STA 314: Statistical Methods for Machine Learning I

Lecture 12 - Unsupervised Learning: K-means clustering and PCA

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Unsupervised learning

- Unsupervised learning is the study of learning without labels. What can we do without labels?
- How can we even define what learning means without labels?
- In some sense, the ML community does not exactly agree on what it means to do unsupervised learning, but intuitively, unsupervised learning is the task of
  - grouping (clustering)
  - explaining
  - finding structured data

Motivating Examples

- Some examples of situations where you'd use unupservised learning
  - You want to understand how a scientific field has changed over time. You want to take a large database of papers and model how the distribution of topics changes from year to year. But what are the topics?
  - You're a biologist studying animal behavior, so you want to infer a high-level description of their behavior from video. You don't know the set of behaviors ahead of time.
  - You want to reduce your energy consumption, so you take a time series of your energy consumption over time, and try to break it down into separate components (refrigerator, washing machine, etc.).
- Common themes: you have some data, and you want to infer some structure underlying the data.
  - Clustering
  - Low-dimensional representation

Clustering

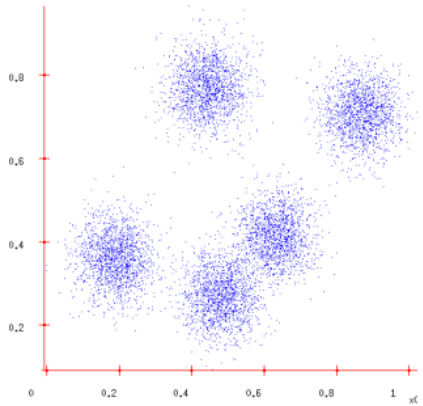
- Clustering is the task of organizing data into groups or clusters.
- We will study the simplest method for doing this: the K-means algorithm.

Example:

- Determine different clothing styles
- Determine groups of people
  - based on clothing styles
  - gender, age, etc

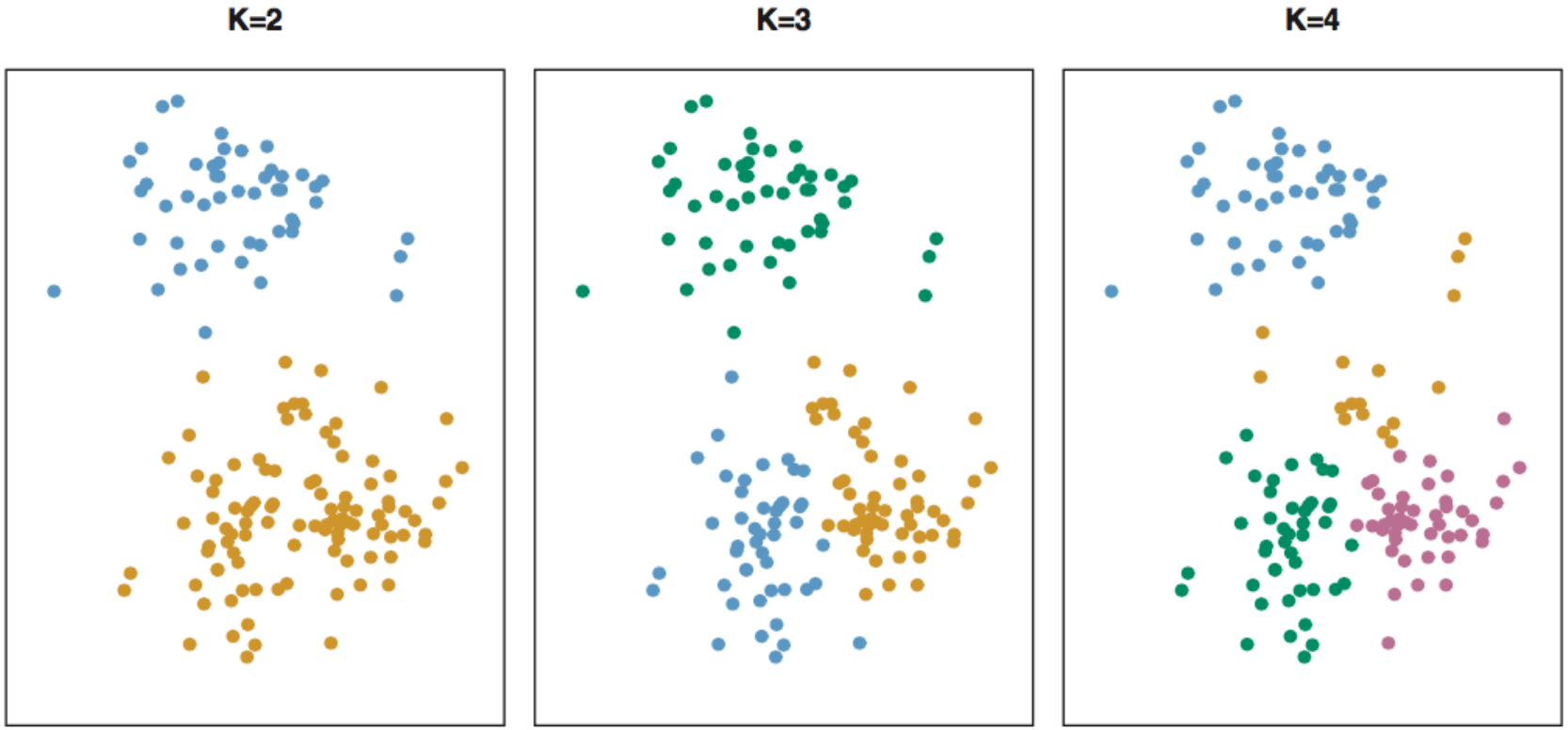
Clustering

- Sometimes the data form clusters, where samples within a cluster are similar to each other, and samples in different clusters are dissimilar:



- Such a distribution is multimodal, since it has multiple modes, or regions of high probability mass.
- Grouping data points into clusters, with no observed labels, is called clustering. It is an unsupervised learning technique.
  - E.g. clustering machine learning papers based on topic (deep learning, Bayesian models, reinforcement learning, etc.)
  - But topics are never observed (unsupervised).

