CS 540 Introduction to Artificial Intelligence

Unsupervised Learning II

University of Wisconsin-Madison

Spring 2023

Announcements

- **Homeworks:**
  - **HW4 due Thursday!**
- **Class roadmap:**

Tuesday, Feb 21	ML Unsupervised II
Thursday, Feb 23	ML Linear Regression
Tuesday, Feb 28	ML: K - Nearest Neighbors & Naive Bayes
Thursday, Mar 2	ML: Neural Networks I
Tuesday, Mar 7	ML: Neural Networks II

Last topic included on midterm!

Unsupervised Learning II Outline

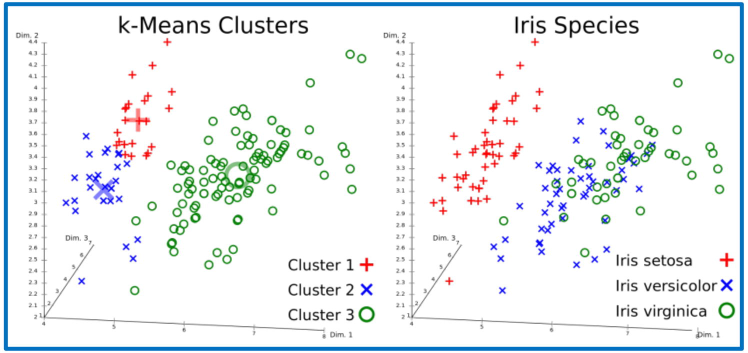
- Finish up Other Clustering Types
  - Graph-based clustering, graph cuts, spectral clustering
- Unsupervised Learning: Visualization
  - t-SNE: algorithm, examples, vs. PCA
- Unsupervised Learning: Density Estimation
  - Kernel density estimation: high-level intro

After today's lecture, you'll be able to..

- Understand graph-based clustering and the steps of the spectral clustering algorithm.
- Describe the purpose of the t-SNE algorithm for data visualization, contrast t-SNE with PCA, and understand the steps of t-SNE.
- Understand the problem of and basic techniques for density estimation.

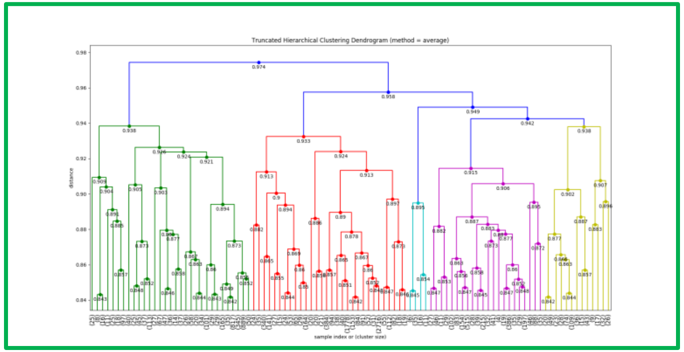
Review: Clustering

- K-means Algorithm:
  - Input: data points, $x_1, x_2, \ldots x_n,$ and desired number of clusters, k.
  - Output: a grouping of the points into k clusters.



Review: Clustering

- Hierarchical Clustering:
  - Input: data points $x_1, x_2, \dots x_n$.
  - Output: a tree that progressively divides data points into smaller and smaller groups.



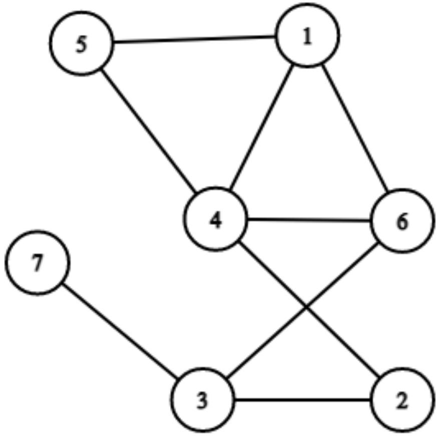
Other Types of Clustering

Graph-based/proximity-based

- Recall: Graph G = (V,E) has vertex set V, edge set E.
  - Edges can be weighted or unweighted
  - Edges encode **similarity** between vertices:

$$w_{ij} = \mathrm{sim}(v_i, v_j)$$

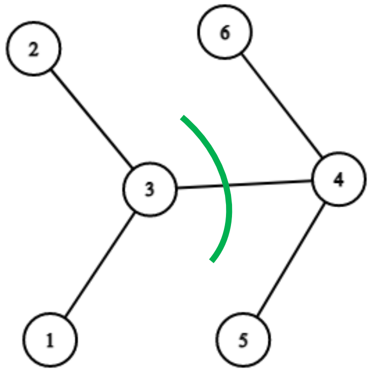
- Don't need to KEEP vectors for each v.
  - Only keep the edges (possibly weighted)



Graph-Based Clustering

Want: partition V into V_1 and V_2

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



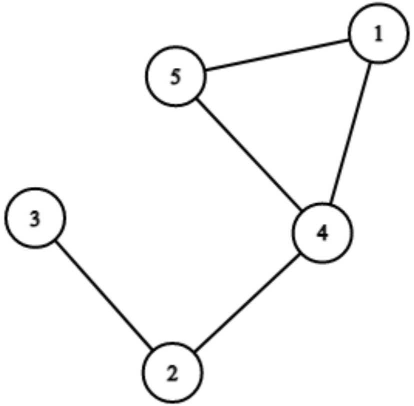
$$W(A,B) = \sum_{i \in A, j \in B} w_{ij}$$

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

Partition-Based Clustering

How do we compute these?

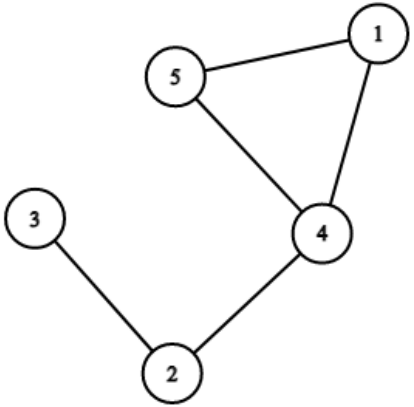
- Hard problem → heuristics
  - Greedy algorithm
  - "Spectral" approaches
- Spectral clustering approach:
  - **Adjacency** matrix



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

Partition-Based Clustering

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

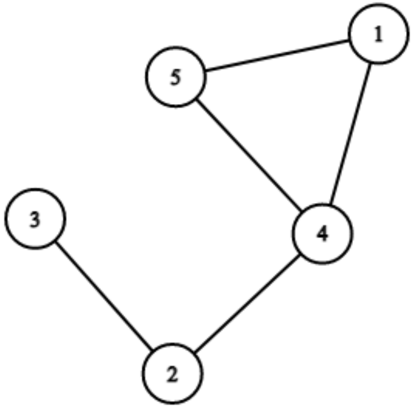


$$D = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{bmatrix} \qquad A = \begin{bmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{bmatrix}$$

Spectral Clustering

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

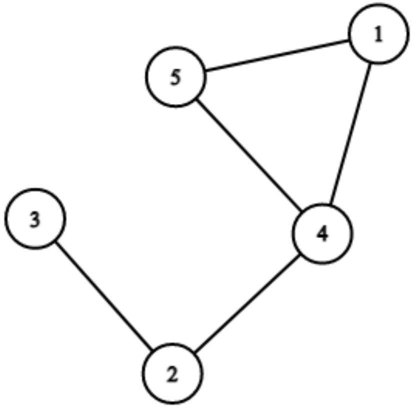
(Important tool in graph theory)



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

Spectral Clustering

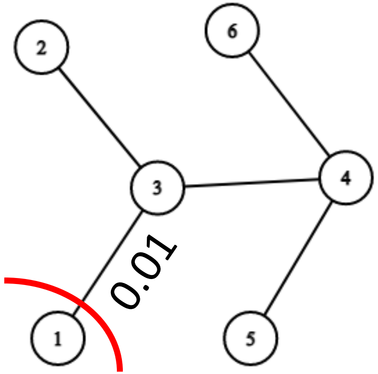
- Spectral clustering approach:
  - 1. Compute **Laplacian** $L = D - A$
  - 1a (optional): compute normalized Laplacian:
    $L = I - D^{-1/2}AD^{-1/2}$, or $L = I - D^{-1}A$
  - 2. Compute j **smallest** eigenvectors of L
  - 3. Set U to be the n x j matrix with $u_1, \ldots, u_j$ as columns. Take the n rows formed as points.
  - 4. Run k-means on the representations.

