Clustering
High Dimensional Data

- **High dim. data**
  - Locality sensitive hashing
  - Clustering
  - Dimensionality reduction

- **Graph data**
  - Community Detection
  - Spam Detection

- **Infinite data**
  - Filtering streams
  - Web advertising on streams

- **Machine learning**
  - Decision Trees
  - Perceptron, kNN

- **Apps**
  - Recommender systems
  - Association Rules
  - Duplicate document detection

Jure Leskovec, Stanford CS246: Mining Massive Datasets
The Problem of Clustering

Given a set of points, with a notion of distance between points, group the points into some number of clusters, so that

- Members of the same cluster are close/similar to each other
- Members of different clusters are dissimilar

Usually:

- Points are in a high-dimensional space
- Similarity is defined using a distance measure
  - Euclidean, Cosine, Jaccard, edit distance, ...
Example: Clusters & Outliers
A catalog of 2 billion “sky objects” represents objects by their radiation in 7 dimensions (frequency bands)

Problem: Cluster similar objects, e.g., galaxies, nearby stars, quasars, etc.

Sloan Digital Sky Survey
Intuitively: Music can be divided into categories, and customers prefer a few genres

- But what are categories really?

Represent a CD by a set of customers who bought it

- Similar CDs have similar sets of customers, and vice-versa
Clustering Problem: Music CDs

Space of all CDs:
- Think of a space with one dim. for each customer
  - Values in a dimension may be 0 or 1 only
  - A CD is a “point” in this space \((x_1, x_2, ..., x_d)\), where \(x_i = 1\) iff the \(i^{th}\) customer bought the CD
- For Amazon, the dimension is tens of millions

Task: Find clusters of similar CDs
Finding topics:

- Represent a document by a vector $(x_1, x_2, ..., x_k)$, where $x_i = 1$ iff the $i$\textsuperscript{th} word (in some order) appears in the document.
  - It actually doesn’t matter if $k$ is infinite; i.e., we don’t limit the set of words.

- Documents with similar sets of words may be about the same topic.
We have a choice when we think of documents as sets of words or shingles:

- **Sets as vectors:** Measure similarity by the cosine distance
- **Sets as sets:** Measure similarity by the Jaccard distance
- **Sets as points:** Measure similarity by Euclidean distance
Clustering is a hard problem!
Why is it hard?

- Clustering in two dimensions looks easy
- Clustering small amounts of data looks easy
- And in most cases, looks are not deceiving

- Many applications involve not 2, but 10 or 10,000 dimensions
- High-dimensional spaces look different: Almost all pairs of points are very far from each other --> The Curse of Dimensionality
Example: Curse of Dimensionality

- Take 10,000 uniform random points on [0,1] line. Assume query point is at the origin.
- To get 10 nearest neighbors we must go to distance $10/10,000 = 0.001$ on the average.
- In 2-dim we must go $\sqrt{0.001} = 0.032$ to get a square that contains 0.001 volume.
- In d-dim we must go $(0.001)^{1/d}$.
- So, in 10-dim to capture 0.1% of the data we need 50% of the range.
Example: Curse of Dimensionality

Curse of Dimensionality: All points are very far from each other.
Overview: Methods of Clustering

- **Hierarchical:**
  - **Agglomerative** (bottom up):
    - Initially, each point is a cluster
    - Repeatedly combine the two “nearest” clusters into one
  - **Divisive** (top down):
    - Start with one cluster and recursively split it

- **Point assignment:**
  - Maintain a set of clusters
  - Points belong to the “nearest” cluster
Hierarchical Clustering
Hierarchical Clustering

- **Key operation:**
  Repeatedly combine two nearest clusters

- **Three important questions:**
  1) How do you represent a cluster of more than one point?
  2) How do you determine the “nearness” of clusters?
  3) When to stop combining clusters?
Which is Better?

- Point assignment good when clusters are nice, convex shapes:
- Hierarchical can win when shapes are weird:
  - Note both clusters have essentially the same centroid.

