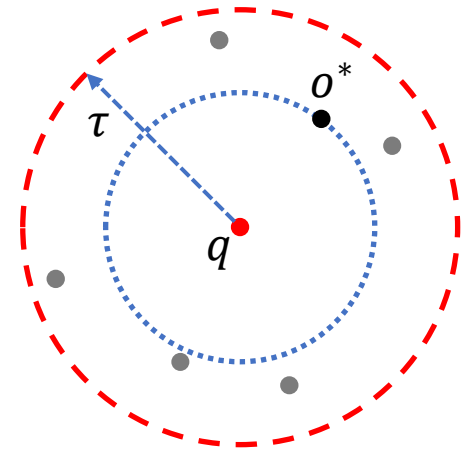


COMP9313: Big Data Management

High Dimensional
Similarity Search

Similarity Search

- Problem Definition:
 - Given a query q and dataset D , find $o \in D$, where o is similar to q
- Two types of similarity search
 - Range search:
 - $dist(o, q) \leq \tau$
 - Nearest neighbor search
 - $dist(o^*, q) \leq dist(o, q), \forall o \in D$
 - Top-k version
- Distance/similarity function varies
 - Euclidean, Jaccard, inner product, ...
- Classic problem, with mutual solutions



High Dimensional Similarity Search

- Applications and relationship to Big Data
 - Almost every object can be and has been represented by a high dimensional vector
 - Words, documents
 - Image, audio, video
 - ...
 - Similarity search is a fundamental process in information retrieval
 - E.g., Google search engine, face recognition system, ...
- High Dimension makes a huge difference!
 - Traditional solutions are no longer feasible
 - This lecture is about why and how
 - We focus on high dimensional vectors in Euclidean space

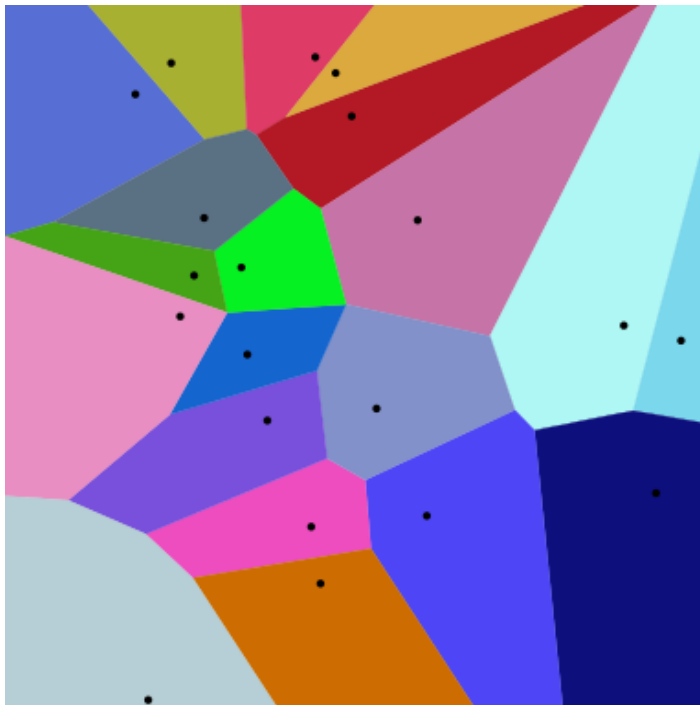
Similarity Search in Low Dimensional Space

Similarity Search in One Dimensional Space

- Just numbers, use binary search, binary search tree, B+ Tree...
- The essential idea behind: objects can be sorted

Similarity Search in Two Dimensional Space

- Why binary search no longer works?
 - No order!
- Voronoi diagram



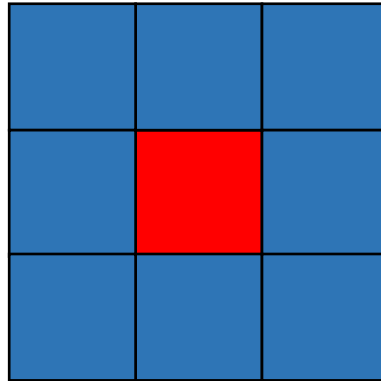
Euclidean distance



Manhattan distance

Similarity Search in Two Dimensional Space

- Partition based algorithms
 - Partition data into “cells”
 - Nearest neighbors are in the same cell with query or adjacent cells



- How many “cells” to probe on 3-dimensional space?

Similarity Search in Metric Space

- Triangle inequality
 - $\text{dist}(x, q) \leq \text{dist}(x, y) + \text{dist}(y, q)$
- Orchard's Algorithm
 - for each $x \in D$, create a list of points in increasing order of distance to x
 - given query q , randomly pick a point x as the initial candidate (i.e., pivot p), compute $\text{dist}(p, q)$
 - walk along the list of p , and compute the distances to q . If found y closer to q than p , then use y as the new pivot (e.g., $p \leftarrow y$).
 - repeat the procedure, and stop when
 - $\text{dist}(p, y) > 2 \cdot \text{dist}(p, q)$

Similarity Search in Metric Space

- Orchard's Algorithm, stop when $\text{dist}(p, y) > 2 \cdot \text{dist}(p, q)$

$$\begin{aligned} & 2 \cdot \text{dist}(p, q) < \text{dist}(p, y) \text{ and} \\ & \text{dist}(p, y) \leq \text{dist}(p, q) + \text{dist}(y, q) \\ \Rightarrow & 2 \cdot \text{dist}(p, q) < \text{dist}(p, q) + \text{dist}(y, q) \\ \Leftrightarrow & \text{dist}(p, q) < \text{dist}(y, q) \end{aligned}$$

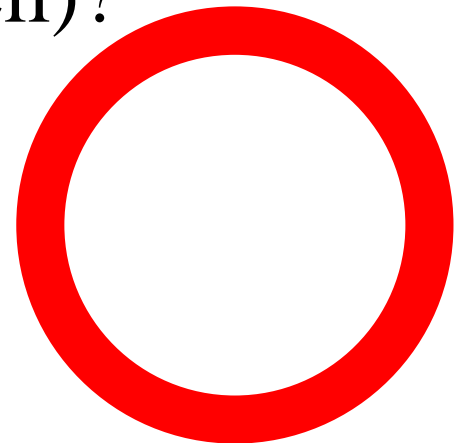
- Since the list of p is in increasing order of distance to p , $\text{dist}(p, y) > 2 \cdot \text{dist}(p, q)$ hold for all the rest y 's.

**None of the Above Works
in
High Dimensional Space!**

Curse of Dimensionality

- Refers to various phenomena that arise in high dimensional spaces that do not occur in low dimensional settings.
- Triangle inequality
 - The pruning power reduces heavily
- What is the volume of a high dimensional “ring” (i.e., hyperspherical shell)?

