DATA MINING LECTURE 6

Min-Hashing, Locality Sensitive Hashing

Clustering

MIN-HASHING AND LOCALITY SENSITIVE HASHING

Thanks to:

Rajaraman and Ullman, “Mining Massive Datasets”

Evimaria Terzi, slides for Data Mining Course.

Motivating problem

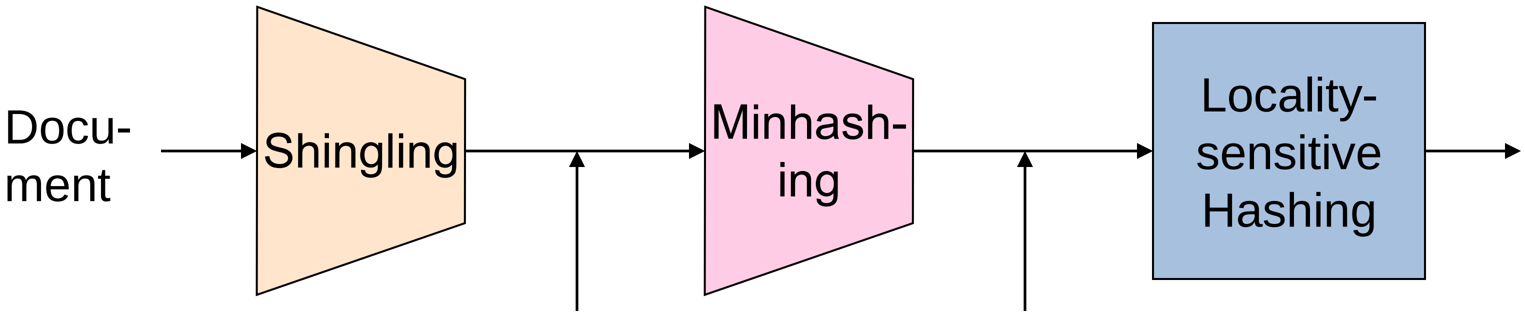
- Find duplicate and near-duplicate documents from a web crawl.

- If we wanted exact duplicates we could do this by hashing
  - We will see how to adapt this technique for near duplicate documents

Main issues

- What is the right representation of the document when we check for similarity?
  - E.g., representing a document as a set of characters will not do (why?)
- When we have billions of documents, keeping the full text in memory is not an option.
  - We need to find a shorter representation
- How do we do pairwise comparisons of billions of documents?
  - If exact match was the issue it would be ok, can we replicate this idea?

The Big Picture



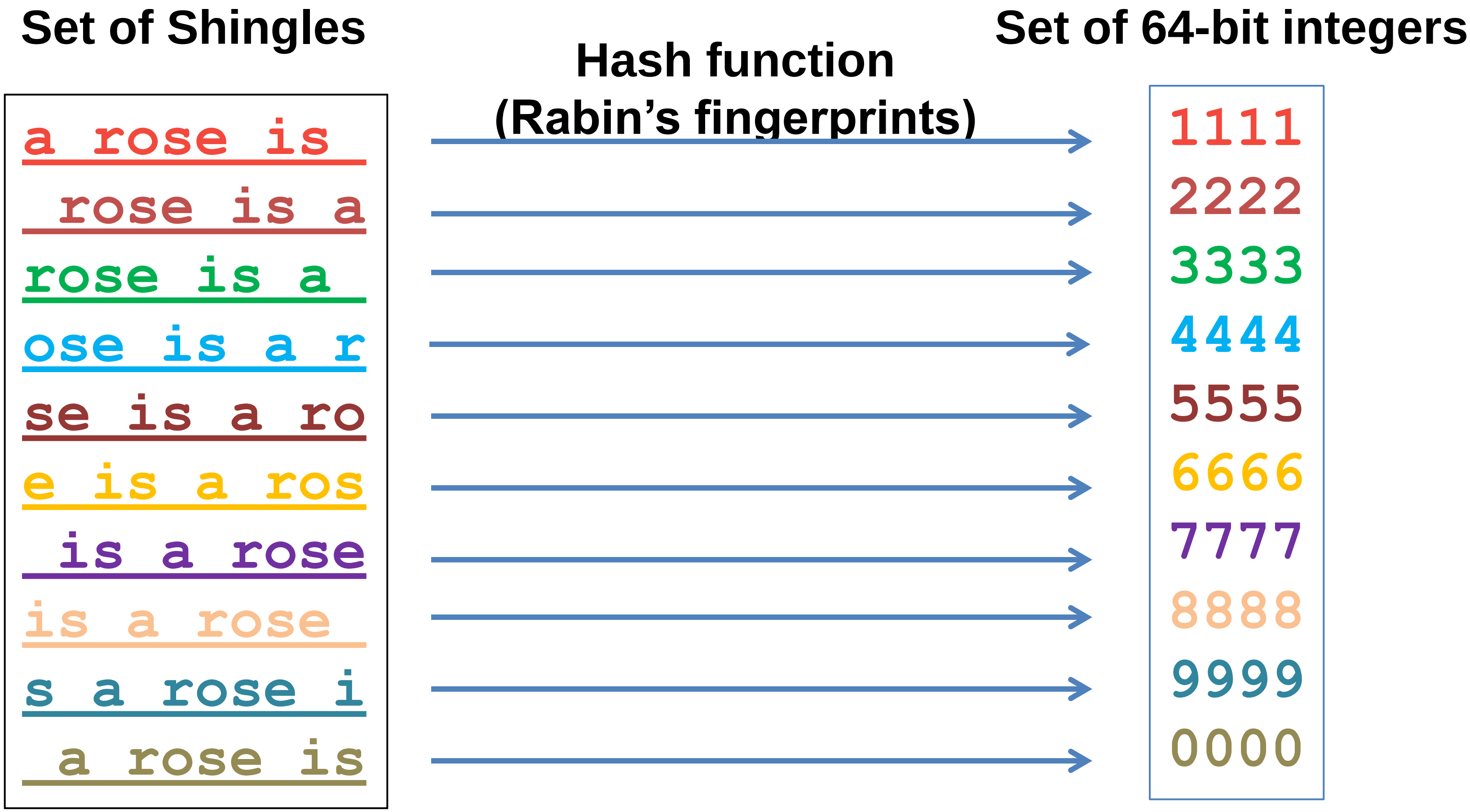
The set of strings of length *k* that appear in the doc- ument

Signatures : short integer vectors that represent the sets, and reflect their similarity

Candidate pairs : those pairs of signatures that we need to test for similarity.

Shingling

- Shingle: a sequence of k contiguous characters



Basic Data Model: Sets

- Document: A document is represented as a set shingles (more accurately, hashes of shingles)

- Document similarity: Jaccard similarity of the sets of shingles.
  - Common shingles over the union of shingles
  - $Sim(C_1, C_2) = |C_1 \cap C_2| / |C_1 \cup C_2|$.

- Applicable to any kind of sets.
  - E.g., similar customers or items.

Signatures

- Key idea: "hash" each set S to a small signature Sig (S), such that:

  1. Sig (S) is small enough that we can fit a signature in main memory for each set.

  2. Sim (S_1, S_2) is (almost) the same as the "similarity" of Sig (S_1) and Sig (S_2). (signature preserves similarity).

- Warning: This method can produce false negatives, and false positives (if an additional check is not made).
  - False negatives: Similar items deemed as non-similar
  - False positives: Non-similar items deemed as similar

From Sets to Boolean Matrices

- Represent the data as a boolean matrix M
  - Rows = the universe of all possible set elements
    - In our case, shingle fingerprints take values in $[0\ldots2^{64}-1]$
  - Columns = the sets
    - In our case, documents, sets of shingle fingerprints
  - M(r,S) = 1 in row r and column S if and only if r is a member of S.

- Typical matrix is sparse.
  - We do not really materialize the matrix

Minhashing

- Pick a random permutation of the rows (the universe U).
- Define "hash" function for set S
  - h(S) = the index of the first row (in the permuted order) in which column S has 1.
  - OR
  - h(S) = the index of the first element of S in the permuted order.
- Use k (e.g., k = 100) independent random permutations to create a signature.

Example of minhash signatures

- Input matrix

	S_1	S_2	S_3	S_4
A	1	0	1	0
B	1	0	0	1
C	0	1	0	1
D	0	1	0	1
E	0	1	0	1
F	1	0	1	0
G	1	0	1	0

A
C
G
F
B
E
D

		S_1	S_2	S_3	S_4
1	**A**	1	0	1	0
2	**C**	0	1	0	1
3	**G**	1	0	1	0
4	**F**	1	0	1	0
5	**B**	1	0	0	1
6	**E**	0	1	0	1
7	**D**	0	1	0	1
		1	**2**	**1**	**2**

Example of minhash signatures

- Input matrix

	S_1	S_2	S_3	S_4
A	1	0	1	0
B	1	0	0	1
C	0	1	0	1
D	0	1	0	1
E	0	1	0	1
F	1	0	1	0
G	1	0	1	0

→

D
B
A
C
F
G
E

→

		S_1	S_2	S_3	S_4
1	D	0	1	0	1
2	B	1	0	0	1
3	A	1	0	1	0
4	C	0	1	0	1
5	F	1	0	1	0
6	G	1	0	1	0
7	E	0	1	0	1
		2	1	3	1

Example of minhash signatures

- Input matrix

	S_1	S_2	S_3	S_4
A	1	0	1	0
B	1	0	0	1
C	0	1	0	1
D	0	1	0	1
E	0	1	0	1
F	1	0	1	0
G	1	0	1	0

→

C
D
G
F
A
B
E

→

		S_1	S_2	S_3	S_4
1	**C**	0	1	0	1
2	**D**	0	1	0	1
3	**G**	1	0	1	0
4	**F**	1	0	1	0
5	**A**	1	0	1	0
6	**B**	1	0	0	1
7	**E**	0	1	0	1
		3	**1**	**3**	**1**

Example of minhash signatures

- Input matrix

	S_1	S_2	S_3	S_4
A	1	0	1	0
B	1	0	0	1
C	0	1	0	1
D	0	1	0	1
E	0	1	0	1
F	1	0	1	0
G	1	0	1	0

$\approx$

Signature matrix

	S_1	S_2	S_3	S_4
h_1	1	2	1	2
h_2	2	1	3	1
h_3	3	1	3	1

- Sig(S) = vector of hash values
  - e.g., $Sig(S_2) = [2,1,1]$
- Sig(S,i) = value of the i-th hash function for set S
  - E.g., $Sig(S_2,3) = 1$

Hash function Property

$$\Pr(h(S_1) = h(S_2)) = Sim(S_1,S_2)$$

- where the probability is over all choices of permutations.

- Why?
  - The first row where one of the two sets has value 1 belongs to the union.
    - Recall that union contains rows with at least one 1.
  - We have equality if both sets have value 1, and this row belongs to the intersection

Example

- Universise: **U = {A,B,C,D,E,F,G}**
- X = {A,B,F,G}
- Y = {A,E,F,G}

Rows C,D could be anywhere
they do not affect the probability

- Union =
  {A,B,E,F,G}
- Intersection =
  {A,F,G}

	X	Y
A	1	1
B	1	0
C	0	0
D	0	0
E	0	1
F	1	1
G	1	1

D
*
*
C
*
*
*

	X	Y
D	0	0
C	0	0

Example

- Universe: **U = {A,B,C,D,E,F,G}**
- X = {A,B,F,G}
- Y = {A,E,F,G}

The * rows belong to the union

- Union = {A,B,E,F,G}
- Intersection = {A,F,G}

	X	Y
A	1	1
B	1	0
C	0	0
D	0	0
E	0	1
F	1	1
G	1	1

D
*
*
C
*
*
*

	X	Y
D	0	0
C	0	0

Example

- Universe: **U = {A,B,C,D,E,F,G}**
- X = {A,B,F,G}
- Y = {A,E,F,G}

The question is what is the value of the **first *** element

- Union = {A,B,E,F,G}
- Intersection = {A,F,G}

	X	Y
A	1	1
B	1	0
C	0	0
D	0	0
E	0	1
F	1	1
G	1	1

D
*
*
C
*
*
*

	X	Y
D	0	0
C	0	0

Example

- Universe: **U = {A,B,C,D,E,F,G}**
- X = {A,B,F,G}
- Y = {A,E,F,G}

If it belongs to the intersection then h(X) = h(Y)

- Union = {A,B,E,F,G}
- Intersection = {A,F,G}

	X	Y
A	1	1
B	1	0
C	0	0
D	0	0
E	0	1
F	1	1
G	1	1

D
*
*
C
*
*
*

	X	Y
D	0	0
C	0	0

Example

- Universe: **U = {A,B,C,D,E,F,G}**
- X = {A,B,F,G}
- Y = {A,E,F,G}

Every element of the union is equally likely to be the * element

$$Pr(h(X) = h(Y)) = \frac{|\{A,F,G\}|}{|\{A,B,E,F,G\}|} = \frac{3}{5} = Sim(X,Y)$$

- Union = {A,B,E,F,G}
- Intersection = {A,F,G}

	X	Y
A	1	1
B	1	0
C	0	0
D	0	0
E	0	1
F	1	1
G	1	1

D
*
*
C
*
*
*

	X	Y
D	0	0
C	0	0

Similarity for Signatures

- The similarity of signatures is the fraction of the hash functions in which they agree.

	S_1	S_2	S_3	S_4
A	1	0	1	0
B	1	0	0	1
C	0	1	0	1
D	0	1	0	1
E	0	1	0	1
F	1	0	1	0
G	1	0	1	0

$\approx$

Signature matrix

S_1	S_2	S_3	S_4
1	2	1	2
2	1	3	1
3	1	3	1

	Actual	**Sig**
(S_1, S_2)	0	0
(S_1, S_3)	3/5	2/3
(S_1, S_4)	1/7	0
(S_2, S_3)	0	0
(S_2, S_4)	3/4	1
(S_3, S_4)	0	0

Zero similarity is preserved
High similarity is well approximated

- With multiple signatures we get a good approximation

Is it now feasible?