Aside: if you realized you had concentric clusters, you could map points based on distance from center, and turn the problem into a simple, one-dimensional case.
Key operation: Repeatedly combine two nearest clusters

(1) How to represent a cluster of many points?
   Key problem: As you merge clusters, how do you represent the “location” of each cluster, to tell which pair of clusters is closest?
   Euclidean case: each cluster has a centroid = average of its (data)points

(2) How to determine “nearness” of clusters?
   Measure cluster distances by distances of centroids
Example: Hierarchical clustering

Data:
- \( \circ \) ... data point
- \( \times \) ... centroid

Dendrogram
What about the Non-Euclidean case?

- The only “locations” we can talk about are the points themselves
  - i.e., there is no “average” of two points

**Approach 1:**

1. (1.1) How to represent a cluster of many points? *clustroid* = (data)point “closest” to other points
2. (1.2) How do you determine the “nearness” of clusters? Treat clustroid as if it were centroid, when computing inter-cluster distances
(1.1) How to represent a cluster of many points? 

clusroid = point “closest” to other points

Possible meanings of “closest”:

- Smallest maximum distance to other points
- Smallest average distance to other points
- Smallest sum of squares of distances to other points
- For distance metric $d$ clustroid $c$ of cluster $C$ is
  \[
  \arg \min_c \sum_{x \in C} d(x, c)^2
  \]

Centroid is the avg. of all (data)points in the cluster. This means centroid is an “artificial” point.

Clustroid is an existing (data)point that is “closest” to all other points in the cluster.
Defining “Nearness” of Clusters

(1.2) How do you determine the “nearness” of clusters? Treat clustroid as if it were centroid, when computing intercluster distances.

**Approach 2:** No centroid, just define distance

*Intercluster distance* = minimum of the distances between any two points, one from each cluster.
Cohesion

**Approach 3:** Pick a notion of *cohesion* of clusters

- Merge clusters whose *union* is most cohesive

**Approach 3.1:** Use the *diameter* of the merged cluster = maximum distance between points in the cluster

**Approach 3.2:** Use the *average distance* between points in the cluster

**Approach 3.3:** Use a *density-based approach*

- Take the diameter or avg. distance, and divide by the number of points in the cluster
When do we stop merging clusters?

- When some number \( k \) of clusters are found (assumes we know the number of clusters)
- When stopping criterion is met
  - Stop if diameter exceeds threshold
  - Stop if density is below some threshold
  - Stop if merging clusters yields a bad cluster
    - E.g., diameter suddenly jumps
- Keep merging until there is only 1 cluster left
It really depends on the shape of clusters.
   Which you may not know in advance.

**Example:** we’ll compare two approaches:

1. Merge clusters with smallest distance between centroids (or clustroids for non-Euclidean)
2. Merge clusters with the smallest distance between two points, one from each cluster
Case 1: Convex Clusters

- Centroid-based merging works well.
- But merger based on closest members might accidentally merge incorrectly.

A and B have closer centroids than A and C, but closest points are from A and C.
Case 2: Concentric Clusters

- Linking based on closest members works well
- But Centroid-based linking might cause errors
$k$-means clustering
Assumes Euclidean space/distance

Start by picking $k$, the number of clusters

Initialize clusters by picking one point per cluster

**Example:** Pick one point at random, then $k-1$ other points, each as far away as possible from the previous points

- OK, as long as there are no outliers (points that are far from any reasonable cluster)
**k-Means++**

- **Basic idea:** Pick a small sample of points $S$, cluster them by any algorithm, and use the centroids as a seed.

- In **k-means++**, sample size $|S| = k$ times a factor that is logarithmic in the total number of points.

- **How to pick sample points:** Visit points in random order, but the probability of adding a point $p$ to the sample is proportional to $D(p)^2$.
  - $D(p) = \text{distance between } p \text{ and the nearest already picked point.}$
1) For each point, place it in the cluster whose current centroid it is nearest

2) After all points are assigned, update the locations of centroids of the \( k \) clusters

3) Reassign all points to their closest centroid
   - Sometimes moves points between clusters

Repeat 2 and 3 until convergence
   - Convergence: Points don’t move between clusters and centroids stabilize
Example: Assigning Clusters

Clusters after round 1

x … data point
☐ … centroid
Example: Assigning Clusters

Clusters after round 2

x … data point
☐ … centroid
Example: Assigning Clusters

- **x** … data point
- **☐** … centroid

Clusters at the end
Getting the $k$ right

How to select $k$?

