CS 760: Machine Learning
Unsupervised Learning II

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Announcements

- **Logistics**:
  - HW6 Due Thursday. HW7 out today
- Class roadmap:

Tuesday, Nov. 16	**Unsupervised Learning I**
Thursday, Nov. 18	Unsupervised Learning II
Tuesday, Nov. 23	Learning Theory
Tuesday, Nov. 30	RL I
Thursday, Dec. 2	RL II

Outline

- **Clustering Review**
  - k-means, hierarchical, spectral clustering
- **Gaussian Mixture Models**
  - Mixtures, Expectation-Maximization algorithm
- **Principal Components Analysis**
  - Definition, Algorithm, Interpretations, Analysis

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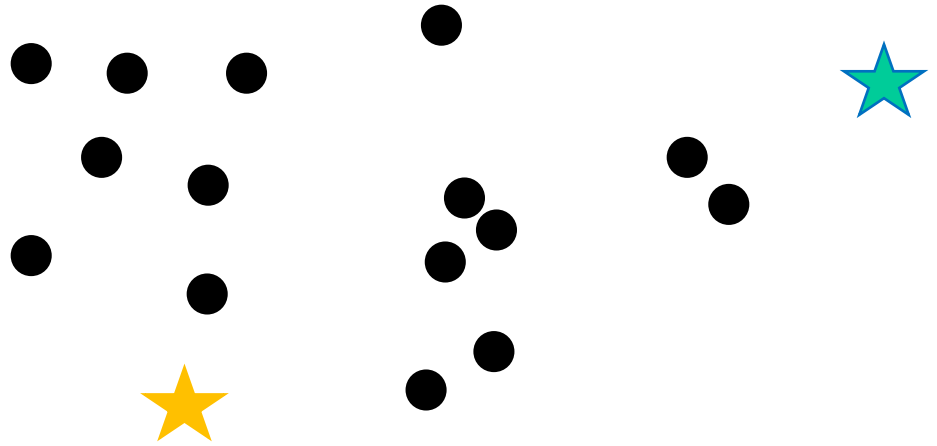
K-Means Clustering

k-means is a type of partitional **centroid-based clustering**

Algorithm:

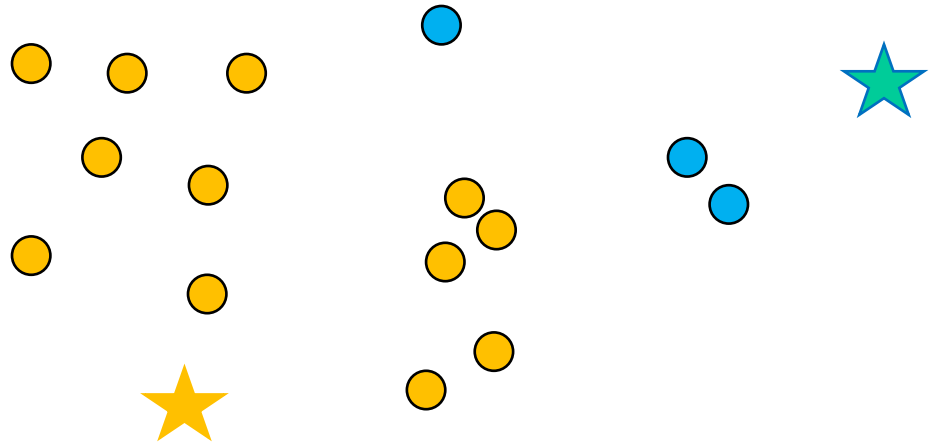
1. Randomly pick k cluster centers



K-Means Clustering: Algorithm

K-Means clustering

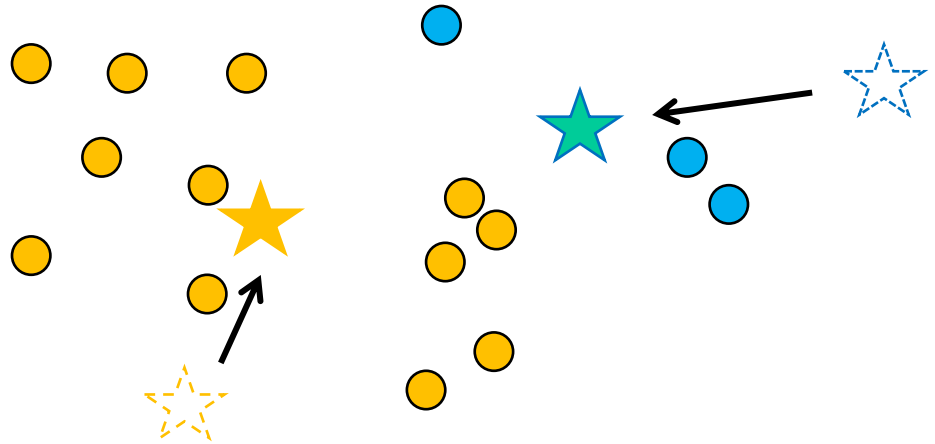
2. Find closest center for each point



K-Means Clustering: Algorithm

K-Means clustering

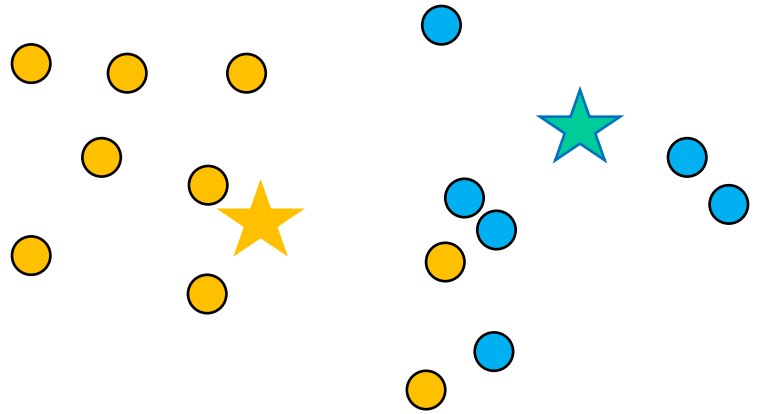
3. Update cluster centers by computing centroids



