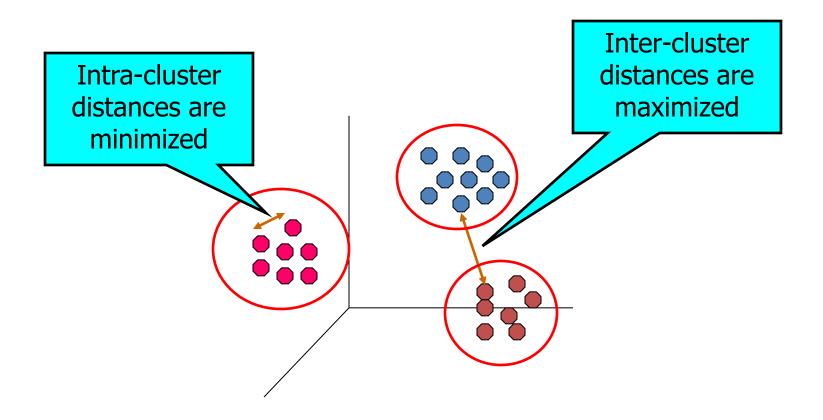
DATA MINING LECTURE 8

Clustering
The k-means algorithm
Hierarchical Clustering
The DBSCAN algorithm

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, genes and proteins

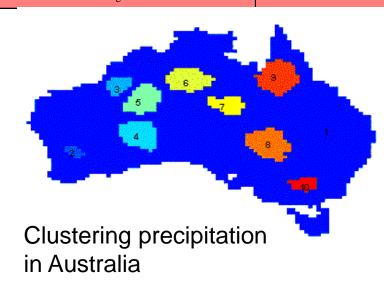
9 , 9		Sull-DOWN	
that have similar functionality, stocks with similar price fluctuations, users with same behavior	2	Apple-Comp-DOWN,Autodesk-DOWN,DEC-DOWN, ADV-Micro-Device-DOWN,Andrew-Corp-DOWN, Computer-Assoc-DOWN,Circuit-City-DOWN, Compaq-DOWN, EMC-Corp-DOWN, Gen-Inst-DOWN, Motorola-DOWN,Microsoft-DOWN,Scientific-Atl-DOWN	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			

oummanzamon

 Reduce the size of large data sets

Applications

- Recommendation systems
- Search Personalization



Industry Group

Technology1-DOWN

Discovered Clusters

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.

Early applications of cluster analysis

John Snow, London 1854

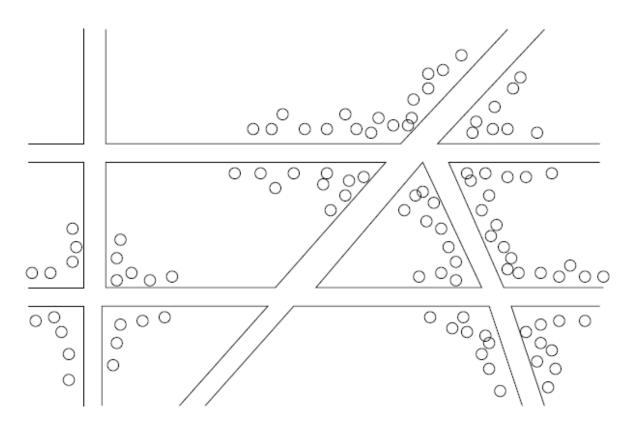
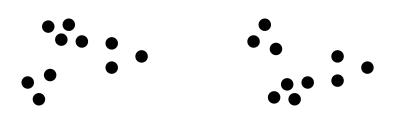
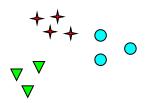


Figure 1.1: Plotting cholera cases on a map of London

Notion of a Cluster can be Ambiguous

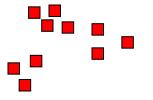


How many clusters?



Six Clusters

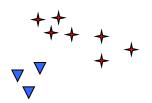




Two Clusters



Four Clusters

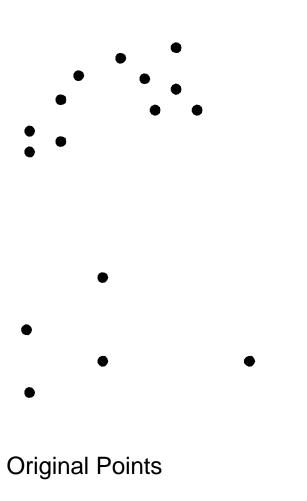


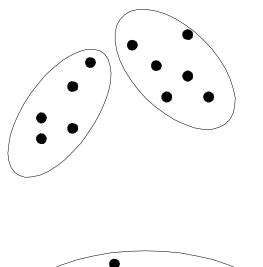


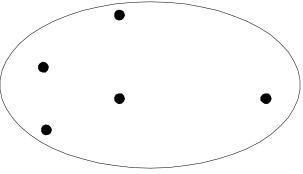
Types of Clusterings

- 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

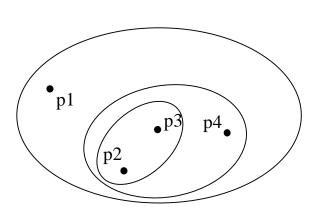




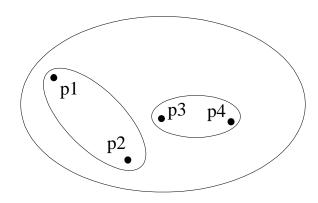


A Partitional Clustering

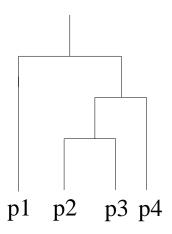
Hierarchical Clustering



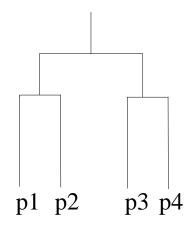
Traditional Hierarchical Clustering



Non-traditional Hierarchical Clustering



Traditional Dendrogram



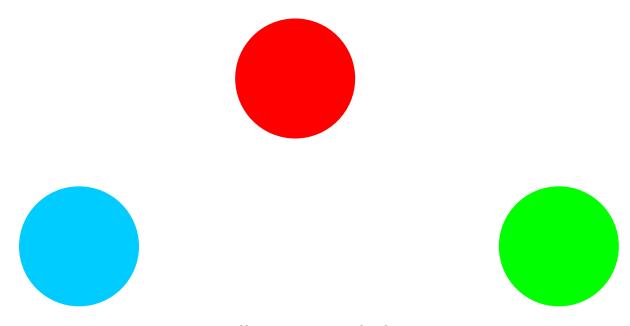
Non-traditional Dendrogram

Other types of clustering

- Exclusive (or non-overlapping) versus nonexclusive (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

