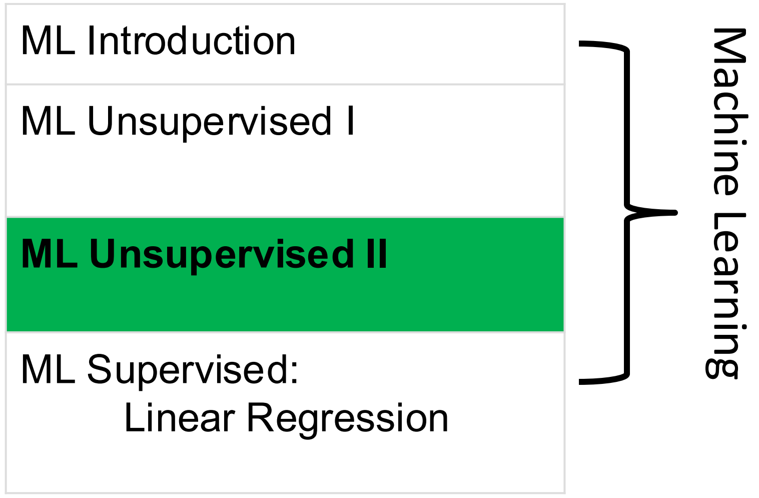
CS 540 Introduction to Artificial Intelligence
Unsupervised Learning II

University of Wisconsin–Madison
Fall 2025, Section 3
September 26, 2025

Announcements

- HW2 due on today at 11:59 PM
- HW3 is out! (due Friday 10/3 at 11:59 pm)
  - PCA & image compression
  - Build a simple language model

- Class roadmap:

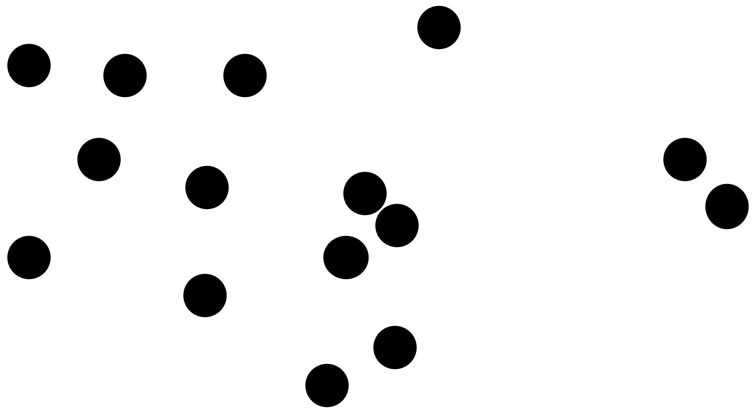


Outline

- Finish up Other Clustering Types
  - Graph-based, cuts, spectral clustering
- Unsupervised Learning: Visualization
  - t-SNE, algorithm, example, vs. PCA
- Unsupervised Learning: Density Estimation
  - Kernel density estimation: high-level intro