Example of results from K-means



- A simulated data set with 150 observations in two-dimensional space. Panels show the results of applying K-means clustering with different values of K.
- The color of each observation indicates the cluster to which it was assigned using the K-means clustering algorithm.
- There is no ordering of the clusters, so the cluster coloring is arbitrary.

K-Means Clustering

K-means clustering is a simple approach for partitioning a data set into K distinct, non-overlapping clusters.

Let $C_1, \ldots, C_K$ denote sets containing the indices of the observations in each cluster. E.g. if the ith observation is in the kth cluster, then $i \in C_k$. These sets $C_1, \ldots, C_K$ satisfy two properties:

- Each observation belongs to at least one of the K clusters.

$$C_1 \cup C_2 \cup \ldots \cup C_K = \{1, \ldots, n\}.$$

- The clusters are non-overlapping: no observation belongs to more than one cluster.

$$C_k \cap C_{k'} = \varnothing, \qquad \text{for all } k \neq k'.$$

- Hence every single observation belongs to one and only one cluster.

The goal is to find good sets $C_1, \ldots, C_K$ for certain purpose.

K-Means Clustering

- The idea behind K-means clustering is that a good clustering ensures the within-cluster variation as small as possible.
- The within-cluster variation for cluster C_k is a measure $W(C_k)$ on the difference among observations within a cluster.
- We aim to find sets $C_1, \ldots, C_K$ by solving

$$\min_{C_1,\ldots,C_K} \left\{ \sum_{k=1}^{K} W(C_k) \right\}.$$

In words, we want to partition the observations into K clusters such that the total within-cluster variation, summed over all K clusters, is as small as possible.

Definition of the within-cluster variation

- It is common to use the Euclidean distance

$$W(C_k) = \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2$$
$$= \frac{1}{|C_k|} \sum_{i,i' \in C_k} \|\mathbf{x}_i - \mathbf{x}_{i'}\|_2^2$$

  where $|C_k|$ denotes the number of observations in the kth cluster.

- Let

$$\bar{\mathbf{x}}_k = \frac{1}{|C_k|} \sum_{i \in C_k} \mathbf{x}_i.$$

  Verify that

$$W(C_k) = \frac{1}{|C_k|} \sum_{i \in C_k} \|\mathbf{x}_i - \bar{\mathbf{x}}_k\|_2^2.$$

Target of the K-means algorithm

- Thus, the optimization problem that defines K-means clustering is to solve

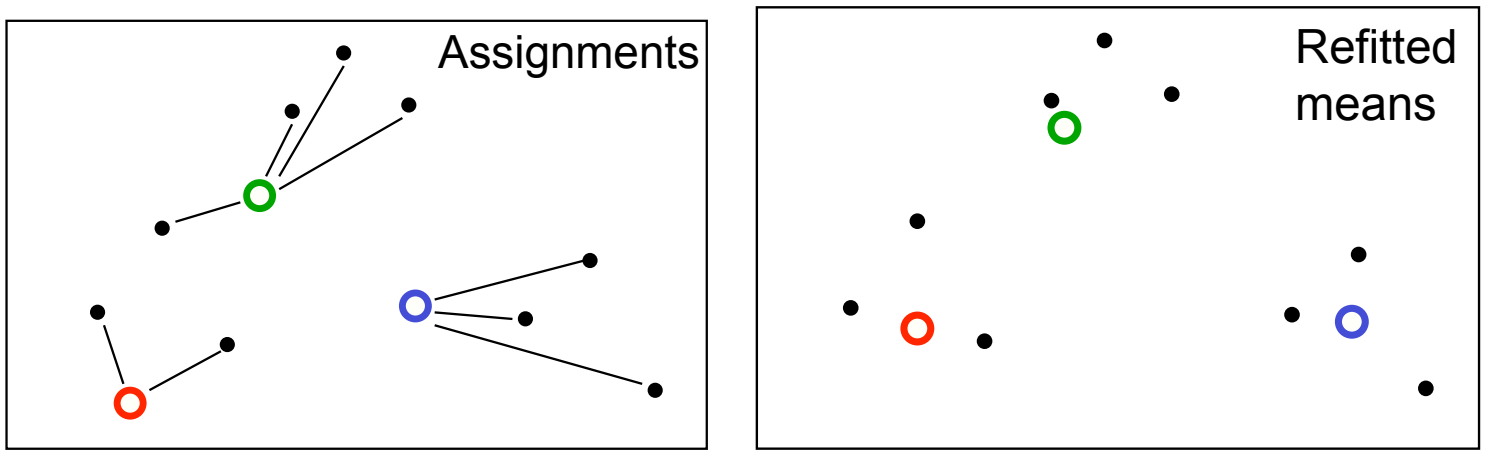
$$\min_{C_1,\ldots,C_K} \sum_{k=1}^{K} W(C_k) \;=\; \min_{C_1,\ldots,C_K} \sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i \in C_k} \|\mathbf{x}_i - \bar{\mathbf{x}}_k\|_2^2.$$

- This is, however, a very difficult problem to solve exactly. There are almost K^n ways to partition n observations into K clusters.

