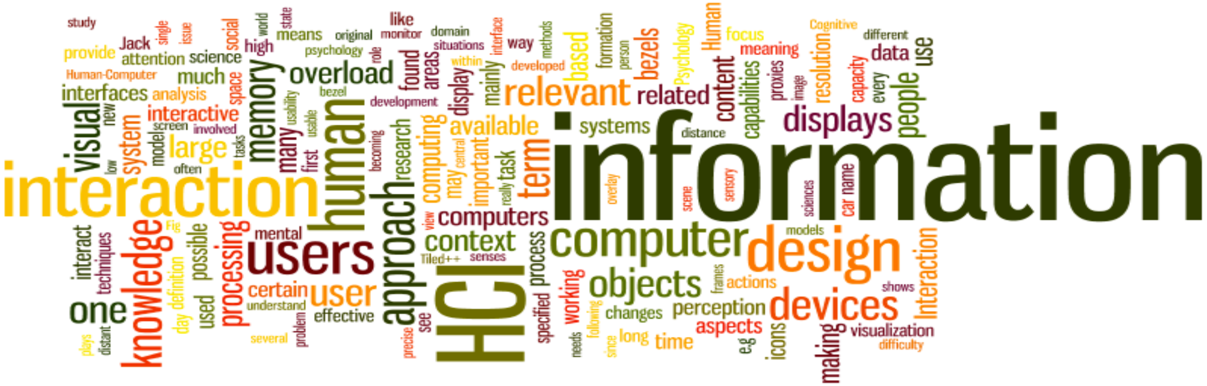
# 机器学习

## ——第10章 聚类——



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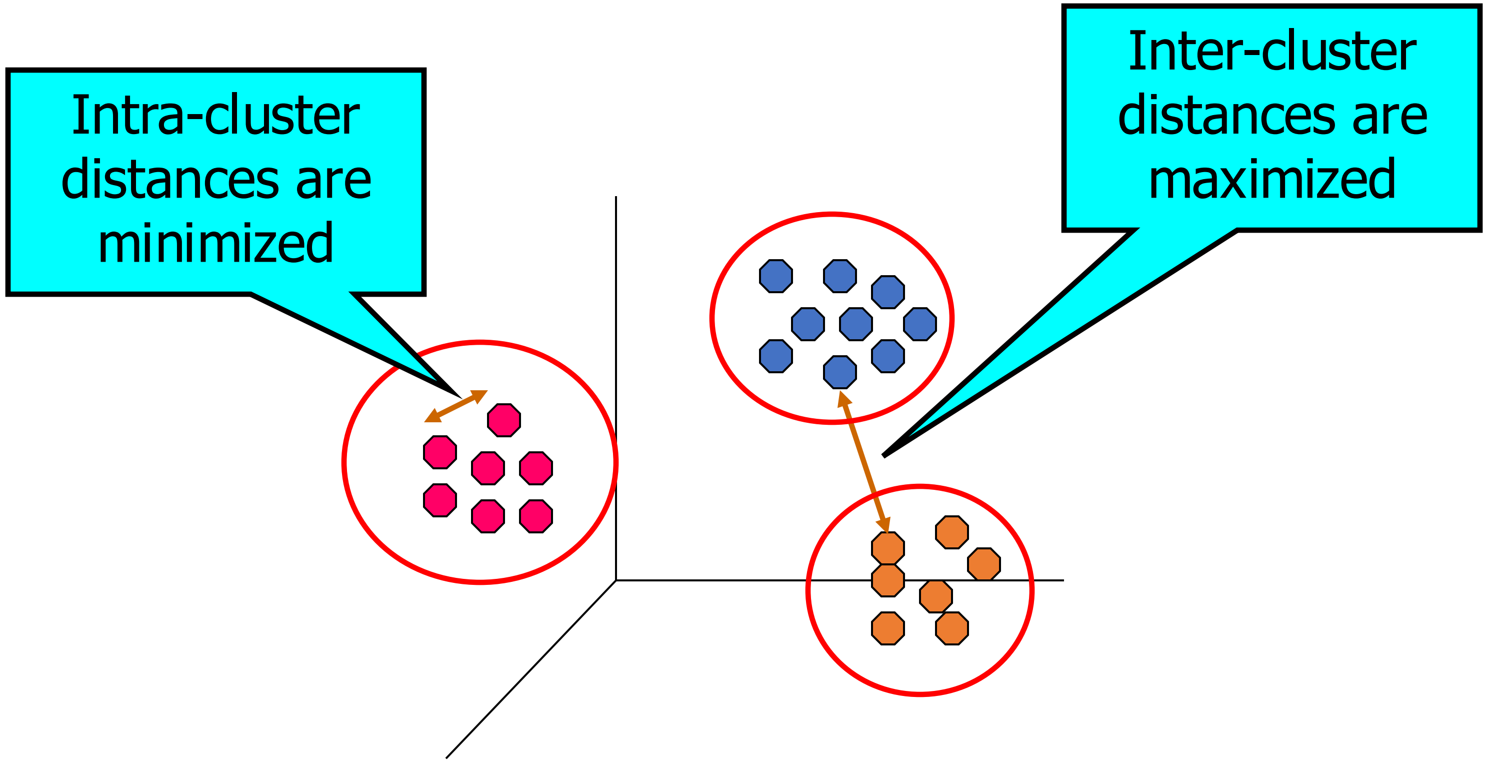
https://eezkni.github.io/

# Machine Learning Problems

| | *Supervised Learning* | *Unsupervised Learning* |
|---|---|---|
| *Discrete* | classification or categorization | clustering |
| *Continuous* | regression | dimensionality reduction |

# What is Cluster Analysis?

- Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups



Intra-cluster distances are minimized

Inter-cluster distances are maximized

# Clustering Applications

Recommender systems and advertising

- Cluster users for item/ad recommendation
- Cluster items for related item suggestion

Text mining

- Cluster documents for related search
- Cluster words for query suggestion

Image search

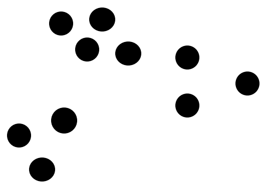
- Cluster images for similar image search and duplication detection

Speech recognition or separation

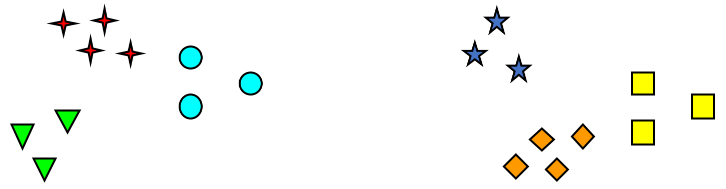
- Cluster phonetical features

…

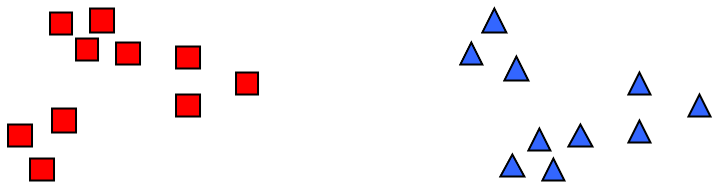
# Notion of a Cluster can be Ambiguous



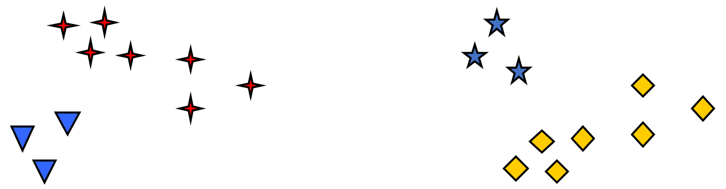
How many clusters?



Six Clusters



Two Clusters



Four Clusters

# Quality: What Is Good Clustering?

- A good clustering method will produce high quality clusters with
  - high intra-class similarity
  - low inter-class similarity
- The quality of a clustering result depends on both the similarity measure used by the method and its implementation
- The quality of a clustering method is also measured by its ability to discover some or all of the hidden patterns

# Major Clustering Approaches

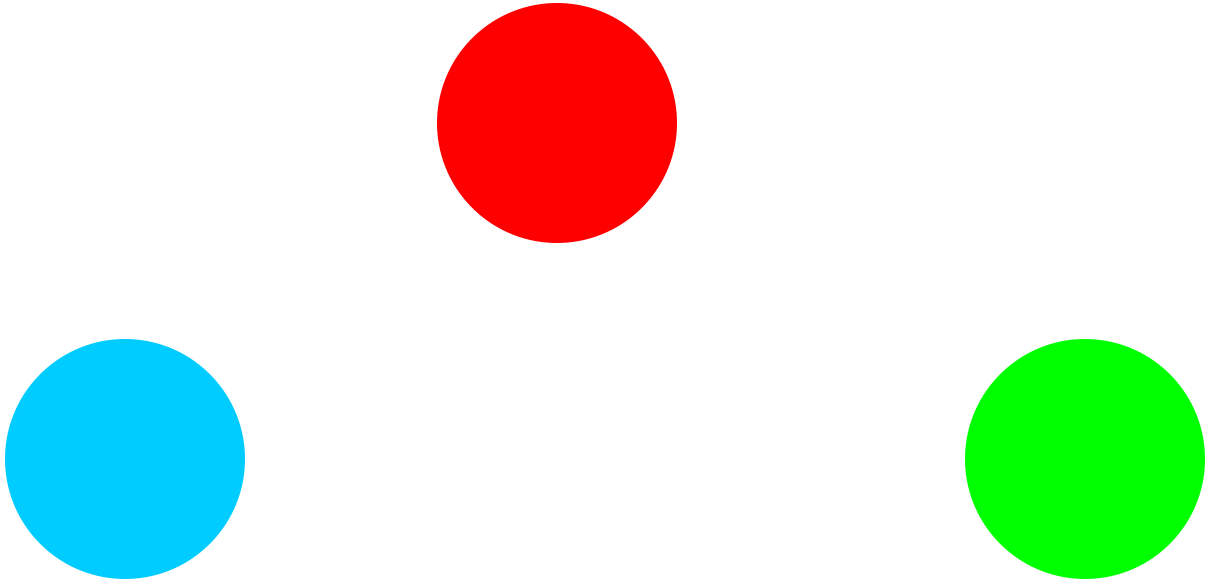
- Partitioning approach:
  - – Construct various partitions and then evaluate them by some criterion, e.g., minimizing the sum of square errors
  - – Typical methods: k-means, ISODATA ,k-medoids, Kernel K-means , CLARANS
- Hierarchical approach:
  - – Create a hierarchical decomposition of the set of data (or objects) using some criterion
  - – Typical methods: Agnes, Diana, BIRCH, ROCK, CAMELEON
- Density-based approach:
  - – Based on connectivity and density functions
  - – Typical methods: DBSCAN, OPTICS, DenClue

# Major Clustering Approaches

- Grid-based approach:
  - based on a multiple-level granularity structure
  - Typical methods: STING, WaveCluster, CLIQUE
- Model-based:
  - A model is hypothesized for each of the clusters and tries to find the best fit of that model to each other
  - Typical methods: EM, SOM, COBWEB
- Frequent pattern-based:
  - Based on the analysis of frequent patterns
  - Typical methods: pCluster
- …

# Types of Clusters: Well-Separated

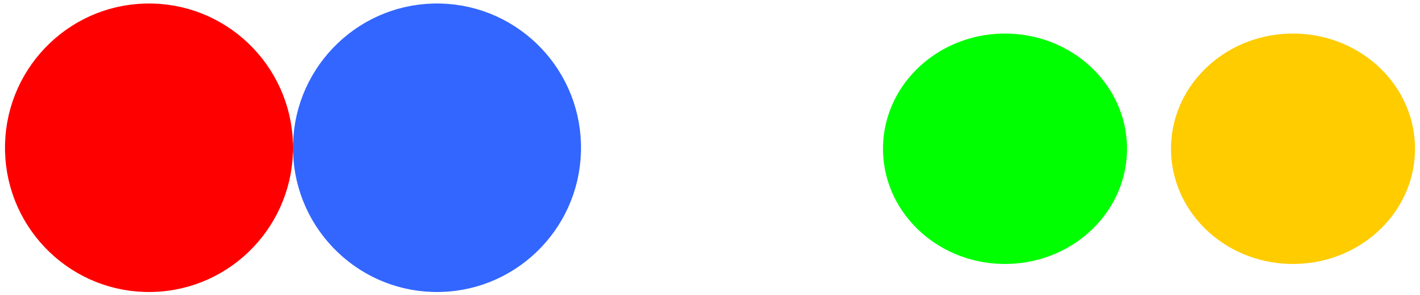
- Well-Separated Clusters:
  - A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.