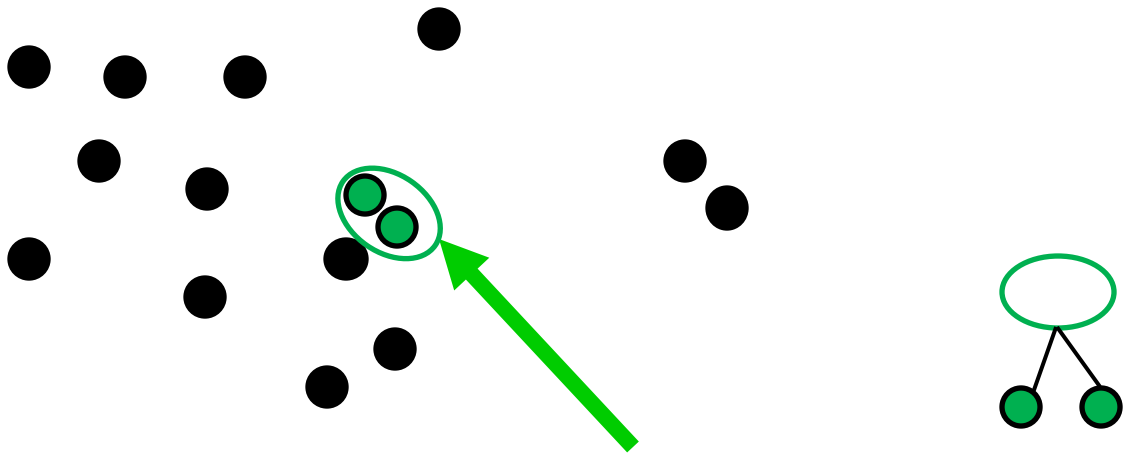
Agglomerative Clustering Example

Agglomerative. Start: every point is its own cluster



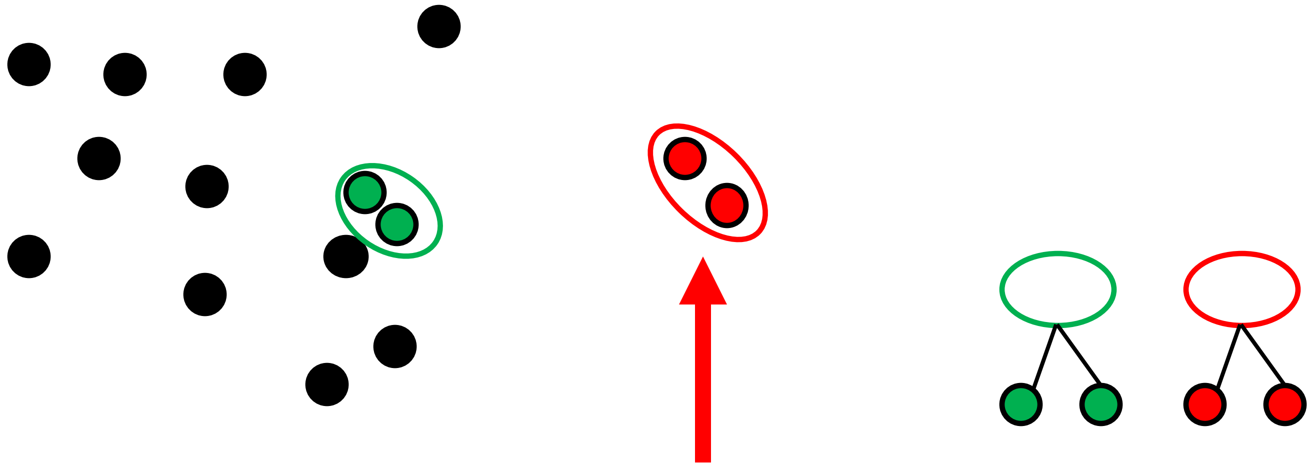
Agglomerative Clustering Example

Get pair of clusters that are closest and merge



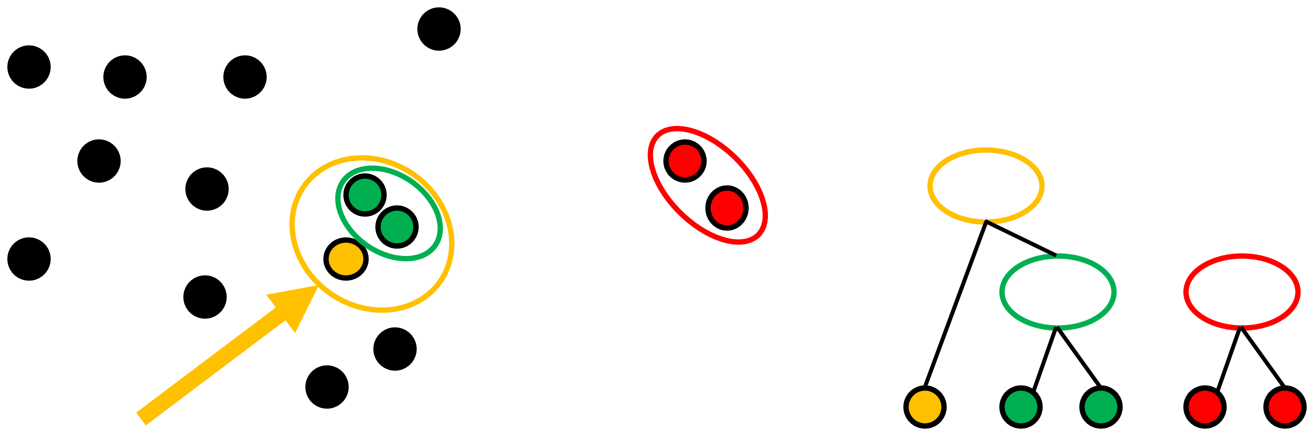
Agglomerative Clustering Example

Repeat: Get pair of clusters that are closest and merge



Agglomerative Clustering Example

Repeat: Get pair of clusters that are closest and merge



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

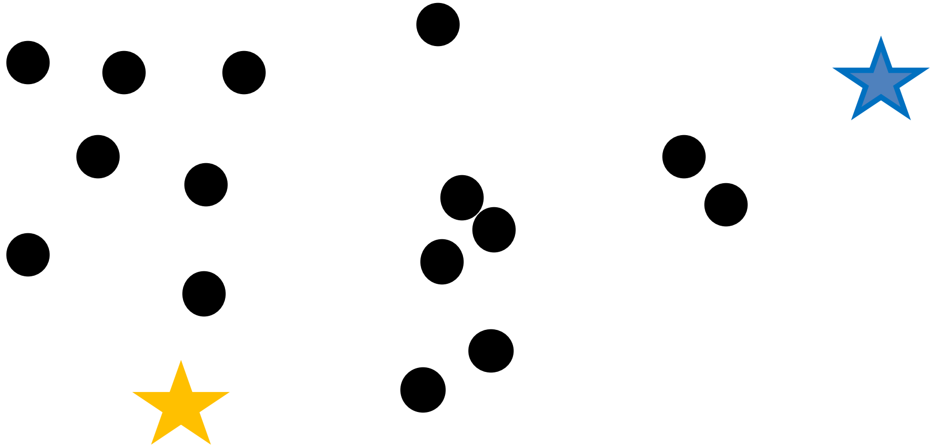
$$d(A,B) = \max_{x_1 \in A, x_2 \in B} d(x_1, x_2)$$

