Data Mining 2025

Clustering Analysis and Unsupervised Learning

Dept. of Computer Science and Information Engineering

National Cheng Kung University

Kun-Ta Chuang

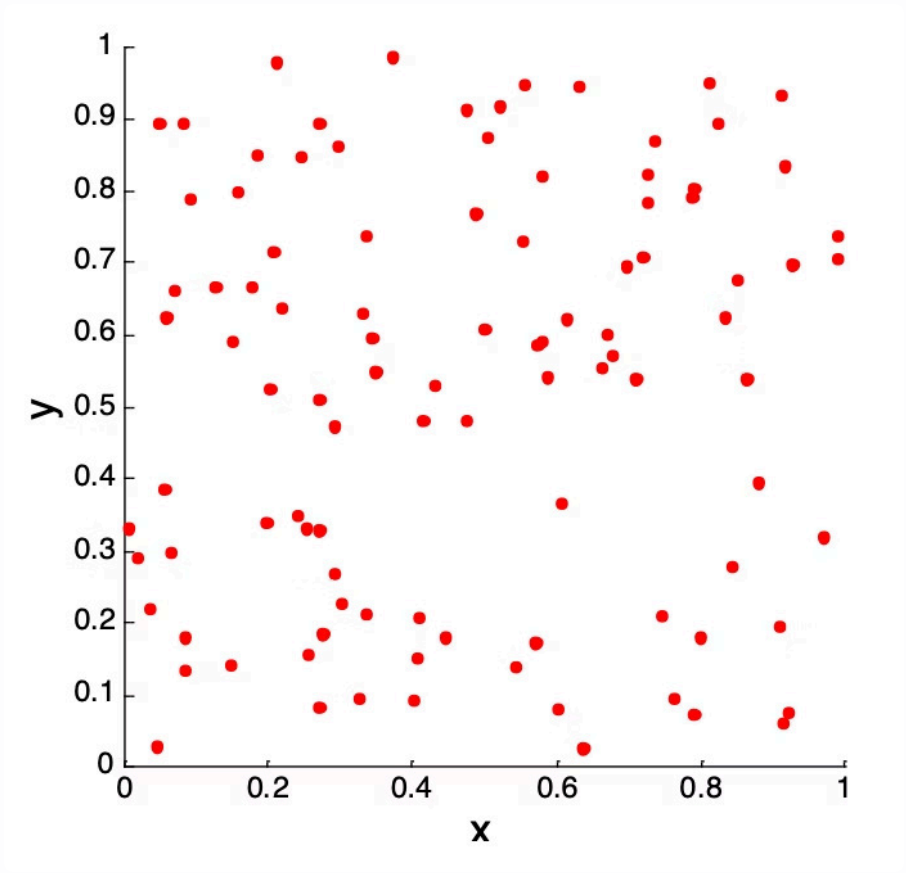
ktchuang@mail.ncku.edu.tw

Cluster Validity

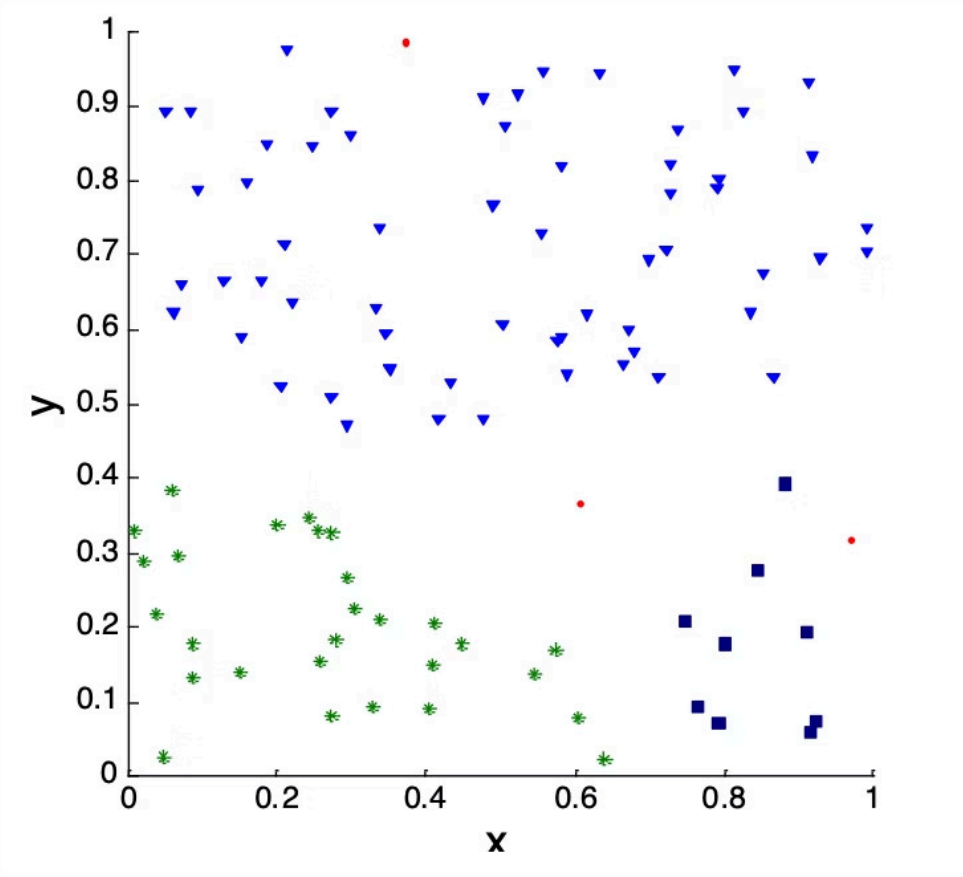
- For supervised classification we have a variety of measures to evaluate how good our model is
  - Accuracy, precision, recall
- For cluster analysis, the analogous question is how to evaluate the "goodness" of the resulting clusters?
- But "clusters are in the eye of the beholder"!
- Then why do we 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