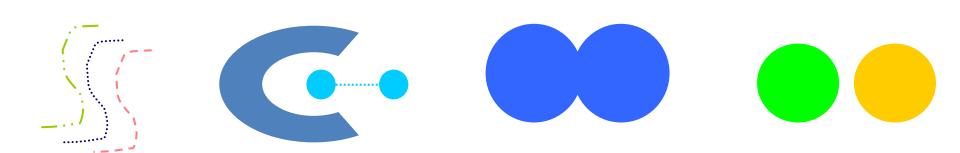
Center-based

- 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



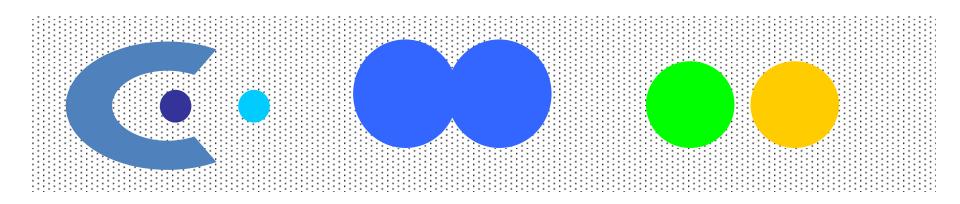
Types of Clusters: Contiguity-Based

- 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.



Types of Clusters: Density-Based

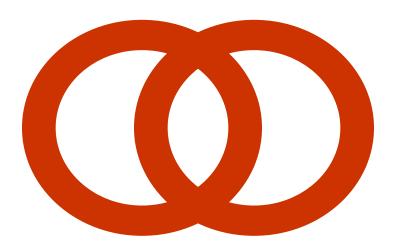
- Density-based
 - A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
 - Used when the clusters are irregular or intertwined, and when noise and outliers are present.



Types of Clusters: Conceptual Clusters

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

.



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 ddimensional space and an integer K group the points into K clusters C= {C₁, C₂,...,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 ddimensional space and an integer K group the points into K clusters C= {C₁, C₂,...,C_k} such that

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

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

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

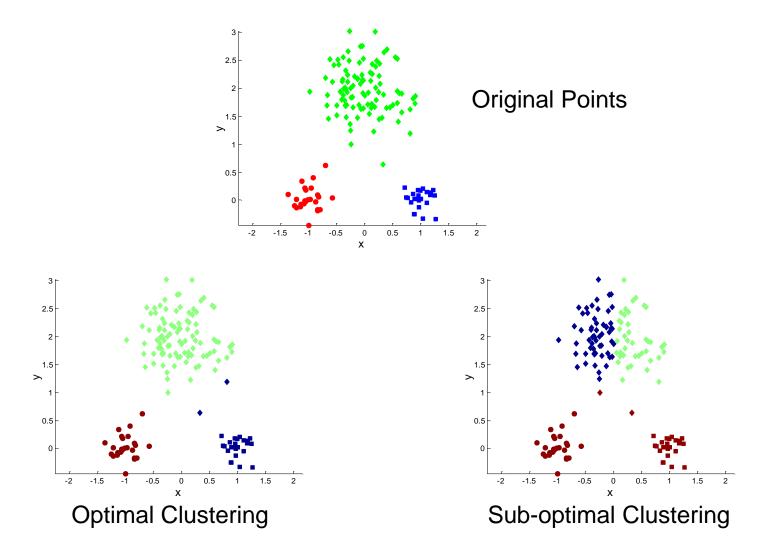
- Also known as Lloyd's algorithm.
- K-means is sometimes synonymous with this algorithm

- 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

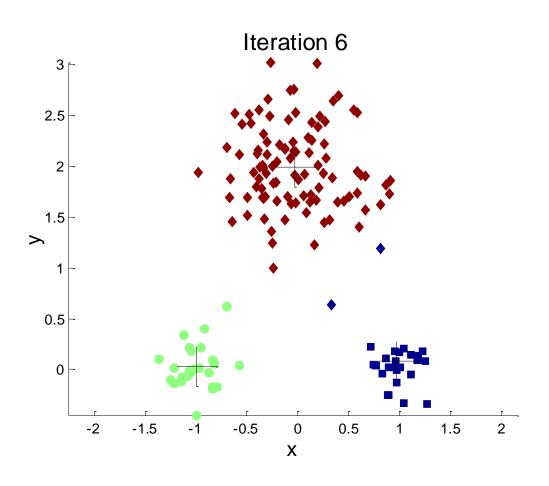
K-means Algorithm — Initialization

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

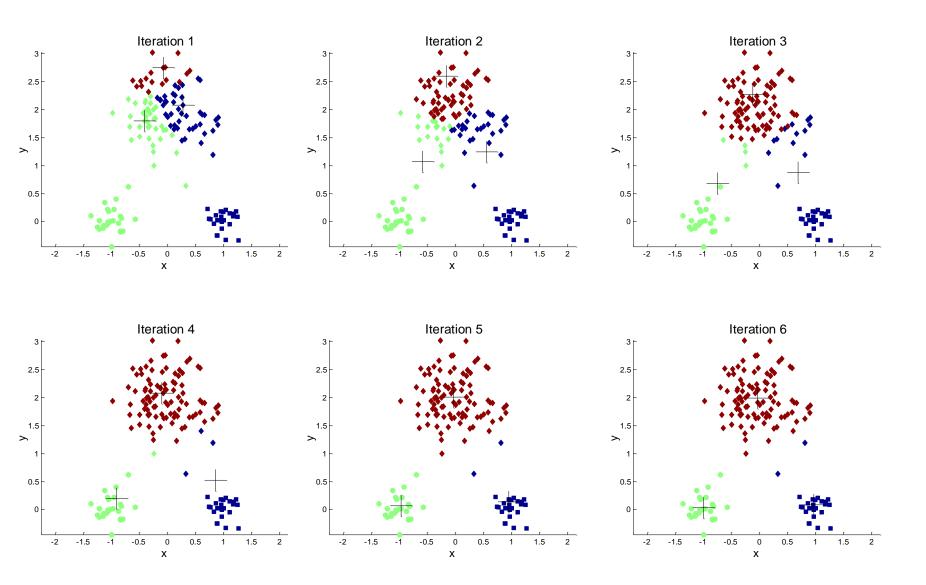
Two different K-means Clusterings



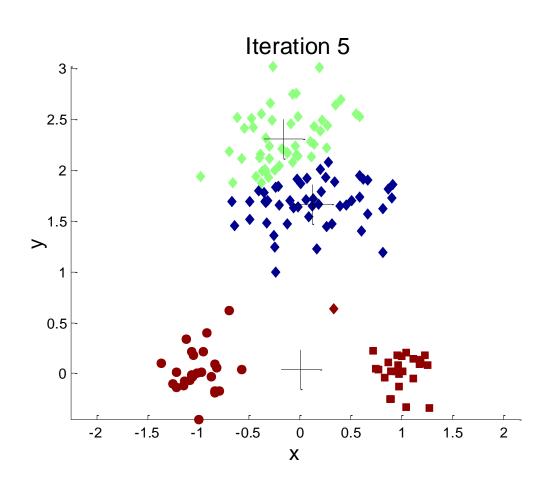
Importance of Choosing Initial Centroids



