Data Mining
Cluster Analysis: Basic Concepts and Algorithms

Lecture Notes for Chapter 7

Introduction to Data Mining, 2nd Edition

by

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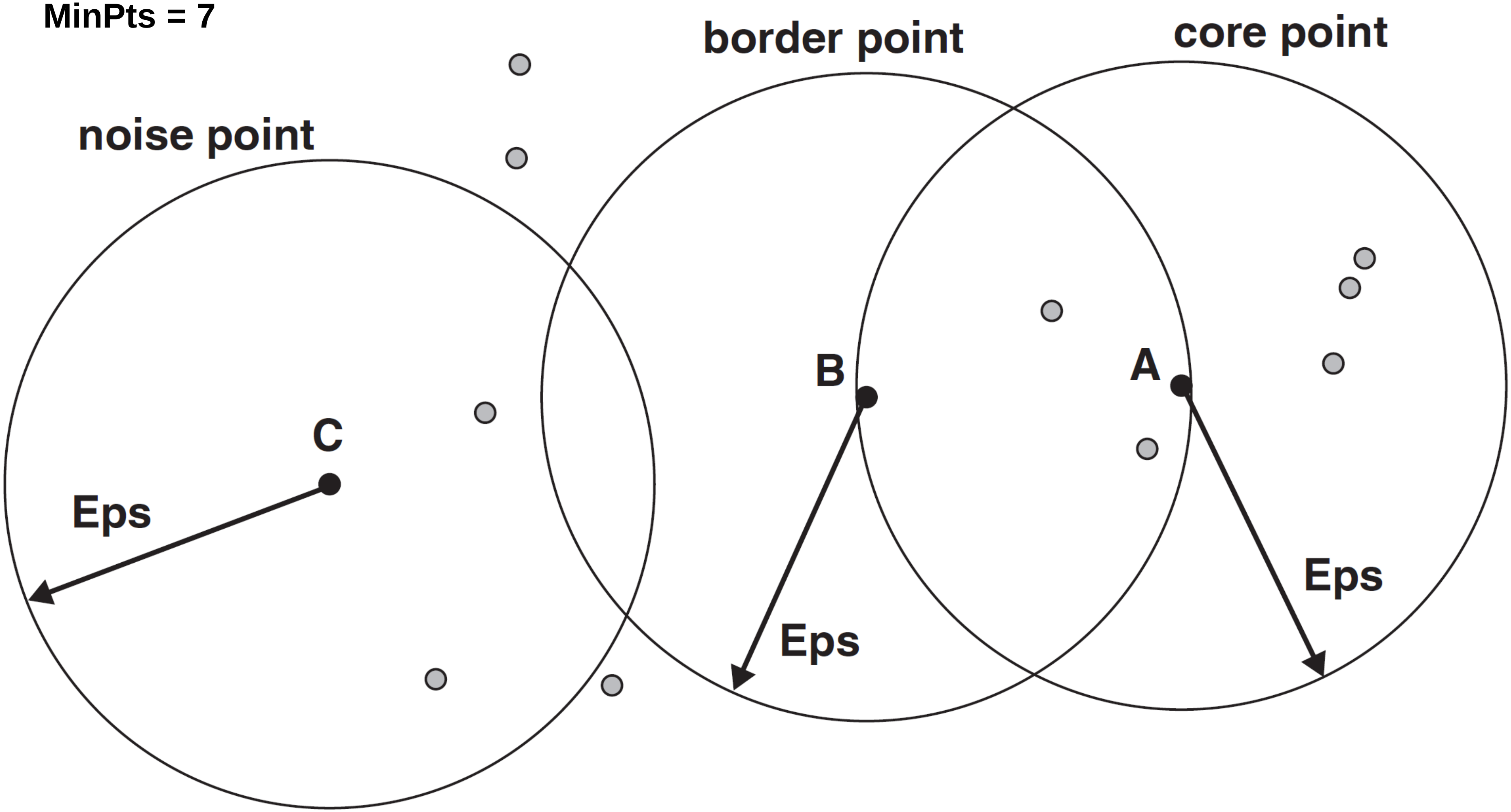
DBSCAN

- DBSCAN is a density-based algorithm.
  - Density = number of points within a specified radius (Eps)
  - A point is a core point if it has at least a specified number of points (MinPts) within Eps
    - These are points that are at the interior of a cluster
    - Counts the point itself
  - A border point is not a core point, 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