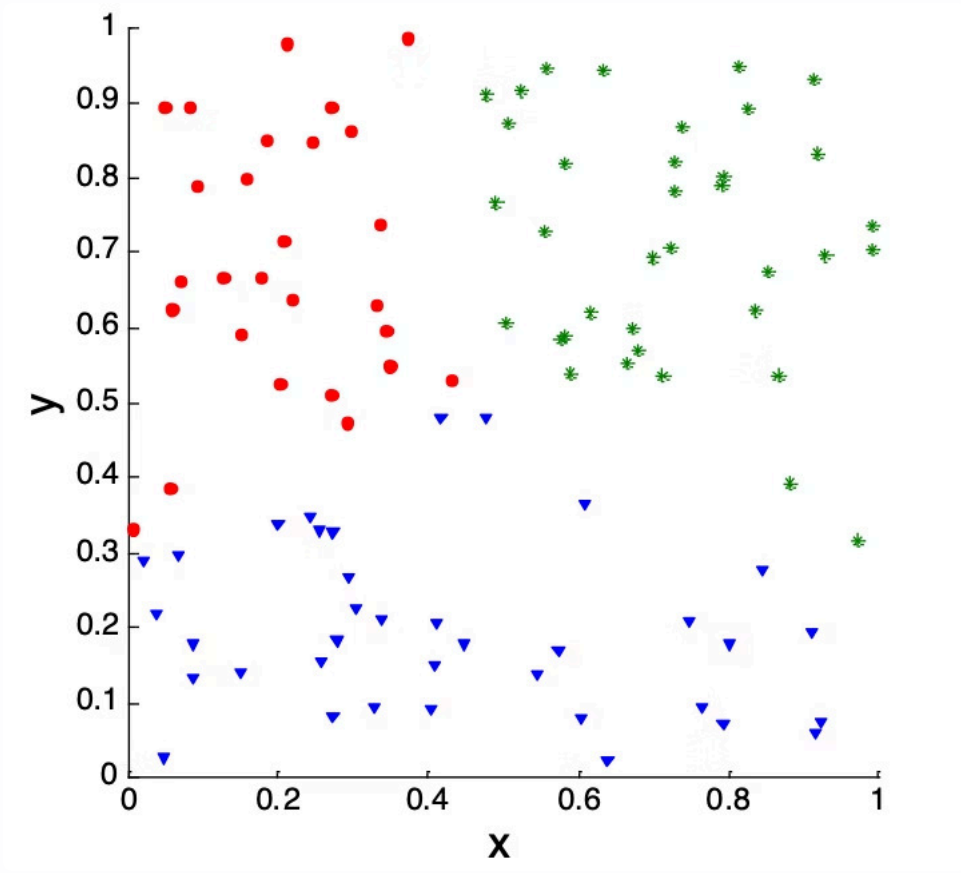
Random Points



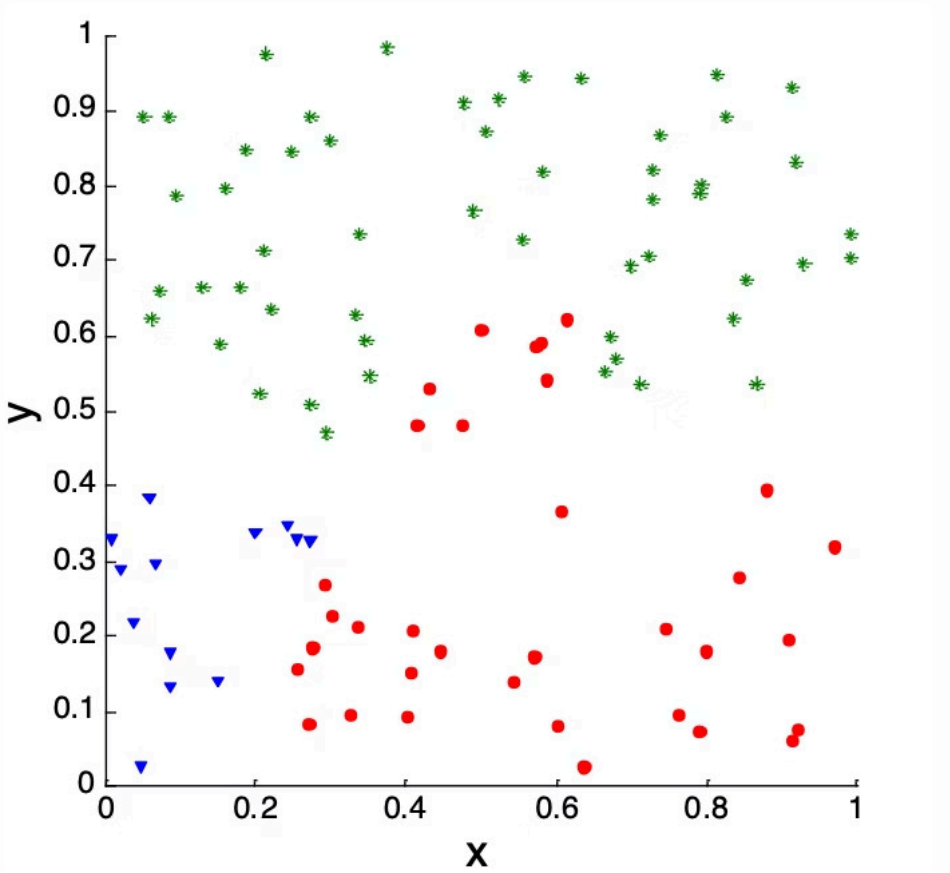
DBSCAN



K-means



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

1. Comparing the results of two different sets of cluster analyses to determine which is better.
