CSE/STAT 416
K-Means Clustering

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Adapted from Hunter Schafer’s slides
We have now finished our study on supervised learning!

**This Week:** Clustering with text data

**Next Week:** Dimensionality Reduction, Recommender Systems

**Next-Next Week:** Course Wrap-Up & Final

**Deadlines:**
- HW5 due TOMORROW, Tues 8/2 11:59PM
  - Submit Concept & Programming on Gradescope
- HW6 Released Wed 8/3
- LR 7 due Fri 8/5 11:59PM

**Notes on the end of the quarter**
- Guest Panel Extra Credit: Mon 8/15 (during lecture)
- HW7 due Tues 8/16, **NO LATE DAYS**
- Take-Home Final Exam: Wed 8/17 – Thurs 8/18
Addressing LR Questions
What is the result of applying a convolution using this kernel on this input image?

Use 1x1 zero padding and a 2x2 stride.

Result: $3 \times 3$
Kernel 3 x 3, stride of 1
Another core operation that is similar to a convolution is a **pool**. 

Idea is to down sample an image using some operation

Combine local pixels using some operation (e.g. max, min, average, median, etc.)

Typical to use **max pool** with 2x2 filter and stride 2

Tends to work better than average pool
Consider solving a digit recognition task on 28x28 images. Suppose I wanted to use a fully connected hidden layer with 84 neurons.

**Weight Sharing**

In a conv layer w/ a KxK kernel, I input channels, and d output channels, the num params to be learnt are $k \cdot k \cdot I \cdot d$

**With Convolutions** (assume $n_1=10$, $n_2=20$)

- **Conv1**: $5 \cdot 5 \cdot 10 = 250$
- **MaxPool1**: 0 weights
- **Conv2**: $5 \cdot 5 \cdot 10 \cdot 20 = 5000$
- **MaxPool2**: 0 weights

**Total**: $250 + 5000 \cdot 27,720 = 32,970 < 66k$

**A inputs flattened**: $4 \cdot 4 \cdot 20 = 320$

**FC component**: $320 \cdot 84 + 84 \cdot 10 = 27,720$
Hyperparameter Optimization

How do we choose hyperparameters to train and evaluate?

Grid search:
- Hyperparameters on 2d uniform grid

Random search:
- Hyperparameters randomly chosen

Bayesian Optimization:
- Hyperparameters adaptively chosen
Transfer Learning

Share the weights for the general part of the network

Neural net trained for Task 1: cat vs. dog

- More generic
  - Can be used as feature extractor

- Very specific
  - To Task 1
  - Should be ignored for other tasks

Keep weights fixed! Re-train

Use simple classifier e.g., logistic regression, SVMs, nearest neighbor,…
Clustering Overview
Recap

For the past 6 weeks, we have covered different **supervised learning** algorithms

Now, we’re going to explore **unsupervised learning** methods where don’t have labels / outputs in your datasets anymore.

Note that several of the concepts you learnt for supervised learning, such as cross-validation, overfitting, bias-variance tradeoff, accuracy, error, etc. no longer apply in unsupervised learning!
Unsupervised Learning

A type of machine learning that detects underlying patterns in unlabeled data.

Examples of unsupervised learning tasks:
- Cluster similar articles together.
- Cluster gene sequences.
- Recommend items, searches, movies, etc.

Coupled indoor navigation for people who are blind
A Nanavati, XZ Tan, A Steinleid - Companion of the 2018 ACM/IEEE ... 2018 - dl.acm.org
This paper presents our design of an autonomous navigation system for a mobile robot that guides people who are blind and low vision in indoor settings. It begins by presenting user …
ML Pipeline (Supervised)

- Historical Bias
- Representation Bias
- Measurement Bias

- Deployment Bias
ML Pipeline (Unsupervised)

- Training Data
- Pre-Processing
- ML model
- Optimization algorithm
- Quality metric

- Historical Bias
- Representation Bias
- Measurement Bias

- Deployment Bias
Note that we’re not talking about learning user preferences (yet – come back next week 😊).

Our case study is document retrieval. Given that someone read a particular article, what similar articles would you recommend (without personalization)?
What if the labels are known? Given labeled training data.

Can do multi-class classification methods to predict label.

However, not all articles fit cleanly into one label.

Further, oftentimes real-world data doesn’t have labels.
In many real world contexts, there aren’t clearly defined labels so we won’t be able to do classification. We will need to come up with methods that uncover structure from the (unlabeled) input data $X$.

**Clustering** is an automatic process of trying to find related groups within the given dataset.
Define Clusters

In their simplest form, a cluster is defined by

- The location of its center (centroid)
- Shape and size of its spread

Clustering is the process of finding these clusters and assigning each example to a particular cluster.