- $\frac{V_{ring}(w=1, d=2)}{V_{ball}(r=10, d=2)} = 29\%$
- $\frac{V_{ring}(w=1, d=100)}{V_{ball}(r=10, d=100)} = 99.997\%$

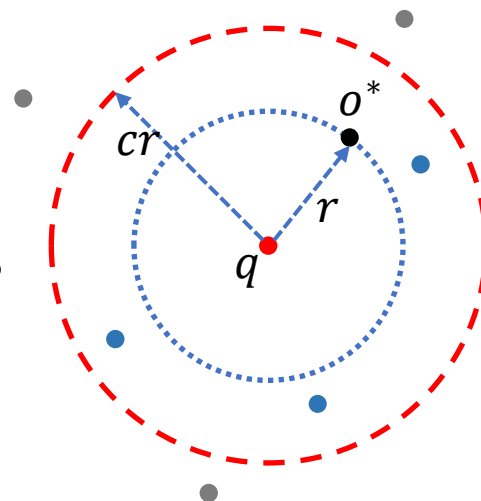


Approximate Nearest Neighbor Search in High Dimensional Space

- There is no sub-linear solution to find the exact result of a nearest neighbor query
 - So we relax the condition
- approximate nearest neighbor search (ANNS)
 - allow returned points to be not the NN of query
 - Success: returns the true NN
 - use success rate (e.g., percentage of succeed queries) to evaluate the method
 - Hard to bound the success rate

c-approximate NN Search

- Success: returns o such that
 - $\text{dist}(o, q) \leq c \cdot \text{dist}(o^*, q)$
- Then we can bound the success probability
 - Usually noted as $1 - \delta$
- Solution: Locality Sensitive Hashing (LSH)



Locality Sensitive Hashing

- Hash function

- Index: Map data/objects to values (e.g., hash key)
 - Same data \Rightarrow same hash key (with 100% probability)
 - Different data \Rightarrow different hash keys (with high probability)
- Retrieval: Easy to retrieve identical objects (as they have the same hash key)
 - Applications: hash map, hash join
- Low cost
 - Space: $O(n)$
 - Time: $O(1)$
- Why it cannot be used in nearest neighbor search?
 - Even a minor difference leads to totally different hash keys

Locality Sensitive Hashing

- Index: make the hash functions error tolerant
 - Similar data \Rightarrow same hash key (with high probability)
 - Dissimilar data \Rightarrow different hash keys (with high probability)
- Retrieval:
 - Compute the hash key for the query
 - Obtain all the data has the same key with query (i.e., candidates)
 - Find the nearest one to the query
 - Cost:
 - Space: $O(n)$
 - Time: $O(1) + O(|cand|)$
- It is not the real Locality Sensitive Hashing!
 - We still have several unsolved issues...

LSH Functions

- Formal definition:
 - Given point o_1, o_2 , distance r_1, r_2 , probability p_1, p_2
 - An LSH function $h(\cdot)$ should satisfy
 - $\Pr[h(o_1) = h(o_2)] \geq p_1$, if $\text{dist}(o_1, o_2) \leq r_1$
 - $\Pr[h(o_1) = h(o_2)] \leq p_2$, if $\text{dist}(o_1, o_2) > r_2$
- What is $h(\cdot)$ for a given distance/similarity function?
 - Jaccard similarity
 - Angular distance
 - Euclidean distance

MinHash - LSH Function for Jaccard Similarity

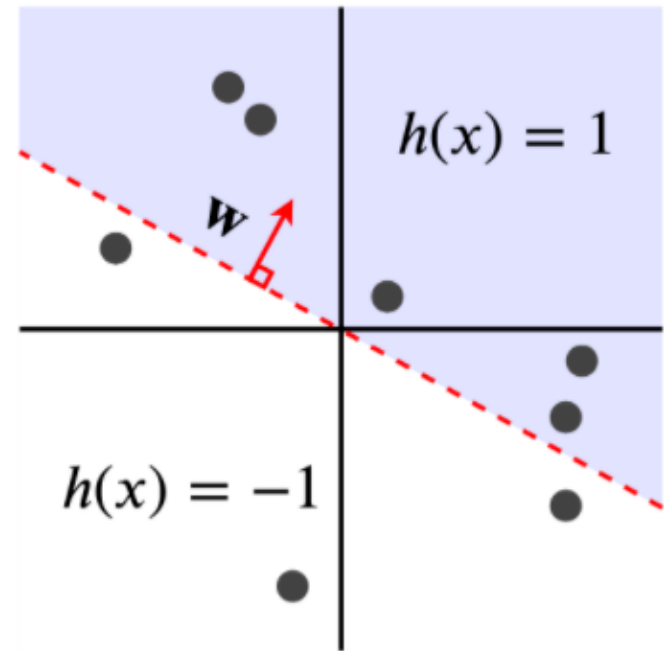
- Each data object is a set
 - $Jaccard(S_1, S_2) = \frac{|S_1 \cap S_2|}{|S_1 \cup S_2|}$
- Randomly generate a global order for all the elements in $C = \bigcup_1^n S_i$
- Let $h(S)$ be the minimal member of S with respect to the global order
 - For example, $S = \{b, c, e, h, i\}$, we use inversed alphabet order, then re-ordered $S = \{i, h, e, c, b\}$, hence $h(S) = i$.

MinHash

- Now we compute $\Pr[h(S_1) = h(S_2)]$
- Every element $e \in S_1 \cup S_2$ has equal chance to be the first element among $S_1 \cup S_2$ after re-ordering
- $e \in S_1 \cap S_2$ if and only if $h(S_1) = h(S_2)$
- $e \notin S_1 \cap S_2$ if and only if $h(S_1) \neq h(S_2)$
- $\Pr[h(S_1) = h(S_2)] = \frac{|\{e_i | h_i(S_1) = h_i(S_2)\}|}{|\{e_i\}|} = \frac{|S_i \cap S_j|}{|S_i \cup S_j|} = Jaccard(S_1, S_2)$