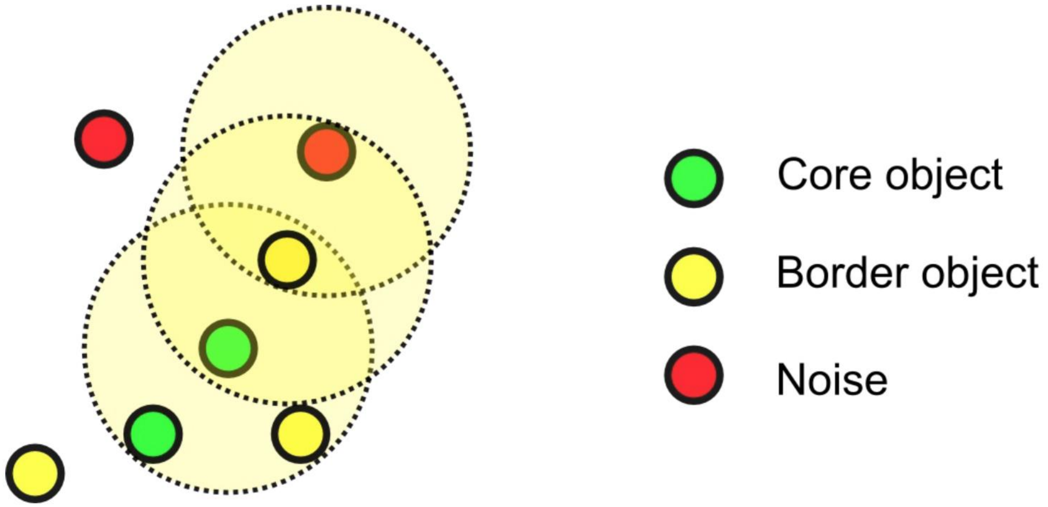
DBSCAN: Core, Border, and Noise Points

MinPts = 7



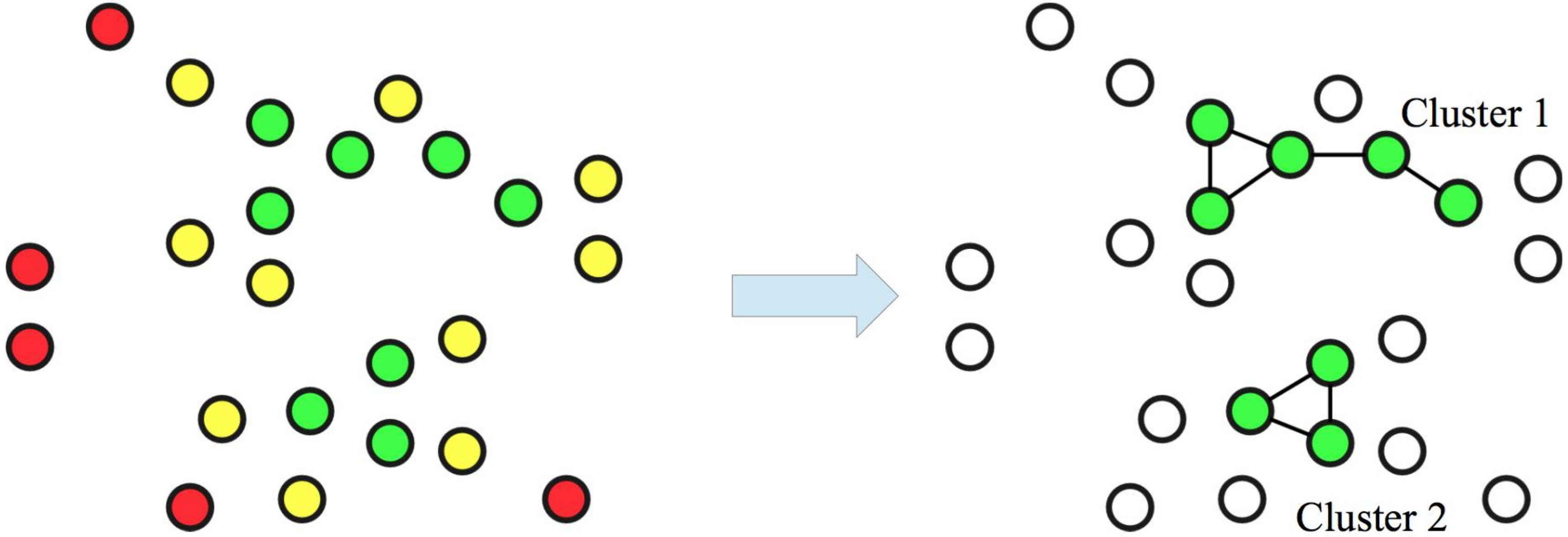
DBSCAN: Step 1

- Label points as **core** (dense), **border** and **noise**
  - Based on thresholds R (radius of neighborhood) and min_pts (min number of neighbors)



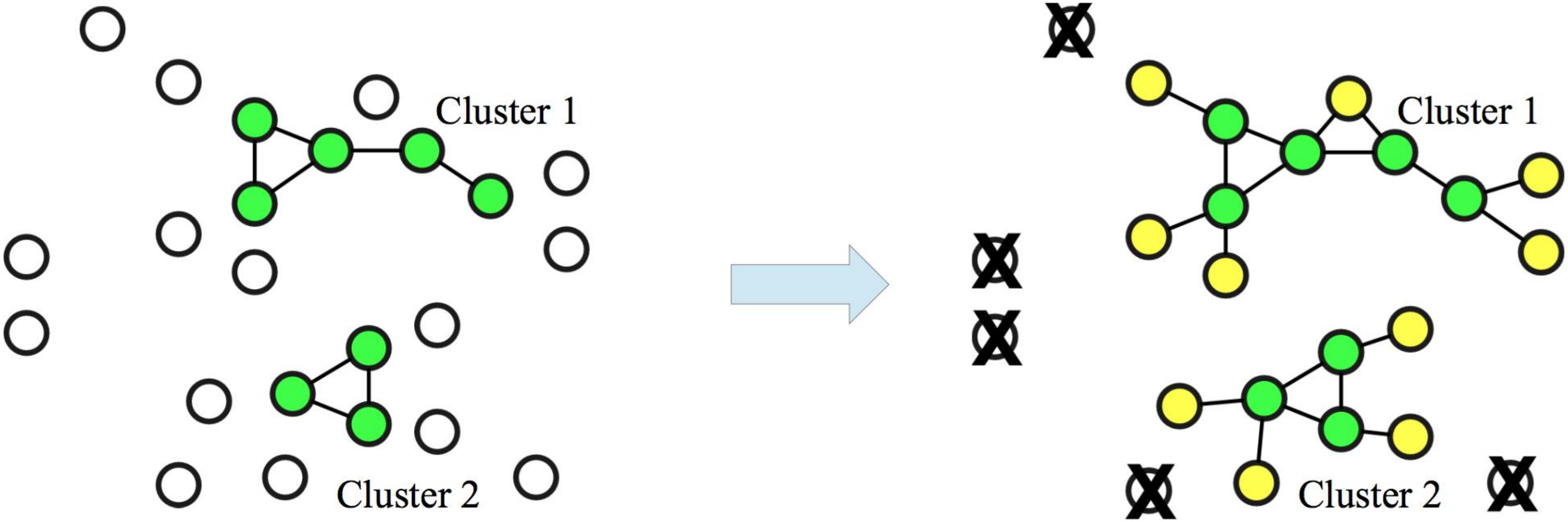
DBSCAN: Step 2

- Connect core objects that are neighbors, and put them in the same cluster



DBSCAN: Step 3

- Associate border objects to (one of) their core(s), and remove noise



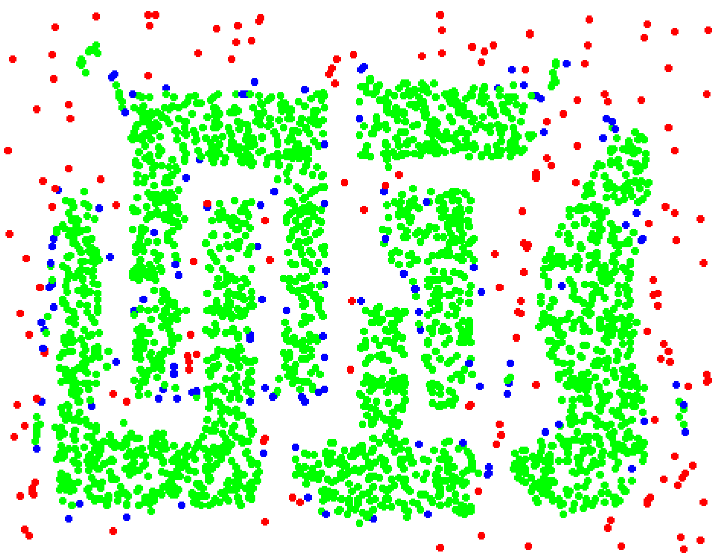
DBSCAN Algorithm

- Eliminate noise points
- Perform clustering on the remaining points

$current\_cluster\_label \leftarrow 0$
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