- Try different $k$, looking at the change in the average distance to centroid as $k$ increases
- Average falls rapidly until right $k$, then changes little
Example: Picking $k$

Too few; many long distances to centroid
Example: Picking $k$

Just right; distances rather short
Example: Picking $k$

Too many; little improvement in average distance
The BFR Algorithm

Extension of $k$-means to large data
BFR Algorithm

- **BFR** [Bradley-Fayyad-Reina] is a variant of *k*-means designed to handle **very large** (disk-resident) data sets.

- **Assumes** that clusters are normally distributed around a centroid in a Euclidean space:
  - Standard deviations in different dimensions may vary
    - Clusters are axis-aligned ellipses

- **Goal** is to find cluster centroids; point assignment can be done in a second pass through the data.
Efficient way to summarize clusters: Want memory required $O(\text{clusters})$ and not $O(\text{data})$

IDEA: Rather than keeping points, BFR keeps summary statistics of groups of points
- 3 sets: Cluster summaries, Outliers, Points to be clustered

Overview of the algorithm:
- 1. Initialize $K$ clusters/centroids
- 2. Load in a bag of points from disk
- 3. Assign new points to one of the $K$ original clusters, if they are within some distance threshold of the cluster
- 4. Cluster the remaining points, and create new clusters
- 5. Try to merge new clusters from step 4 with any of the existing clusters
- 6. Repeat steps 2-5 until all points are examined
Points are read from disk one main-memory-full at a time

Most points from previous memory loads are summarized by simple statistics

Step 1) From the initial load we select the initial \( k \) centroids by some sensible approach:

- Take \( k \) random points
- Take a small random sample and cluster optimally
- Take a sample; pick a random point, and then \( k-1 \) more points, each as far from the previously selected points as possible
Three Classes of Points

3 sets of points which we keep track of:

- **Discard set (DS):**
  - Points close enough to a centroid to be summarized

- **Compression set (CS):**
  - Groups of points that are close together but not close to any existing centroid
  - These points are summarized, but not assigned to a cluster

- **Retained set (RS):**
  - Isolated points waiting to be assigned to a compression set
A cluster. Its points are in the **DS**.

**Compressed sets.** Their points are in the **CS**.

Points in the **RS**

**Discard set (DS):** Close enough to a centroid to be summarized

**Compression set (CS):** Summarized, but not assigned to a cluster

**Retained set (RS):** Isolated points
For each cluster, the discard set (DS) is summarized by:

- The number of points, \( N \)
- The vector \( \text{SUM} \), whose \( i^{\text{th}} \) component is the sum of the coordinates of the points in the \( i^{\text{th}} \) dimension
- The vector \( \text{SUMSQ} \): \( i^{\text{th}} \) component = sum of squares of coordinates in \( i^{\text{th}} \) dimension
2d + 1 values represent any size cluster
- d = number of dimensions

Average in each dimension (the centroid) can be calculated as \( \text{SUM}_i / N \)
- \( \text{SUM}_i = i^{\text{th}} \) component of SUM

Variance of a cluster’s discard set in dimension \( i \) is: \( (\text{SUMSQ}_i / N) - (\text{SUM}_i / N)^2 \)
- And standard deviation is the square root of that

Next step: Actual clustering

Note: Dropping the “axis-aligned” clusters assumption would require storing full covariance matrix to summarize the cluster. So, instead of \( \text{SUMSQ} \) being a \( d \)-dim vector, it would be a \( d \times d \) matrix, which is too big!
The “Memory-Load” of Points

Steps 3-5) Processing “Memory-Load” of points:

- **Step 3)** Find those points that are “sufficiently close” to a cluster centroid and add those points to that cluster and the DS
  - These points are so close to the centroid that they can be summarized and then discarded
- **Step 4)** Use any in-memory clustering algorithm to cluster the remaining points and the old RS
  - Clusters go to the CS; outlying points to the RS

Discard set (DS): Close enough to a centroid to be summarized.
Compression set (CS): Summarized, but not assigned to a cluster
Retained set (RS): Isolated points
Steps 3-5) Processing “Memory-Load” of points:

- **Step 5) DS set:** Adjust statistics of the clusters to account for the new points
  - Add $N_s$, $SUM_s$, $SUMSQ_s$
  - Consider merging compressed sets in the DS

- **If this is the last round**, merge all compressed sets in the CS and all RS points into their nearest cluster

**Discard set (DS):** Close enough to a centroid to be summarized.
**Compression set (CS):** Summarized, but not assigned to a cluster
**Retained set (RS):** Isolated points
A cluster. Its points are in the **DS**.

