



CS 540 Introduction to Artificial Intelligence
Unsupervised Learning II
University of Wisconsin-Madison

Spring 2024

Announcements

- **Homeworks:**
 - HW4 deadline on **Thursday Feb. 22nd at 11 AM**
- Midterm 13th of March
- Class roadmap:

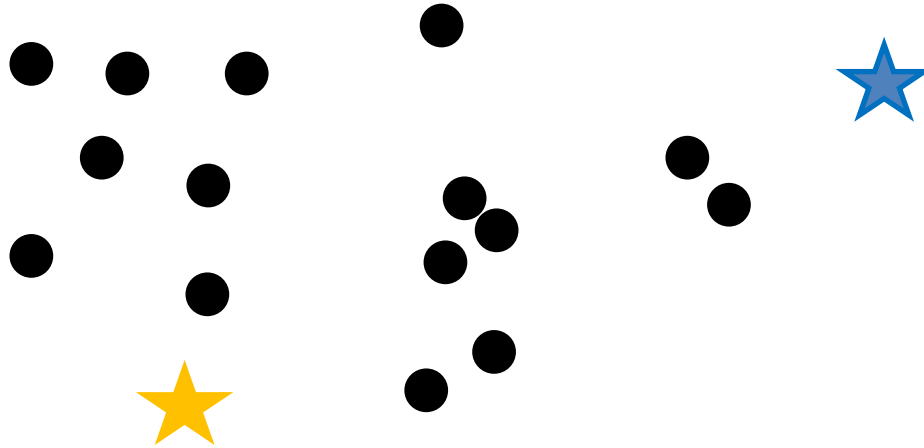
Tuesday, Feb. 20	ML Unsupervised II	Machine Learning
Thursday, Feb. 22	ML Linear Regression	
Tuesday, Feb. 27	Machine Learning: K - Nearest Neighbors & Naive Bayes	
Thursday, Feb. 29	Machine Learning: Neural Networks I (Perceptron)	