\( x_i \) gets assigned \( z_i \in [1, 2, \ldots, k] \)

Usually based on closest centroid

Will define some kind of objective function for a clustering that determines how good the assignments are

Based on distance of assigned examples to each cluster.

Close distance reflects strong similarity between datapoints.
When Might This Work?

Clustering is easy when distance captures the clusters.

Ground Truth (not visible)                      Given Data

Easy?

Impossible?

Maybe?
Not Always Easy

There are many clusters that are harder to learn with this setup. Distance does not determine clusters.
Think of 1-2 problems that you might want to use clustering for. For each problem, describe:

- Why unsupervised learning is the right approach.
- What the input features are for the clustering algorithm.
- What clusters you hypothesize would emerge.
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Embedding
Text Data
Revisited

TF-IDF
Converting Text to Numbers (Vectorizing):

**Bag of Words**

**Idea**: One feature per word!

Example: "Sushi was great, the food was awesome, but the service was terrible"

<table>
<thead>
<tr>
<th>sushi</th>
<th>was</th>
<th>great</th>
<th>the</th>
<th>food</th>
<th>awesome</th>
<th>but</th>
<th>service</th>
<th>terrible</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3</td>
<td>1</td>
<td>2</td>
<td>1</td>
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This has to be too simple, right?

Stay tuned (today and Wed) for issues that arise and how to address them 😊
Bag of Words

Pros
- Very simple to describe
- Very simple to compute

Cons
- Common words like “the” and “a” dominate counts of uncommon words
- Often it’s the uncommon words that uniquely define a doc.
TF-IDF (Term Frequency Inverse Document Frequency)

**Goal:** Emphasize important words

- Appear frequently in the document (common locally)
- Appears rarely in the corpus (rare globally)

\[
\text{TF} = \frac{\text{word counts}}{\text{num words}}
\]

\[
\text{IDF} = \log \frac{\text{# docs}}{1 + \text{# docs using word}}
\]

 Corpus of 1000 documents
 "the" occurs in doc \# 200 times

Do a pair-wise multiplication to compute the TF-IDF for each word

Words that appear in every document will have a small IDF making the TF-IDF small!
Understanding IDF

IDF goes from 0, when all documents have the word, to \( \log(\# \text{docs}) \), when no docs have the word.

\[
\text{IDF} = \log \left( \frac{\# \text{docs}}{1 + \# \text{docs w/ word}} \right)
\]

Assume \( \# \text{ docs} \) is large
Recall the Bag of Words Example from Lecture 5

<table>
<thead>
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<th></th>
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Review

“Sushi was great, the food was awesome, but the service was terrible”

“Terrible food; the sushi was rancid.”

Note that if we divide the Bag of Words embedding by the num words in the document, we get the TF!
Think

1 min

Which word(s) have the largest IDF? Which word(s) have the smallest IDF?

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| Sushi was great the food awesome but service terrible rancid |
|-----------------|-----------------|----------------|----------------|-----------------|-----------------|----------------|
| 1 3  1  2  1  1 1 1 1 1 0 |
| 1 1 0 1  1  0 0 0 1 1 1 |
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Brain Break

3:29
K-Means Clustering
K-Means Clustering Algorithm

We define the criterion of assigning point to a cluster based on its distance.
Shorter distance => Better Clustering

Algorithm
Given a dataset of n datapoints and a particular choice of k

Step 0: Initialize cluster centroids randomly

Repeat until convergence:
  Step 1: Assign each example to its closest cluster centroid
  Step 2: Update the centroids to be the average of all the points assigned to that cluster
Step 0

Start by choosing the initial cluster centroids

A common default choice is to choose centroids $\mu_1, \ldots, \mu_k$ randomly

Will see later that there are smarter ways of initializing
Step 1

Assign each example to its closest cluster centroid

For \( i = 1 \) to \( n \)

\[
\begin{align*}
z_i &\leftarrow \arg\min_{j \in [k]} \left\| \mu_j - x_i \right\|_2^2
\end{align*}
\]
Step 2

Update the centroids to be the mean of points assigned to that cluster.

$$\mu_j = \frac{\sum_{i=1}^{n} 1\{z_i = j\}x_i}{\sum_{i=1}^{n} 1\{z_i = j\}} = \text{sum of datapoints assigned to cluster } j \over \text{number of datapoints assigned to cluster } j$$

Computes center of mass for cluster!
Repeat until convergence

Repeat Steps 1 and 2 until convergence
k-Means Stopping Condition

Stopping conditions
- Cluster assignments haven’t changed
- Centroids haven’t changed
- Some number of max iterations have been passed

What will it converge to?
- Local optima
- Global optima
- Neither
Visualizing k-Means
What cluster assignment would result from these centroids?

(A)  
(B)  
(C)  
(D)
What cluster assignment would result from these centroids?

(A) X  
(B) ✓  
(C) X
In what direction would each of the centroids (roughly) move?