Compressed sets. Their points are in the **CS**.

Points in the **RS**.

**Discard set (DS):** Close enough to a centroid to be summarized

**Compression set (CS):** Summarized, but not assigned to a cluster

**Retained set (RS):** Isolated points
Q1) How do we decide if a point is “close enough” to a cluster that we will add the point to that cluster?

Q2) How do we decide whether two compressed sets (CS) deserve to be combined into one?
Q1) We need a way to decide whether to put a new point into a cluster (and discard)

- **BFR suggests two ways:**
  - The *Mahalanobis distance* is less than a threshold
  - High likelihood of the point belonging to currently nearest centroid
**Mahalanobis Distance**

- **Normalized Euclidean distance from centroid**

- For point \((x_1, \ldots, x_d)\) and centroid \((c_1, \ldots, c_d)\)
  1. Normalize in each dimension: \(y_i = (x_i - c_i) / \sigma_i\)
  2. Take sum of the squares of the \(y_i\)
  3. Take the square root

\[
d(x, c) = \sqrt{\sum_{i=1}^{d} \left( \frac{x_i - c_i}{\sigma_i} \right)^2}
\]

\(\sigma_i \ldots\) standard deviation of points in the cluster in the \(i^{th}\) dimension
If clusters are normally distributed in \( d \) dimensions, then after transformation, one standard deviation = \( \sqrt{d} \)

- i.e., 68% of the points of the cluster will have a Mahalanobis distance < \( \sqrt{d} \)

Accept a point for a cluster if its M.D. is < some threshold, e.g. 2 standard deviations
Euclidean vs. Mahalanobis distance

Contours of equidistant points from the origin

Uniformly distributed points, Euclidean distance

Normally distributed points, Euclidean distance

Normally distributed points, Mahalanobis distance
Q2) Should 2 CS clusters be combined?

- Compute the variance of the combined subcluster
  - \( N, \text{SUM}, \) and \( \text{SUMSQ} \) allow us to make that calculation quickly
- Combine if the combined variance is below some threshold

- Many alternatives: Treat dimensions differently, consider density
The CURE Algorithm

Extension of $k$-means to clusters of arbitrary shapes
The CURE Algorithm

- **Problem with BFR/k-means:**
  - Assumes clusters are normally distributed in each dimension
  - And axes are fixed – ellipses at an angle are *not OK*

- **CURE (Clustering Using REpresentatives):**
  - Assumes a Euclidean distance
  - Allows clusters to assume any shape
  - *Uses a collection of representative points to represent clusters*
Example: Stanford Salaries

salary

age

Jure Leskovec, Stanford CS246: Mining Massive Datasets
2 Pass algorithm. Pass 1:

0) Pick a random sample of points that fit in main memory

1) Initial clusters:
   - Cluster these points hierarchically – group nearest points/clusters

2) Pick representative points:
   - For each cluster, pick a sample of points, as dispersed as possible
   - From the sample, pick representatives by moving them (say) 20% toward the centroid of the cluster
Example: Initial Clusters

salary

age
Example: Pick Dispersed Points

Pick (say) 4 remote points for each cluster.
Move points (say) 20% toward the centroid.
Pass 2:

- Now, rescan the whole dataset and visit each point \( p \) in the data set

- Place it in the “closest cluster”
  - Normal definition of “closest”: Find the closest representative point to \( p \) and assign it to representative’s cluster
Why the 20% Move Inward?

Intuition:

- A large, dispersed cluster will have large moves from its boundary.
- A small, dense cluster will have little move.
- Favors a small, dense cluster that is near a larger dispersed cluster.
**Summary**

- **Clustering:** Given a set of points, with a notion of distance between points, group the points into some number of *clusters*

- **Algorithms:**
  - Agglomerative *hierarchical clustering*:
    - Centroid and clustroid
  - *k*-means:
    - Initialization, picking *k*
  - BFR
  - CURE