CS 540 Introduction to Artificial Intelligence
Unsupervised Learning II

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October 7, 2021

Slides created by Fred Sala [modified by Josiah Hanna]

Announcements

- **Homeworks**:
  - HW4 due Tuesday
- Class roadmap:

Tuesday, Sept 28	Natural Language Processing	Slides	HW 2 Due, HW 3 Released
Thursday, Sept 30	Machine Learning: Introduction		
Tuesday, Oct 5	Machine Learning: Unsupervised Learning I		HW 3 Due, HW 4 Released
Thursday, Oct 7	Machine Learning: Unsupervised Learning II		
Tuesday, Oct 12	Machine Learning: Linear Regression		HW 4 Due, HW 5 Released
Thursday, Oct 14	Machine Learning: K-Nearest Neighbors & Naive Bayes		
Everything below here is tentative and subject to change.			
Tuesday, Oct 19	Machine Learning: Neural Network I (Perceptron)		HW 5 Due, HW 6 Released
Thursday, Oct 21	Machine Learning: Neural Network II		
Tuesday, Oct 26	Machine Learning: Neural Network III		
MIDTERM EXAM October 28			

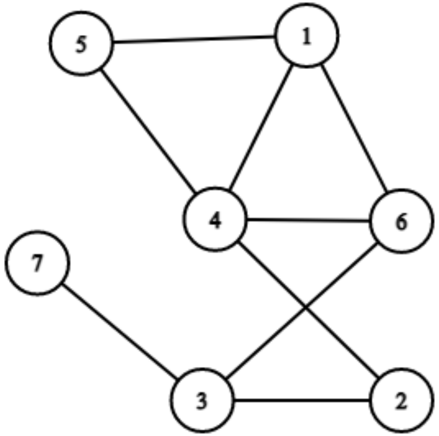
Outline

- 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

Other Types of Clustering

Graph-based/proximity-based

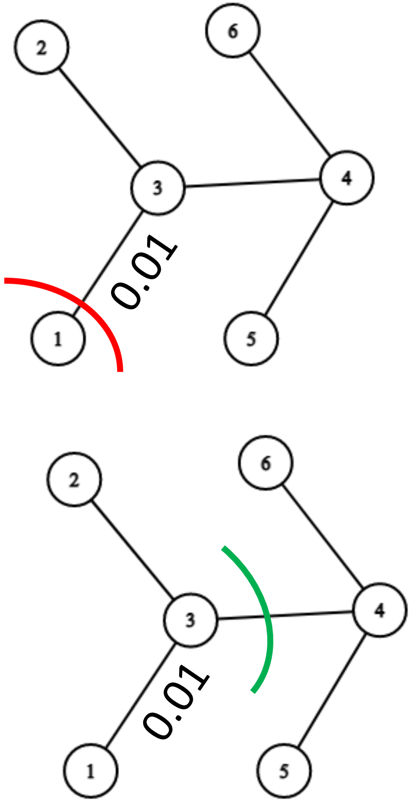
- Recall: Graph G = (V,E) has vertex set V, edge set E.
  - Edges can be weighted or unweighted
  - Encode **similarity**
- Don’t need vectors here
  - Just edges (and maybe weights)



Graph-Based Clustering

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



Partition-Based Clustering

Want: partition V into V_1 and V_2

- Just minimizing weight isn't good… want **balance!**
- **Approaches:**

$$\mathrm{Cut}(V_1,V_2)=\frac{\mathrm{Cut}(V_1,V_2)}{|V_1|}+\frac{\mathrm{Cut}(V_1,V_2)}{|V_2|}$$

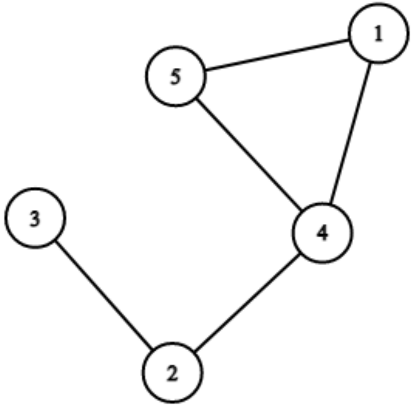
$$\mathrm{NCut}(V_1,V_2)=\frac{\mathrm{Cut}(V_1,V_2)}{\sum_{i\in V_1} d_i}+\frac{\mathrm{Cut}(V_1,V_2)}{\sum_{i\in V_2} d_i}$$

Sum of edge weights at vertex

Partition-Based Clustering

How do we compute these?