- Assume a billion rows
- Hard to pick a random permutation of 1…billion
- **Even representing a random permutation requires 1 billion entries!!!**
- How about accessing rows in permuted order? ☹

Being more practical

- Instead of permuting the rows we will apply a hash function that maps the rows to a new (possibly larger) space
  - The value of the hash function is the position of the row in the new order (permutation).
  - Each set is represented by the smallest hash value among the elements in the set

- The space of the hash functions should be such that if we select one at random each element (row) has equal probability to have the smallest value
  - Min-wise independent hash functions

Algorithm – One set, one hash function

Computing **Sig(S,i)** for a single column S and single hash function h_i

In practice only the rows (shingles) that appear in the data

for each row **r**

compute h_i **(r)**

h_i **(r)** = index of row r in permutation

if column **S** that has **1** in row **r**

S contains row r

if h_i **(r)** is a smaller value than **Sig(S,i) then**

Sig(S,i) = h_i **(r);**

Find the row r with minimum index

Sig(S,i) will become the smallest value of h_i**(r)** among all rows (shingles) for which column **S** has value **1** (shingle belongs in S); *i*.e., h_i **(r)** gives the min index for the **i-**th permutation

Algorithm – All sets, k hash functions

Pick k=100 hash functions $(h_1,\ldots,h_k)$

In practice this means selecting the hash function parameters

for each row r

  for each hash function h_i

    compute $h_i(r)$

Compute $h_i(r)$ only once for all sets

    for each column S that has 1 in row r

      if $h_i(r)$ is a smaller value than Sig(S,i) **then**

        $Sig(S,i) = h_i(r)$;

Example

x	Row	S1	S2	h(x)	g(x)
0	A	1	0	1	3
1	B	0	1	2	0
2	C	1	1	3	2
3	D	1	0	4	4
4	E	0	1	0	1

$h(x) = x+1 \bmod 5$
$g(x) = 2x+3 \bmod 5$

h(Row)	Row	S1	S2
0	E	0	1
1	A	1	0
2	B	0	1
3	C	1	1
4	D	1	0

g(Row)	Row	S1	S2
0	B	0	1
1	E	0	1
2	C	1	0
3	A	1	1
4	D	1	0

	Sig1	Sig2
$h(0) = 1$	1	-
$g(0) = 3$	3	-
$h(1) = 2$	1	2
$g(1) = 0$	3	0
$h(2) = 3$	1	2
$g(2) = 2$	2	0
$h(3) = 4$	1	2
$g(3) = 4$	2	0
$h(4) = 0$	1	0
$g(4) = 1$	2	0

Implementation

- Often, data is given by column, not row.
  - E.g., columns = documents, rows = shingles.
- If so, sort matrix once so it is by row.
- And always compute $h_i(r)$ only once for each row.

Finding similar pairs

- Problem: Find all pairs of documents with similarity at least t = 0.8
- While the signatures of all columns may fit in main memory, comparing the signatures of all pairs of columns is quadratic in the number of columns.
- Example: 10^6 columns implies $5*10^{11}$ column-comparisons.
- At 1 microsecond/comparison: 6 days.

Locality-Sensitive Hashing

- What we want: a function f(X,Y) that tells whether or not X and Y is a candidate pair: a pair of elements whose similarity must be evaluated.

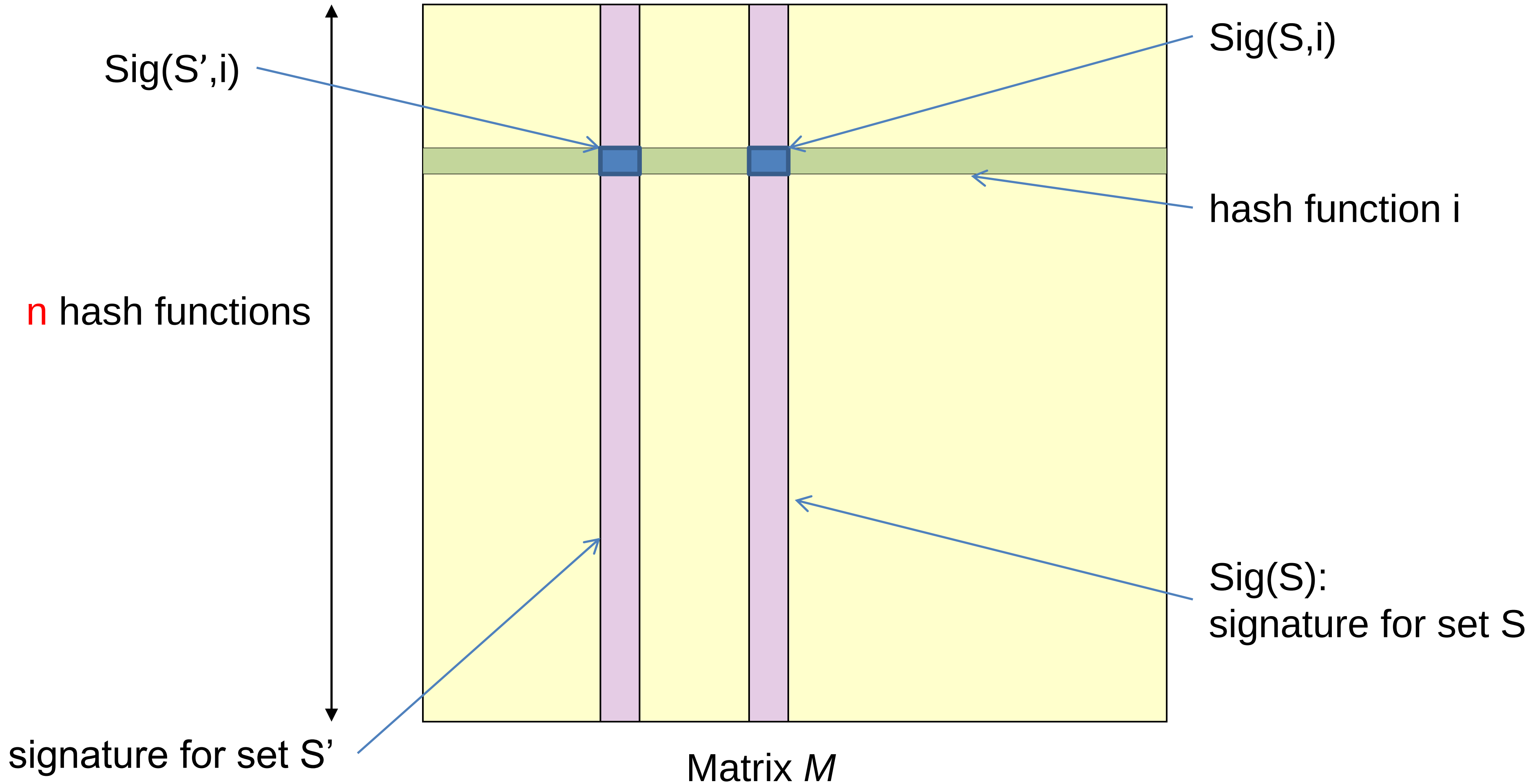
- A simple idea: X and Y are a candidate pair if they have the same min-hash signature.
  - Easy to test by hashing the signatures.
  - Similar sets are more likely to have the same signature.
  - Likely to produce many false negatives.
    - Requiring full match of signature is strict, some similar sets will be lost.

! Multiple levels of Hashing!

- Improvement: Compute multiple signatures; candidate pairs should have at least one common signature.
  - Reduce the probability for false negatives.

Signature matrix reminder

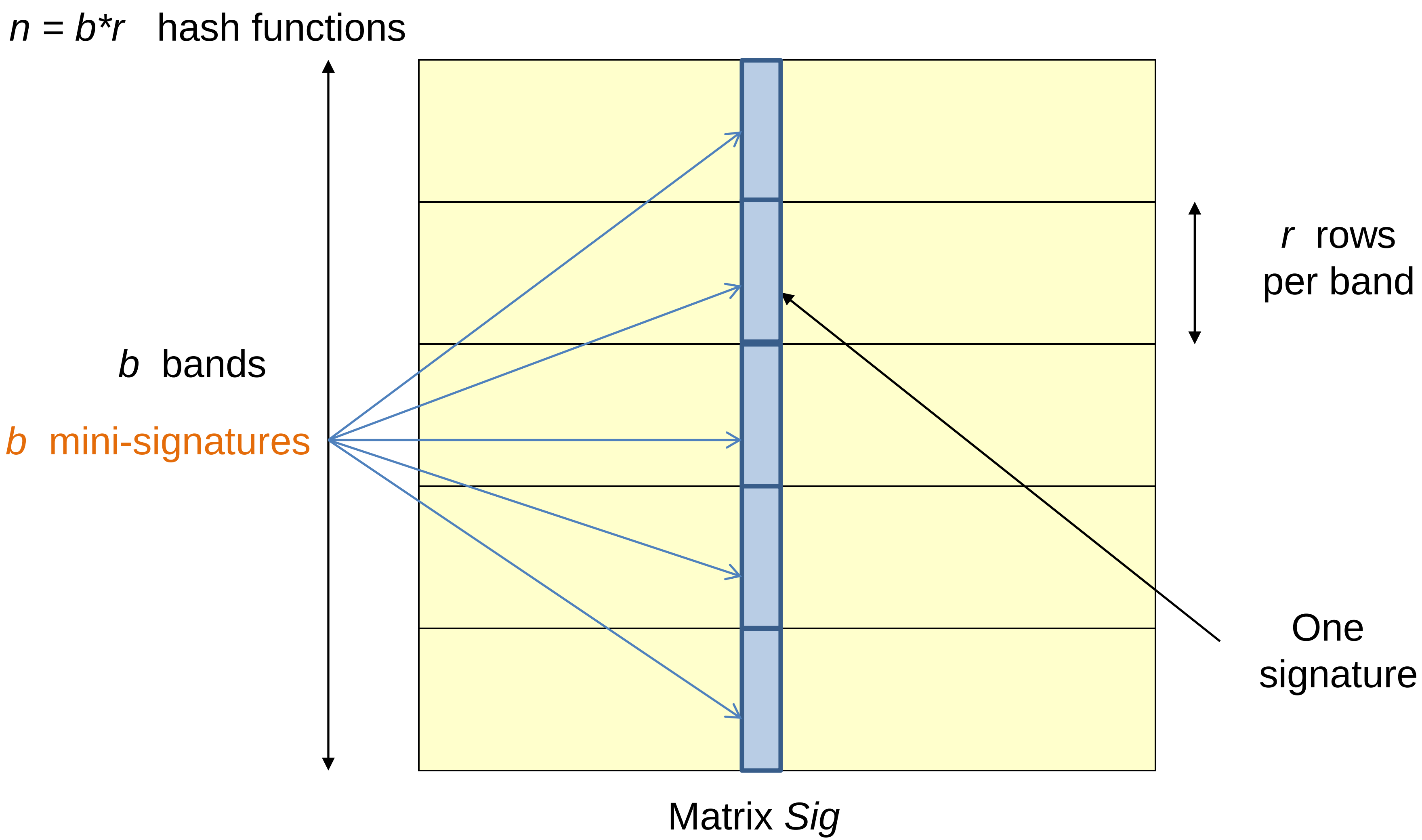
Prob(Sig(S,i) == Sig(S',i)) = sim(S,S')



Partition into Bands – (1)

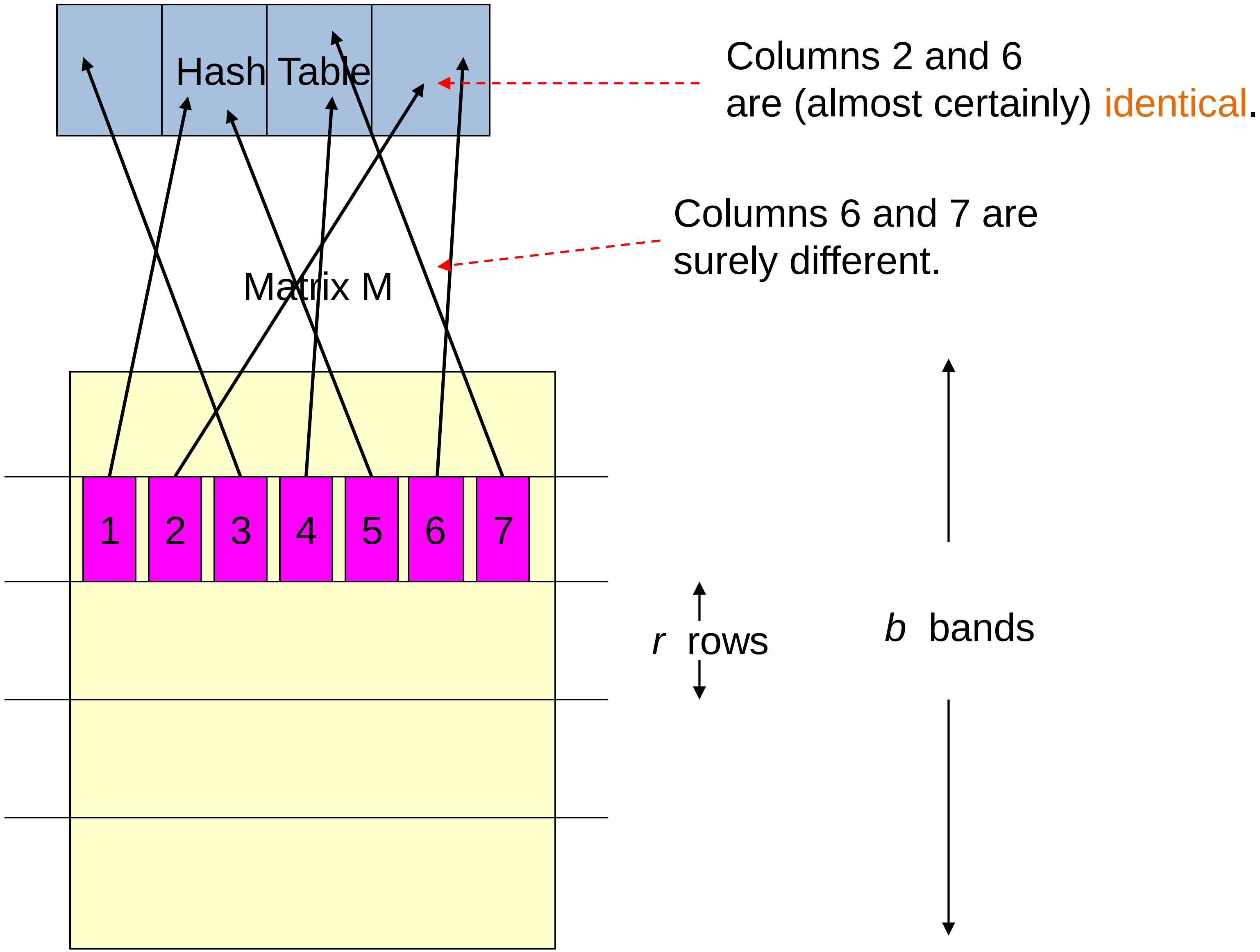
- Divide the signature matrix Sig into *b* bands of *r* rows.
  - Each band is a mini-signature with r hash functions.