K-Means Clustering: Algorithm

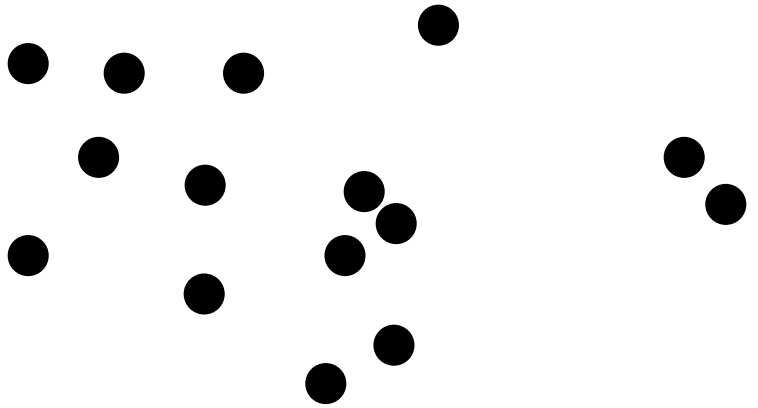
K-Means clustering

Repeat Steps 2 & 3 until convergence



HC: Agglomerative Clustering Example

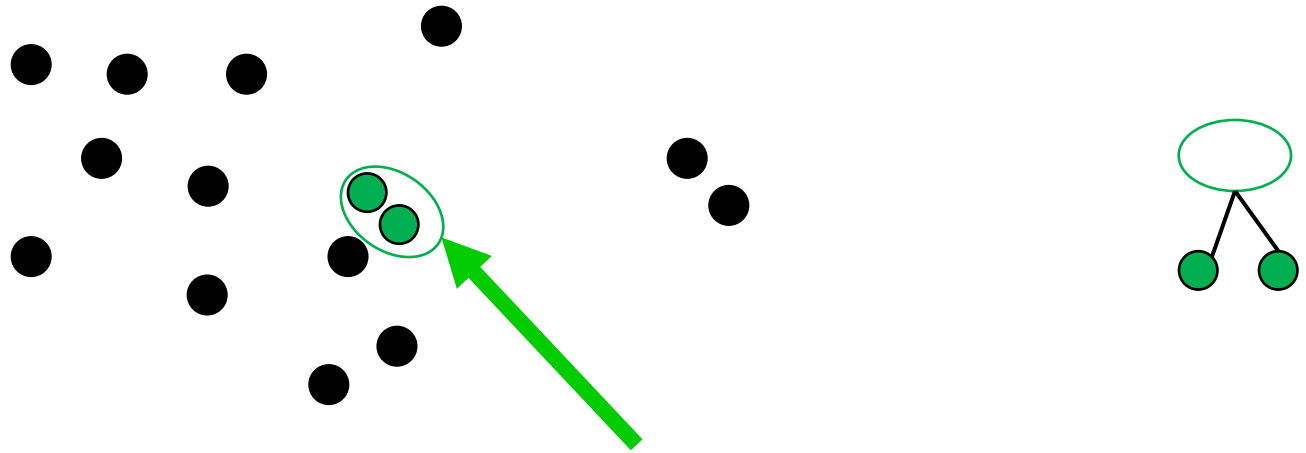
Agglomerative: Start: every point is its own cluster



HC: Agglomerative Clustering Example

Basic idea: build a “hierarchy”

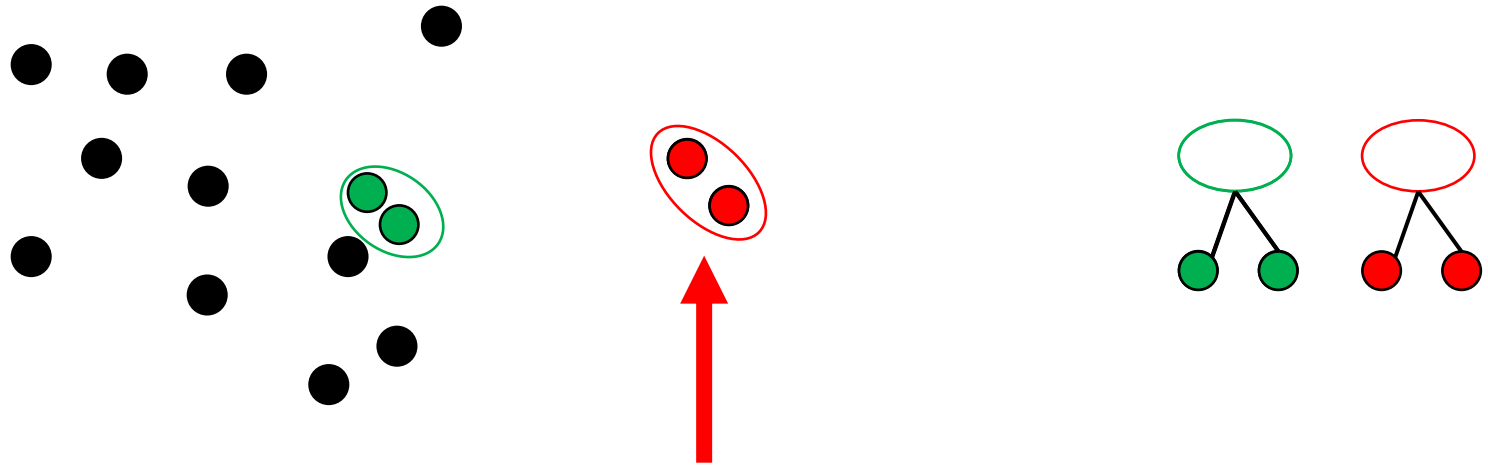
- Get pair of clusters that are closest and merge