DBSCAN: Core, Border and Noise Points

Original Points

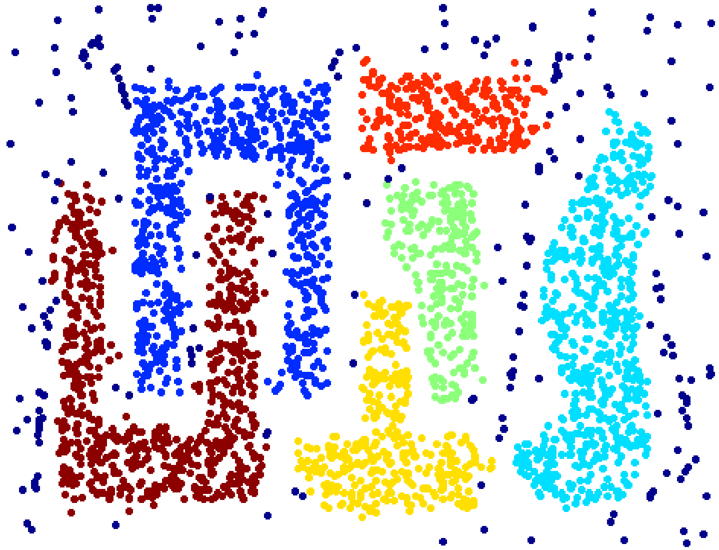


Point types: core, border and noise

Eps = 10, MinPts = 4

When DBSCAN Works Well

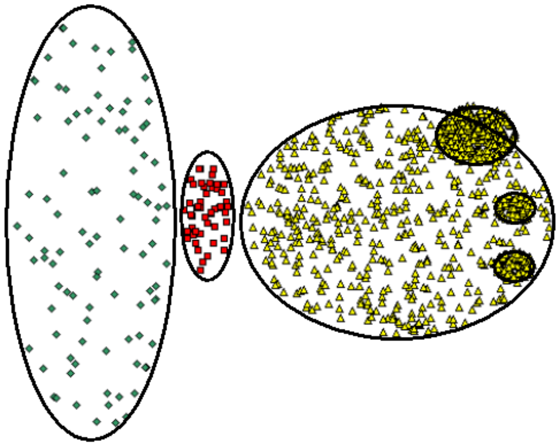
Original Points



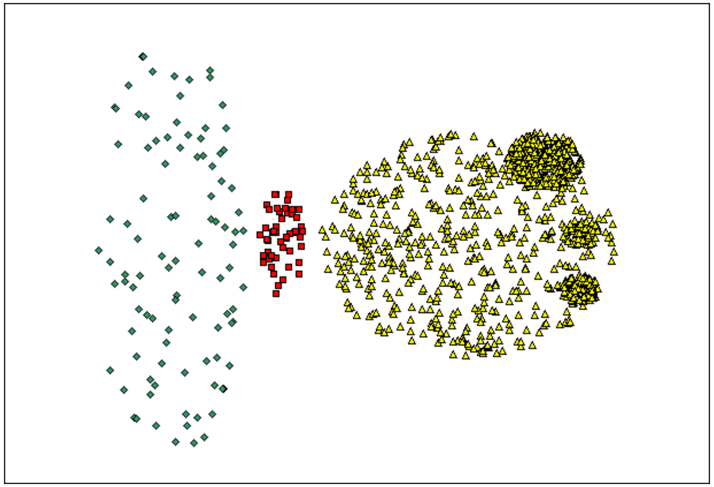
Clusters

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

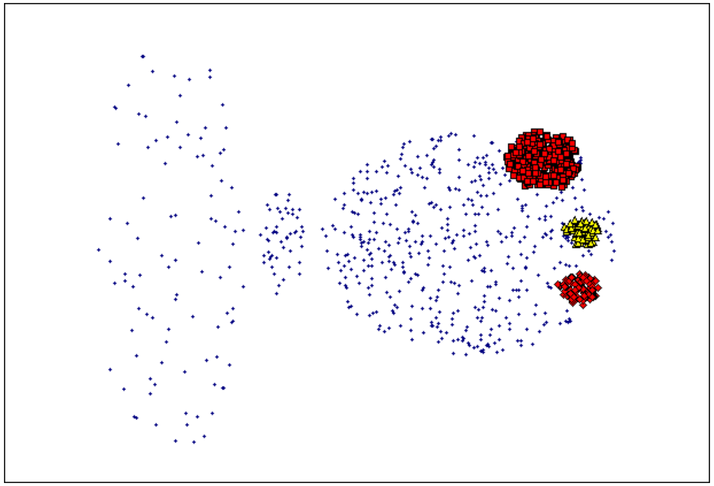
When DBSCAN Does NOT Work Well



Original Points



(MinPts=4, Eps=9.75).

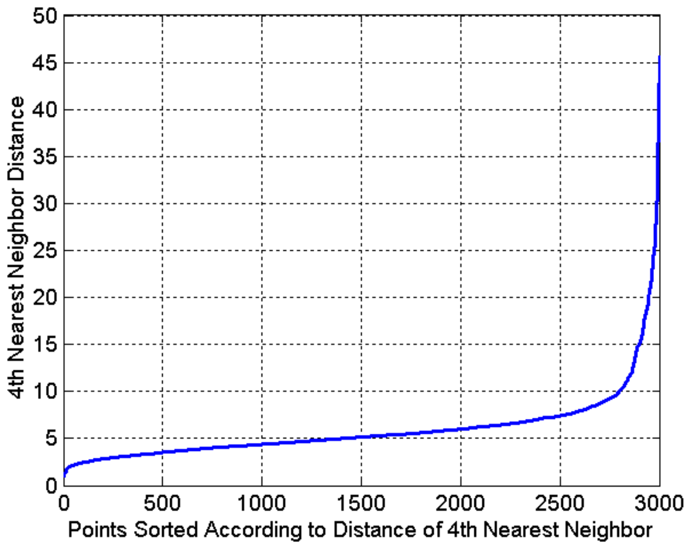


(MinPts=4, Eps=9.92)

- Varying densities
- High-dimensional data where density it is harder to define

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

Cluster Validity

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

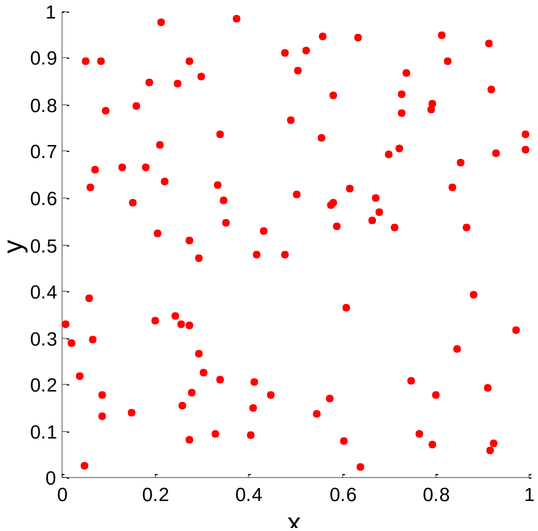
- For cluster analysis, the analogous question is how to evaluate the “goodness” of the resulting clusters?

- But “clusters are in the eye of the beholder”!