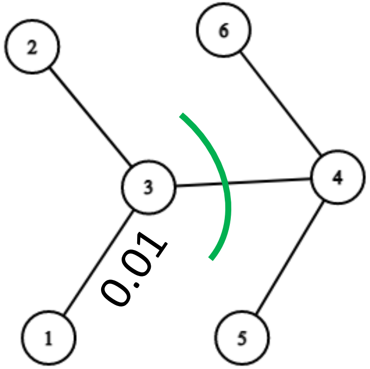


Why normalized Laplacian?

Want: partition V into V_1 and V_2

- Implies a graph "cut"
- One idea: minimize the **weight** of the cut
  - Downside: might only get 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!**

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

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

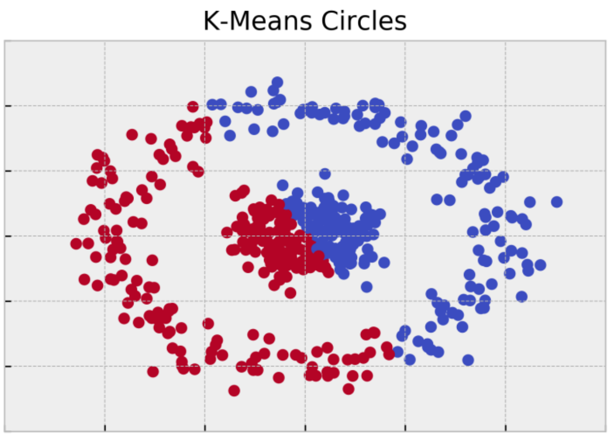
Spectral Clustering

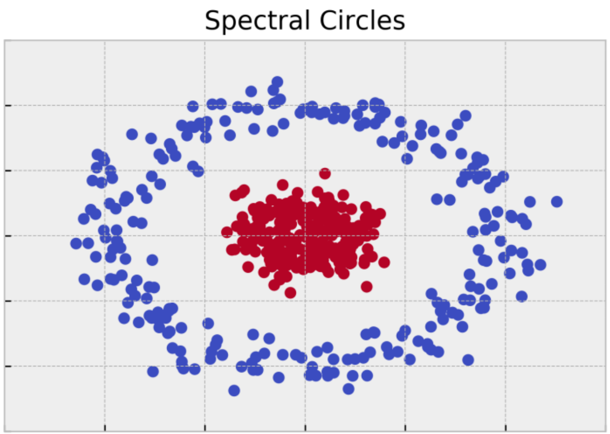
- Compare/contrast to **PCA**:
  - Use an **eigendecomposition /** dimensionality reduction
    - But, run on Laplacian (not covariance); use smallest eigenvectors, not largest
- Intuition: Laplacian encodes structure information
  - “Lower” eigenvectors give partitioning information

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

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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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 **(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

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

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- A. Only (i)
- B. Only (ii) and (iii)
- C. Only (i) and (ii)
- **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?