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

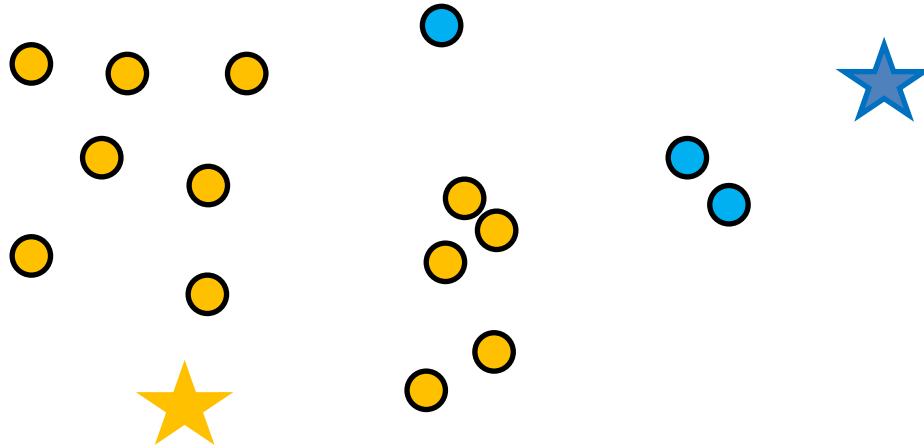
K-Means Clustering

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



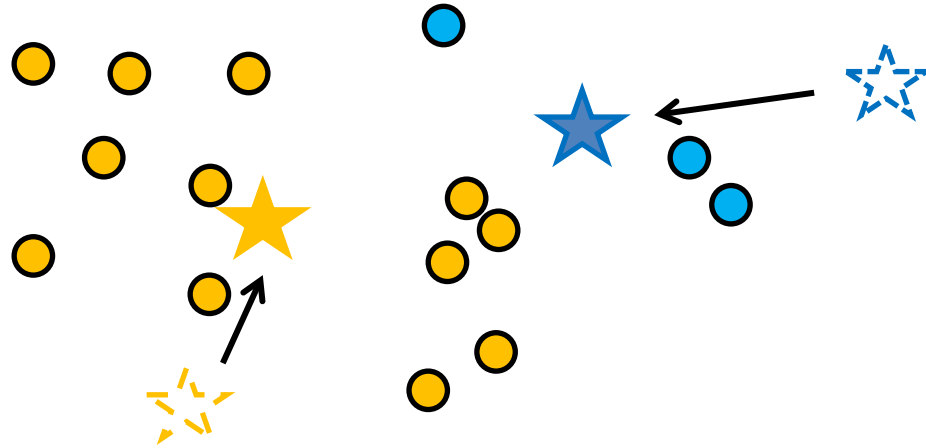
K-Means Clustering

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



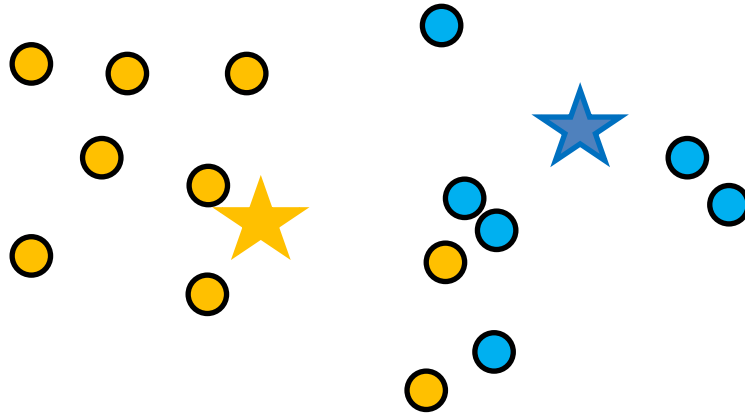
K-Means Clustering

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



K-Means Clustering

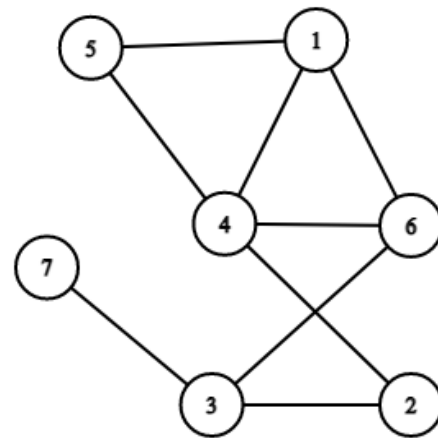
- Repeat Steps 2 & 3 until convergence



Other Types of Clustering

Graph-based/proximity-based

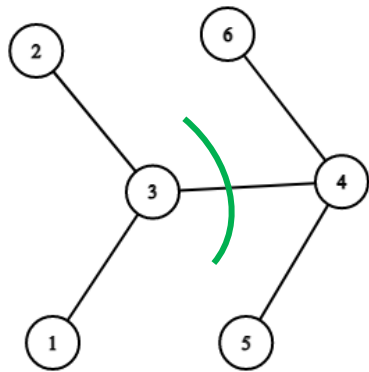
- Recall: Graph $G = (V, E)$ has vertex set V , edge set E .
 - Edges can be weighted or unweighted
 - Encode **similarity**: $w_{ij} = \text{sim}(v_i, v_j)$
- Don't need to KEEP vectors v
 - Only keep the edges (possibly weighted)



Graph-Based Clustering

Want: partition V into V_1 and V_2

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



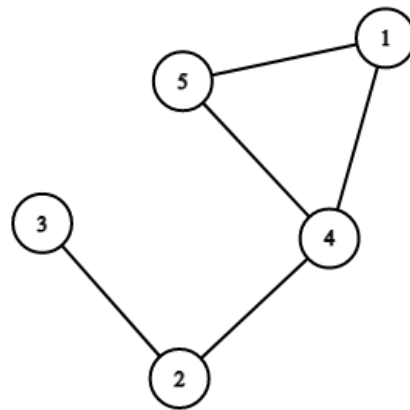
$$W(A, B) = \sum_{i \in A, j \in B} w_{ij}$$

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

Partition-Based Clustering

How do we compute these?

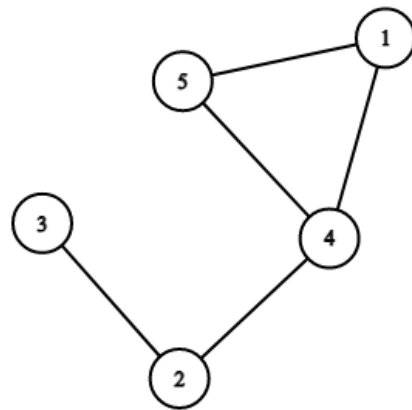
- Hard problem → heuristics
 - Greedy algorithm
 - “Spectral” approaches
- Spectral clustering approach:
 - **Adjacency** matrix



