DATA MINING CLUSTERING

The k-means algorithm

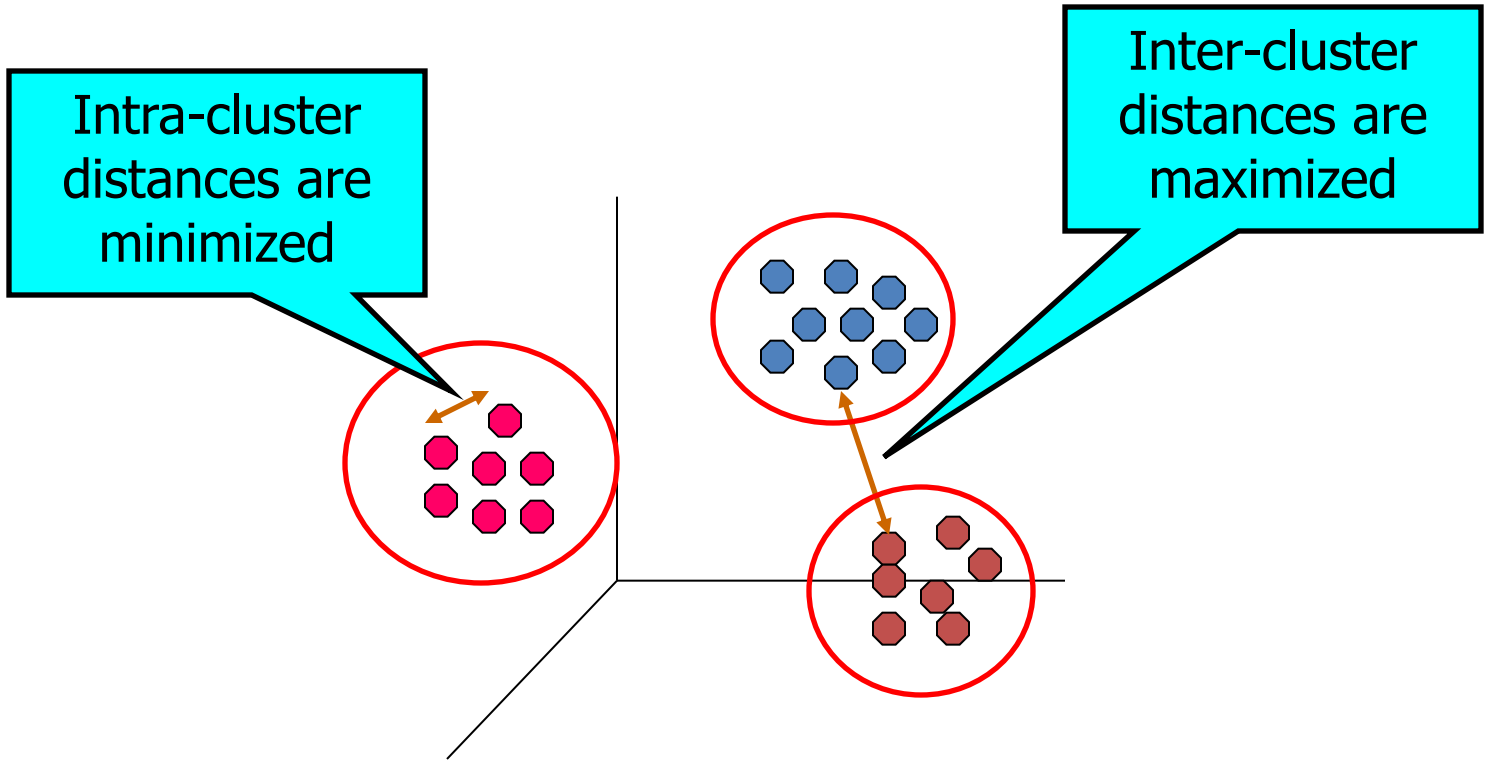
Hierarchical Clustering

The DBSCAN algorithm

Evaluation

What is a Clustering?

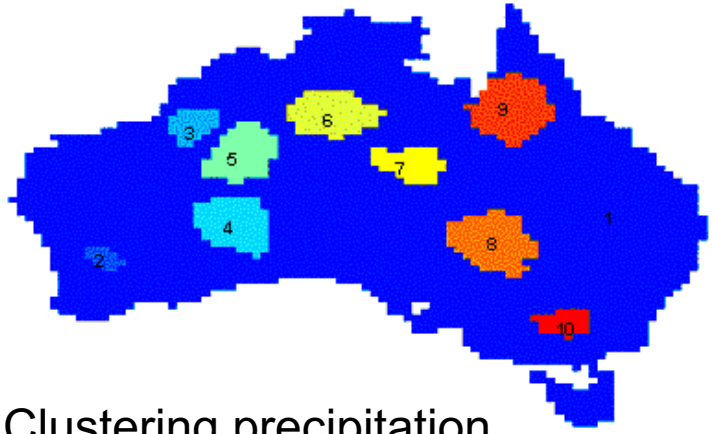
A grouping of objects such that the objects in a group (cluster) are similar (or related) to one another and different from (or unrelated to) the objects in other groups (clusters)



Why Cluster Analysis

- **Understanding**
  - Group related documents for browsing, genes and proteins that have similar functionality, stocks with similar price fluctuations, users with same behavior
- **Summarization**
  - Reduce the size of large data sets
- **Applications**
  - Recommendation systems
  - Search Personalization

	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



Clustering precipitation in Australia

Early applications of cluster analysis

- John Snow, London 1854

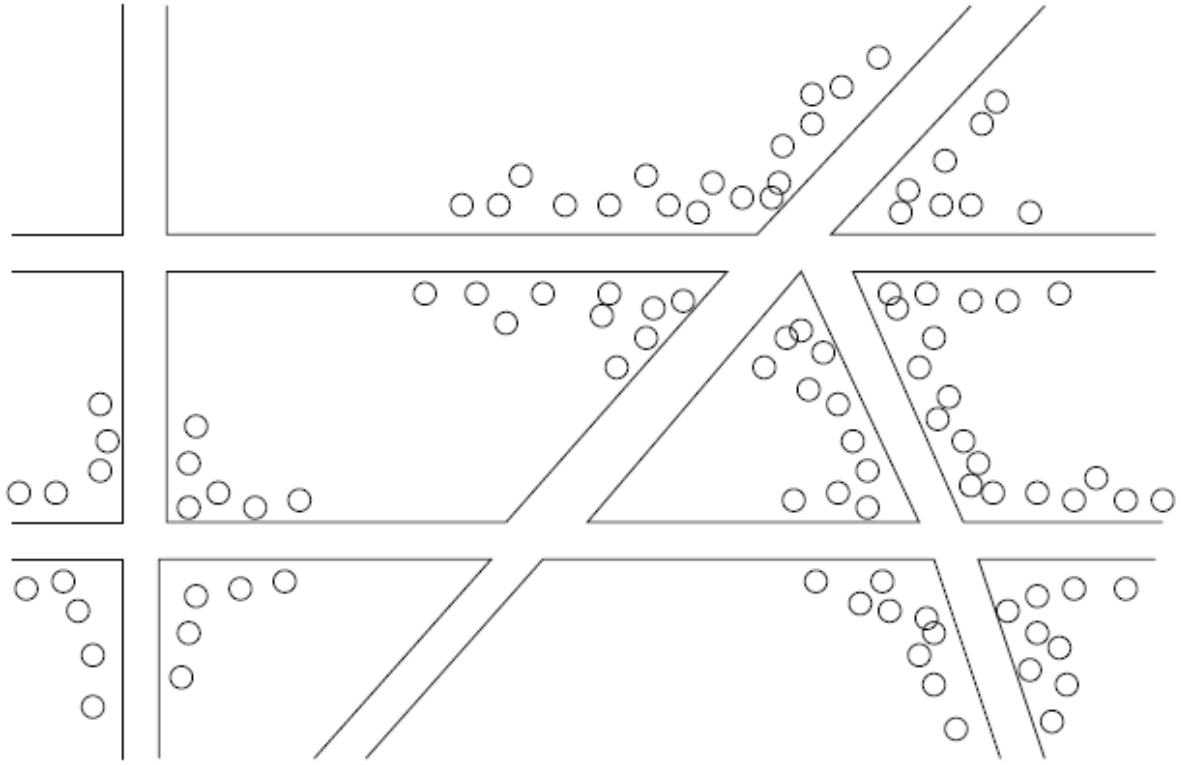


Figure 1.1: Plotting cholera cases on a map of London

Notion of a Cluster can be Ambiguous

How many clusters?

Six Clusters

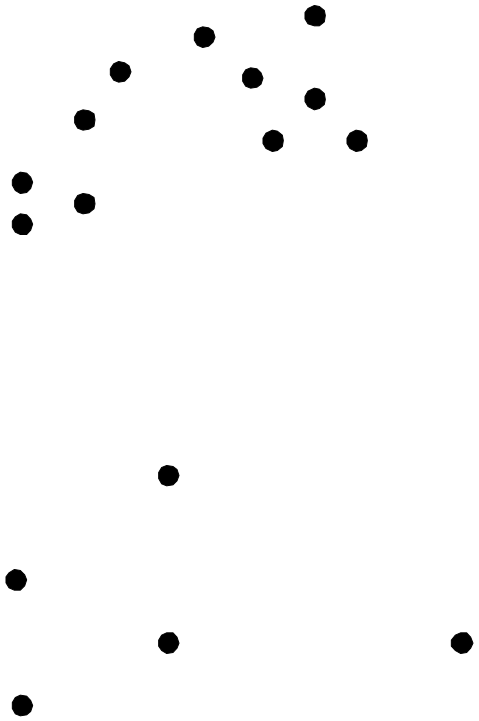
Two Clusters

Four Clusters

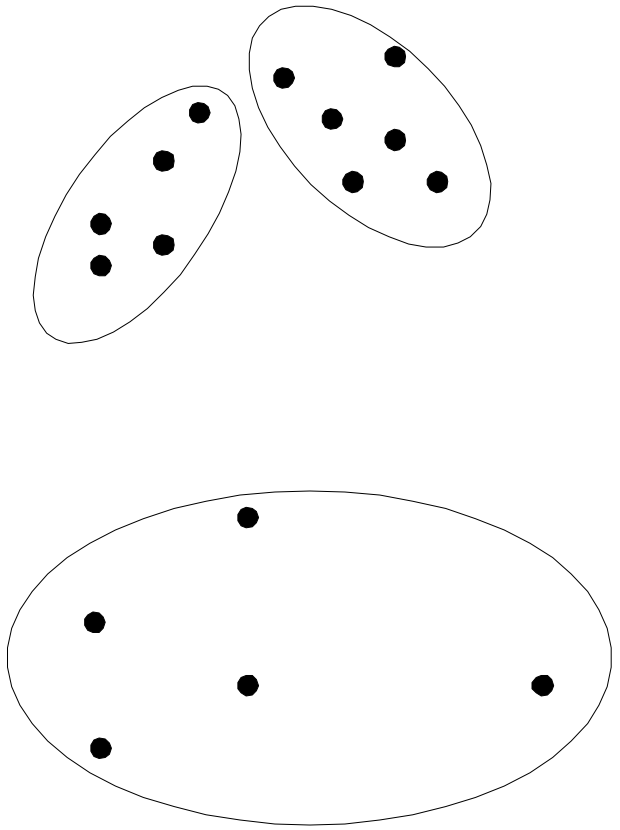
Types of Clusterings

- Important distinction between hierarchical and partitional sets of clusters
- Partitional Clustering
  - A division of 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

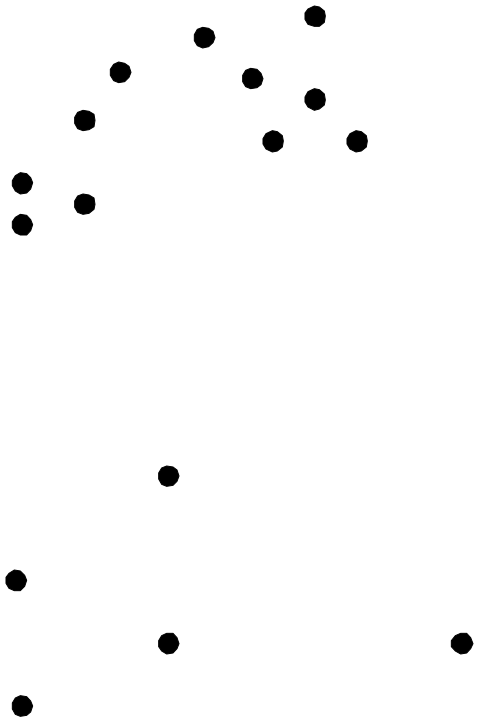


Original Points

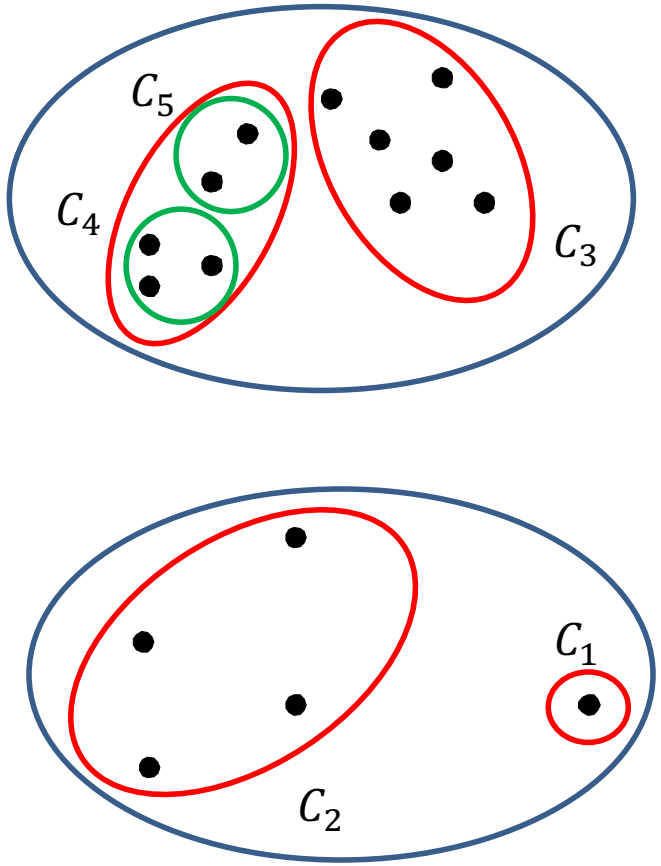


A Partitional Clustering

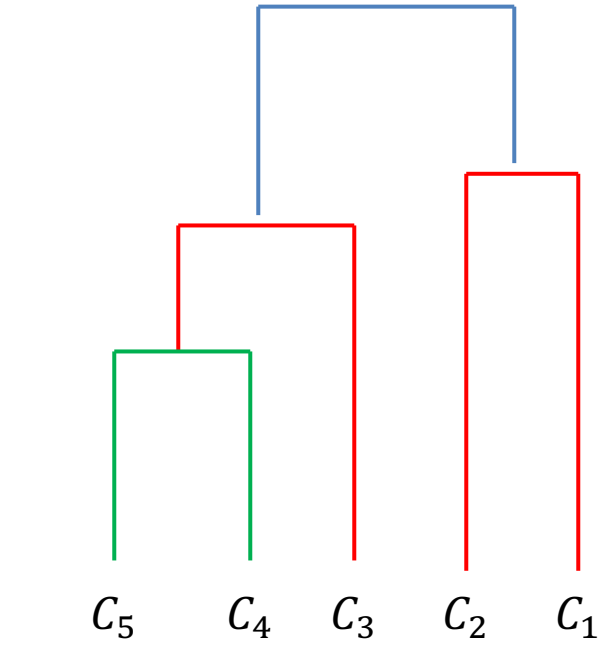
Hierarchical Clustering



Original Points



Hierarchical Clustering



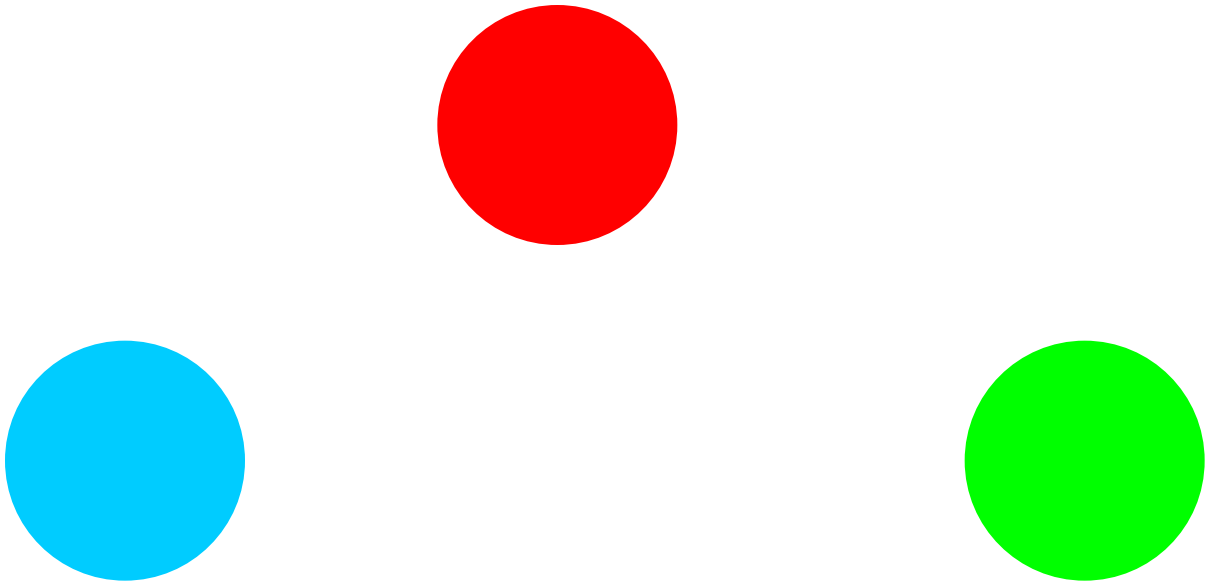
Hierarchical Clustering dendrogram

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

Clustering objectives

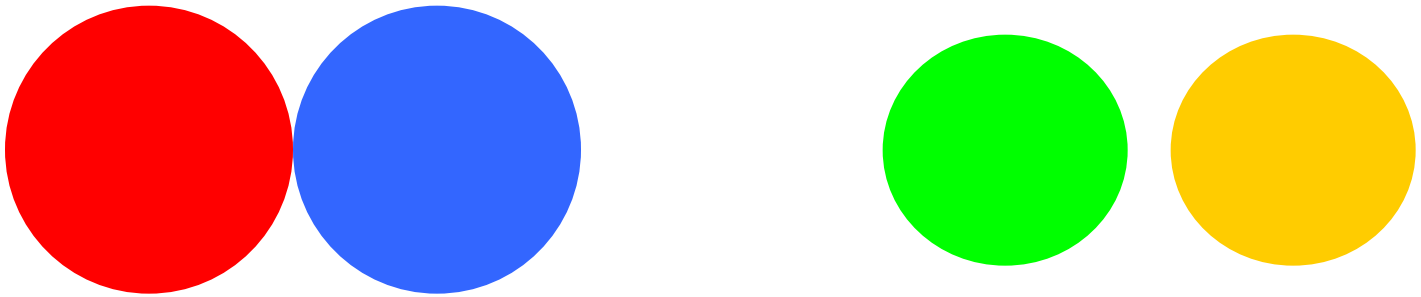
- Well-Separated Clusters:
  - A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.



3 well-separated clusters

Clustering objectives

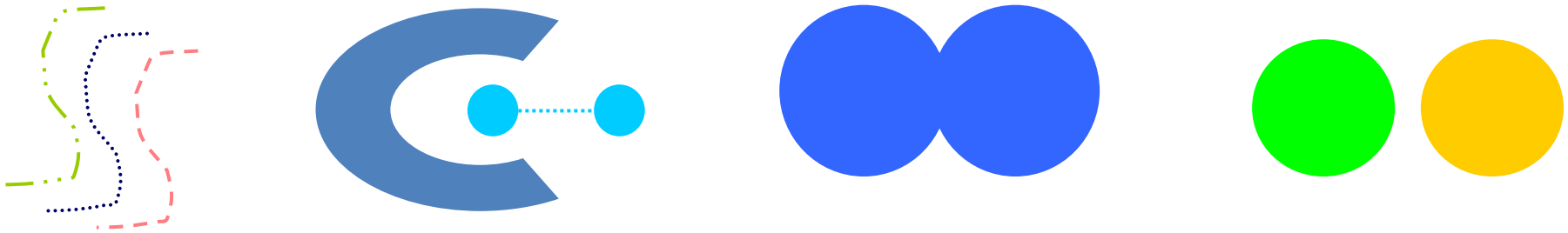
- Center-based Clusters:
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the “center” of a cluster, than to the center of any other cluster
  - The center of a cluster is often a centroid, the minimizer of distances from all the points in the cluster, or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



4 center-based clusters

Clustering objectives

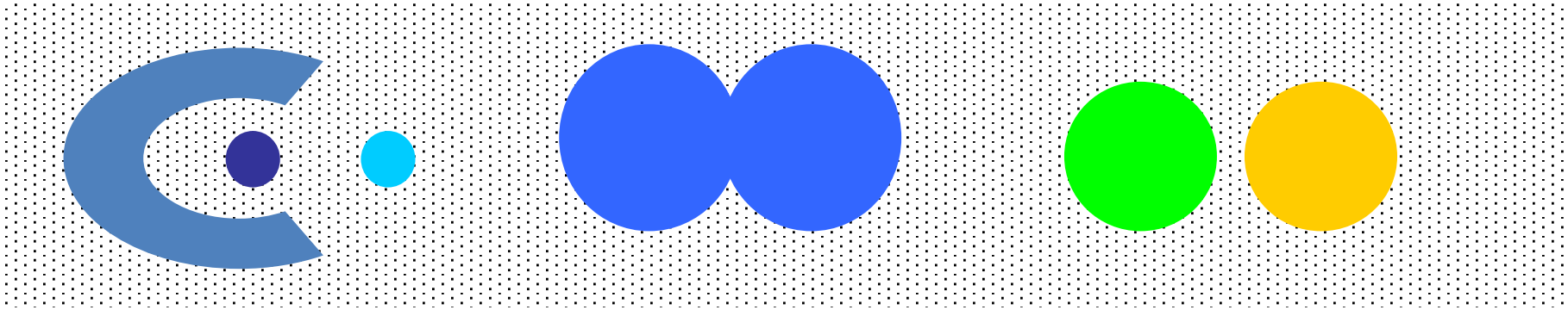
- Contiguous Clusters (Nearest neighbor or Transitive)
  - A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.



