CS 446/ECE 449: Machine Learning

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L20: Principal Component Analysis, Singular Value Decomposition

Goals of this lecture

- Transition from supervised to unsupervised learning
- Getting to know the Principal Component Analysis (PCA)
- Relating PCA to the Singular Value Decomposition

Reading material:

- K. Murphy; Machine Learning: A Probabilistic Perspective; Chapter 12

Recap: Supervised learning

Given a dataset $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}$ of data-label pairs, construct a mapping $F(w, x, y)$.

Examples:

- KNN
- Least squares
- Logistic regression
- Support vector machine
- Deep net
- Structured prediction

What if we don't have labels?

Without labels, we can still find structure in unlabeled data

$$\mathcal{D} = \{(x^{(i)})\}$$

Goal of unsupervised learning?
Less clear but generally:

- Recover hidden structure
- Data compression or dimensionality reduction
- Explore or explain data (generate data)
- Construct features for supervised learning (e.g., word embeddings)

Methods:

- PCA
- k-means
- Gaussian Mixture Models
- Hidden Markov Models
- Variational Auto-encoders
- Generative Adversarial Nets

PCA

Goal: find that lower dimensional **linear** subspace in which the projected data has highest variance

$$\text{(data)} \quad X = \begin{bmatrix} | & & | \\ x^{(1)} & \dots & x^{(|\mathcal{D}|)} \\ | & & | \end{bmatrix}$$

$$\text{(centered data)} \quad \bar{X} = \begin{bmatrix} | & & | \\ x^{(1)} - \mu & \dots & x^{(|\mathcal{D}|)} - \mu \\ | & & | \end{bmatrix} \quad \text{where } \mu = \frac{1}{|\mathcal{D}|} \sum_{x \in \mathcal{D}} x$$

Never forget to center data! Symmetric matrix $\Sigma = \frac{1}{|\mathcal{D}|} \bar{X} \bar{X}^T$

$$\max_{w : \|w\|_2^2 = 1} \text{Var}(w^T \bar{X}) = \max_{w : \|w\|_2^2 = 1} \mathbb{E}[w^T \bar{X} \bar{X}^T w] = \max_{w : \|w\|_2^2 = 1} w^T \Sigma w$$

How to solve

$$\max_{w:\|w\|_2^2=1} \quad w^T \Sigma w$$

Lagrangian:

$$L() = w^T \Sigma w - \lambda(w^T w - 1)$$

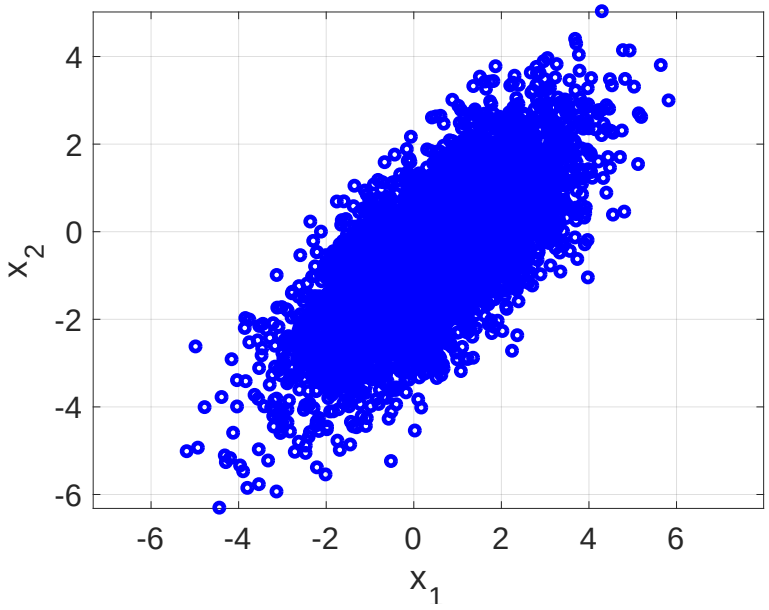
Derivative of L w.r.t. w set to zero:

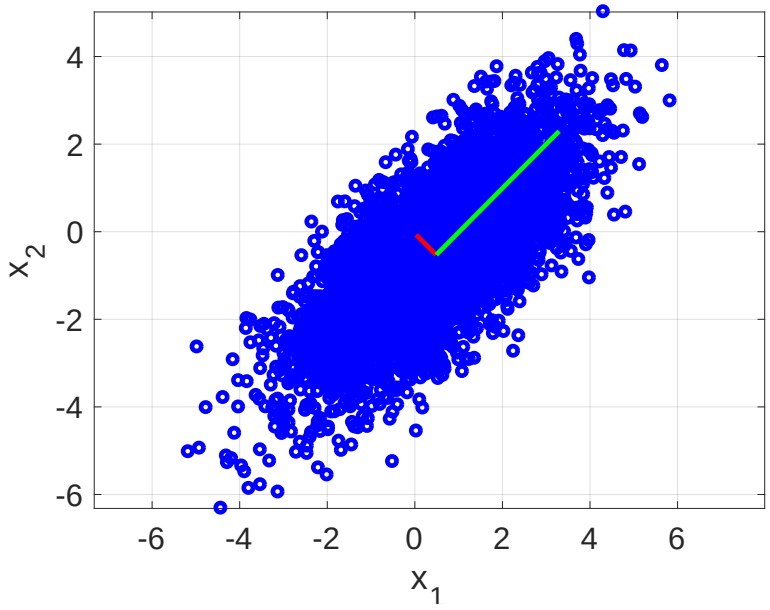
$$\Sigma w = \lambda w \qquad \text{(eigenvalue problem)}$$

Which eigenvector/eigenvalue should we take?

We want to maximize $w^T \Sigma w = \lambda w^T w = \lambda$. Hence, w is the eigenvector corresponding to the largest eigenvalue.

Example:





What if we want to find the direction with second, third largest variance that's orthogonal to the first, first and second?

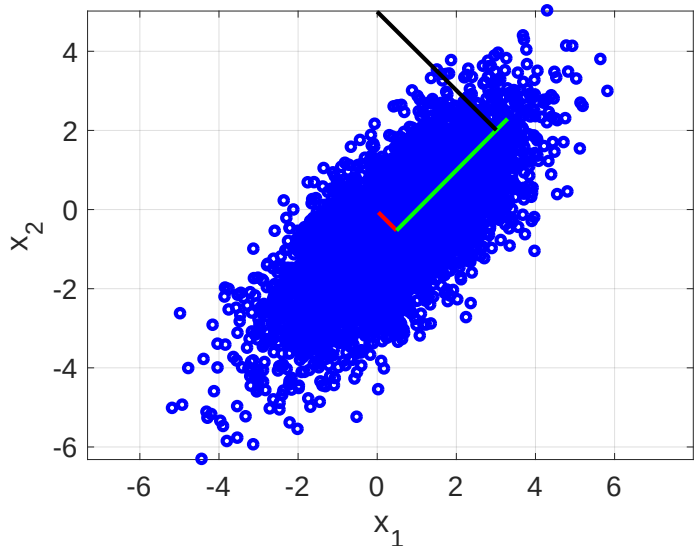
Finding that d-dimensional subspace that captures the largest variance?

$$\max_{w_1,\ldots,w_d : w_i^T w_j = \delta_{ij}} \sum_{i=1}^{d} w_i^T \Sigma w_i$$

Algorithm:

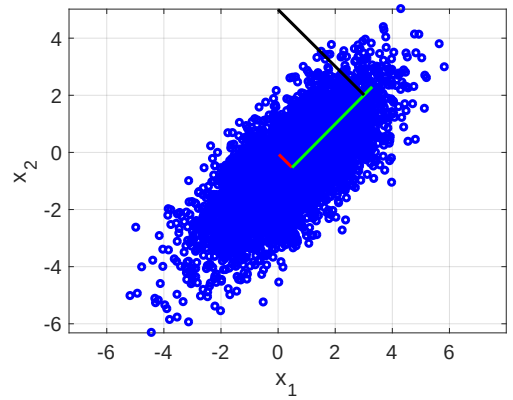
- Work sequentially one vector at a time
- Compute a matrix eigenvalue decomposition

How to project data into low-dimensional space?



1. Collect all subspace directions:

$$U = \begin{bmatrix} | & & | \\ w_1 & \cdots & w_d \\ | & & | \end{bmatrix}$$



2. Project points into subspace (compressed space)

$$\hat{x} = U^T(x - \mu)$$

3. Approximately reconstructed data

$$\tilde{x} = U\hat{x} + \mu$$

Alternative view of PCA:

PCA finds the axis which minimizes the sum of squared distances from points to their orthogonal projections on that axis (we assume $\mu = 0$ for notational convenience):

$$\min_{w:\|w\|_2^2=1} \frac{1}{|\mathcal{D}|} \sum_{i=1}^{|\mathcal{D}|} \|x^{(i)} - ww^T x^{(i)}\|_2^2$$

(see previous slide & lin reg)