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

Partition-Based Clustering

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

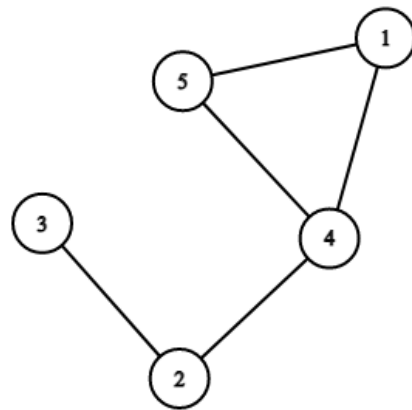


$$D = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{bmatrix}$$

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

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** $\mathbf{L} = \mathbf{D} - \mathbf{A}$

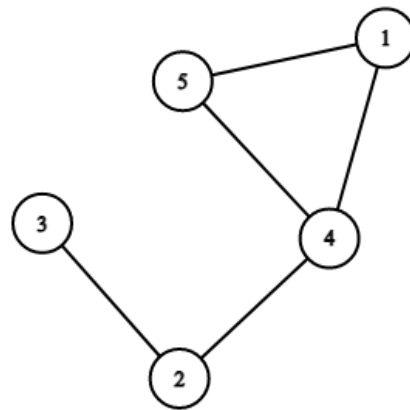
- 1a (optional): compute normalized Laplacian:

$$\mathbf{L} = \mathbf{I} - \mathbf{D}^{-1/2} \mathbf{A} \mathbf{D}^{-1/2}, \text{ or } \mathbf{L} = \mathbf{I} - \mathbf{D}^{-1} \mathbf{A}$$

- 2. Compute k **smallest** eigenvectors of \mathbf{L}

- 3. Set U to be the $n \times k$ matrix with u_1, \dots, u_k as columns. Take the n rows formed as points

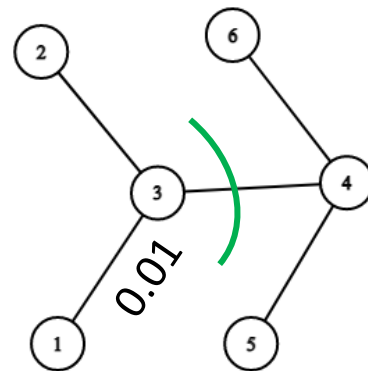
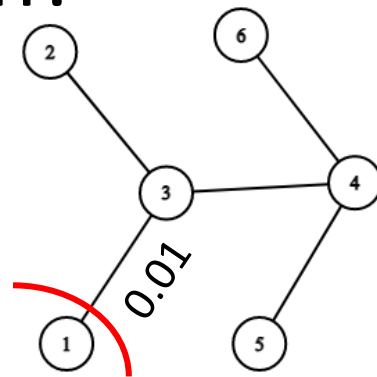
- 4. Run k-means on the representations



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**!

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

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

Spectral Clustering

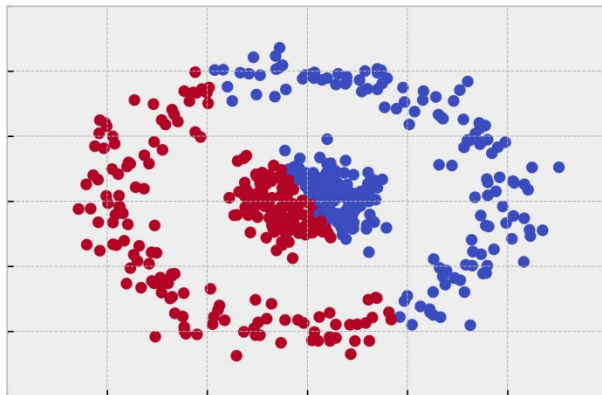
- Compare/contrast to **PCA**:
 - Use an **eigendecomposition** / dimensionality reduction
 - But, run on Laplacian (not covariance); use smallest eigenvectors, not largest
- Intuition: Laplacian encodes structure information
 - “Lower” eigenvectors give partitioning information

Spectral Clustering

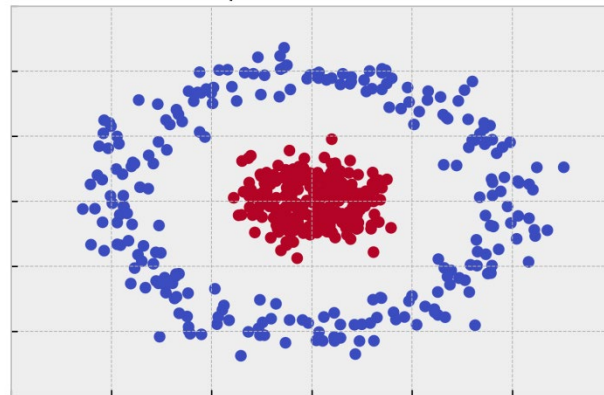
Q: Why do this?