2. 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.

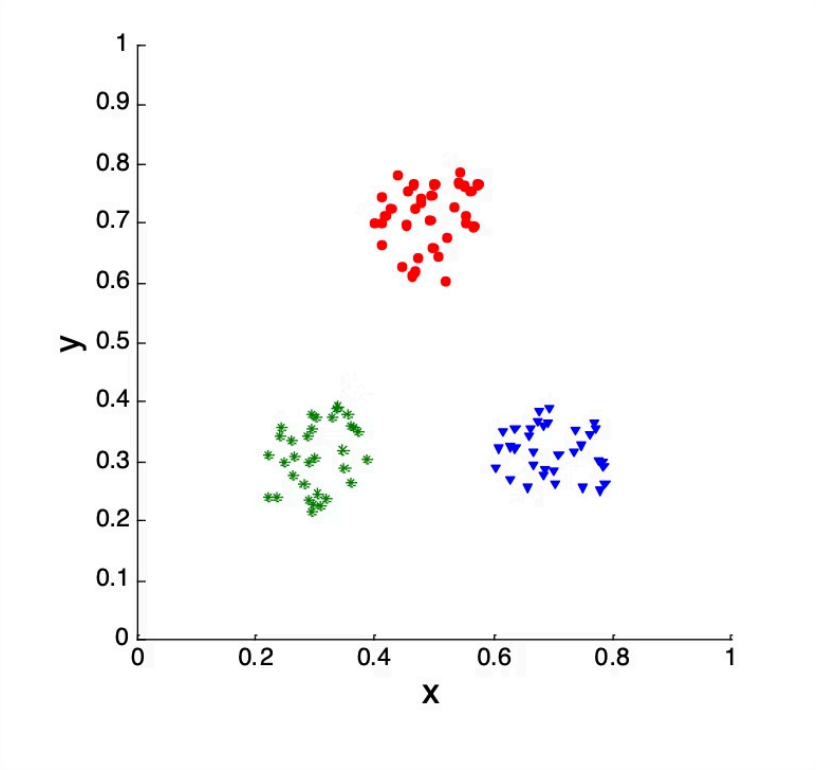
Measuring Cluster Validity Via Correlation

- Two matrices
  - Proximity Matrix
  - "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 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.