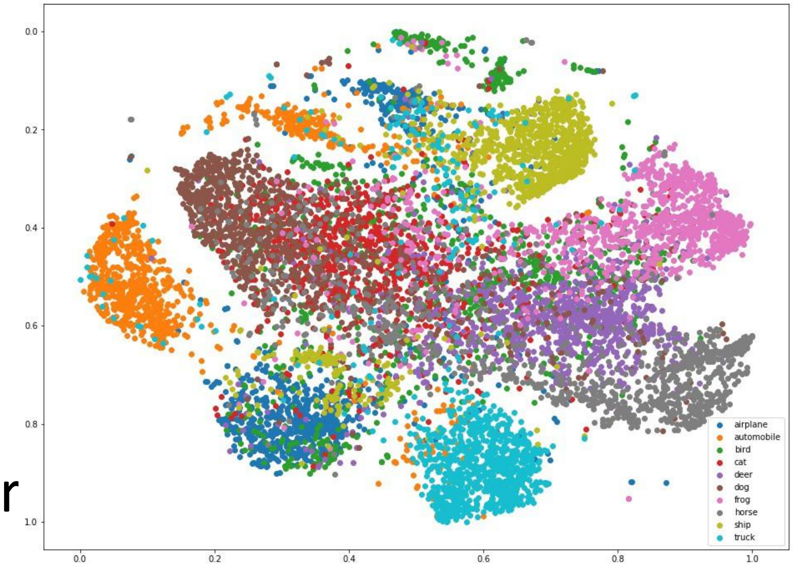
(i) Supervised learning (ii) PCA (iii) k-means clustering

- (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 are **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?
  - Reducing dimensionality to 2-3 dimensions allows people to visualize data points and their relationships.