Partitioning into bands



Partition into Bands – (2)

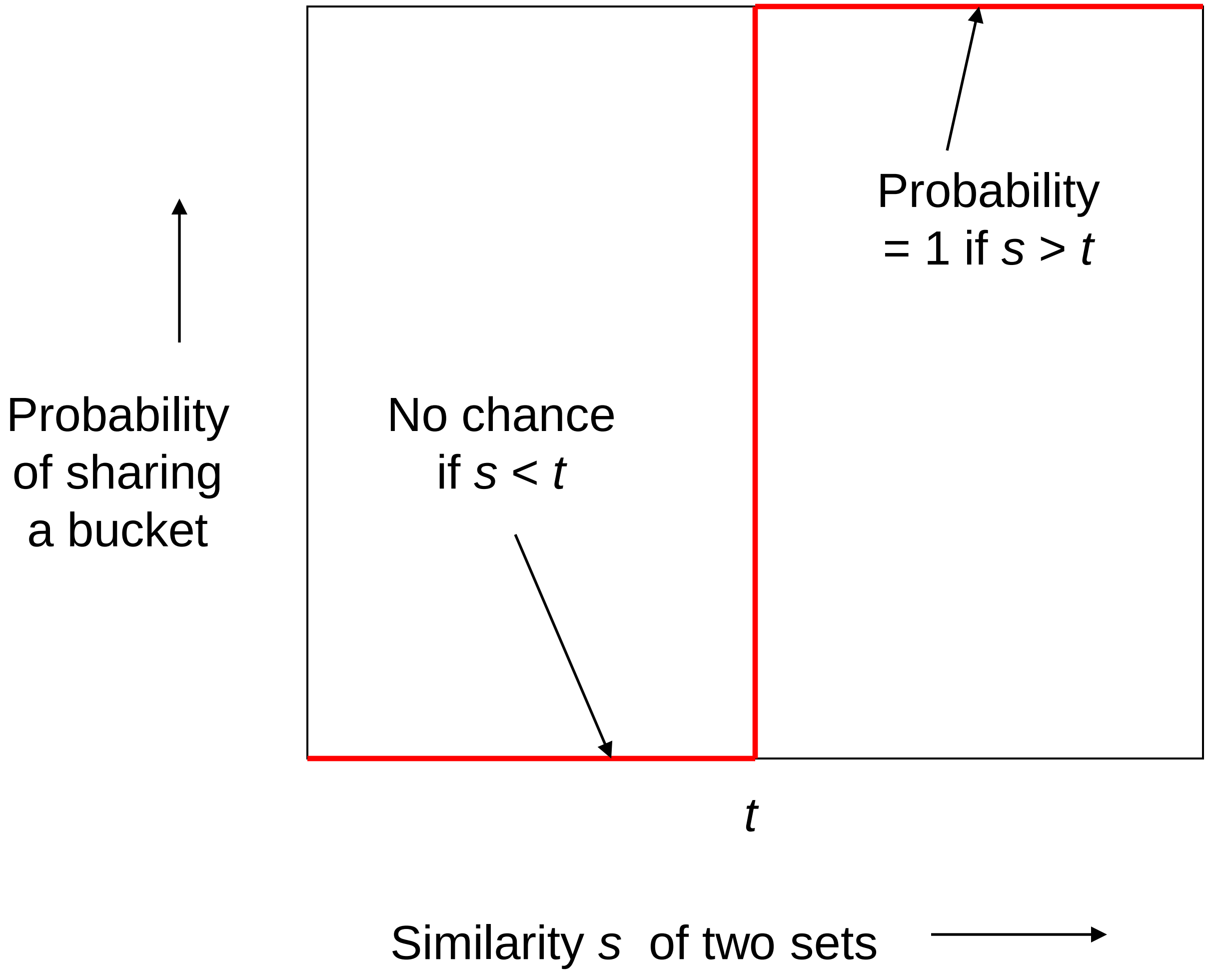
- Divide the signature matrix Sig into *b* bands of *r* rows.
  - Each band is a mini-signature with r hash functions.
- For each band, hash the mini-signature to a hash table with *k* buckets.
  - Make *k* as large as possible so that mini-signatures that hash to the same bucket are almost certainly identical.


Hash Table
Columns 2 and 6
are (almost certainly) identical.
Columns 6 and 7 are
surely different.
Matrix M
1
2
3
4
5
6
7
r rows
b bands

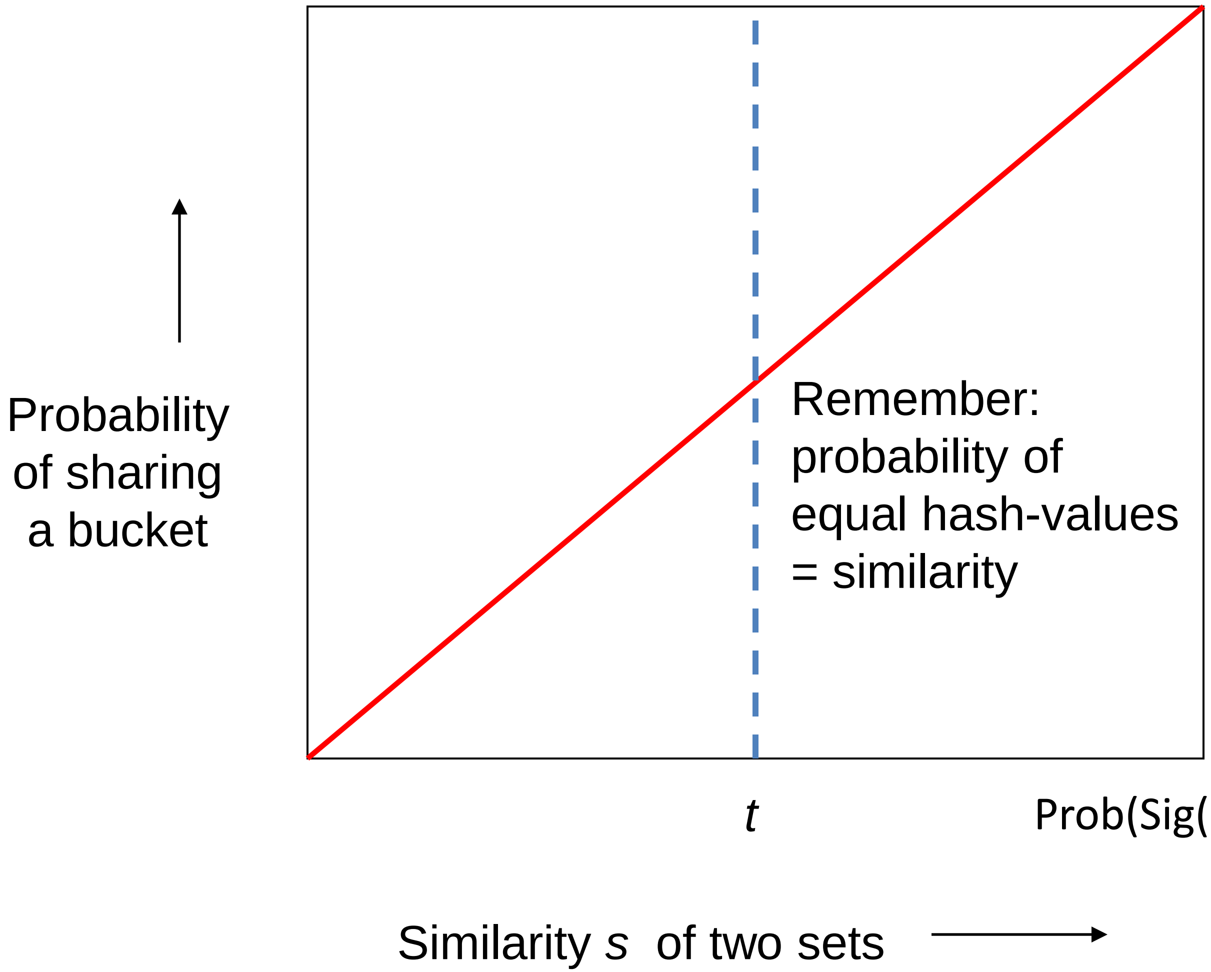
Partition into Bands – (3)

- Divide the signature matrix Sig into *b* bands of *r* rows.
  - Each band is a mini-signature with r hash functions.
- For each band, hash the mini-signature to a hash table with *k* buckets.
  - Make *k* as large as possible so that mini-signatures that hash to the same bucket are almost certainly identical.
- Candidate column pairs are those that hash to the same bucket for at least 1 band.
- Tune *b* and *r* to catch most similar pairs, but few non-similar pairs.

Analysis of LSH – What We Want



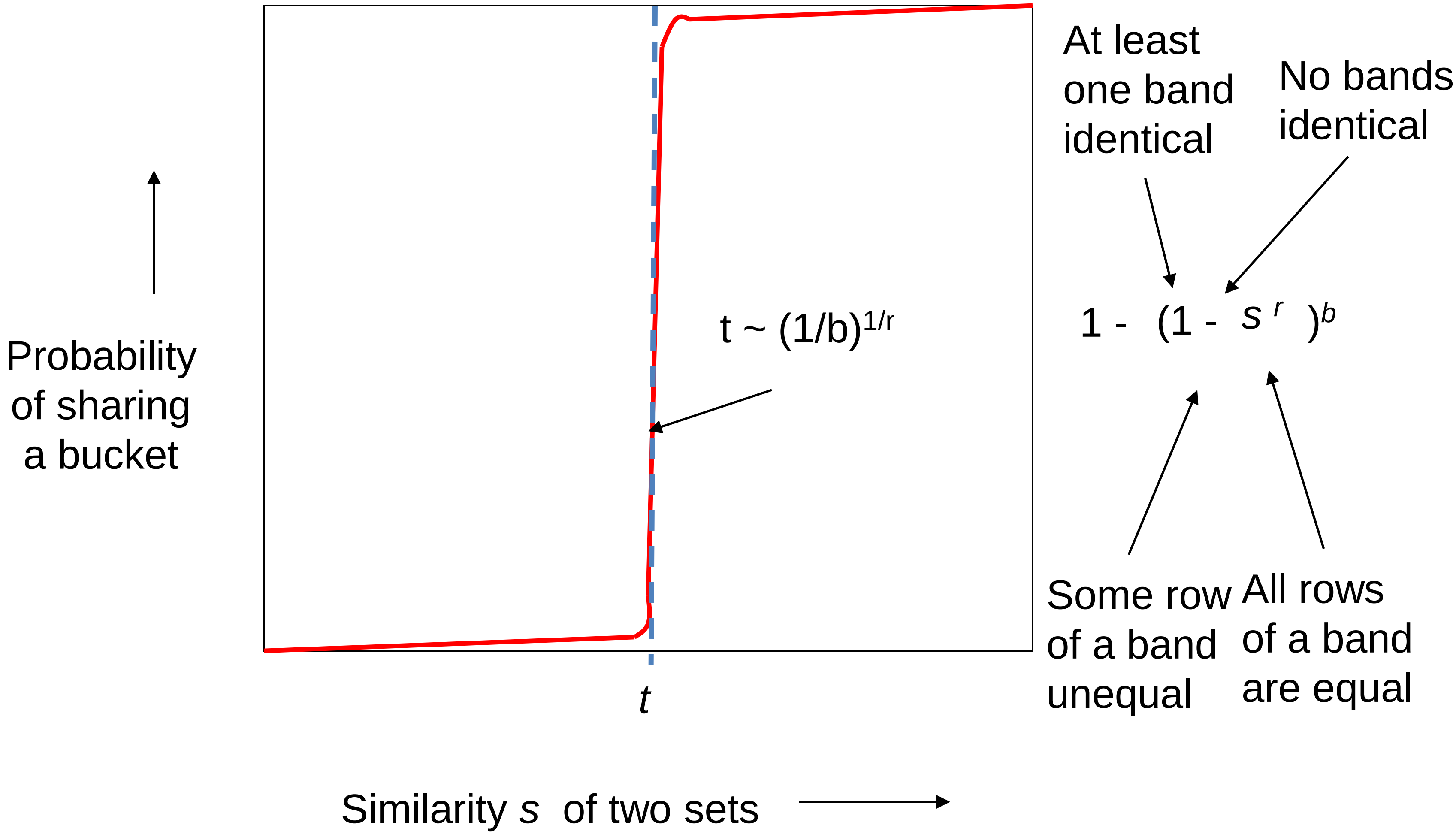
What One Band of One Row Gives You



Single hash signature

Prob(Sig(S,i) == Sig(S',i)) = sim(S,S')

What *b* Bands of *r* Rows Gives You



Example: $b = 20; r = 5$

s	$1-(1-s^r)^b$
.2	.006
.3	.047
.4	.186
.5	.470
.6	.802
.7	.975
.8	.9996

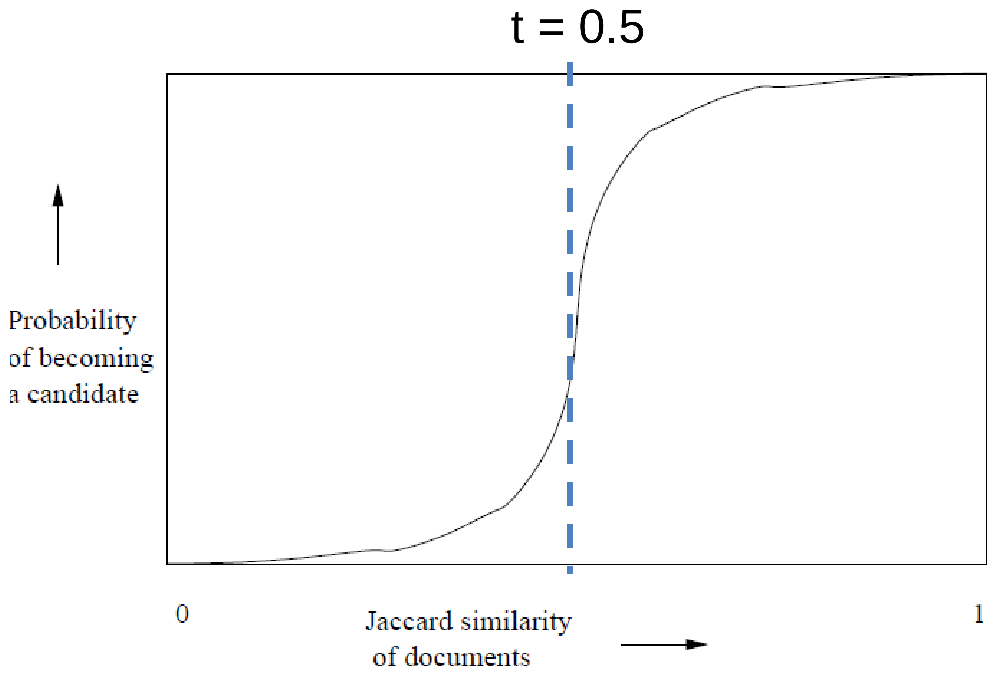


Figure 3.7: The S-curve

Suppose S_1, S_2 are 80% Similar

- We want all 80%-similar pairs. Choose 20 bands of 5 integers/band.