8 contiguous clusters

Clustering Objectives

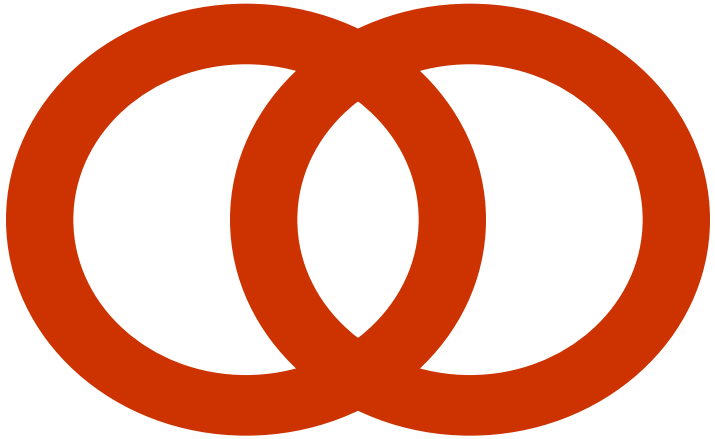
- Density-based clusters
  - A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
  - Used when the clusters are irregular or intertwined, and when noise and outliers are present.



6 density-based clusters

Clustering objectives

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



A cluster is defined as a set of points that lie on a circle

Clustering objectives

- Clustering as an optimization problem
  - Finds clusters that minimize or maximize an objective function.
  - Consider all possible ways of dividing the points into clusters and compute the `goodness' of each clustering using the objective function to find the best one.
    - Usually, finding the best is NP-hard (no polynomial algorithm).
  - 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 (probabilistic) 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:
  - find K centroids and
  - the assignment of points to clusters/centroids
  - so as to minimize the sum of distances of the points to their respective centroid

K-means Clustering as an optimization problem

- Problem: Given a set X of n objects and an integer K, group the points into K clusters $C = \{C_1, C_2, \ldots, Ck\}$ such that

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

  is minimized, where c_i is the centroid of the points in cluster C_i
- Note: We need to find both the grouping into clusters and the centroids per cluster.

K-means Clustering

- Most common definition is with euclidean distance, minimizing the Sum of Squares Error (SSE) – distance 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 $C = \{C_1, C_2, \dots, Ck\}$ such that

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

Sum of Squares Error (SSE)

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 ($d \geq 2$)
  - 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

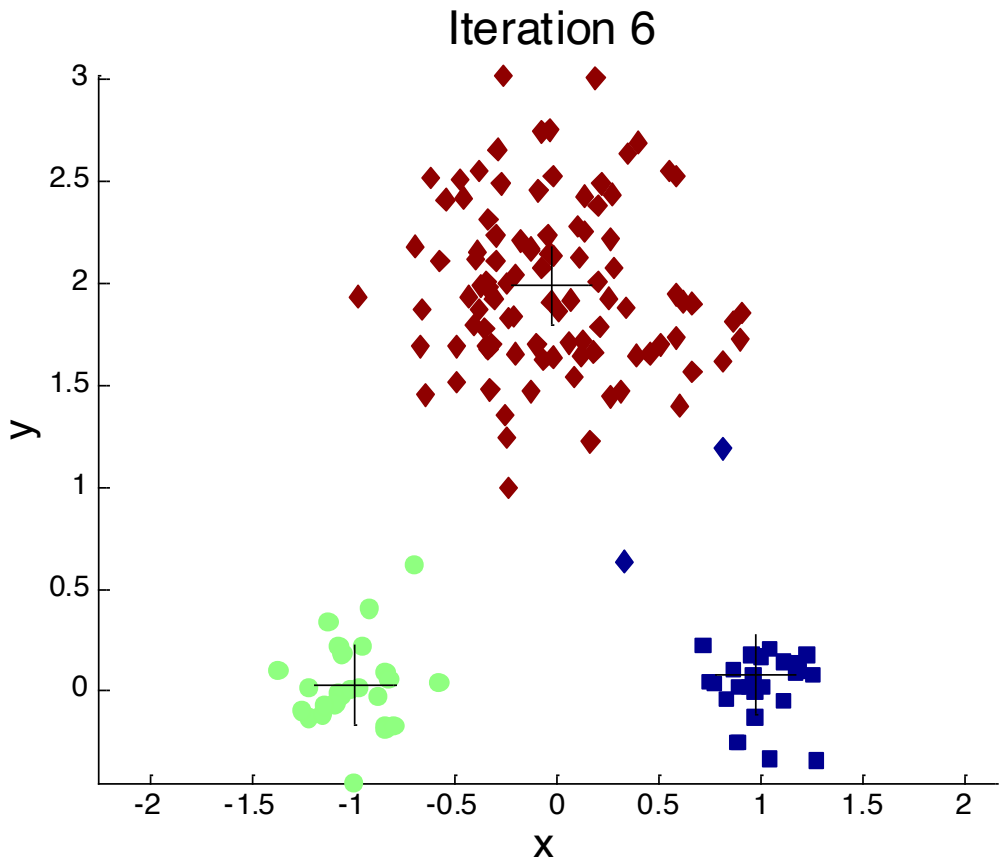
K-means Algorithm

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

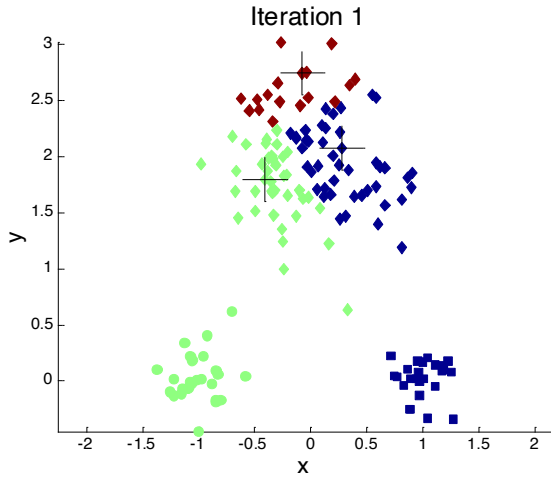
1. Select K points as the initial centroids
2. **repeat**
3. Form K clusters by assigning each point to the closest centroid
4. Compute the new centroid* of each cluster
5. **until** The centroids do not change

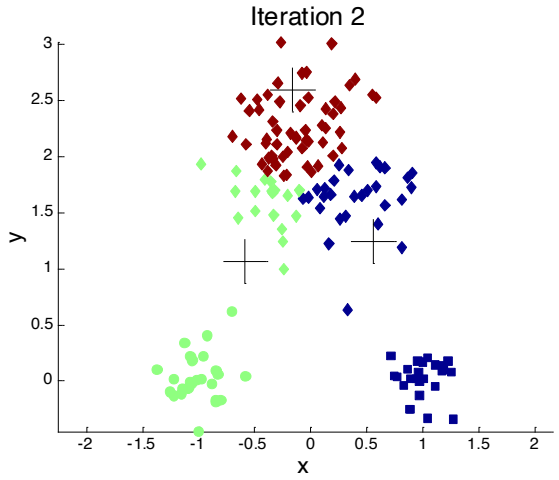
*The centroid of a set of points is the point that is minimizes the sum of distances from the points in the set

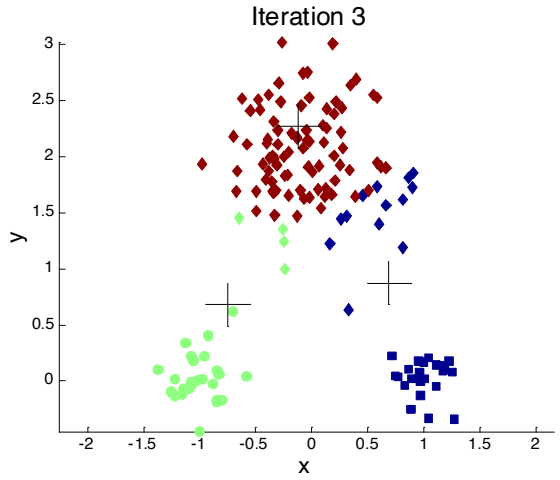
Example

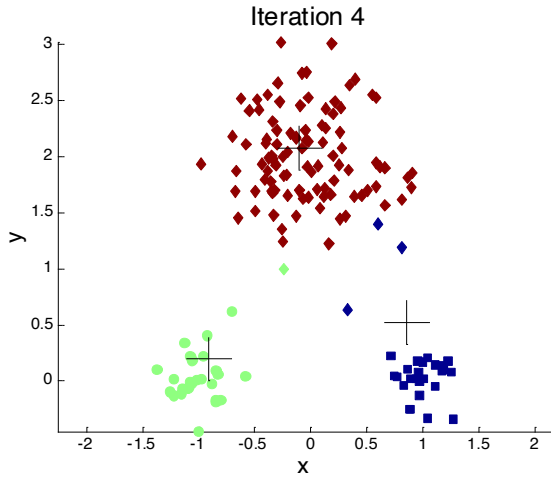


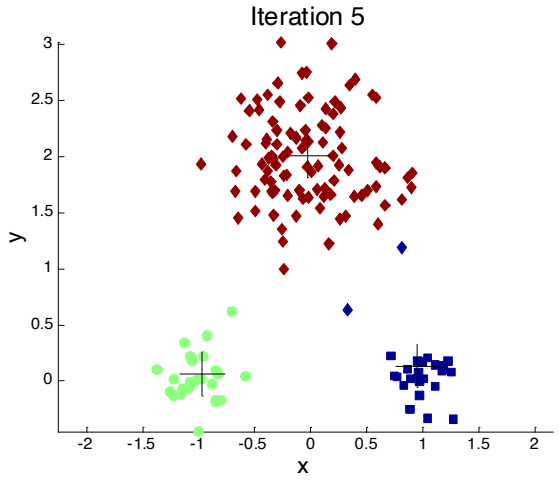
Example

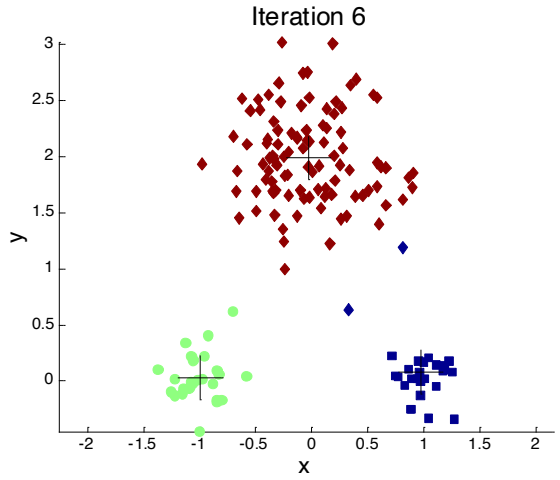

Iteration 1
x
y


Iteration 2
x
y


Iteration 3
x
y


Iteration 4
x
y

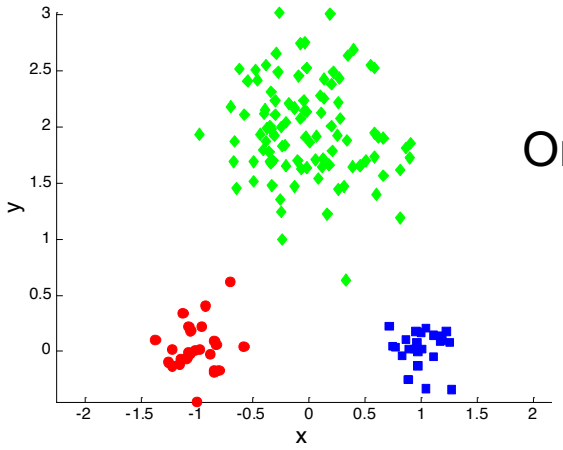

Iteration 5
x
y


Iteration 6
x
y

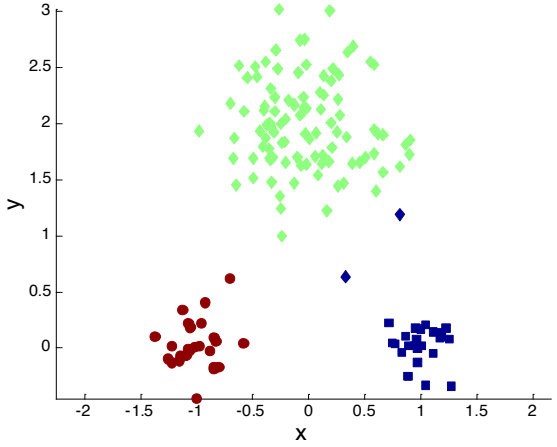
K-means Algorithm – Initialization

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

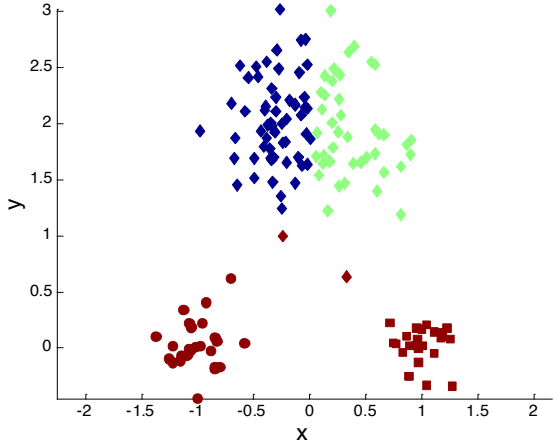
Two different K-means Clusterings



Original Points

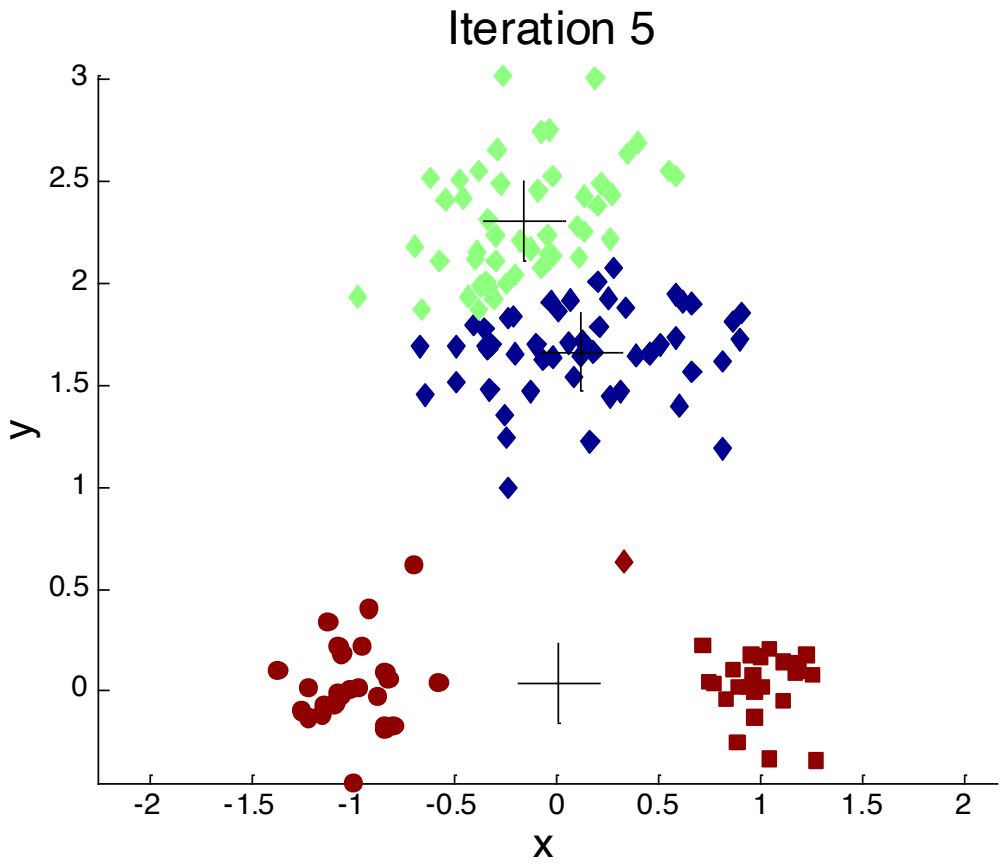


Optimal Clustering

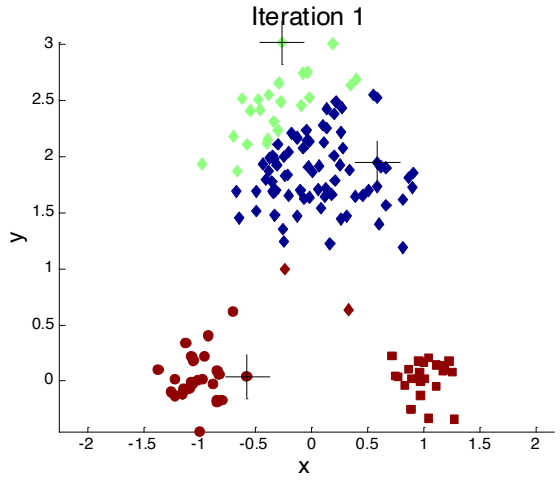


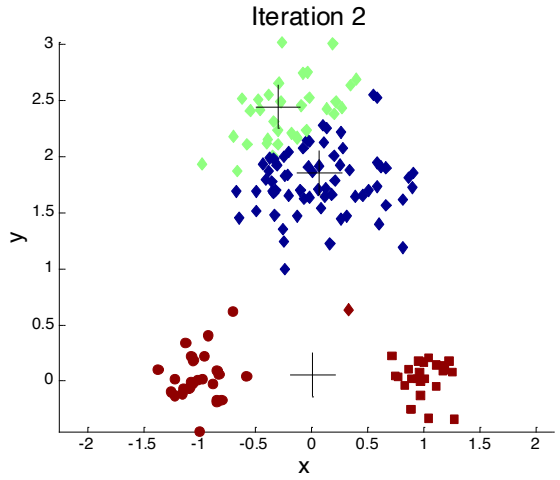
Sub-optimal Clustering

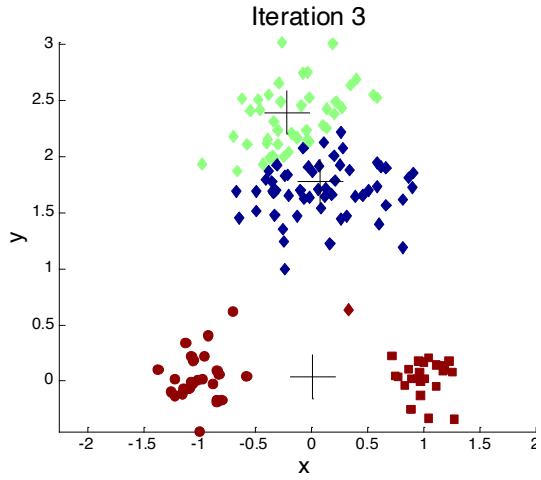
Importance of Choosing Initial Centroids

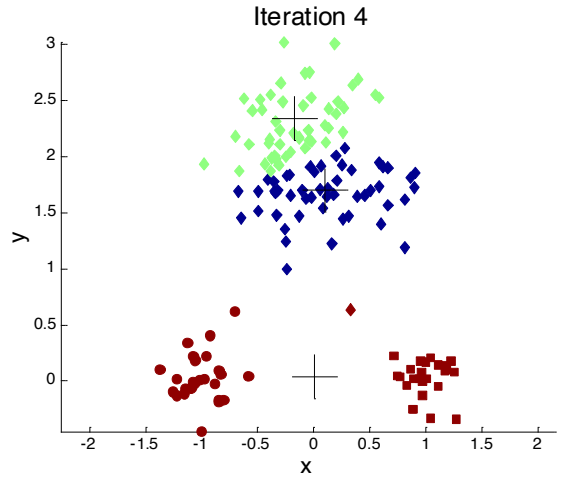


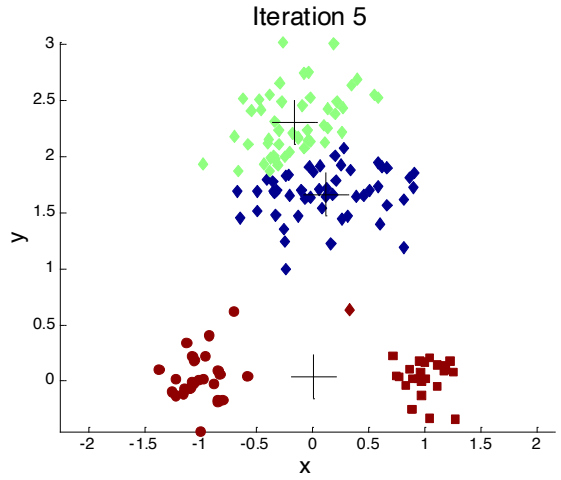
Importance of Choosing Initial Centroids …











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

- 'Closeness' is measured by some similarity or distance function
  - E.g., Euclidean distance (SSE), cosine similarity, correlation, etc.
- The centroid depends on the distance function
  - The minimizer for the distance function
- 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 for multiple dimensions

K-means Algorithm – Convergence

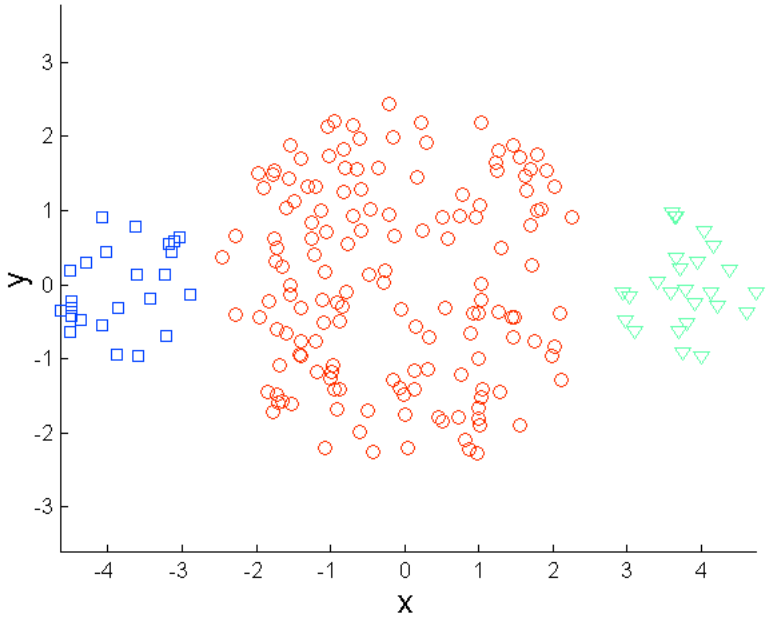
- K-means will converge for common similarity measures mentioned above.
  - Most of the convergence happens in the first few iterations.
  - Often the stopping condition is changed to 'Until relatively few points change clusters'
- Complexity is O(n * K * I * d)
  - n = number of points,
  - K = number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

