbf{v}^{(2)} & \mathbf{v}^{(3)} & \cdots & \mathbf{v}^{(k)} \\ \vdots & \vdots & \vdots & & \vdots \end{bmatrix} \in \mathbb{R}^{d \times k}$$

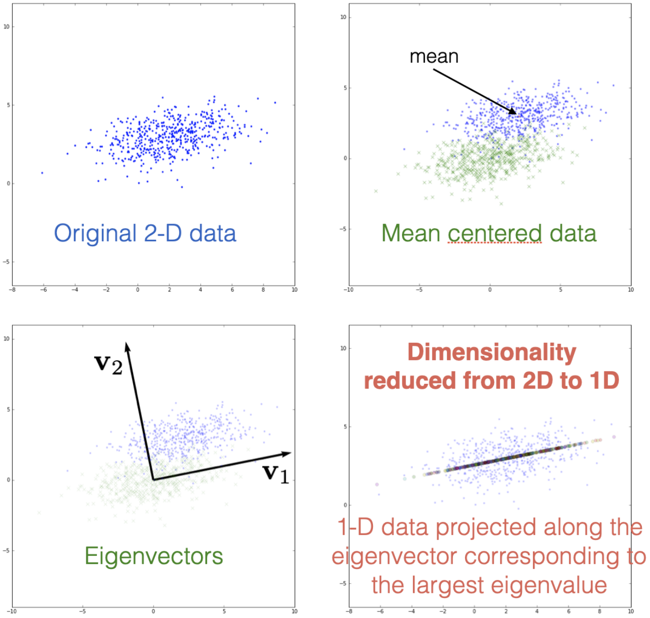
- **Project data to achieve dimensionality reduction**

$$\mathbf{x}_{\text{proj}} = \mathbf{P}^T \mathbf{x}, \text{ where } \mathbf{x} \in \mathbb{R}^n \text{ and } \mathbf{x}_{\text{proj}} \in \mathbb{R}^k$$

- **Lossy reconstruction**

$$\mathbf{x}_{\text{recon}} = \mathbf{P} \mathbf{x}_{\text{proj}} + \mu, \text{ where } \mathbf{x}_{\text{recon}} \in \mathbb{R}^n$$

PCA (4)


Original 2-D data
mean
Mean centered data
$\mathbf{v}_2$
$\mathbf{v}_1$
Eigenvectors
Dimensionality reduced from 2D to 1D
1-D data projected along the eigenvector corresponding to the largest eigenvalue

Singular Value Decomposition (SVD)

SVD theorem states

$$\mathbf{A}_{d\times n} = \mathbf{U}_{d\times d}\Sigma_{d\times n}\mathbf{V}^T_{n\times n},$$

where $\mathbf{U}$ columns are left singular vectors, Σ are singular values, and $\mathbf{V}^T$ rows are right singular vectors. For our case, rows of $\mathbf{A}$ represent dimensions (or features) and columns of $\mathbf{A}$ represent samples.

- SVD represents an expansion of the original data into a coordinate system where covariance matrix is diagonal.
- The eigenvectors of $\mathbf{A}\mathbf{A}^T$ make up columns of $\mathbf{U}$.
- The eigenvectors of $\mathbf{A}^T\mathbf{A}$ make up columns of $\mathbf{V}$.
- The singular values are squareroot of eigenvalues of $\mathbf{A}\mathbf{A}^T$ or $\mathbf{A}^T\mathbf{A}$.

Eigenfaces (Application of PCA)

Eigenfaces for Recognition

Matthew Turk and Alex Pentland
Vision and Modeling Group
The Media Laboratory
Massachusetts Institute of Technology

M. A. Turk and A. P. Pentland, "Face recognition using eigenfaces," Proceedings. 1991 IEEE Computer Society Conference on Computer Vision and Pattern Recognition, Maui, HI, 1991, pp. 586-591.

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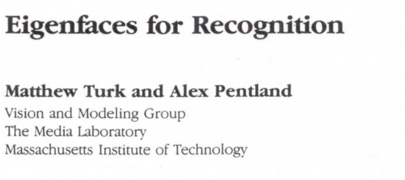

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Why does it work?

Takeaway

- PCA
  - Data can be represented in different spaces
  - Sometimes less is more
- A working knowledge of fundamental ideas from statistics and linear algebra is useful for 1) understanding machine learning theory and 2) informing machine learning practice

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