3 well-separated clusters

# Types of Clusters: Center-Based

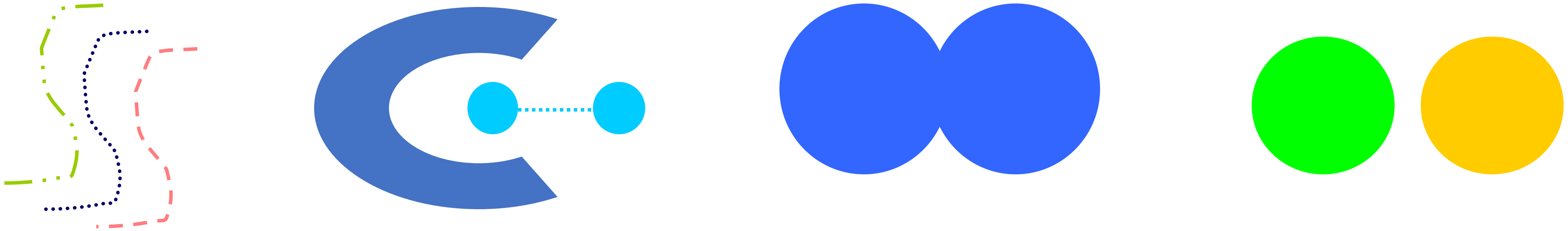
- Center-based
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the "center" of a cluster, than to the center of any other cluster
  - The center of a cluster is often a centroid, the average of all the points in the cluster, or a medoid, the most "representative"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



4 center-based clusters

# Types of Clusters: Contiguity-Based

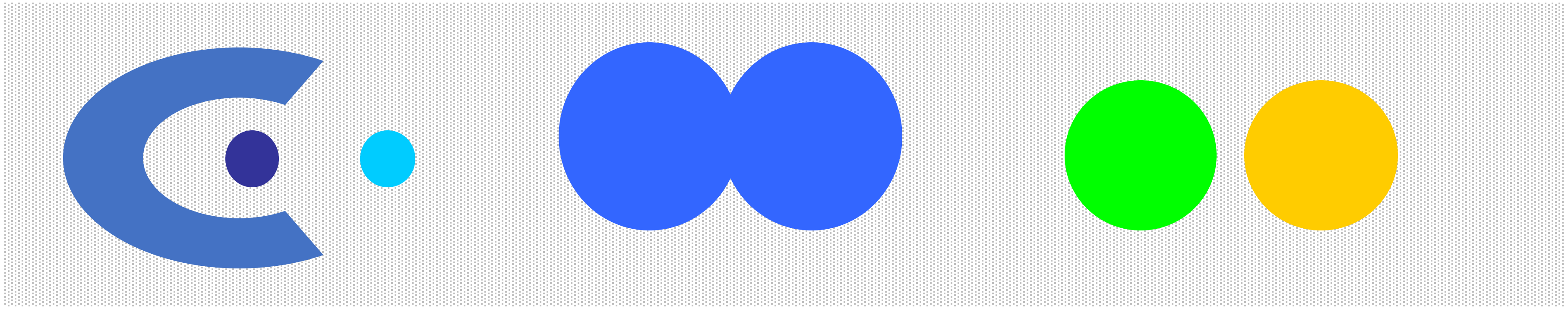
- Contiguous Cluster (Nearest neighbor or Transitive)
  - – A cluster can be defined as a connected component: a group of objects that are connected to each other but not to objects outside the group.
  - – A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.



8 contiguous clusters

# Types of Clusters: Density-Based

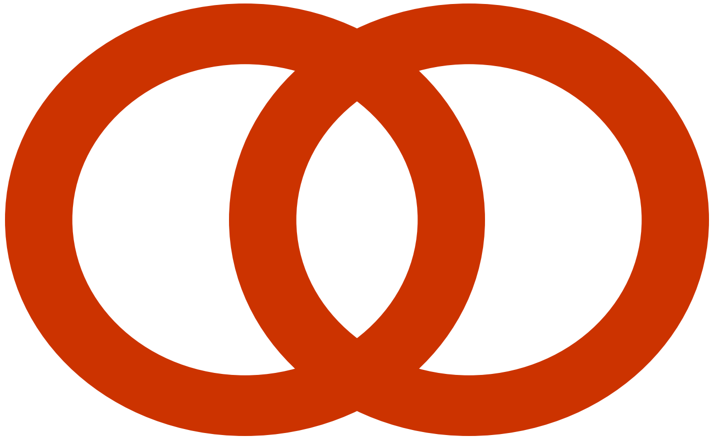
- Density-based
  - A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
  - Used when the clusters are irregular or intertwined, and when noise and outliers are present.



6 density-based clusters

# Types of Clusters: Conceptual Clusters

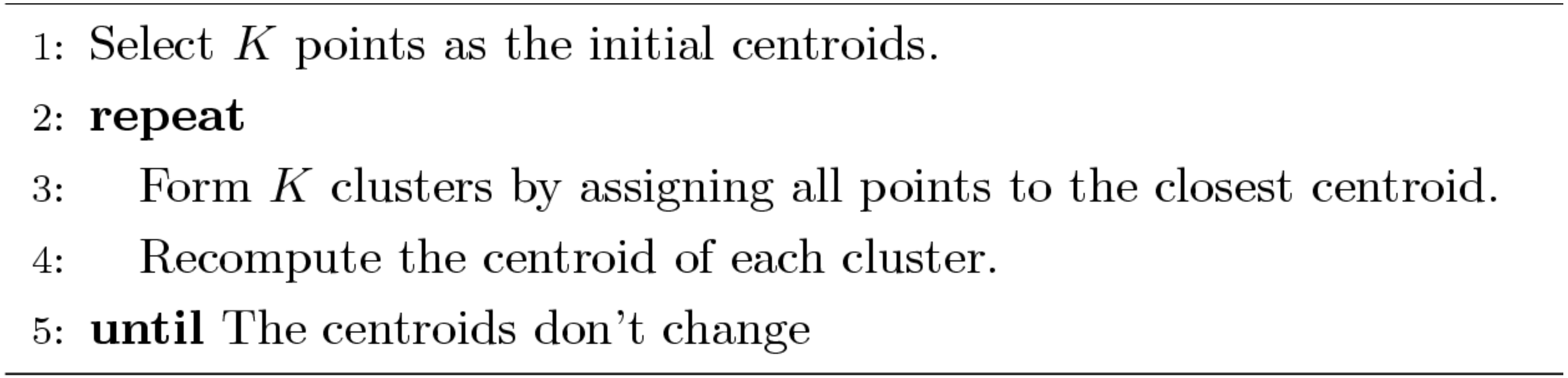
- Shared Property or Conceptual Clusters
  - – Finds clusters that share some common property or represent a particular concept.



2 Overlapping Circles

# 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 basic algorithm is very simple



```
Select $K$ points as the initial centroids.
**repeat**
    Form $K$ clusters by assigning all points to the closest centroid.
    Recompute the centroid of each cluster.
**until** The centroids don't change
```

# K-means Clustering – Details

- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.
- The centroid is (typically) the mean of the points in the cluster.
- ‘Closeness’ is measured by Euclidean distance, cosine similarity, etc.
- 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 = number of attributes

# Euclidean Distance

Euclidean Distance

$$d(x,y)=\sqrt{\sum_{k=1}^{n}(x_k-y_k)^2}$$

# Cosine Similarity

- If $d_1$ and $d_2$ are two document vectors, then

$$\cos(x, y) = (x \bullet y) / ||x|| \; ||y|| \, ,$$

- Example:

$x =$ 3 2 0 5 0 0 0 2 0 0

$y =$ 1 0 0 0 0 0 0 1 0 2

$x \bullet y =$ 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5

$||x|| = (3*3+2*2+0*0+5*5+0*0+0*0+0*0+2*2+0*0+0*0)^{0.5} = (42)^{0.5} = 6.481$

$||y|| = (1*1+0*0+0*0+0*0+0*0+0*0+0*0+1*1+0*0+2*2)^{0.5} = (6)^{0.5} = 2.245$

$\cos(d_1, d_2) = 0.3150$

# Problems with Selecting Initial Points

- If there are K ‘real’ clusters then the chance of selecting one centroid from each cluster is small.
  - Chance is relatively small when K is large
  - If clusters are the same size, n, then

$$P = \frac{\text{number of ways to select one centroid from each cluster}}{\text{number of ways to select } K \text{ centroids}} = \frac{K!n^K}{(Kn)^K} = \frac{K!}{K^K}$$

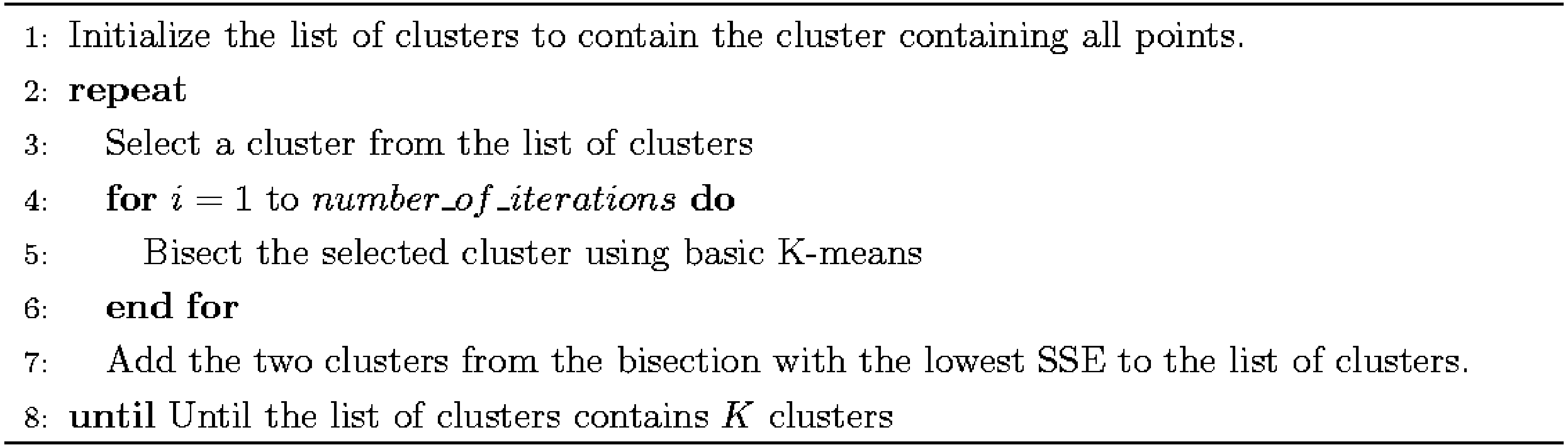
  - For example, if K = 10, then probability = 10!/1010 = 0.00036
  - Sometimes the initial centroids will readjust themselves in ‘right’ way, and sometimes they don’t
  - Consider an example of five pairs of clusters

# Solutions to Initial Centroids Problem

- Multiple runs
  - Helps, but probability is not on your side
- Sample and use hierarchical clustering to determine initial centroids
- Select more than k initial centroids and then select among these initial centroids
  - Select most widely separated
- K-means and its variants
- Bisecting K-means
  - Not as susceptible to initialization issues
- Postprocessing

# Bisecting K-means

- Bisecting K-means algorithm
  - Variant of K-means that can produce a partitional or a hierarchical clustering



```
Initialize the list of clusters to contain the cluster containing all points.
repeat
    Select a cluster from the list of clusters
    for $i = 1$ to $number\_of\_iterations$ do
        Bisect the selected cluster using basic K-means
    end for
    Add the two clusters from the bisection with the lowest SSE to the list of clusters.
until Until the list of clusters contains $K$ clusters
```

Sum of Squared Error (SSE)

$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(m_i, x)$$

# Evaluating K-means Clusters

- Most common measure is Sum of Squared Error (SSE)
  - For each point, the error is the distance to the nearest cluster
  - To get SSE, we square these errors and sum them.

$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(m_i, x)$$

  - x is a data point in cluster Ci and mi is the representative point for cluster Ci
    - can show that mi corresponds to the center (mean) of the cluster
  - Given two clusters, we can choose the one with the smallest error
  - One easy way to reduce SSE is to increase K, the number of clusters
    - A good clustering with smaller K can have a lower SSE than a poor clustering with higher K

# Handling Empty Clusters

- Basic K-means algorithm can yield empty clusters

- Several strategies
  - Choose the point that contributes most to SSE
  - Choose a point from the cluster with the highest SSE
  - If there are several empty clusters, the above can be repeated several times.

# Updating Centers Incrementally

- In the basic K-means algorithm, centroids are updated after all points are assigned to a centroid

- An alternative is to update the centroids after each assignment (incremental approach)
  - Each assignment updates zero or two centroids
  - More expensive
  - Introduces an order dependency
  - Never get an empty cluster
  - Can use “weights” to change the impact

# Pre-processing and Post-processing

- Pre-processing
  - Normalize the data
  - Eliminate outliers
- Post-processing
  - Eliminate small clusters that may represent outliers
  - Split ‘loose’ clusters, i.e., clusters with relatively high SSE
  - Merge clusters that are ‘close’ and that have relatively low SSE
  - Can use these steps during the clustering process.