Limitations of K-means

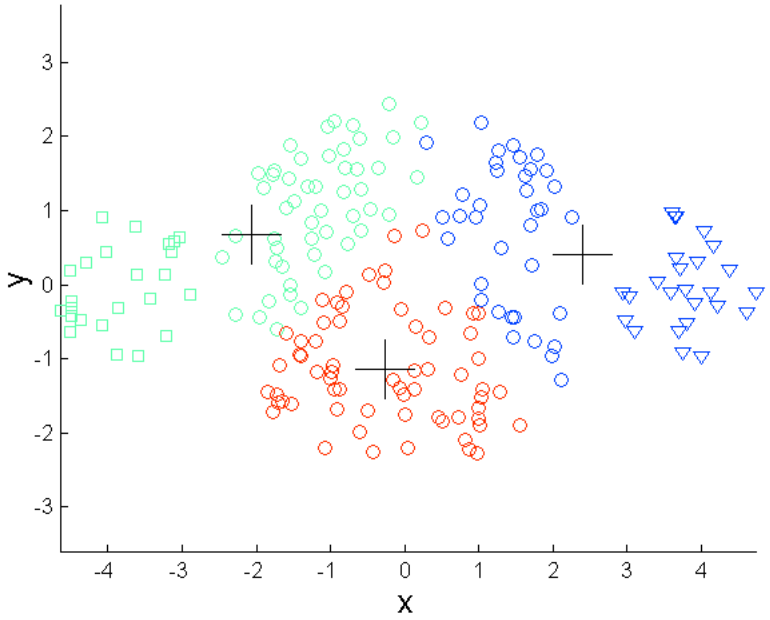
- K-means has problems when clusters are of different:
  - sizes
  - densities
  - non-globular shapes

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

Limitations of K-means: Differing Sizes

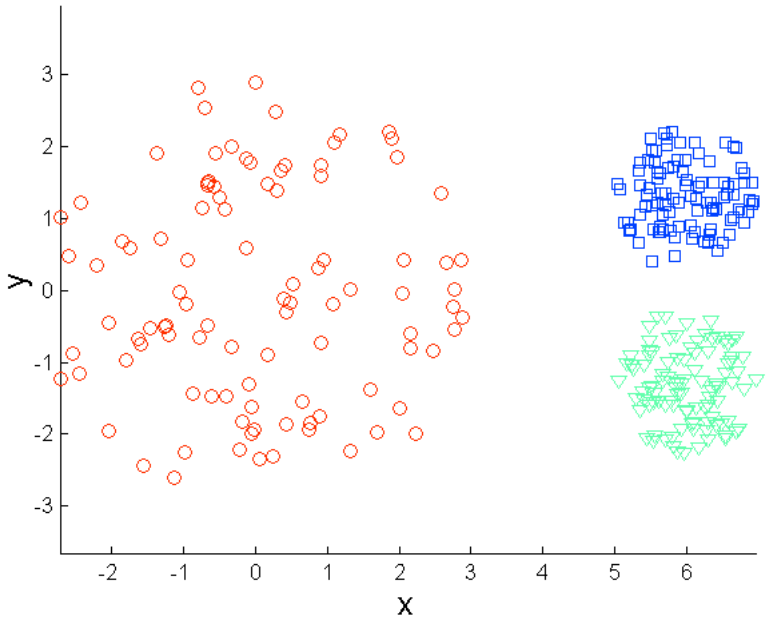


Original Points



K-means (3 Clusters)

Limitations of K-means: Differing Density



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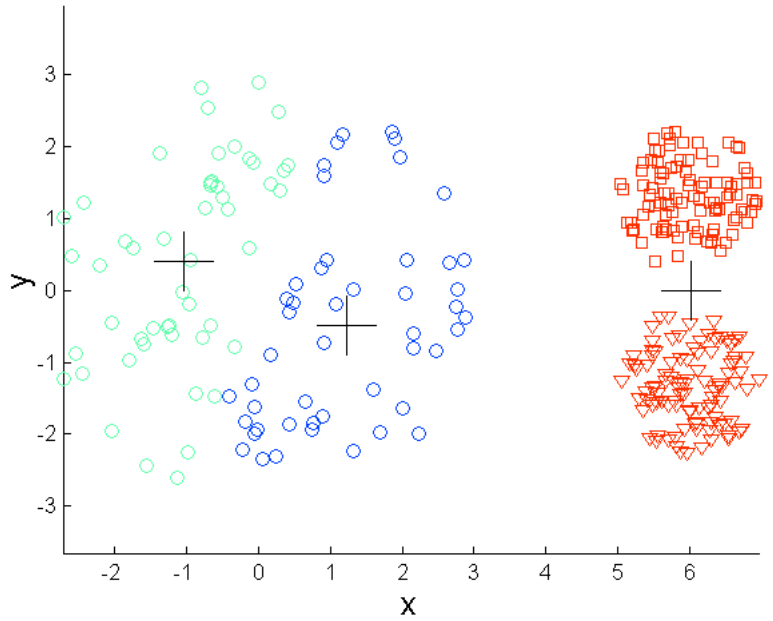
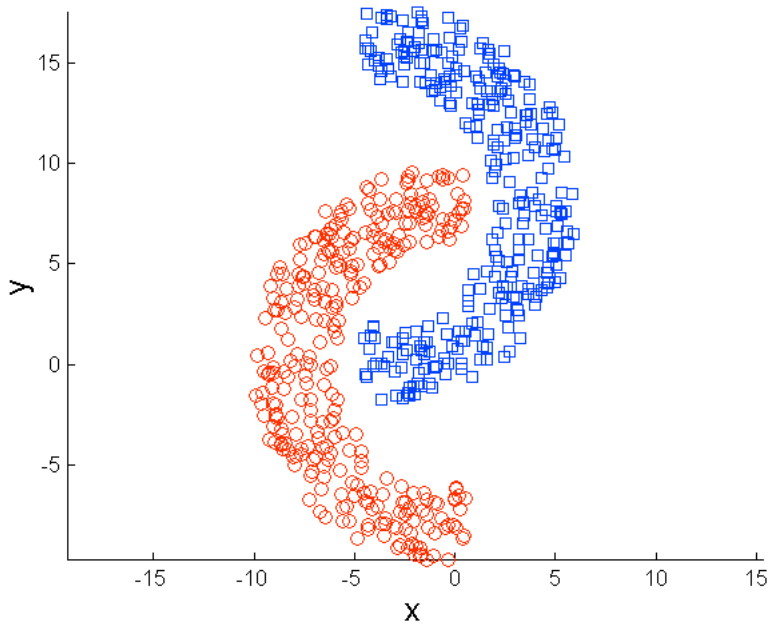
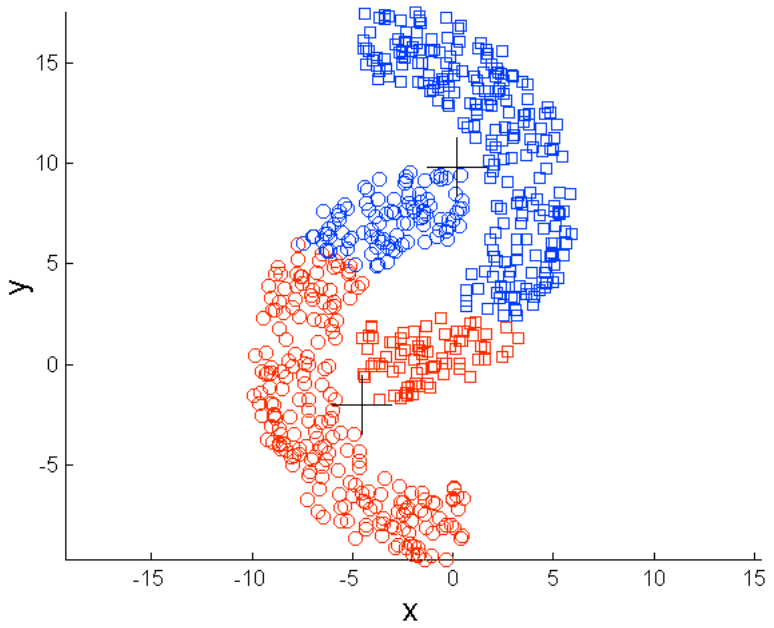


K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes

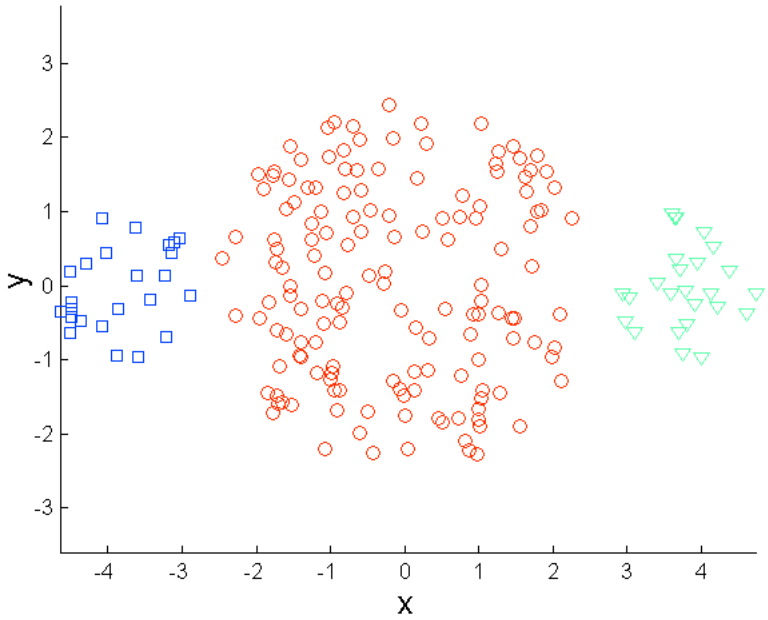


Original Points

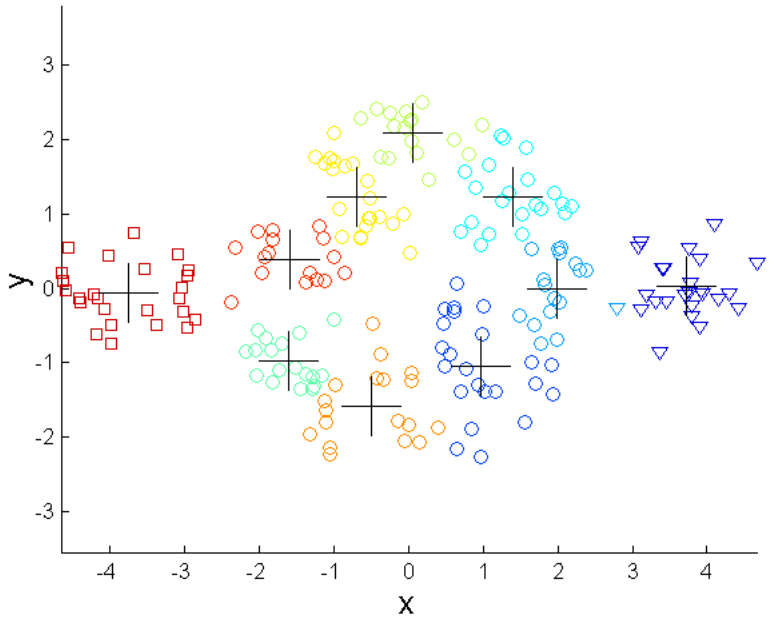


K-means (2 Clusters)

Overcoming K-means Limitations



Original Points

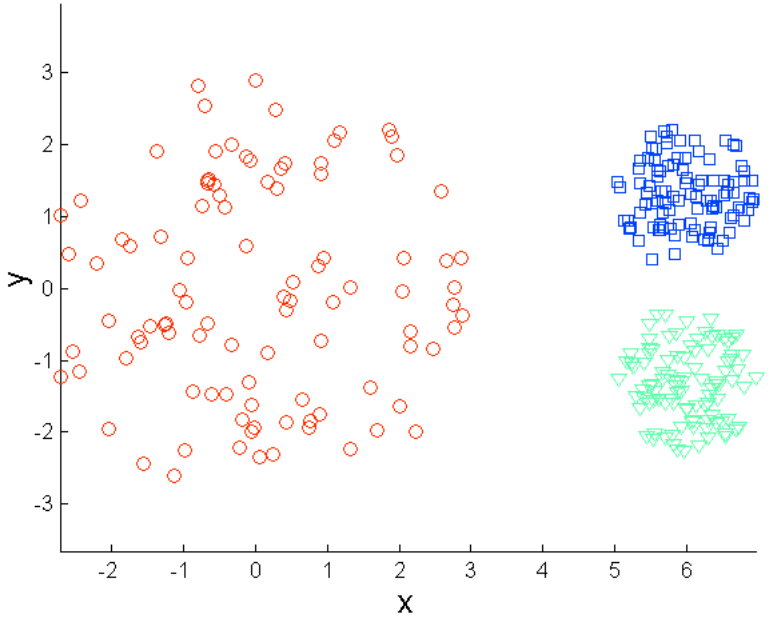


K-means Clusters

One solution is to use many clusters.

Find parts of clusters, but need to put together.

Overcoming K-means Limitations



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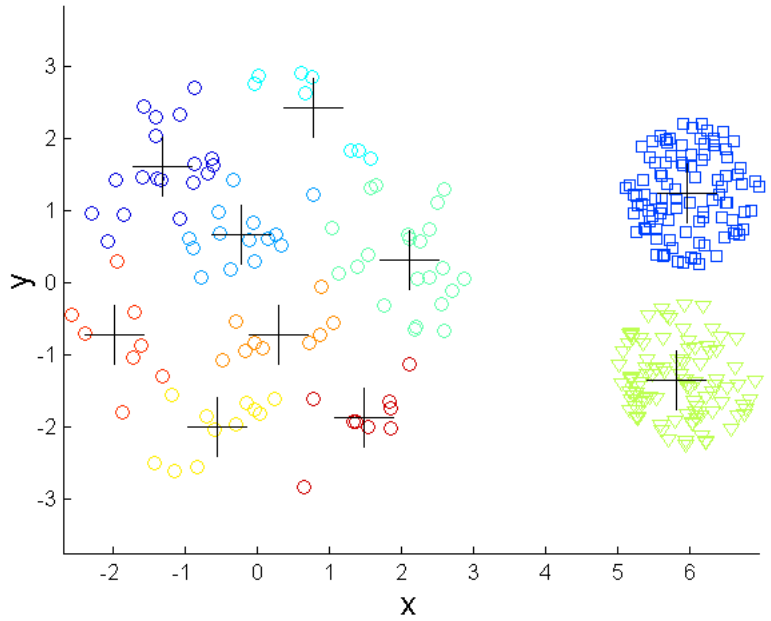
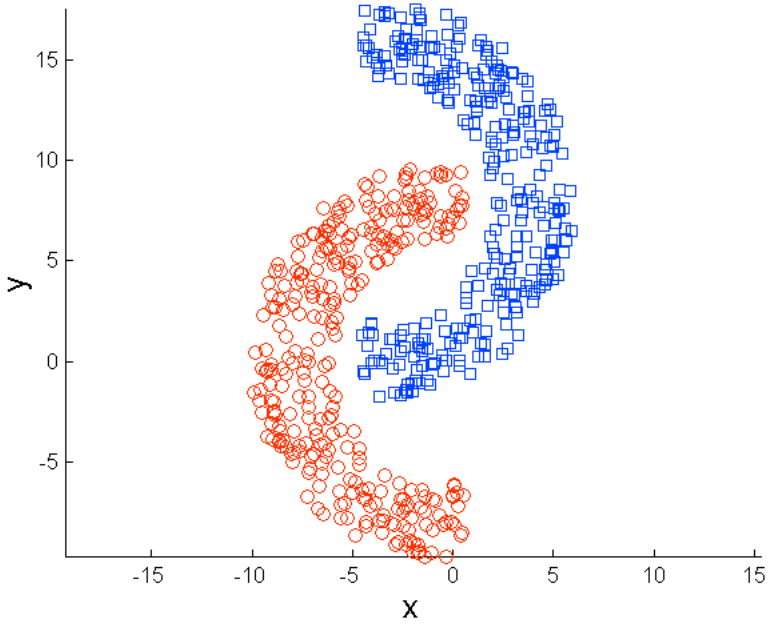


K-means Clusters

Overcoming K-means Limitations



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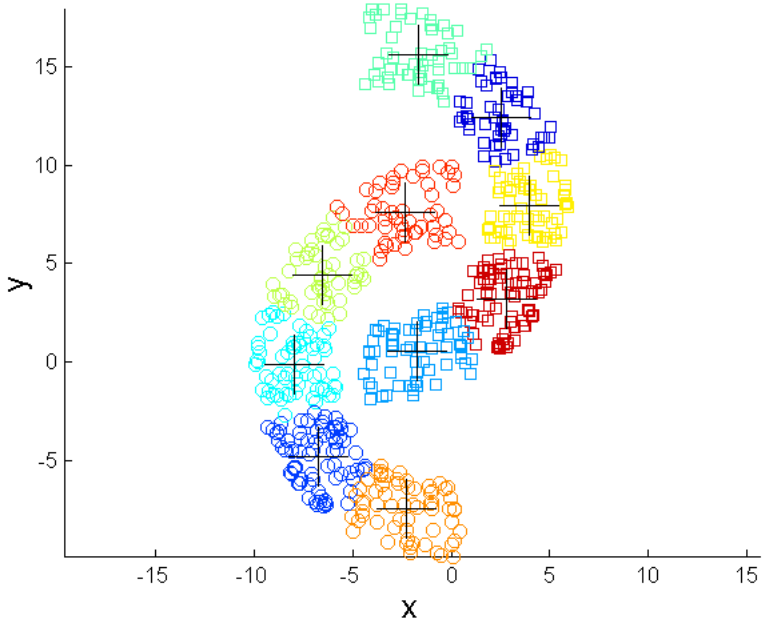
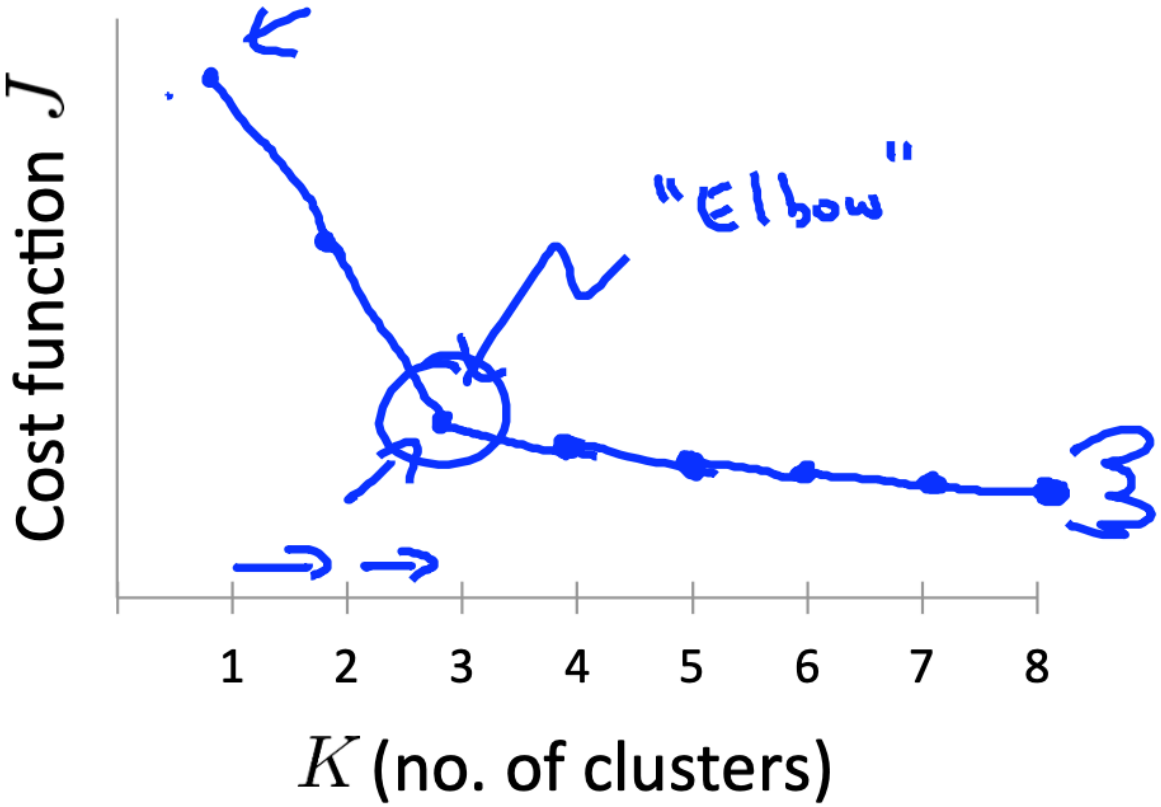
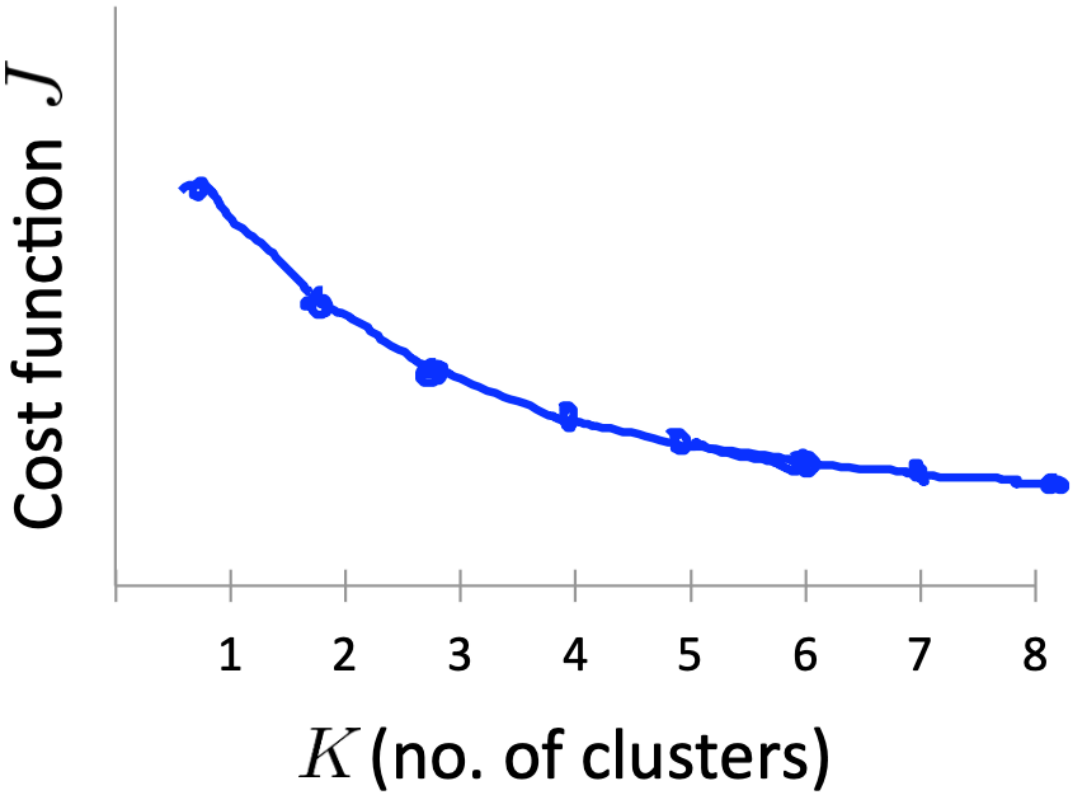