HC: Agglomerative Clustering Example

Basic idea: build a “hierarchy”

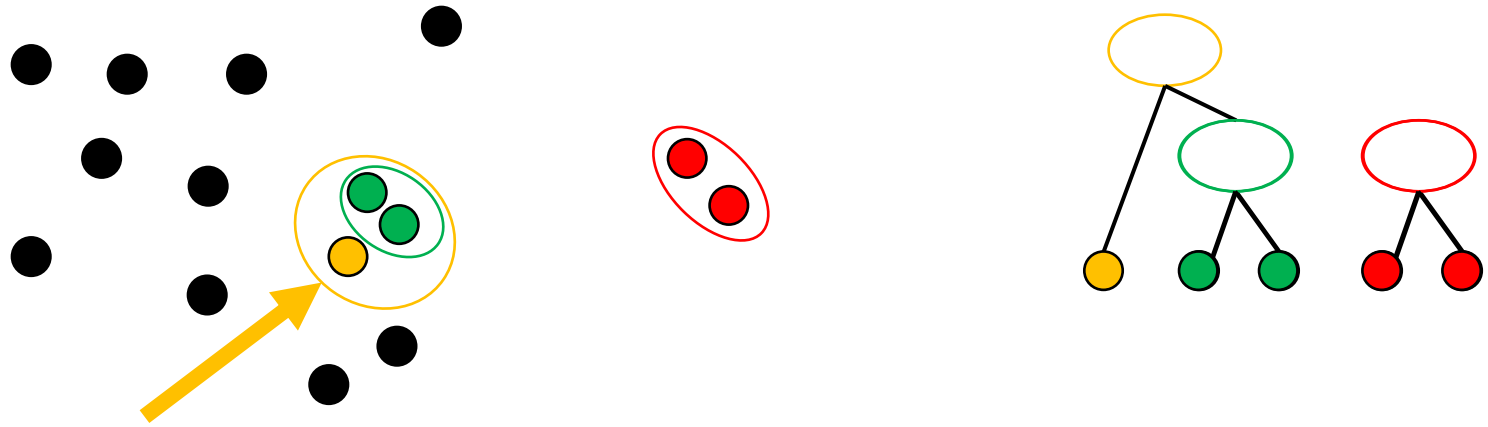
- **Repeat:** Get pair of clusters that are closest and merge



HC: Agglomerative Clustering Example

Basic idea: build a “hierarchy”

- **Repeat:** Get pair of clusters that are closest and merge



HC: Merging Criteria

Merge: use closest clusters. Define closest?

- Single-linkage $$d(A,B) = \min_{x_1 \in A, x_2 \in B} d(x_1, x_2)$$
- Complete-linkage $$d(A,B) = \max_{x_1 \in A, x_2 \in B} d(x_1, x_2)$$
- Average-linkage $$d(A,B) = \frac{1}{|A||B|} \sum_{x_1 \in A, x_2 \in B} d(x_1, x_2)$$

Break & Quiz

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- **Gaussian Mixture Models**
  - Mixtures, Expectation-Maximization algorithm
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Mixture Models

- Let's get back to modeling densities in unsupervised learning.
- Have dataset:

$$\{(x^{(1)}, x^{(2)}, \ldots, x^{(n)}\}$$

- One type of model: **mixtures**
  - A function of the **latent variable** z
  - We did something similar with flows
  - Model:

$$p(x^{(i)}|z^{(i)})p(z^{(i)})$$

Mixture Models: Gaussians

- Lots of different kinds of mixtures, but let's focus on Gaussians.
- What does this mean?
- Latent variable z has some multinomial distribution, $\sum_{i=1}^{k} \phi_i = 1$

$$z^{(i)} \sim \text{Multinomial}(\phi)$$

- Then, let's make x be conditional Gaussian

$$x^{(i)} | (z^{(i)} = j) \sim \mathcal{N}(\mu_j, \Sigma_j)$$

Mean Covariance Matrix

Gaussian Mixture Models: Likelihood

- How should we learn the parameters? ϕ, μ_j, Σ_j
- Could try our usual way: maximum likelihood
  - Log likelihood:

$$\ell(\phi, \mu, \Sigma) = \sum_{i=1}^{n} \log \sum_{z^{(i)}=1}^{k} p(x^{(i)}|z^{(i)}; \mu, \Sigma) p(z^{(i)}; \phi)$$

  - Turns out to be **hard** to solve… inner sum leads to problems!