- Average-linkage

$$d(A,B) = \frac{1}{|A||B|} \sum_{x_1 \in A, x_2 \in B} d(x_1, x_2)$$

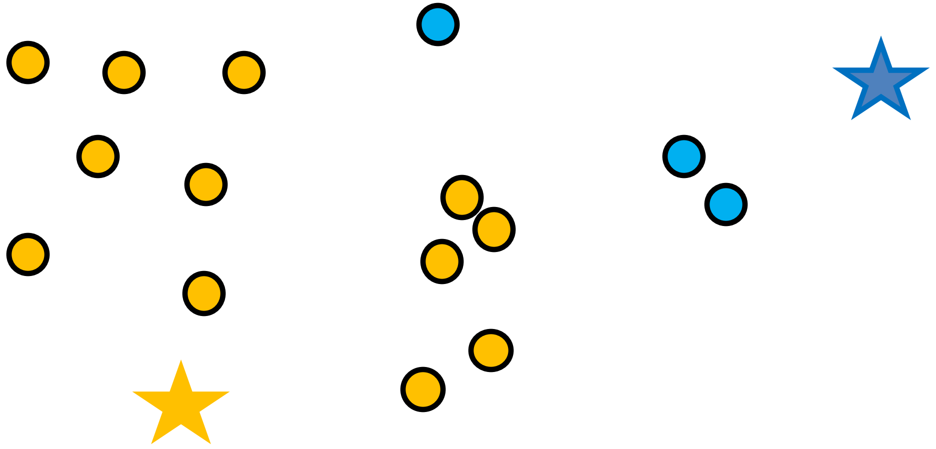
K-Means Clustering

- Steps: **1**. Randomly pick k cluster centers



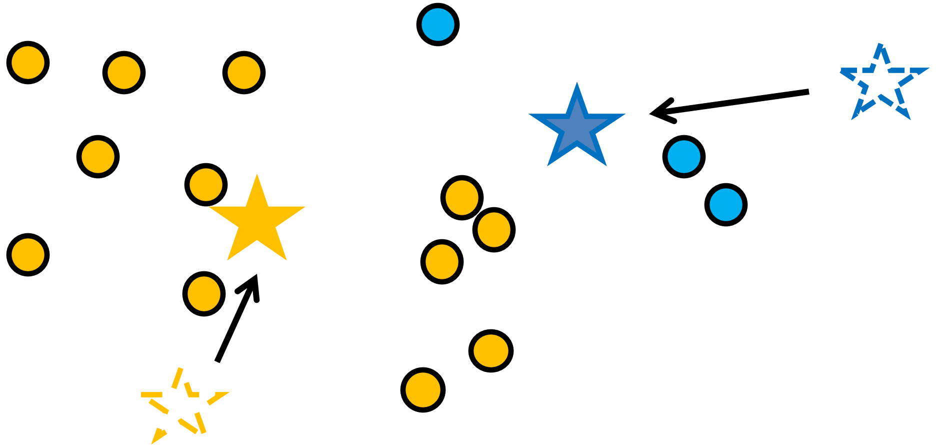
K-Means Clustering

- **2.** Find closest center for each point



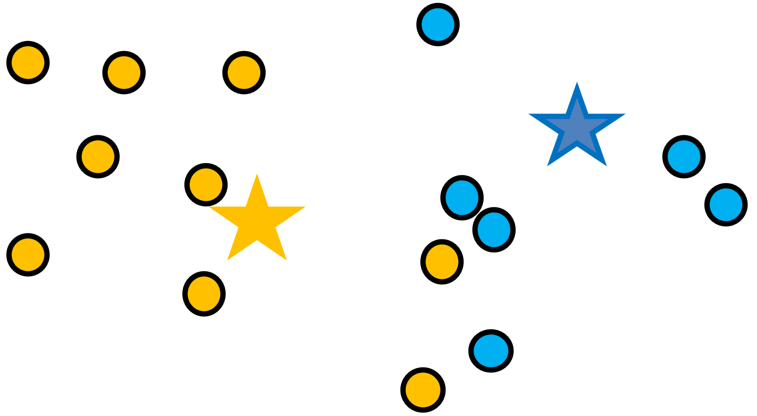
K-Means Clustering

- **3.** Update cluster centers by computing centroids



K-Means Clustering

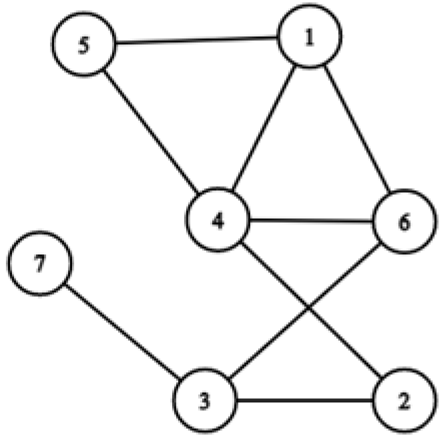
- Repeat Steps 2 & 3 until convergence



Other Types of Clustering

Graph-based/proximity-based

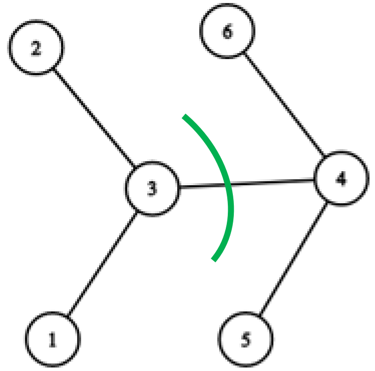
- Recall: Graph G = (V,E) has vertex set V, edge set E.
  - Edges can be weighted or unweighted
  - Encode **similarity:** $w_{ij} = \mathrm{sim}(v_i, v_j)$
- Don't need to KEEP vectors v
  - Only keep the edges (possibly weighted)