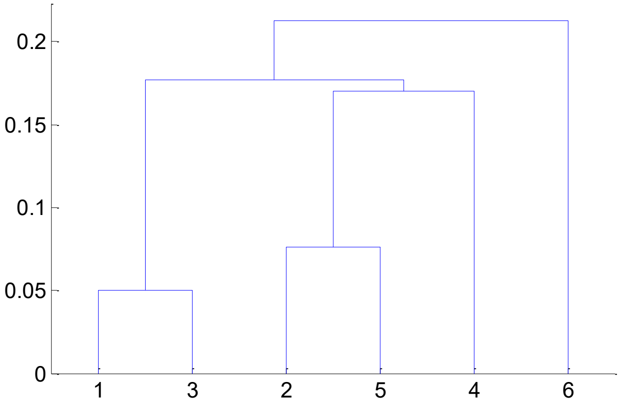
# Limitations of K-means

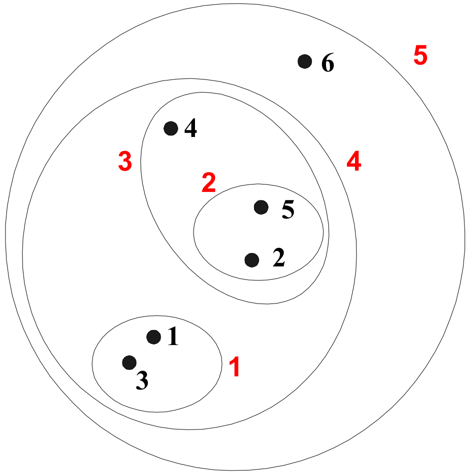
- K-means has problems when clusters are of differing
    - Sizes
    - Densities
    - Non-globular shapes

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

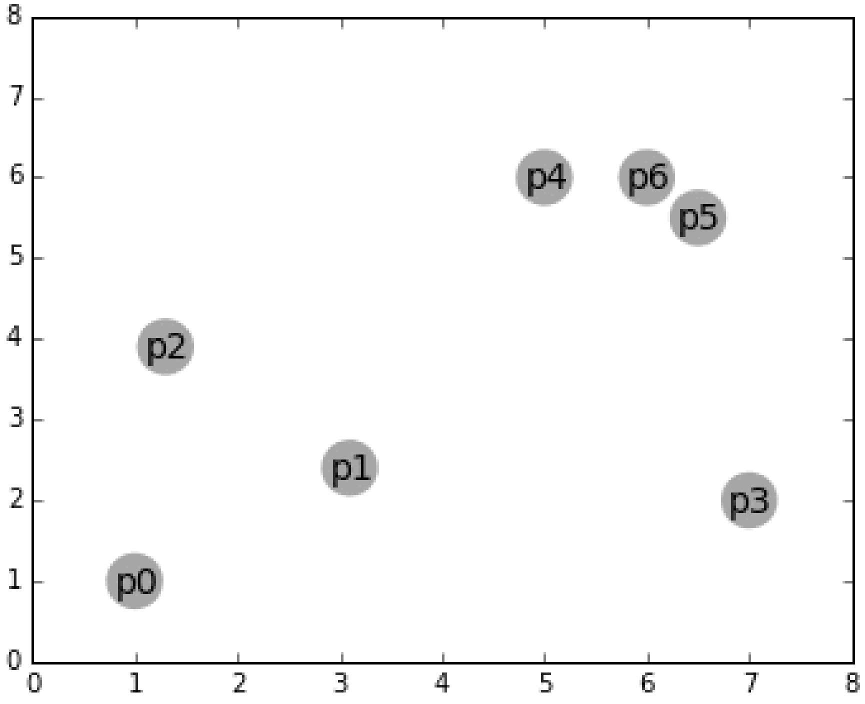
# Hierarchical Clustering

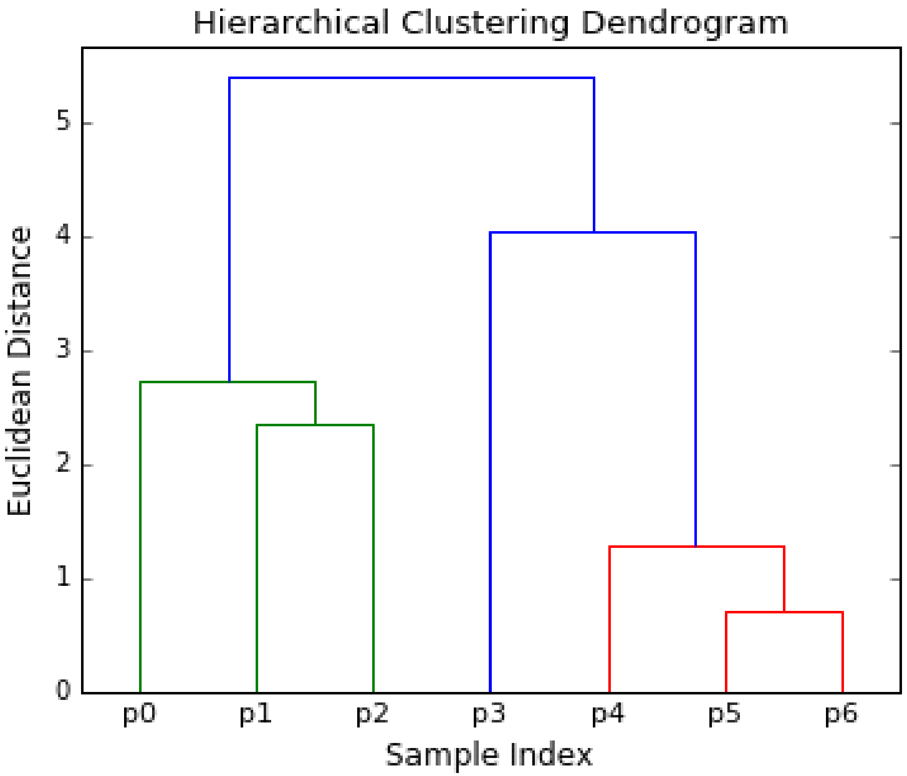
- Produces a set of nested clusters organized as a hierarchical tree
- Can be visualized as a dendrogram(树图)
    - A tree like diagram that records the sequences of merges or splits





# Hierarchical Clustering





# 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, …)

# Hierarchical Clustering

- Two main types of hierarchical clustering
  - Agglomerative (凝聚):
    - 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(分裂):
    - 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