K-means Clusters

Choosing the value of K

Elbow method:





Andrew Ng

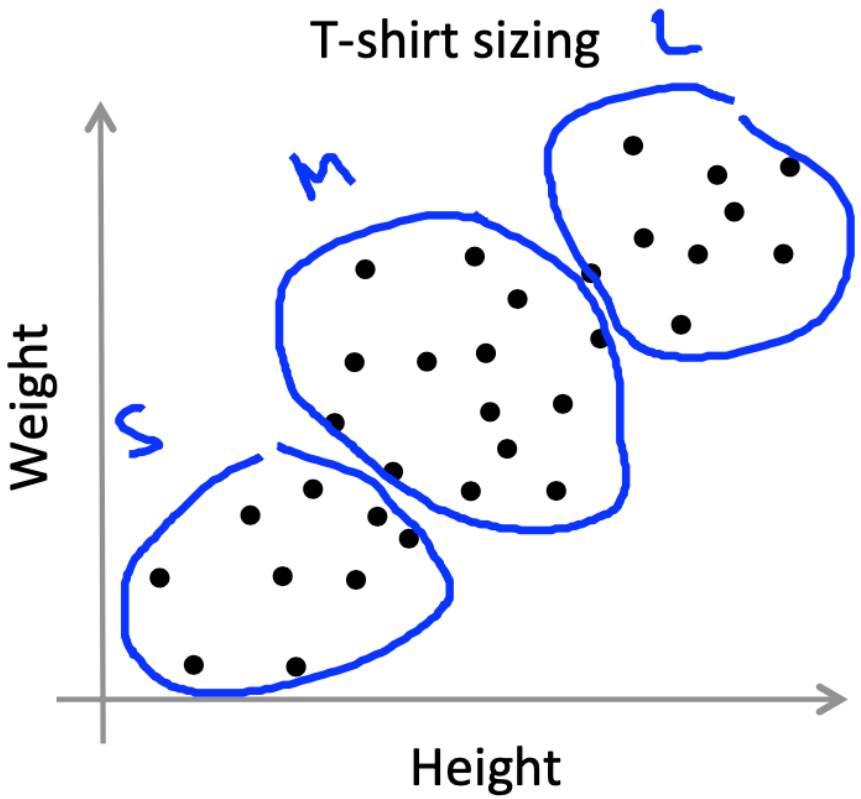
Choosing the value of K

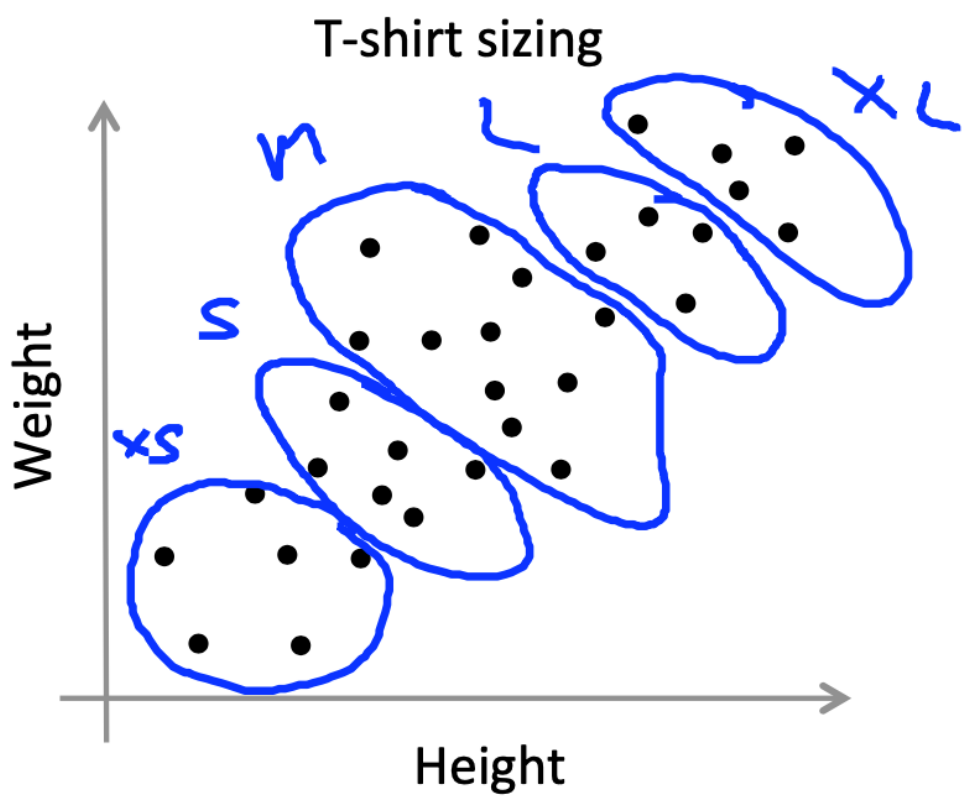
Sometimes, you're running K-means to get clusters to use for some later/downstream purpose. Evaluate K-means based on a metric for how well it performs for that later purpose.

K=3 S, M, L

K=5 XS, S, M, L, XL

E.g.





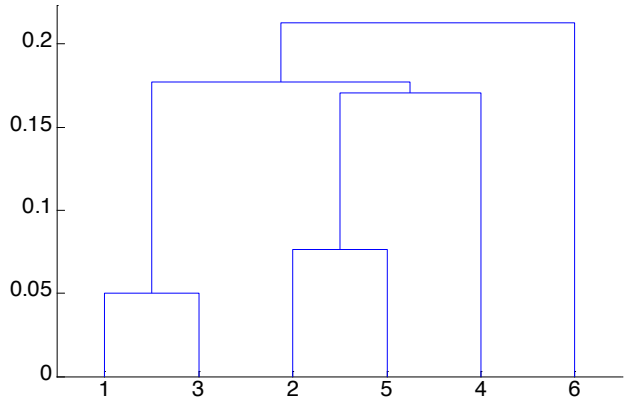
HIERARCHICAL CLUSTERING

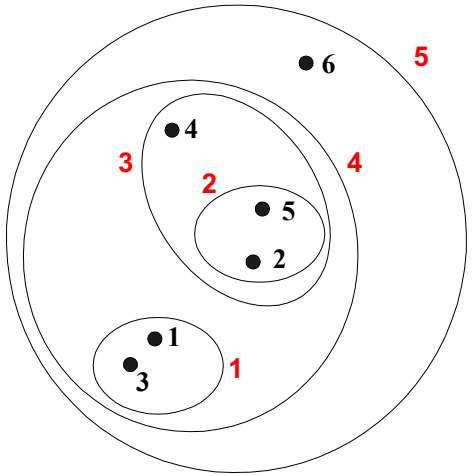
Hierarchical Clustering

- 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

- Dendrograms may correspond to meaningful taxonomies
  - Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, …)

Agglomerative Clustering Algorithm

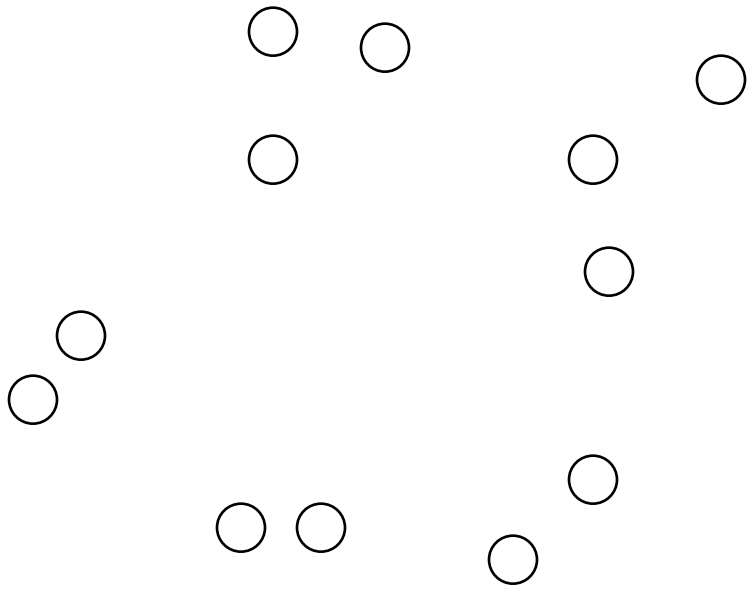
- Most popular hierarchical clustering technique
- Basic algorithm is straightforward

1. Compute the proximity matrix
2. 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 single-point clusters and a proximity matrix between points

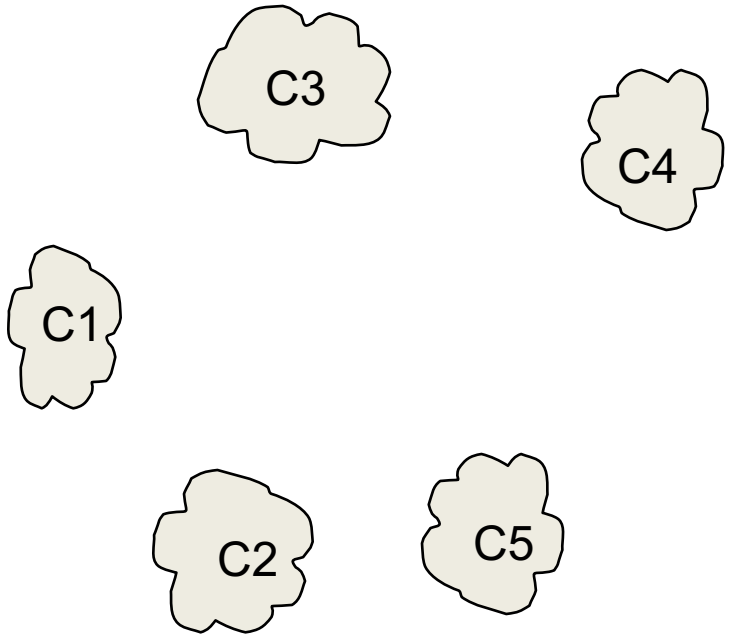


	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

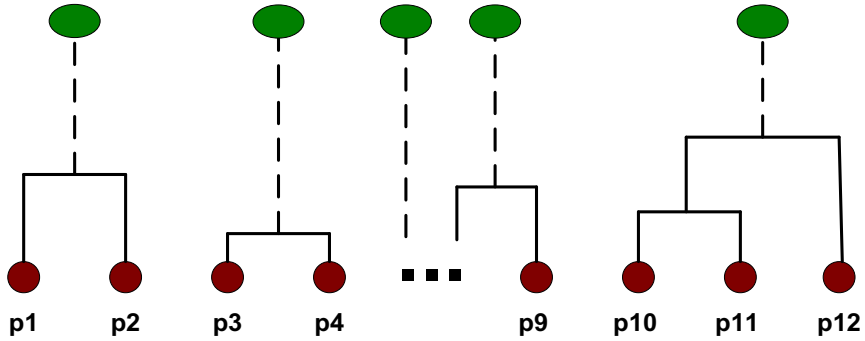
Intermediate Situation

- After some merging steps, we have some clusters and a proximity matrix between clusters



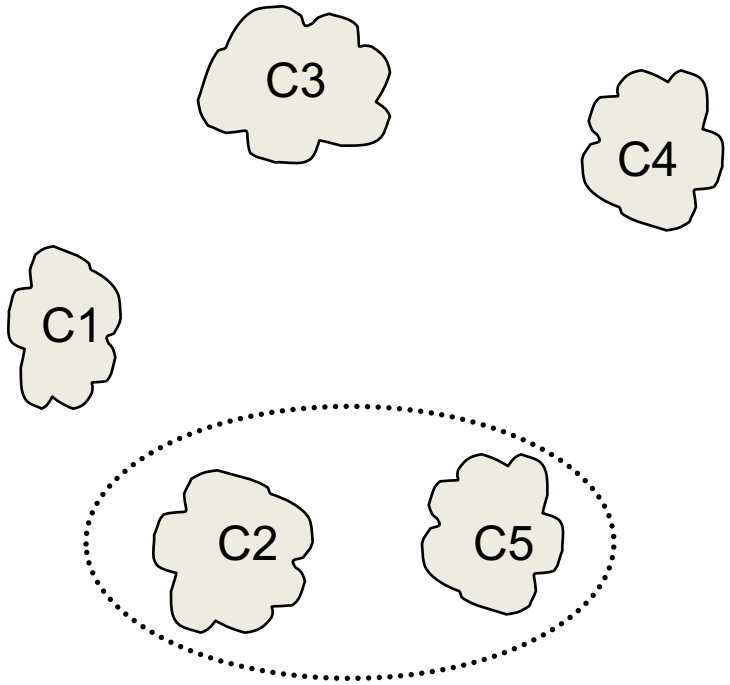
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Proximity Matrix



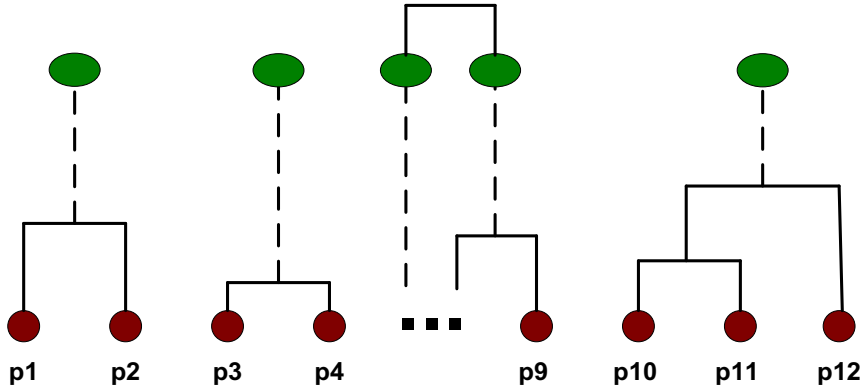
Intermediate Situation

- We want to merge the two closest clusters (C2 and C5) and update the proximity matrix.



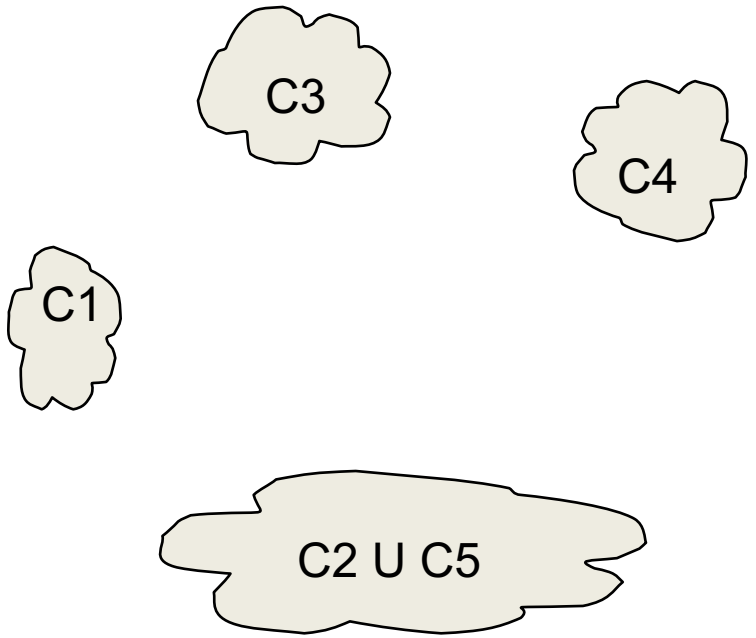
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Proximity Matrix



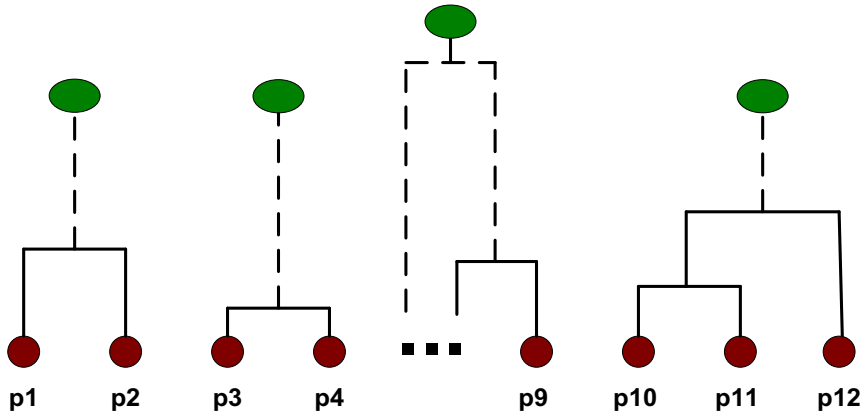
After Merging

- The question is “How do we update the proximity matrix?”

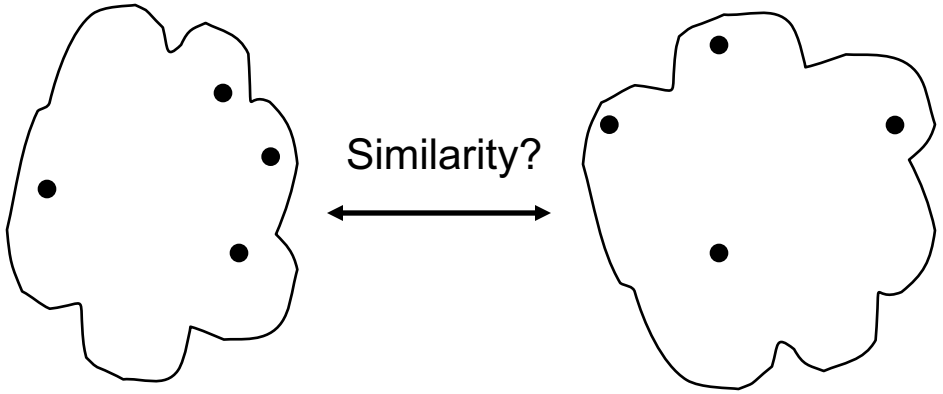


	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		

Proximity Matrix



How to Define Inter-Cluster Similarity

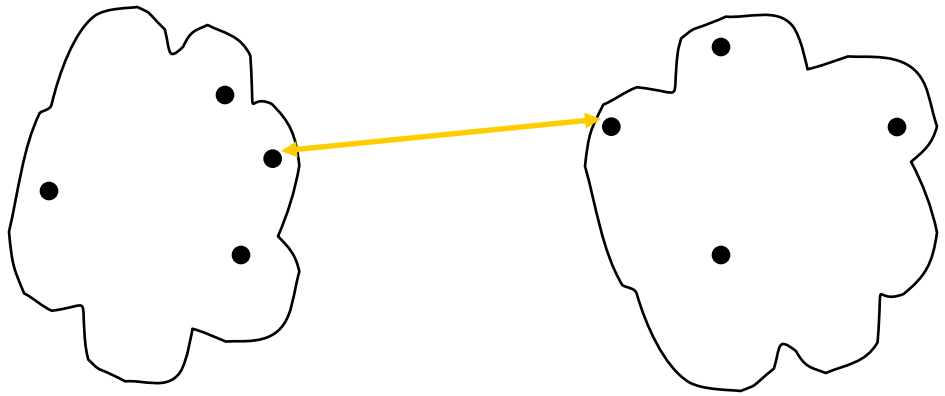


	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

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

How to Define Inter-Cluster Similarity



	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
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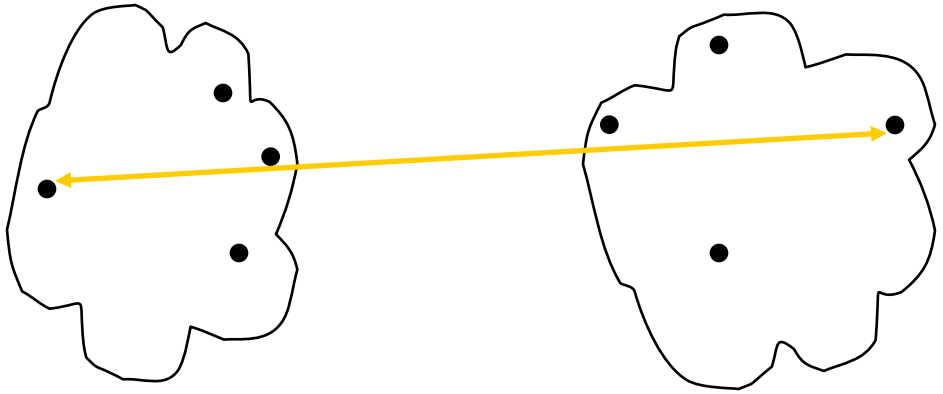
How to Define Inter-Cluster Similarity



	p1	p2	p3	p4	p5	. . .
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p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

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- MAX
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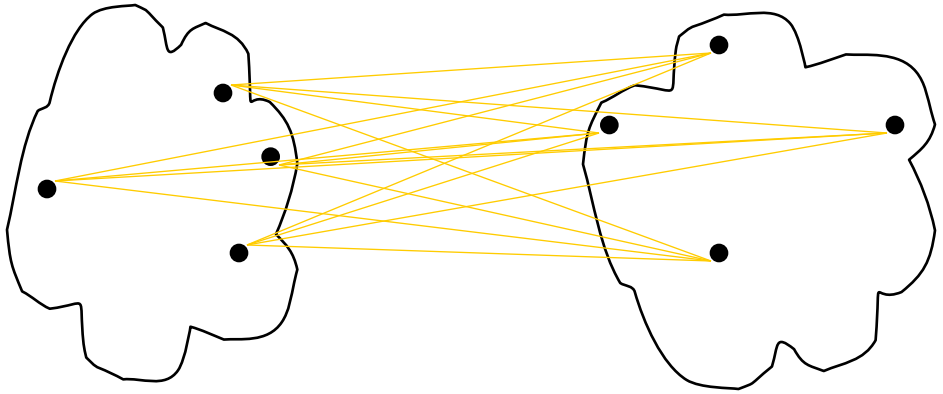
How to Define Inter-Cluster Similarity



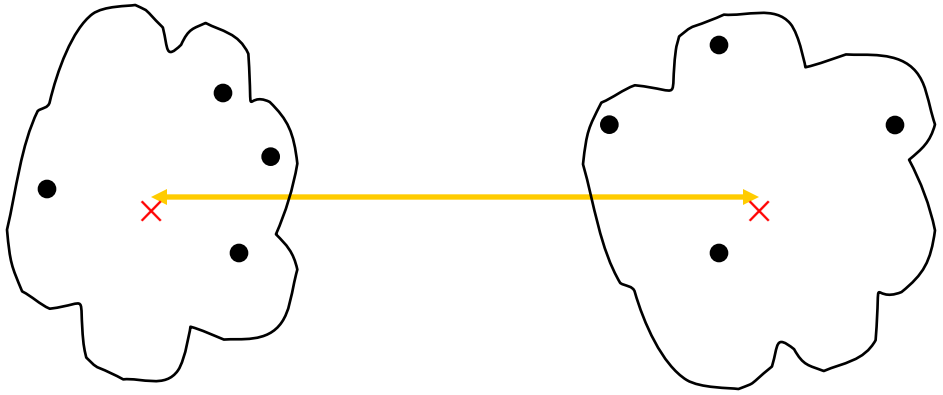
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

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

$$\text{proximity}(\text{Cluster}_i, \text{Cluster}_j) = \frac{\sum_{\substack{p_i \in \text{Cluster}_i \\ p_j \in \text{Cluster}_j}} \text{proximity}(p_i, p_j)}{|\text{Cluster}_i| * |\text{Cluster}_j|}$$

How to Define Inter-Cluster Similarity



	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

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

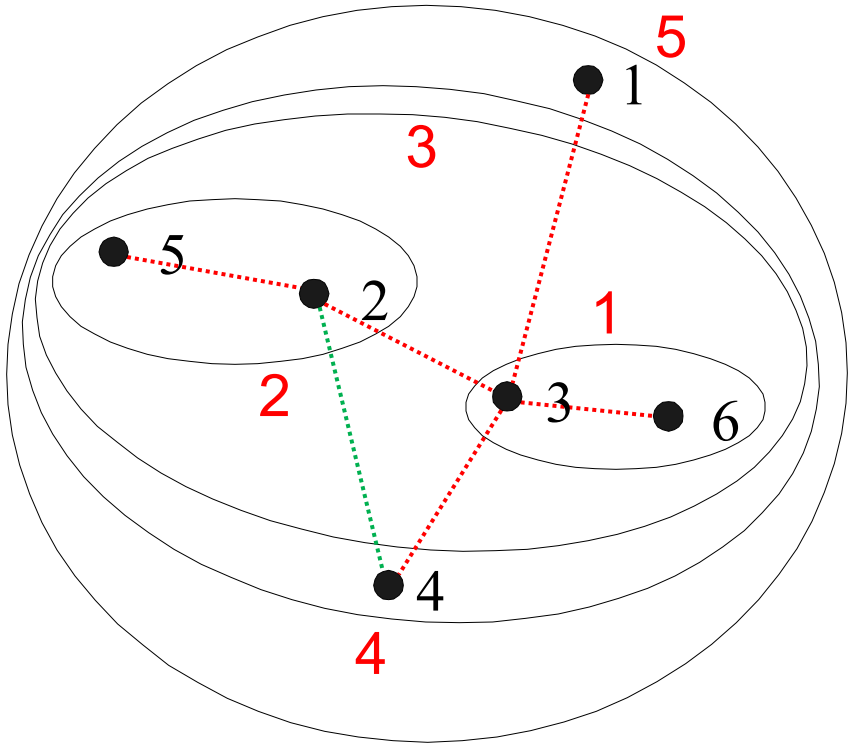
Single Link – Complete Link

- 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.