Graph-Based Clustering

Want: partition V into V_1 and V_2

- Implies a graph "cut"
- One idea: minimize the **weight** of the cut



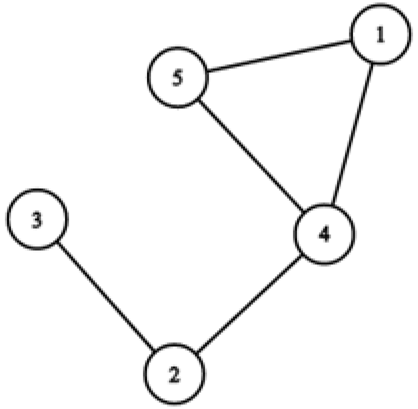
$$W(A,B) = \sum_{i \in A, j \in B} w_{ij}$$

$$\mathrm{cut}(A_1, \ldots, A_k) := \frac{1}{2} \sum_{i=1}^{k} W(A_i, \overline{A}_i).$$

Partition-Based Clustering

How do we compute these?

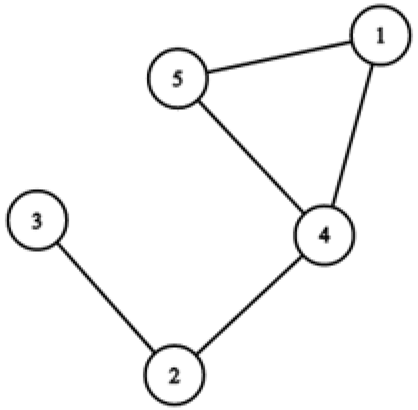
- Hard problem → heuristics
  - Greedy algorithm
  - "Spectral" approaches
- Spectral clustering approach:
  - **Adjacency** matrix



$$A = \begin{bmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{bmatrix}$$

Partition-Based Clustering

- Spectral clustering approach:
  - **Adjacency** matrix
  - **Degree** matrix

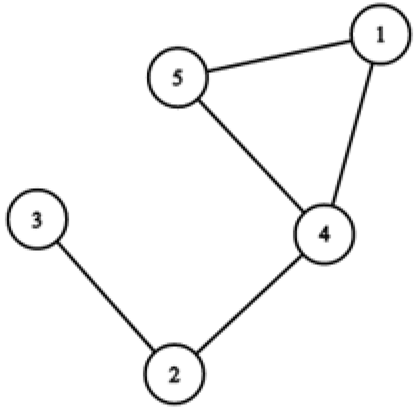


$$D = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{bmatrix} \qquad A = \begin{bmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{bmatrix}$$

Spectral Clustering

- Spectral clustering approach:
  - 1. Compute **Laplacian** L = D – A

(Important tool in graph theory)

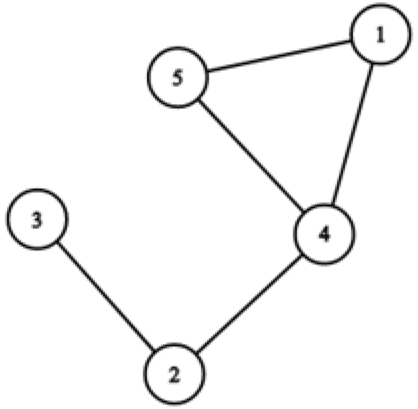


$$L = \underbrace{\begin{bmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{bmatrix}}_{\text{Degree Matrix}} - \underbrace{\begin{bmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{bmatrix}}_{\text{Adjacency Matrix}} = \underbrace{\begin{bmatrix} 2 & 0 & 0 & -1 & -1 \\ 0 & 2 & -1 & -1 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ -1 & -1 & 0 & 3 & -1 \\ -1 & 0 & 0 & -1 & 2 \end{bmatrix}}_{\text{Laplacian}}$$

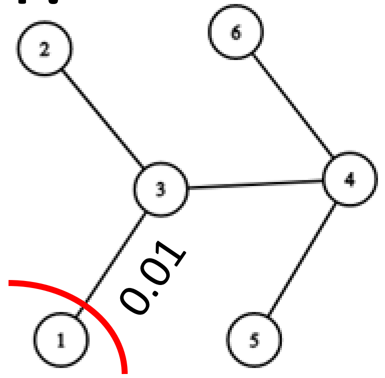
Spectral Clustering

- Spectral clustering approach:
  - 1. Compute **Laplacian** $\mathbf{L} = \mathbf{D} - \mathbf{A}$
  - 1a (optional): compute normalized Laplacian:

    $\mathbf{L} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$
  - 2. Compute k **smallest** eigenvectors of $\mathbf{L}$
  - 3. Set U to be the n x k matrix with $u_1, \ldots, u_k$ as columns. Take the n rows formed as points
  - 4. Run k-means on the representations

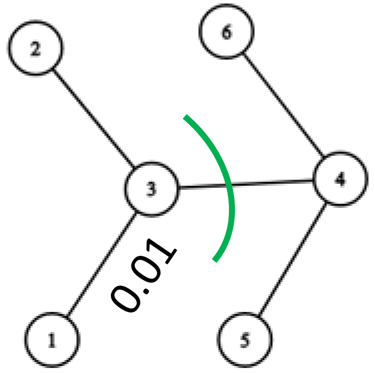


Why normalized Laplacian?