# Agglomerative Clustering Algorithm

- More popular hierarchical clustering technique

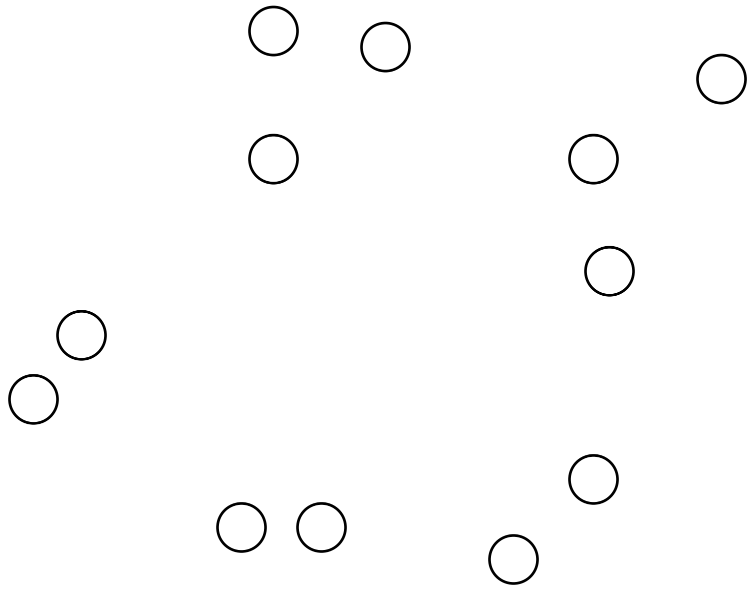
- Basic algorithm is straightforward

```
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 clusters of individual points and a proximity matrix



|  | p1 | p2 | p3 | p4 | p5 | . . . |
|---|---|---|---|---|---|---|
| p1 |  |  |  |  |  |  |
| p2 |  |  |  |  |  |  |
| p3 |  |  |  |  |  |  |
| p4 |  |  |  |  |  |  |
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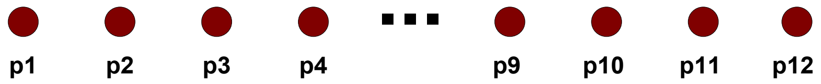
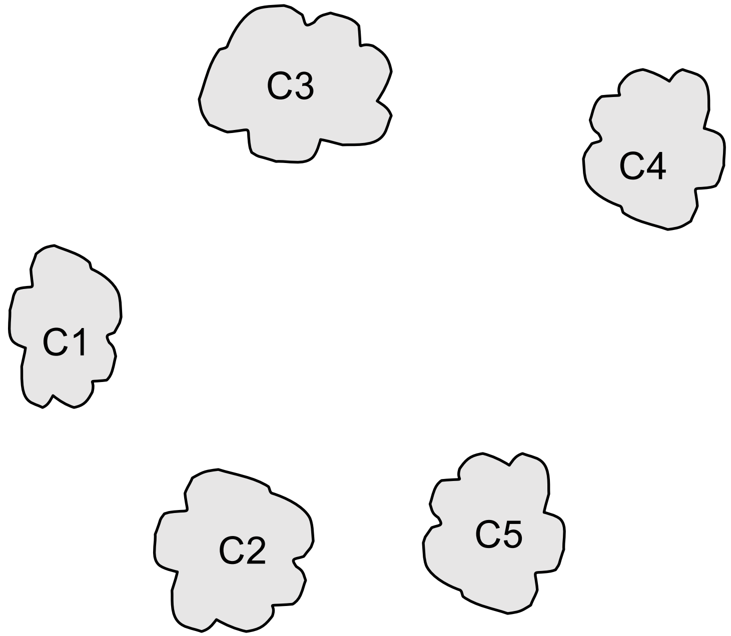
Proximity Matrix



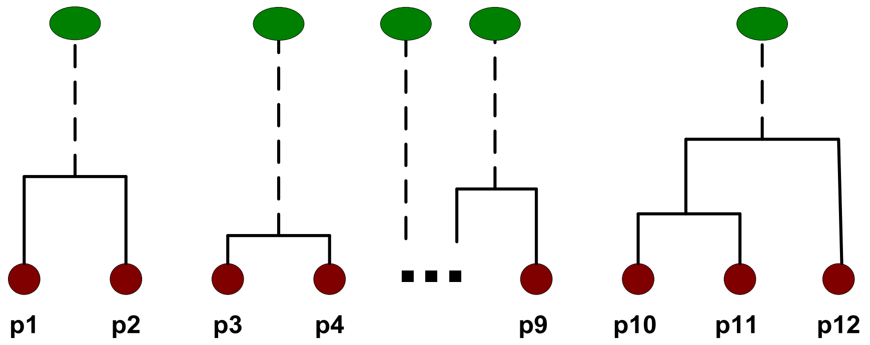
# Intermediate Situation

- After some merging steps, we have some clusters



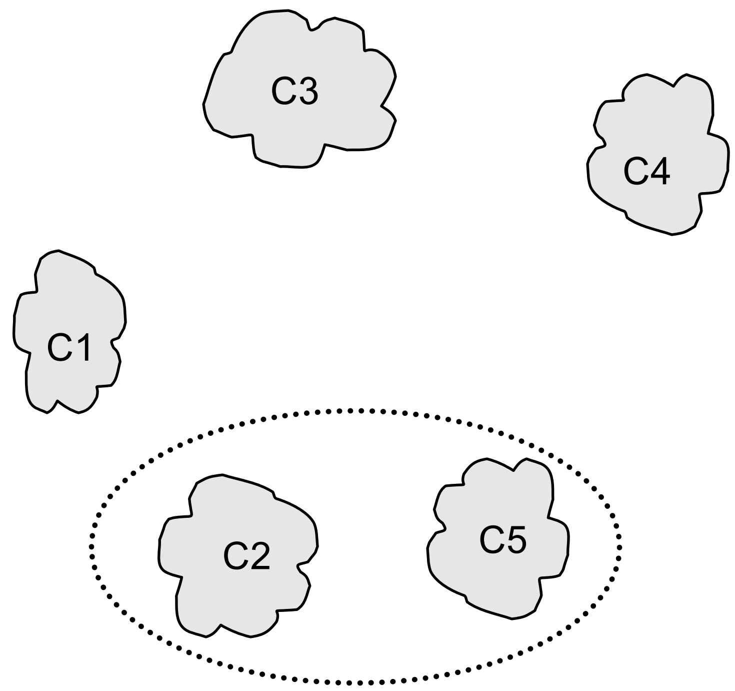
|  | C1 | C2 | C3 | C4 | C5 |
|---|---|---|---|---|---|
| C1 |  |  |  |  |  |
| C2 |  |  |  |  |  |
| C3 |  |  |  |  |  |
| C4 |  |  |  |  |  |
| C5 |  |  |  |  |  |

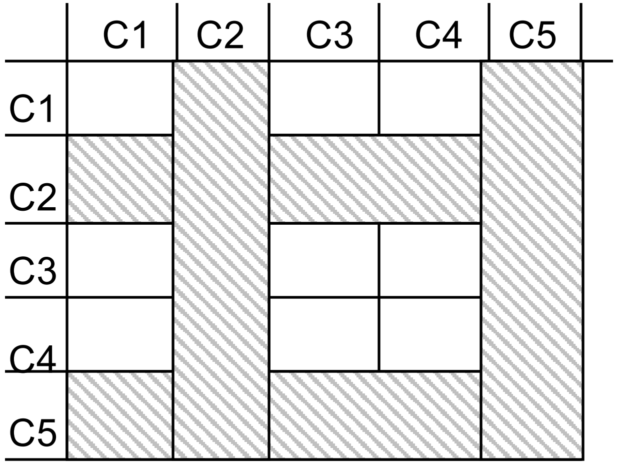
Proximity Matrix



# Intermediate Situation

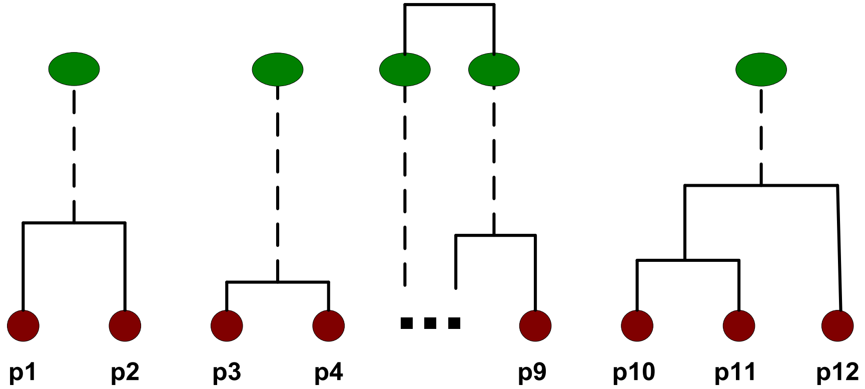
- We want to merge the two closest clusters (C2 and C5) and update the proximity matrix.





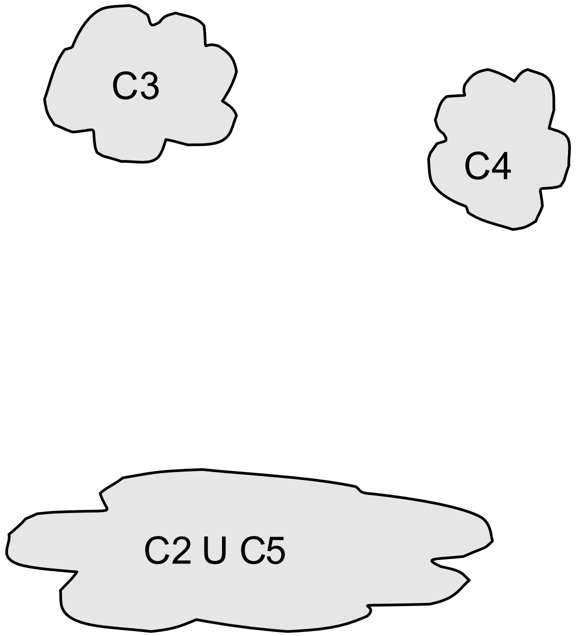
| | C1 | C2 | C3 | C4 | C5 |
|---|---|---|---|---|---|
| C1 | | ▨ | | | ▨ |
| C2 | ▨ | ▨ | ▨ | ▨ | ▨ |
| C3 | | ▨ | | | ▨ |
| C4 | | ▨ | | | ▨ |
| C5 | ▨ | ▨ | ▨ | ▨ | ▨ |

Proximity Matrix



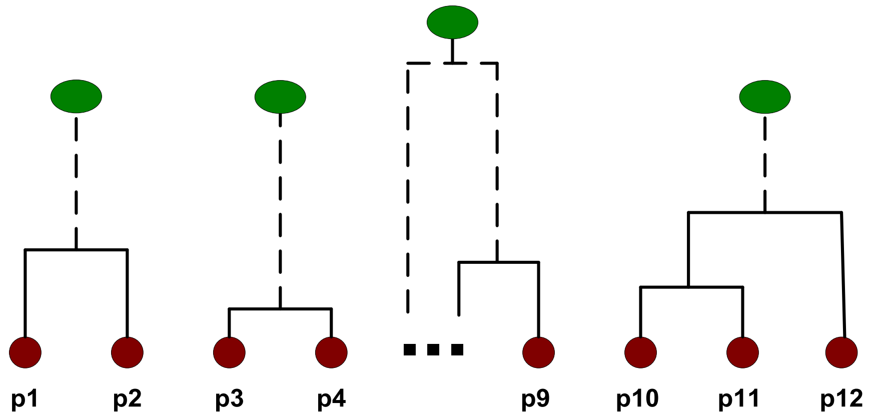
# After Merging

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

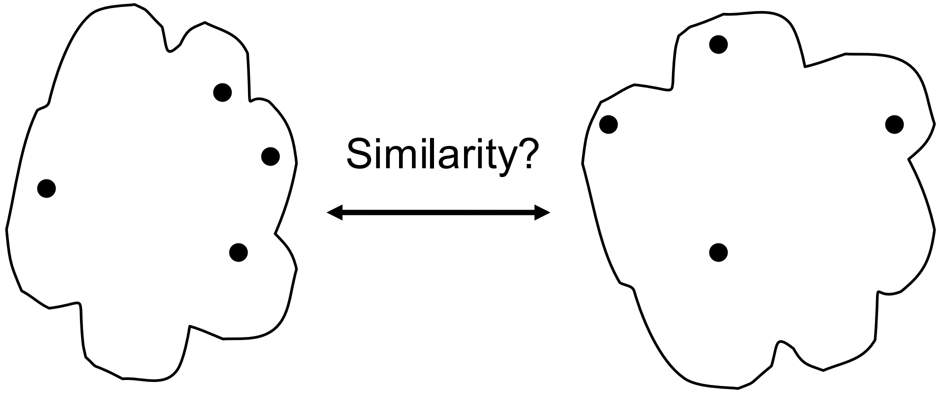


| | C1 | C2 U C5 | C3 | C4 |
|---|---|---|---|---|