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

K-Means Circles



Spectral Clustering



Credit: William Fleshman

Break & Quiz

Q 1.1: We have two datasets: a social network dataset S_1 which shows which individuals are friends with each other along with image dataset S_2 .

What kind of clustering can we do? Assume we do not make additional data transformations.

- A. k-means on both S_1 and S_2
- B. graph-based on S_1 and k-means on S_2
- C. k-means on S_1 and graph-based on S_2
- D. hierarchical on S_1 and graph-based on S_2

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- A. k-means on both S_1 and S_2
- **B. graph-based on S_1 and k-means on S_2**
- C. k-means on S_1 and graph-based on S_2
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Break & Quiz

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What kind of clustering can we do? Assume we do not make additional data transformations.

- A. k-means on both S_1 and S_2 **(No: can't do k-means on graph)**
- **B. graph-based on S_1 and k-means on S_2**
- C. k-means on S_1 and graph-based on S **(Same as A)**
- D. hierarchical on S_1 and graph-based on S_2 **(No: S_2 is not a graph)**

Break & Quiz

Q 1.2: The CIFAR-10 dataset contains 32x32 images labeled with one of 10 classes. What could we use it for?

(i) Supervised learning (ii) PCA (iii) k-means clustering

- A. Only (i)
- B. Only (ii) and (iii)
- C. Only (i) and (ii)
- D. All of them



Break & Quiz

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- **D. All of them**

Break & Quiz

Q 1.2: The CIFAR-10 dataset contains 32x32 images labeled with one of 10 classes. What could we use it for?

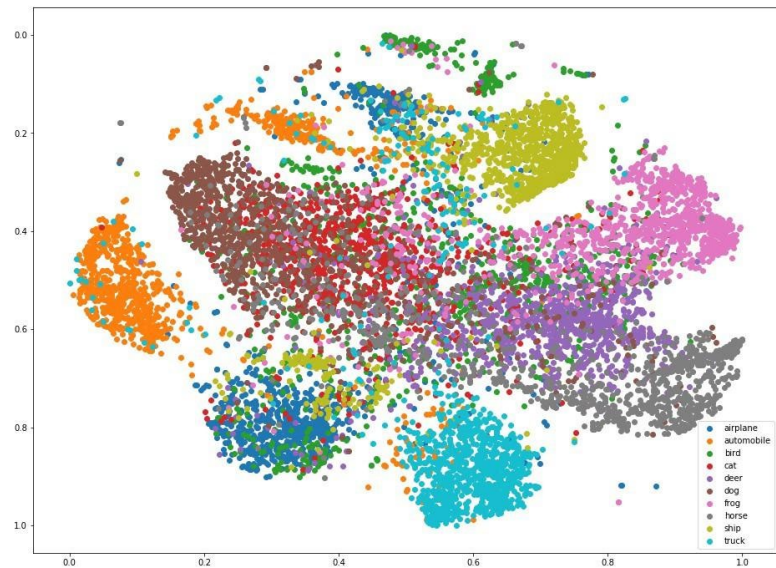
(i) Supervised learning (ii) PCA (iii) k-means clustering

- (i) **Yes: train an image classifier; have labels**
- (ii) **Yes: run PCA on image vectors to reduce dimensionality**
- (iii) **Yes: can cluster image vectors with k-means**
- **D. All of them**