SimHash – LSH Function for Angular Distance

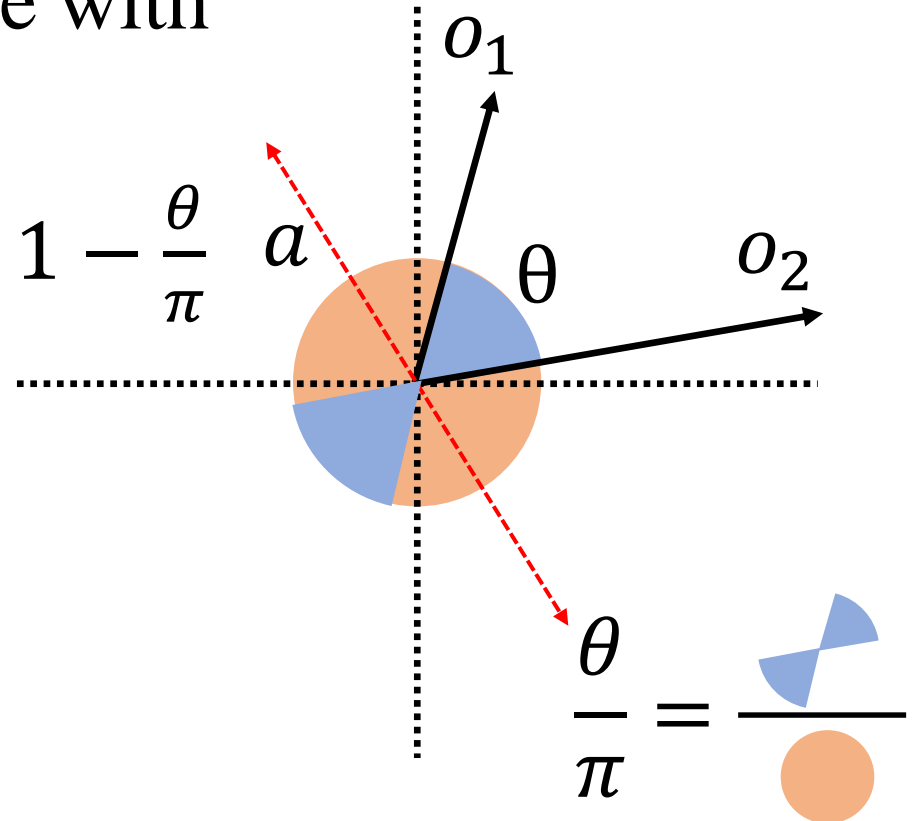
- Each data object is a d dimensional vector
 - $\theta(x, y)$ is the angle between x and y
- Randomly generate a normal vector a , where $a_i \sim N(0, 1)$
- Let $h(x; a) = \text{sgn}(a^T x)$
 - $\text{sgn}(o) = \begin{cases} 1; & \text{if } o \geq 0 \\ -1; & \text{if } o < 0 \end{cases}$
 - x lies on which side of a 's corresponding hyperplane



SimHash

- Now we compute $\Pr[h(o_1) = h(o_2)]$
- $h(o_1) \neq h(o_2)$ iff o_1 and o_2 are on different sides of the hyperplane with a as its normal vector

- $\Pr[h(o_1) = h(o_2)] = 1 - \frac{\theta}{\pi}$

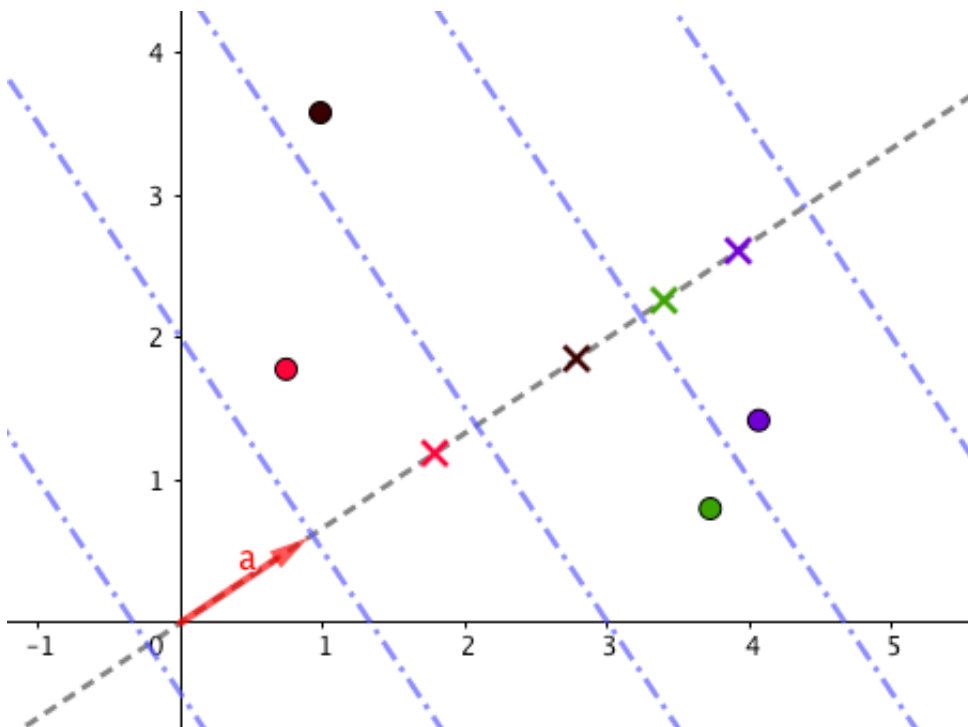


p-stable LSH - LSH function for Euclidean distance

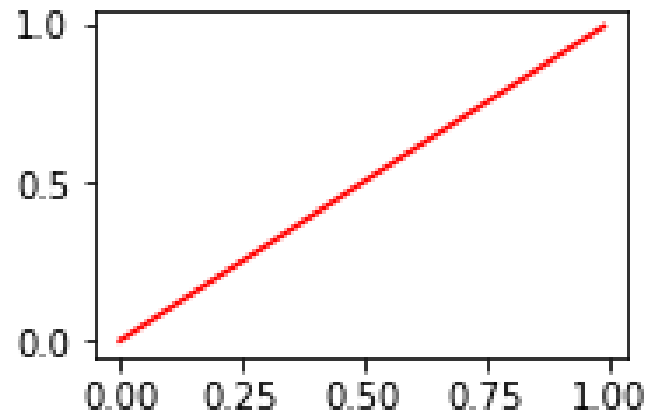
- Each data object is a d dimensional vector
 - $dist(x, y) = \sqrt{\sum_1^d (x_i - y_i)^2}$
- Randomly generate a normal vector a , where $a_i \sim N(0, 1)$
 - Normal distribution is 2-stable, i.e., if $a_i \sim N(0, 1)$, then $\sum_1^d a_i \cdot x_i \sim N(0, \|x\|_2^2)$
- Let $h(x; a, b) = \left\lfloor \frac{a^T x + b}{w} \right\rfloor$, where $b \sim U(0, 1)$ and w is user specified parameter
 - $\Pr[h(o_1; a, b) = h(o_2; a, b)] = \int_0^w \frac{1}{\|o_1, o_2\|} f_p\left(\frac{t}{\|o_1, o_2\|}\right) \left(1 - \frac{t}{w}\right) dt$
 - $f_p(\cdot)$ is the pdf of the absolute value of normal variable

p-stable LSH

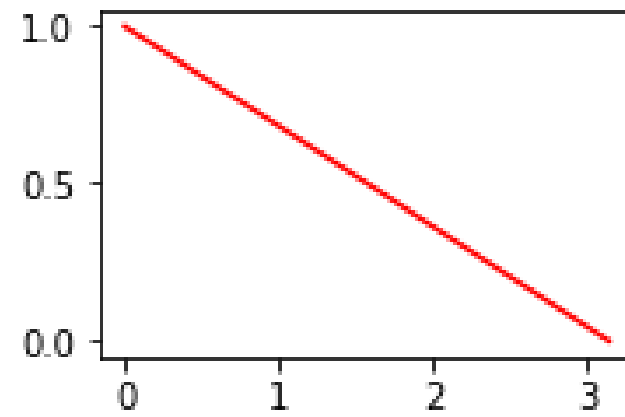
- Intuition of p-stable LSH
 - Similar points have higher chance to be hashed together