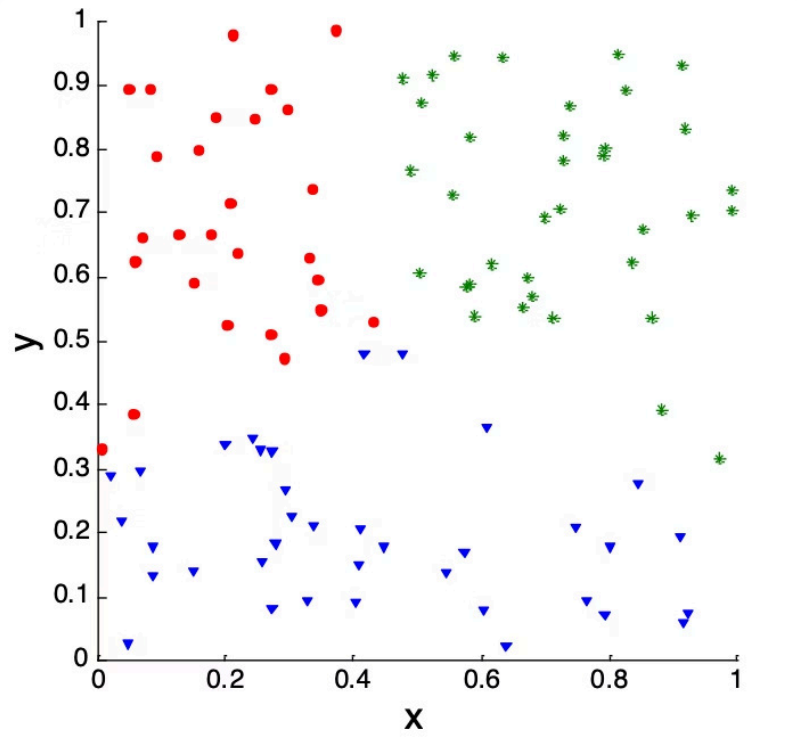
Measuring Cluster Validity Via Correlation