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



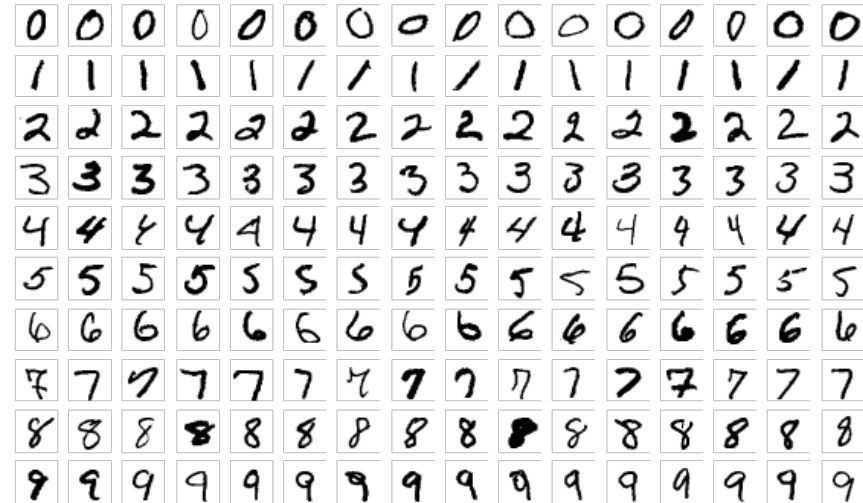
Philip Slingerland

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)

3 6 8 1 7 9 6 6 9 1
6 7 5 7 8 6 3 4 8 5
2 1 7 9 7 1 2 8 4 5
4 8 1 9 0 1 8 8 9 4
7 6 1 8 6 4 1 5 6 0
7 5 9 2 6 5 8 1 9 7
1 2 2 2 2 3 4 4 8 0
0 2 3 8 0 7 3 8 5 7
0 1 4 6 4 6 0 2 4 3
7 1 2 8 7 6 9 8 6 1