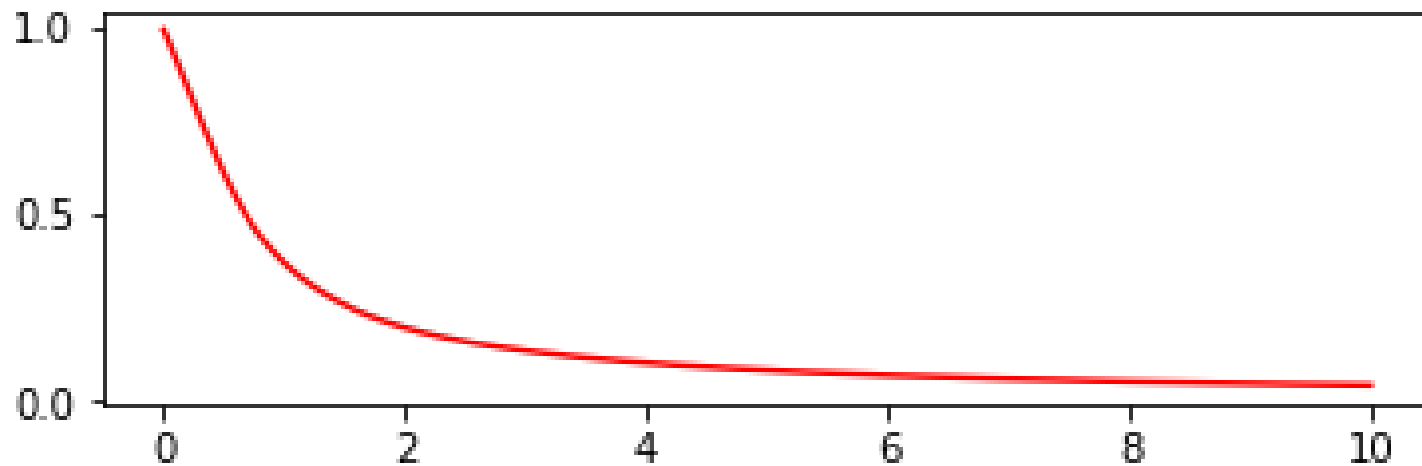
$\Pr[h(x) = h(y)]$ for different Hash Functions



MinHash



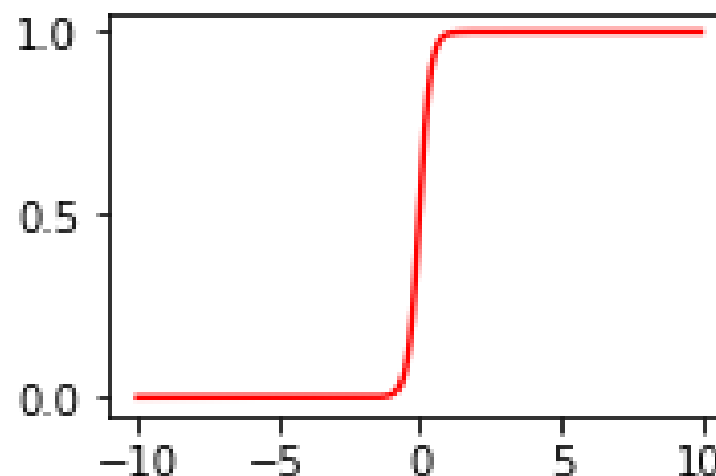
SimHash



p-stable LSH

Problem of Single Hash Function

- Hard to distinguish if two pairs have distances close to each other
 - $\Pr[h(o_1) = h(o_2)] \geq p_1$, if $\text{dist}(o_1, o_2) \leq r_1$
 - $\Pr[h(o_1) = h(o_2)] \leq p_2$, if $\text{dist}(o_1, o_2) > r_2$
- We also want to control where the drastic change happens...
 - Close to $\text{dist}(o^*, q)$
 - Given range

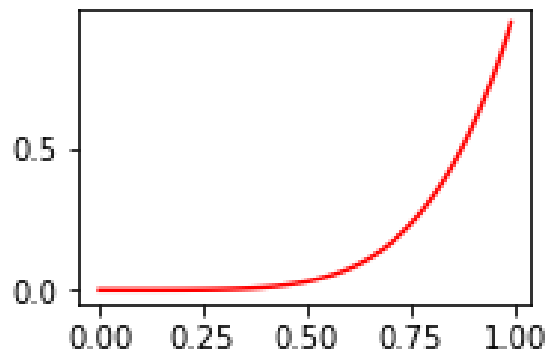
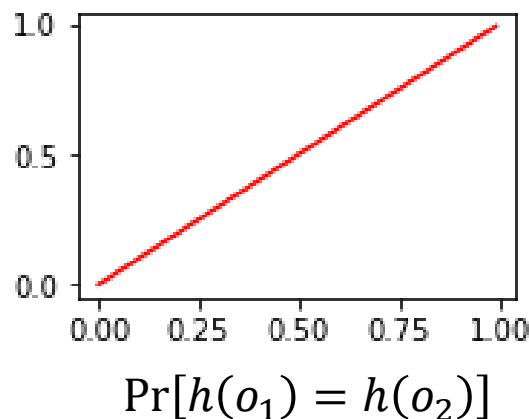


AND-OR Composition

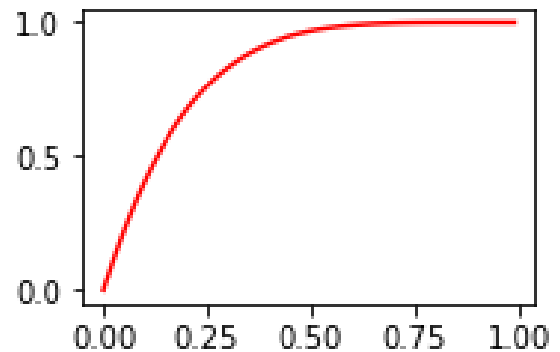
- Recall for a single hash function, we have
 - $\Pr[h(o_1) = h(o_2)] = p(\text{dist}(o_1, o_2))$, denoted as p_{o_1, o_2}
- Now we consider two scenarios:
 - Combine k hashes together, using AND operation
 - One must match all the hashes
 - $\Pr[H_{AND}(o_1) = H_{AND}(o_2)] = p_{o_1, o_2}^k$
 - Combine l hashes together, using OR operation
 - One need to match at least one of the hashes
 - $\Pr[H_{OR}(o_1) = H_{OR}(o_2)] = 1 - (1 - p_{o_1, o_2})^l$
 - Not match only when all the hashes don't match

AND-OR Composition

- Example with minHash, $k = 5, l = 5$



$\Pr[H_{AND}(o_1) = H_{AND}(o_2)]$



$\Pr[H_{OR}(o_1) = H_{OR}(o_2)]$

AND-OR Composition in LSH

- Let $h_{i,j}$ be LSH functions, where $i \in \{1, 2, \dots, l\}, j \in \{1, 2, \dots, k\}$
- Let $H_i(o) = [h_{i,1}(o), h_{i,2}(o), \dots, h_{i,k}(o)]$
 - super-hash
 - $H_i(o_1) = H_i(o_2) \Leftrightarrow \forall j \in \{1, 2, \dots, k\}, h_{i,j}(o_1) = h_{i,j}(o_2)$
- Consider query q and any data point o , o is a nearest neighbor candidate of q if
 - $\exists i \in \{1, 2, \dots, l\}, H_i(o) = H_i(q)$
- The probability of o is a nearest neighbor candidate of q is
 - $1 - (1 - p_{q,o}^k)^l$