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

Corr = -0.9235

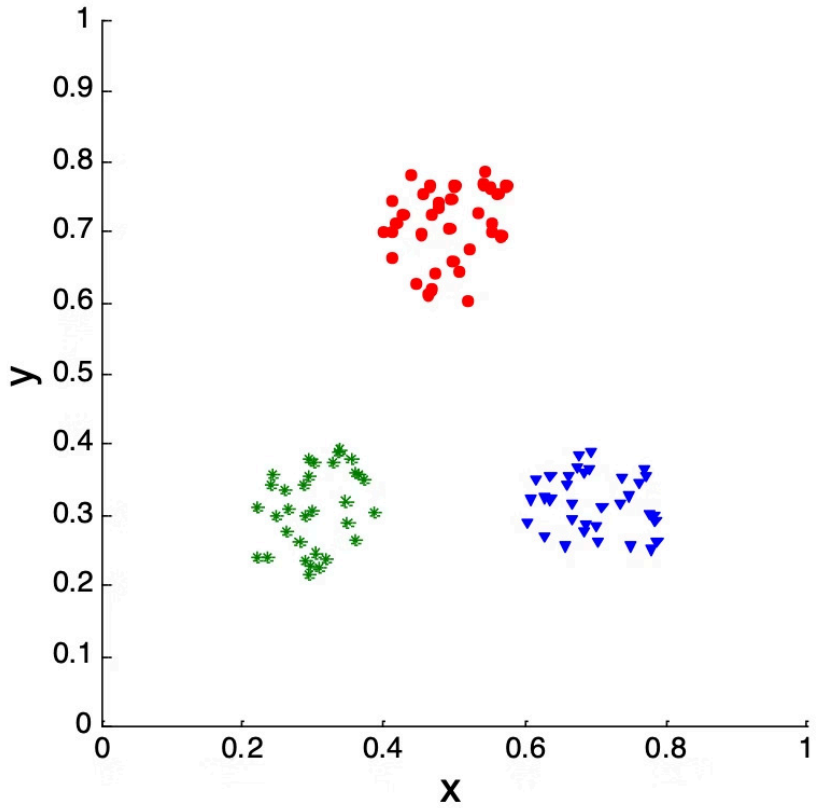


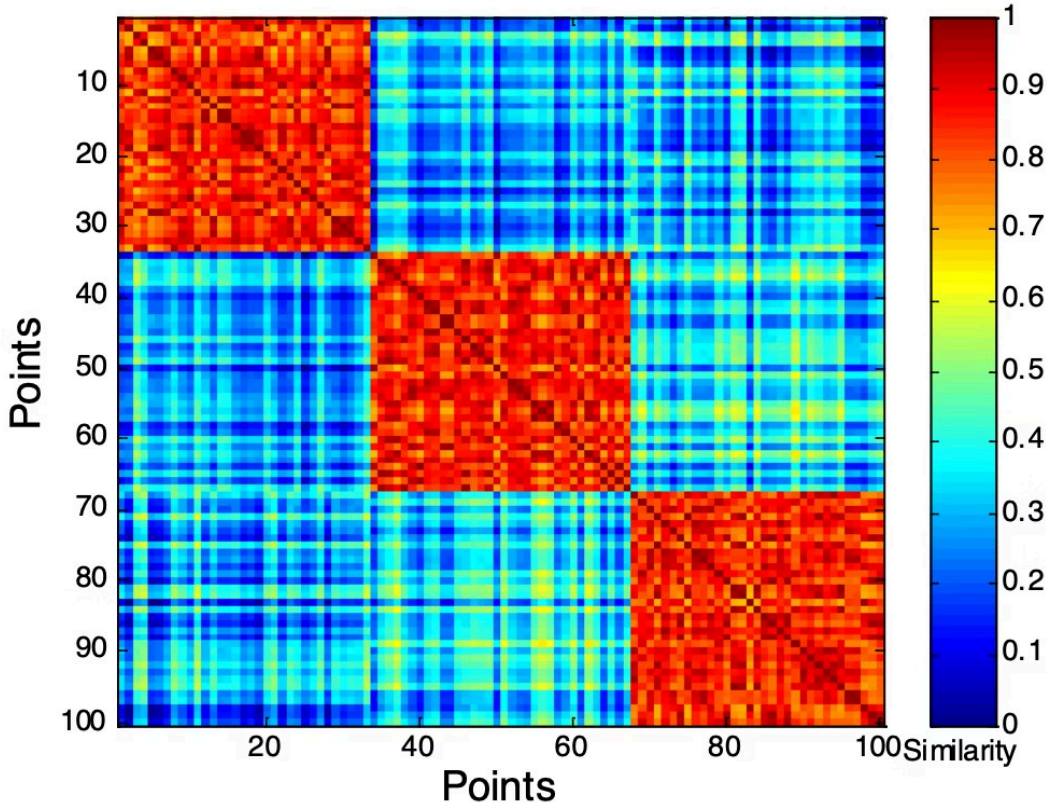
Corr = -0.5810



Using Similarity Matrix for Cluster Validation

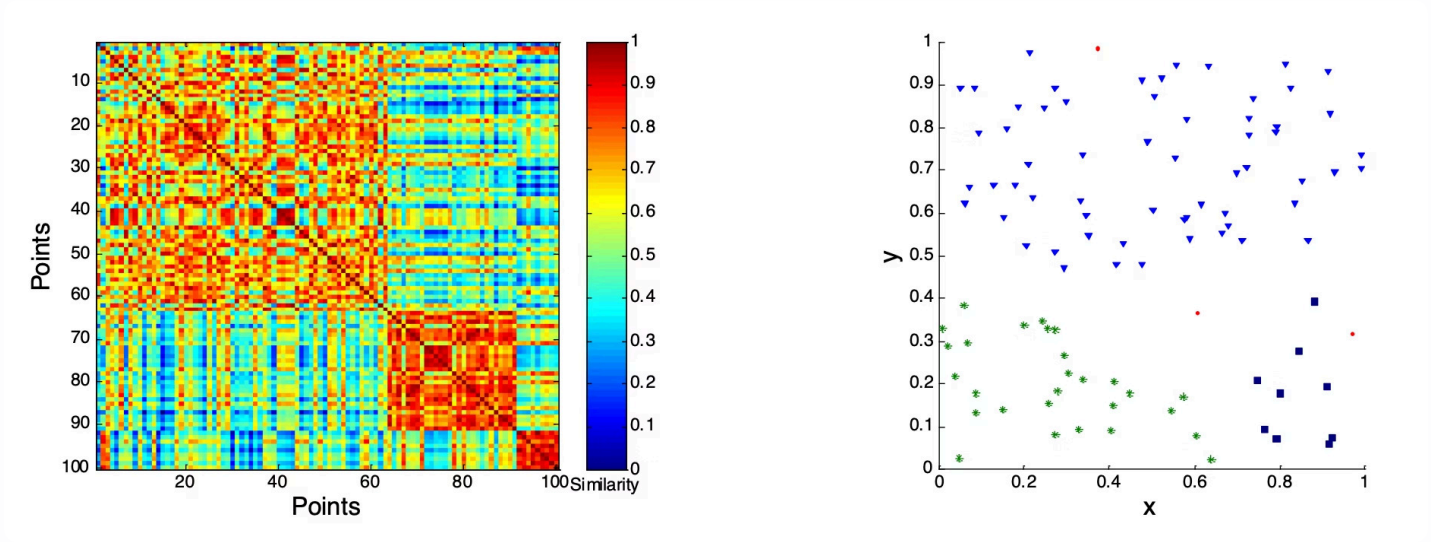
- Order the similarity matrix with respect to cluster labels and inspect visually.