GMMs: Supervised Setting

- What if we knew the z's?
  - "Supervised" setting… very similar to Gaussian Naïve Bayes
- First, empirically estimate the z parameters:

$$\phi_j = \frac{1}{n}\sum_{i=1}^{n} 1\{z^{(i)} = j\}$$

- Next the Gaussian components:

$$\mu_j = \frac{\sum_{i=1}^{n} 1\{z^{(i)} = j\}x^{(i)}}{\sum_{i=1}^{n} 1\{z^{(i)} = j\}}$$

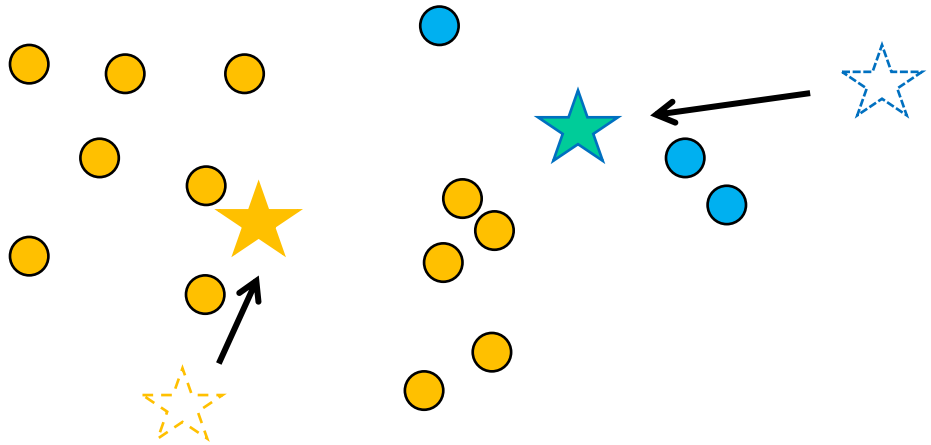
Average of x's where z = j

$$\Sigma_j = \frac{\sum_{i=1}^{n} 1\{z_j^{(i)} = j\}(x^{(i)} - \mu_j)(x^{(i)} - \mu_j)^T}{\sum_{i=1}^{n} 1\{z_j^{(i)} = j\}}$$

GMMs: Back to Latent Setting

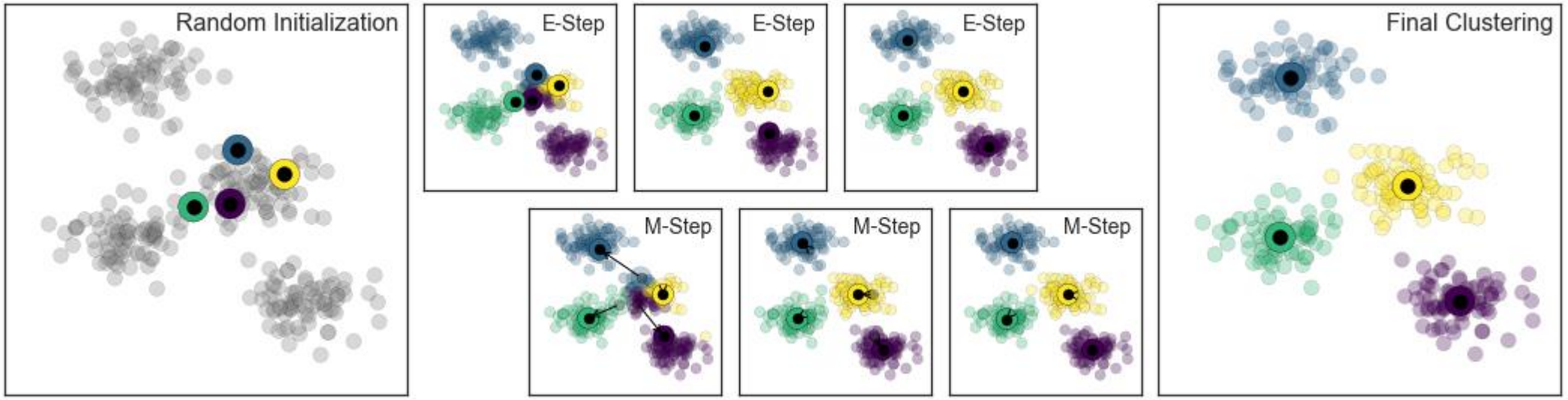
- But, we don't get to see the z's
  - Similar to the weak supervision setting from last time.

- What could we do instead?
- Recall our **k-means** approach: we don't know the centers, but we pretend we do, perform a clustering, re-center, iterate



GMMs: Expectation Maximization

- EM :an algorithm for dealing with latent variable problems
- Iterative, alternating between two steps:
  - **E**-step (expectation): guess the latent variables
  - **M**-step (maximization): update the parameters of the model
  - Note similarity to k-means clustering.



Jake VanderPlas

GMM EM: E-Step

- Let's write down the formulas.
- **E-step**: fix parameters, compute posterior:

$$w_j^{(i)} = p(z^{(i)} = j | x^{(i)}; \phi, \mu, \Sigma)$$

- These w's are "soft" assignments of the z terms… probabilities over the values z could take. Concretely:

$$w_j^{(i)} = p(z^{(i)} = j | x^{(i)}; \phi, \mu, \Sigma) = \frac{p(x^{(i)} | z^{(i)} = j; \mu, \Sigma) p(z^{(i)} = j; \phi)}{\sum_{\ell=1}^{k} p(x^{(i)} | z^{(i)} = \ell; \mu, \Sigma) p(z^{(i)} = \ell; \phi)}$$

GMM EM: M-Step

- Let's write down the formulas.
- **M-step**: fix w, update parameters:

$$\phi_j = \frac{1}{n}\sum_{i=1}^{n} w_j^{(i)}$$

Soft version of our counting estimator for the supervised case.

$$\mu_j = \frac{\sum_{i=1}^{n} w_j^{(i)} x^{(i)}}{\sum_{i=1}^{n} w_j^{(i)}}$$

Soft version of our empirical mean and covariances.