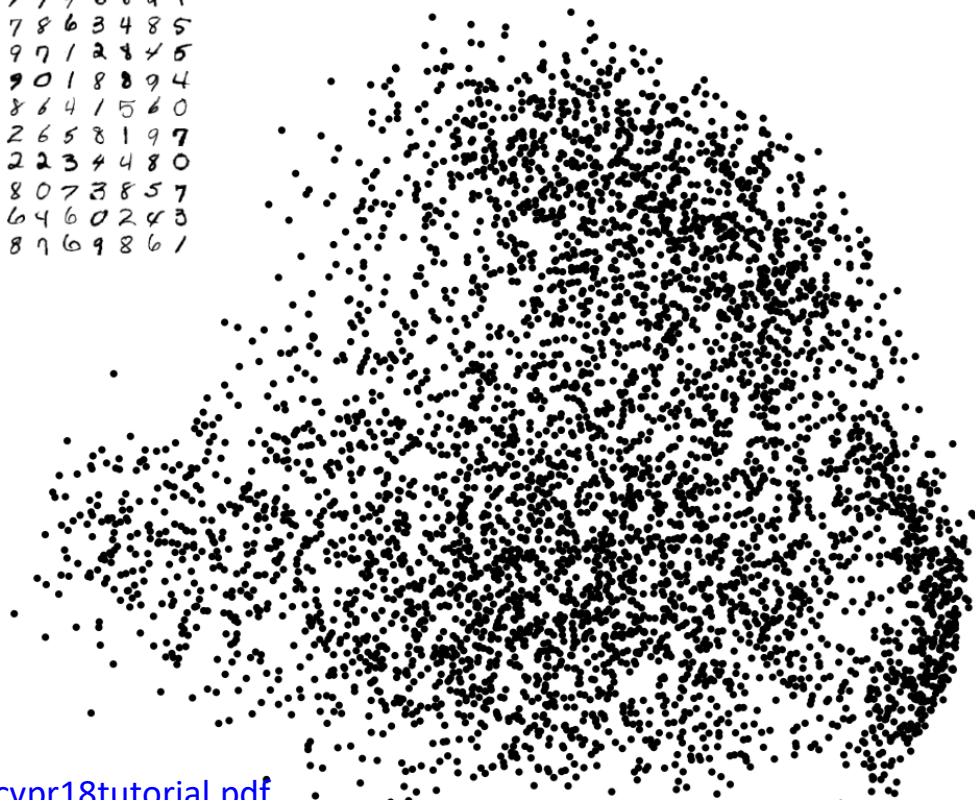


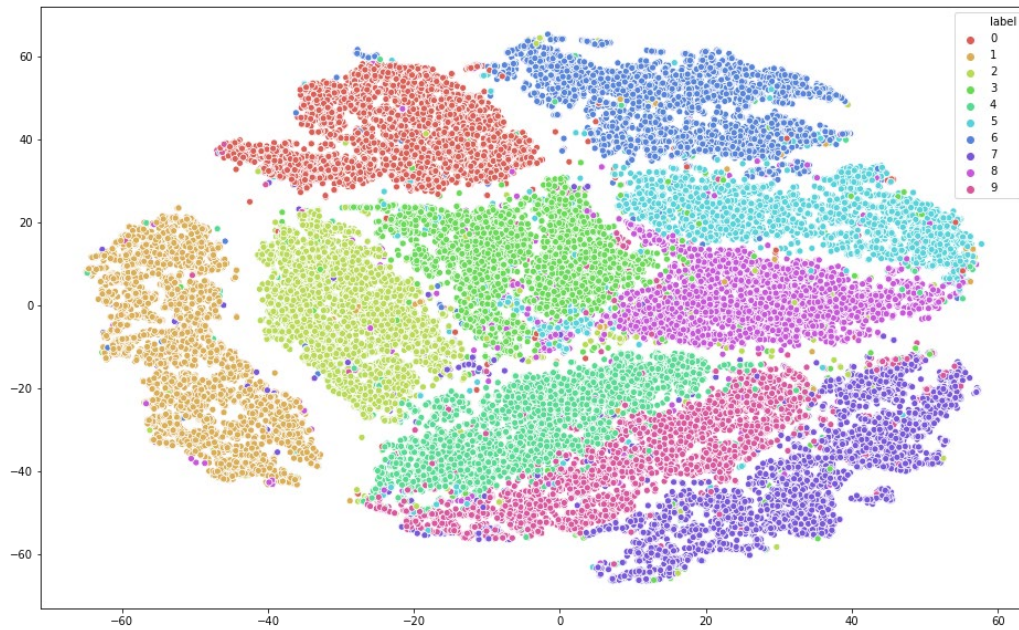
Image source:

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

Visualization: T-SNE

Typical dataset: MNIST

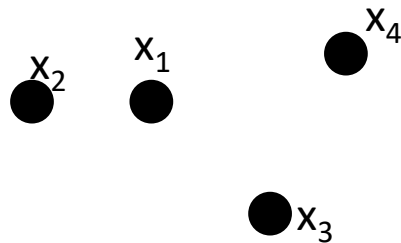
- **T-SNE**: project data into just 2 dimensions
- Try to maintain structure
- MNIST Example
- **Input**: x_1, x_2, \dots, x_n
- **Output**: 2D/3D y_1, y_2, \dots, y_n



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

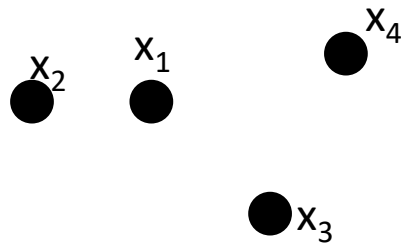
$$q_{ij} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_{k \neq \ell} (1 + \|y_k - y_\ell\|^2)^{-1}}$$

and minimize

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



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

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



KL Divergence
between p and q

T-SNE Examples

- Examples: (from Laurens van der Maaten)

- **Movies:**

https://lvdmaaten.github.io/tsne/examples/netflix_tsne.jpg



T-SNE Examples

- Examples: (from Laurens van der Maaten)
- **NORB:**
https://lvdmaaten.github.io/tsne/examples/norb_tsne.jpg



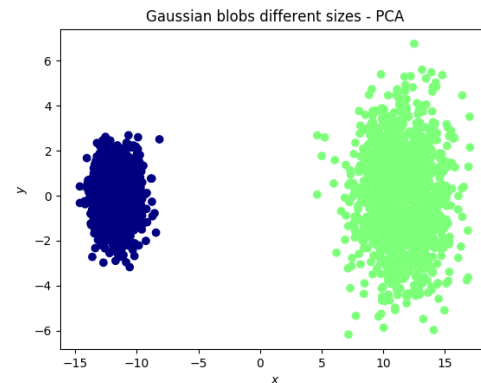
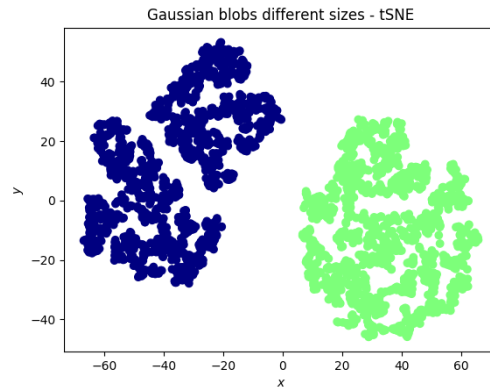
Visualization: T-SNE

t-SNE vs PCA?