| C1 | | ? | | |
| C2 U C5 | ? | ? | ? | ? |
| C3 | | ? | | |
| C4 | | ? | | |

Proximity Matrix



# How to Define Inter-Cluster Similarity



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

|  | p1 | p2 | p3 | p4 | p5 | . . . |
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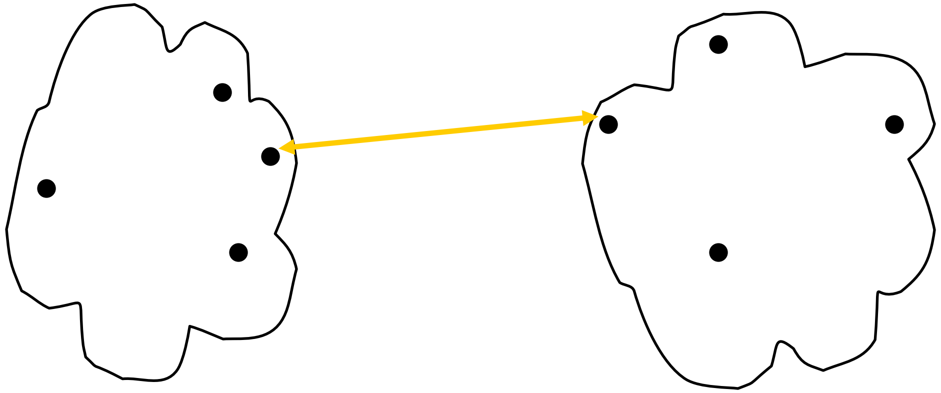
Proximity Matrix

# How to Define Inter-Cluster Similarity



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Proximity Matrix

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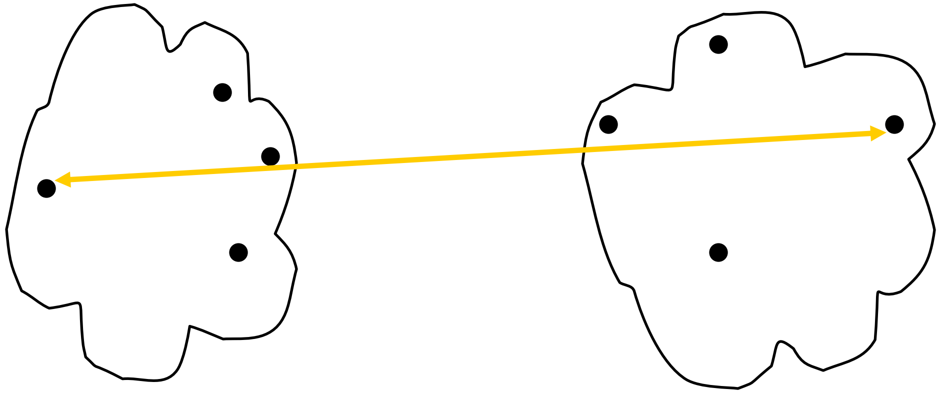
# How to Define Inter-Cluster Similarity



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| p1 | | | | | | |
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| p3 | | | | | | |
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| p5 | | | | | | |
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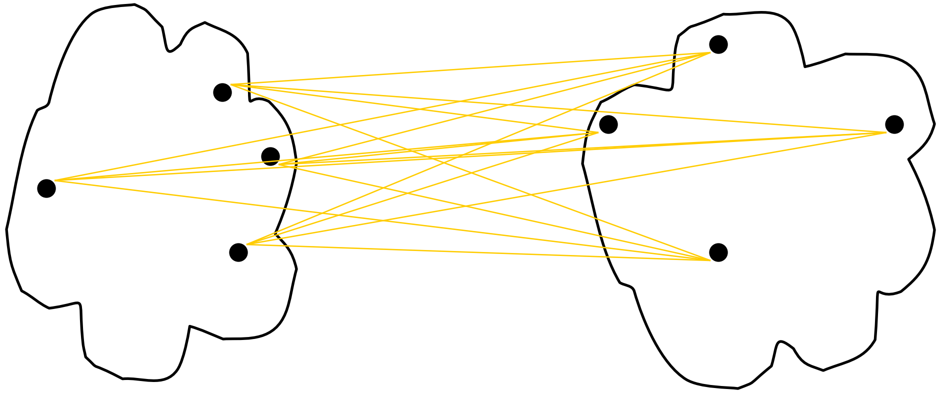
Proximity Matrix

# How to Define Inter-Cluster Similarity



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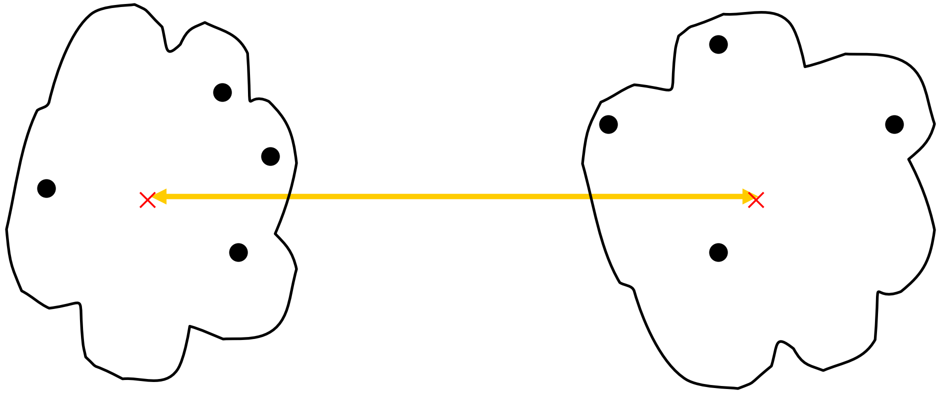
Proximity Matrix

# How to Define Inter-Cluster Similarity



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|---|---|---|---|---|---|---|
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Proximity Matrix

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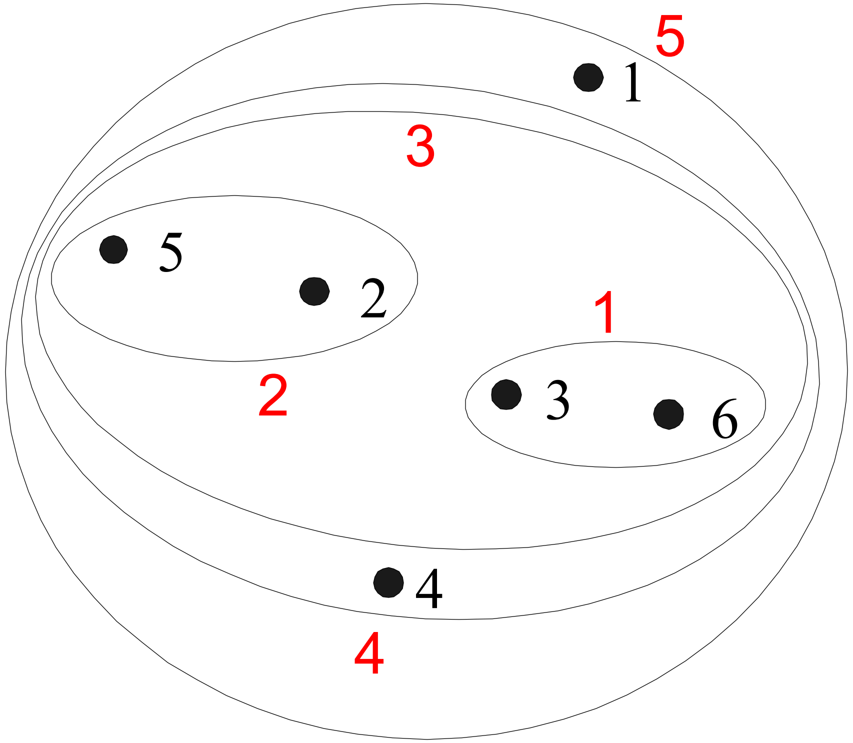
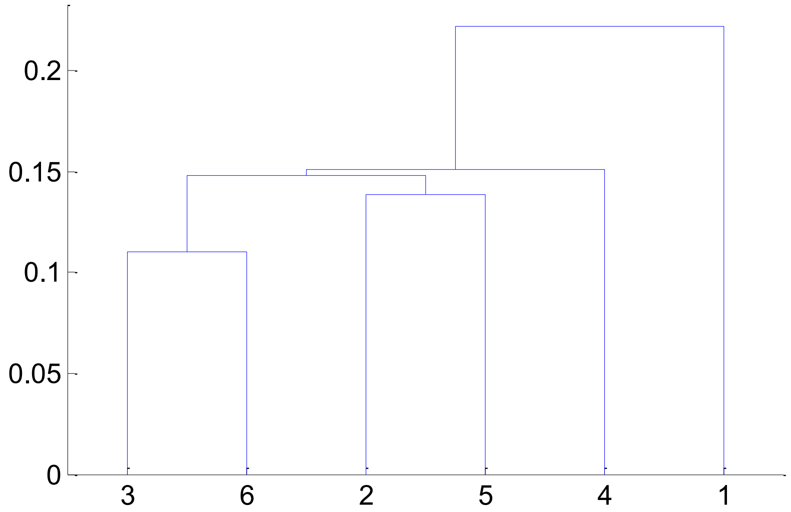
# Hierarchical Clustering: MIN

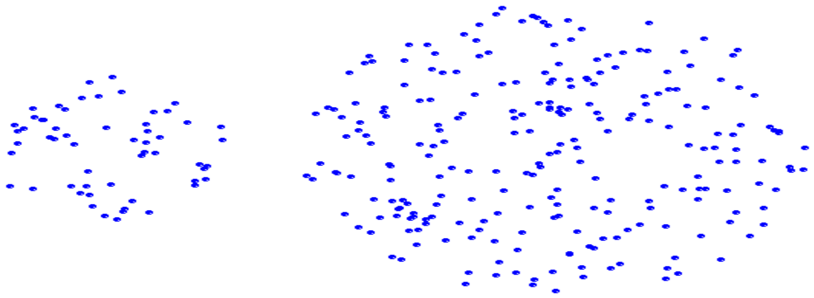


Nested Clusters

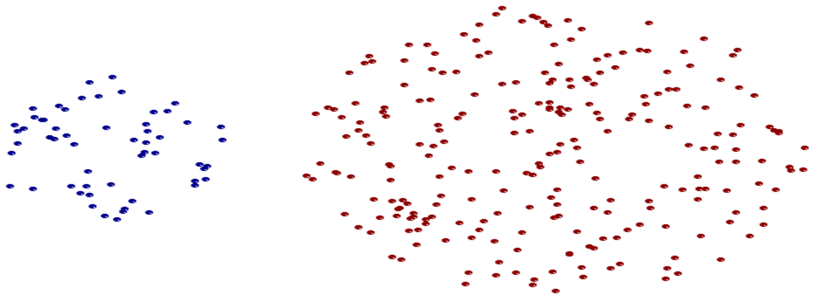


Dendrogram

# Strength of MIN



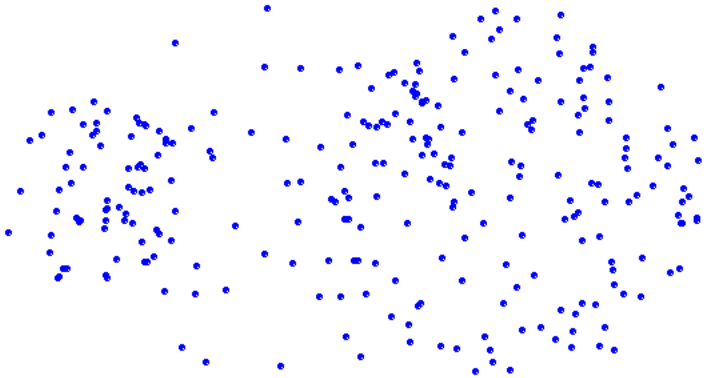