Want: partition V into V_1 and V_2

- Implies a graph “cut”
- One idea: minimize the **weight** of the cut
  - Downside: might just cut of one node
  - Need: “**balanced**” cut



Why Normalized Laplacian?

Want: partition V into V_1 and V_2

- Just minimizing weight is not always a good idea.
- We want **balance!**

$$\mathrm{Ncut}(A_1, \ldots, A_k) := \frac{1}{2} \sum_{i=1}^{k} \frac{W(A_i, \overline{A}_i)}{\mathrm{vol}(A_i)}$$

$$\mathrm{vol}(A) = \sum_{i \in A} \mathrm{degree}(i)$$

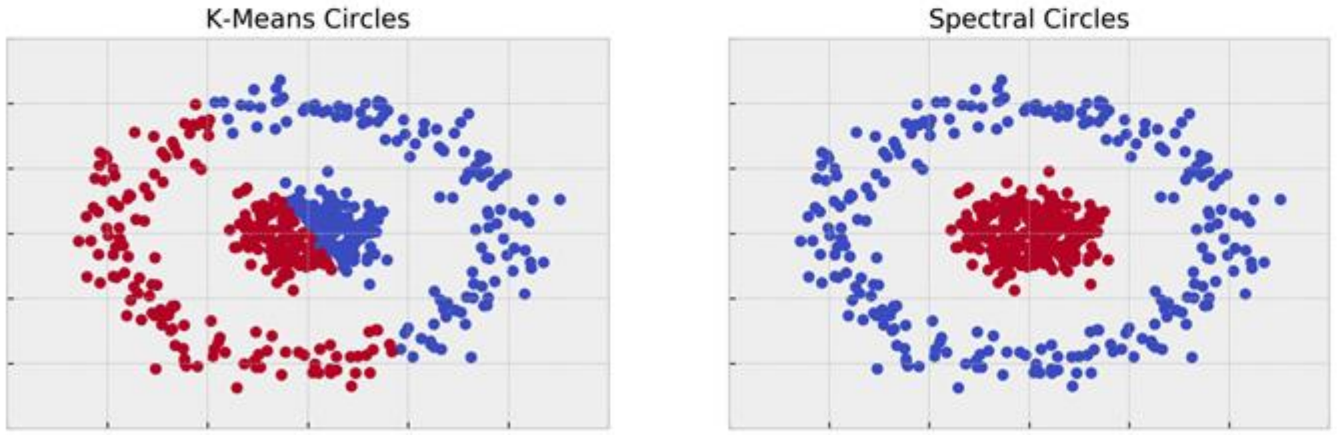
Spectral Clustering

- Compare/contrast to **PCA**:
  - Use an **eigendecomposition /** dimensionality reduction
    - But, run on Laplacian (not covariance); use smallest eigenvectors, not largest
- Intuition: Laplacian encodes structure information
  - "Lower" eigenvectors give partitioning information

Spectral Clustering

Q: Why do this?

- 1. No need for points or distances as input
- 2. Can handle intuitive separation (k-means can't!)

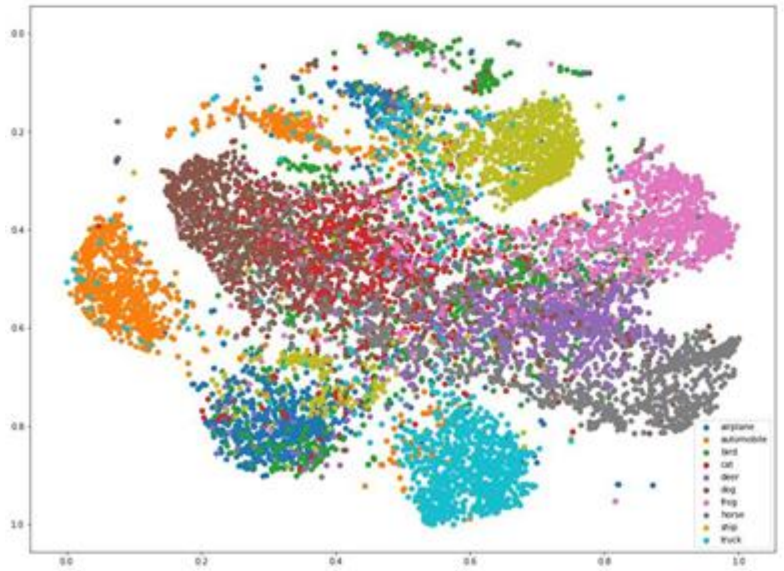


Credit: William Fleshman

Unsupervised Learning Beyond Clustering

Data analysis, dimensionality reduction, etc

- Already talked about PCA
- Note: PCA can be used for visualization, but not specifically designed for it
- Some algorithms **specifically** for visualization



Philip Slingerland

Dimensionality Reduction & Visualization

Typical dataset: MNIST

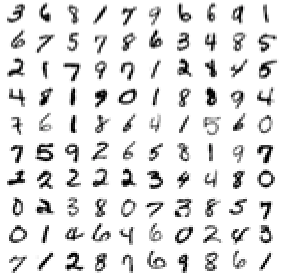
- Handwritten digits 0-9
  - 60,000 images (small by ML standards)
  - 28×28 pixel (784 dimensions)
  - Standard for image experiments

- Dimensionality reduction?