The Effectiveness of LSH

- $1 - (1 - p_{q,o}^k)^l$ changes with $p_{q,o}$, ($k = 20, l = 5$)

| $p_{q,o}$ | $1 - (1 - p_{q,o}^k)^l$ |
|-----------|-------------------------|
| 0.2 | 0.002 |
| 0.4 | 0.050 |
| 0.6 | 0.333 |
| 0.7 | 0.601 |
| 0.8 | 0.863 |
| 0.9 | 0.988 |

- E.g., we are expected to retrieve 98.8% of the data with Jaccard > 0.9

False Positives and False Negatives

- False Positive:
 - returned data with $\text{dist}(o, q) > r_2$
- False Negative
 - not returned data with $\text{dist}(o, q) < r_1$
- They can be controlled by carefully chosen k and l
 - It's a trade-off between space/time and accuracy

The Framework of NNS using LSH

- Pre-processing
 - Generate LSH functions
 - minHash: random permutations
 - simHash: random normal vectors
 - p-stable: random normal vectors and random uniform values
- Index
 - Compute $H_i(o)$ for each data object o , $i \in \{1, \dots, l\}$
 - Index o using $H_i(o)$ as key in the i -th hash table
- Query
 - Compute $H_i(q)$ for query q , $i \in \{1, \dots, l\}$
 - Generate candidate set $\{o | \exists i \in \{1, \dots, l\}, H_i(q) = H_i(o)\}$
 - Compute the actual distance for all the candidates and return the nearest one to the query

The Drawback of LSH

- Concatenate k hashes is too “strong”
 - $h_{i,j}(o_1) \neq h_{i,j}(o_2) \Rightarrow H_i(q) \neq H_i(o)$ for any j
- Not adaptive to the distribution of the distances
 - What if not enough candidates?
 - Need to tune w (or build indexes different w 's) to handle different cases

Multi-Probe LSH

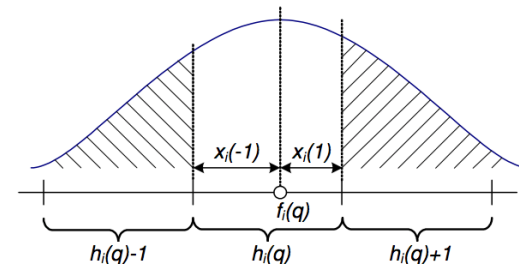


Figure 3: Probability of q 's nearest neighbors falling into the neighboring slots.

- Observation:

- If q 's nearest neighbor does not fall into q 's hash bucket, then most likely it will fall into the adjacent bucket to q 's
- Why? $\sum_1^d a_i \cdot x_i - \sum_1^d a_i \cdot q_i \sim N(0, \|x, q\|_2^2)$

- Idea:

- Not only look at the hash bucket where q falls into, but also those adjacent to it

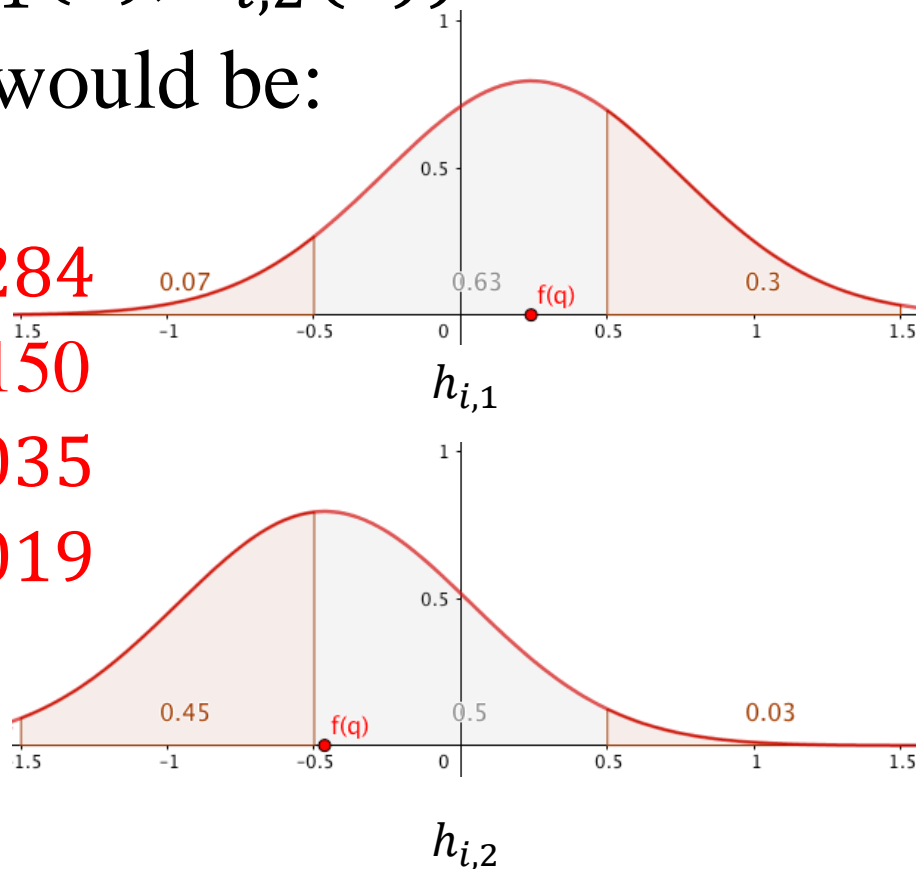
- Problem:

- How many such bucket? 2^k
- And they are not equally important!

Multi-Probe LSH

- Consider the case when $k = 2$:
- Note that $H_i(o) = (h_{i,1}(o), h_{i,2}(o))$
- The ideal probe order would be:
 - $h_{i,1}(q), h_{i,2}(q)$: **0.315**
 - $h_{i,1}(q), h_{i,2}(q) - 1$: **0.284**
 - $h_{i,1}(q) + 1, h_{i,2}(q)$: **0.150**
 - $h_{i,1}(q) - 1, h_{i,2}(q)$: **0.035**
 - $h_{i,1}(q), h_{i,2}(q) + 1$: **0.019**

We don't have to compute the integration, but use the offset between $f(q)$ and the boundaries.



Multi Probe LSH

- Pros:

- Requires less l

- Because we use hash tables more efficiently

- More robust against the unlucky points

- Cons:

- Lose the theoretical guarantee about the results

- Not parallel-friendly

Collision Counting LSH (C2LSH)

- C2LSH (SIGMOG'12 paper)
 - Which one is closer to q ?

| q | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
|-------|---|---|---|---|---|---|---|---|---|---|---|---|
| o_1 | 1 | 1 | 1 | 2 | 1 | 2 | 1 | 1 | 2 | 1 | 1 | 1 |
| o_2 | 1 | 1 | 1 | 1 | 2 | 2 | 3 | 4 | 1 | 2 | 3 | 4 |

- We will omit the theoretical parts hence leads to a slightly different version to the paper.
 - But the essential ideas are the same
- Project 1 is to implement C2LSH using PySpark!