A pratical alternating algorithm

High level overview of algorithm:

- Initialization: randomly initialize cluster centers
- The algorithm iteratively alternates between two steps:
  - Assignment step: Assign each data point to the closest cluster
  - Re-center step: Move each cluster center to the mean of the data assigned to it



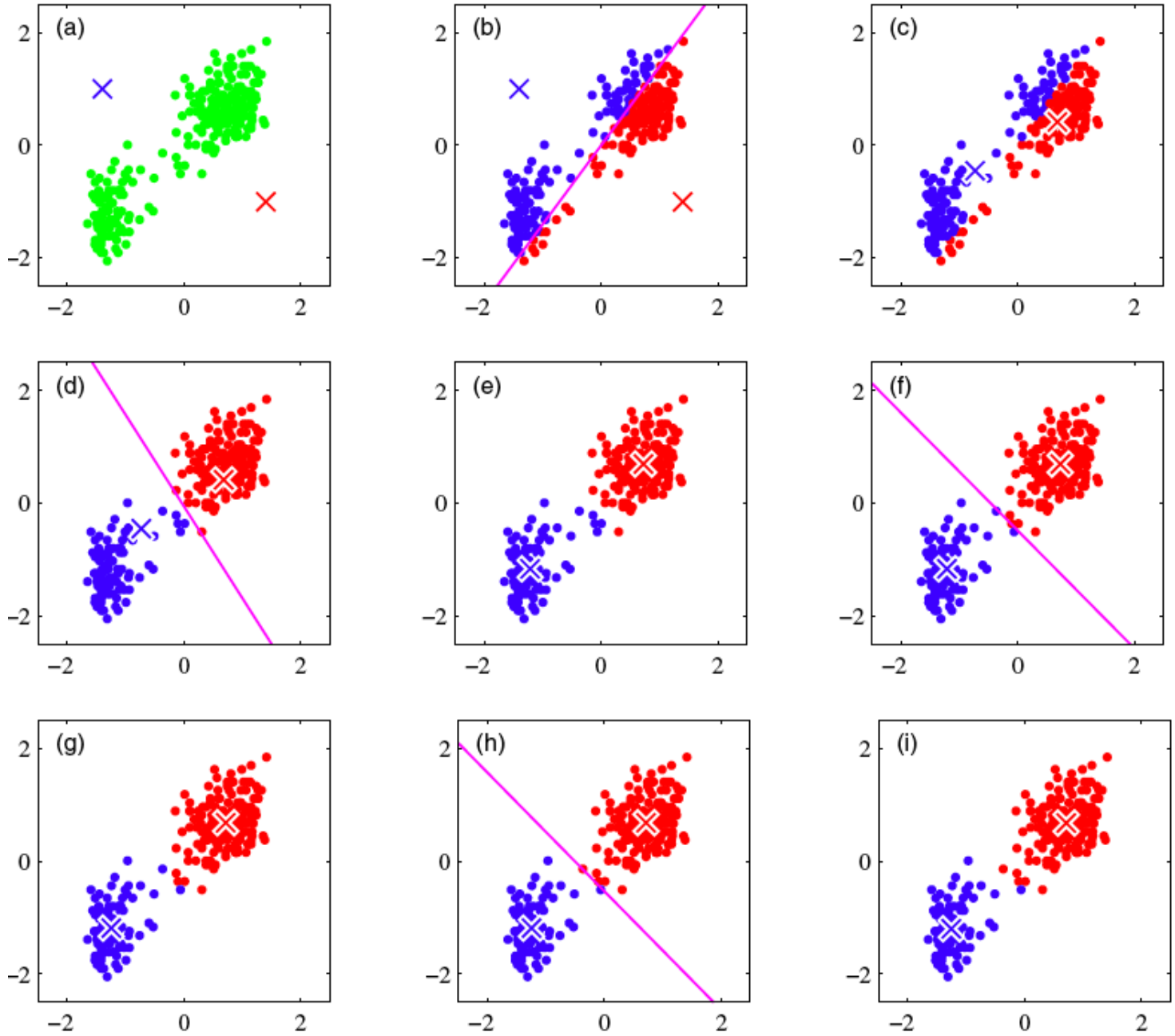


Figure from Bishop

Simple demo: http://syskall.com/kmeans.js/

K-means algorithm

Algorithm 10.1 *K-Means Clustering*

1. Randomly assign a number, from 1 to K, to each of the observations. These serve as initial cluster assignments for the observations.
2. Iterate until the cluster assignments stop changing:
   (a) For each of the K clusters, compute the cluster *centroid*. The kth cluster centroid is the vector of the p feature means for the observations in the kth cluster.
   (b) Assign each observation to the cluster whose centroid is closest (where *closest* is defined using Euclidean distance).

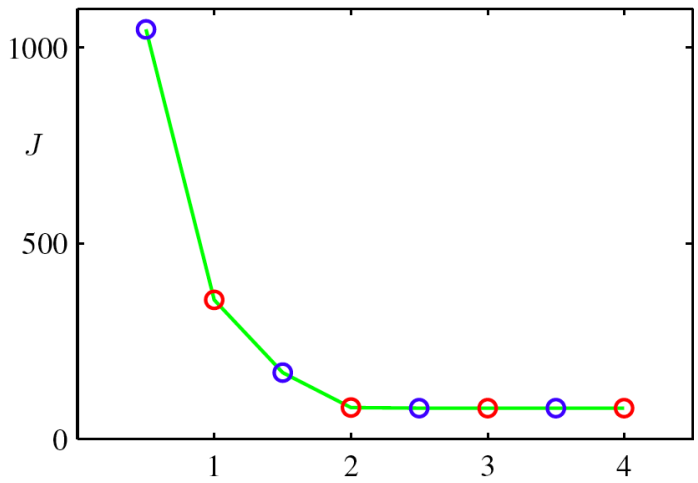
Animation of the algorithm: `http://shabal.in/visuals/kmeans/5.html`.

Why K-means Converges

- K-means algorithm reduces the cost at each iteration.
  - Assignment step: fixing the centers, re-assignment will decrease the total within-cluster variation.
  - Re-center step: fixing the assignments, re-centering the data within clusters will reduce the total within-cluster variation.
- Stopping criterion for convergence: when the assignments do not change in the assignment step, we have converged (to at least a local minimum).