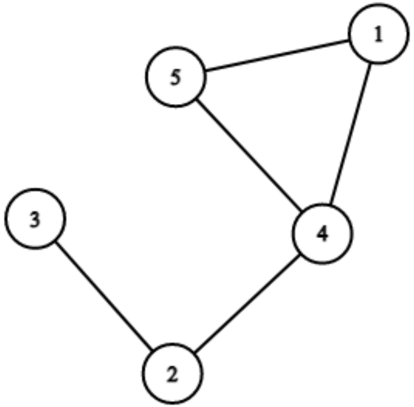
- Hard problem → heuristics
  - Greedy algorithm
  - "Spectral" approaches
- Spectral clustering approach:
  - **Adjacency** matrix



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

Partition-Based Clustering

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

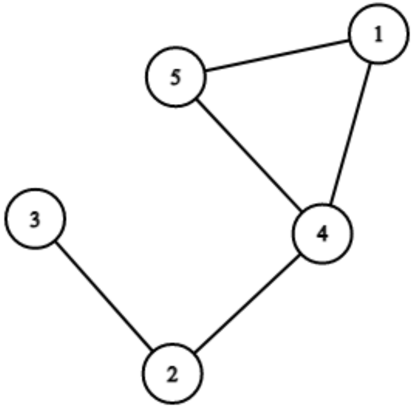


$$D = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{bmatrix} \quad A = \begin{bmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{bmatrix}$$

Spectral Clustering

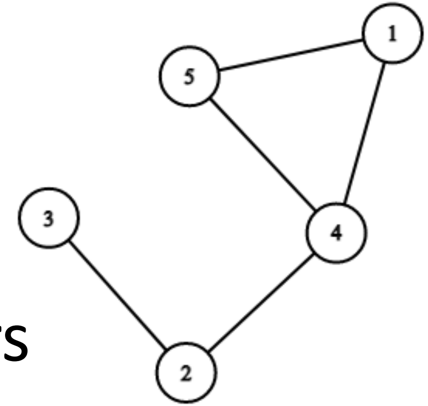
- Spectral clustering approach:
  - 1. Compute **Laplacian** L = D – A

(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** L = D – A
  - 2. Compute *k* **smallest** eigenvectors
  - 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

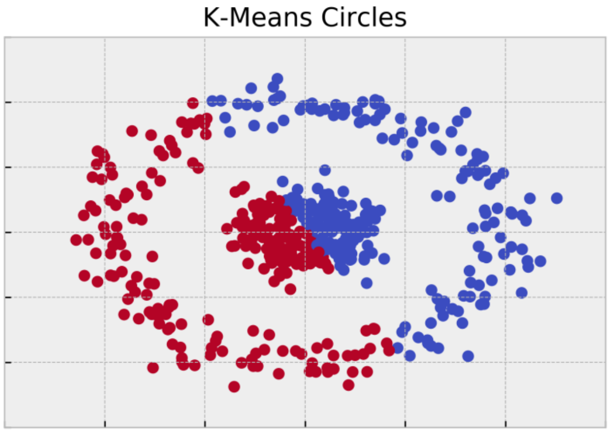
Spectral Clustering

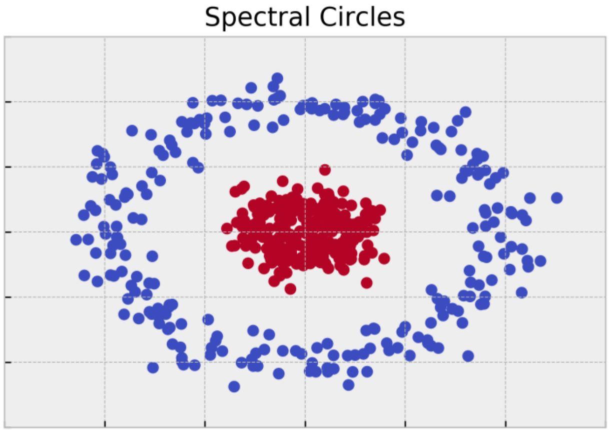
- Compare/contrast to **PCA**:
  - Use an **eigendecomposition /** dimensionality reduction
    - But, run on Laplacian (not covariance); use smallest eigenvectors, not largest
- Intuition: Laplacian encodes structure information
  - “Lower” eigenvectors give partitioning information