- Probability S_1, S_2 identical in one particular band:

  $$(0.8)^5 = 0.328.$$

- Probability S_1, S_2 are not similar in any of the 20 bands:

  $$(1-0.328)^{20} = 0.00035$$

  - i.e., about 1/3000-th of the 80%-similar column pairs are false negatives.

- Probability S_1, S_2 are similar in at least one of the 20 bands:

  $$1-0.00035 = 0.999$$

Suppose S_1, S_2 Only 40% Similar

- Probability S_1, S_2 identical in any one particular band:

  $$(0.4)^5 = 0.01 .$$

- Probability S_1, S_2 identical in at least 1 of 20 bands:

  $$\leq 20 * 0.01 = 0.2 .$$

- But false positives much lower for similarities << 40%.

LSH Summary

- Tune to get almost all pairs with similar signatures, but eliminate most pairs that do not have similar signatures.
- Check in main memory that candidate pairs really do have similar signatures.
- Optional: In another pass through data, check that the remaining candidate pairs really represent similar *sets* .

Locality-sensitive hashing (LSH)

- Big Picture: Construct hash functions **$h: R^d \rightarrow U$** such that for any pair of points **p,q**, for distance function **D** we have:
  - If **$D(p,q) \leq r$**, then **$Pr[h(p)=h(q)] \geq \alpha$** is high
  - If **$D(p,q) \geq cr$**, then **$Pr[h(p)=h(q)] \leq \beta$** is small
- Then, we can find close pairs by hashing

- LSH is a general framework: for a given distance function **D** we need to find the right **h**
  - **h** is **(r, cr, α, β)-**sensitive

LSH for Cosine Distance

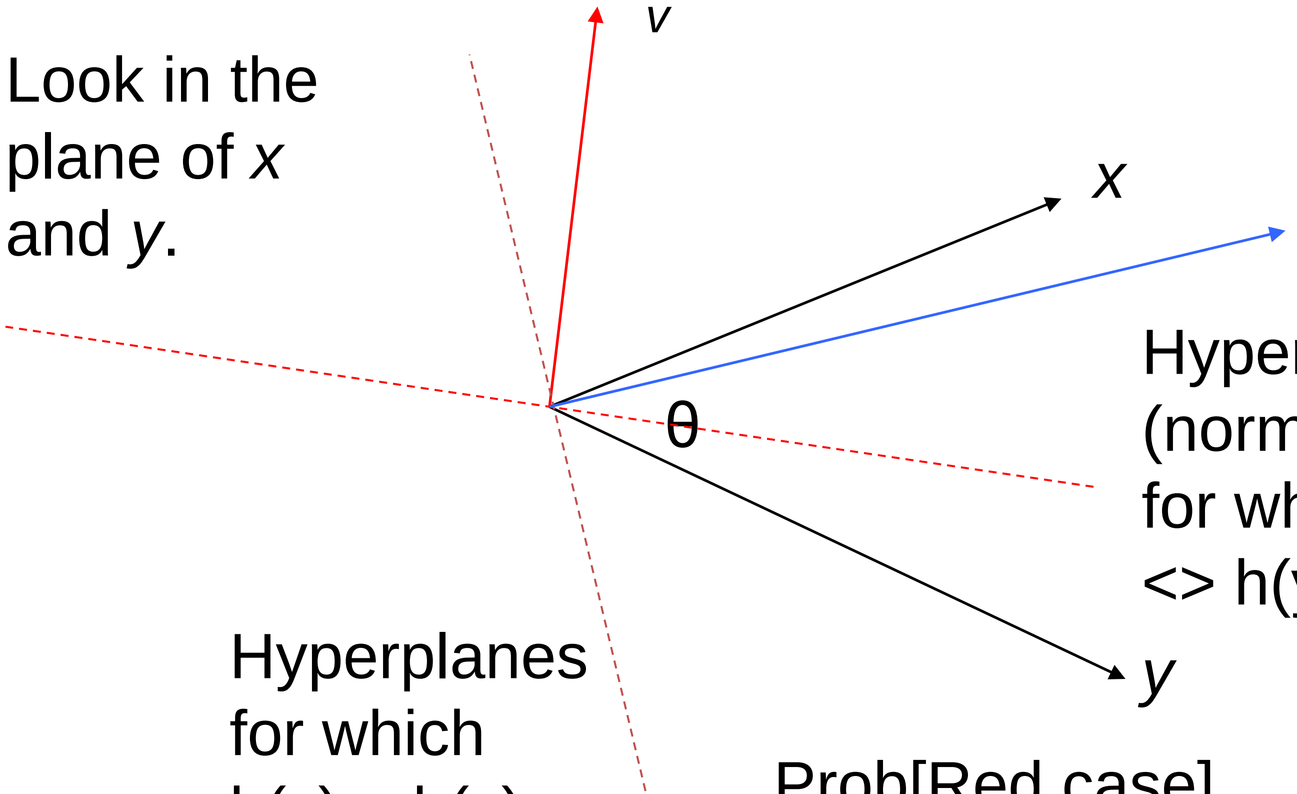
- For cosine distance, there is a technique analogous to minhashing for generating a $(d_1, d_2, (1-d_1/180), (1-d_2/180))$- sensitive family for any d_1 and d_2.
- Called *random hyperplanes*.

Random Hyperplanes

- Pick a random vector *v*, which determines a hash function h_v with two buckets.
- $h_v(x) = +1$ if $v.x > 0$; $= -1$ if $v.x < 0$.
- LS-family **H** = set of all functions derived from any vector.
- Claim: Prob[h(x)=h(y)] = 1 – (angle between *x* and *y* divided by 180).

Proof of Claim

Look in the plane of *x* and *y*.



Hyperplanes (normal to *v*) for which h(x) <> h(y)

Hyperplanes for which h(x) = h(y)

Prob[Red case] = θ/180

Signatures for Cosine Distance

- Pick some number of vectors, and hash your data for each vector.
- The result is a signature (*sketch*) of +1's and –1's that can be used for LSH like the minhash signatures for Jaccard distance.

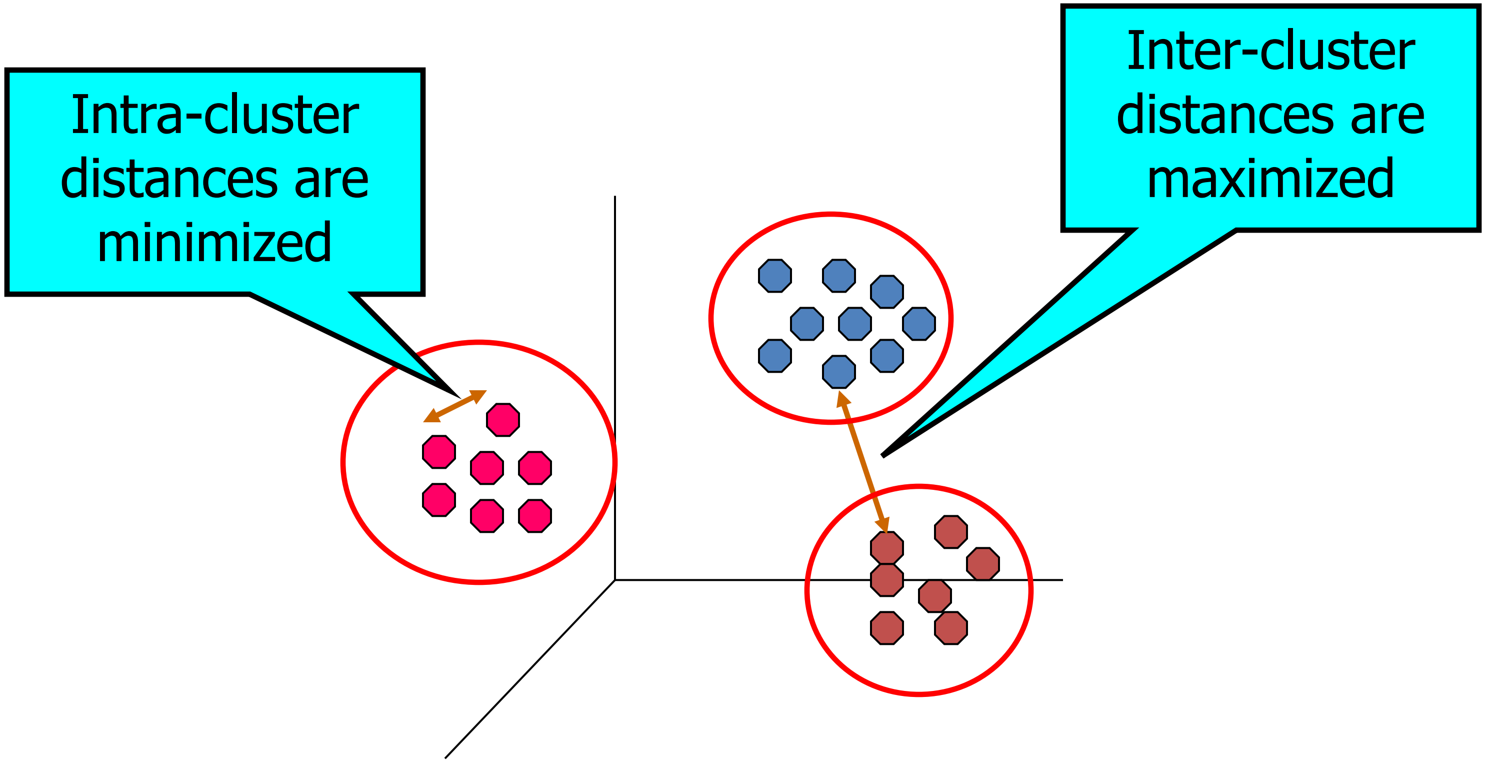
Simplification

- We need not pick from among all possible vectors v to form a component of a sketch.
- It suffices to consider only vectors v consisting of +1 and –1 components.

CLUSTERING

What is a Clustering?

- In general a grouping of objects such that the objects in a group (cluster) are similar (or related) to one another and different from (or unrelated to) the objects in other groups

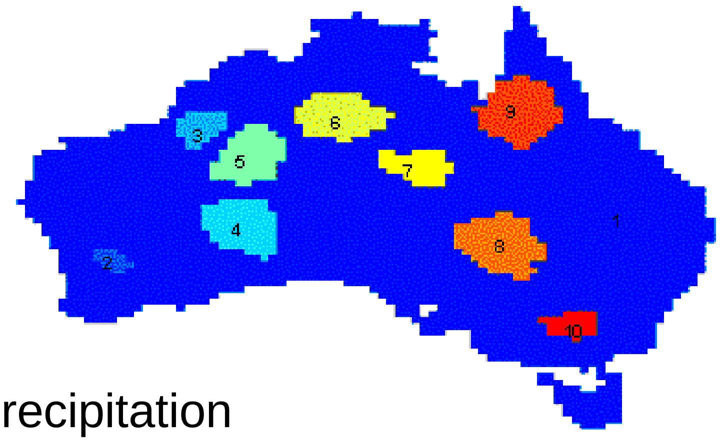


Applications of Cluster Analysis

- **Understanding**
  - Group related documents for browsing, group genes and proteins that have similar functionality, or group stocks with similar price fluctuations

	Discovered Clusters	*Industry Group*
1	Applied-Matl-DOWN,Bay-Network-Down,3-COM-DOWN, Cabletron-Sys-DOWN,CISCO-DOWN,HP-DOWN, DSC-Comm-DOWN,INTEL-DOWN,LSI-Logic-DOWN, Micron-Tech-DOWN,Texas-Inst-Down,Tellabs-Inc-Down, Natl-Semiconduct-DOWN,Oracl-DOWN,SGI-DOWN, Sun-DOWN	Technology1-DOWN
2	Apple-Comp-DOWN,Autodesk-DOWN,DEC-DOWN, ADV-Micro-Device-DOWN,Andrew-Corp-DOWN, Computer-Assoc-DOWN,Circuit-City-DOWN, Compaq-DOWN, EMC-Corp-DOWN, Gen-Inst-DOWN, Motorola-DOWN,Microsoft-DOWN,Scientific-Atl-DOWN	Technology2-DOWN
3	Fannie-Mae-DOWN,Fed-Home-Loan-DOWN, MBNA-Corp-DOWN,Morgan-Stanley-DOWN	Financial-DOWN
4	Baker-Hughes-UP,Dresser-Inds-UP,Halliburton-HLD-UP, Louisiana-Land-UP,Phillips-Petro-UP,Unocal-UP, Schlumberger-UP	Oil-UP