$$\Sigma_j = \frac{\sum_{i=1}^{n} w_j^{(i)} (x^{(i)} - \mu_j)(x^{(i)} - \mu_j)^T}{\sum_{i=1}^{n} w_j^{(i)}}$$

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High-Dimensional Data

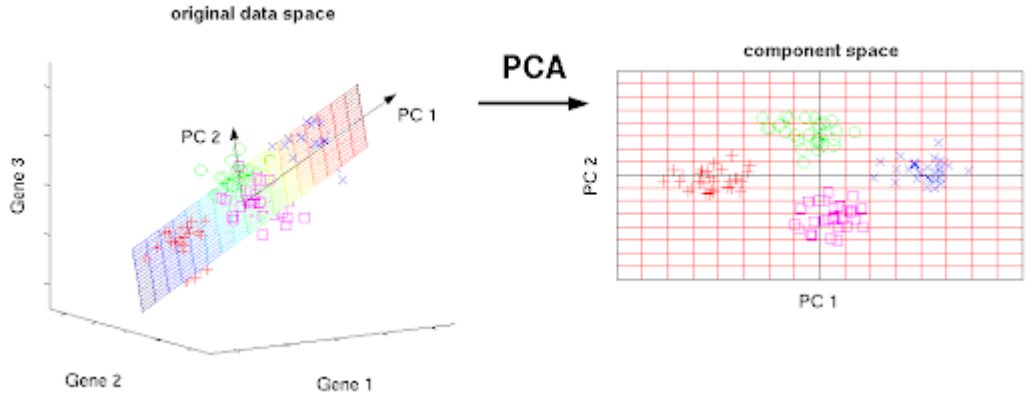
- High-dimensions = lots of features
- We've seen this repeatedly, but some examples:
- Document classification
  - Features per document = thousands of words/unigrams millions of bigrams, contextual information
- **Example**: Surveys - Netflix

  480189 users x 17770 movies

	movie 1	movie 2	movie 3	movie 4	movie 5	movie 6
Tom	5	?	?	1	3	?
George	?	?	3	1	2	5
Susan	4	3	1	?	5	1
Beth	4	3	?	2	4	2

Dealing with Dimensionality

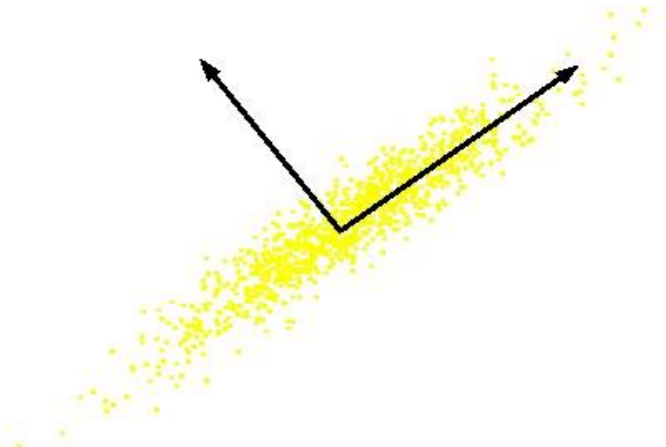
- **PCA, Kernel PCA, ICA**: Powerful unsupervised learning techniques for extracting hidden (potentially lower dimensional) structure from high dimensional datasets.
- Some uses:
  - Visualization
  - More efficient use of resources (e.g., time, memory, communication)
  - Noise removal (improving data quality)
  - Further processing by machine learning algorithms