Original Points



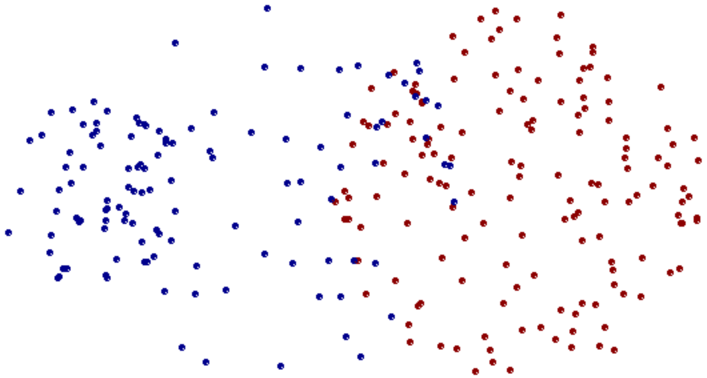
Two Clusters

- Can handle non-elliptical shapes

# Limitations of MIN



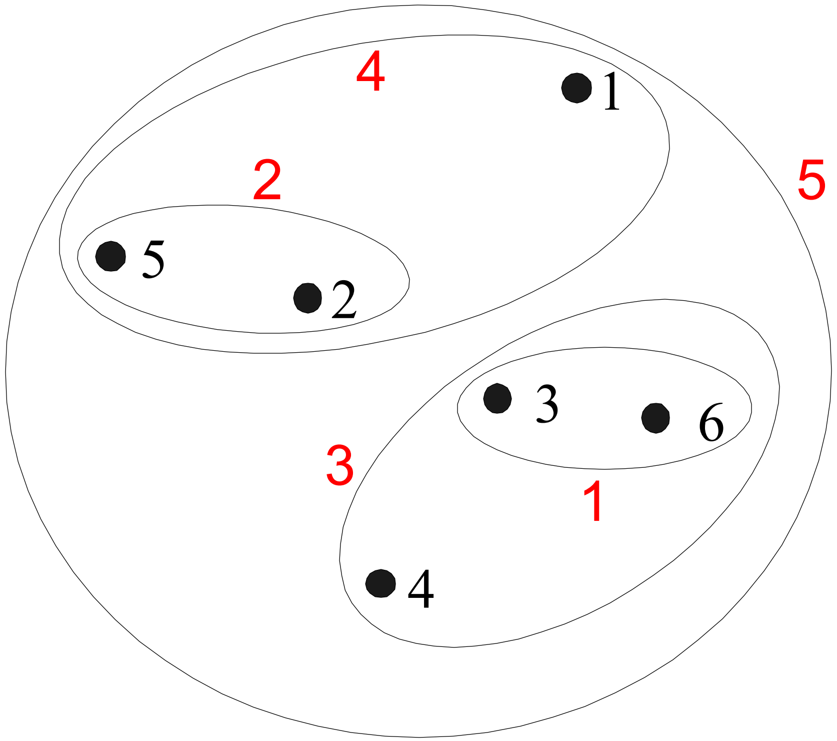
Original Points



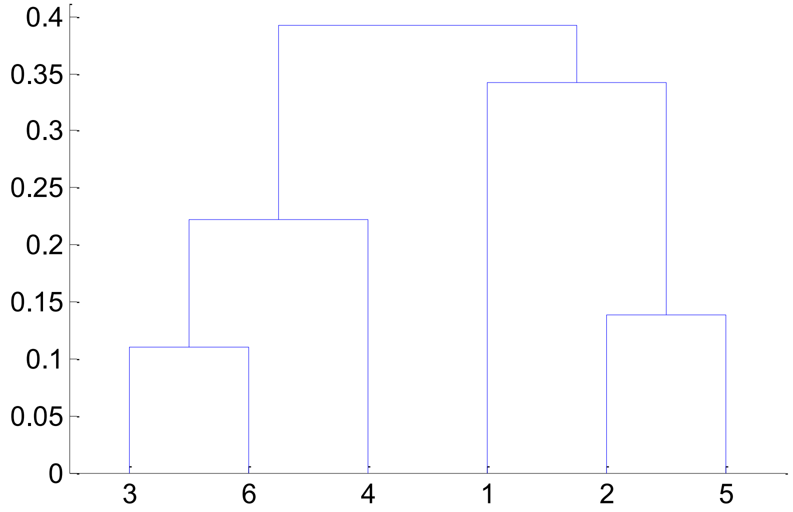
Two Clusters

- Sensitive to noise and outliers

# Hierarchical Clustering: MAX

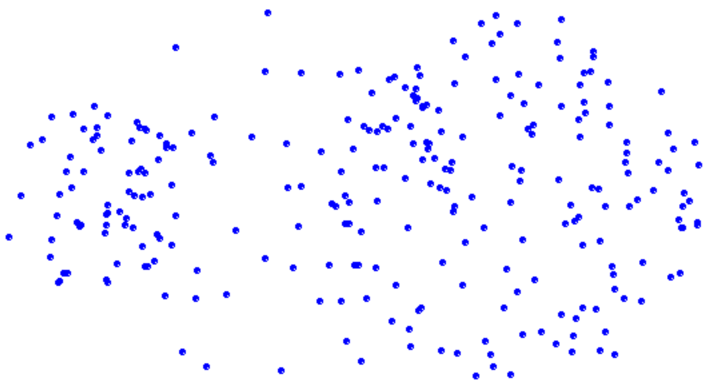


Nested Clusters

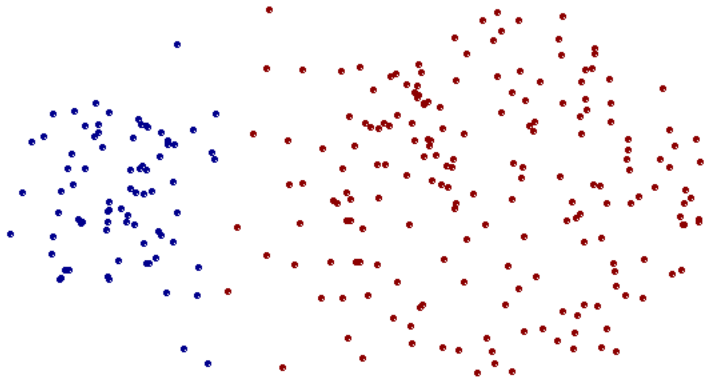


Dendrogram

# Strength of MAX



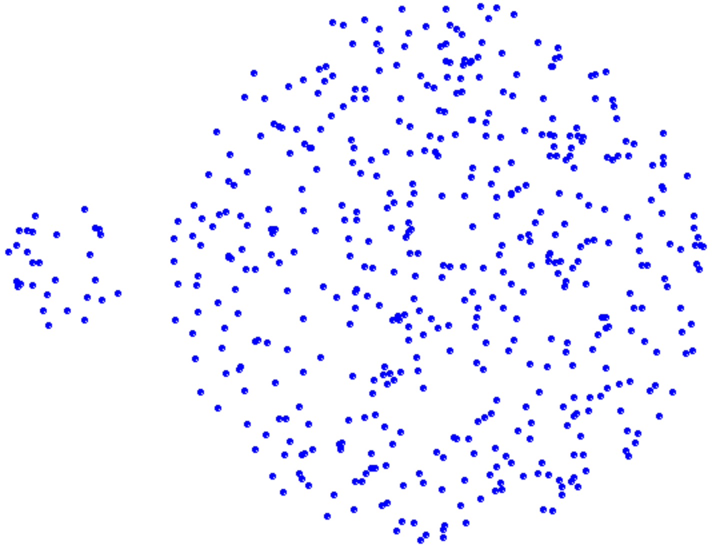
Original Points



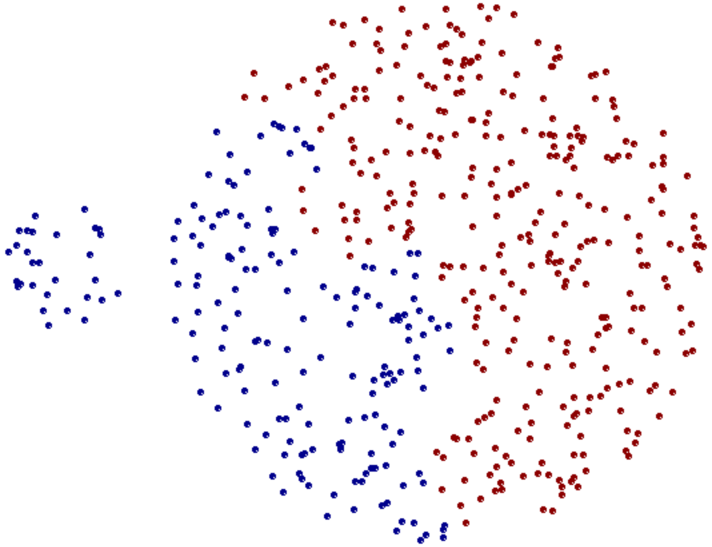
Two Clusters

- 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

- Compromise between Single and Complete Link

- Strengths
  - Less susceptible to noise and outliers

- Limitations
  - Biased towards globular clusters

# Cluster Similarity: Ward's Method

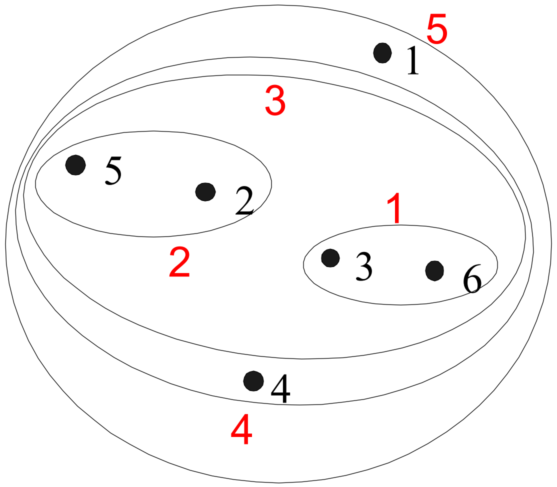
- Similarity of two clusters is based on the increase in squared error when two clusters are merged
  - Similar to group average if distance between points is distance squared

- Less susceptible to noise and outliers

- Biased towards globular clusters

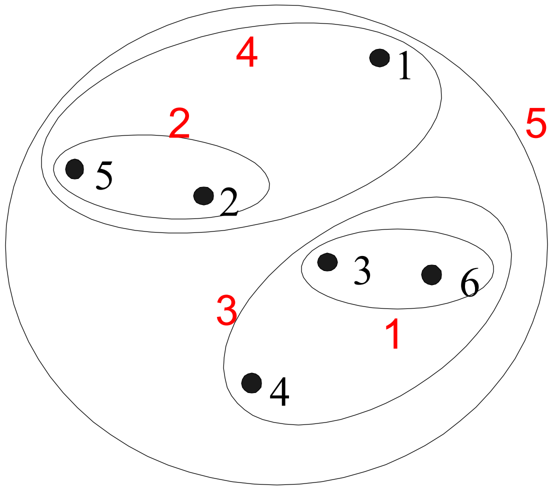
- Hierarchical analogue of K-means
  - Can be used to initialize K-means

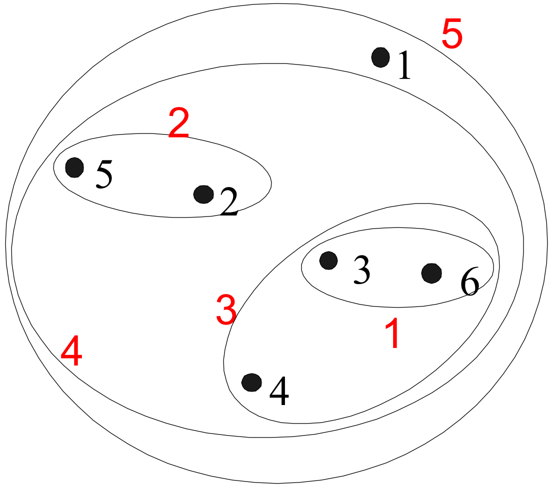
# Hierarchical Clustering: Comparison



MIN

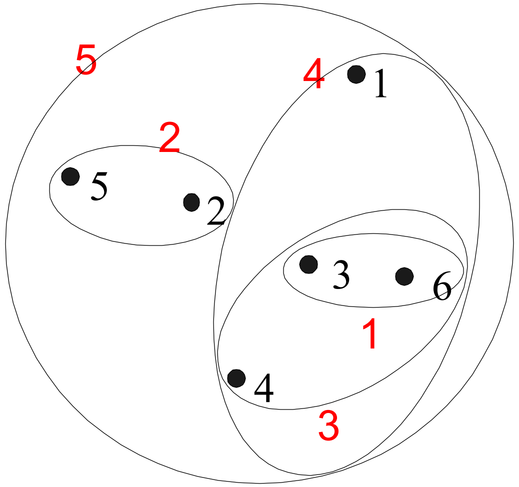
MAX





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.

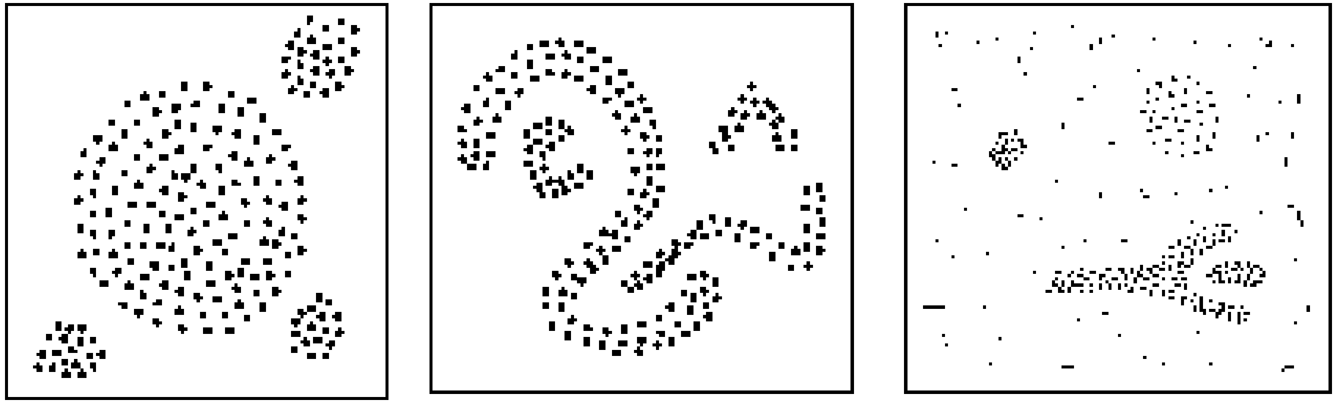
- O($N^3$) time in many cases
  - There are N steps and at each step the size, $N^2$, proximity matrix must be updated and searched