- **Summarization**
  - Reduce the size of large data sets



Clustering precipitation in Australia

Early applications of cluster analysis

- John Snow, London 1854

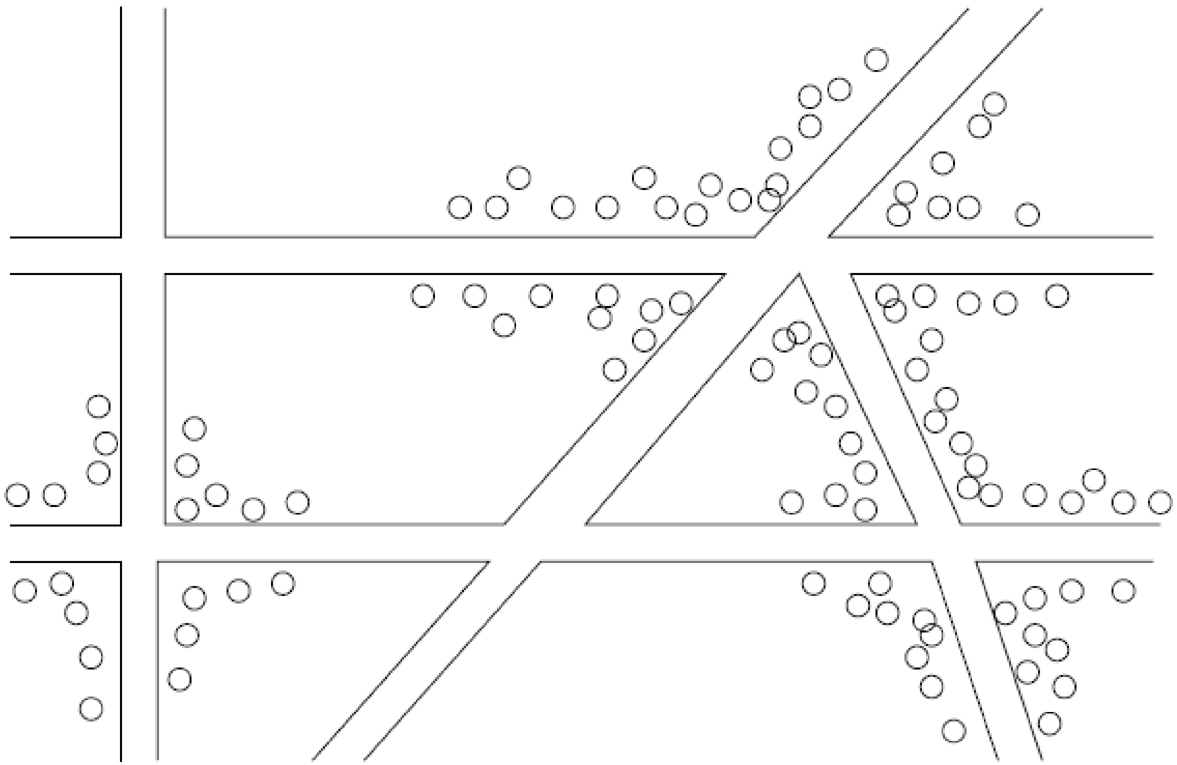
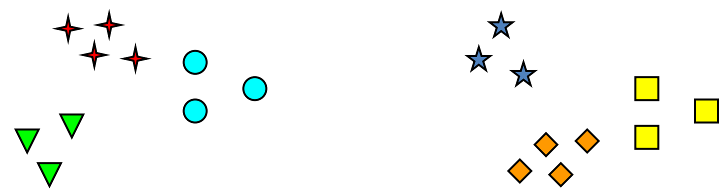


Figure 1.1: Plotting cholera cases on a map of London

Notion of a Cluster can be Ambiguous

How many clusters?



Six Clusters

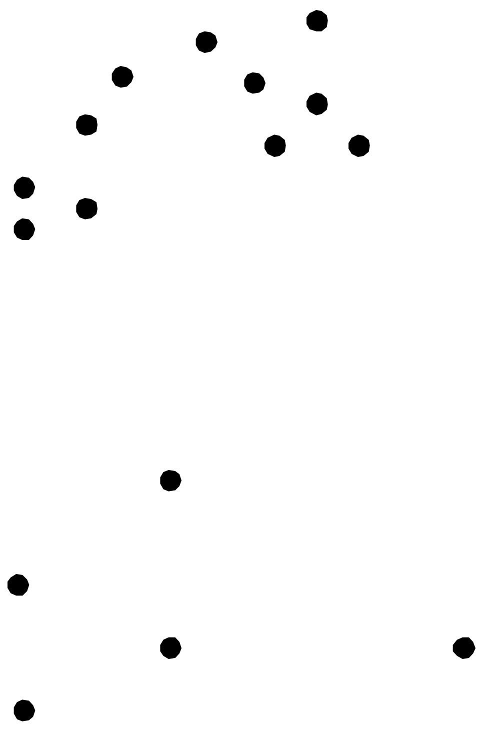
Two Clusters

Four Clusters

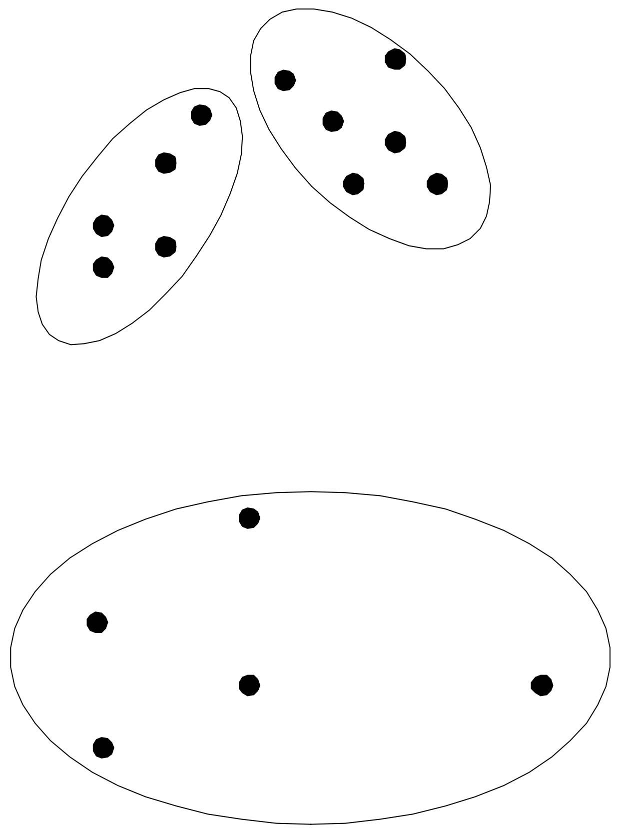
Types of Clusterings

- A clustering is a set of clusters
- Important distinction between hierarchical and partitional sets of clusters
- Partitional Clustering
  - A division data objects into subsets (clusters) such that each data object is in exactly one subset
- Hierarchical clustering
  - A set of nested clusters organized as a hierarchical tree

Partitional Clustering

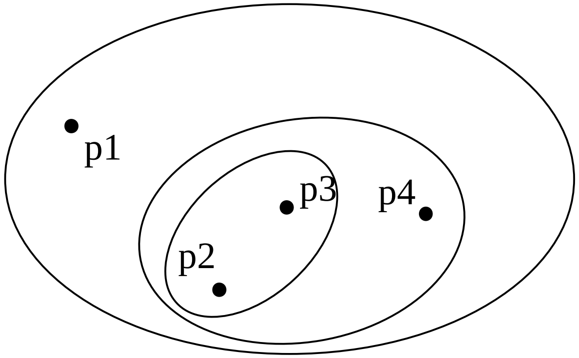


Original Points

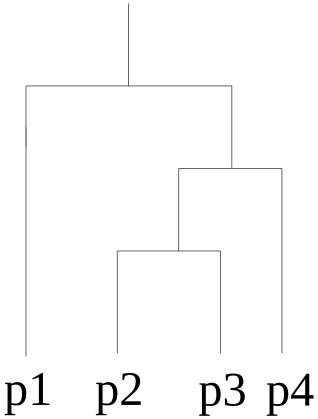


A Partitional Clustering

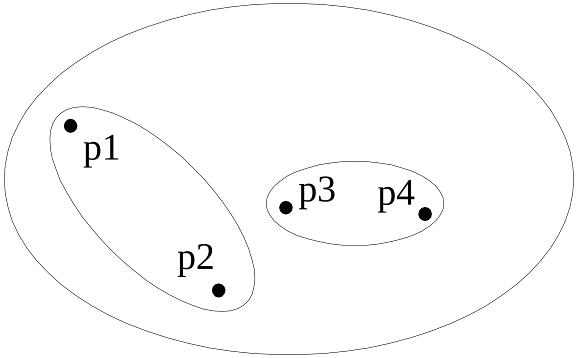
Hierarchical Clustering



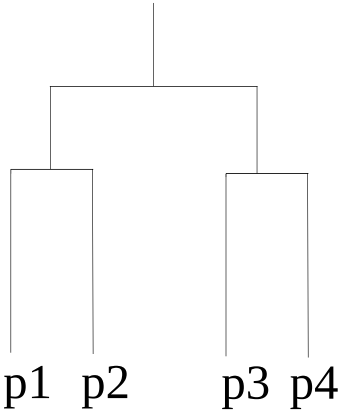
Traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Hierarchical Clustering



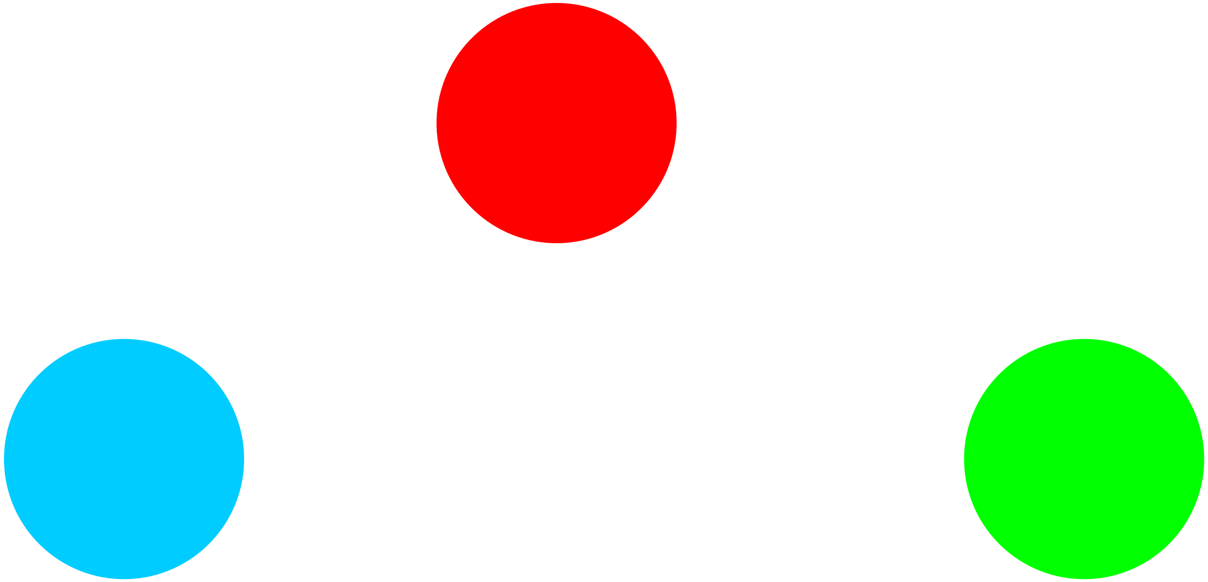
Non-traditional Dendrogram

Other types of clustering

- Exclusive (or non-overlapping) versus non-exclusive (or overlapping)
  - In non-exclusive clusterings, points may belong to multiple clusters.
    - Points that belong to multiple classes, or ‘border’ points
- Fuzzy (or soft) versus non-fuzzy (or hard)
  - In fuzzy clustering, a point belongs to every cluster with some weight between 0 and 1
    - Weights usually must sum to 1 (often interpreted as probabilities)
- Partial versus complete
  - In some cases, we only want to cluster some of the data

Types of Clusters: Well-Separated

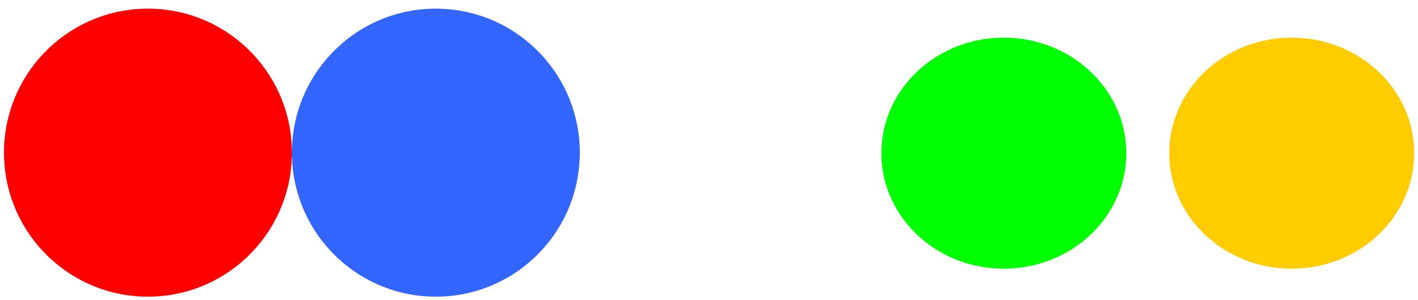
- Well-Separated Clusters:
  - A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.