Counting the Collisions

- Collision: match on a single hash function
 - Use number of collisions to determine the candidates
 - Match one of the super hash with $q \rightarrow$ collides at least αm hash values with q
- Recall in LSH, The probability of o with $\text{dist}(o, q) \leq r_1$ is a nearest neighbor candidate of q is $1 - (1 - p_1^k)^l$
- Now we compute the case with collision counting...

The Collision Probability

- $\forall o$ with $\text{dist}(o, q) \leq r_1$, we have
 - $\Pr[\#collision(o) \geq \alpha m] = \sum_{i=\alpha m}^m \binom{m}{i} p^i (1-p)^{m-i}$
 - $p = \Pr[h_j(o) = h_j(q)] \geq p_1$
- We define m Bernoulli random variables $X_i \sim B(m, 1-p)$ with $1 \leq i \leq m$.
 - Let X_i equal 1 if o does not collide with q
 - i.e., $\Pr[X_i = 1] = 1-p$
 - Let X_i equal 0 if o collides with q
 - i.e., $\Pr[X_i = 0] = p$
 - Hence $E[X_i] = 1-p$
 - Thus $E(\bar{X}) = 1-p$, where $\bar{X} = \frac{\sum_{i=1}^m X_i}{m}$.
- Let $t = p - \alpha > 0$, we have:
 - $\Pr[\bar{X} - E(\bar{X}) \geq t] = \Pr\left[\frac{\sum_{i=1}^m X_i}{m} - (1-p) \geq t\right] = \Pr[\sum X_i \geq (1-\alpha)m]$

The Collision Probability

- From Hoeffding's Inequality, we have
 - $\Pr[\bar{X} - E(\bar{X}) \geq t] = \Pr[\sum X_i \geq (1 - \alpha)m] \leq \exp\left(-\frac{2(p-\alpha)^2 m^2}{\sum_{i=1}^m (1-0)^2}\right) = \exp(-2(p - \alpha)^2 m) \leq \exp(-2(p_1 - \alpha)^2 m)$
- Since the event “ $\#collision(o) \geq \alpha m$ ” is equivalent to the event “ o misses the collision with q less than $(1 - \alpha)m$ times”,
 - $\Pr[\#collision(o) \geq \alpha m] = \Pr[\sum X_i < (1 - \alpha)m] \geq 1 - \exp(-2(p_1 - \alpha)^2 m)$
- Now you can compute the case for o with $\text{dist}(o, q) \geq r_2$ in a similar way...
- Then we can accordingly set α to control false positives and false negatives

Virtual Rehashing

- When we are not getting enough candidates...
 - E.g., # of candidates < top-k
- Observation:
 - A close point o usually falls into adjacent hash buckets of q 's if it does not collide with q
 - Why?
 - $\sum_1^d a_i \cdot x_i - \sum_1^d a_i \cdot q_i \sim N(0, \|x, q\|_2^2)$
- Idea:
 - Include the adjacent hash buckets into consideration
 - So you don't need to re-hash them again...

Virtual Rehashing

- At first consider $h(o) = h(q)$

| | | | | | | | | | | |
|-------|---|---|---|----|---|---|---|----|---|----|
| q | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| o_1 | 1 | 0 | 2 | -1 | 1 | 2 | 4 | -3 | 0 | -1 |

- Consider $h(o) = h(q) \pm 1$ if not enough candidates

| | | | | | | | | | | |
|-------|---|---|---|----|---|---|---|----|---|----|
| q | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| o_1 | 1 | 0 | 2 | -1 | 1 | 2 | 4 | -3 | 0 | -1 |

- Then $h(o) = h(q) \pm 2$ and so on...

| | | | | | | | | | | |
|-------|---|---|---|----|---|---|---|----|---|----|
| q | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| o_1 | 1 | 0 | 2 | -1 | 1 | 2 | 4 | -3 | 0 | -1 |

The Framework of NNS using C2LSH

- Pre-processing
 - Generate LSH functions
 - Random normal vectors and random uniform values
- Index
 - Compute and store $h_i(o)$ for each data object o , $i \in \{1, \dots, m\}$
- Query
 - Compute $h_i(q)$ for query q , $i \in \{1, \dots, m\}$
 - Take those o that shares at least αm hashes with q as candidates
 - Relax the collision condition (e.g., virtual rehashing) and repeat the above step, until we got enough candidates

Pseudo code of Candidate Generation in C2LSH

```
candGen(data_hashes, query_hashes,  $\alpha m$ ,  $\beta n$ ):  
    offset  $\leftarrow$  0  
    cand  $\leftarrow \emptyset$   
    while true:  
        for each (id, hashes) in data_hashes:  
            if count(hashes, query_hashes, offset)  $\geq \alpha m$ :  
                cand  $\leftarrow$  cand  $\cup$  {id}  
        if |cand|  $< \beta n$ :  
            offset  $\leftarrow$  offset + 1  
        else:  
            break  
    return cand
```

Pseudo code of Candidate Generation in C2LSH

```
count(hashes_1, hashes_2, offset):  
    counter  $\leftarrow$  0  
    for each  $hash_1, hash_2$  in hashes_1, hashes_2:  
        if  $|hash_1 - hash_2| \leq \text{offset}$ :  
            counter  $\leftarrow$  counter + 1  
    return counter
```

Project 1

- Spec has been released, deadline: 18 Jul, 2020
 - Late Penalty: 10% on day 1 and 30% on each subsequent day.
- Implement a light version of C2LSH (i.e., the one we introduced in the lecture)
- Start working ASAP
- Evaluation: **Correctness** and **Efficiency**
- Must use PySpark, some python modules and PySpark functions are banned.
 - E.g., numpy, pandas, collect(), take(), ...
 - Use transformations!

Project 1

- There will be a **bonus** part (max 20 points) to encourage efficient implementations.
 - Details in the spec
- Make sure you have valid output
- **Make your own test cases**, a real dataset would be more desirable
 - Toy example in the spec is a real “toy” (e.g., for babies...)
- Won’t accept excuses like “it works on my own computer”
- **Don’t violate the Student Conduct!!!**

产品量化

Product Quantization

and K-Means Clustering

K均值聚类

Recall: NNS in High Dimensional Euclidean Space

- Naïve (but exact) solution:
 - Linear scan: compute $\text{dist}(o, q)$ for all $o \in D$
 - $\text{dist}(o, q) = \sqrt{\sum_{i=1}^d (o_i - q_i)^2}$
 - $O(nd)$
 - n times (d subtractions + $d - 1$ additions + d multiplications)
 - Storage is also costly: $O(nd)$
 - Could be problematic in DBMS and distributed systems
在DBMS和分布式系统中可能会出现问题
- This motivates the idea of **compression**
这激发了压缩的想法

向量量化

Vector Quantization

向量的压缩表示形式

- Idea: compressed representation of vectors
 - Each vector o is represented by a representative^{代表}
 - Denoted as $QZ(o)$
 - We will discuss how to get the representatives later
 - We control the total number of representatives for the dataset (denoted as k)^{表示为k}
 - One representative represents multiple vectors
 - Instead of store o , we store its representative id
 - d floats \Rightarrow 1 integer
 - Instead of compute $dist(o, q)$, we compute $dist(QZ(o), q)$
 - We only need k computations of distance!