Using Similarity Matrix for Cluster Validation

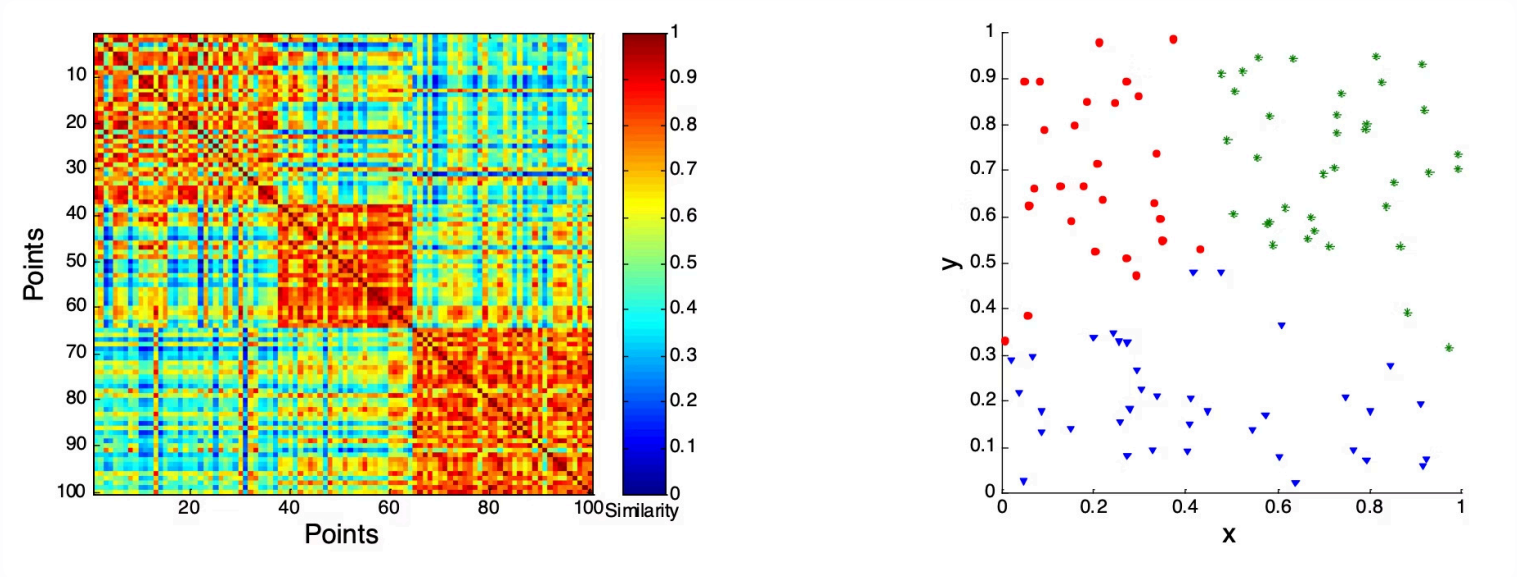
- Clusters in random data are not so crisp



DBSCAN

Using Similarity Matrix for Cluster Validation

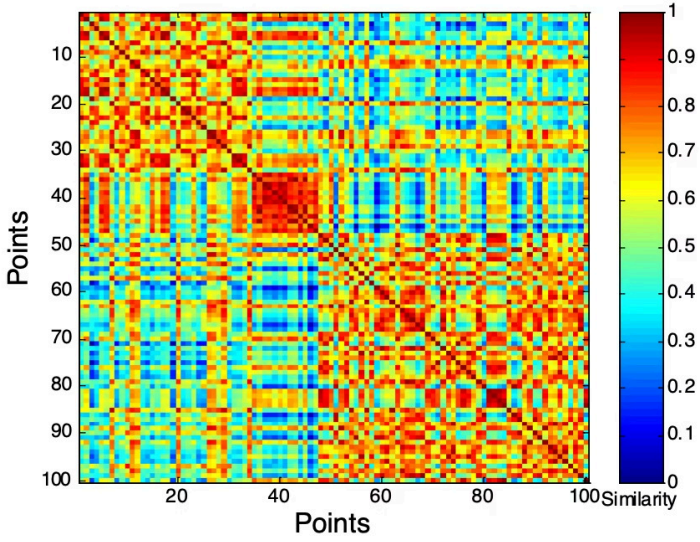
- Clusters in random data are not so crisp