3 well-separated clusters

Types of Clusters: Center-Based

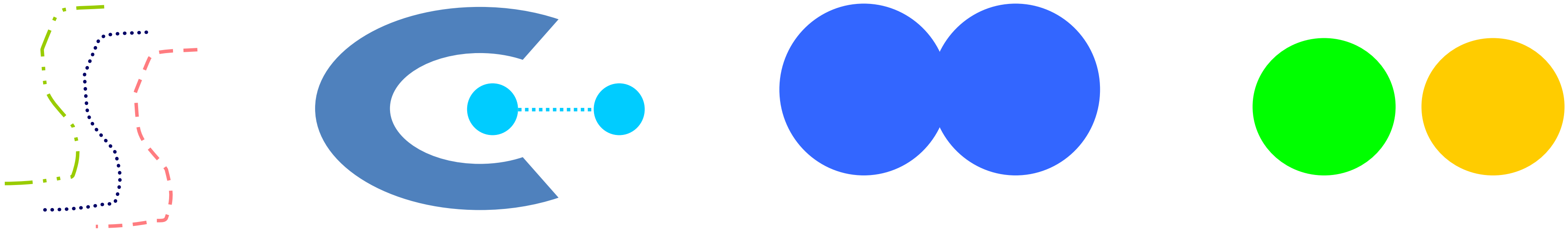
- Center-based
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the "center" of a cluster, than to the center of any other cluster
  - The center of a cluster is often a centroid, the minimizer of distances from all the points in the cluster, or a medoid, the most "representative" point of a cluster



4 center-based clusters

Types of Clusters: Contiguity-Based

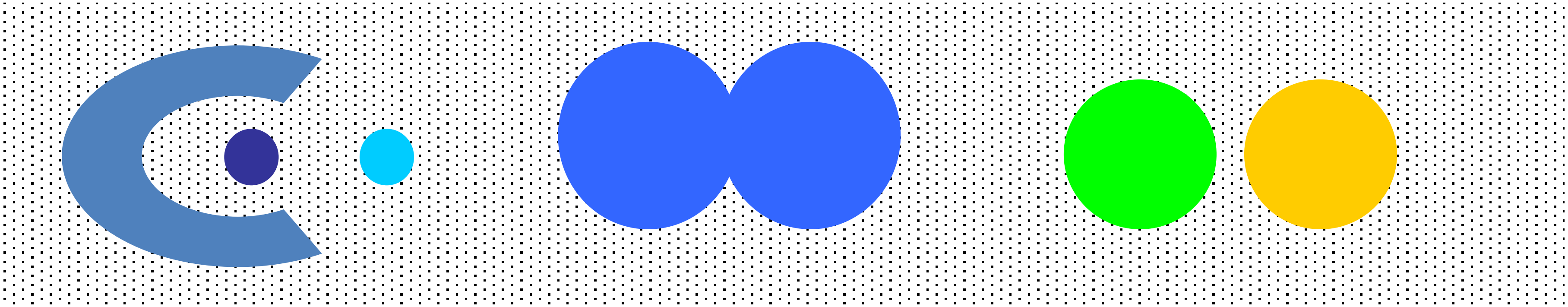
- Contiguous Cluster (Nearest neighbor or Transitive)
  - A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.



8 contiguous clusters

Types of Clusters: Density-Based

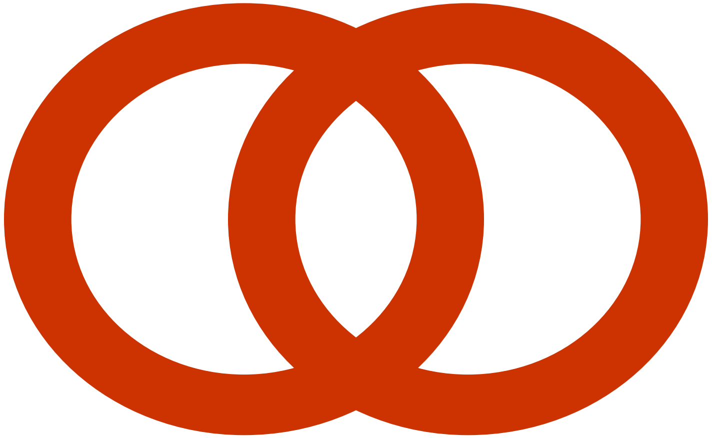
- Density-based
  - A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
  - Used when the clusters are irregular or intertwined, and when noise and outliers are present.



6 density-based clusters

Types of Clusters: Conceptual Clusters

- Shared Property or Conceptual Clusters
  - Finds clusters that share some common property or represent a particular concept.
  - .



2 Overlapping Circles

Types of Clusters: Objective Function

- Clustering as an optimization problem
  - Finds clusters that minimize or maximize an objective function.
  - Enumerate all possible ways of dividing the points into clusters and evaluate the `goodness' of each potential set of clusters by using the given objective function. (NP Hard)
  - Can have global or local objectives.
    - Hierarchical clustering algorithms typically have local objectives
    - Partitional algorithms typically have global objectives
  - A variation of the global objective function approach is to fit the data to a parameterized model.
    - The parameters for the model are determined from the data, and they determine the clustering
    - E.g., Mixture models assume that the data is a ‘mixture' of a number of statistical distributions.

Clustering Algorithms

- K-means and its variants
- Hierarchical clustering
- DBSCAN

K-MEANS

K-means Clustering

- Partitional clustering approach
- Each cluster is associated with a centroid (center point)
- Each point is assigned to the cluster with the closest centroid
- Number of clusters, K, must be specified
- The objective is to minimize the sum of distances of the points to their respective centroid

K-means Clustering

- **Problem:** Given a set X of n points in a d-dimensional space and an integer K group the points into K clusters $C = \{C_1, C_2, \ldots, C_k\}$ such that

$$Cost(C) = \sum_{i=1}^{k} \sum_{x \in C_i} dist(x, c)$$

is minimized, where c_i is the centroid of the points in cluster C_i

K-means Clustering

- Most common definition is with euclidean distance, minimizing the Sum of Squares Error (SSE) function
  - Sometimes K-means is defined like that

- **Problem:** Given a set X of n points in a d-dimensional space and an integer K group the points into K clusters $C = \{C_1, C_2, \ldots, C_k\}$ such that

$$Cost(C) = \sum_{i=1}^{k} \sum_{x \in C_i} (x - c_i)^2$$

is minimized, where c_i is the mean of the points in cluster C_i

Sum of Squares Error (SSE)

Complexity of the k-means problem

- NP-hard if the dimensionality of the data is at least 2 (**d>=2**)
  - Finding the best solution in polynomial time is infeasible
- For **d=1** the problem is solvable in polynomial time (how?)
- A simple iterative algorithm works quite well in practice

K-means Algorithm

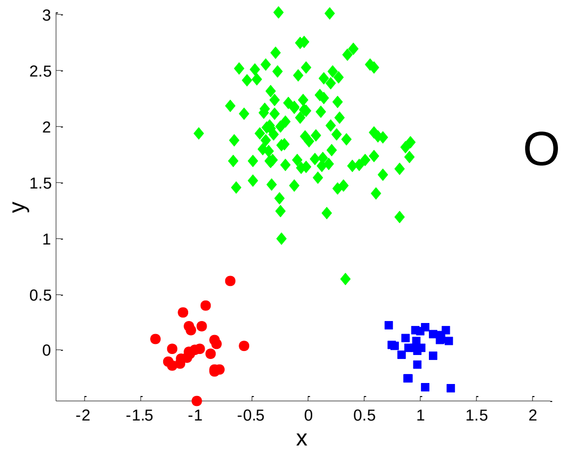
- Also known as Lloyd's algorithm.
- K-means is sometimes synonymous with this algorithm

1: Select K points as the initial centroids.
2: **repeat**
3: Form K clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: **until** The centroids don't change

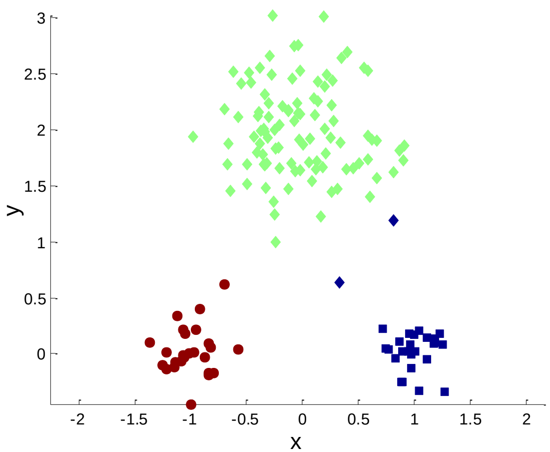
K-means Algorithm – Initialization

- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.