Dimensionality Reduction & Visualization

Run PCA on MNIST

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

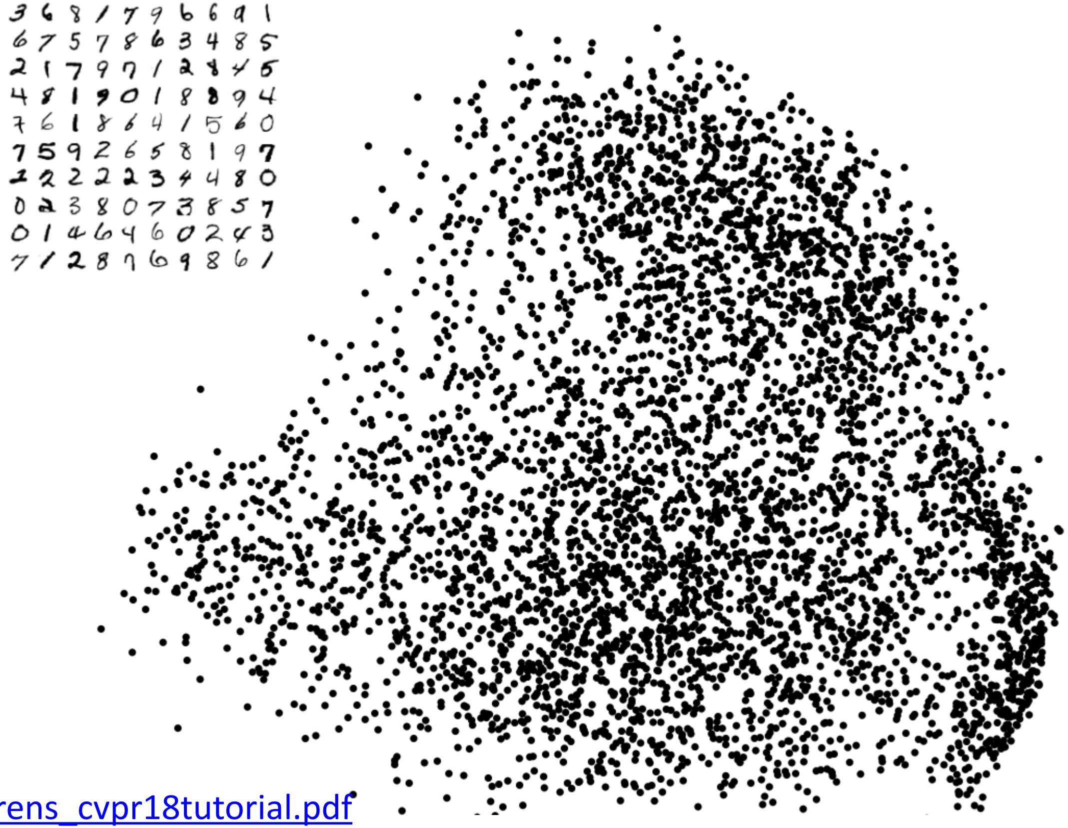


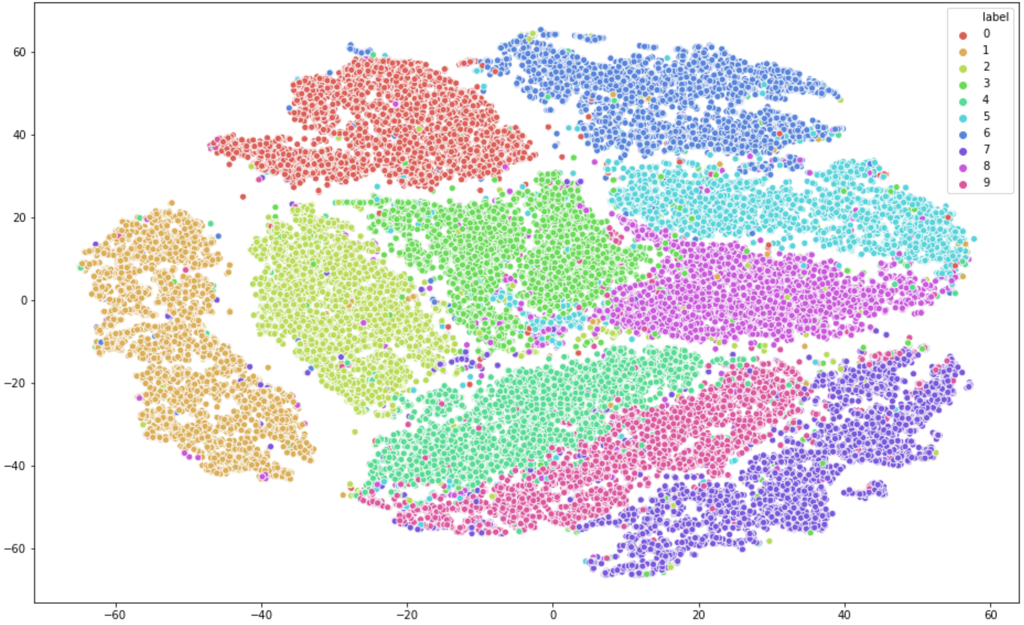
Image source:
http://deeplearning.csail.mit.edu/slide_cvpr2018/laurens_cvpr18tutorial.pdf

Visualization: **T-SNE**

Typical dataset: MNIST

- **T-SNE**: project data into just 2 dimensions
- Try to maintain structure

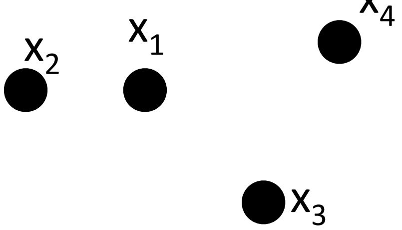
- MNIST Example
- **Input**: $x_1, x_2, \ldots, x_n$
- **Output**: 2D/3D $y_1, y_2, \ldots, y_n$



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:

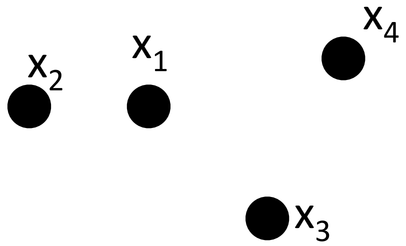
$$p_{j|i} = \frac{\exp(-\|x_i - x_j\|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|x_i - x_k\|^2 / 2\sigma_i^2)} \quad p_{ij} = \frac{1}{2n}(p_{j|i} + p_{i|j})$$

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

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

KL Divergence
between p and q
(Measures dissimilarity between probability distributions)

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 lectures.