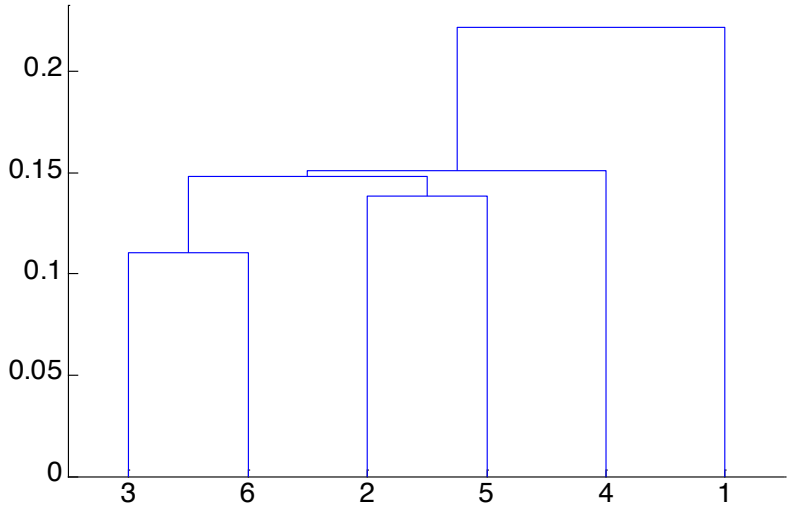
Hierarchical Clustering: MIN

The MIN – Single Link, will merge two clusters when a single pair of elements is linked

	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

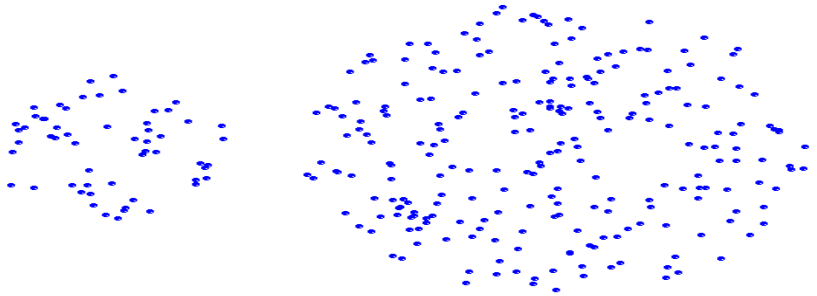


Nested Clusters

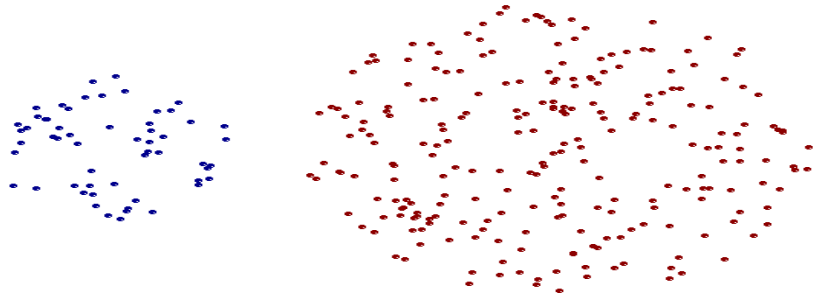


Dendrogram

Strength of MIN



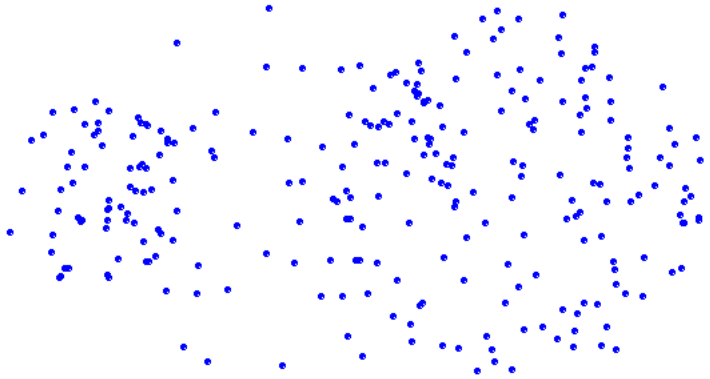
Original Points



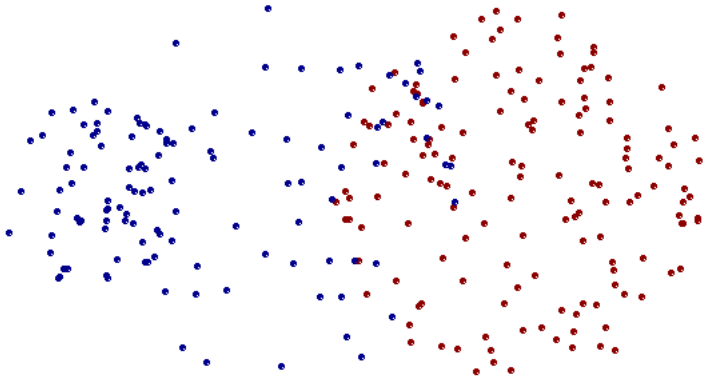
Two Clusters

- Can handle non-elliptical shapes

Limitations of MIN



Original Points

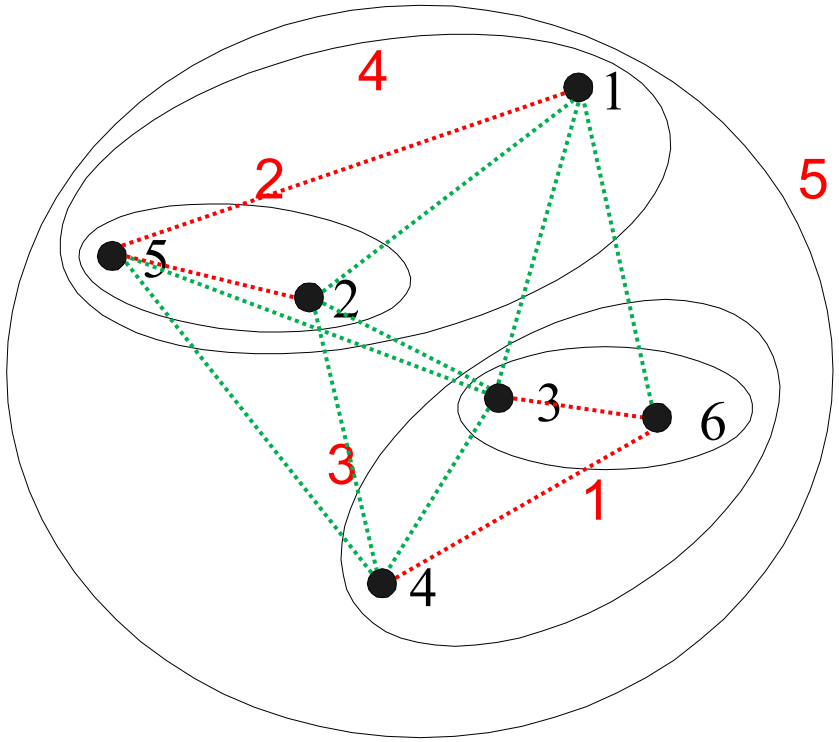


Two Clusters

- Sensitive to noise and outliers

Hierarchical Clustering: MAX

The MAX – Complete Linkage will merge two clusters when all pairs of elements have been linked.



Nested Clusters

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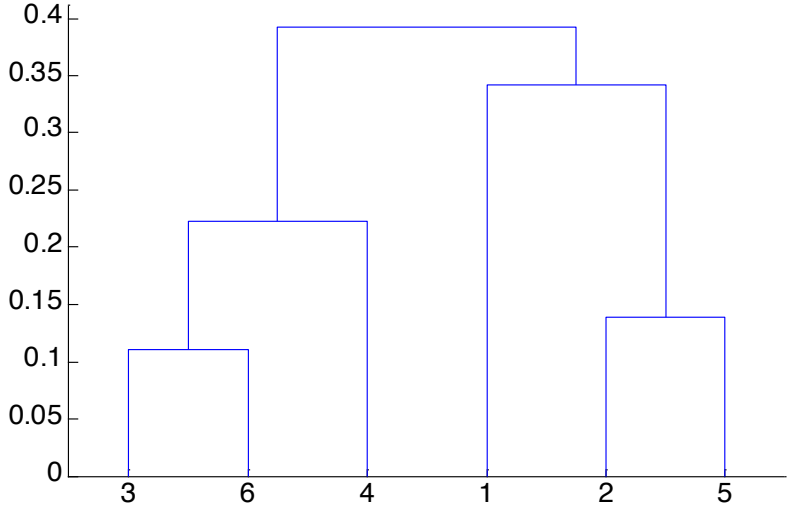
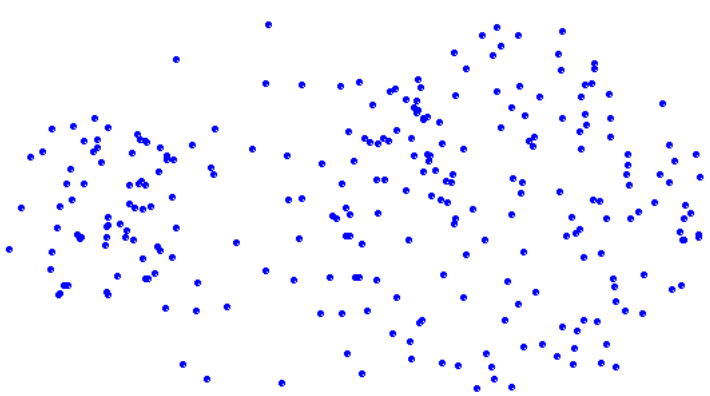
4	.37	.20	.15	0	.29	.22
5	.34	.14	.28	.29	0	.39
6	.23	.25	.11	.22	.39	0

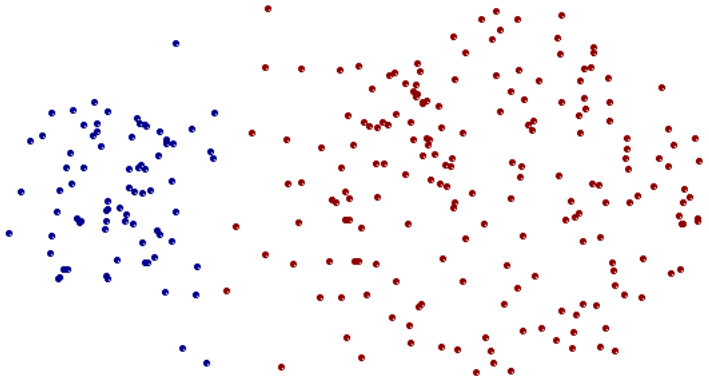


Dendrogram

Strength of MAX



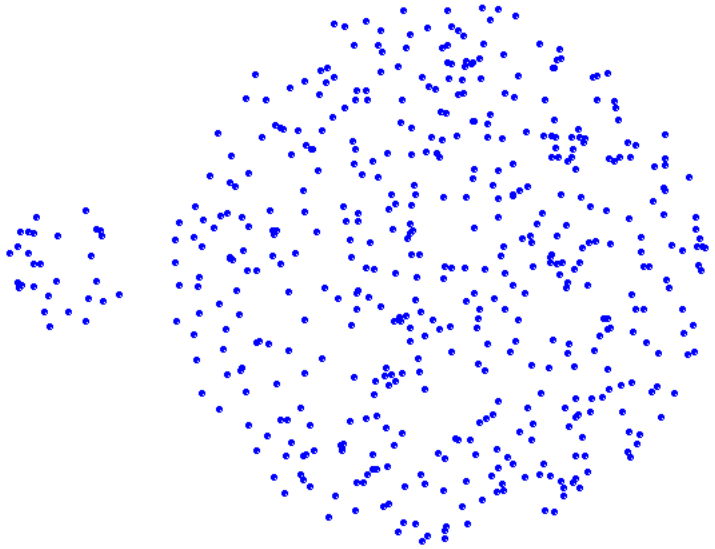
Original Points



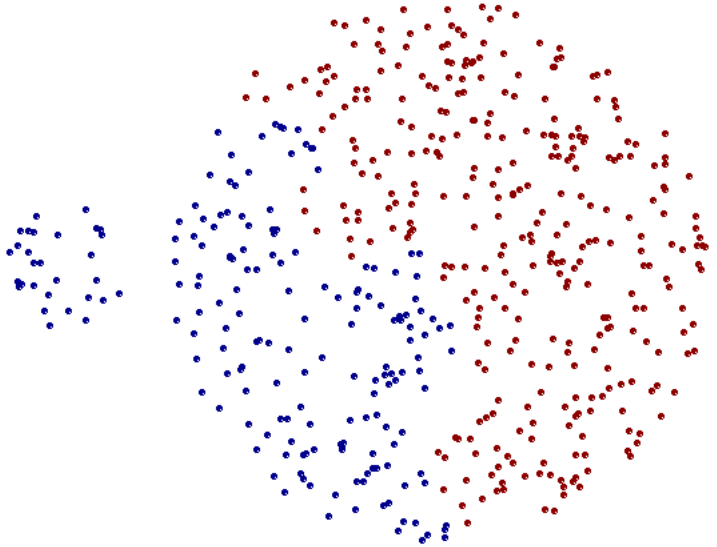
Two Clusters

- Less susceptible to noise and outliers

Limitations of MAX



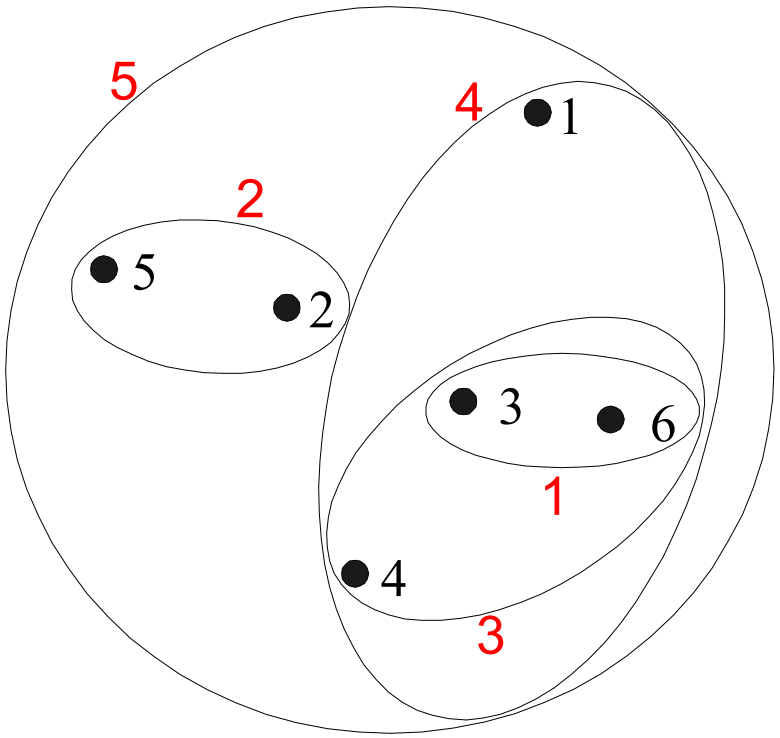
Original Points



Two Clusters

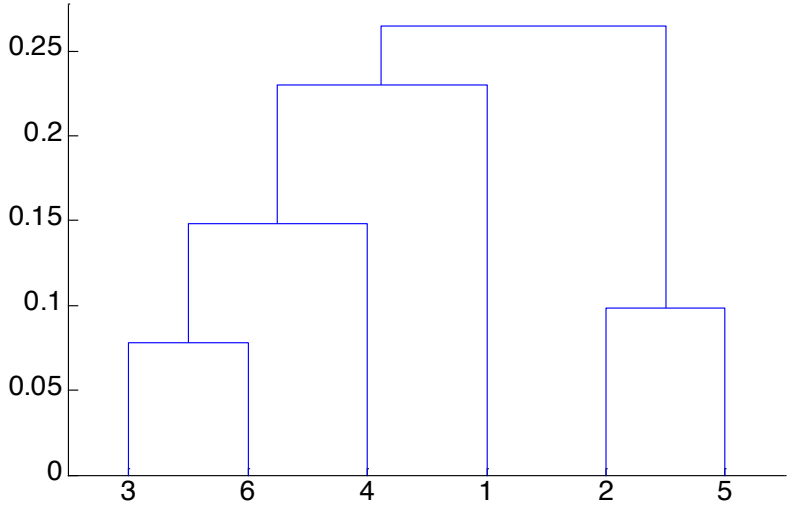
- Tends to break large clusters
- Biased towards globular clusters

Hierarchical Clustering: Group Average



Nested 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



Dendrogram

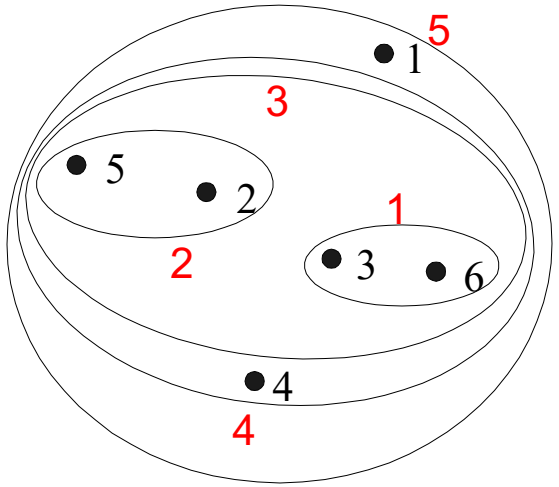
Hierarchical Clustering: Group Average

- Compromise between Single and Complete Link
- Strengths
  - Less susceptible to noise and outliers
- Limitations
  - Biased towards globular clusters

Cluster Similarity: Ward's Method

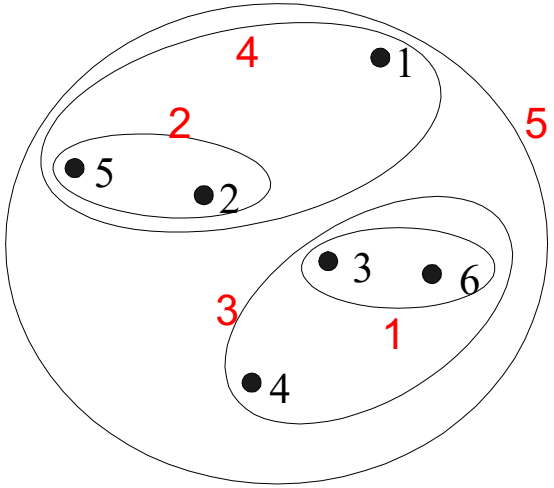
- Similarity of two clusters is based on the increase in squared error (SSE) when two clusters are merged
  - Similar to group average if distance between points is sum of squared distance
- Hierarchical analogue of K-means
  - Can be used to initialize K-means
- Less susceptible to noise and outliers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

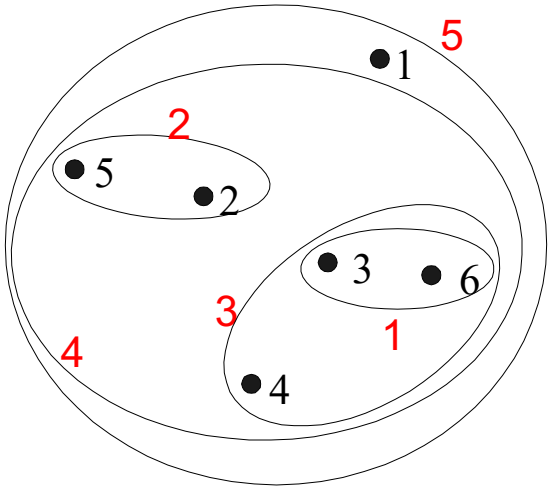
Hierarchical Clustering: Comparison



MIN

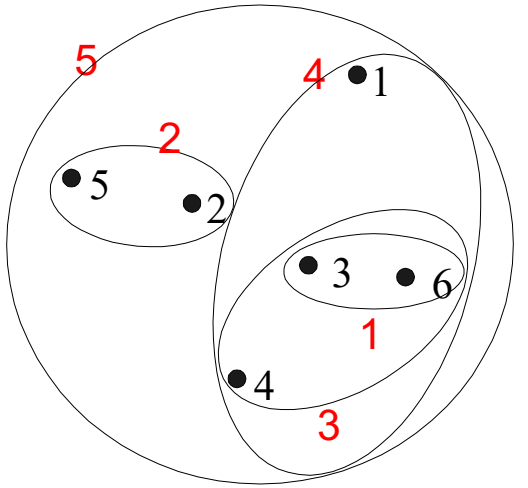
MAX





Group Average

Ward's Method



Hierarchical Clustering: Time and Space requirements

- $O(N^2)$ space since it uses the proximity matrix.
  - N is the number of points.