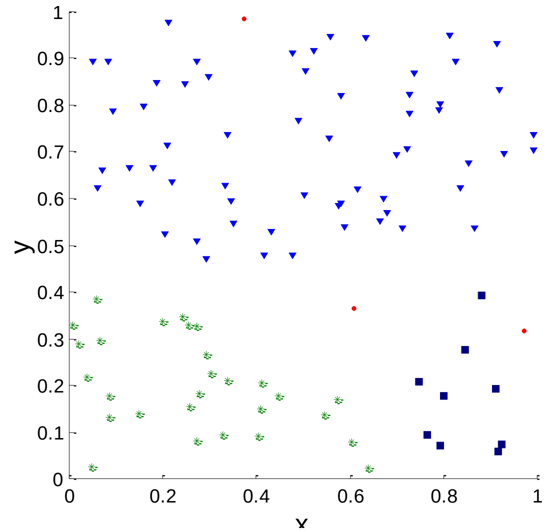
- Then why do we want to evaluate them?
  - To avoid finding patterns in noise
  - To compare clustering algorithms
  - To compare two sets of clusters
  - To compare two clusters

Clusters found in Random Data

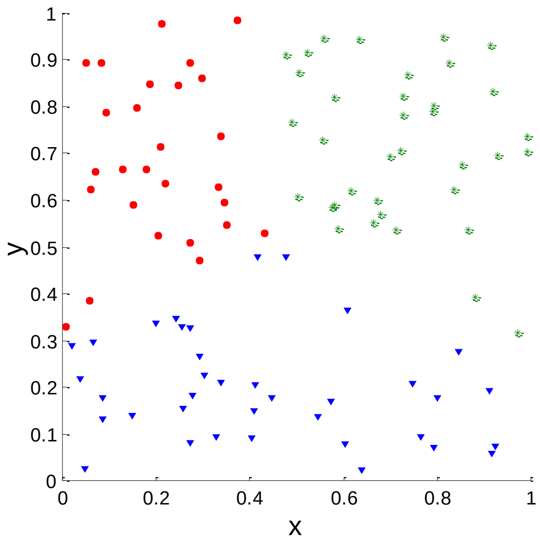
Random Points



DBSCAN



K-means



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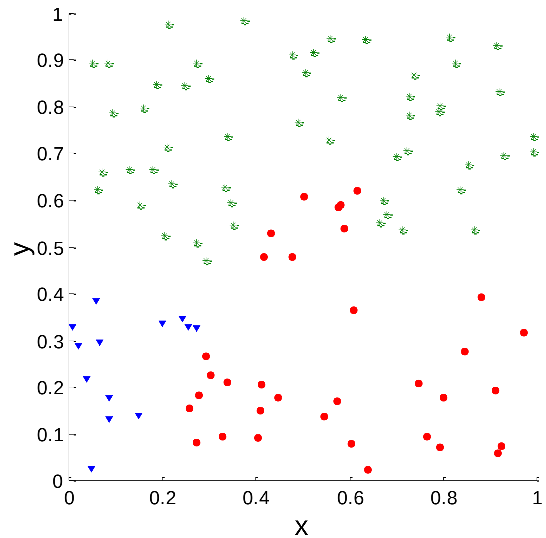


Different Aspects of Cluster Validation

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

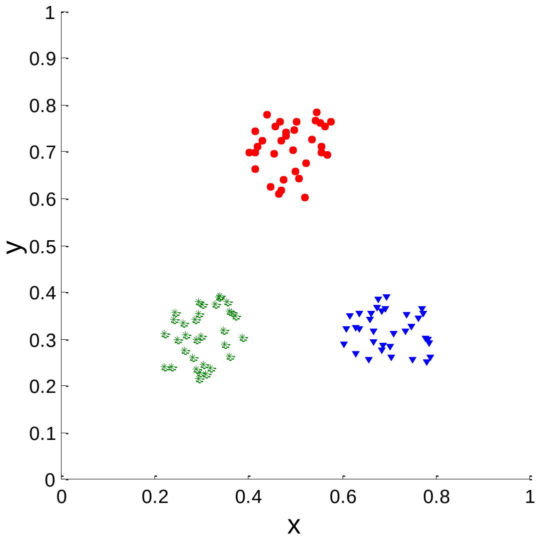
- Numerical measures that are applied to judge various aspects of cluster validity, are classified into the following three types.
  - External Index: Used to measure the extent to which cluster labels match externally supplied class labels.
    - Entropy
  - Internal Index: Used to measure the goodness of a clustering structure *without* respect to external information.
    - 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.

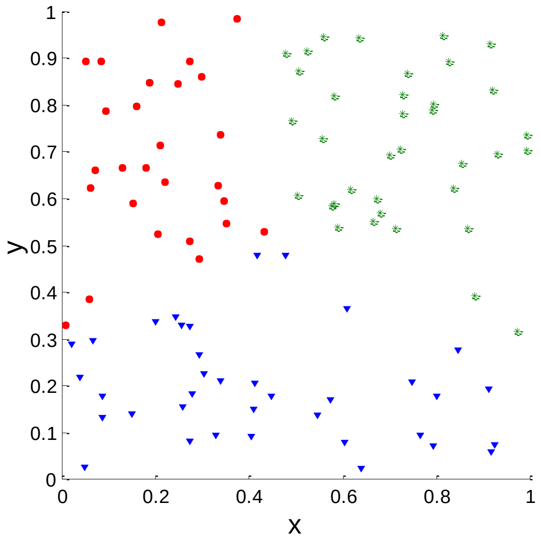
Measuring Cluster Validity Via Correlation

- Two matrices
  - Proximity Matrix
  - Ideal Similarity 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 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.