Convergence of the K-means algorithm

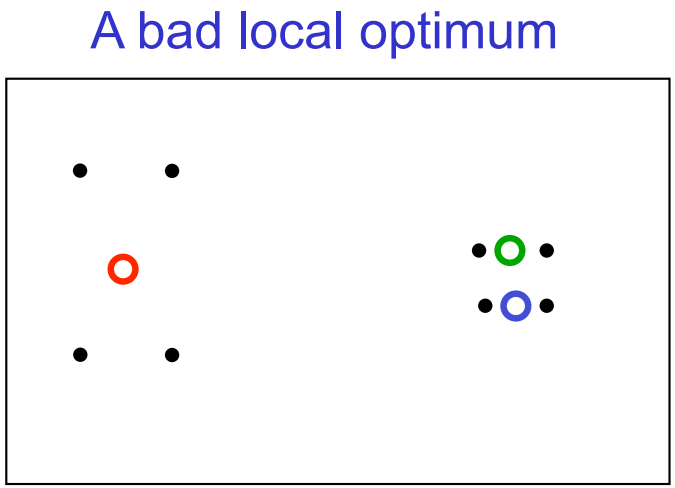
- Convergence will always happen after a finite number of iterations, since the number of possible cluster assignments is finite



- K-means cost function after each assignment step (blue) and refitting step (red). The algorithm has converged after the third refitting step.

Local Minima

- The cost function is non-convex (so convergence is not equivalent to the global minimum)
- There is nothing to prevent K-means getting stuck at local minima.
- Possible remedy: could try many random starting points

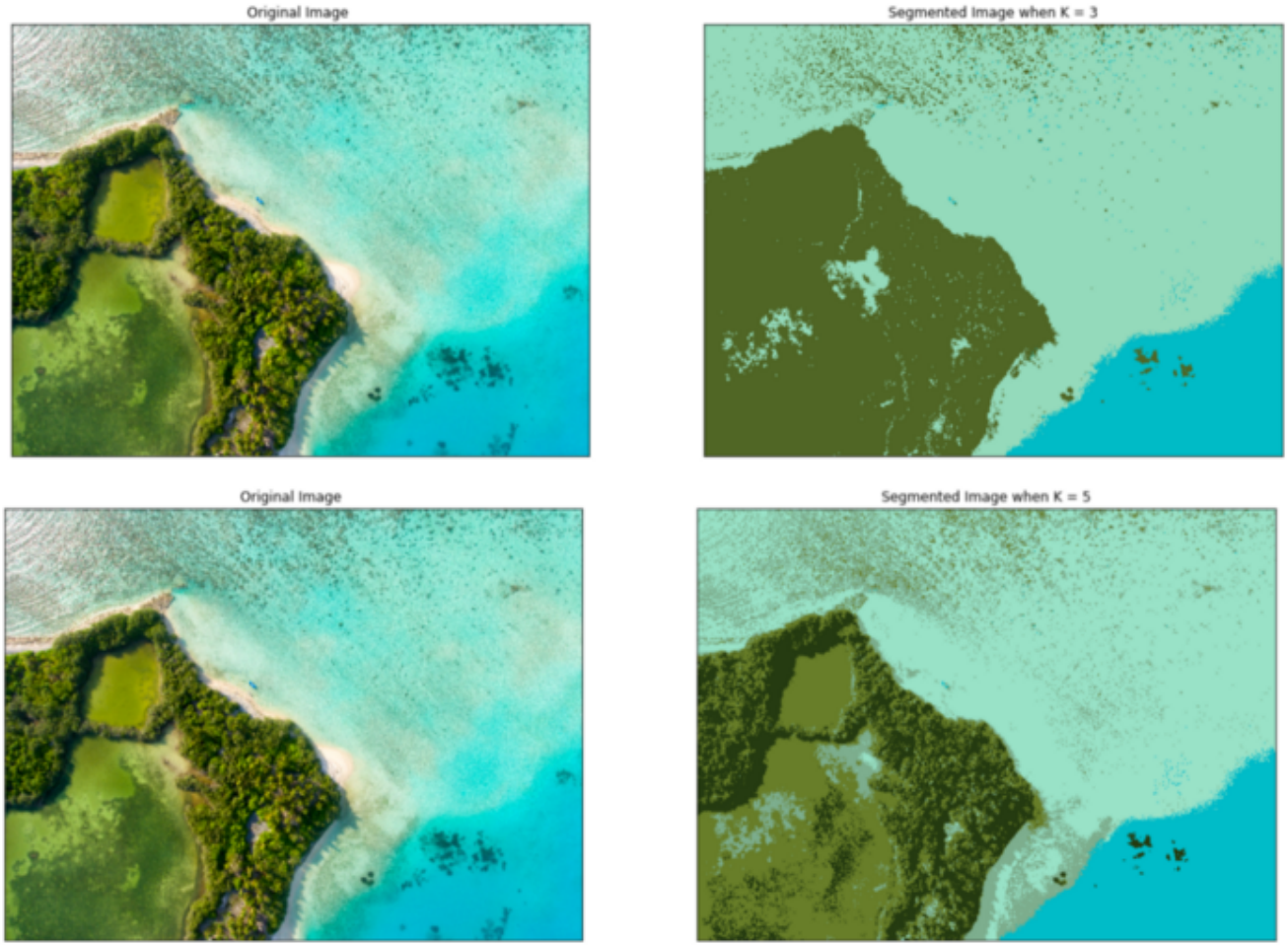


K-means for Vector Quantization

Figure from Bishop

- Given image, construct "dataset" of pixels represented by their RGB pixel intensities
- Run K-means, replace each pixel by its cluster center

K-means for Image Segmentation



- Given image, construct "dataset" of pixels, represented by their HSV pixel intensities
- Run k-means to get superpixels

Extensions

- Non-exhaustive clustering. Allow some of the data points not to belong to any cluster.
- Overlapping clustering. Allow some of the data points to belong to more than one clusters.
  - Soft K-means
- Clustering features rather than data points. Previously, we consider the clustering for data points.