- $O(N^3)$ time in many cases
  - There are N steps and at each step the size, N^2, proximity matrix must be updated and searched
  - Complexity can be reduced to $O(N^2 \log(N))$ 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.

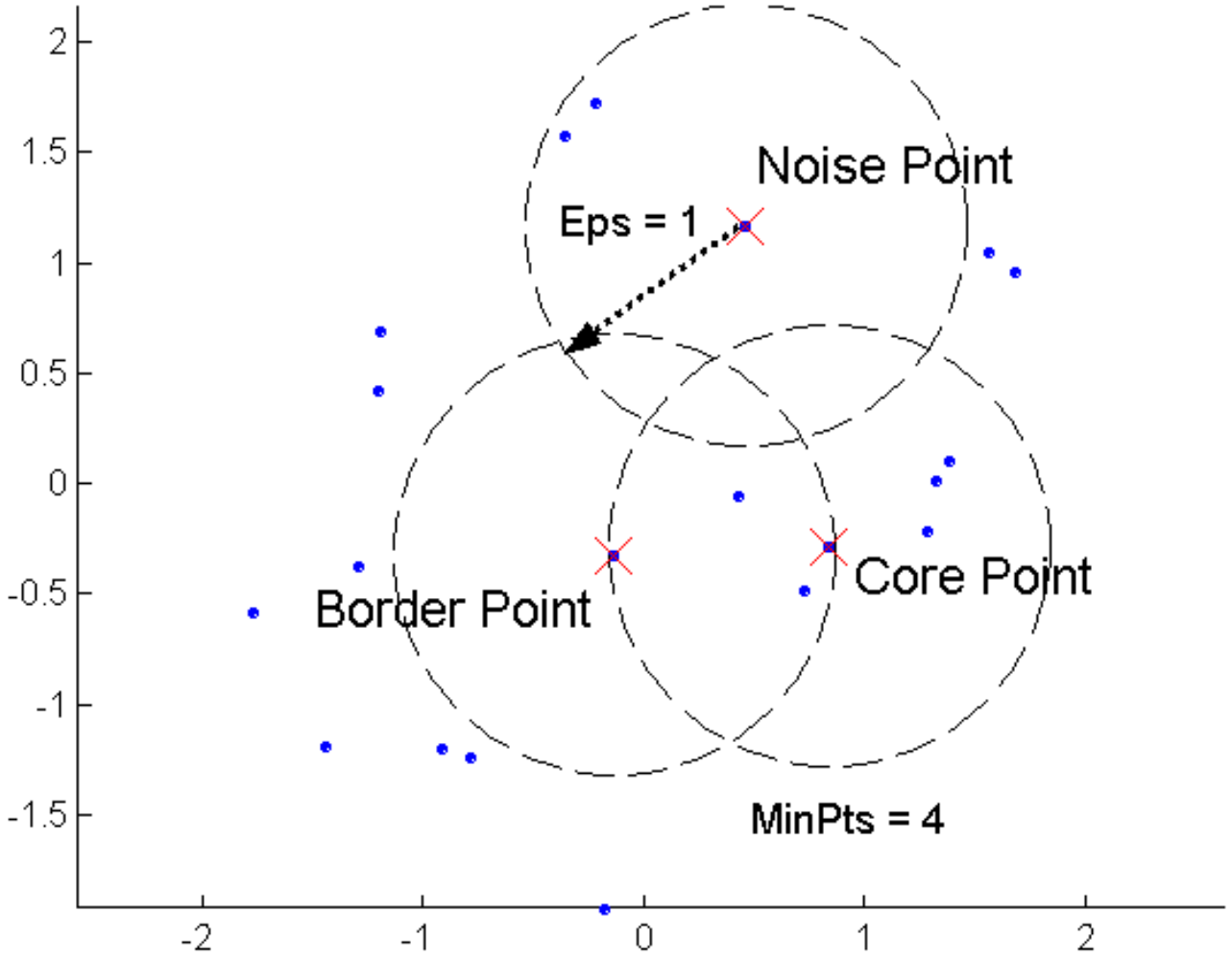
- Important Questions:
  - How do we measure density?
  - What is a dense region?

- 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

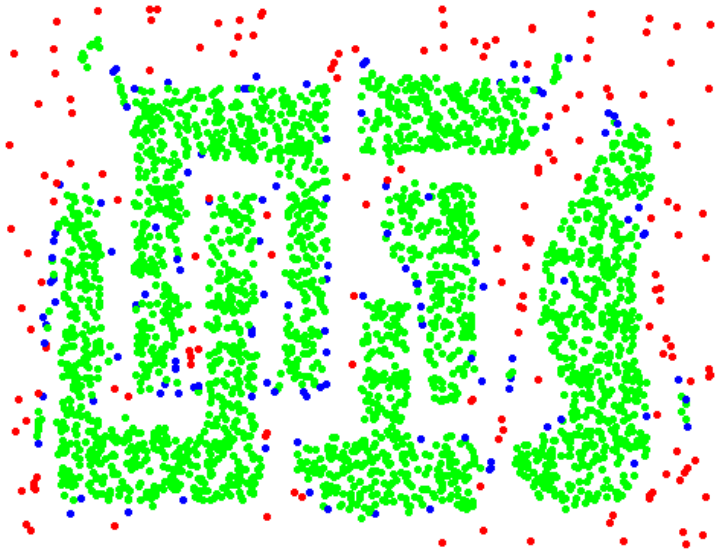
- Characterization of points
  - A point is a core point if it has more than a specified number of points (MinPts) within Eps
    - These points belong in a dense region and are at the interior of a cluster
  - A border point has fewer than MinPts within Eps, but is in the neighborhood of a core point.
  - 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

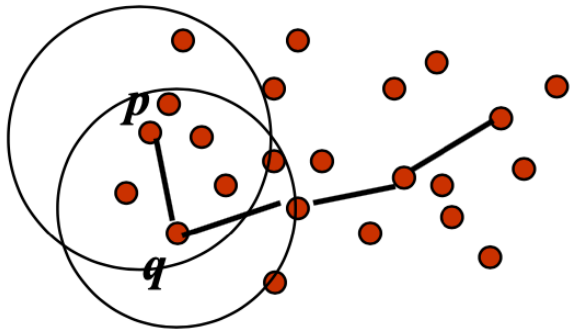


Point types: core, border and noise

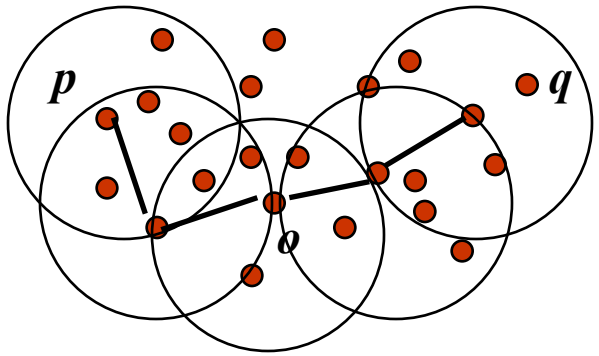
Eps = 10, MinPts = 4

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

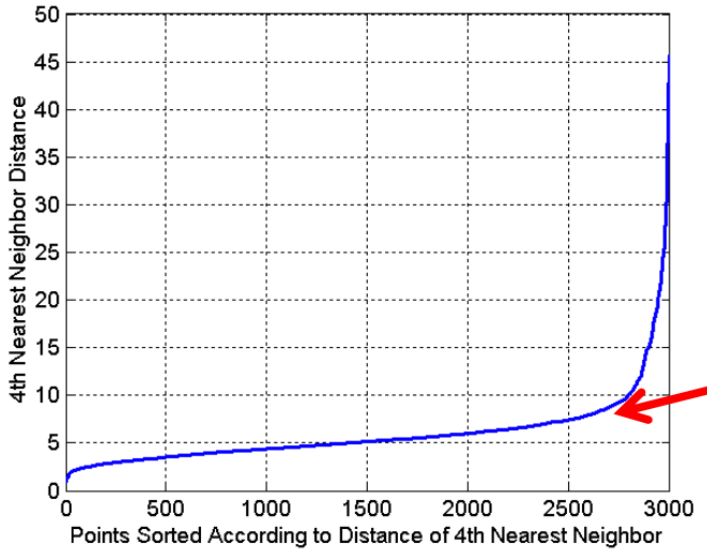


DBSCAN Algorithm

- 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

- Try different minPts= k
- So, plot sorted distance of every point to its k^{th} nearest neighbor
- Find the distance d where there is a "knee" in the curve
  - Eps = d, MinPts = k

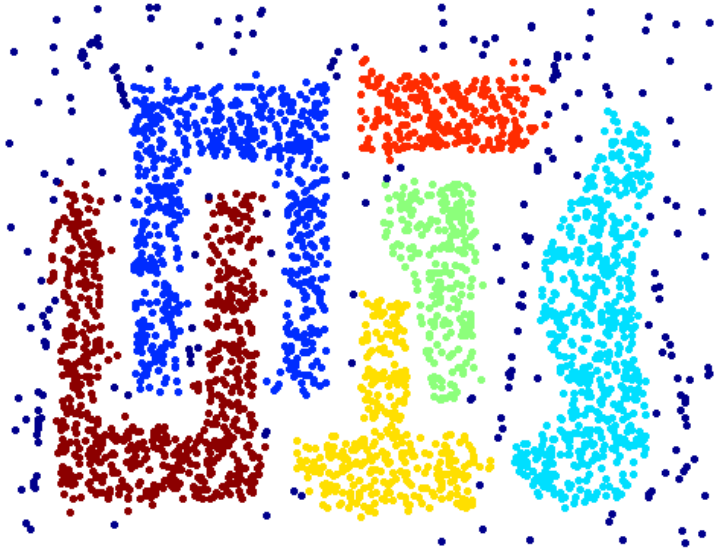


Noise points have the k^{th} nearest neighbor at farther distance

Eps ~ 7-10
MinPts = 4

When DBSCAN Works Well

Original Points



Clusters

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

DBSCAN: Sensitive to Parameters

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

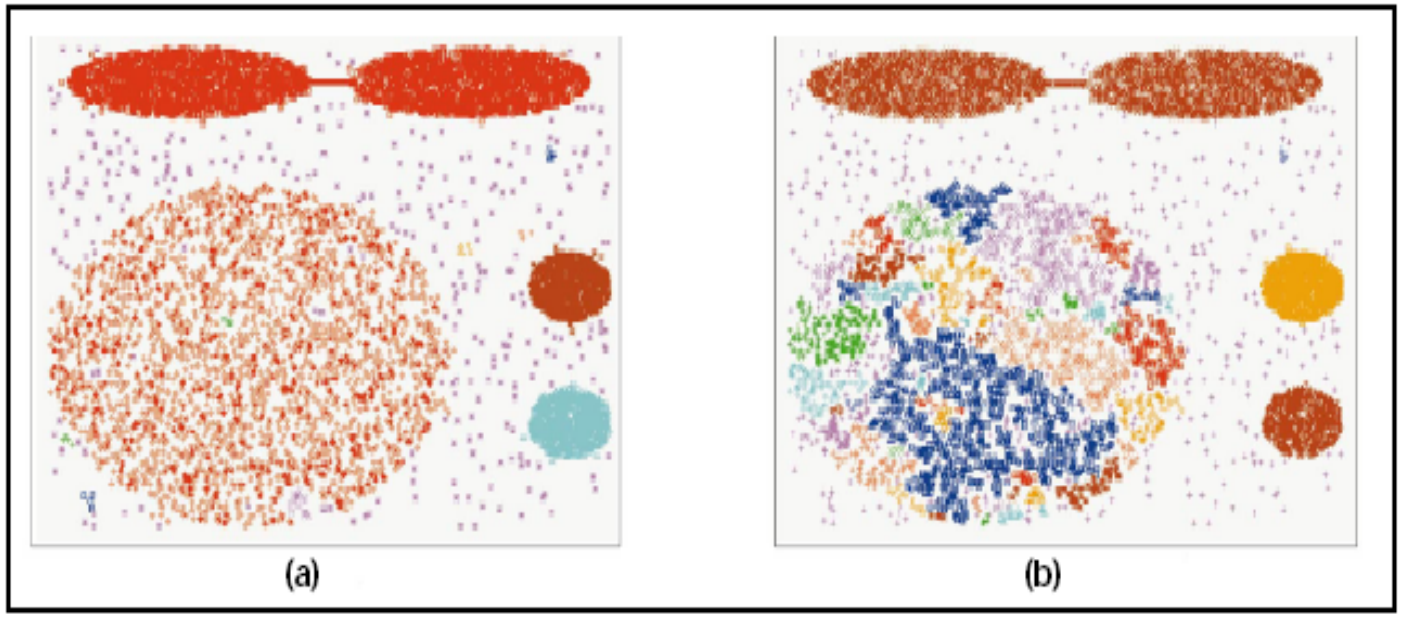
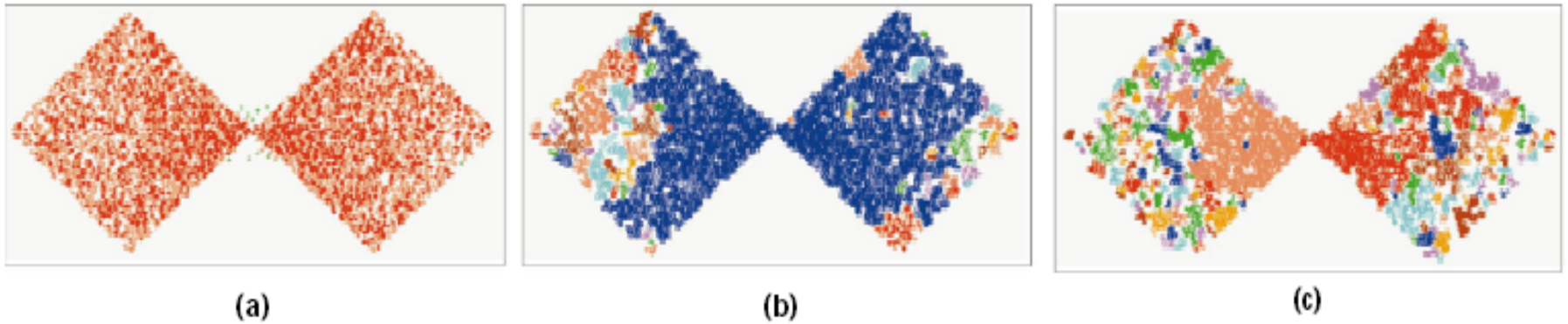
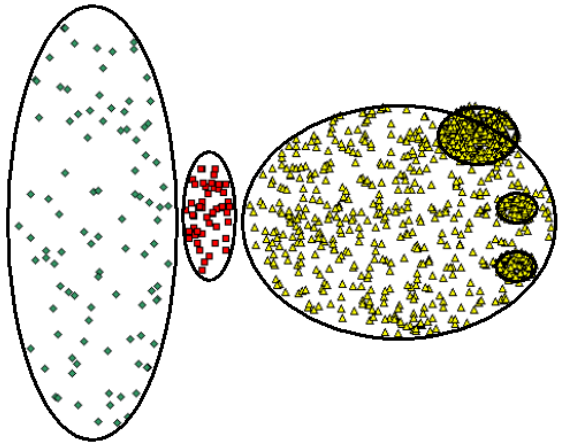


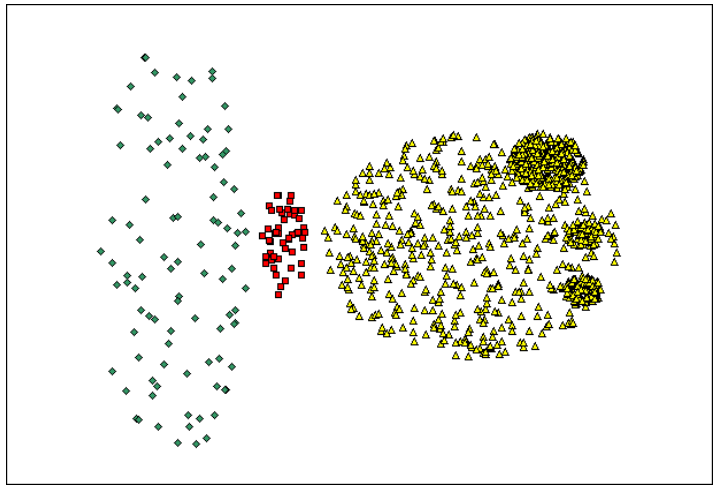
Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.



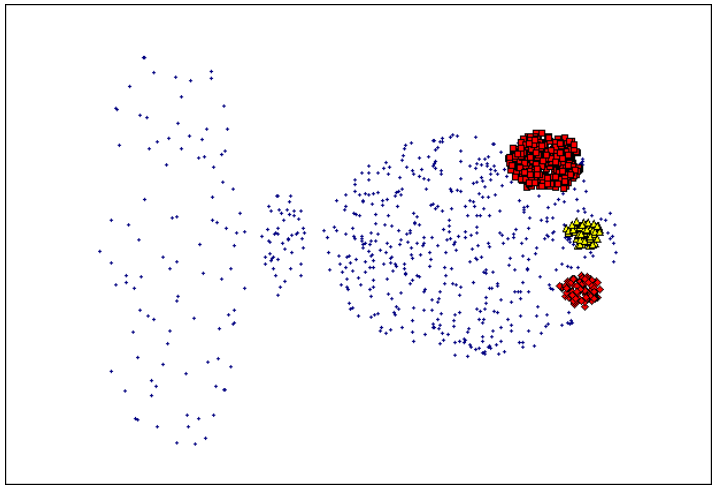
When DBSCAN Does NOT Work Well



Original Points



(MinPts=4, Eps=9.75).



(MinPts=4, Eps=9.92)

- Varying densities
- High-dimensional data

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

CLUSTERING EVALUATION

Clustering Evaluation

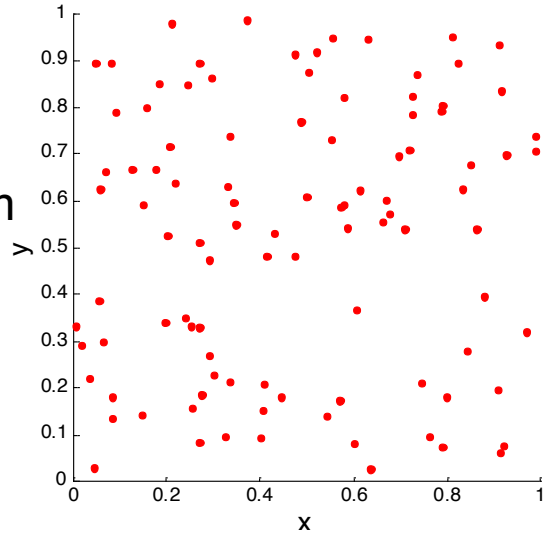
- We need to evaluate the "goodness" of the resulting clusters?

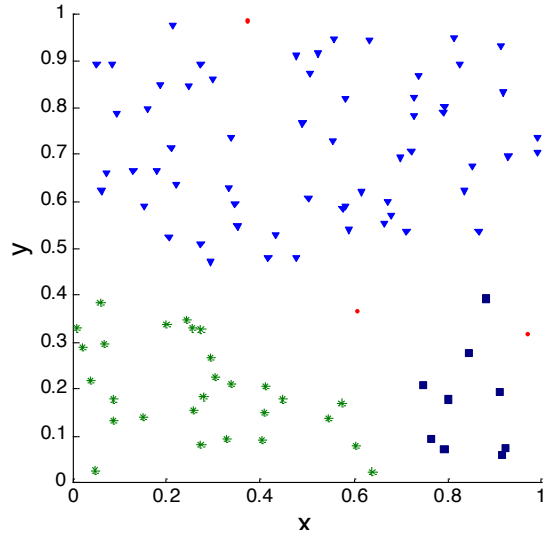
- But "clustering lies in the eye of the beholder"!

- Then why do we want to evaluate them?
  - To avoid finding patterns in noise
  - To compare clusterings, or clustering algorithms
  - To compare against a "ground truth"

Clusters found in Random Data

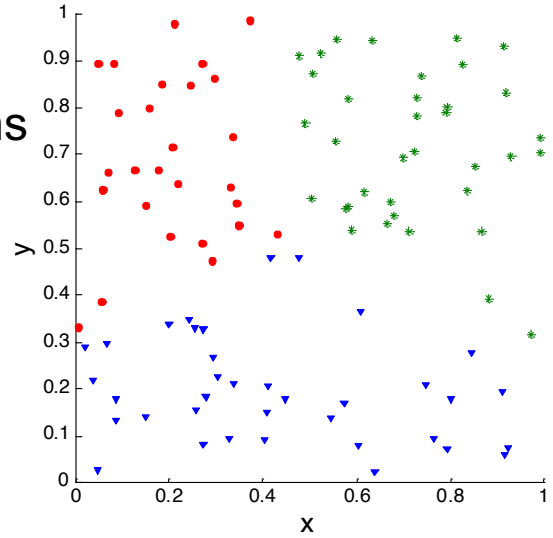
Random Points

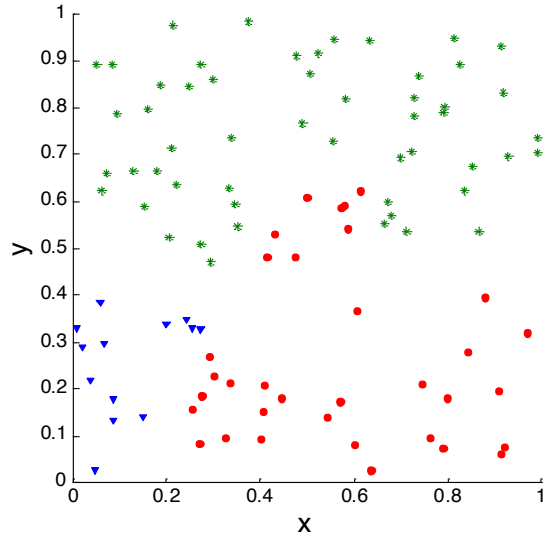




DBSCAN

K-means





Complete Link

Different Aspects of Cluster Validation

1. Determining the clustering tendency of a set of data, i.e., distinguishing whether non-random structure actually exists in the data.
2. Comparing the results of a cluster analysis to externally known results, e.g., to externally given class labels.
3. Evaluating how well the results of a cluster analysis fit the data *without* reference to external information.
    - Use only the data
4. Comparing the results of two different sets of cluster analyses to determine which is better.
5. Determining the 'correct' number of clusters.