Measuring Cluster Validity Via Correlation

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

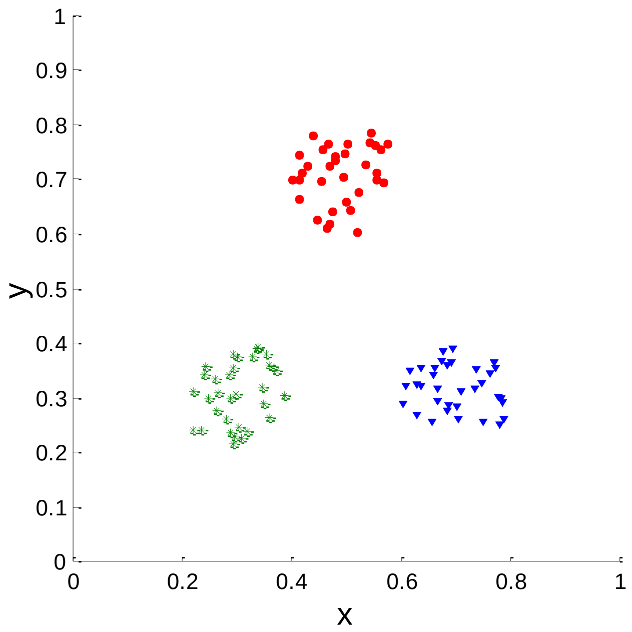


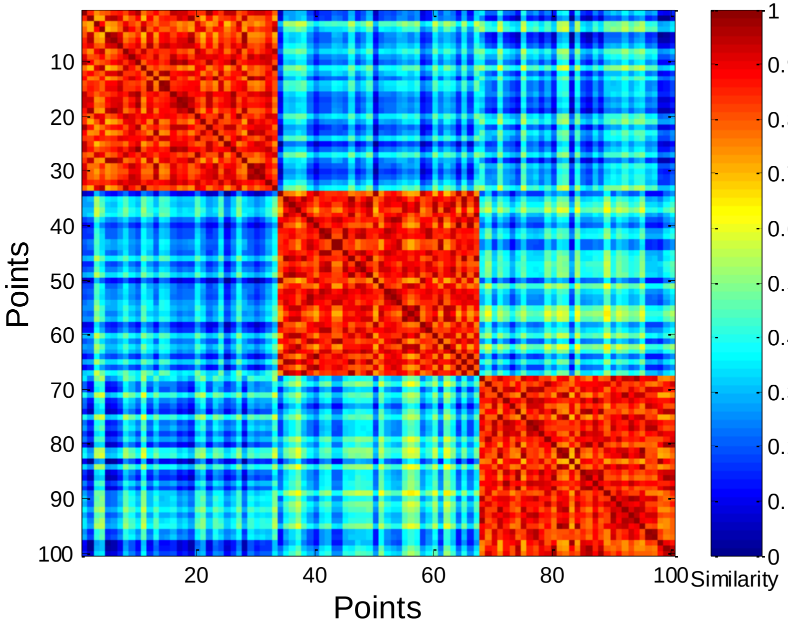


Corr = -0.9235 **Corr = -0.5810**

Using Similarity Matrix for Cluster Validation

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

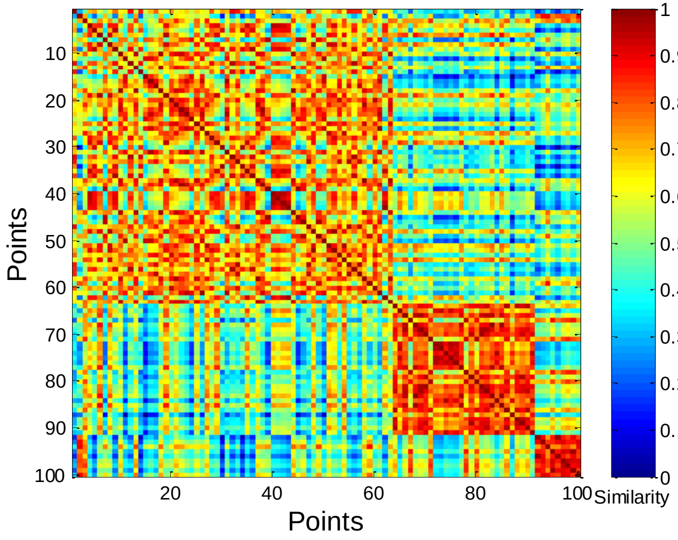


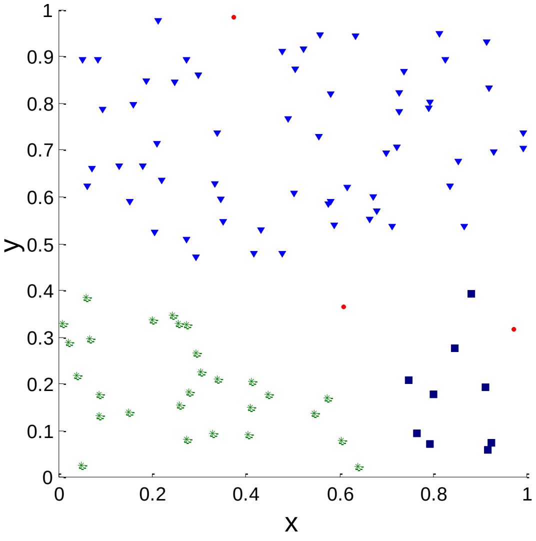


If we have well-separated clusters, then the similarity matrix should be roughly block-diagonal

Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp





DBSCAN

Using Similarity Matrix for Cluster Validation

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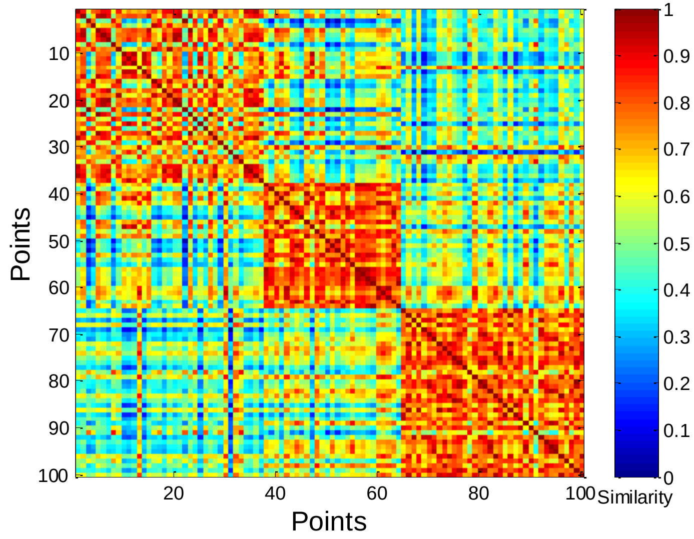
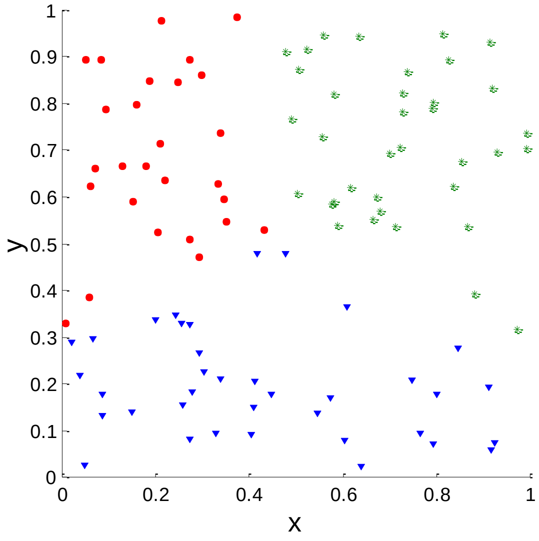
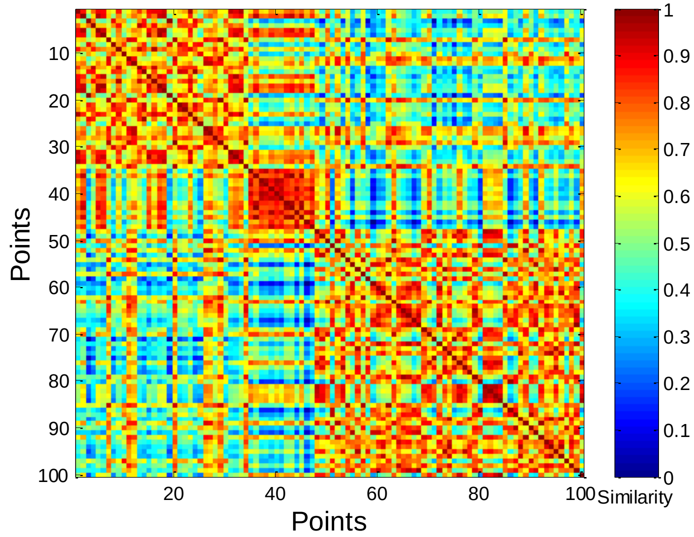