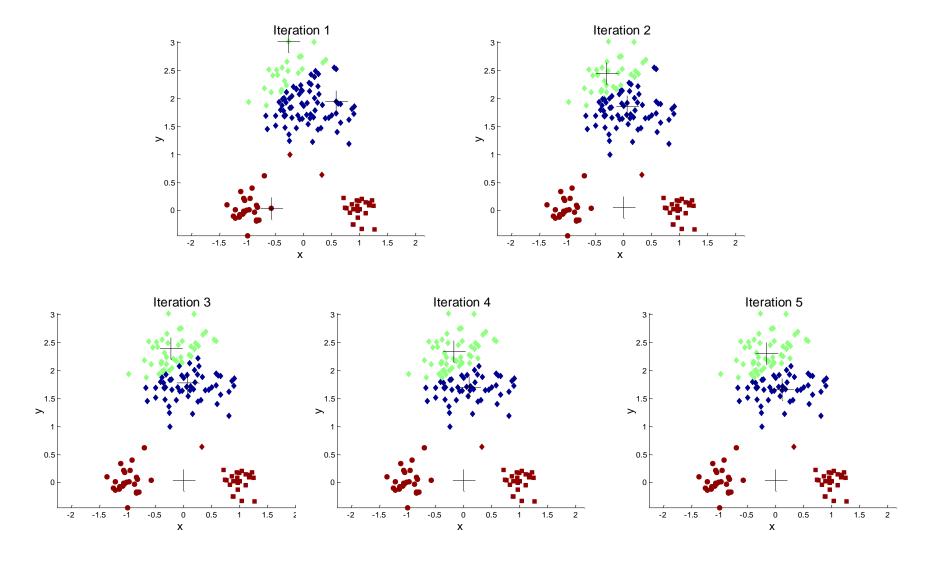
Importance of Choosing Initial Centroids



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

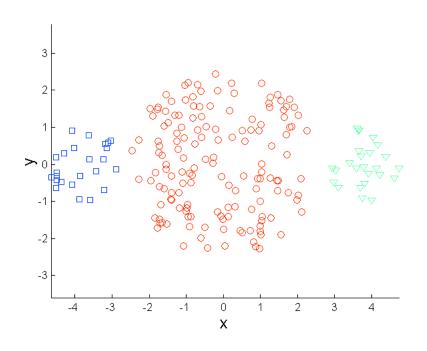
- K-means will converge for common similarity measures mentioned above.
 - Most of the convergence happens in the first few iterations.
 - Often the stopping condition is changed to 'Until relatively few points change clusters'
- Complexity is O(n * K * I * d)
 - n = number of points, K = number of clusters,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

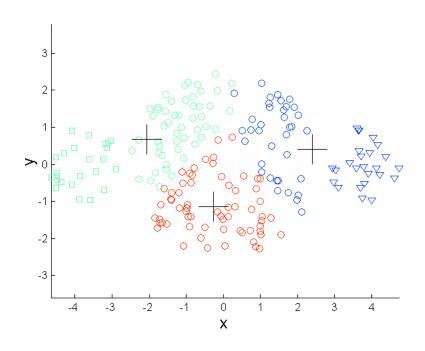
Limitations of K-means

- 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

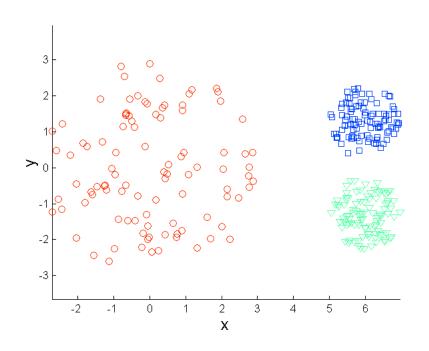


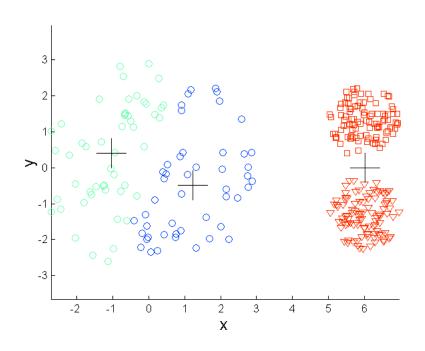


Original Points

K-means (3 Clusters)

Limitations of K-means: Differing Density

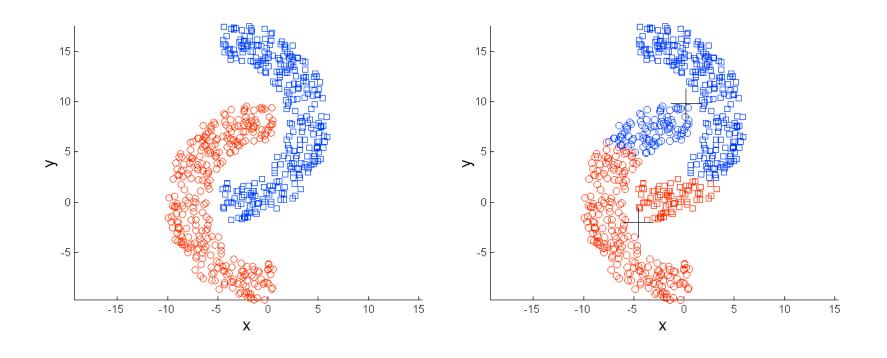




Original Points

K-means (3 Clusters)

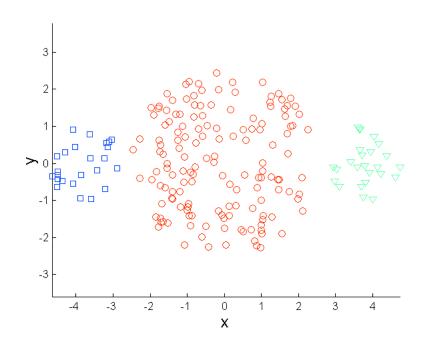
Limitations of K-means: Non-globular Shapes