Principal Components Analysis

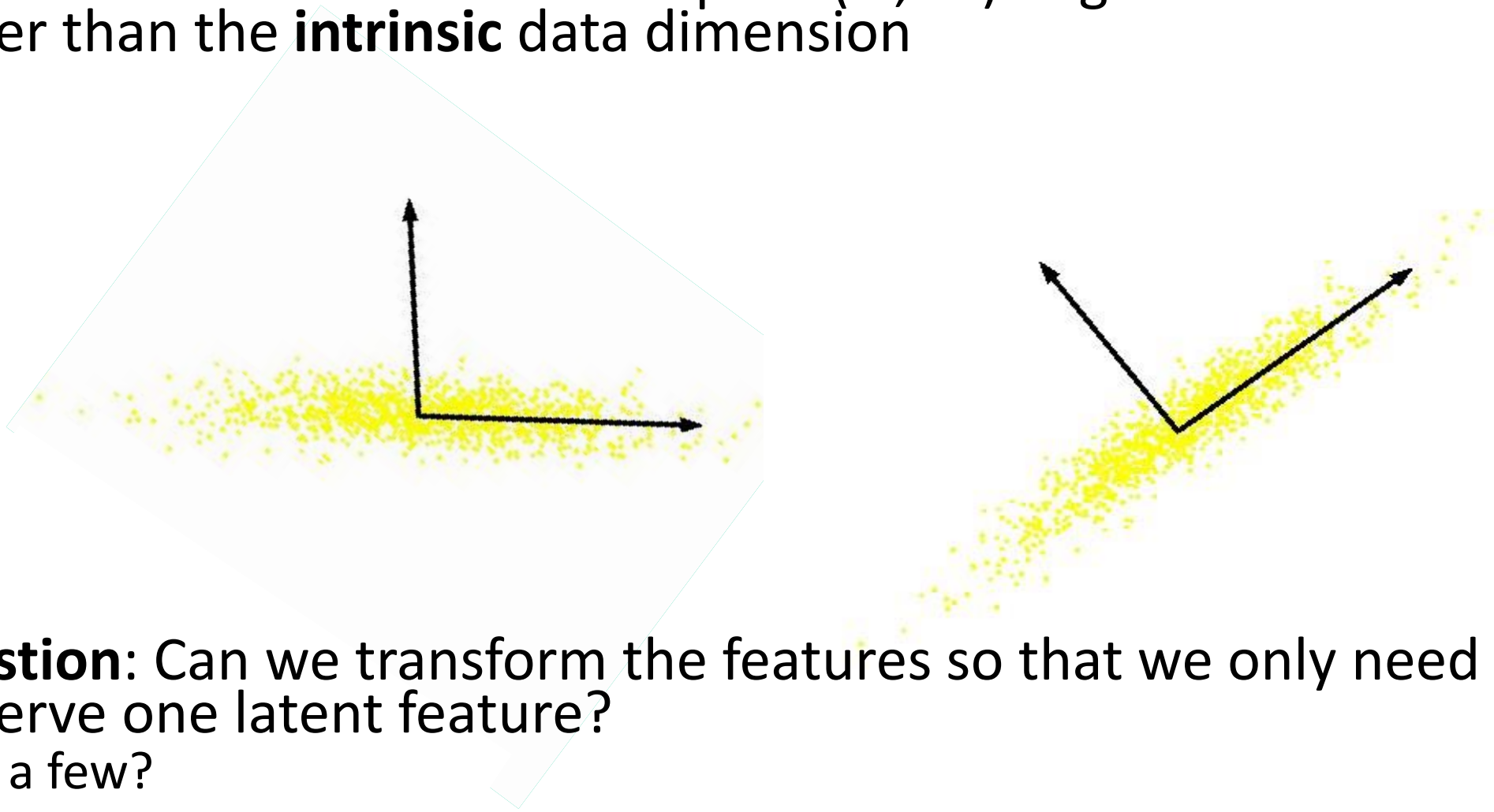
- Unsupervised technique for extracting variance structure from high dimensional datasets
  - And also reduces dimensionality

- PCA: orthogonal projection / transformation of the data
  - Into a (possibly lower dimensional) subspace
  - So that the variance of the projected data is maximized.



PCA Intuition

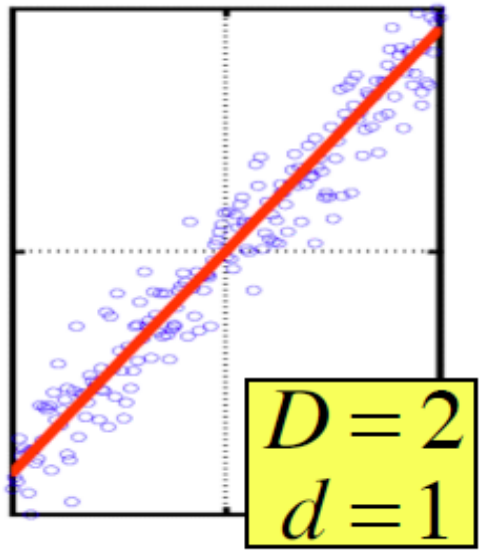
- The dimension of the ambient space (ie, R^d) might be much higher than the **intrinsic** data dimension

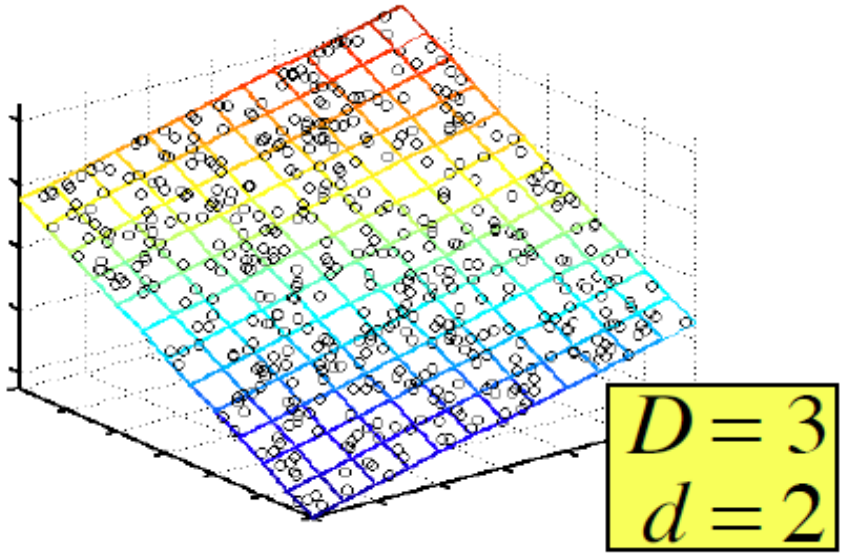


- **Question**: Can we transform the features so that we only need to preserve one latent feature?
  - Or a few?

PCA Intuition

- Some more visualizations

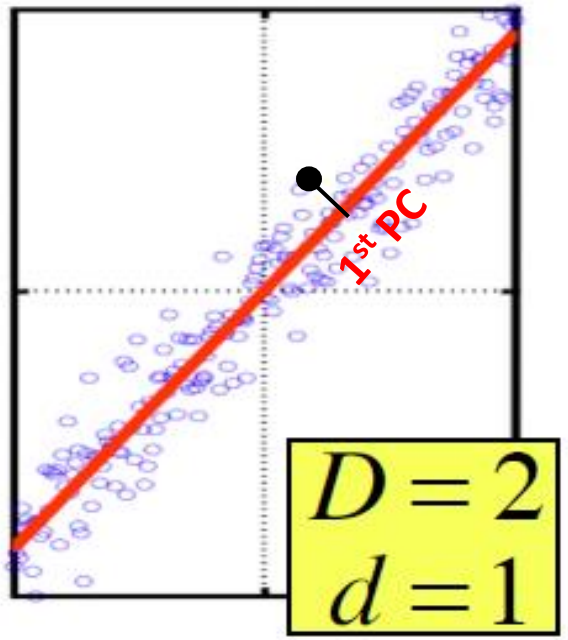




- In case where data lies on or near a low d-dimensional linear subspace, axes of this subspace are an effective representation of the data.