PCA Overview

- We now turn to the second unsupervised learning algorithm for this course: principal component analysis (PCA)
- PCA is used for dimensionality reduction: map data to a lower dimensional space
- PCA finds linear low-dimensional representations of the data by preserving as much variation (in the original data) as possible.
- PCA is useful for understanding lots of other algorithms.
  - Autoencoders
  - Matrix factorizations

Low dimensional representation

- In practice, even though data is very high dimensional, its important features can be accurately captured in a low dimensional subspace.

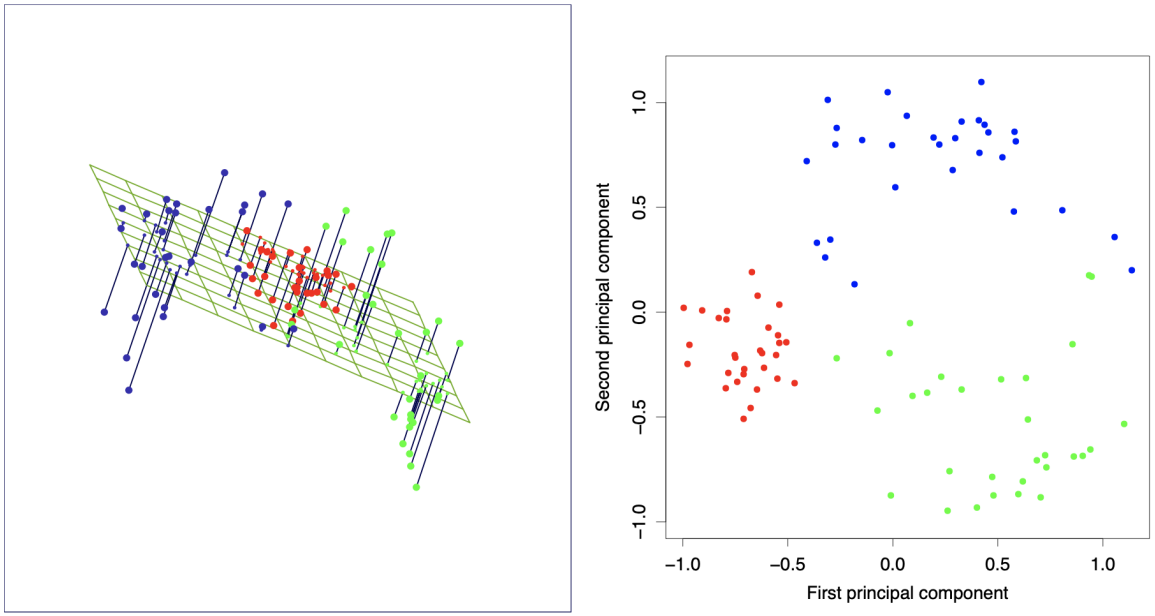


Image credit: Elements of Statistical Learning

- Find a low dimensional representation of your data.
  - Computational benefits
  - Interpretability, visualization
  - Generalization

Principal Components Analysis

- PCA construct linear combinations of p features $X_1, X_2, \ldots, X_p$.
- The first principal component(PC) is the linear combination of the features

$$Z_1 = u_{11}X_1 + u_{21}X_2 + \cdots + u_{p1}X_p$$

where the coefficients

$$\mathbf{u}_1 = \begin{bmatrix} u_{11} \\ u_{21} \\ \vdots \\ u_{p1} \end{bmatrix}$$

are chosen such that

  - Z_1 has the largest variance;
  - $\mathbf{u}_1$ is normalized such that $\sum_{j=1}^{p} u_{j1}^2 = 1$, i.e. $\|\mathbf{u}_1\|_2 = 1$.

- We refer to the coefficients $\mathbf{u}_1$ as the **loading** of the first PC.

More Principal Components

- The second PC is again the linear combination of $X_1, \ldots, X_p$

$$Z_2 = u_{12}X_1 + u_{22}X_2 + \cdots + u_{p2}X_p$$

where the loading

$$\mathbf{u}_2 = \begin{bmatrix} u_{12} \\ u_{22} \\ \vdots \\ u_{p2} \end{bmatrix}$$

are chosen such that

  - Z_2 has the largest variance,
  - $\|\mathbf{u}_2\|_2 = 1$,
  - $\mathbf{u}_2^\top \mathbf{u}_1 = 0$. This implies Z_2 is uncorrelated with Z_1.

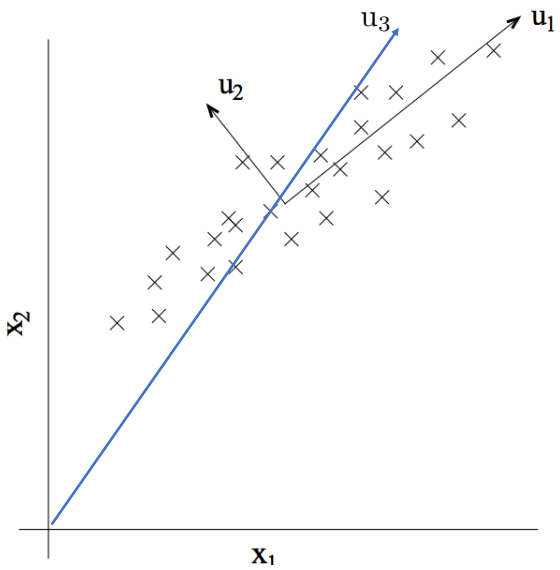
- This successively defines the first K PCs, $Z_1, \ldots, Z_K$, with corresponding loadings $\mathbf{u}_1, \ldots, \mathbf{u}_K$.