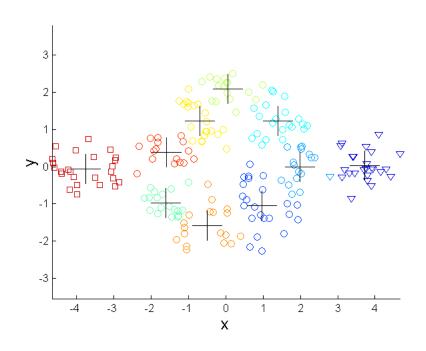


Original Points

K-means (2 Clusters)

Overcoming K-means Limitations



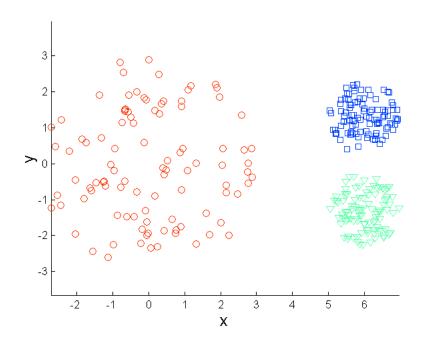


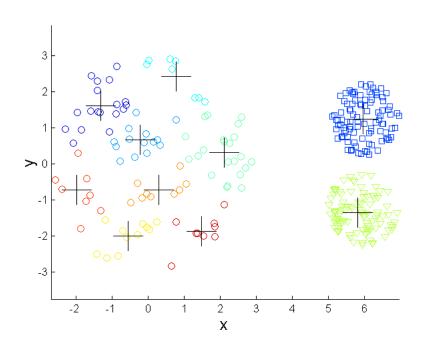
Original Points

K-means Clusters

One solution is to use many clusters. Find parts of clusters, but need to put together.

Overcoming K-means Limitations

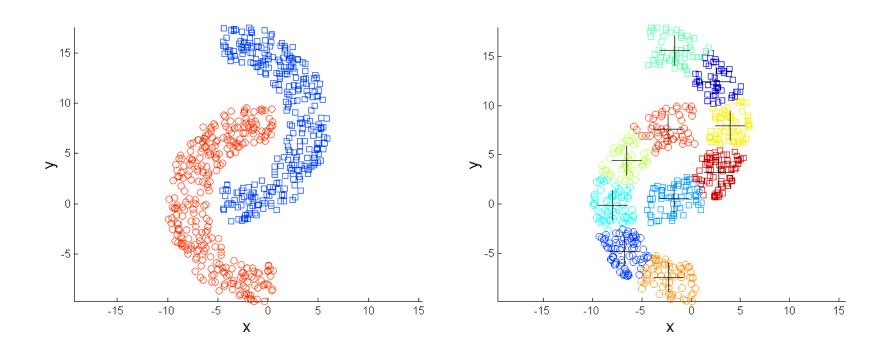




Original Points

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).

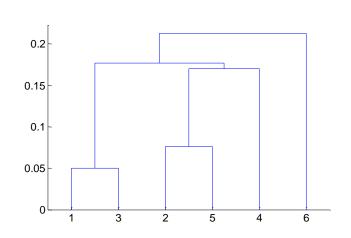
HIERARCHICAL CLUSTERING

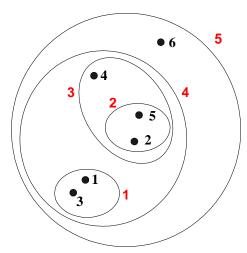
Hierarchical Clustering

- Two main types of hierarchical clustering
 - Agglomerative:
 - Start with the points as individual clusters
 - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
 - Divisive:
 - Start with one, all-inclusive cluster
 - At each step, split a cluster until each cluster contains a point (or there are k clusters)
- Traditional hierarchical algorithms use a similarity or distance matrix
 - Merge or split one cluster at a time

Hierarchical Clustering

- Produces a set of nested clusters organized as a hierarchical tree
- Can be visualized as a dendrogram
 - A tree like diagram that records the sequences of merges or splits





Strengths of Hierarchical Clustering

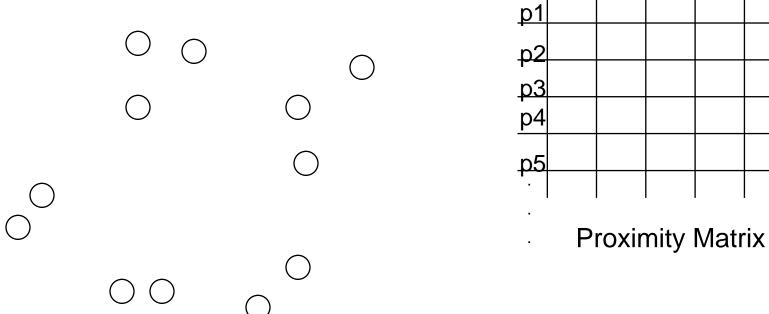
- Do not have to assume any particular number of clusters
 - Any desired number of clusters can be obtained by 'cutting' the dendogram at the proper level
- They may correspond to meaningful taxonomies
 - Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, ...)

Agglomerative Clustering Algorithm

- More popular hierarchical clustering technique
- Basic algorithm is straightforward
 - Compute the proximity matrix
 - Let each data point be a cluster
 - 3. Repeat
 - 4. Merge the two closest clusters
 - 5. Update the proximity matrix
 - 6. Until only a single cluster remains
- Key operation is the computation of the proximity of two clusters
 - Different approaches to defining the distance between clusters distinguish the different algorithms