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

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

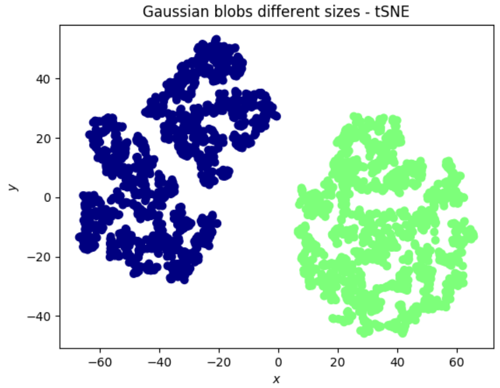
Visualization: **T-SNE**

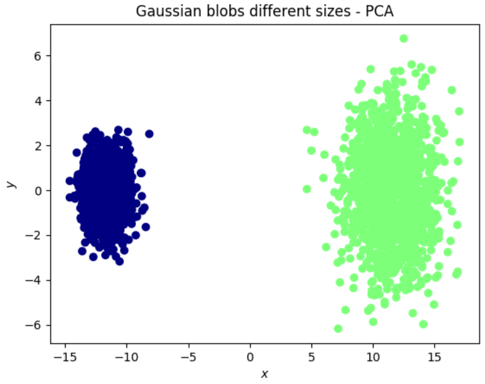
t-SNE vs PCA?

- "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 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

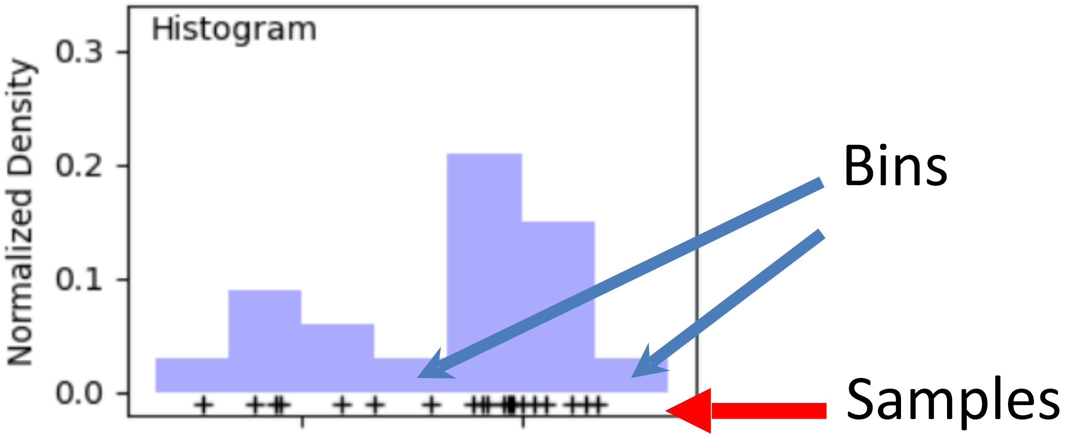
Goal: given samples $x_1, \ldots, x_n$ from some distribution *P,* estimate P.

- 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

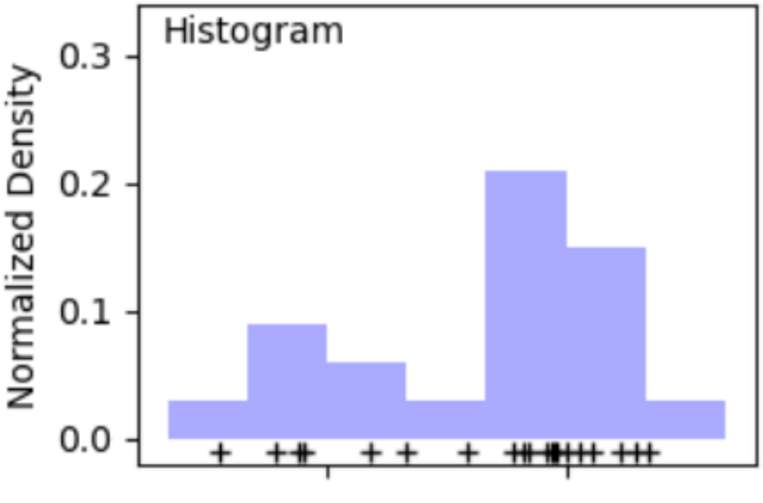
Goal: given samples $x_1, \ldots, x_n$ from some distribution P, estimate P.

Downsides:

i) High-dimensions: most bins are empty.

ii) Not continuous.

iii) How to choose bins?



Kernel Density Estimation

Goal: given samples x_1, …, 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