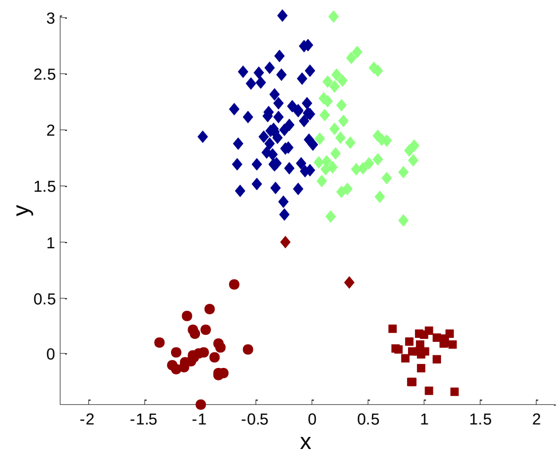
Two different K-means Clusterings



Original Points

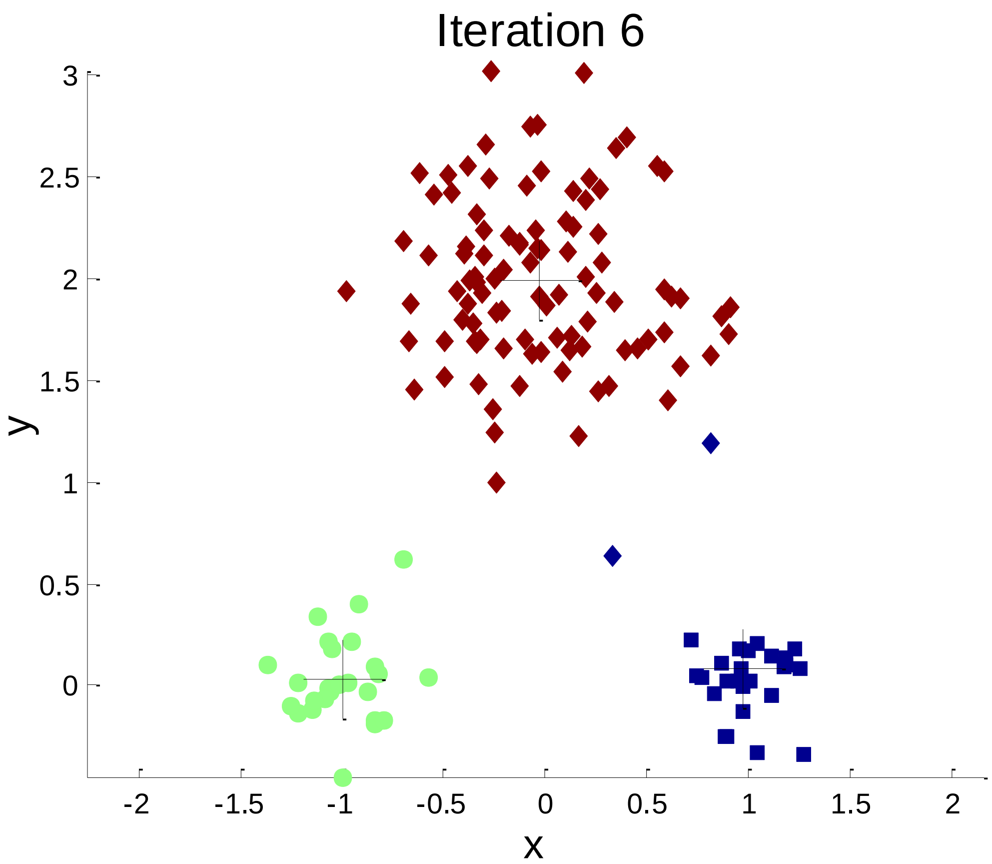


Optimal Clustering

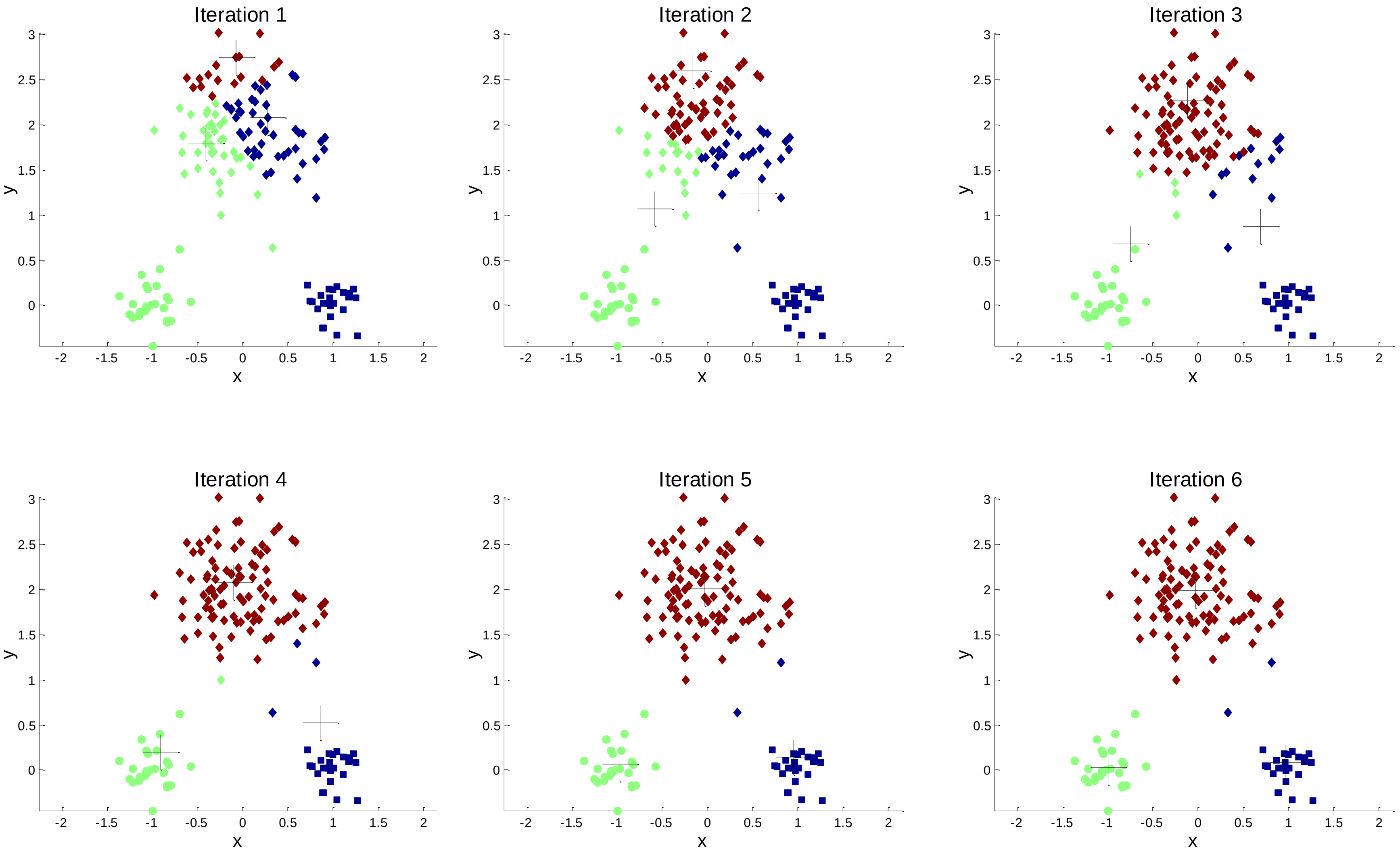


Sub-optimal Clustering

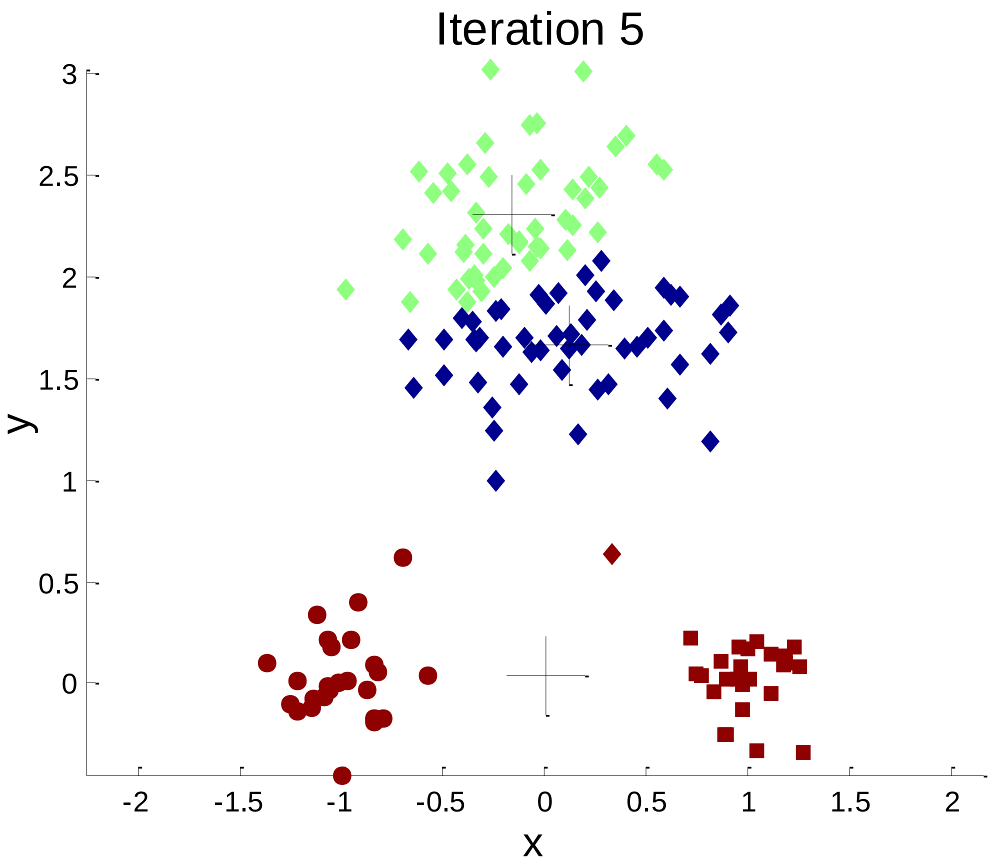
Importance of Choosing Initial Centroids



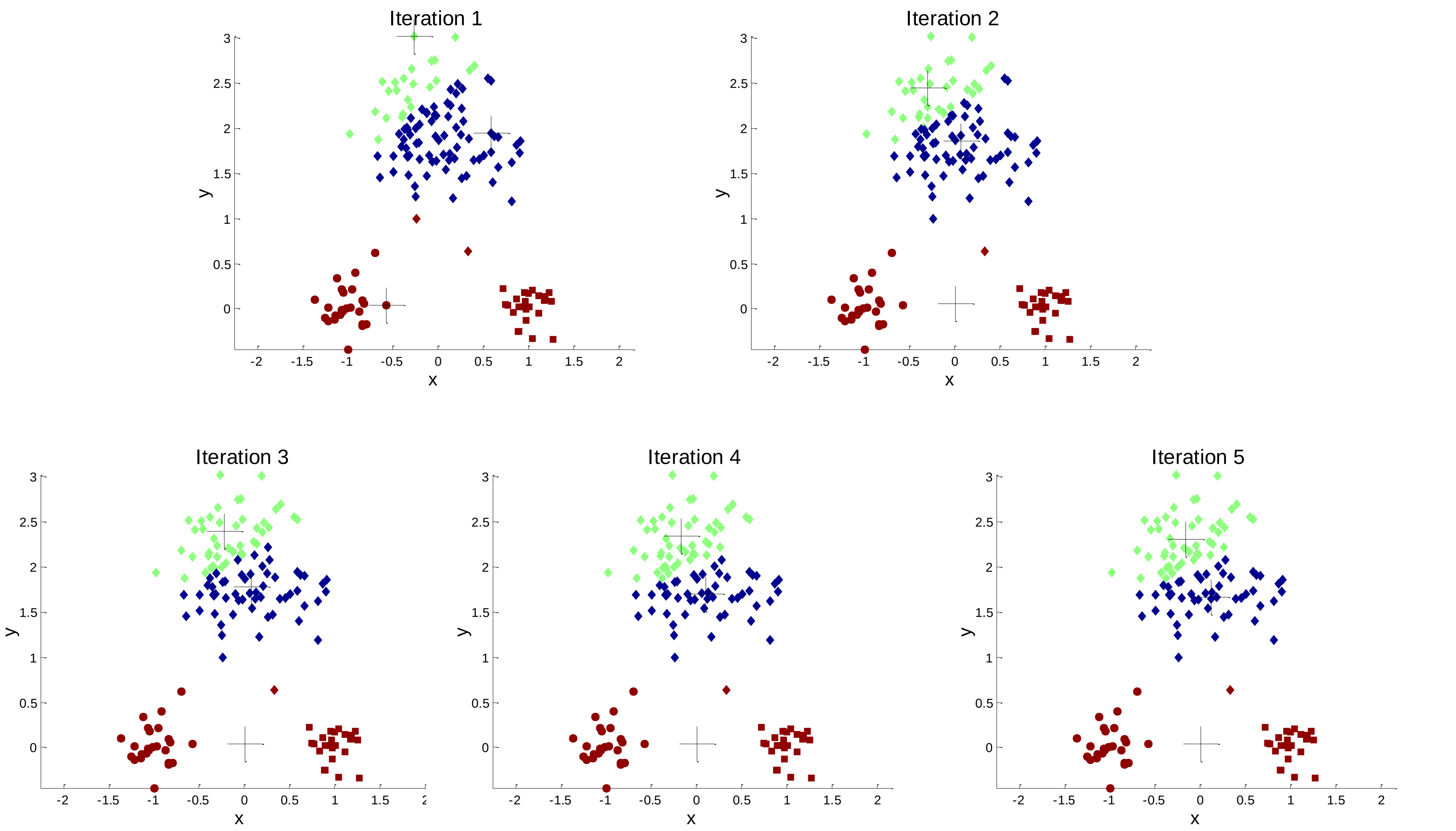
Importance of Choosing Initial Centroids



Importance of Choosing Initial Centroids



Importance of Choosing Initial Centroids …



Dealing with Initialization

- Do multiple runs and select the clustering with the smallest error

- Select original set of points by methods other than random . E.g., pick the most distant (from each other) points as cluster centers (K-means++ algorithm)

K-means Algorithm – Centroids

- The centroid depends on the distance function
  - The minimizer for the distance function
- ‘Closeness’ is measured by Euclidean distance (SSE), cosine similarity, correlation, etc.
- Centroid:
  - The mean of the points in the cluster for SSE, and cosine similarity
  - The median for Manhattan distance.

- Finding the centroid is not always easy
  - It can be an NP-hard problem for some distance functions
    - E.g., median form multiple dimensions

K-means Algorithm – Convergence

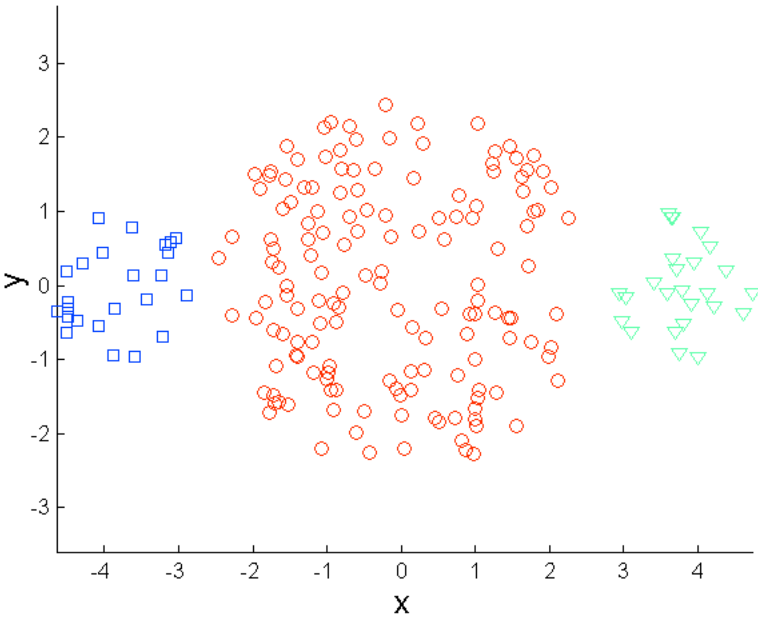
- K-means will converge for common similarity measures mentioned above.
  - Most of the convergence happens in the first few iterations.
  - Often the stopping condition is changed to ‘Until relatively few points change clusters’
- Complexity is O(n * K * I * d)
  - n = number of points, K = number of clusters, I = number of iterations, d = dimensionality
- In general a fast and efficient algorithm

Limitations of K-means

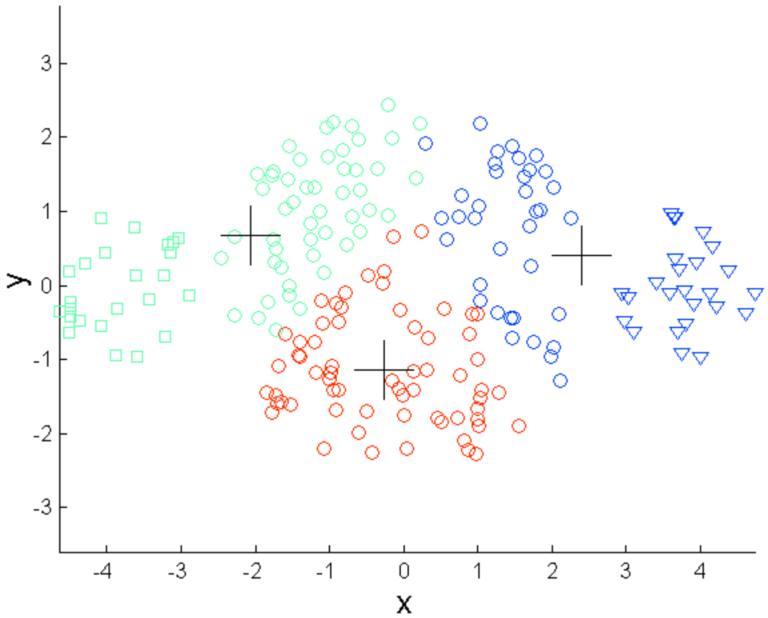
- K-means has problems when clusters are of different
  - Sizes
  - Densities
  - Non-globular shapes

- K-means has problems when the data contains outliers.

Limitations of K-means: Differing Sizes

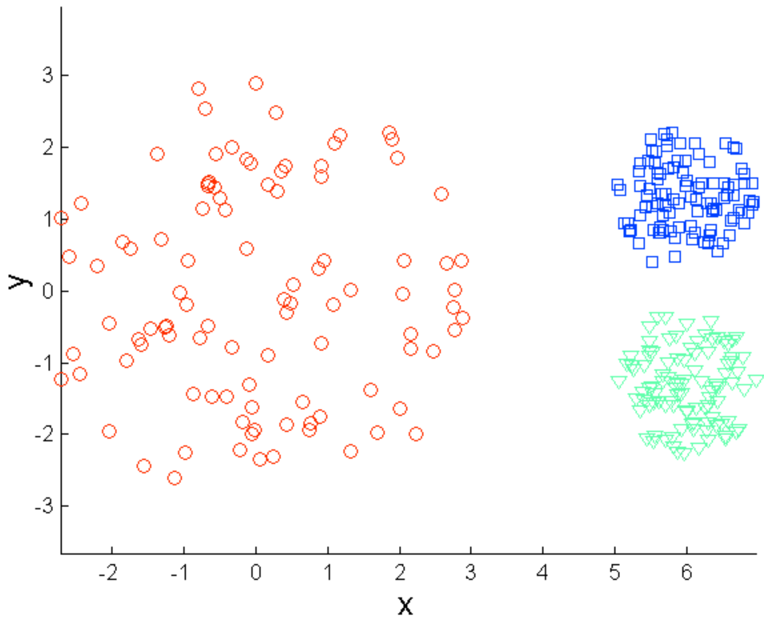


Original Points

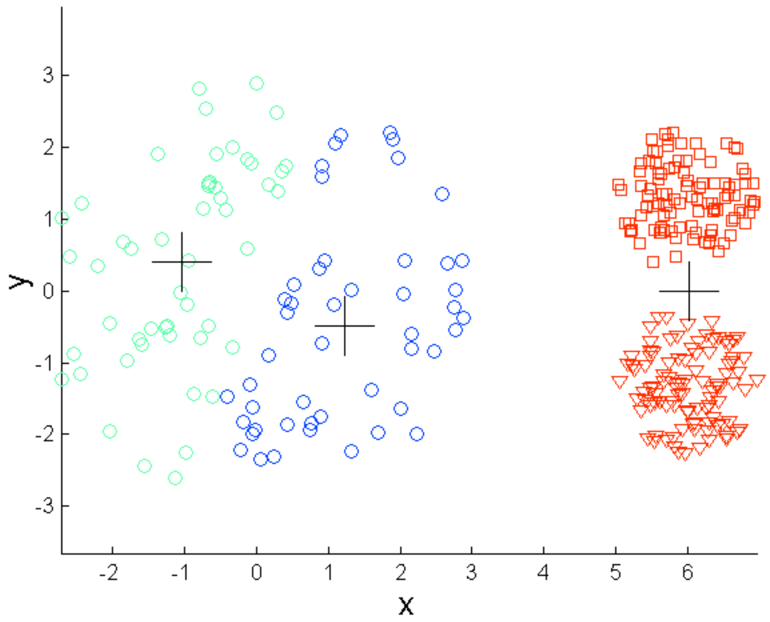


K-means (3 Clusters)