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

Break & Quiz

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

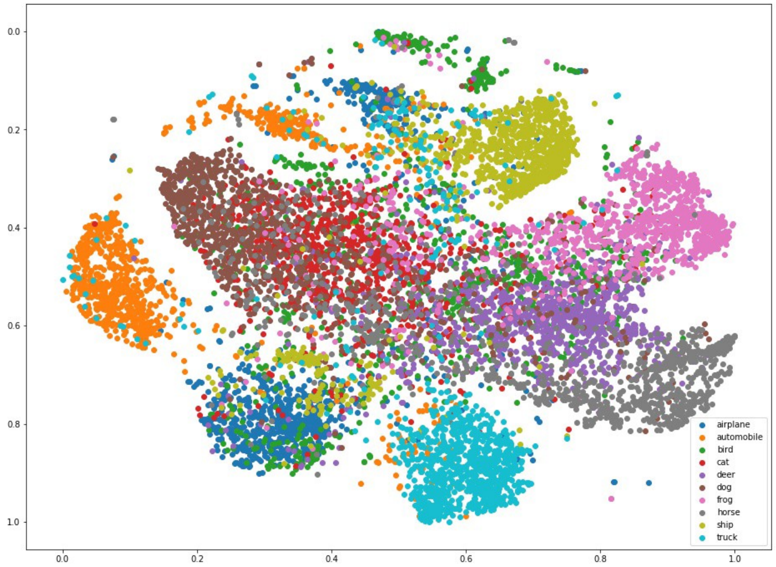
(i) Supervised learning (ii) PCA (iii) k-means clustering

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

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

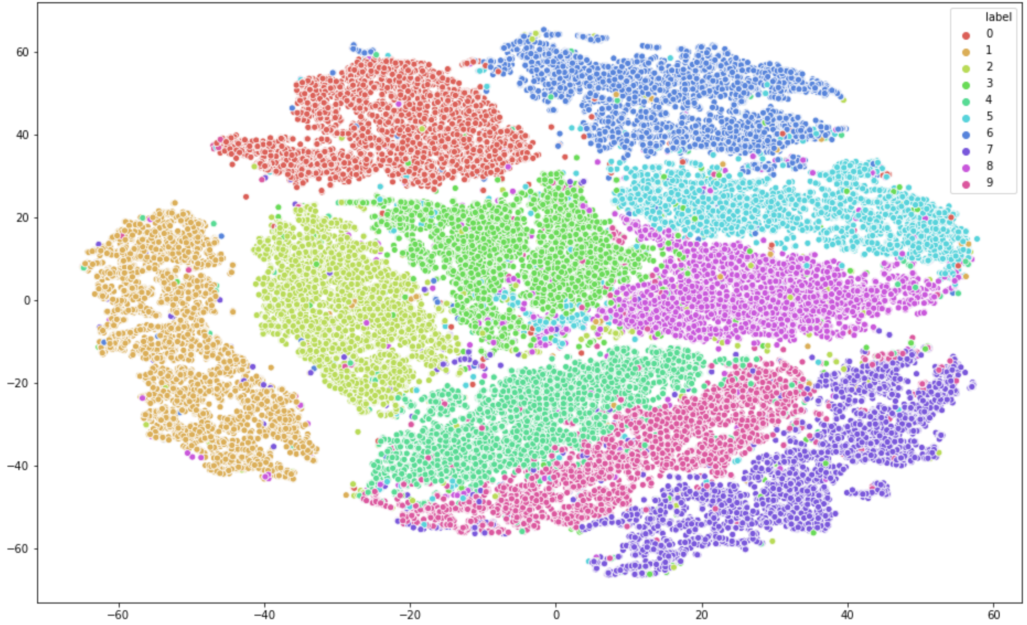
- Dimensionality reduction?