产生

How to Generate Representatives

- Assigning representatives is essentially a partition 划分问题 problem
 - Construct a “good” partition of a database of n objects into a set of k clusters 集群
- How to measure the “goodness” of a given partitioning scheme?
 - Cost of a cluster 集群成本
 - $Cost(C_i) = \sum_{o_j \in C_i} \|o_j - center(C_i)\|_2^2$
 - Cost of k clusters: sum of $Cost(C_i)$

Partitioning Problem: Basic Concept

优化问题

- It's an optimization problem!

全局最优

- Global optimal:

- NP-hard (for a wide range of cost functions)
- Requires exhaustively ^{详尽的列举} enumerate all $\binom{n}{k}$ partitions
 - Stirling numbers of the second kind
 - $\binom{n}{k} \sim \frac{k^n}{k!}$ when $n \rightarrow \infty$

启发式方法

- Heuristic methods:

- k-means
- Many variants

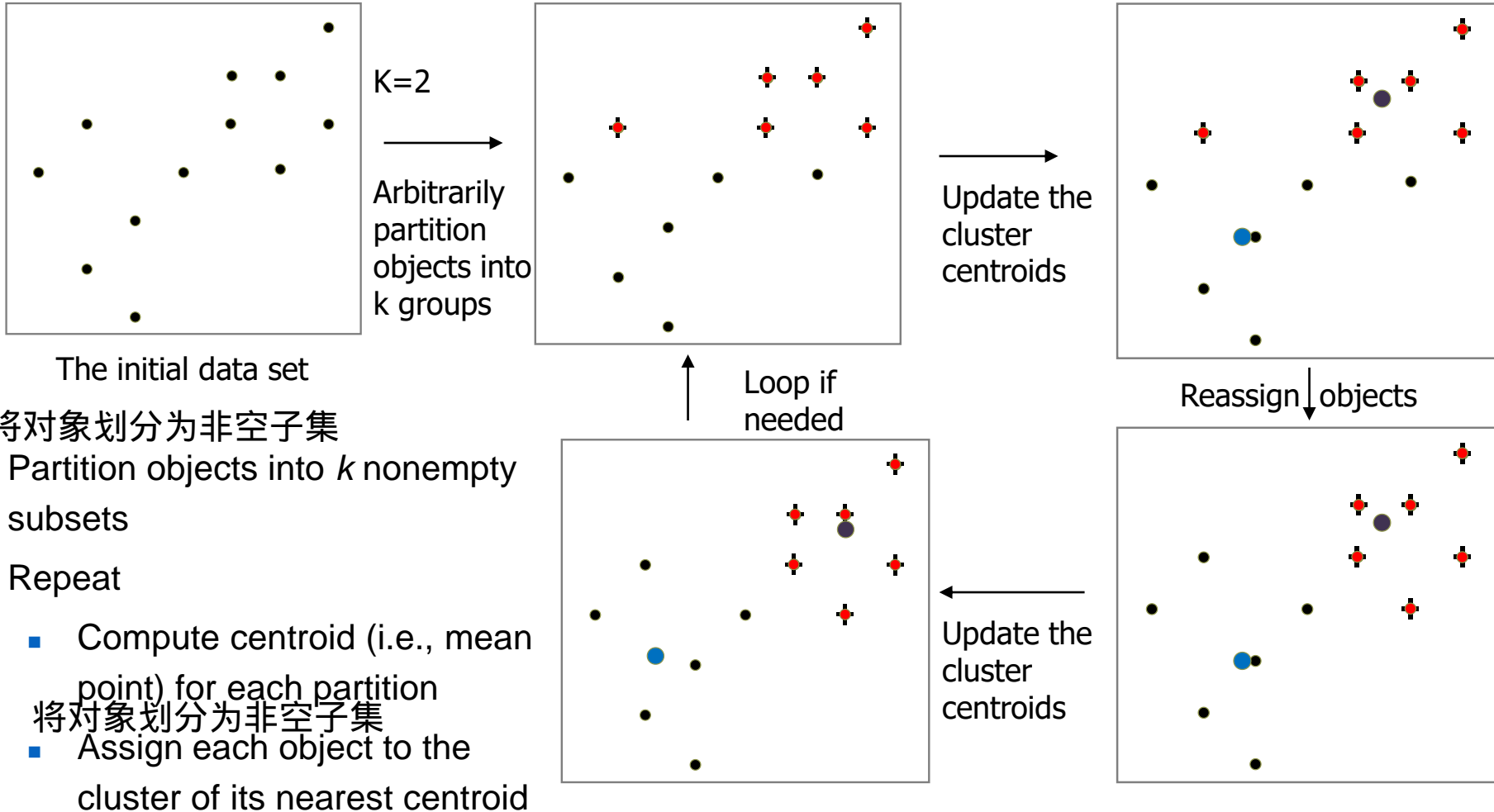
The k-Means Clustering Method

- Given k , the k-means algorithm is implemented in four steps:

非空的子集

1. Partition objects into k nonempty subsets (randomly)
将种子点计算为当前分区的群集的质心（质心是群集的中心，即均值）
2. Compute seed points as the centroids of the clusters of the current partitioning (the centroid is the center, i.e., **mean point**, of the cluster)
3. ^{用最近的种子点将每个对象分配给集群.} Assign each object to the cluster with the nearest seed point
4. Go back to Step 2, stop when the assignment does not change

An Example of k-Means Clustering



The initial data set

将对象划分为非空子集

- Partition objects into k nonempty subsets

- Repeat

- Compute centroid (i.e., mean point) for each partition

将对象划分为非空子集

- Assign each object to the cluster of its nearest centroid

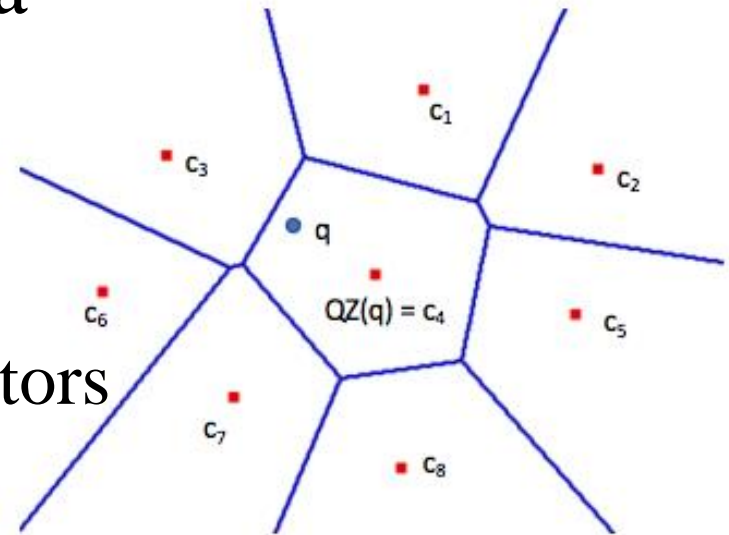
- Until no change

Vector Quantization

- Encode the vectors
 - Generate a codebook $W = \{c_1, \dots, c_k\}$ via k-means
 - Assign o to its nearest codeword in W
 - E.g., $QZ(o) = c_i$ ($i \in 1 \dots k$) such that $dist(o, c_i) \leq dist(o, c_j) \forall j$
 - Represent each vector o by its assigned codeword
- Assume $d = 256, k = 2^{16}$
 - Before: 4 bytes * 256 = 1024 bytes for each vector
 - Now:
 - data: 16 bits = 2 bytes
 - codebook: $4 * 256 * 2^{16}$