Limitations of K-means: Differing Density

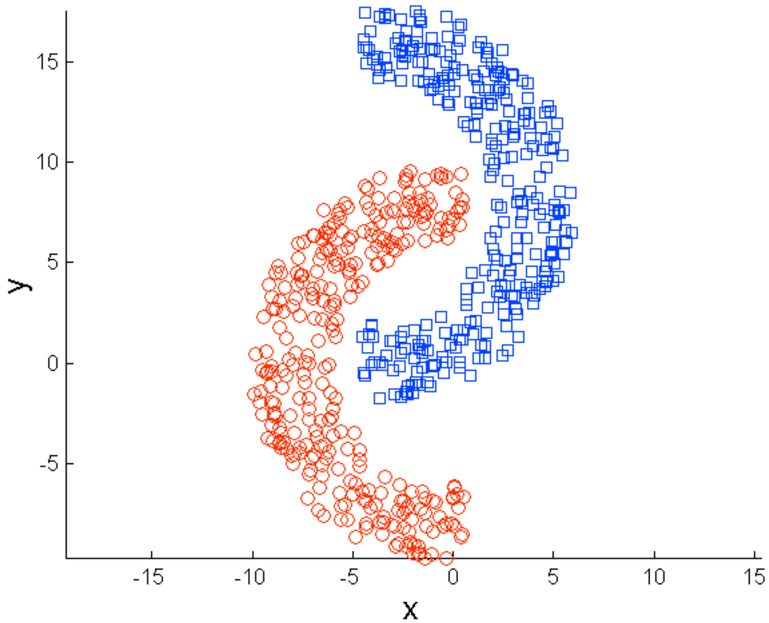


Original Points

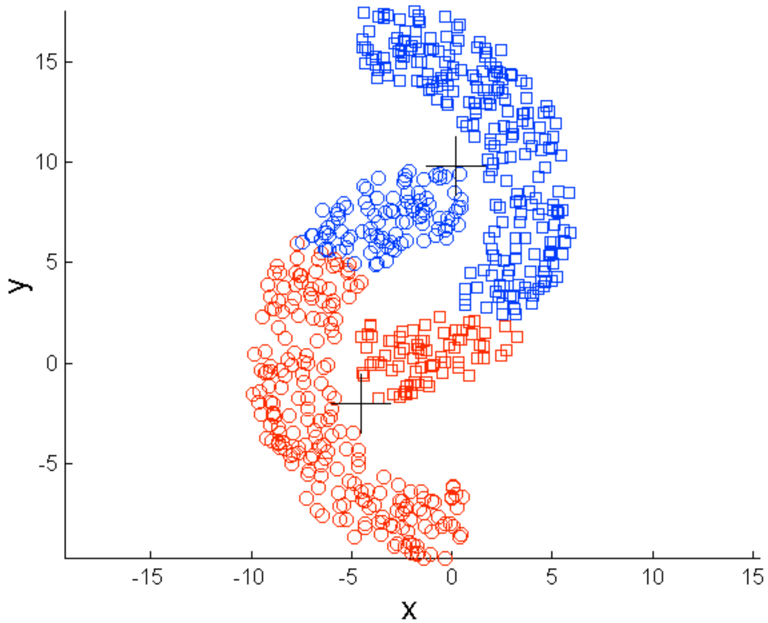


K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes

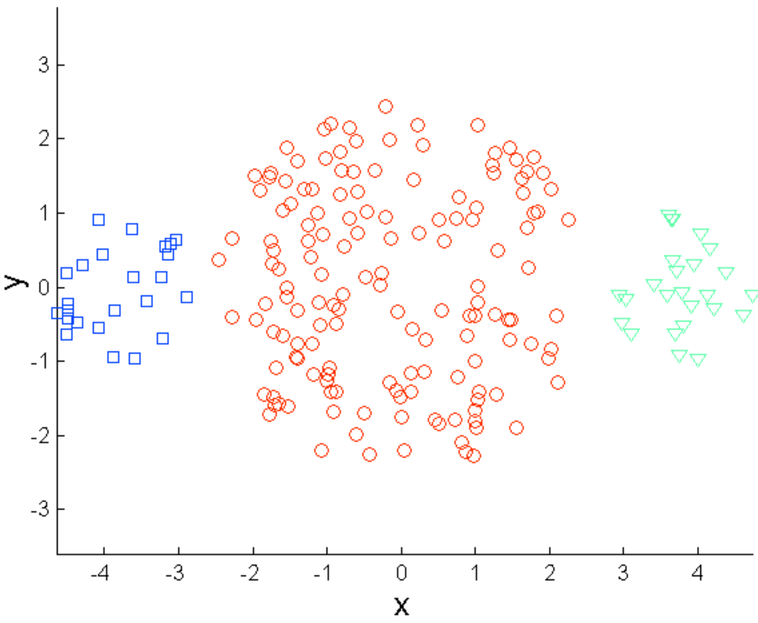


Original Points

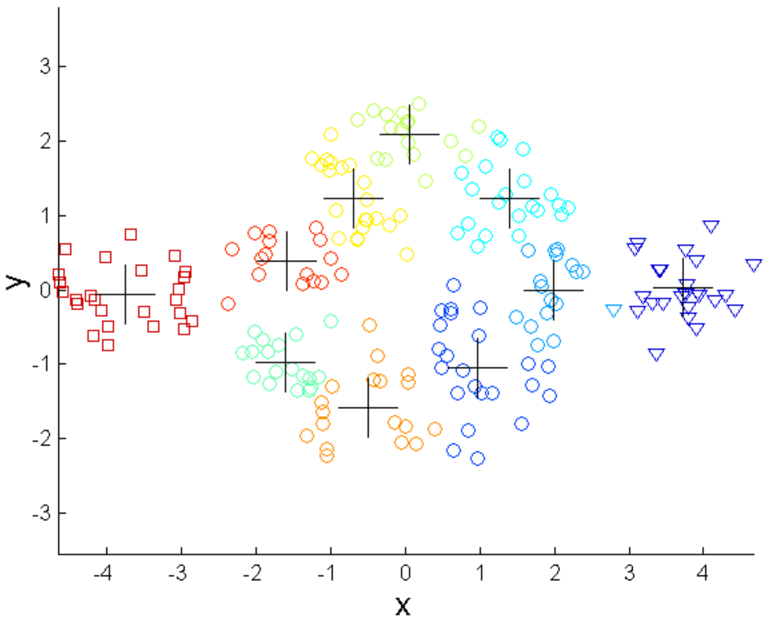


K-means (2 Clusters)

Overcoming K-means Limitations



Original Points

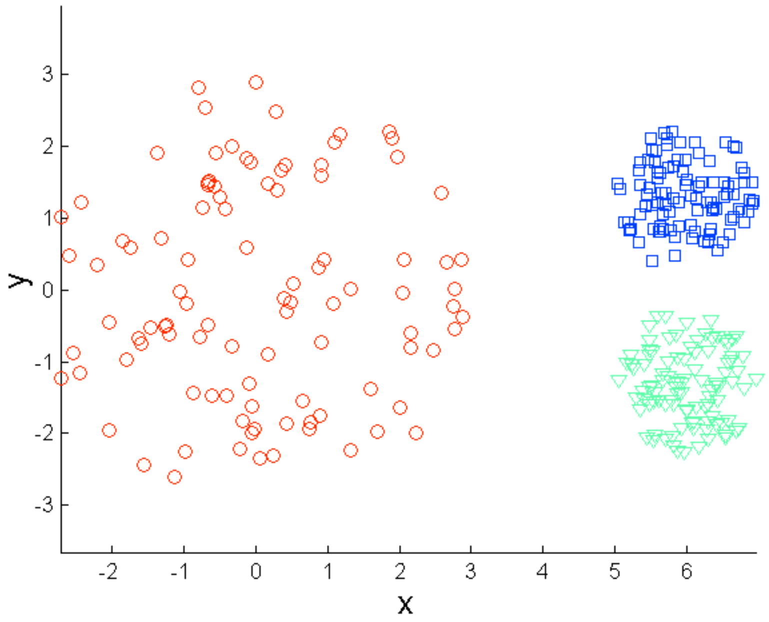


K-means Clusters

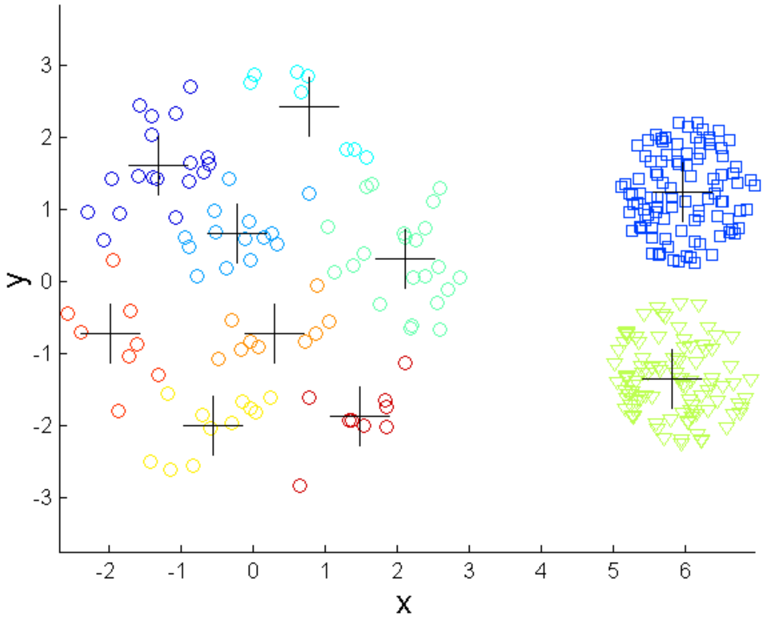
One solution is to use many clusters.

Find parts of clusters, but need to put together.

Overcoming K-means Limitations

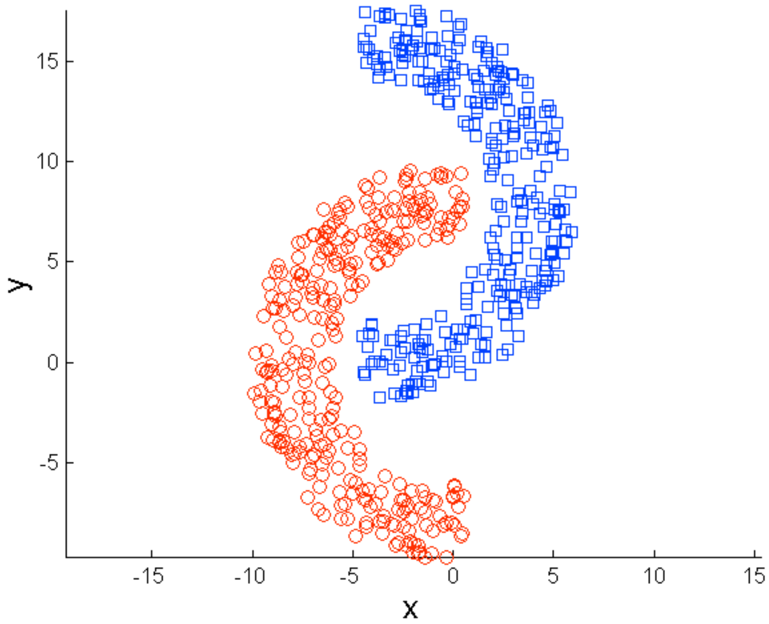


Original Points

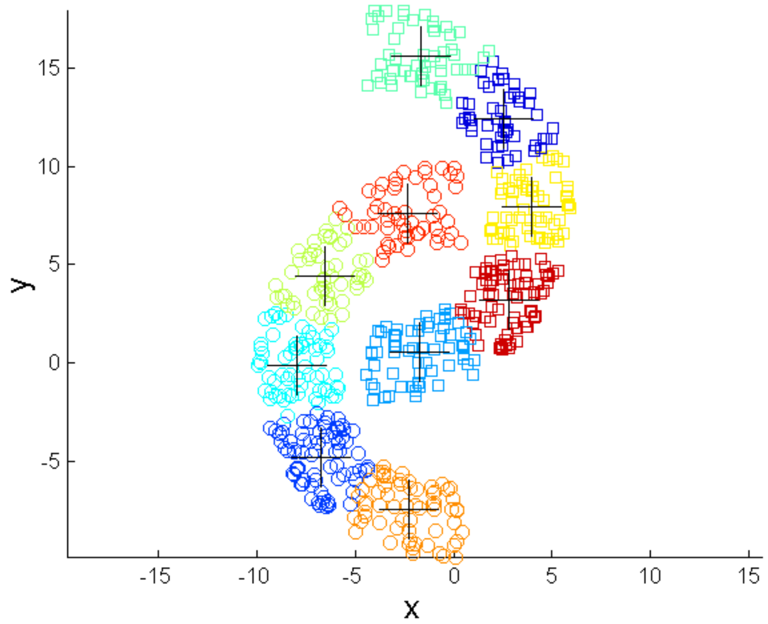


K-means Clusters

Overcoming K-means Limitations



Original Points



K-means Clusters

Variations

- K-medoids: Similar problem definition as in K-means, but the centroid of the cluster is defined to be one of the points in the cluster (the medoid).

- K-centers: Similar problem definition as in K-means, but the goal now is to minimize the maximum diameter of the clusters (diameter of a cluster is maximum distance between any two points in the cluster).