Visualization: **T-SNE**

Typical dataset: MNIST

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

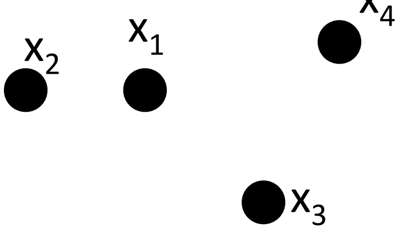
- MNIST Example
- **Input**: $x_1, x_2, \ldots, x_n$
- **Output**: 2D/3D $y_1, y_2, \ldots, y_n$



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:

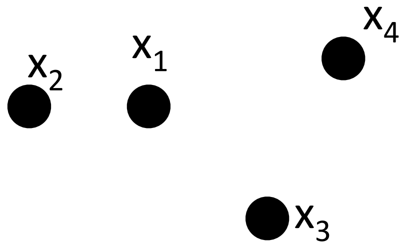
$$p_{j|i} = \frac{\exp(-\|x_i - x_j\|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|x_i - x_k\|^2 / 2\sigma_i^2)} \qquad p_{ij} = \frac{1}{2n}(p_{j|i} + p_{i|j})$$

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

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

Low dim representation

and minimize

$$\sum_i \sum_j p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}$$

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!

$$\sum_i \sum_j p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}$$

KL Divergence between p and q

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

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

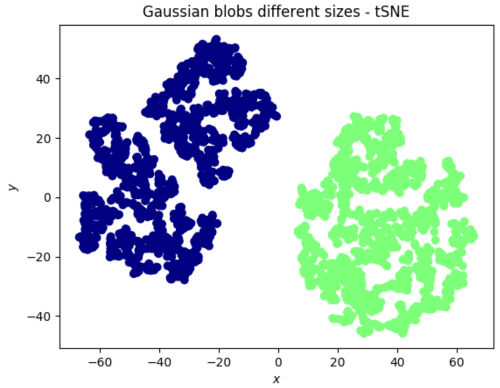
Visualization: **T-SNE**

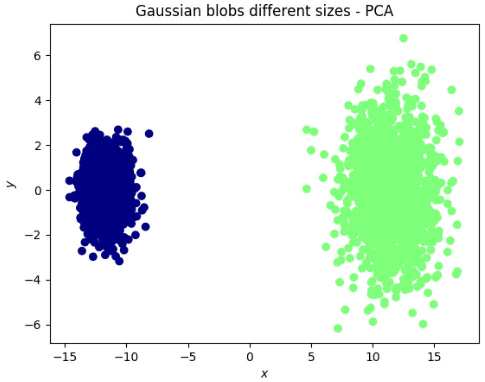
t-SNE vs PCA?

- “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

Short Intro to Density Estimation

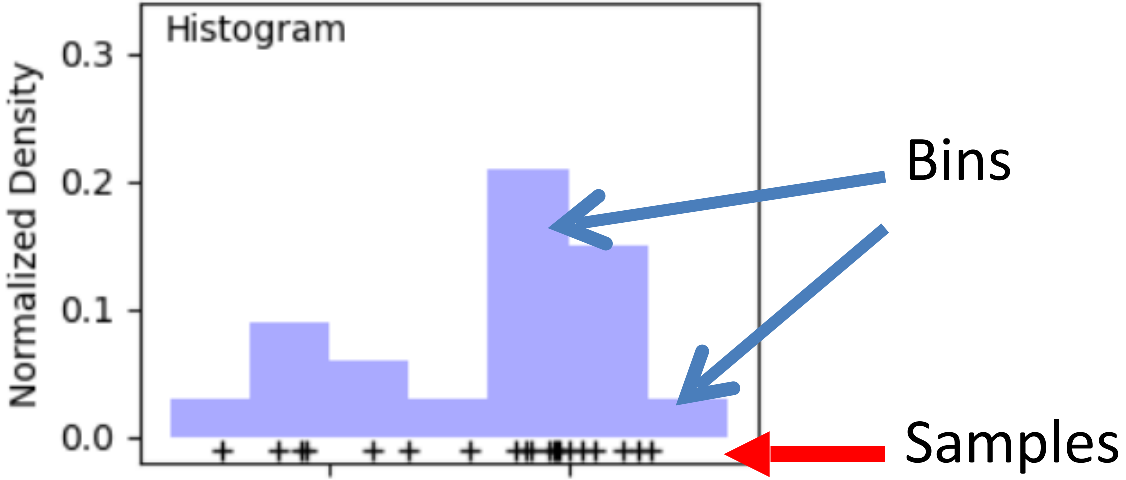
Goal: given samples $x_1, \ldots, x_n$ from some distribution P, estimate P.