Starting Situation

Start with clusters of individual points and a proximity matrix



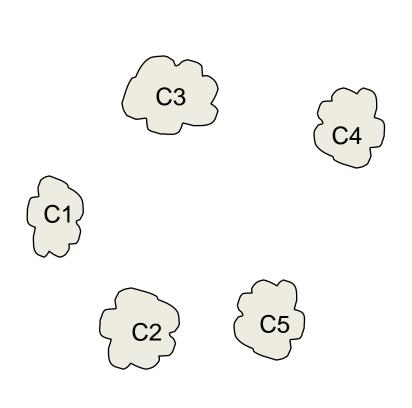


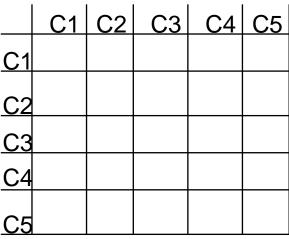
p1

p3 p4 p5

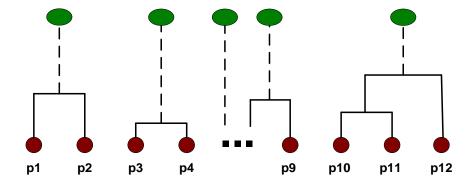
Intermediate Situation

After some merging steps, we have some clusters





Proximity Matrix

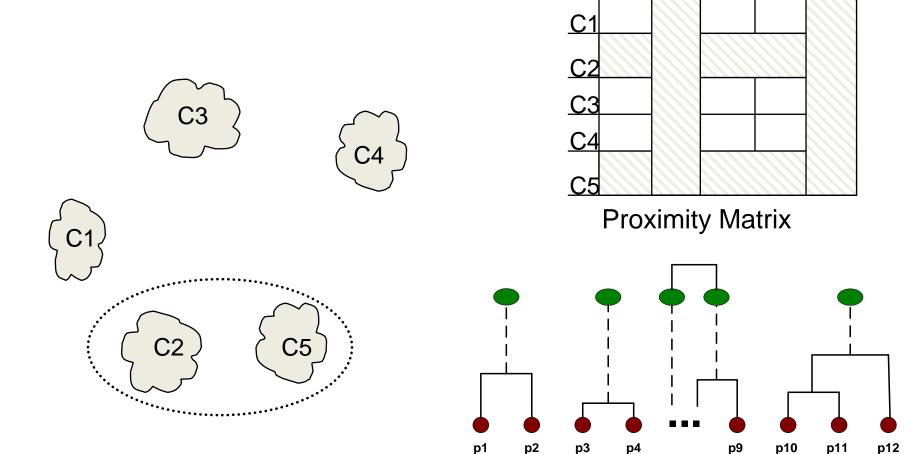


Intermediate Situation

We want to merge the two closest clusters (C2 and C5) and

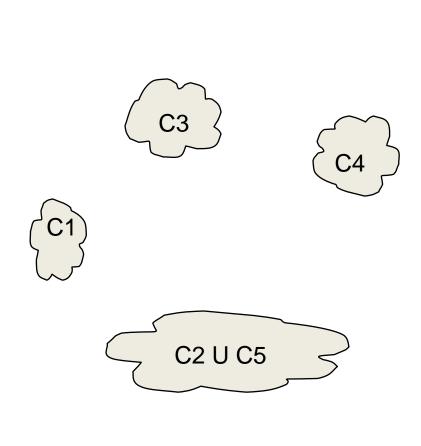
C1 C2 C3 C4 C5

update the proximity matrix.

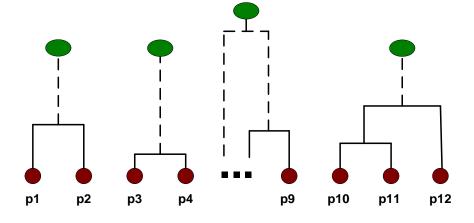


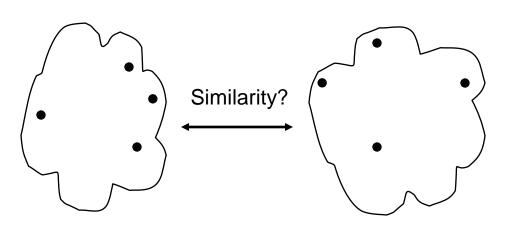
After Merging

• The question is "How do we update the proximity matrix?"



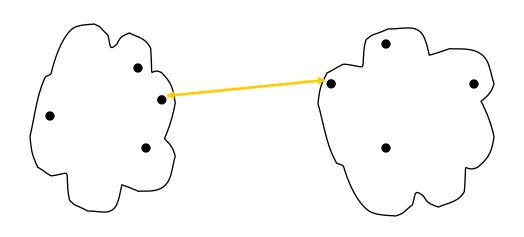
•		C2 U		
	C1	C5	C3	C4
<u>C1</u>		?		
C2 U C5	?	?	?	?
<u>C</u> 3		?		
<u>C4</u>		?		





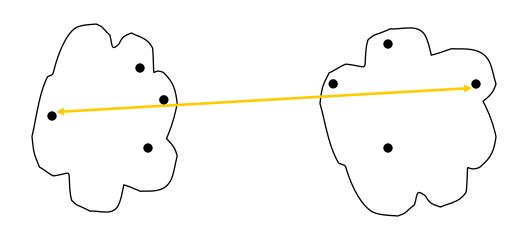
	p1	p2	р3	p4	p5	<u>.</u>
p1						
<u>p2</u>						
<u>p2</u> <u>p3</u>						
р4 р5						

- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
 - Ward's Method uses squared error



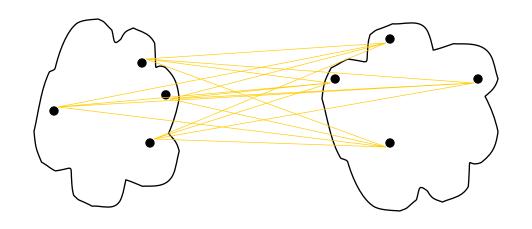
	p1	p2	р3	p4	p5	<u> </u>
<u>p1</u>						
<u>p2</u>						
<u>p2</u> p3						
<u>p4</u> <u>p5</u>						
_						

- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
 - Ward's Method uses squared error



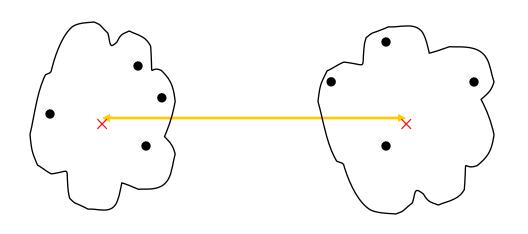
	p1	p2	р3	p4	p5	<u>.</u>
p1						
<u>p2</u>						
<u>p2</u> <u>p3</u>						
<u>p4</u>						
<u>р4</u> <u>р5</u>						
•						

- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
 - Ward's Method uses squared error



	p1	p2	р3	p4	p5	<u> </u>
<u>p1</u>						
<u>p2</u>						
<u>p2</u> p3						
<u>р4</u> <u>р5</u>						

- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
 - Ward's Method uses squared error



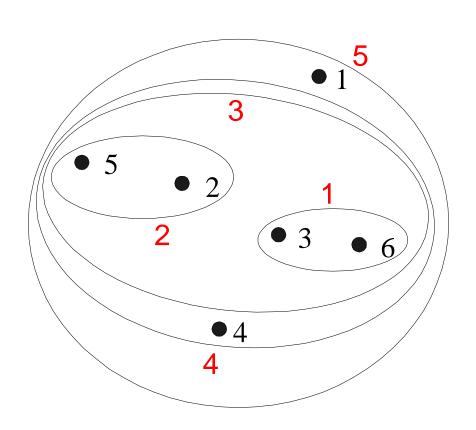
	p1	p2	р3	p4	р5	<u>.</u>
p1						
<u>p2</u>						
<u>p2</u> <u>p3</u>						
<u>p4</u> <u>p5</u>						

- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
 - Ward's Method uses squared error

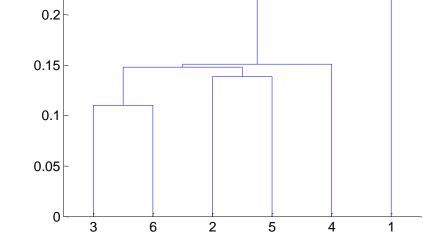
Single Link – Complete Link

- Another way to view the processing of the hierarchical algorithm is that we create links between the elements in order of increasing distance
 - The MIN Single Link, will merge two clusters when a single pair of elements is linked
 - The MAX Complete Linkage will merge two clusters when all pairs of elements have been linked.