Dimensionality Reduction & Visualization

Run PCA on MNIST

- PCA is a linear mapping, (can be restrictive)



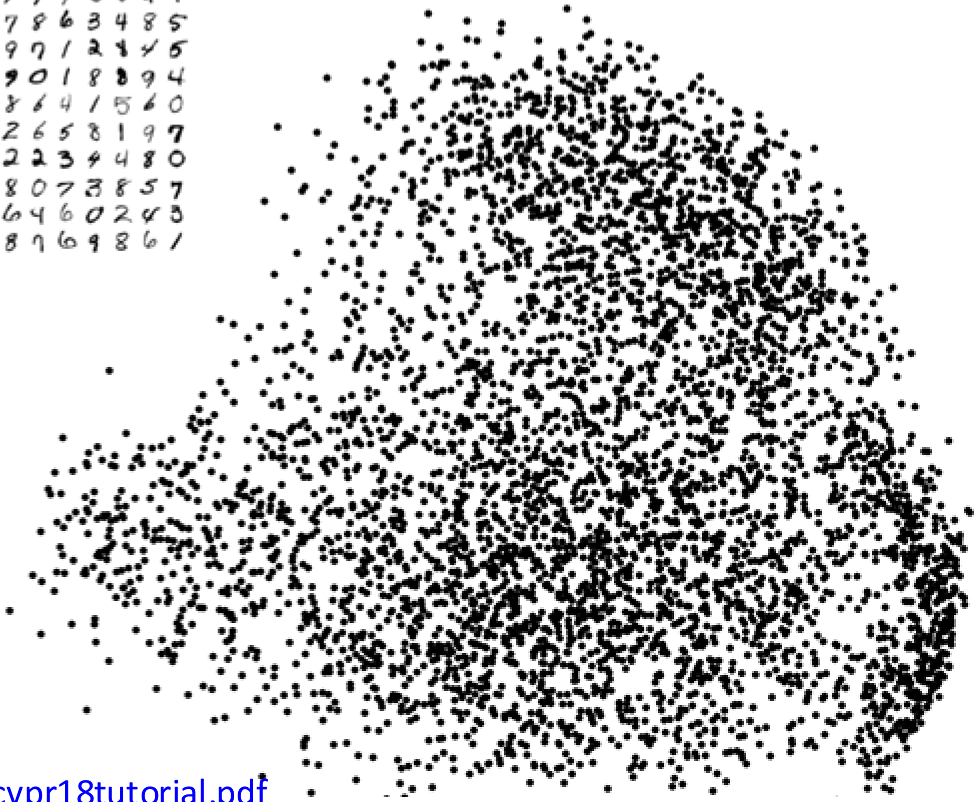


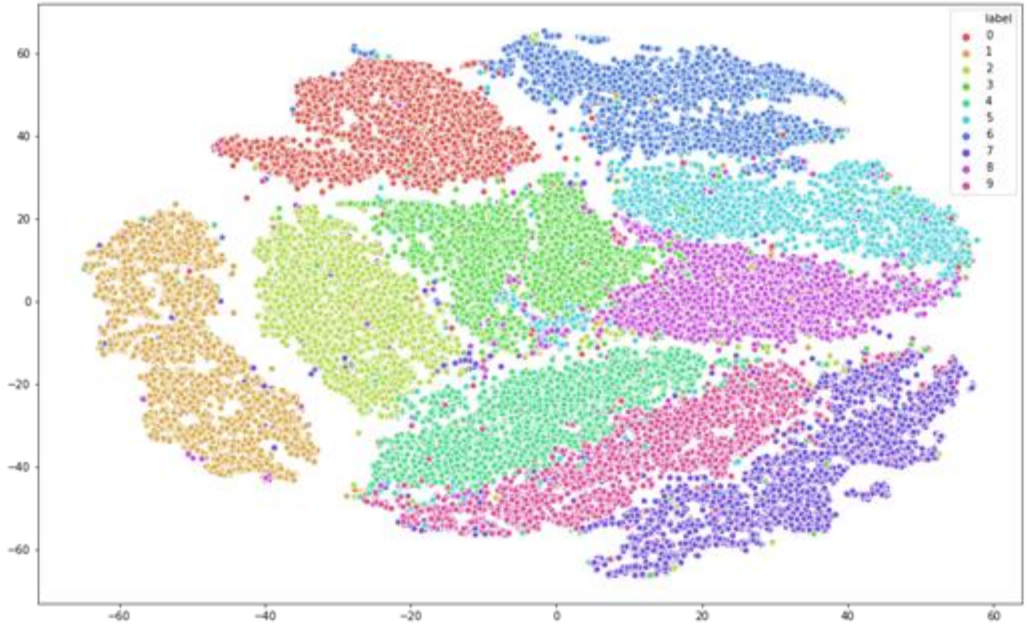
Image source: http://deeplearning.csail.mit.edu/slide_cvpr2018/laurens_cvpr18tutorial.pdf