- 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

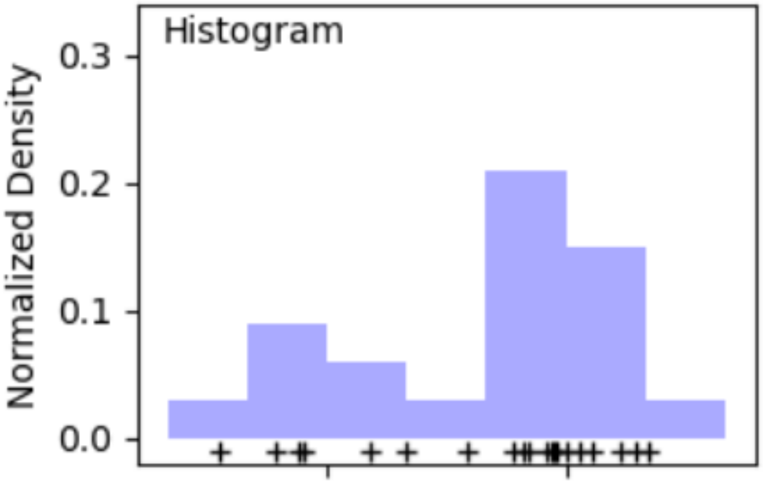
Goal: given samples $x_1, \ldots, x_n$ from some distribution P, estimate P.

Downsides:

i) High-dimensions: most bins 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

Gaussian kernels

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

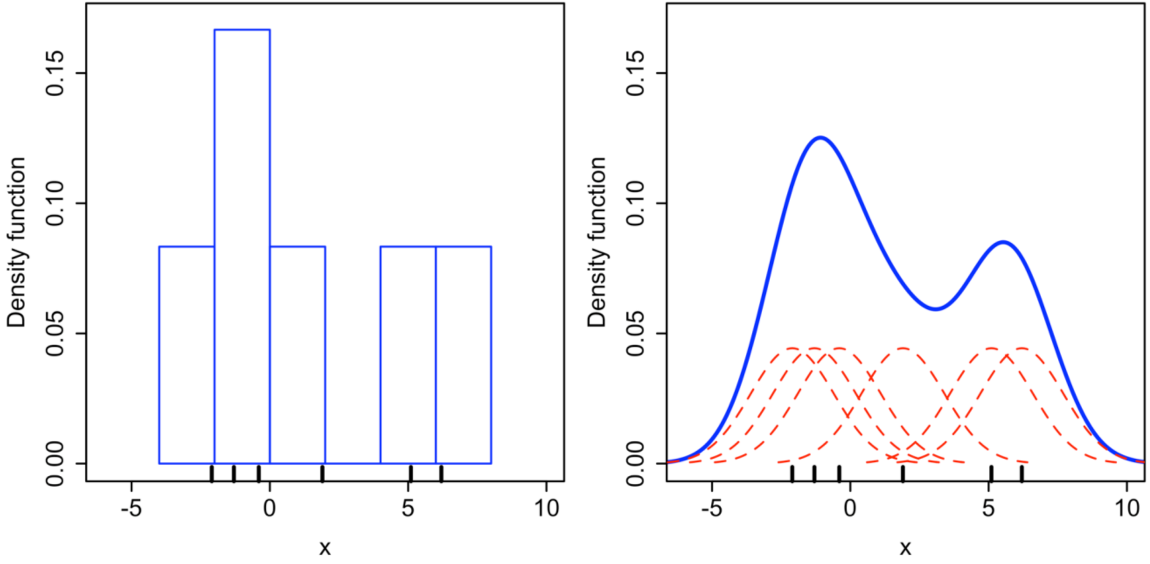
Mean at each point

Variance parameter

Kernel Density Estimation

Idea: represent density as combination of kernels

- "Smooth" out the histogram



Break & Quiz

Q 1.1: Which of the following is not true?

- A. Using a Gaussian kernel for KDE, all possible values for x_i will have non-zero probability.
- B. The goal of KDE is to approximate the true probability distribution function of X.
- C. When using a histogram, every bucket must be represented explicitly in memory
- D. With some kernels, KDE can assign zero probability to some subset of values for x_i.