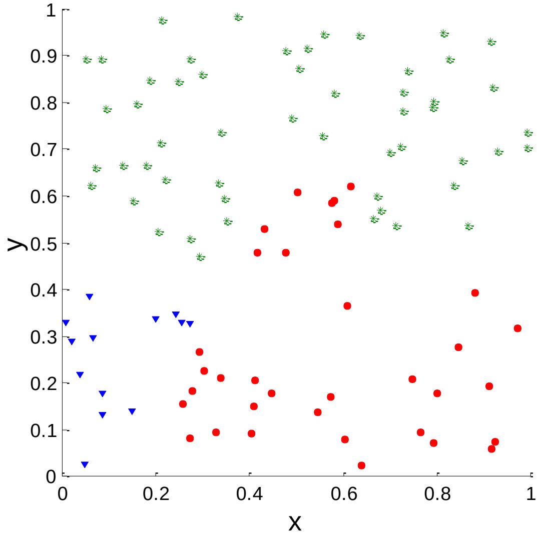


K-means

Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp





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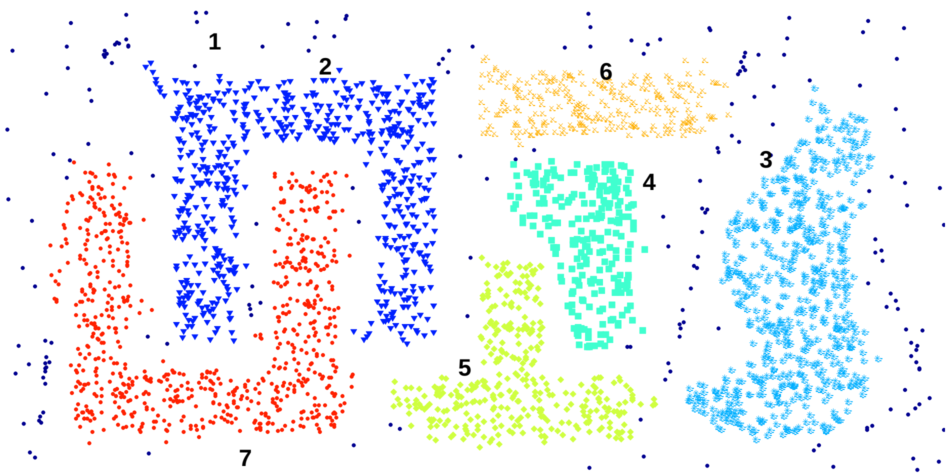
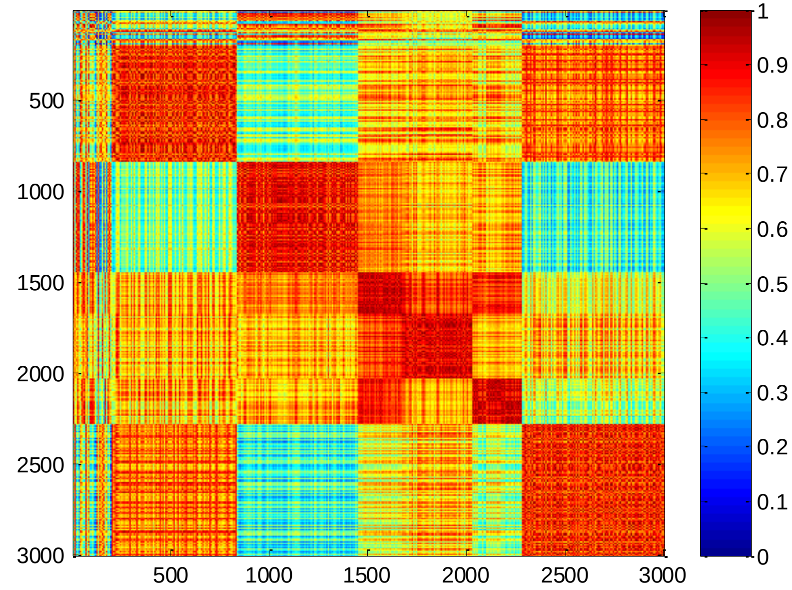
Using Similarity Matrix for Cluster Validation