Frobenius norm:

$$\|A\|_F^2 = \sum_{i,j} a_{i,j}^2 = \text{Tr}(A^T A)$$

Rewriting the objective:

$$\frac{1}{|\mathcal{D}|}\sum_{i=1}^{|\mathcal{D}|}\|x^{(i)}-ww^Tx^{(i)}\|_2^2=\frac{1}{|\mathcal{D}|}\|\bar{X}-ww^T\bar{X}\|_F^2$$

$$=\frac{1}{|\mathcal{D}|}\mathrm{Tr}((P\bar{X})^T(P\bar{X})) \quad \text{where} \quad P=I-ww^T$$

$$=\frac{1}{|\mathcal{D}|}\mathrm{Tr}(\bar{X}\bar{X}^TP^TP)$$

$$= \mathrm{Tr}(\Sigma P) \qquad \text{since for projection } P^TP=P$$

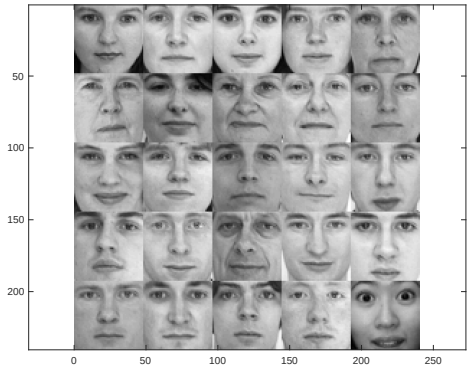
Hence:

$$\arg\min_{w:\|w\|_2^2=1}\frac{1}{|\mathcal{D}|}\sum_{i=1}^{|\mathcal{D}|}\|x^{(i)}-ww^Tx^{(i)}\|_2^2 := \mathrm{Tr}(\Sigma)-\mathrm{Tr}(\Sigma ww^T)$$

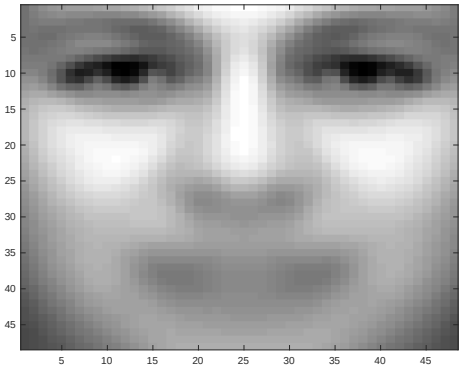
$$= \arg\max_{w:\|w\|_2^2=1} w^T\Sigma w$$

Applications

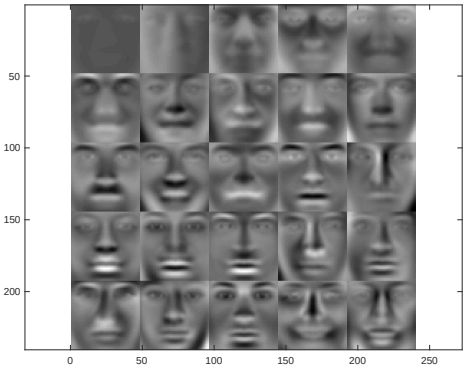
Compressing high-dimensional data



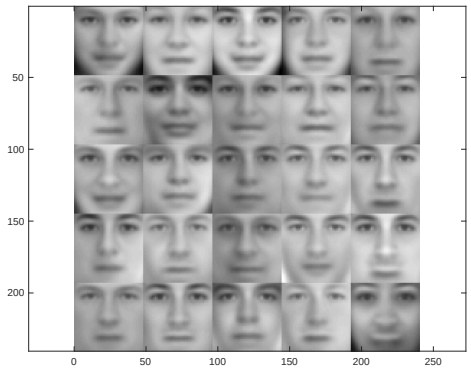
Original x



Mean μ



25 eigenvectors U



Reconstruction $\tilde{x}$

Singular Value Decomposition to compute PCA

Currently we compute the eigenvalues of $\Sigma = \frac{1}{|\mathcal{D}|}\bar{X}\bar{X}^T$
Instead of first computing the outer product and then computing its eigenvalues we can use the singular value decomposition.

How?

Given the singular value decomposition

$$\frac{1}{\sqrt{|\mathcal{D}|}}\bar{X} = USV^T$$

We obtain

$$\Sigma = USV^T VSU^T$$

The left singular vectors U of $\frac{1}{\sqrt{|\mathcal{D}|}}\bar{X}$ are needed

Quiz:

- What is PCA?
- What are the two views of PCA?
- Which two approaches can be used to compute principal components?
- How is data compressed and reconstructed?

Important topics of this lecture

- Understanding PCA
- Getting to know different ways to compute PCA

Up next:

- k-means