PCA: Principal Components

- **Principal Components (PCs)** are orthogonal directions that capture most of the variance in the data.
  - First PC – direction of greatest variability in data.
  - Projection of data points along first PC discriminates data most along any one direction



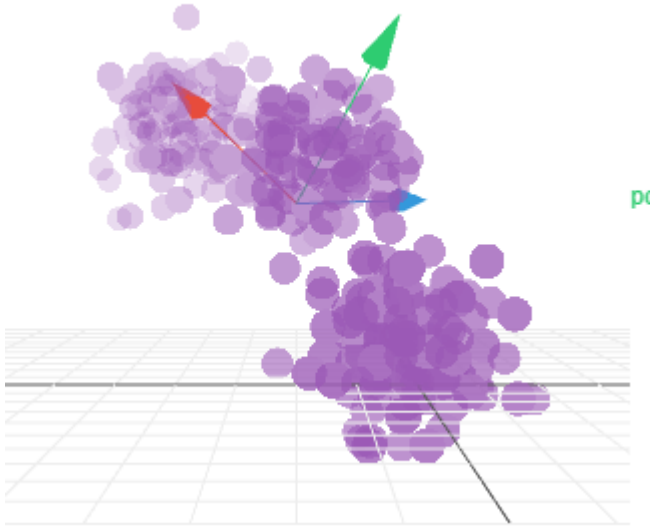
PCA: Principal Components and Projection

- How does dimensionality reduction work? From *d* dimensions to *r* dimensions:
  - Get
  - Orthogonal!

$$v_1, v_2, \ldots, v_r \in \mathbb{R}^d$$

- Maximizing variability
  - Equivalent to **minimizing reconstruction error**

- Then project data onto PCs → d-dimensional



Victor Powell

PCA Approach Overview

- Want directions/components (unit vectors) so that
  - Projecting data maximizes variance
  - Specifically, for centered data $\sum_{i=1}^{n} \langle x_i, v \rangle = \|Xv\|^2$

- Do this **recursively**
  - Get orthogonal directions $v_1, v_2, \ldots, v_r \in \mathbb{R}^d$

PCA First Step

- First component,

$$v_1 = \arg\max_{\|v\|=1} \sum_{i=1}^{n} \langle v, x_i \rangle^2$$

- Same as getting

$$v_1 = \arg\max_{\|v\|=1} \|Xv\|^2$$

PCA Recursion

- Once we have *k-1* components, next?

$$\hat{X}_k = X - \sum_{i=1}^{k-1} X v_i v_i^T$$

Deflation

- Then do the same thing

$$v_k = \arg \max_{\|v\|=1} \|\hat{X}_k w\|^2$$

PCA Interpretations

- The v's are eigenvectors of XX^T **(Gram matrix)**
  - We'll see why in a second

- XX^T (proportional to) sample covariance matrix
  - When data is 0 mean!
  - I.e., PCA is eigendecomposition of sample covariance

- Nested subspaces *span(v1), span(v1,v2),…,*

PCA Interpretations: First Component

- Two specific ways to think about the first component
- **Maximum variance direction**
  - What we saw so far

$$\sum_{i=1}^{n} (\mathbf{v}^T \mathbf{x}_i)^2 = \mathbf{v}^T \mathbf{X} \mathbf{X}^T \mathbf{v}$$

- **Minimum reconstruction error**
  - A direction so that projection yields minimum MSE in reconstruction

$$\sum_{i=1}^{n} \|\mathbf{x}_i - (\mathbf{v}^T \mathbf{x}_i)\mathbf{v}\|^2$$

PCA Interpretations: Equivalence

- Interpretation 1.

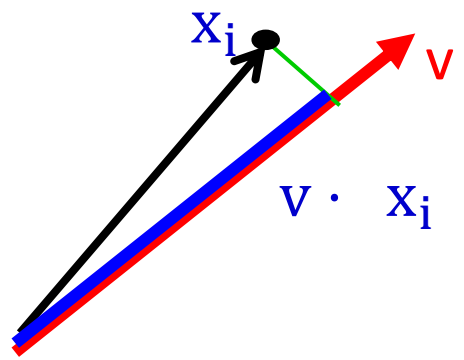
Maximum variance direction

$$\sum_{i=1}^{n} (\mathbf{v}^T \mathbf{x}_i)^2 = \mathbf{v}^T \mathbf{X}\mathbf{X}^T \mathbf{v}$$

$$\sum_{i=1}^{n} \|\mathbf{x}_i - (\mathbf{v}^T \mathbf{x}_i)\mathbf{v}\|^2$$

- Interpretation 2.