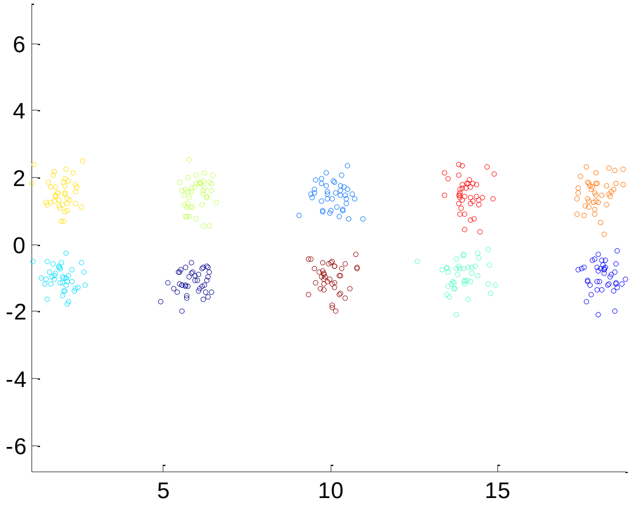


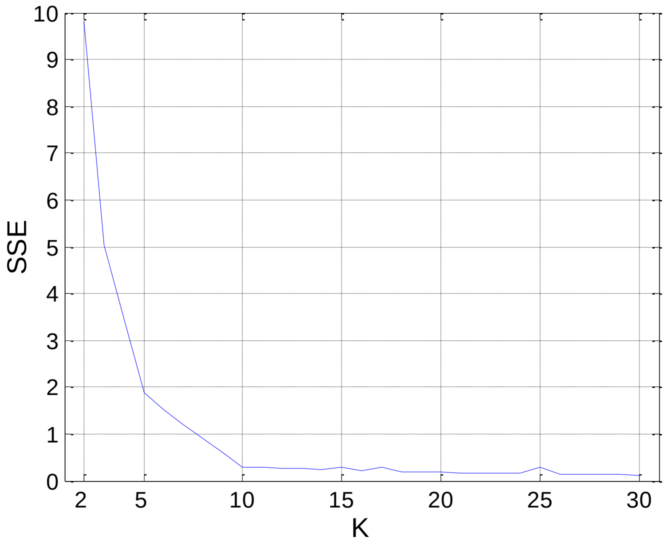


DBSCAN

Internal Measures: SSE

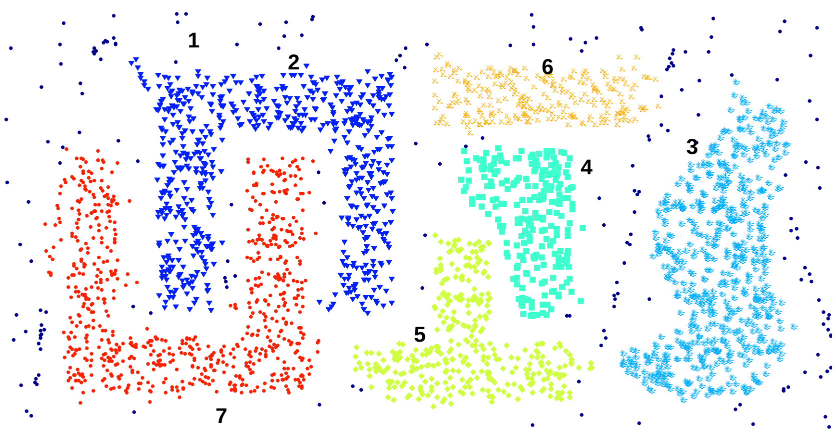
- Clusters in more complicated figures aren't well separated
- Internal Index: Used to measure the goodness of a clustering structure without respect to external information
  – SSE
- SSE is good for comparing two clusterings or two clusters (average SSE).
- Can also be used to estimate the number of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

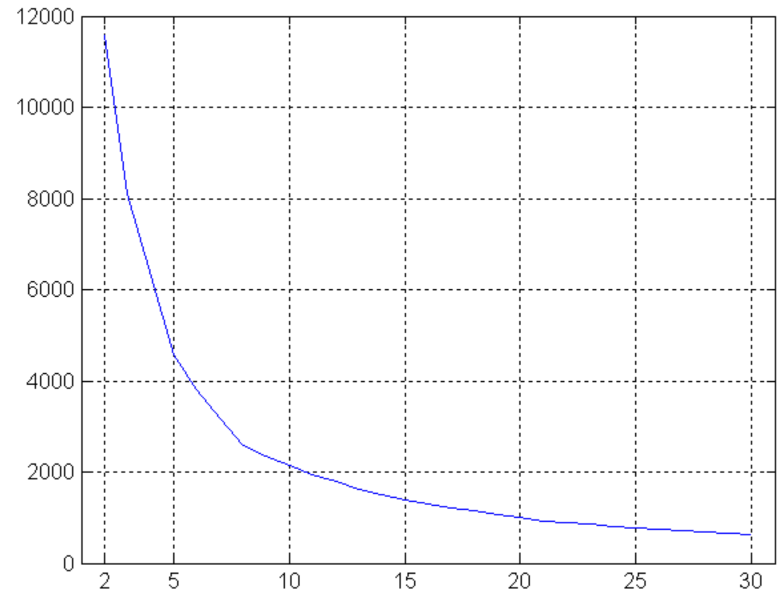




Internal Measures: SSE

- SSE curve for a more complicated data set

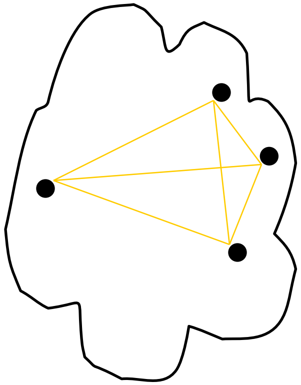




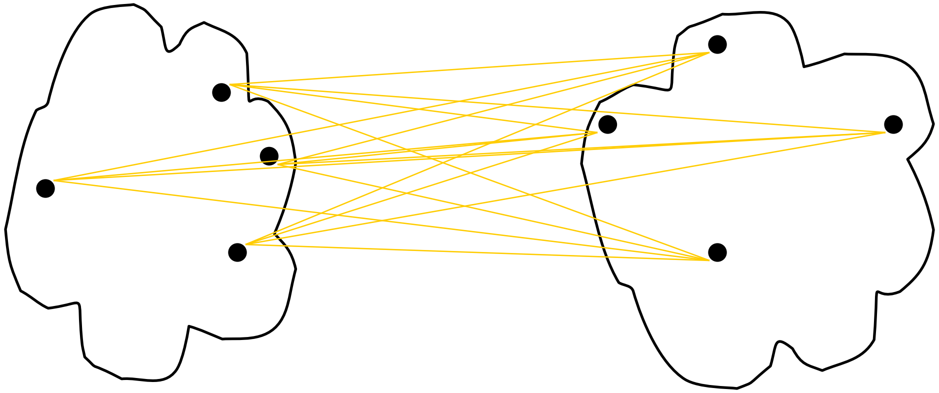
SSE of clusters found using K-means

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: Cohesion and Separation

- Cluster Cohesion: Measures how closely related are objects in a cluster
  - Example: SSE
- 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)

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

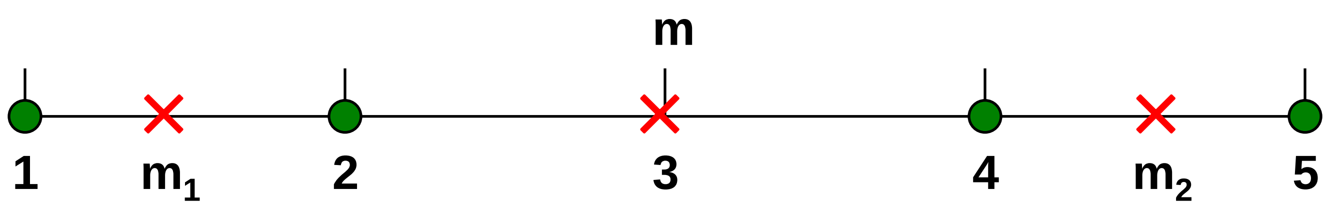
  - Separation is measured by the between cluster sum of squares

$$BSS = \sum_{i} |C_i| (m - m_i)^2$$

  - Where $|C_i|$ is the size of cluster i

Internal Measures: Cohesion and Separation

- Example: SSE
  - BSS + WSS = constant



K=1 cluster:

$$SSE = WSS = (1-3)^2 + (2-3)^2 + (4-3)^2 + (5-3)^2 = 10$$

$$BSS = 4 \times (3-3)^2 = 0$$

$$Total = 10 + 0 = 10$$

K=2 clusters:

$$SSE = WSS = (1-1.5)^2 + (2-1.5)^2 + (4-4.5)^2 + (5-4.5)^2 = 1$$

$$BSS = 2 \times (3-1.5)^2 + 2 \times (4.5-3)^2 = 9$$

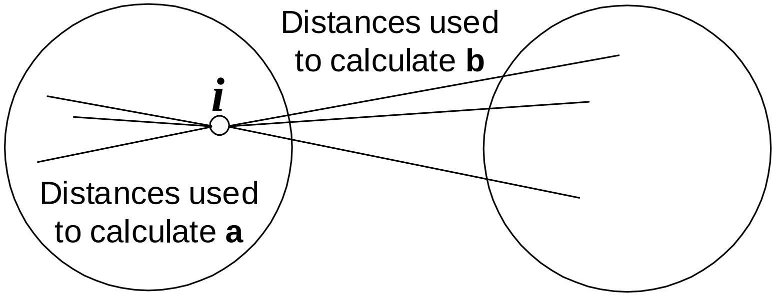
$$Total = 1 + 9 = 10$$

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 = average distance of i to the points in its cluster
  - Calculate b = min (average distance of i to points in another cluster)
  - The silhouette coefficient for a point is then given by

    s = (b – a) / max(a,b)

  - Typically between 0 and 1.
  - The closer to 1 the better.