Hierarchical Clustering: MIN



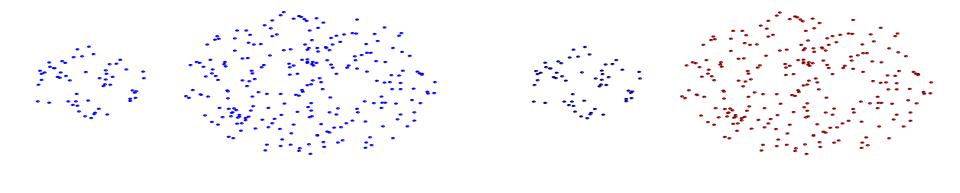
	1	2	3	4	5	6
1	0	.24	.22	.37	.34	.23
2	.24	0	.15	.20	.14	.25
3	.22	.15	0	.15	.28	.11
4	.37	.20	.15	0	.29	.22
5	.34	.14	.28	.29	0	.39
6	.23	.25	.11	.22	.39	0



Nested Clusters

Dendrogram

Strength of MIN

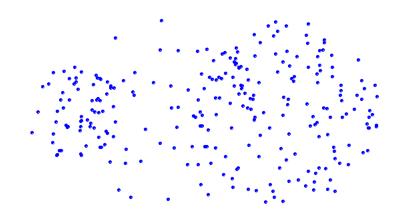


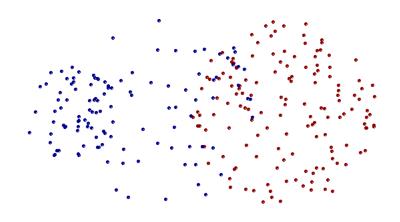
Original Points

Two Clusters

Can handle non-elliptical shapes

Limitations of MIN



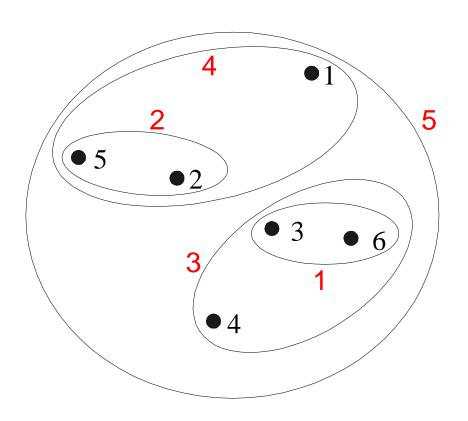


Original Points

Two Clusters

Sensitive to noise and outliers

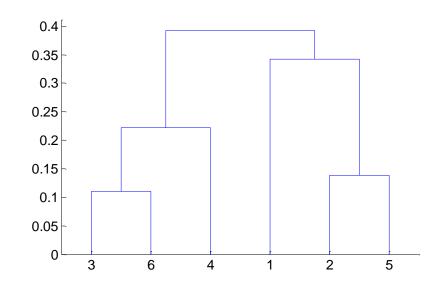
Hierarchical Clustering: MAX



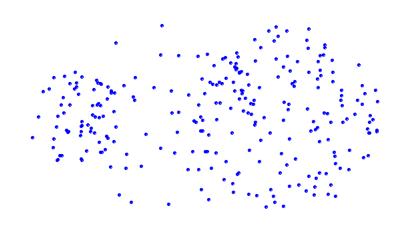
Nested Clusters

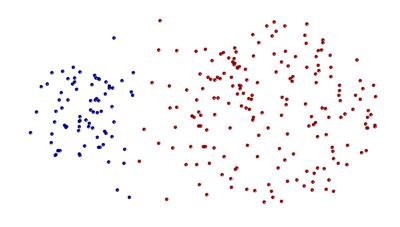
Dendrogram

	1	2	3	4	5	6
1	0	.24	.22	.37	.34	.23
2	.24	0	.15	.20	.14	.25
3	.22	.15	0	.15	.28	.11
4	.37	.20	.15	0	.29	.22
5	.34	.14	.28	.29	0	.39
6	.23	.25	.11	.22	.39	0



Strength of MAX



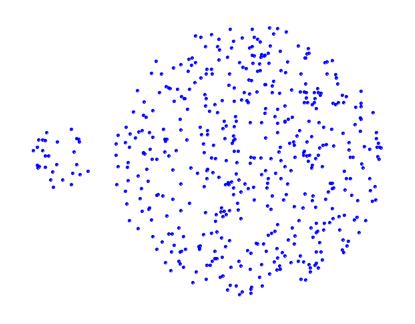


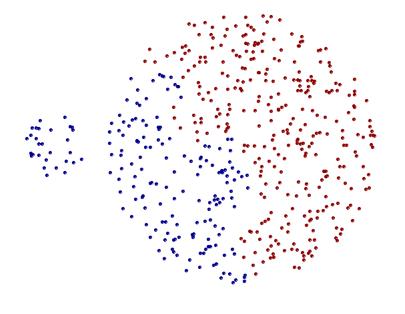
Original Points

Two Clusters

• Less susceptible to noise and outliers

Limitations of MAX





Original Points

Two Clusters

- Tends to break large clusters
- •Biased towards globular clusters

Cluster Similarity: Group Average

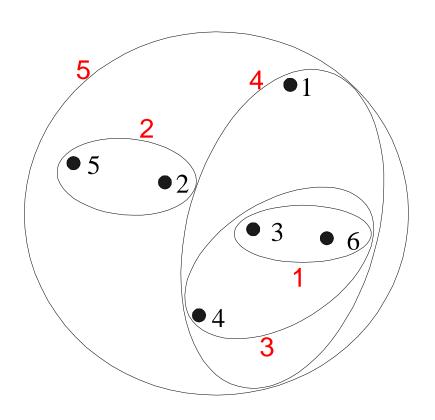
 Proximity of two clusters is the average of pairwise proximity between points in the two clusters.