Vector Quantization – Query Processing

- Given query q , how to find a point close to q ?
- Algorithm:
 - Compute $QZ(q)$
 - Candidate set C = all data vectors associated with $QZ(q)$
 - 验证; 检验 Verification: compute distance between q and $o_i \in C$
 - Requires loading the vectors in C
- Any problem/improvement?



Inverted index: a hash table that maps c_j to a list of o_i that are associated with c_j

Limitations of VQ 向量量化

- To achieve better accuracy, fine-grained quantizer with large k is needed
- Large k
 - Costly to run K-means
 - Computing $QZ(q)$ is expensive: $O(kd)$
 - May need to look beyond $QZ(q)$ cell
- Solution:
 - Product Quantization
产品量化

Product Quantization 产品量化

- Idea

将维度划分为 m 个分区

- Partition the dimension into m partitions

- Accordingly a vector \Rightarrow subvectors

- Use separate VQ with k codewords for each chunk 每个块的码字

- Example:

分解的

- 8-dim vector decomposed into $m = 2$ subvectors

- Each codebook has $k = 4$ codewords, (i.e., $c_{i,j}$)

- Total space in bits:

- Data: $n \cdot m \cdot \log(k)$

- Codebook: $m \cdot \frac{d}{m} \cdot k \cdot 32$

Example of PQ

| | | | | | | | |
|----------|----------|----------|----------|-----------|-----------|----------|----------|
| 2 | 4 | 6 | 5 | -2 | 6 | 4 | 1 |
| 1 | 2 | 1 | 4 | 9 | -1 | 2 | 0 |
| ... | ... | ... | ... | ... | ... | ... | ... |
| ... | ... | ... | ... | ... | ... | ... | ... |
| ... | ... | ... | ... | ... | ... | ... | ... |

| | |
|-----------|-----------|
| 00 | 00 |
| 01 | 11 |
| ... | ... |
| ... | ... |
| ... | ... |

| | | | | |
|-----------|------------|------------|------------|------------|
| $c_{1,0}$ | 2.1 | 3.6 | 5.3 | 6.6 |
| $c_{1,1}$ | 1.2 | 1.5 | 2.4 | 3.3 |
| $c_{1,2}$ | ... | ... | ... | ... |
| $c_{1,3}$ | ... | ... | ... | ... |
| $c_{2,0}$ | 3.3 | 4.1 | 2.7 | 1.4 |
| $c_{2,1}$ | ... | ... | ... | ... |
| $c_{2,2}$ | ... | ... | ... | ... |
| $c_{2,3}$ | ... | ... | ... | ... |

Distance Estimation

- Euclidean distance between a query point q and a data point encoded as t

- Restore the virtual joint center by looking up each partition of t in the corresponding codebooks $\Rightarrow p$

- $d^2(q, t) = \sum_{i=1}^d (q_i - p_i)^2$

非对称距离的计算

- Known as Asymmetric Distance Computation (ADC)

- $d^2(q, t) = \sum_{i=1}^m (q_{(i)} - c_{i,t(i)})^2$

| | | | | | | | | |
|---|---|---|---|---|----|---|---|---|
| q | 1 | 3 | 5 | 4 | -3 | 7 | 3 | 2 |
|---|---|---|---|---|----|---|---|---|

| | | |
|---|----|----|
| t | 01 | 00 |
|---|----|----|

| | | | | |
|-----------|-----|-----|-----|-----|
| $c_{1,0}$ | 2.1 | 3.6 | 5.3 | 6.6 |
| $c_{1,1}$ | 1.2 | 1.5 | 2.4 | 3.3 |
| $c_{1,2}$ | ... | ... | ... | ... |
| $c_{1,3}$ | ... | ... | ... | ... |
| $c_{2,0}$ | 3.3 | 4.1 | 2.7 | 1.4 |
| $c_{2,1}$ | ... | ... | ... | ... |
| $c_{2,2}$ | ... | ... | ... | ... |
| $c_{2,3}$ | ... | ... | ... | ... |

| | | | | | | | | |
|---|-----|-----|-----|-----|-----|-----|-----|-----|
| p | 1.2 | 1.5 | 2.4 | 3.3 | 3.3 | 4.1 | 2.7 | 1.4 |
|---|-----|-----|-----|-----|-----|-----|-----|-----|

Query Processing

- Compute ADC for every point in the database
 - How?
- Candidate = those with the l smallest AD
- [Optional] Reranking (if $l > 1$):
 - Load the data vectors and compute the actual Euclidean distance
 - Return the one with the smallest distance

Query Processing

| | | | | | | | | |
|---|---|---|---|---|----|---|---|---|
| q | 1 | 3 | 5 | 4 | -3 | 7 | 3 | 2 |
|---|---|---|---|---|----|---|---|---|

| | | |
|----------------|----|----|
| t ₁ | 01 | 00 |
|----------------|----|----|

$$(q_{(1)} - c_{1,t_1(1)})^2 + (q_{(2)} - c_{2,t_1(2)})^2$$

| | | |
|----------------|----|----|
| t ₂ | 11 | 10 |
|----------------|----|----|

$$(q_{(1)} - c_{1,t_2(1)})^2 + (q_{(2)} - c_{2,t_2(2)})^2$$

| | |
|-----|-----|
| ... | ... |
|-----|-----|

| | |
|-----|-----|
| ... | ... |
|-----|-----|

| | | | | |
|------------------|-----|-----|-----|-----|
| c _{1,0} | 2.1 | 3.6 | 5.3 | 6.6 |
| c _{1,1} | 1.2 | 1.5 | 2.4 | 3.3 |
| c _{1,2} | ... | ... | ... | ... |
| c _{1,3} | ... | ... | ... | ... |
| c _{2,0} | 3.3 | 4.1 | 2.7 | 1.4 |
| c _{2,1} | ... | ... | ... | ... |
| c _{2,2} | ... | ... | ... | ... |
| c _{2,3} | ... | ... | ... | ... |

Framework of PQ

- Pre-processing:
 - Step 1: partition data vectors
 - Step 2: generate codebooks (e.g., k-means)
 - Step 3: encode data
- Query
 - Step 1: compute distance between q and codewords
 - Step 2: compute AD for each point and return the candidates
 - Step 3: re-ranking (optional)