Visualization: **T-SNE**

Typical dataset: MNIST

- **T-SNE**: project data into low dimensions
- Try to maintain structure

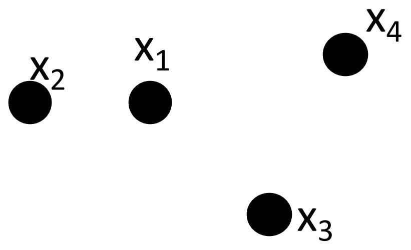
- MNIST Example
- **Input**: $x_1, x_2, \ldots, x_n$
- **Output**: 2D/3D $y_1, y_2, \ldots, y_n$



T-SNE Algorithm: Step 1

How does it work? Two steps

- **1.** Turn vectors into probability pairs
- **2**. Turn pairs back into **(lower-dim)** vectors



Step 1:

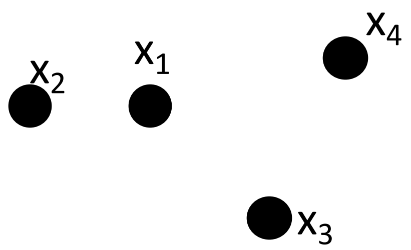
$$p_{j|i} = \frac{\exp(-\|x_i - x_j\|^2/2\sigma_i^2)}{\sum_{k\neq i}\exp(-\|x_i - x_k\|^2/2\sigma_i^2)} \quad p_{ij} = \frac{1}{2n}(p_{j|i} + p_{i|j})$$

Intuition: probability that x_i would pick x_j as its neighbor under a Gaussian probability

T-SNE Algorithm: Step 2

How does it work? Two steps

- **1.** Turn vectors into probability pairs
- **2**. Turn pairs back into **(lower-dim)** vectors



Step 2: set

$$q_{ij} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_{k \neq \ell}(1 + \|y_k - y_\ell\|^2)^{-1}}$$

and minimize

$$\sum_{i,j} p_{ij} \log \frac{p_{ij}}{q_{ij}} \longleftarrow$$

KL Divergence between p and q

T-SNE Algorithm: Step 2

More on step 2:

- We have two distributions *p*, *q*. *p* is fixed
- *q* is a function of the y_i which we move around
- Move y_i around until the KL divergence is small
  - So we have a good representation!

$$\sum_{i,j} p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

$$\uparrow$$

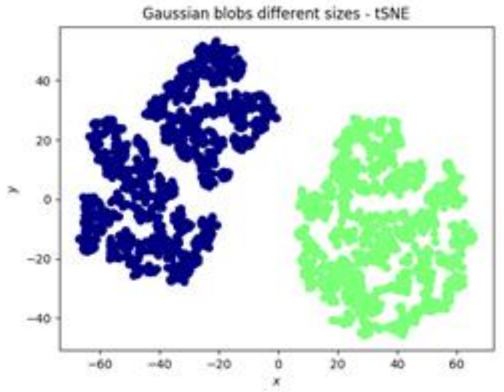
KL Divergence between p and q

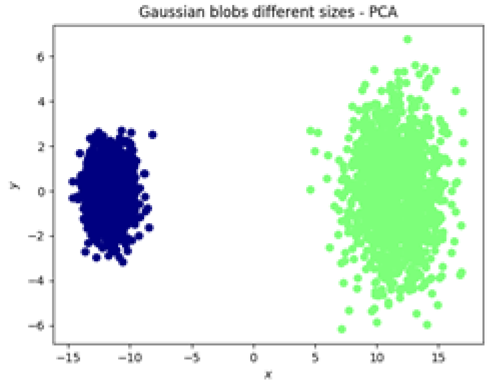
- **Optimizing a loss function**---we'll see more in supervised learning.

Visualization: **T-SNE**

t-SNE vs PCA?

- Local vs Global
- Nonlinear vs Linear
- Lose information in t-SNE
  - not a bad thing necessarily





https://www.thekerneltrip.com/statistics/tsne-vs-pca/
https://priceless-hamilton-1e6ee1.netlify.app/statistics/tsne-vs-pca/

Short Intro to Density Estimation

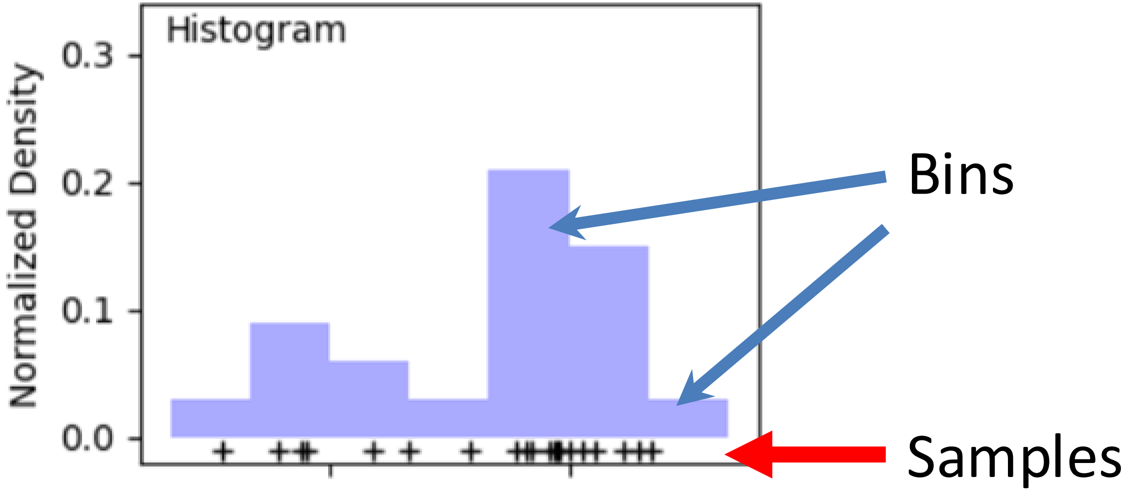
Goal: given samples x_1, …, x_n from some distribution P, estimate P.