(A)

(B)

(C)

(D)
In what direction would each of the centroids (roughly) move?
No more changes
Different $k$ gives different results
Effect of Initialization
Different initialization can give different results

Initialization

Final Clusters
You are clustering news articles using the features “# sport” and “# injury.” How would you interpret these clusters?

“This is a cluster of ...[some characterization]... articles.”
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“This is a cluster of …[some characterization]… articles.”
Effect of initialization

What does it mean for something to converge to a local optima?

Some initialization can be bad and affect the quality of clustering

Initialization will greatly impact results!
Making sure the initialized centroids are “good” is critical to finding quality local optima. Our purely random approach was wasteful since it’s very possible that initial centroids start close together.

**Idea:** Try to select a set of points farther away from each other.

**k-means++** does a slightly smarter random initialization

1. Choose first cluster $\mu_1$ from the data uniformly at random
2. For each datapoint $x_i$, compute the distance between $x_i$ and the closest centroid from the current set of centroids (starting with just $\mu_i$). Denote that distance $d(x_i)$.
3. Choose a new centroid from the remaining data points, where the probability of $x_i$ being chosen is proportional to $d(x_i)^2$.
4. Repeat 2 and 3 until we have selected $k$ centroids.
k-means++

Example

Start by picking a point at random

Then pick points proportional to their distances to their centroids

This tries to maximize the spread of the centroids!
k-means++

Pros / Cons

Pros
- Improves quality of local minima
- Faster convergence to local minima

Cons
- Computationally more expensive at beginning when compared to simple random initialization
Assessing Performance
Which clustering would I prefer?

Don’t know, there is no “right answer” in clustering 🤷‍♂️. Depends on the practitioner’s domain-specific knowledge and interpretation of results!
k-means is trying to optimize the **heterogeneity** objective

\[
\arg\min_{\mu} \sum_{j=1}^{k} \sum_{i=1}^{n} 1\{z_i = j\} \left\| \mu_j - x_i \right\|_2^2
\]

**total distance between points in that cluster and the centroid**
**sum over clusters**
Coordinate Descent

$k$-means is trying to minimize the heterogeneity objective

\[
\arg\min_{\mathbf{z}, \mathbf{\mu}} \sum_{j=1}^{k} \sum_{i=1}^{n} \mathbf{1}\{z_i = j\} \left\| \mu_j - x_i \right\|_2^2
\]

Step 0: Initialize cluster centers

Repeat until convergence:

Step 1: Assign each example to its closest cluster centroid

Step 2: Update the centroids to be the mean of all the points assigned to that cluster

\textbf{Coordinate Descent} alternates how it updates parameters to find minima. On each of iteration of Step 1 and Step 2, heterogeneity decreases or stays the same.

=> Will converge in finite time
Consider training k-means to convergence for different values of k. Which of the following graphs shows how the heterogeneity objective will change based on the value of k?
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How to Choose k?

No right answer! Depends on your application.

General, look for the “elbow” in the graph.

Note: You will usually have to run k-means multiple times for each k.
k-means works well for well-separated hyper-spherical clusters of the same size
Think

1 min

Identify the similarities and differences between the following:

- k-means & k nearest neighbors
- clustering & classification
Identify the similarities and differences between the following:

- **k-means & k nearest neighbors**
- **clustering & classification**
Clustering vs Classification

Clustering looks like we assigned labels (by coloring or numbering different groups) but we didn’t use any labeled data.

In clustering, the “labels” don’t have meaning. To give meaning to the labels, human inputs is required.

Classification learns from minimizing the error between a prediction and an actual label.

Clustering learns by minimizing the distance between points in a cluster.

Classification quality metrics (accuracy / loss) do not apply to clustering (since there is no label).

You can’t use validation set / cross-validation to choose the best choice of k for clustering.
Curse of Dimensionality
High Dimensions

Methods like k-NN and k-means that rely on computing distances start to struggle in high dimensions.

As the number of dimensions grow, the data gets sparser!

Need more data to make sure you cover all the space in high dim.
Data Moves Farther Apart in Higher Dimensions

It’s believable with more dimensions the data becomes more sparse, but what’s even weirder is the sparsity is not uniform!

As $D$ increases, the “mass” of the space goes towards the corners.

Most of the points aren’t in the center.

The distance between points gets really high!
Practicalities

Have to pay attention to the number of dimensions with distance-based methods (k-means clustering, also k nearest neighbors).

Very tricky if \( n < D \)

Can run into some strange results if \( D \) is very large

Later, we will talk about ways of trying to do dimensionality reduction in order to reduce the number of dimensions here.
Recap

Differences between classification and clustering
What types of clusters can be formed by k-means
K-means algorithm
Convergence of k-means
How to choose k
Better initialization using k-means++