$$proximity(Cluster_{i}, Cluster_{j}) = \frac{\sum_{p_{i} \in Cluster_{i}} proximity(p_{i}, p_{j})}{|Cluster_{i}| * |Cluster_{i}|}$$

 Need to use average connectivity for scalability since total proximity favors large clusters

	1	2	3	4	5	6
1	0	.24	.22	.37	.34	.23
2	.24	0	.15	.20	.14	.25
3	.22	.15	0	.15	.28	.11
4	.37	.20	.15	0	.29	.22
5	.34	.14	.28	.29	0	.39
6	.23	.25	.11	.22	.39	0

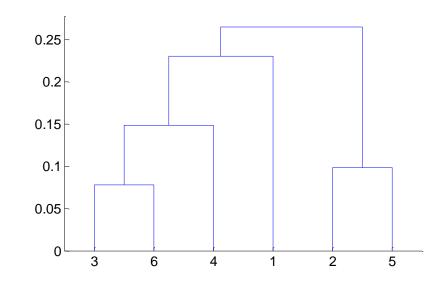
Hierarchical Clustering: Group Average



Nested Clusters

Dendrogram

	1	2	3	4	5	6
1	0	.24	.22	.37	.34	.23
2	.24	0	.15	.20	.14	.25
3	.22	.15	0	.15	.28	.11
4	.37	.20	.15	0	.29	.22
5	.34	.14	.28	.29	0	.39
6	.23	.25	.11	.22	.39	0



Hierarchical Clustering: Group Average

 Compromise between Single and Complete Link

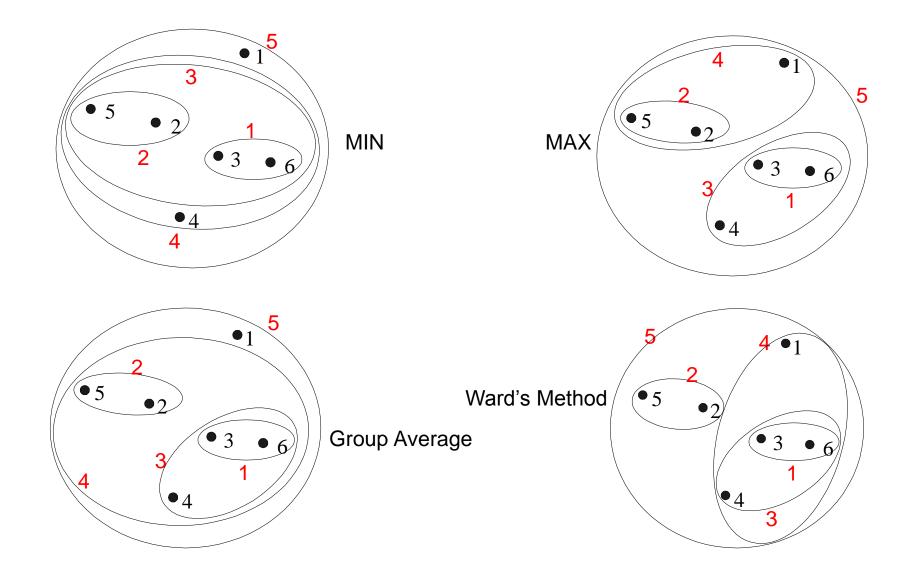
- Strengths
 - Less susceptible to noise and outliers

- Limitations
 - Biased towards globular clusters

Cluster Similarity: Ward's Method

- Similarity of two clusters is based on the increase in squared error (SSE) when two clusters are merged
 - Similar to group average if distance between points is distance squared
- Less susceptible to noise and outliers
- Biased towards globular clusters
- Hierarchical analogue of K-means
 - Can be used to initialize K-means

Hierarchical Clustering: Comparison



Hierarchical Clustering: Time and Space requirements

- O(N²) space since it uses the proximity matrix.
 - N is the number of points.
- O(N³) time in many cases
 - There are N steps and at each step the size, N², proximity matrix must be updated and searched
 - Complexity can be reduced to O(N² log(N)) time for some approaches

Hierarchical Clustering: Problems and Limitations

- Computational complexity in time and space
- Once a decision is made to combine two clusters, it cannot be undone
- No objective function is directly minimized
- Different schemes have problems with one or more of the following:
 - Sensitivity to noise and outliers
 - Difficulty handling different sized clusters and convex shapes
 - Breaking large clusters

DBSCAN

DBSCAN: Density-Based Clustering

- DBSCAN is a Density-Based Clustering algorithm
- Reminder: In density based clustering we partition points into dense regions separated by not-so-dense regions.
- Important Questions:
 - How do we measure density?
 - What is a dense region?

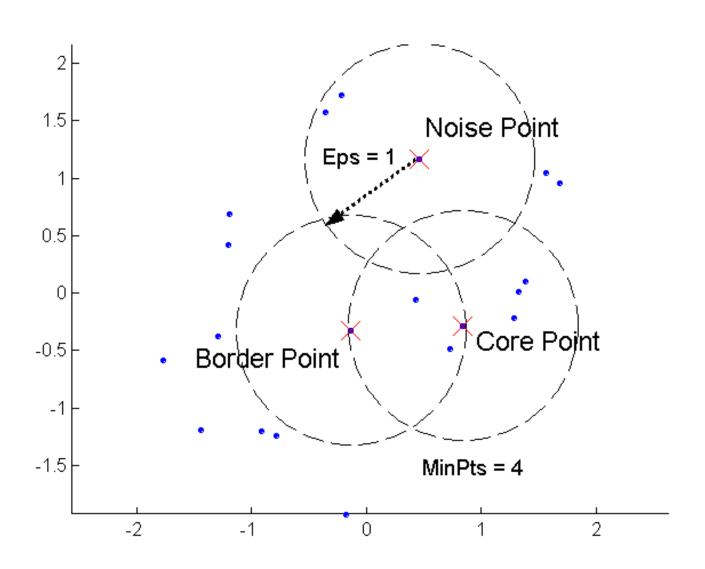
DBSCAN:

- Density at point p: number of points within a circle of radius Eps
- Dense Region: A circle of radius Eps that contains at least MinPts points

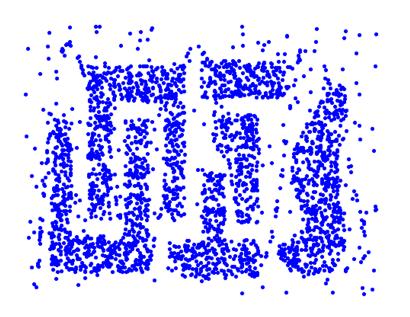
DBSCAN

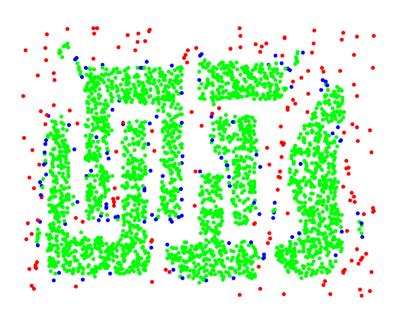
- Characterization of points
 - A point is a core point if it has more than a specified number of points (MinPts) within Eps
 - These points belong in a dense region and are at the interior of a cluster
 - A border point has fewer than MinPts within Eps, but is in the neighborhood of a core point.
 - A noise point is any point that is not a core point or a border point.