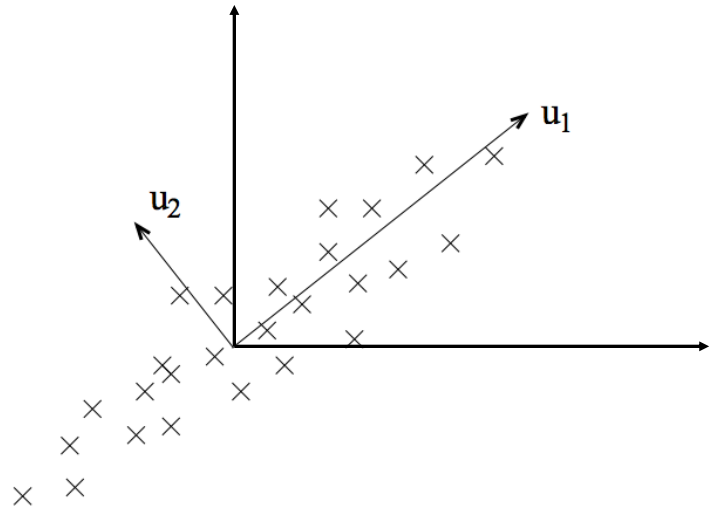
Computation

Suppose we have a data matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$ and we want to construct K PCs with $K \in \{1, 2, \ldots, p\}$.

1. Center $\mathbf{X}$ such that the columns have zero mean, that is,
$$\tilde{\mathbf{X}} = \mathbf{X} - 1_n \bar{\mathbf{X}}^\top.$$
2. Compute the first K loadings
$$\mathbf{U}_K = (\mathbf{u}_1, \ldots, \mathbf{u}_K)$$
from the centered data, $\tilde{\mathbf{X}}$.
3. Obtain the first K PCs
$$\tilde{\mathbf{Z}} = \tilde{\mathbf{X}}\mathbf{U}_K \in \mathbb{R}^{n \times K}.$$
4. Add the centers back to the PCs
$$\mathbf{Z} = \tilde{\mathbf{Z}} + 1_n \bar{\mathbf{X}}^\top \mathbf{U}_K = (\tilde{\mathbf{X}} + 1_n \bar{\mathbf{X}}^\top)\mathbf{U}_K = \mathbf{X}\mathbf{U}_K.$$

Centering the data





- Directions we compute will pass through origin, and should represent the direction of the highest variation.
- We need to center our data since we don't want location of data to influence calculation of the loadings. That is, we are **not** interested in $\mathbf{u}_3$.

Computation of the first loading

Let $\mathbf{X} \in \mathbb{R}^{n \times p}$ be the centered data.

- The first loading vector $\mathbf{u}_1$ is obtained via the optimization problem

$$\mathbf{u}_1 = \arg\max_{\mathbf{u}} \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=1}^{p} u_j x_{ij} \right)^2, \quad \text{subject to} \quad \sum_{j=1}^{p} u_j^2 = 1.$$

- In the matrix notation,

$$\mathbf{u}_1 = \arg\max_{\mathbf{u}} \frac{1}{n} \mathbf{u}^\top \mathbf{X}^\top \mathbf{X} \mathbf{u}, \quad \text{subject to} \quad \mathbf{u}^\top \mathbf{u} = 1.$$

- The problem can be solved via the eigen decomposition of $\hat{\mathbf{\Sigma}} := \mathbf{X}^\top \mathbf{X}/n$, a standard technique in linear algebra. More specifically, $\mathbf{u}_1$ is nothing but the first eigenvector of $\hat{\mathbf{\Sigma}}$.

Computation of the second loading

Let $\mathbf{X} \in \mathbb{R}^{n \times p}$ be the centered data and $\mathbf{u}_1$ be the first loading.

- The second loading vector $\mathbf{u}_2$ is obtained via the optimization problem

$$\mathbf{u}_2 = \arg\max_{\mathbf{u}} \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=1}^{p} u_j x_{ij} \right)^2, \quad \text{s.t.} \quad \sum_{j=1}^{p} u_j^2 = 1, \sum_{j=1}^{p} u_j u_{j1} = 0.$$