- Can calculate the average silhouette coefficient for a cluster or a clustering

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.

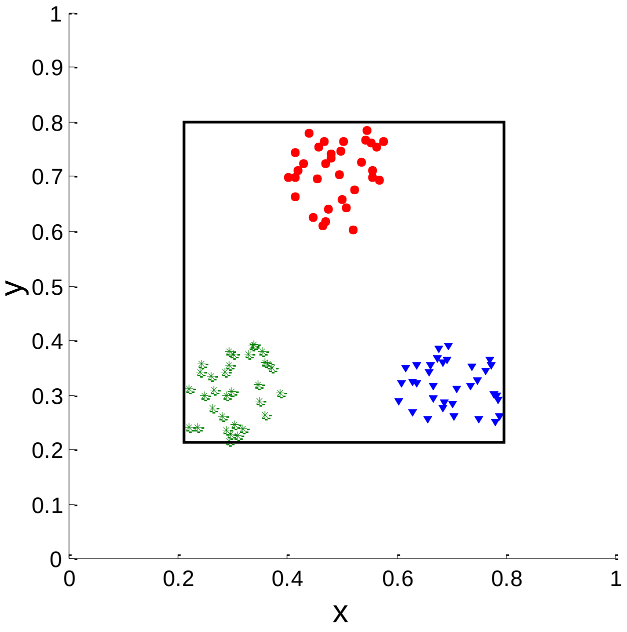
purity Using the terminology derived for entropy, the purity of cluster j, is given by $purity_j = \max p_{ij}$ and the overall purity of a clustering by $purity = \sum_{i=1}^{K} \frac{m_i}{m} purity_j$.

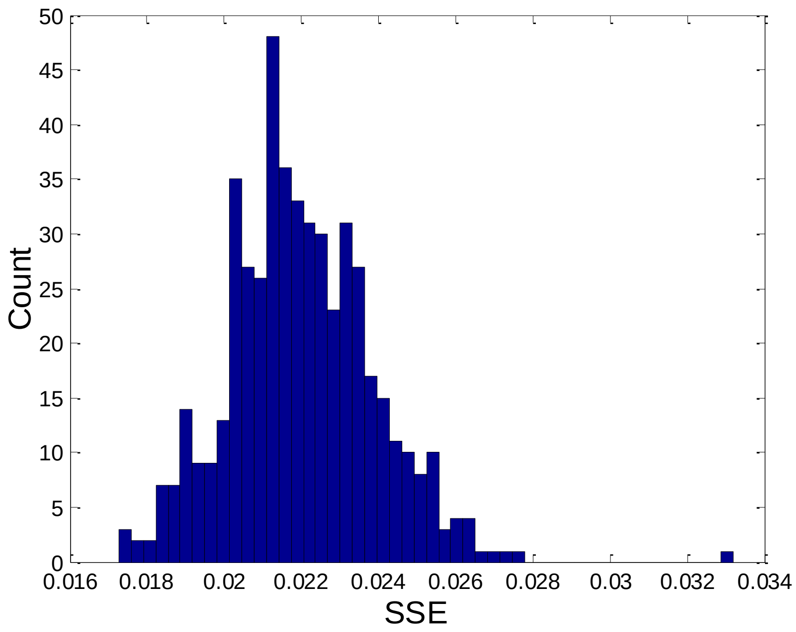
Framework for Cluster Validity

- 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 “atypical” 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
  - These approaches are more complicated and harder to understand.
- 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

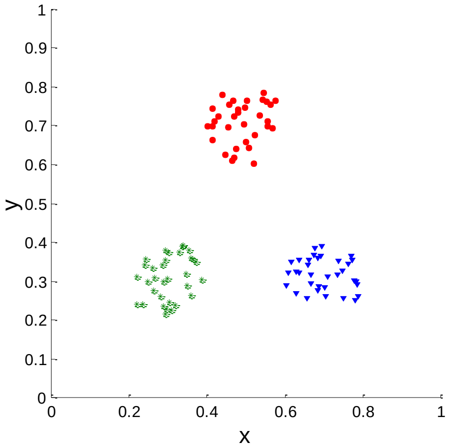
- Example
  - Compare SSE of 0.005 against three clusters in random data
  - Histogram shows SSE of three clusters in 500 sets of random data points of size 100 distributed over the range 0.2 – 0.8 for x and y values

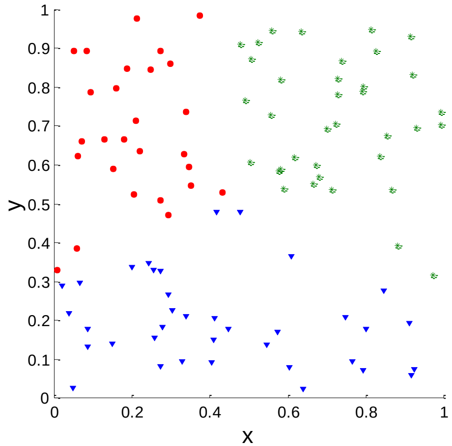


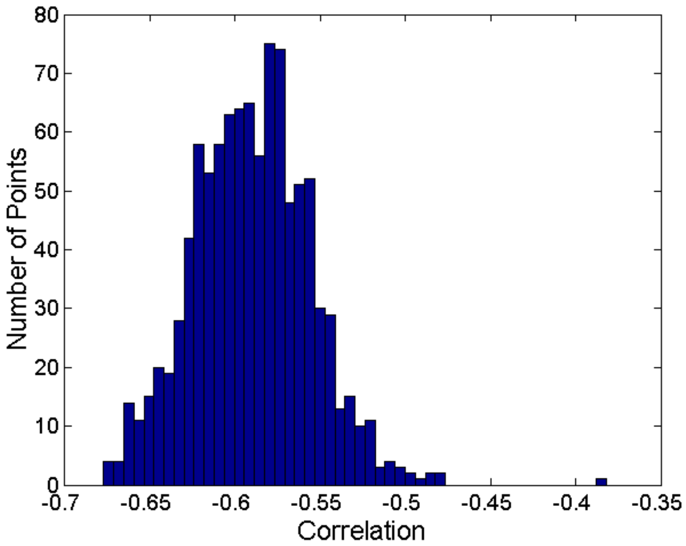


Statistical Framework for Correlation

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







Corr = -0.9235

Corr = -0.5810

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