- “Local” vs “Global”
- Lose information in t-SNE
 - not a bad thing necessarily
- Downstream use

Good resource/credit:

<https://www.thekerneltrip.com/statistics/tsne-vs-pca/>



Break & Quiz

Q 2.1: Can we do t-SNE on NLP (words) or graph datasets?

- A. Never
- B. Yes, after running PCA on them
- C. Yes, after mapping them into \mathbb{R}^d (ie, embedding)
- D. Yes, after running hierarchical clustering on them

Break & Quiz

Q 2.1: Can we do t-SNE on NLP (words) or graph datasets?

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Break & Quiz

Q 2.1: Can we do t-SNE on NLP (words) or graph datasets?

- A. Never **(No: too strong)**
- B. Yes, after running PCA on them **(No: can't run PCA on words or graphs directly. Need vectors)**
- **C. Yes, after mapping them into R^d (ie, embedding)**
- D. Yes, after running hierarchical clustering on them **(No: hierarchical clustering gives us a graph)**

Short Intro to Density Estimation

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

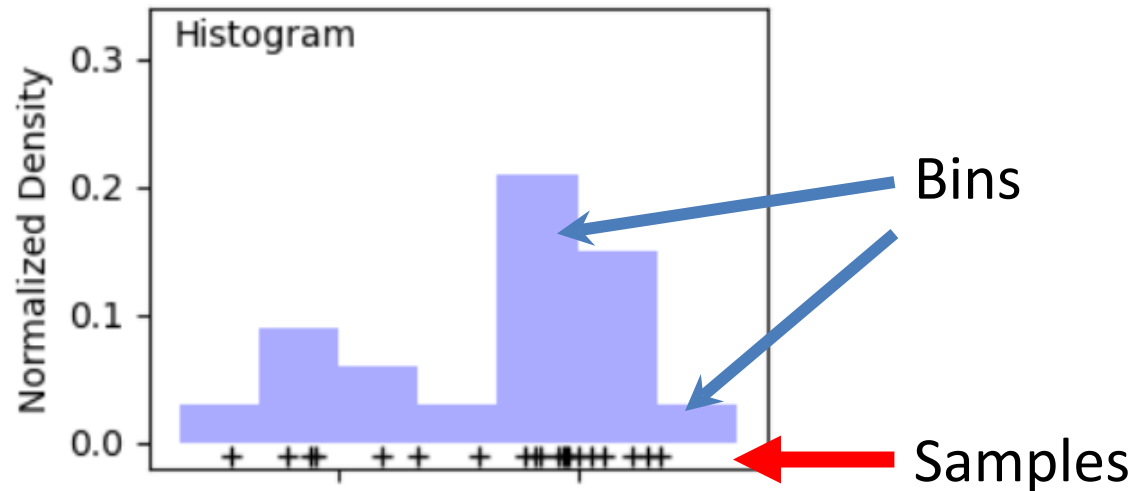
- Compute statistics (mean, variance)
- Generate samples from P
- Run inference



Zach Monge

Simplest Idea: Histograms

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



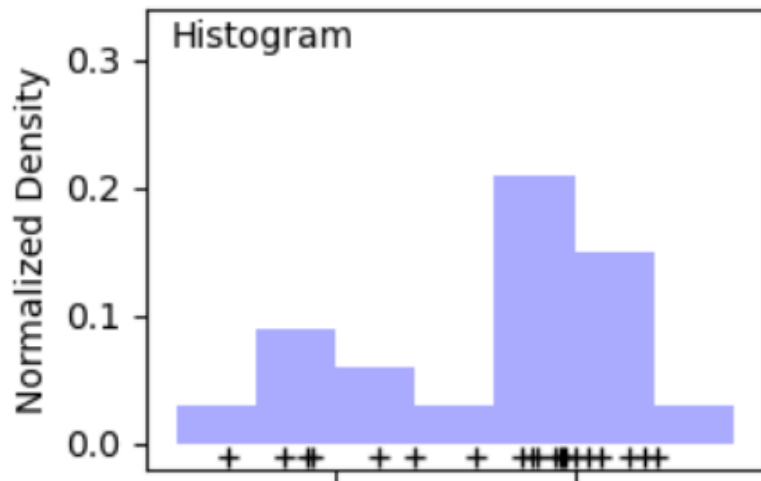
Define bins; count # of samples in each bin, normalize

Simplest Idea: Histograms

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

Downsides:

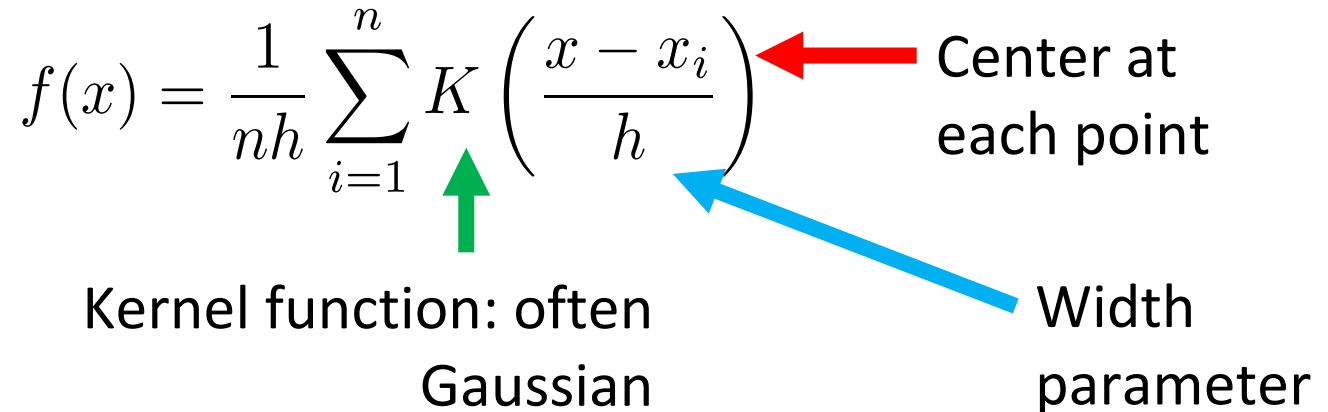
- i) High-dimensions: most bins empty
- ii) Not continuous
- iii) How to choose bins?



Kernel Density Estimation

Goal: given samples x_1, \dots, 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

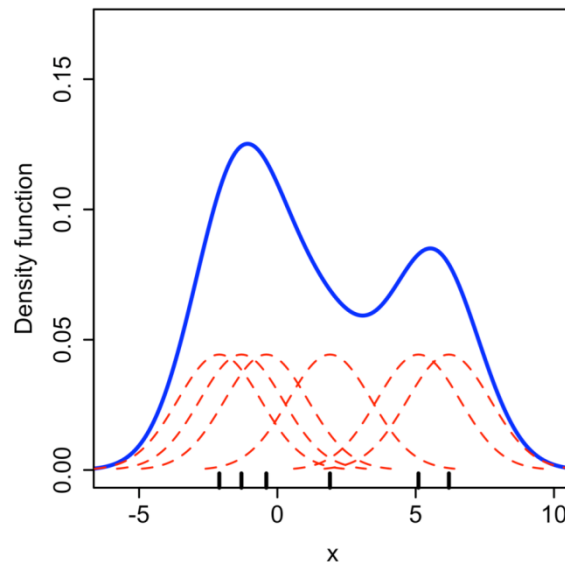
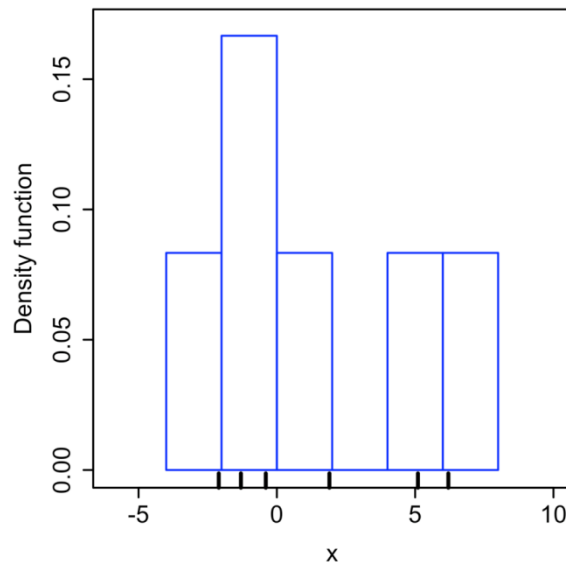
Kernel function: often Gaussian

Width parameter

Kernel Density Estimation

Idea: represent density as combination of kernels

- “Smooth” out the histogram



Readings

Suggested reading:

A Tutorial on Spectral Clustering, Ulrike von Luxburg

https://people.csail.mit.edu/dsontag/courses/ml14/notes/Luxburg07_tutorial_spectral_clustering.pdf