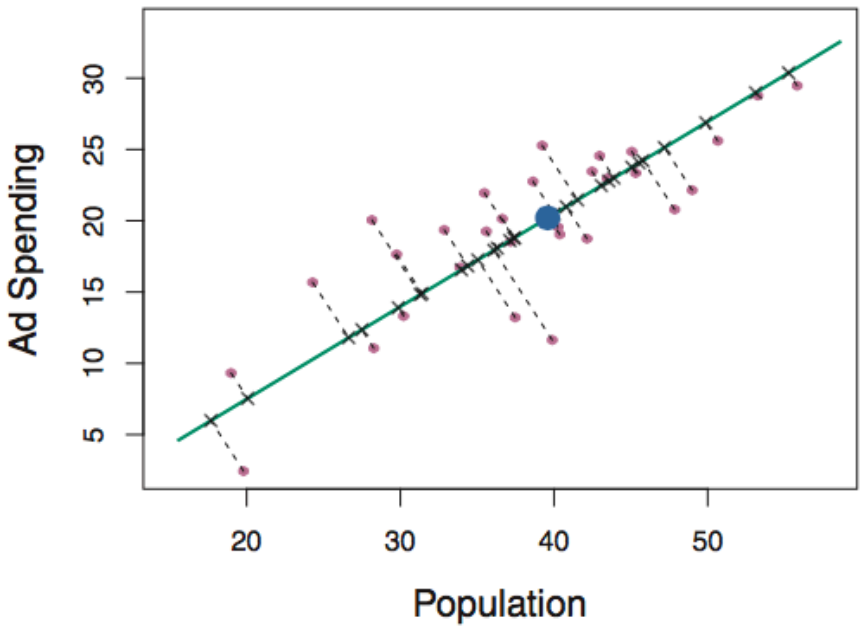
- In the matrix notation,

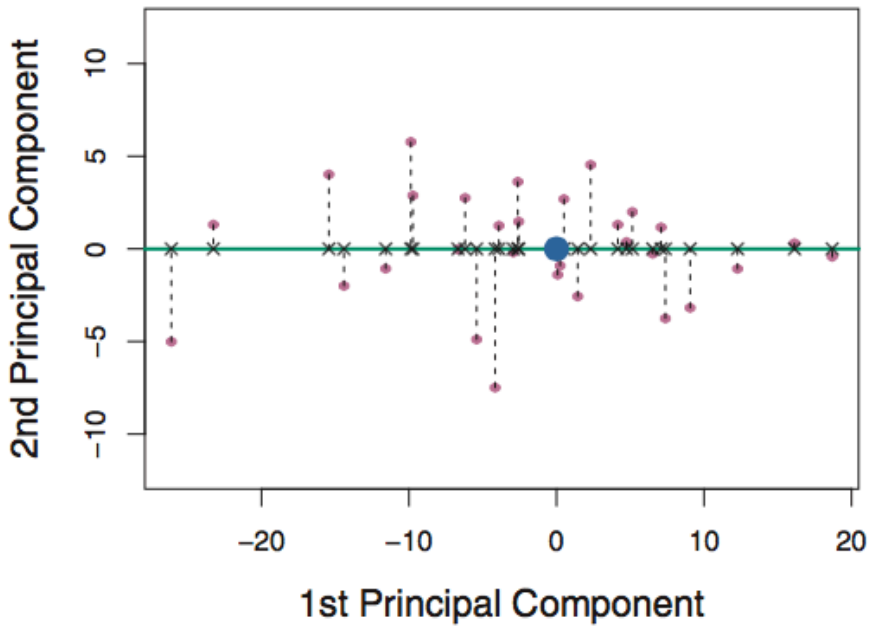
$$\mathbf{u}_2 = \arg\max_{\mathbf{u}} \frac{1}{n} \mathbf{u}^\top \mathbf{X}^\top \mathbf{X} \mathbf{u}, \quad \text{s.t.} \quad \mathbf{u}^\top \mathbf{u} = 1, \mathbf{u}^\top \mathbf{u}_1 = 0.$$

- $\mathbf{u}_2$ is simply the second eigenvector of $\hat{\mathbf{\Sigma}}$.
- Similarly, $\mathbf{u}_1, \ldots, \mathbf{u}_K$ are the first K eigenvectors of $\hat{\mathbf{\Sigma}}$.

Geometry of PCA

- The loading vector $\mathbf{u}_1$ with elements $u_{11}, u_{21}, \ldots, u_{p1}$ defines a direction in feature space along which the data vary the most.
- If we project the n data points $\mathbf{x}_1, \ldots, \mathbf{x}_n$ onto this direction, the projected values are the first PC with coordinates $z_{11}, \ldots, z_{n1}$.

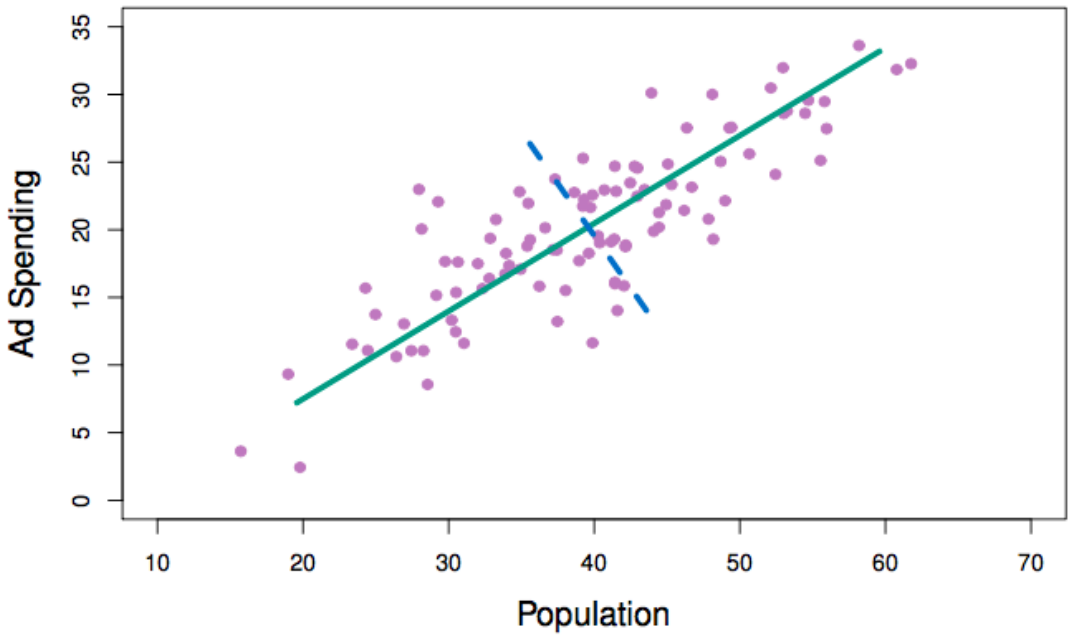




$$z_{i1} = 0.839 \times (\text{population}_i - \overline{\text{population}}) + 0.544 \times (\text{ad}_i - \overline{\text{ad}}).$$

Advertising Data

Consider two features: population size and ad spending for a particular company (ad).



The green solid line indicates $\mathbf{u}_1$, the first loading, and the blue dashed line indicates $\mathbf{u}_2$, the second loading.