- Compute statistics (mean, variance)
- Generate samples from P
- Run inference

Zach Monge

Simplest Idea: Histograms

Goal: given samples $x_1, \ldots, x_n$ from some distribution P, estimate P.



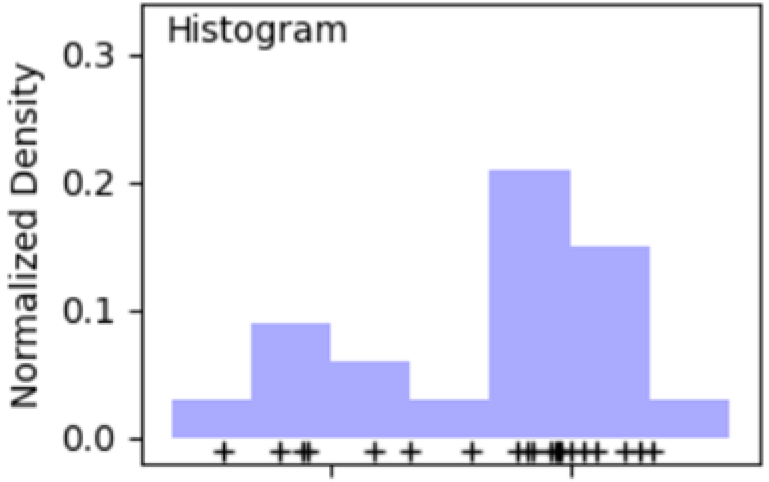
Define bins; count # of samples in each bin, normalize

Simplest Idea: Histograms

Goal: given samples $x_1, \ldots, x_n$ from some distribution P, estimate P.

Downsides:

i) High-dimensions: most bins empty
ii) Not continuous
iii) How to choose bins?



Kernel Density Estimation

Goal: given samples $x_1, \ldots, x_n$ from some distribution P, estimate P.

Idea: represent density as combination of "kernels"

$$f(x) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right)$$

Center at each point

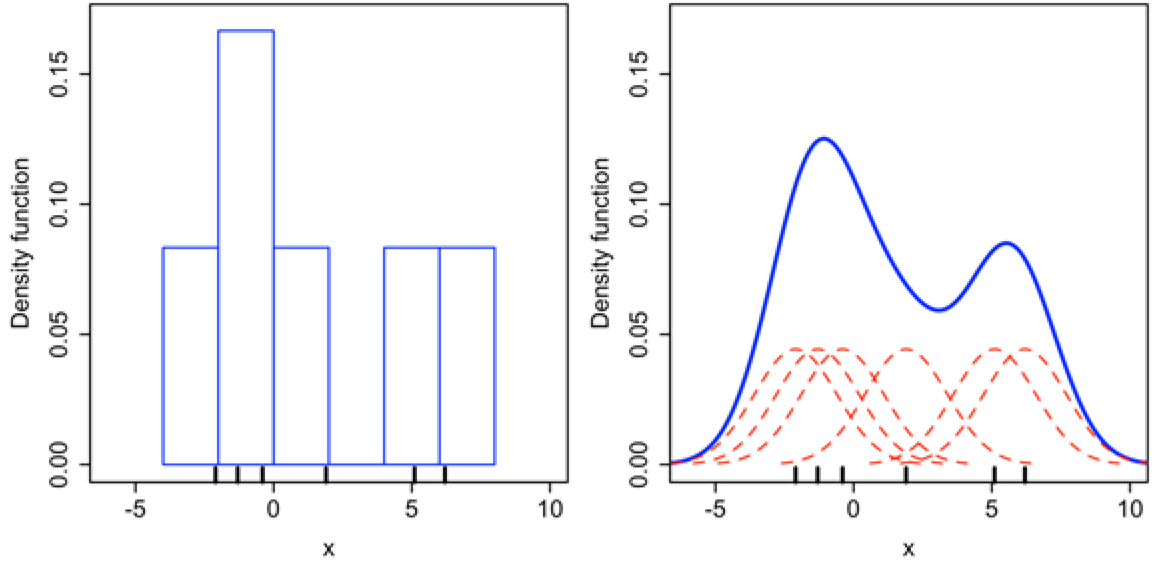
Kernel function: often Gaussian

Width parameter

Kernel Density Estimation

Idea: represent density as combination of kernels

- "Smooth" out the histogram


Density function
x
Density function
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