For 2, 3, and 4, we can further distinguish whether we want to evaluate the entire clustering or just individual clusters.

Measures of Cluster Validity

- Numerical measures that are applied to judge various aspects of cluster validity, are classified into the following three types.
  - External Index: Used to measure the extent to which cluster labels match externally supplied class labels.
    - E.g., entropy, precision, recall
  - Internal Index: Used to measure the goodness of a clustering structure without reference to external information.
    - E.g., Sum of Squared Error (SSE)
  - Relative Index: Used to compare two different clusterings or clusters.
    - Often an external or internal index is used for this function, e.g., SSE or entropy
- Sometimes these are referred to as criteria instead of indices
  - However, sometimes criterion is the general strategy and index is the numerical measure that implements the criterion.

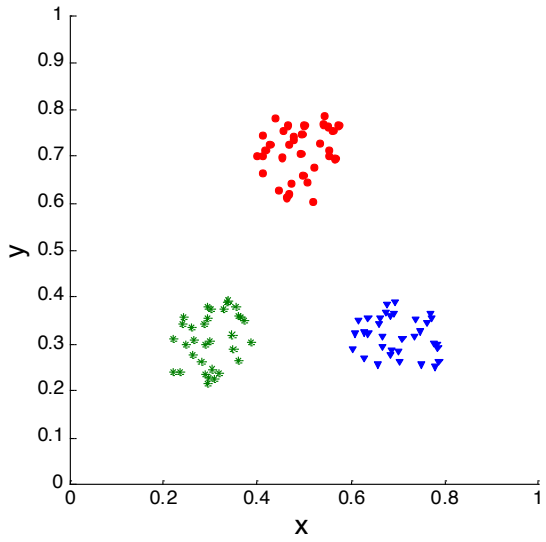
Measuring Cluster Validity Via Correlation

- Two matrices
  - Similarity or Distance Matrix
    - One row and one column for each data point
    - An entry is the similarity or distance of the associated pair of points
  - "Incidence" Matrix
    - One row and one column for each data point
    - An entry is 1 if the associated pair of points belong to the same cluster
    - An entry is 0 if the associated pair of points belongs to different clusters
- Compute the correlation between the two matrices
  - Since the matrices are symmetric, only the correlation between n(n-1) / 2 entries needs to be calculated.
- High correlation (positive for similarity, negative for distance) indicates that points that belong to the same cluster are close to each other.
- Not a good measure for some density or contiguity-based clusters.

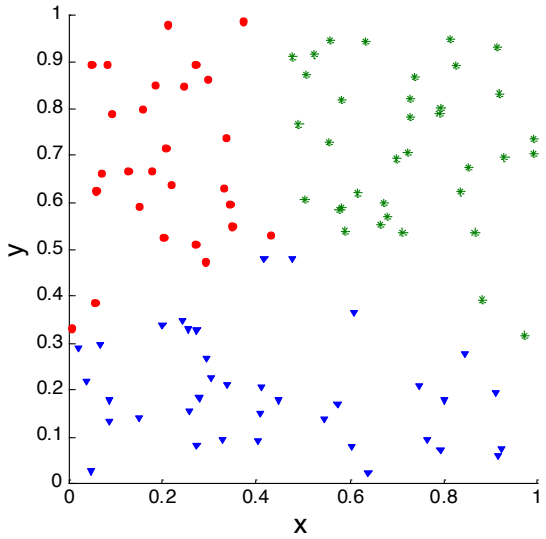
$$CorrCoeff(X,Y) = \frac{\sum_i (x_i - \mu_X)(y_i - \mu_Y)}{\sqrt{\sum_i (x_i - \mu_X)^2}\sqrt{\sum_i (y_i - \mu_Y)^2}}$$

Measuring Cluster Validity Via Correlation

- Correlation of incidence and proximity matrices for the K-means clusterings of the following two data sets.



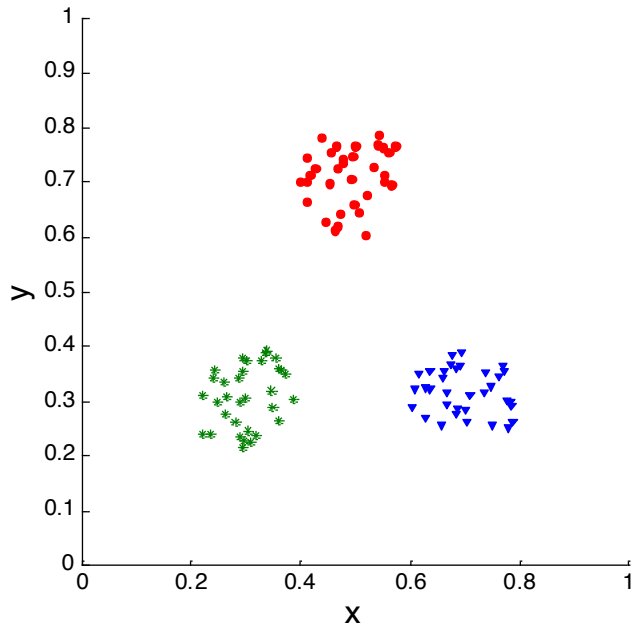
Corr = -0.9235

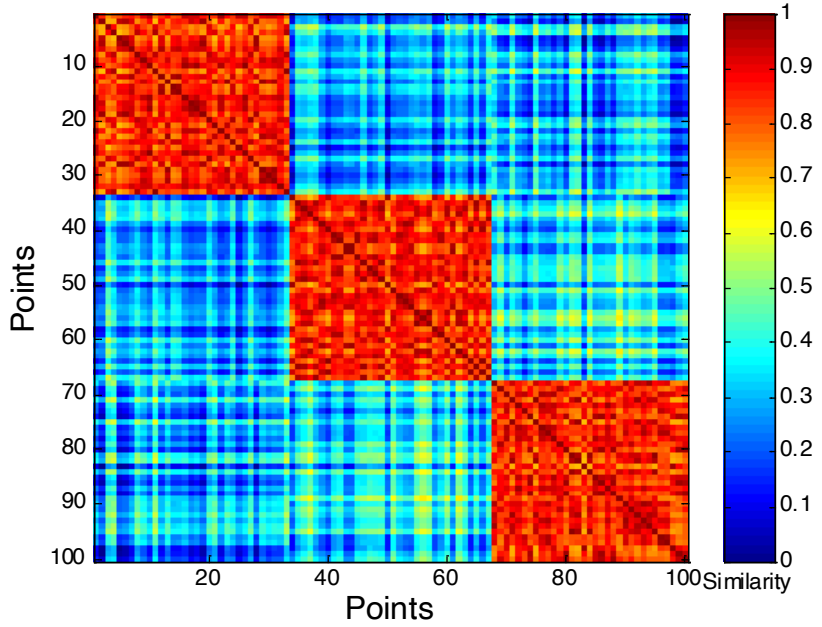


Corr = -0.5810

Using Similarity Matrix for Cluster Validation

- Order the similarity matrix with respect to cluster labels and inspect visually.

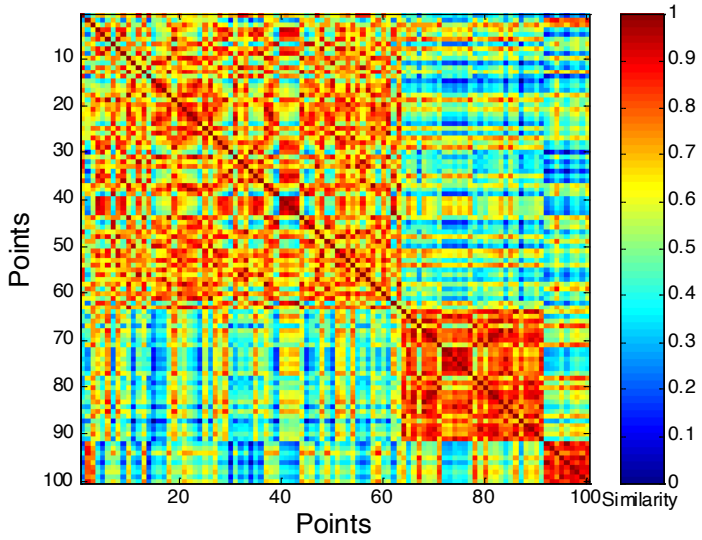


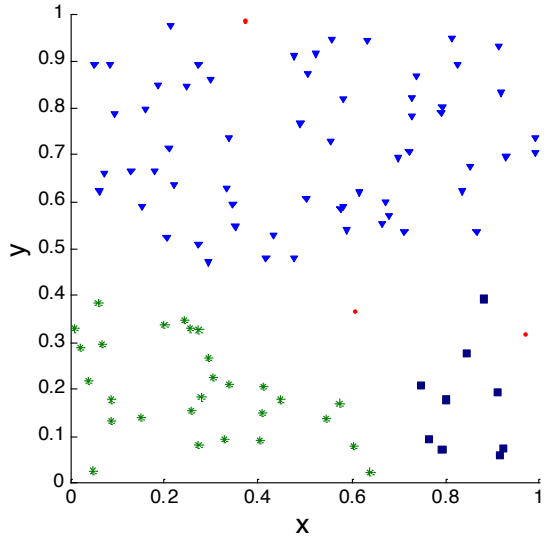


$$sim(i,j) = 1 - \frac{d_{ij} - d_{min}}{d_{max} - d_{min}}$$

Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp

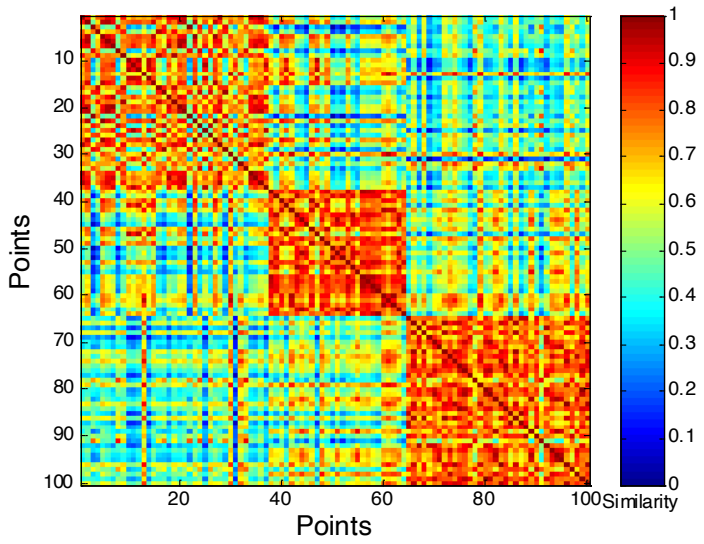


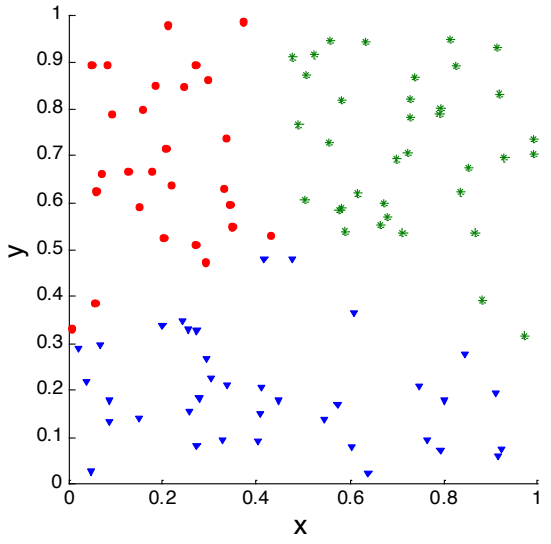


DBSCAN

Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp

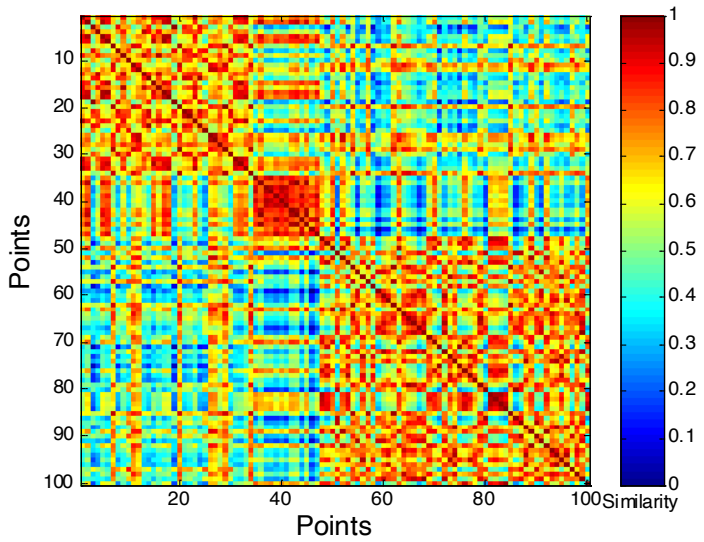


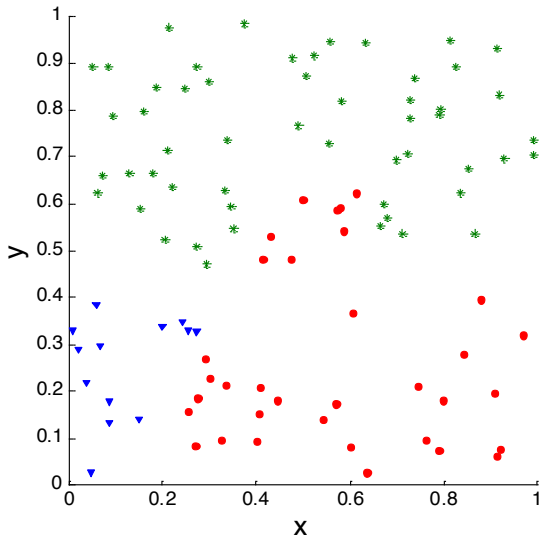


K-means

Using Similarity Matrix for Cluster Validation

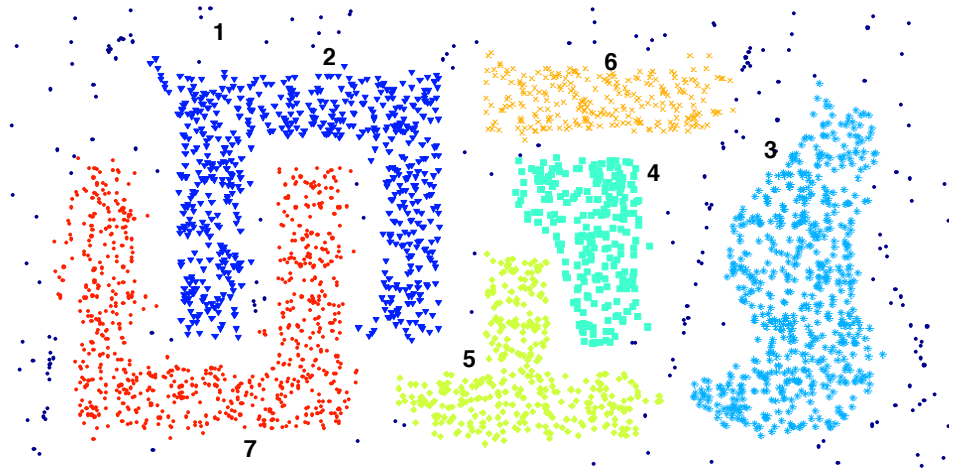
- Clusters in random data are not so crisp

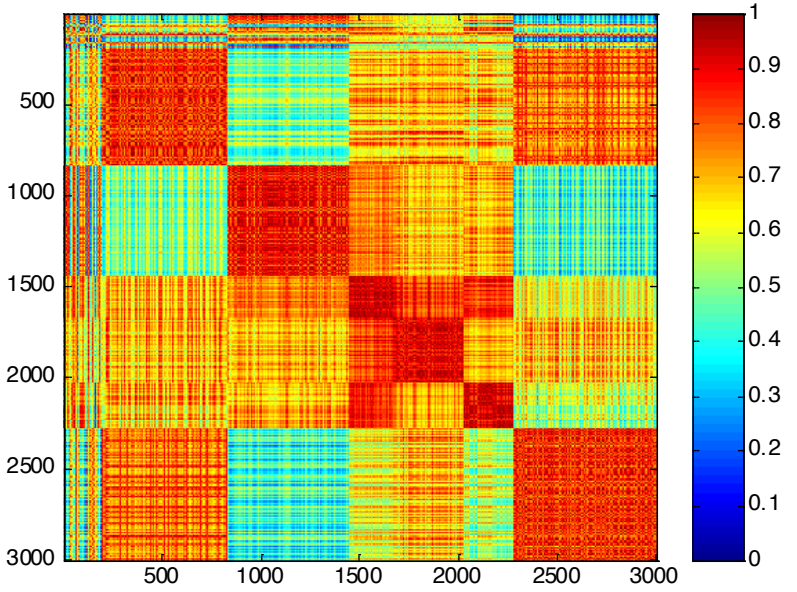




Complete Link

Using Similarity Matrix for Cluster Validation



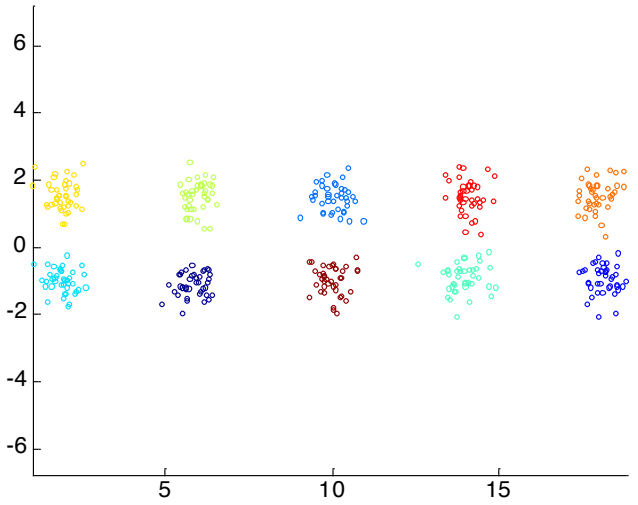


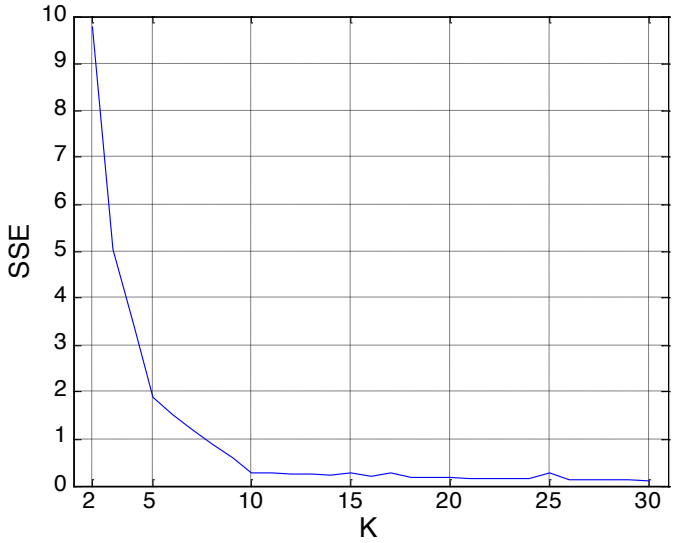
DBSCAN

- Clusters in more complicated figures are not well separated
- This technique can only be used for small datasets since it requires a quadratic computation

Internal Measures: SSE

- Internal Index: Used to measure the goodness of a clustering structure without reference to external information
  - Example: SSE
- SSE is good for comparing two clusterings or two clusters (average SSE).
- Can also be used to estimate the number of clusters





Internal Measures: Cohesion and Separation

- Cluster Cohesion: Measures how closely related are objects in a cluster
- Cluster Separation: Measure how distinct or well-separated a cluster is from other clusters
- Example: Squared Error
  - Cohesion is measured by the within cluster sum of squares (SSE)

$$WSS = \sum_{i} \sum_{x \in C_i} (x - c_i)^2$$

We want this to be small

  - Separation is measured by the between cluster sum of squares

$$BSS = \sum_{i} m_i (c - c_i)^2$$

We want this to be large

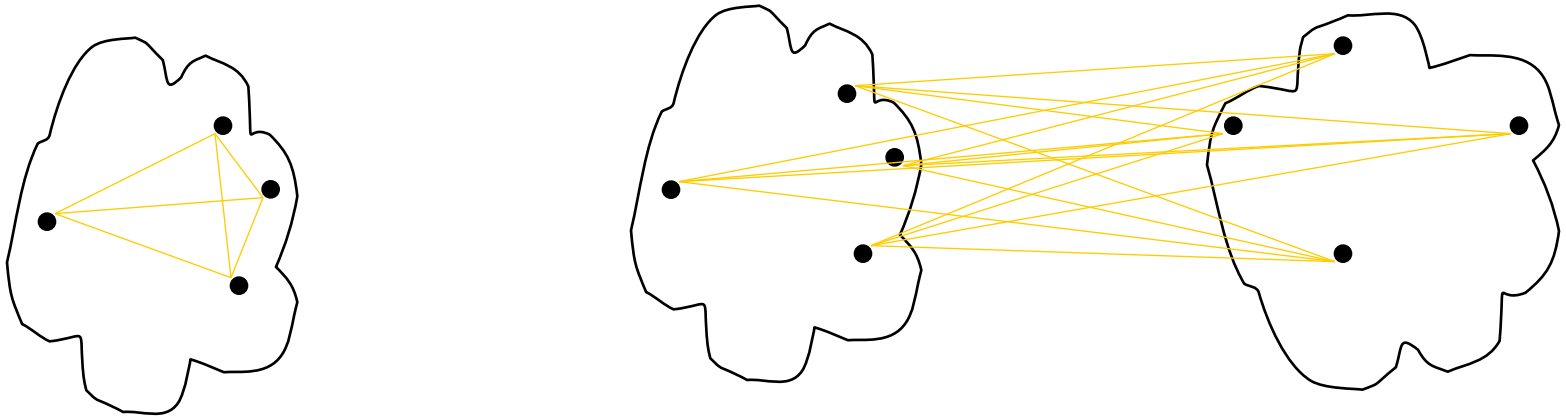
  - Where m_i is the size of cluster i , c the overall mean

$$BSS = \sum_{x \in C_i} \sum_{y \in C_j} (x - y)^2$$

  - Interesting observation: WSS+BSS = constant

Internal Measures: Cohesion and Separation

- A proximity graph-based approach can also be used for cohesion and separation.
  - Cluster cohesion is the sum of the weight of all links within a cluster.
  - Cluster separation is the sum of the weights between nodes in the cluster and nodes outside the cluster.