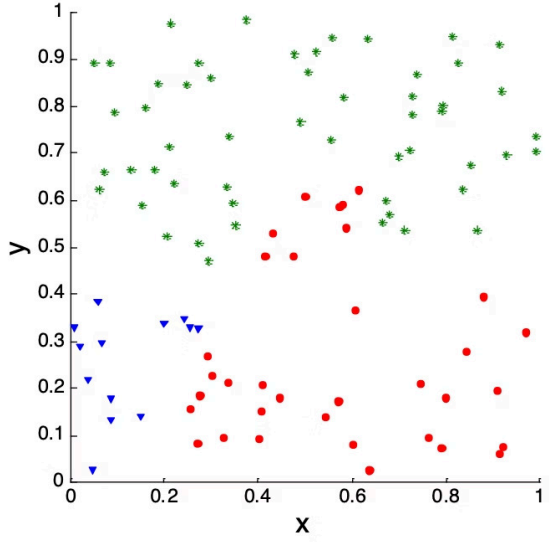


K-means

Using Similarity Matrix for Cluster Validation

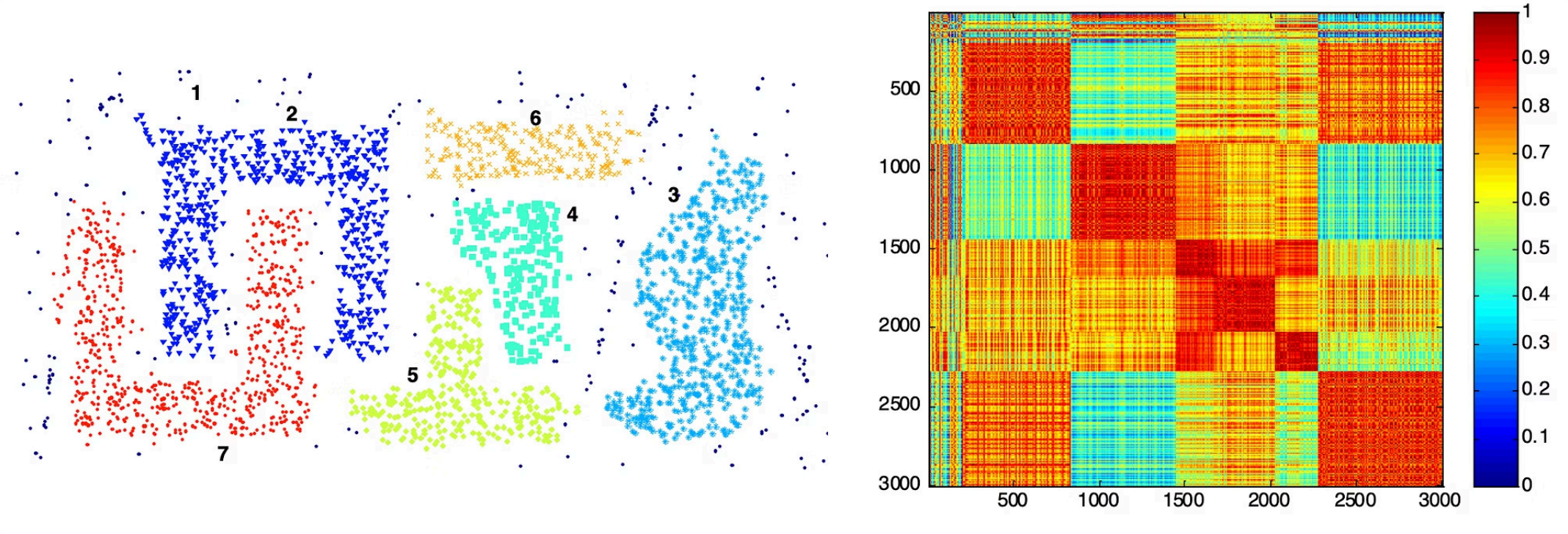
- Clusters in random data are not so crisp