  - Complexity can be reduced to O($N^2$ log(N) ) time for some approaches

# Hierarchical Clustering: Problems and Limitations

- Once a decision is made to combine two clusters, it cannot be undone

- 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

# Density-Based Clustering



- Clustering based on density (local cluster criterion), such as density-connected points
- Each cluster has a considerable higher density of points than outside of the cluster

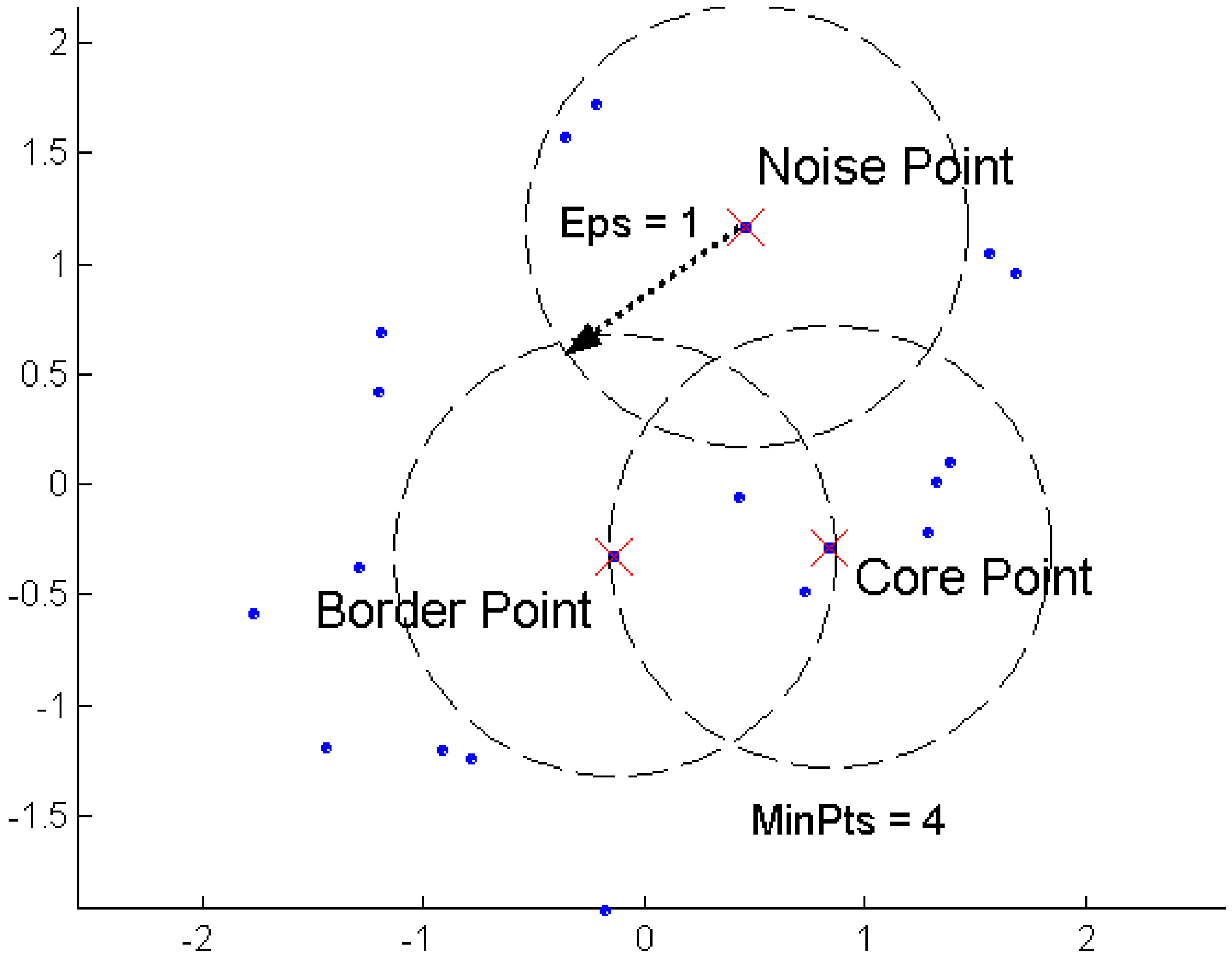
# Density-Based Clustering

- Major features:
  - Discover clusters of arbitrary shape
  - Handle noise
  - One scan
- Several interesting studies:
  - **DBSCAN**: **Ester, et al.** (KDD’**96**)
  - GDBSCAN: Sander, et al. (KDD’98)
  - OPTICS: Ankerst, et al (SIGMOD’99).
  - DENCLUE: Hinneburg & D. Keim (KDD’98)
  - CLIQUE: Agrawal, et al. (SIGMOD’98)

# DBSCAN

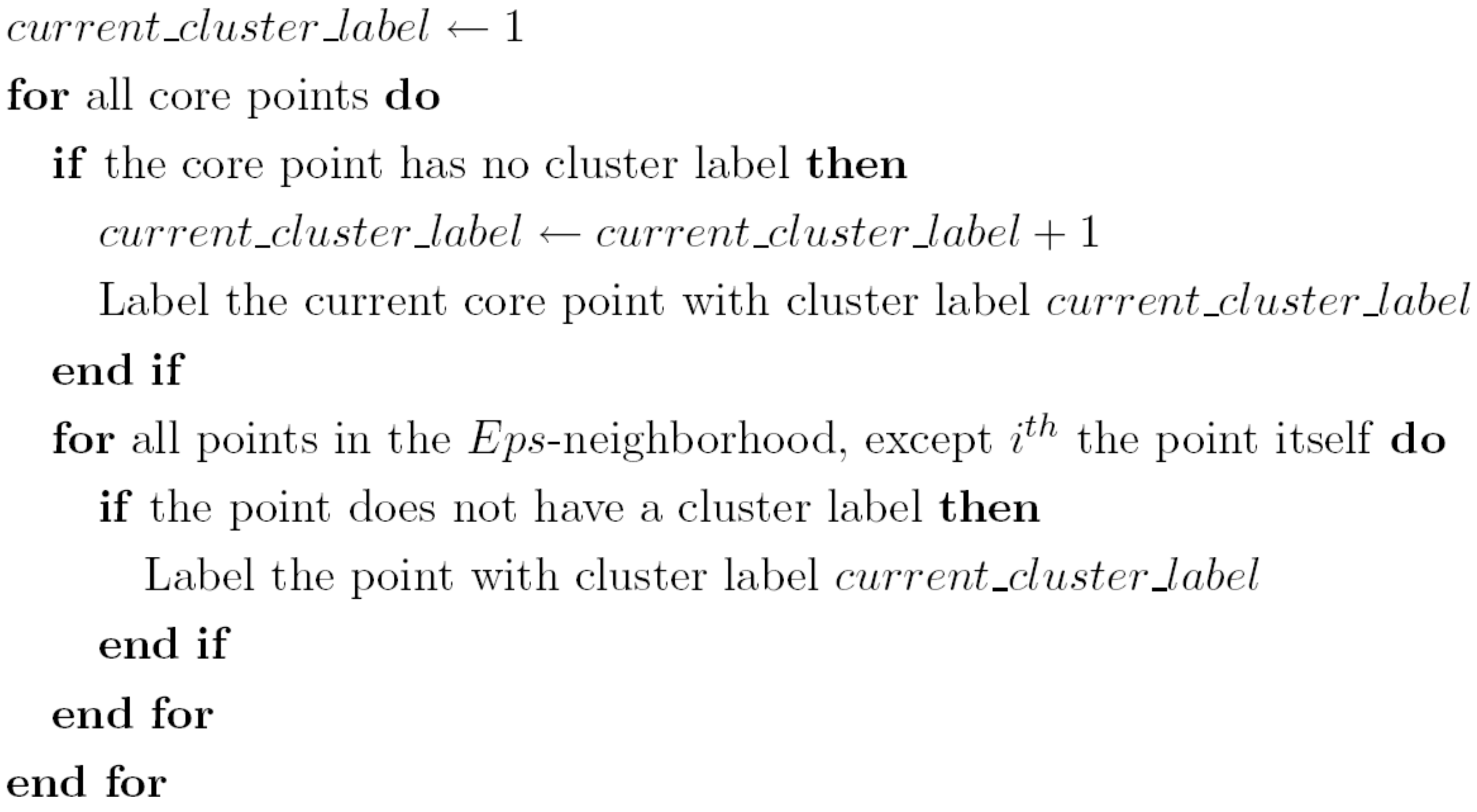
- DBSCAN is a density-based algorithm.
  - Density = number of points within a specified radius (Eps)
  - A point is a core point if it has more than a specified number of points (MinPts) within Eps
    - These are points that are at the interior of a cluster
  - A border point has fewer than MinPts 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.
  - does not require one to specify the number of clusters.
  - requires few parameters .

# DBSCAN: Core, Border, and Noise Points



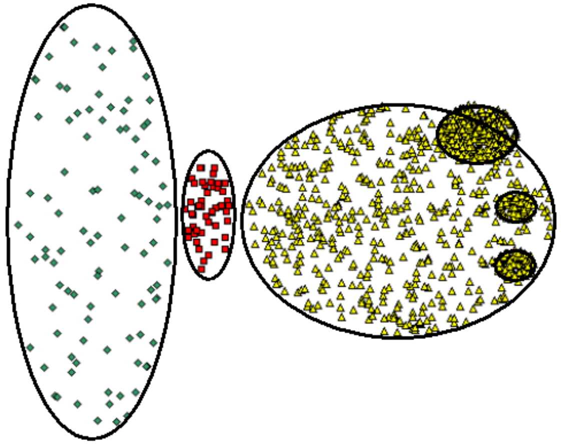
# DBSCAN Algorithm

- Eliminate noise points
- Perform clustering on the remaining points

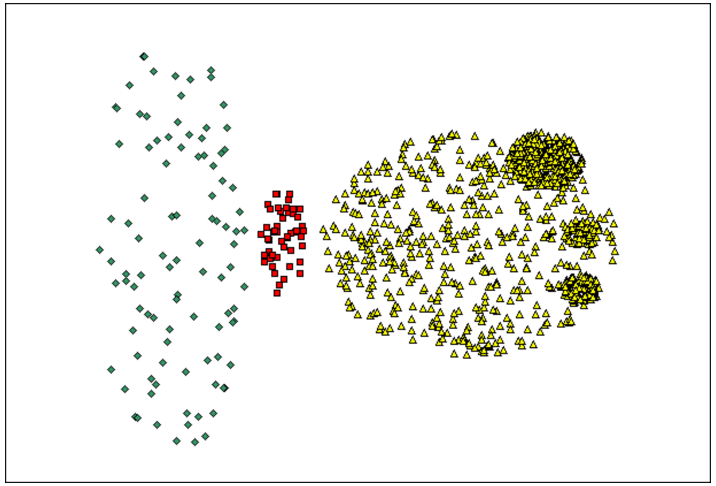