DBSCAN: Core, Border, and Noise Points



DBSCAN: Core, Border and Noise Points





Original Points

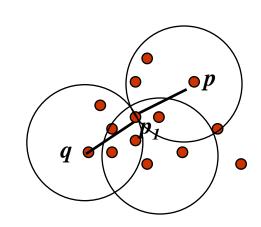
Point types: core, border and noise

Eps = 10, MinPts = 4

Density-Connected points

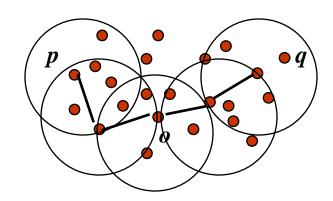
Density edge

 We place an edge between two core points q and p if they are within distance Eps.



Density-connected

 A point p is density-connected to a point q if there is a path of edges from p to q

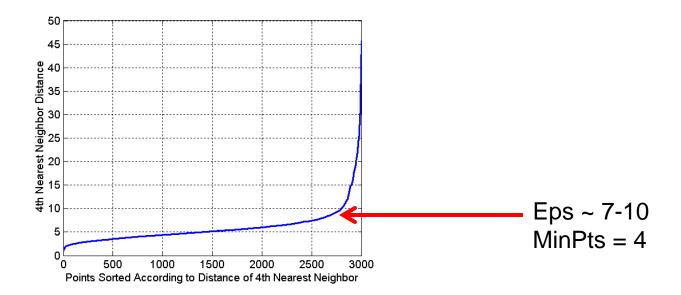


DBSCAN Algorithm

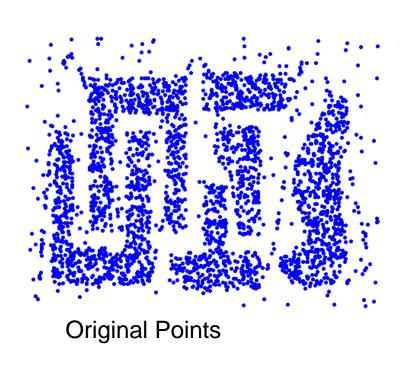
- Label points as core, border and noise
- Eliminate noise points
- For every core point p that has not been assigned to a cluster
 - Create a new cluster with the point p and all the points that are density-connected to p.
- Assign border points to the cluster of the closest core point.

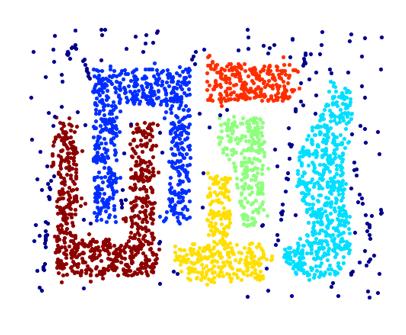
DBSCAN: Determining Eps and MinPts

- Idea is that for points in a cluster, their kth nearest neighbors are at roughly the same distance
- Noise points have the kth nearest neighbor at farther distance
- So, plot sorted distance of every point to its kth nearest neighbor
- Find the distance d where there is a "knee" in the curve
 - Eps = d, MinPts = k



When DBSCAN Works Well

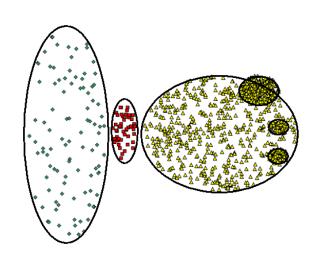




Clusters

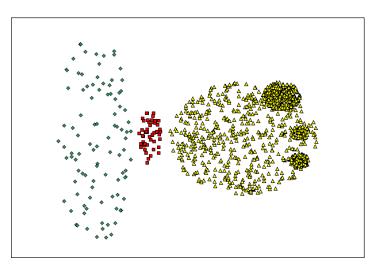
- Resistant to Noise
- Can handle clusters of different shapes and sizes

When DBSCAN Does NOT Work Well

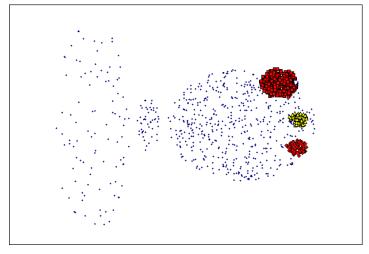


Original Points

- Varying densities
- High-dimensional data



(MinPts=4, Eps=9.75).



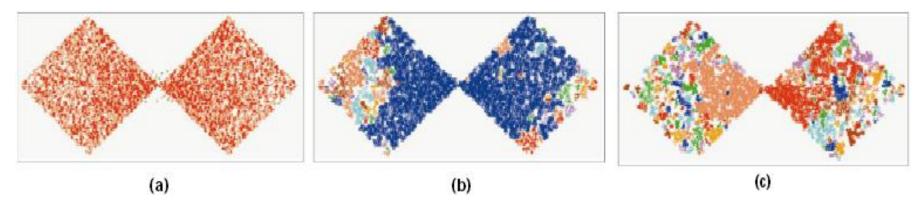
(MinPts=4, Eps=9.92)

DBSCAN: Sensitive to Parameters

Figure 8. DBScan results for DS1 with MinPts at 4 and Eps at (a) 0.5 and (b) 0.4.

(a) (b)

Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.



Other algorithms

- PAM, CLARANS: Solutions for the k-medoids problem
- BIRCH: Constructs a hierarchical tree that acts a summary of the data, and then clusters the leaves.
- MST: Clustering using the Minimum Spanning Tree.
- ROCK: clustering categorical data by neighbor and link analysis
- LIMBO, COOLCAT: Clustering categorical data using information theoretic tools.
- CURE: Hierarchical algorithm uses different representation of the cluster
- CHAMELEON: Hierarchical algorithm uses closeness and interconnectivity for merging