Data-Intensive Distributed Computing
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Part 7: Data Mining (4/4)

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These slides are available at https://www.student.cs.uwaterloo.ca/~cs451
High Dimensional Data

- Given a cloud of data points we want to understand its structure
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 a 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
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 at about the same distance
Clustering Problem: Galaxies

- A catalog of 2 billion “sky objects” represents objects by their radiation in 7 dimensions (frequency bands)
- **Problem:** Cluster into similar objects, e.g., galaxies, nearby stars, quasars, etc.
- Sloan Digital Sky Survey
Clustering Problem: Music CDs

- Intuitively: Music divides into categories, and customers prefer a few categories
  - 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 \((x_1, x_2, ..., x_k)\), 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 \((x_1, x_2, \ldots, x_k)\), where \(x_i = 1\) iff the \(i^{th}\) 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**
As with CDs 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
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 “nearest” cluster
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?
**Hierarchical Clustering**

- **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:
- o ... data point
- x ... centroid

Dendrogram
And in the Non-Euclidean Case?

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

- **Clustroid** = 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: $\min_c \sum_{x \in C} d(x, c)^2$

**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.
(2) How do you determine the “nearness” of clusters?

- **Approach 2:**
  Intercluster distance = minimum of the distances between any two points, one from each cluster

- **Approach 3:**
  Pick a notion of “cohesion” of clusters, e.g., maximum distance from the clustroid
  - Merge clusters whose union is most cohesive
**Cohesion**

- **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, e.g., and divide by the number of points in the cluster
### Implementation

- **Naïve implementation of hierarchical clustering:**
  - At each step, compute pairwise distances between all pairs of clusters, then merge
  - $O(N^3)$

- Careful implementation using priority queue can reduce time to $O(N^2 \log N)$
  - **Still too expensive for really big datasets that do not fit in memory**
$k$-means clustering
**k-means Algorithm(s)**

- 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
Populating Clusters

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

- \( \times \): data point
- \( \square \): 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.
class Mapper {
    def setup() = {
        clusters = loadClusters()
    }

    def map(id: Int, vector: Vector) = {
        emit(clusters.findNearest(vector), vector)
    }
}

class Reducer {
    def reduce(clusterId: Int, values: Iterable[Vector]) = {
        for (vector <- values) {
            sum += vector
            cnt += 1
        }
        emit(clusterId, sum/cnt)
    }
}