```
$current\_cluster\_label \leftarrow 1$
for all core points do
  if the core point has no cluster label then
    $current\_cluster\_label \leftarrow current\_cluster\_label + 1$
    Label the current core point with cluster label $current\_cluster\_label$
  end if
  for all points in the $Eps$-neighborhood, except $i^{th}$ the point itself do
    if the point does not have a cluster label then
      Label the point with cluster label $current\_cluster\_label$
    end if
  end for
end for
```

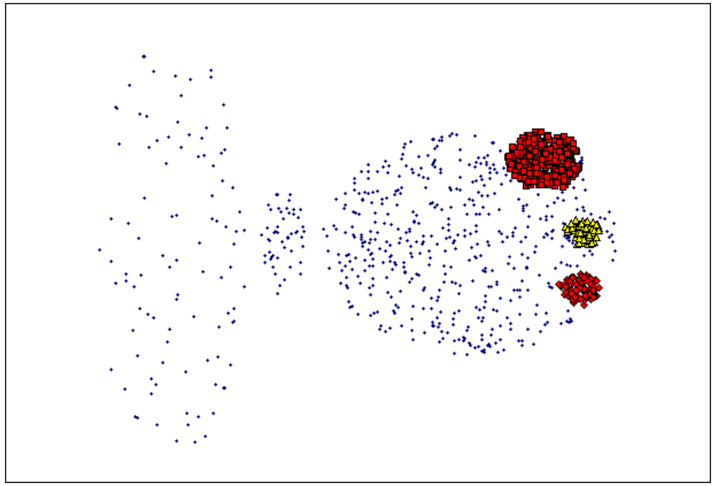
# When DBSCAN Does NOT Work Well



Original Points



(MinPts=4, Eps=9.75).

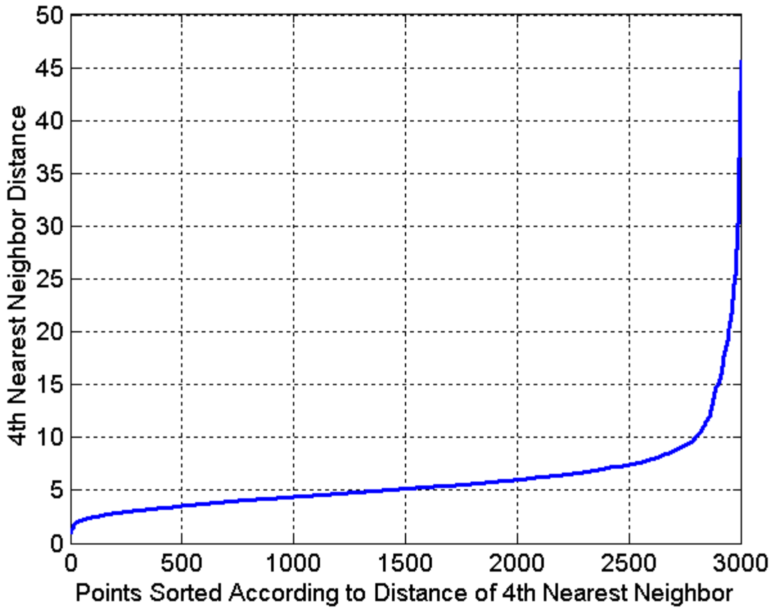


(MinPts=4, Eps=9.92)

- Varying densities
- High-dimensional data

# DBSCAN: Determining EPS and MinPts

- Idea is that for points in a cluster, their k$^{th}$ nearest neighbors are at roughly the same distance
- Noise points have the k$^{th}$ nearest neighbor at farther distance
- So, plot sorted distance of every point to its k$^{th}$ nearest neighbor



# Cluster Validity

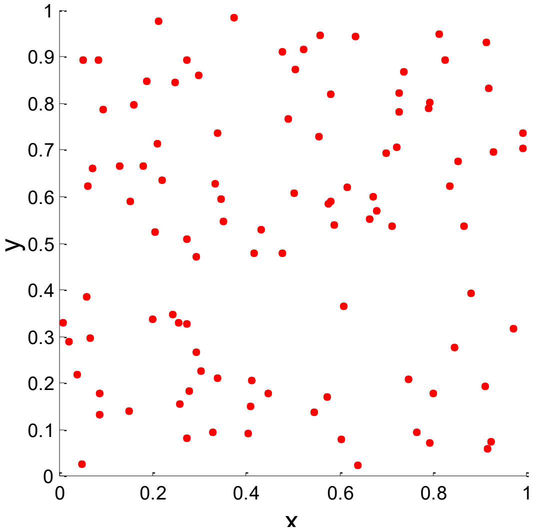
- For supervised classification we have a variety of measures to evaluate how good our model is
  - Accuracy, precision, recall

- For cluster analysis, the analogous question is how to evaluate the “goodness” of the resulting clusters?

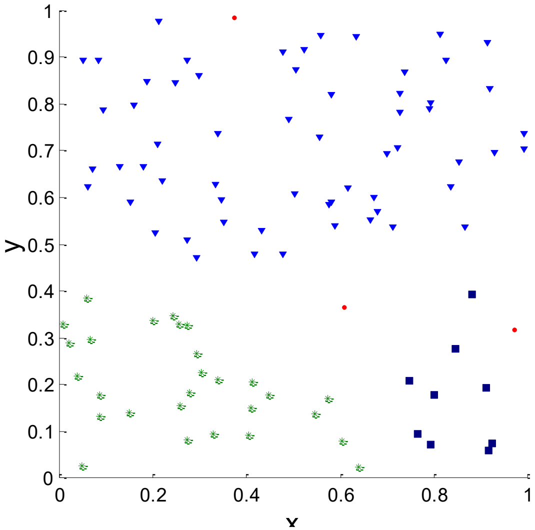
- Then why do we want to evaluate them?
  - To compare clustering algorithms
  - To compare two sets of clusters
  - To compare two clusters

# Clusters found in Random Data

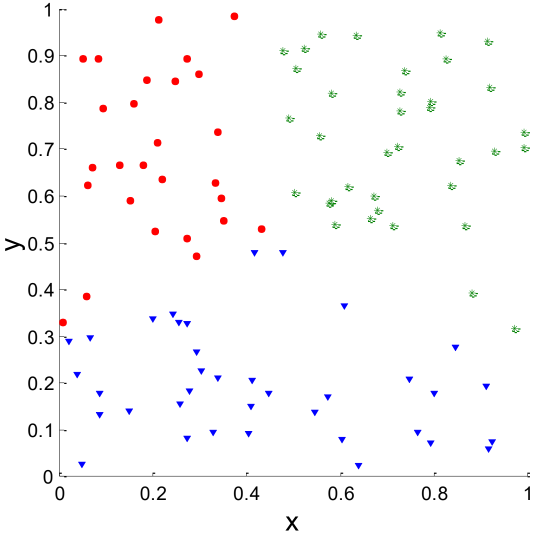
Random Points



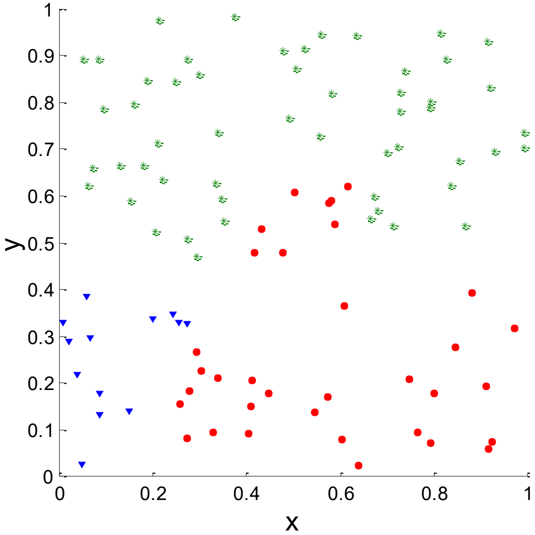
DBSCAN



K-means



Complete Link



# Measures of Cluster Validity

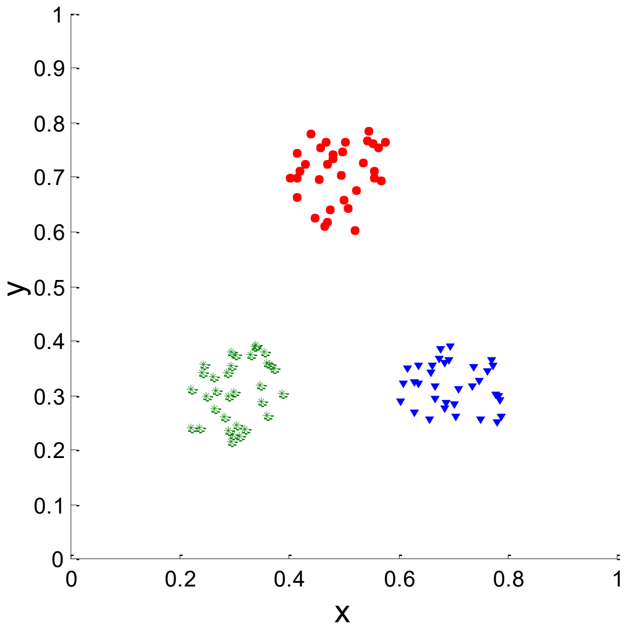
- Numerical measures that are applied to judge various aspects of cluster validity, are classified into the following three types.
  - External Index: Used to measure the extent to which cluster labels match externally supplied class labels.
    - Jaccard Coefficient, Mutual Information, Fowlkes and Mallows Index, Rand Index, Entropy
  - Internal Index:  Used to measure the goodness of a clustering structure without respect to external information.
    - Silhouette Coefficient, Calinski-Harabasz, Sum of Squared Error (SSE), Davies-Bouldin Index, Dunn Index
  - 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

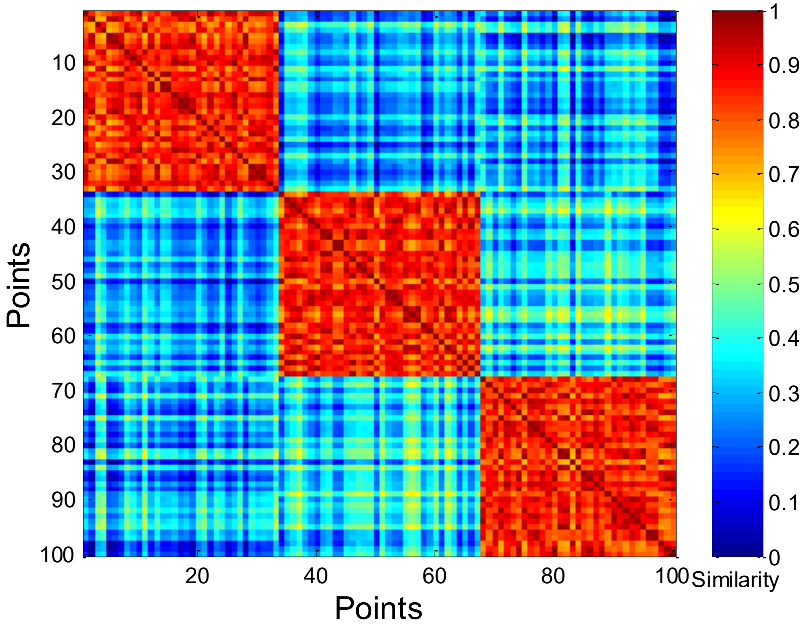
# Measuring Cluster Validity Via Correlation

- Two matrices
  - – Proximity Matrix (邻接矩阵)– actual similarity matrix
  - – incidence Matrix(关联矩阵)
    - 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 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.

# Using Similarity Matrix for Cluster Validation

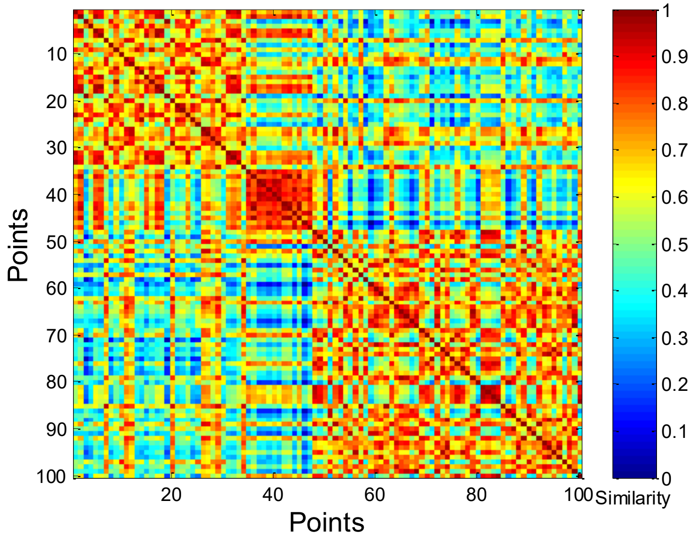
- Order the similarity matrix with respect to cluster labels and inspect visually.

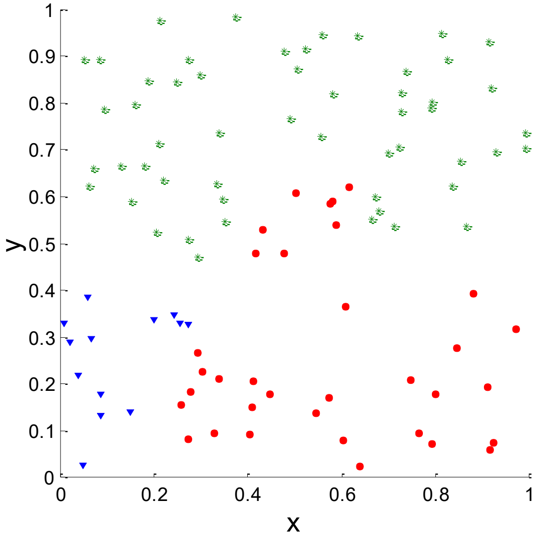




# Using Similarity Matrix for Cluster Validation

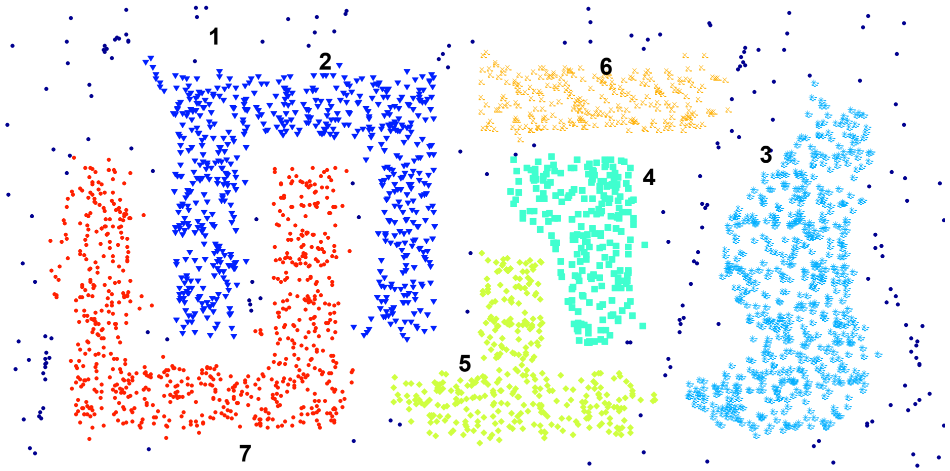
- Clusters in random data

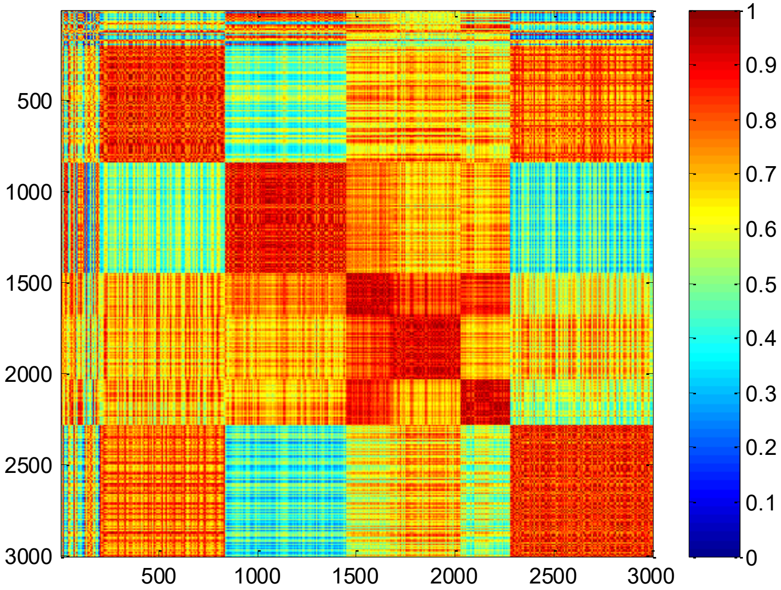




Complete Link

# Using Similarity Matrix for Cluster Validation

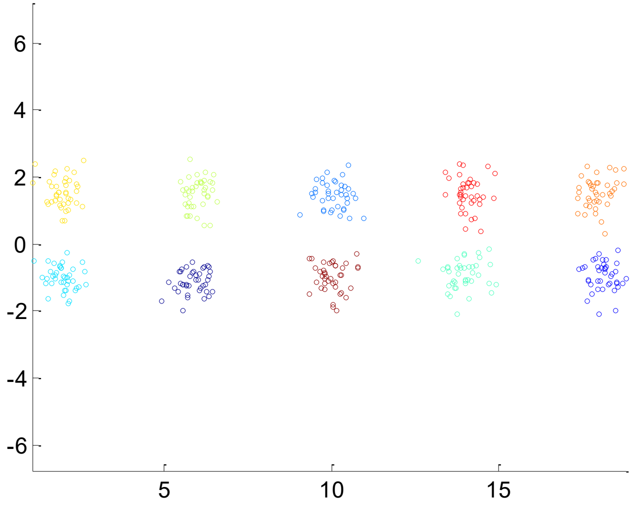


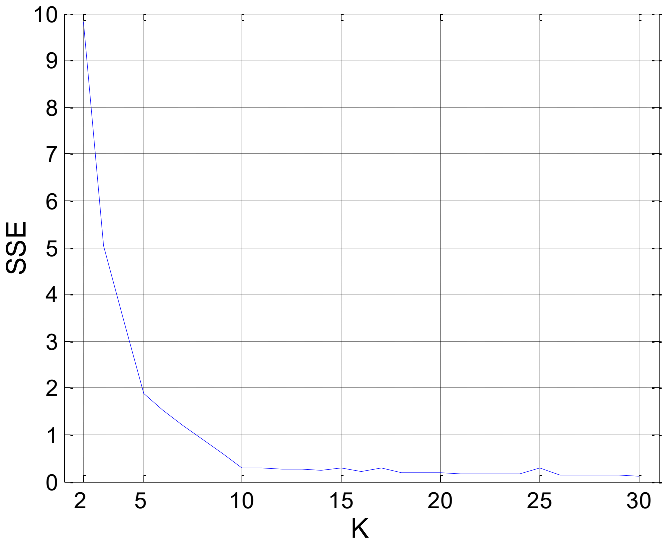


DBSCAN

# Internal Measures: SSE

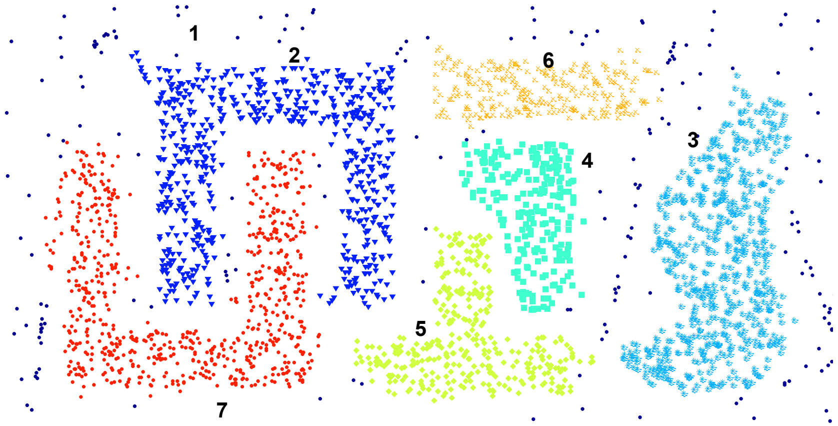
- Clusters in more complicated figures aren’t well separated
- Internal Index:  Used to measure the goodness of a clustering structure without respect to external information
  - SSE
- SSE is good for comparing two clusterings or two clusters (average SSE).
- Can also be used to estimate the number of clusters

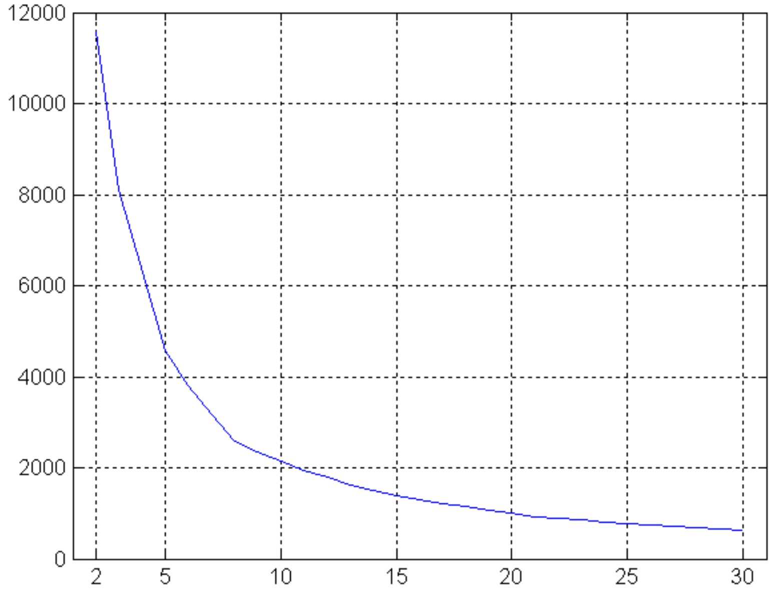




# Internal Measures: SSE

- SSE curve for a more complicated data set





SSE of clusters found using K-means

# Conclusion

- Clustering Method
  - Unsupervised, discrete
- Algorithm
  - Partitioning approach: CATA ,k-medoids, Kernel K-means , CLARANS
  - Hierarchical approach: Agnes, Diana, BIRCH, ROCK, CAMELEON
  - Density-based approach: DBSCAN, OPTICS, DenClue
- Measures of Cluster Validity
  - External Index: Jaccard Coefficient, Fowlkes and Mallows Index, Rand Index, Entropy
  - Internal Index: Silhouette Coefficient , Sum of Squared Error (SSE)， Davies-Bouldin Index， Dunn Index
  - Relative Index: SSE or entropy