Minimum reconstruction error



- Why are these equivalent?
  - Use Pythagorean theorem.
  - Maximizing **blue** segment is the same as minimizing the **green**

PCA Gram Matrix Interpretation

- Recall our first PC, maximized variance:

$$\max_{\mathbf{v}} \ \mathbf{v}^T\mathbf{X}\mathbf{X}^T\mathbf{v} \quad \text{s.t.} \quad \mathbf{v}^T\mathbf{v} = 1$$

- Constrained optimization
  - Recall our usual approach: Lagrangian + KKT conditions

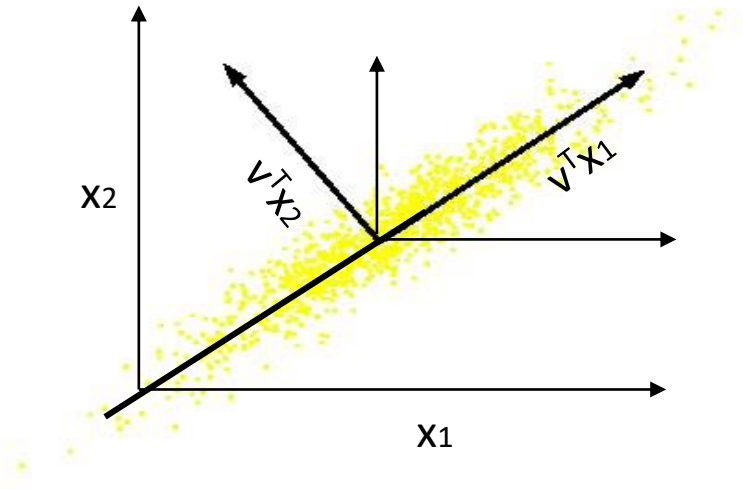
$$\text{Lagrangian: } \max_{\mathbf{v}} \mathbf{v}^T\mathbf{X}\mathbf{X}^T\mathbf{v} - \lambda\mathbf{v}^T\mathbf{v}$$

$$\partial/\partial\mathbf{v} = 0 \ \ (\mathbf{X}\mathbf{X}^T - \lambda\mathbf{I})\mathbf{v} = 0 \ \ \Rightarrow \boxed{(\mathbf{X}\mathbf{X}^T)\mathbf{v} = \lambda\mathbf{v}}$$

PCA Covariance Matrix Interpretation

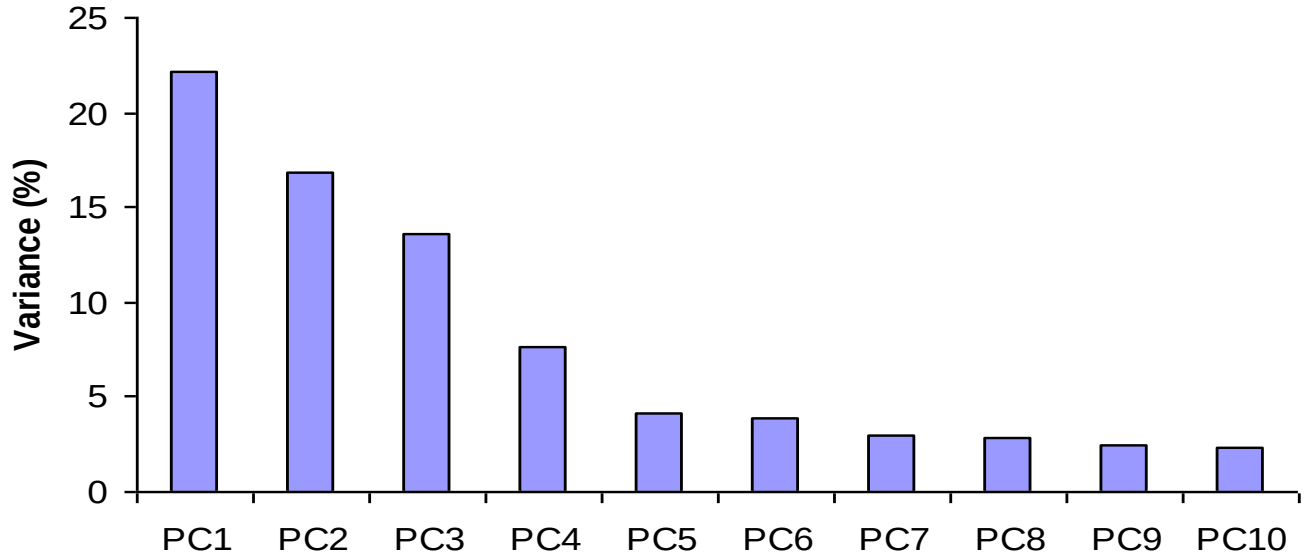
- So… $\Rightarrow (\mathbf{X}\mathbf{X}^T)\mathbf{v} = \lambda\mathbf{v}$
- Means that v (the first PC) is an eigenvector of XX^T
- Its eigenvalue λ denotes the amount of variability captured along that dimension

- PCs are just the eigenvectors…
  - How to find them? Eigendecompositio
- Don't need to keep all eigenvectors
  - Just the ones for largest eigenvalues



PCA Dimensionality Reduction

- In high-dimensional problems, data sometimes lies near a linear subspace, as noise introduces small variability
- Only keep data projections onto principal components with **large** eigenvalues
- Can *ignore* the components of smaller significance.



Application: Image Compression

- Start with image; divide into 12x12 patches
  - I.E., 144-D vector
  - **Original image:**

Application: Image Compression

- Project to 6D,

Compressed

Original

Thanks Everyone!

Some of the slides in these lectures have been adapted/borrowed from materials developed by Mark Craven, David Page, Jude Shavlik, Tom Mitchell, Nina Balcan, Elad Hazan, Tom Dietterich, Pedro Domingos, Jerry Zhu, Yingyu Liang, Volodymyr Kuleshov