Another Interpretation of PCA

- The first K loadings

$$\mathbf{U} \in \mathbb{R}^{p \times K}$$

are obtained via

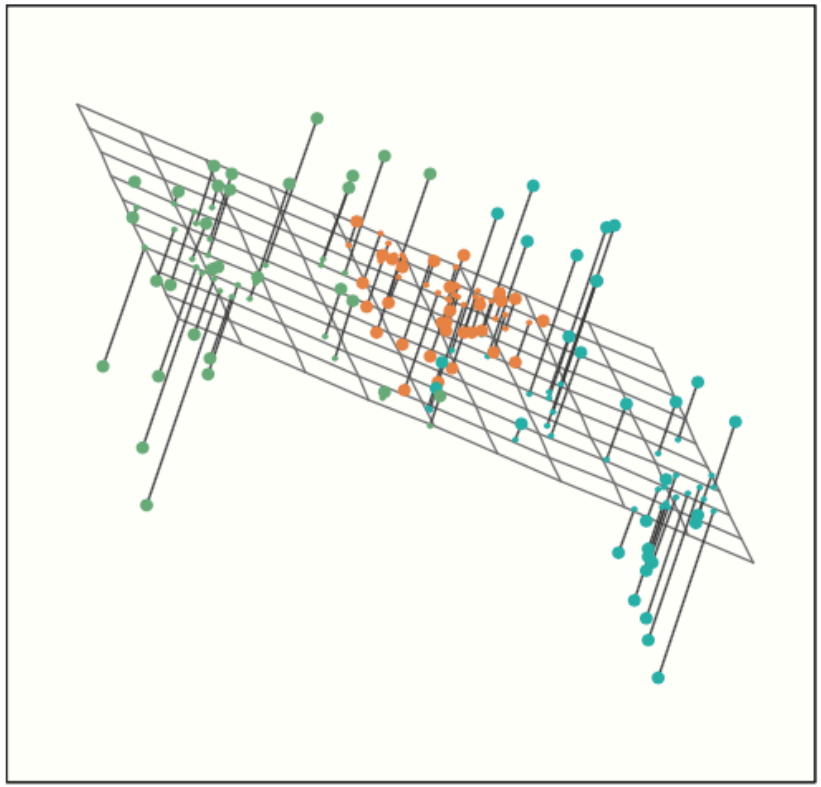
$$\arg\max_{\mathbf{U}} \frac{1}{n} \mathrm{tr}\left(\mathbf{U}^\top \mathbf{X}^\top \mathbf{X} \mathbf{U}\right), \quad \text{s.t.} \quad \mathbf{U}^\top \mathbf{U} = \mathbf{I}_K.$$

- It can also be obtained by

$$\arg\min_{\mathbf{U}} \frac{1}{n} \sum_{i=1}^{n} \|\mathbf{x}_i - \mathbf{U}\mathbf{U}^\top \mathbf{x}_i\|^2, \quad \text{s.t.} \quad \mathbf{U}^\top \mathbf{U} = \mathbf{I}_K.$$

- PCA finds the subspace such that the projected data points in this subspace are closest to the original data points.

Another Interpretation of PCA



The first two loading vectors span the plane that best fits the data.

Some practical considerations

- In general, in addition to centering, standardizing each variable to have unit standard deviation is recommended.
- Each principal component loading vector is unique, up to a sign flip.
- How many PCs to retain?
  - No simple answer to this question, as cross-validation is not available for this purpose.
  - There are several ad-hoc procedures.

Applying PCA to faces

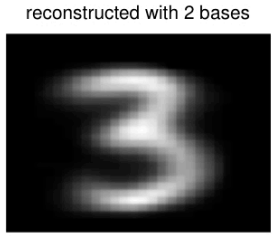
- Consider running PCA on 2429 19x19 grayscale images (CBCL data)
- Can get good reconstructions with only 3 components

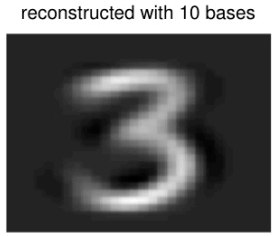
- PCA for pre-processing: can apply classifier to latent representation
  - Original data is 361 dimensional
  - For face recognition PCA with 3 components obtains 79% accuracy on face/non-face discrimination on test data vs. 76.8% for a Gaussian mixture model (GMM) with 84 states. (We'll cover GMMs later in the course.)
- Can also be good for visualization

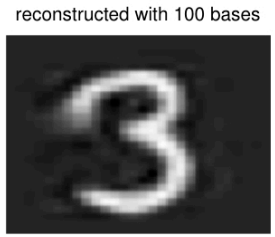
Applying PCA to faces: Learned basis

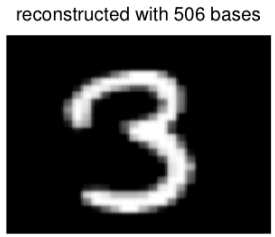
Principal components of face images ("eigenfaces")

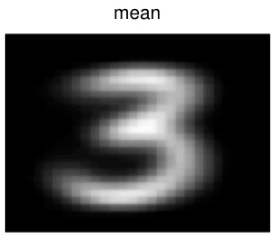
Applying PCA to digits

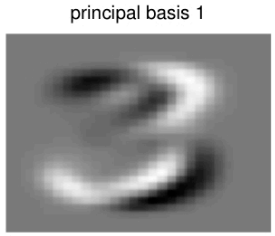


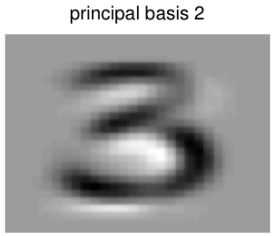


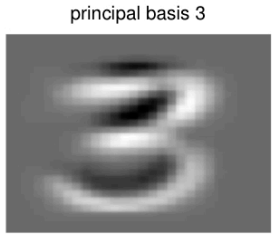












Summary

- 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 (linear) in the original features.