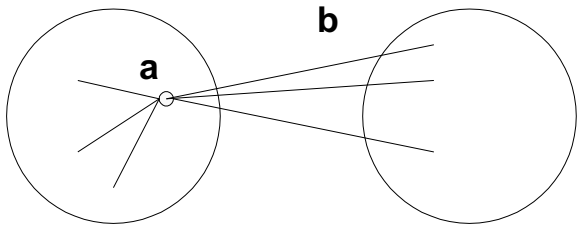
cohesion

separation

Internal Measures: Silhouette Coefficient

- Silhouette Coefficient combines ideas of both cohesion and separation, but for individual points, as well as clusters and clusterings
- For an individual point i
  - Calculate a_i = average distance of i to the points in its own cluster
  - Calculate b_i = min (over clusters) of the average distance of i to points in other clusters
  - The silhouette coefficient for a point i is then given by

$$s_i = 1 - a_i / b_i$$



  - Typically between 0 and 1, the closer to 1 the better.
  - Can be less than 0 but this is a problematic case

- Can calculate the Average Silhouette coefficient for a cluster, or for a clustering

Silhouette Coefficient Example

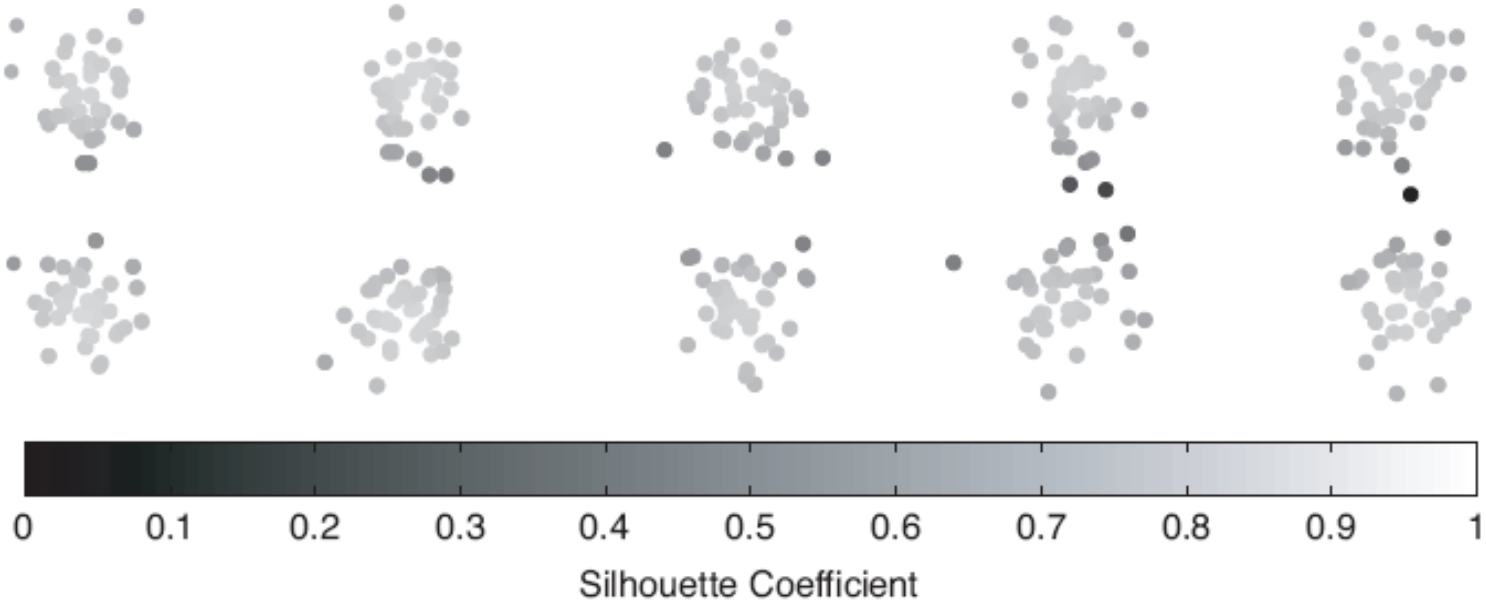


Figure 8.29. Silhouette coefficients for points in ten clusters.

Internal measures – caveats

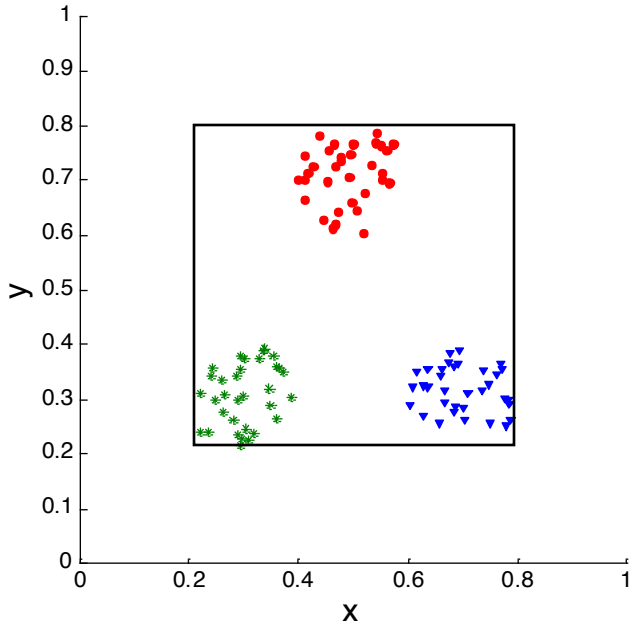
- Internal measures have the problem that the clustering algorithm did not set out to optimize this measure, so it is will not necessarily do well with respect to the measure.
  - Essentially, we check whether one criterion correlates well with another
- An internal measure can also be used as an objective function for clustering
- The algorithm that optimizes this criterion is expected to do well.

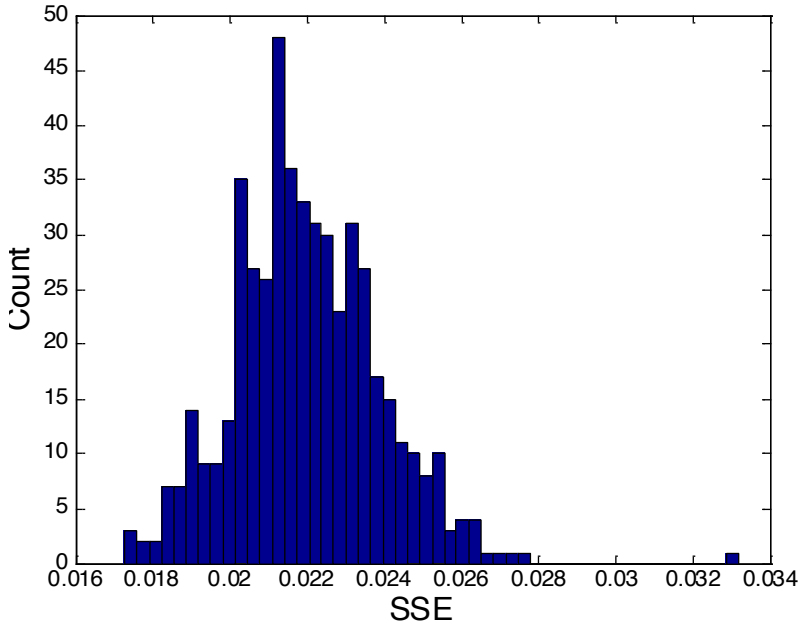
Framework for Cluster Validity

- Need a framework to interpret any measure.
  - For example, if our measure of evaluation has the value, 10, is that good, fair, or poor?
- Statistics provide a framework for cluster validity
  - The more "non-random" a clustering result is, the more likely it represents valid structure in the data
  - Can compare the values of an index that result from random data or clusterings to those of a clustering result.
    - If the value of the index is unlikely, then the cluster results are valid
- For comparing the results of two different sets of cluster analyses, a framework is less necessary.
  - However, there is the question of whether the difference between two index values is significant

Statistical Framework for SSE

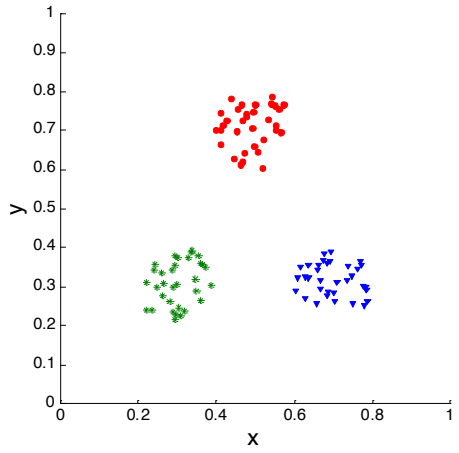
- Example
  - Compare SSE of 0.005 against three clusters in random data
  - Histogram of SSE for three clusters in 500 random data sets of 100 random points distributed in the range 0.2 – 0.8 for x and y
    - Value 0.005 is very unlikely

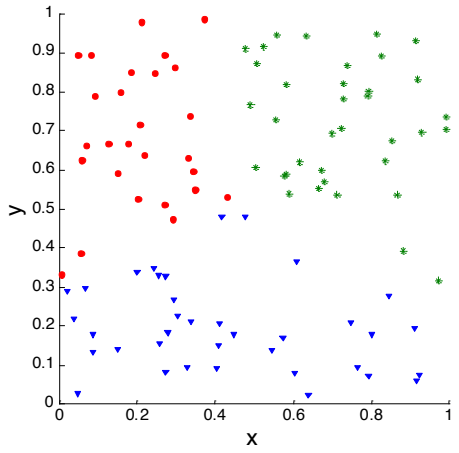


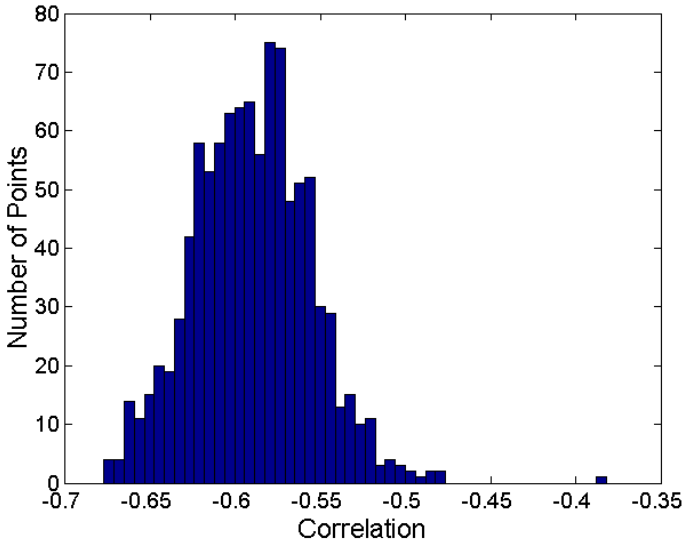


Statistical Framework for Correlation

- Correlation of incidence and proximity matrices for the K-means clusterings of the following two data sets.







Corr = -0.9235

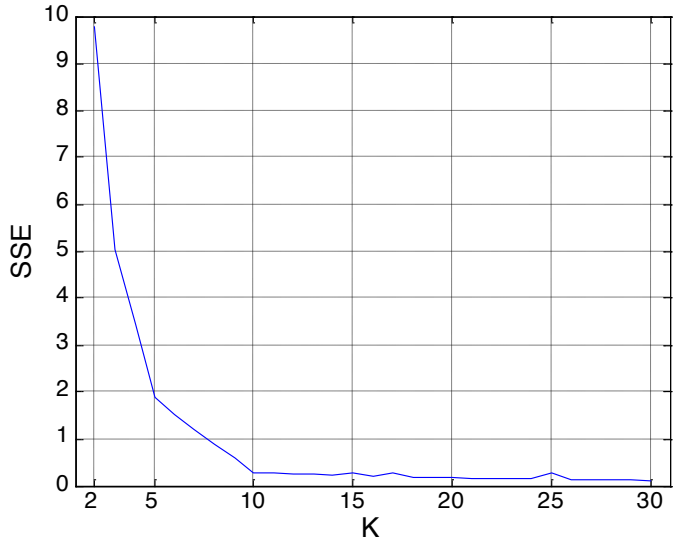
Corr = -0.5810

Empirical p-value

- If we have a measurement v (e.g., the SSE value)
- ..and we have N measurements on random datasets
- …the empirical p-value is the fraction of measurements in the random data that have value less or equal than value v (or greater or equal if we want to maximize)
  - i.e., the value in the random dataset is at least as good as that in the real data
- We usually require that p-value ≤ 0.05
- Hard question: what is the right notion of a random dataset?

Estimating the “right” number of clusters

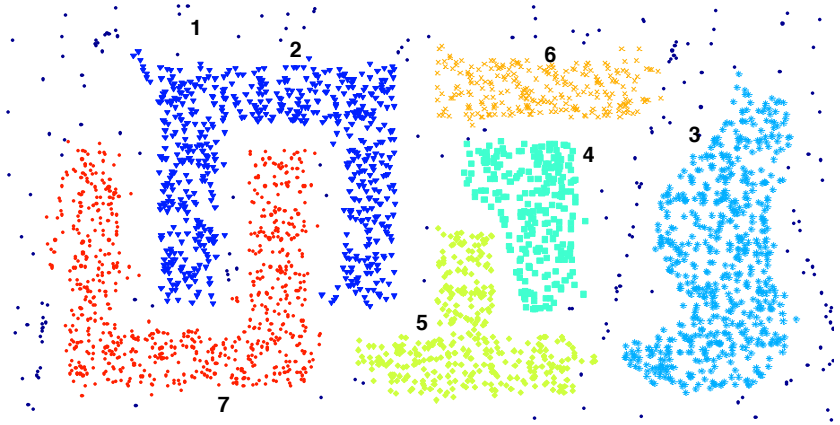
- Typical approach: find a “knee” in an internal measure curve.

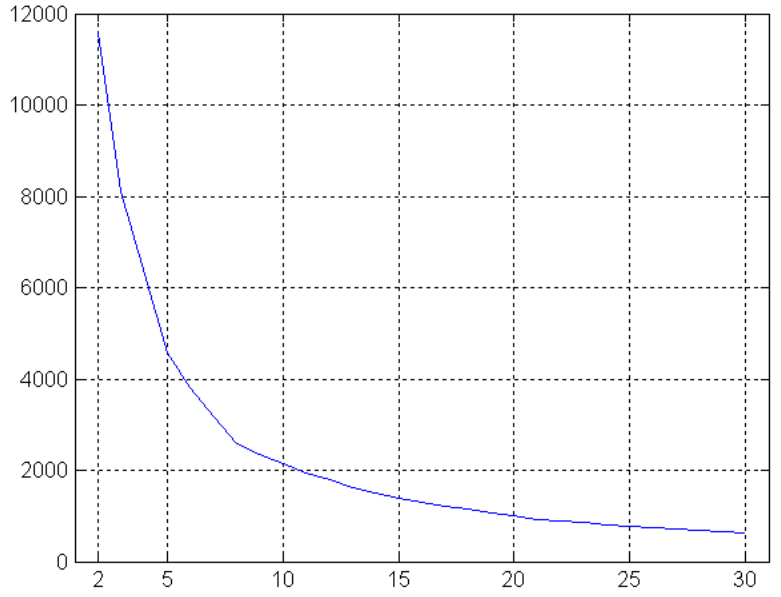


- Question: why not the k that minimizes the SSE?
  - Forward reference: minimize a measure, but with a “simple” clustering
- Desirable property: the clustering algorithm does not require the number of clusters to be specified (e.g., DBSCAN)

Estimating the “right” number of clusters

- SSE curve for a more complicated data set





SSE of clusters found using K-means

External Measures for Clustering Validity

- Assume that the data is labeled with some class labels
  - E.g., documents are classified into topics, people classified according to their income, politicians classified according to the political party.
  - This is called the "ground truth"
- In this case we want the clusters to be homogeneous with respect to classes
  - Each cluster should contain elements of mostly one class
  - Each class should ideally be assigned to a single cluster
- This does not always make sense
  - Clustering is not the same as classification
  - …but this is what people use most of the time

Confusion matrix

- Rows: clusters
- Columns: classes
- Entries: counts/probability of cluster-class pair
- n = number of points
- m_i = points in cluster i
- c_j = points in class j
- n_{ij}= points in cluster i coming from class j
- $p_{ij} = n_{ij}/m_i$= probability of element from cluster i to be assigned in class j

Confusion matrix of clusters/classes (counts)

	Class 1	Class 2	Class 3	
Cluster 1	n_{11}	n_{12}	n_{13}	m_1
Cluster 2	n_{21}	n_{22}	n_{23}	m_2
Cluster 3	n_{31}	n_{32}	n_{33}	m_3
	c_1	c_2	c_3	n

Joint distribution of clusters/classes

	Class 1	Class 2	Class 3	
Cluster 1	p_{11}	p_{12}	p_{13}	m_1
Cluster 2	p_{21}	p_{22}	p_{23}	m_2
Cluster 3	p_{31}	p_{32}	p_{33}	m_3
	c_1	c_2	c_3	n

Measures

- Entropy:
  - Of a cluster i: $e_i = -\sum_{j=1}^{L} p_{ij} \log p_{ij}$
    - Highest when uniform, zero when single class
  - Of a clustering: $e = \sum_{i=1}^{K} \frac{m_i}{n} e_i$
- Purity:
  - Of a cluster i: $p_i = \max_j p_{ij}$
  - Of a clustering: $p(C) = \sum_{i=1}^{K} \frac{m_i}{n} p_i$

	Class 1	Class 2	Class 3	
Cluster 1	p_{11}	p_{12}	p_{13}	m_1
Cluster 2	p_{21}	p_{22}	p_{23}	m_2
Cluster 3	p_{31}	p_{32}	p_{33}	m_3
	c_1	c_2	c_3	n

Measures

- Precision:
  - Of cluster i with respect to class j: $Prec(i,j) = \frac{n_{ij}}{m_i} = p_{ij}$
- Recall:
  - Of cluster i with respect to class j: $Rec(i,j) = \frac{n_{ij}}{c_j}$
- F-measure:
  - Harmonic Mean of Precision and Recall:

$$F(i,j) = \frac{2 * Prec(i,j) * Rec(i,j)}{Prec(i,j) + Rec(i,j)}$$

	Class 1	Class 2	Class 3	
Cluster 1	n_{11}	n_{12}	n_{13}	m_1
Cluster 2	n_{21}	n_{22}	n_{23}	m_2
Cluster 3	n_{31}	n_{32}	n_{33}	m_3
	c_1	c_2	c_3	n

	Class 1	Class 2	Class 3	
Cluster 1	p_{11}	p_{12}	p_{13}	m_1
Cluster 2	p_{21}	p_{22}	p_{23}	m_2
Cluster 3	p_{31}	p_{32}	p_{33}	m_3
	c_1	c_2	c_3	n

Measures

Precision/Recall for clusters and clusterings

- Assign to cluster i the class k_i such that $k_i = \arg\max_j n_{ij}$
- Precision:
  - Of cluster i: $Prec(i) = \frac{n_{ik_i}}{m_i}$
  - Of the clustering: $Prec(C) = \sum_i \frac{m_i}{n} Prec(i)$
- Recall:
  - Of cluster i: $Rec(i) = \frac{n_{ik_i}}{c_{k_i}}$
  - Of the clustering: $Rec(C) = \sum_i \frac{m_i}{n} Rec(i)$
- F-measure:
  - Harmonic Mean of Precision and Recall

	Class 1	Class 2	Class 3	
Cluster 1	n_{11}	n_{12}	n_{13}	m_1
Cluster 2	n_{21}	n_{22}	n_{23}	m_2
Cluster 3	n_{31}	n_{32}	n_{33}	m_3
	c_1	c_2	c_3	n

Good and bad clustering

	Class 1	Class 2	Class 3	
Cluster 1	2	3	85	90
Cluster 2	90	12	8	110
Cluster 3	8	85	7	100
	100	100	100	300

Purity: (0.94, 0.81, 0.85)
– overall 0.86
Precision: (0.94, 0.81, 0.85)
– overall 0.86
Recall: (0.85, 0.9, 0.85)
- overall 0.87

	Class 1	Class 2	Class 3	
Cluster 1	20	35	35	90
Cluster 2	30	42	38	110
Cluster 3	38	35	27	100
	100	100	100	300

Purity: (0.38, 0.38, 0.38)
– overall 0.38
Precision: (0.38, 0.38, 0.38)
– overall 0.38
Recall: (0.35, 0.42, 0.38)
– overall 0.39

Another clustering

	Class 1	Class 2	Class 3	
Cluster 1	0	0	35	35
Cluster 2	50	77	38	165
Cluster 3	38	35	27	100
	100	100	100	300

Cluster 1:

Purity: 1

Precision: 1

Recall: 0.35

External Measures of Cluster Validity: Entropy and Purity

Table 5.9. K-means Clustering Results for LA Document Data Set

Cluster	Entertainment	Financial	Foreign	Metro	National	Sports	Entropy	Purity
1	3	5	40	506	96	27	1.2270	0.7474
2	4	7	280	29	39	2	1.1472	0.7756
3	1	1	1	7	4	671	0.1813	0.9796
4	10	162	3	119	73	2	1.7487	0.4390
5	331	22	5	70	13	23	1.3976	0.7134
6	5	358	12	212	48	13	1.5523	0.5525
Total	354	555	341	943	273	738	1.1450	0.7203

entropy For each cluster, the class distribution of the data is calculated first, i.e., for cluster j we compute p_{ij}, the 'probability' that a member of cluster j belongs to class i as follows: $p_{ij} = m_{ij}/m_j$, where m_j is the number of values in cluster j and m_{ij} is the number of values of class i in cluster j. Then using this class distribution, the entropy of each cluster j is calculated using the standard formula $e_j = \sum_{i=1}^{L} p_{ij} \log_2 p_{ij}$, where the L is the number of classes. The total entropy for a set of clusters is calculated as the sum of the entropies of each cluster weighted by the size of each cluster, i.e., $e = \sum_{i=1}^{K} \frac{m_i}{m} e_j$, where m_j is the size of cluster j, K is the number of clusters, and m is the total number of data points.

purity Using the terminology derived for entropy, the purity of cluster j, is given by $purity_j = \max p_{ij}$ and the overall purity of a clustering by $purity = \sum_{i=1}^{K} \frac{m_i}{m} purity_j$.

Final Comment on Cluster Validity

"The validation of clustering structures is the most difficult and frustrating part of cluster analysis.

Without a strong effort in this direction, cluster analysis will remain a black art accessible only to those true believers who have experience and great courage."

Algorithms for Clustering Data, Jain and Dubes