Complete Link

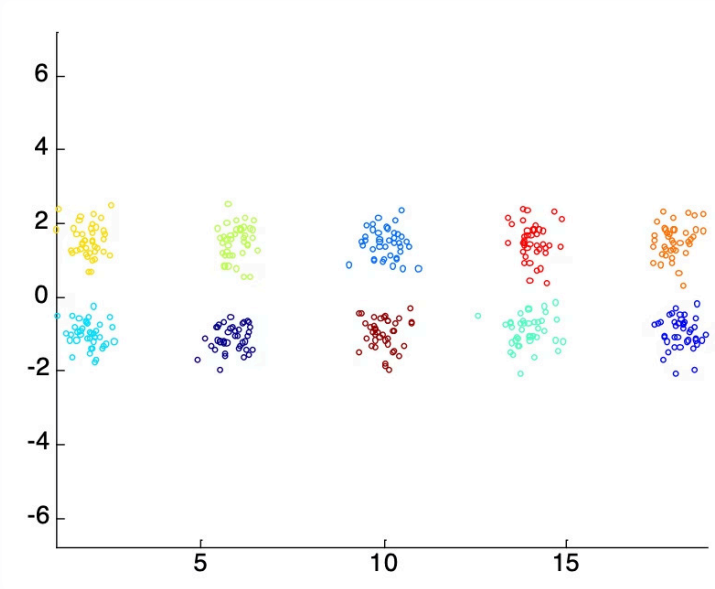
Using Similarity Matrix for Cluster Validation

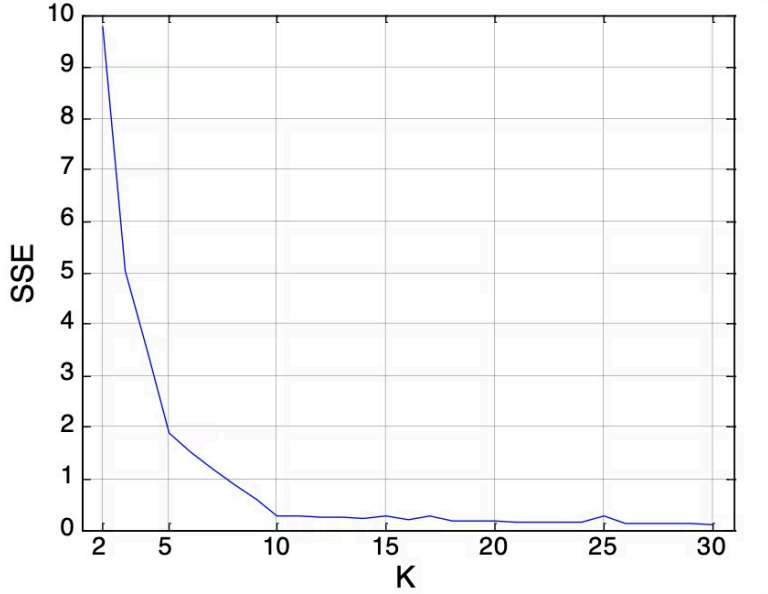


DBSCAN

Internal Measures: SSE

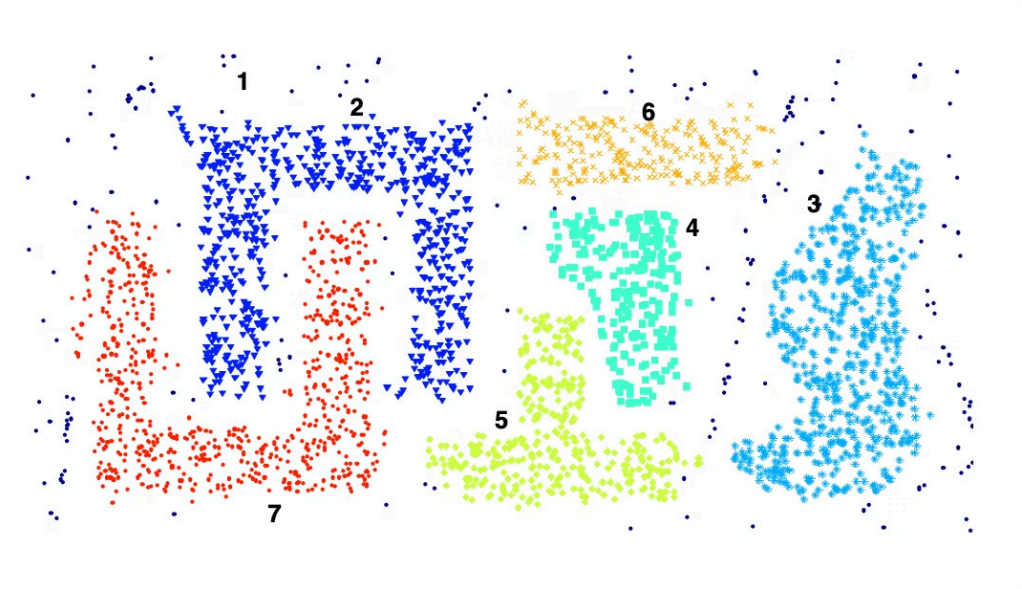
- Clusters in more complicated figures aren't well separated
- Internal Index: Used to measure the goodness of a clustering structure without respect to external information
  - SSE
- SSE is good for comparing two clusterings or two clusters (average SSE).
- Can also be used to estimate the number of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

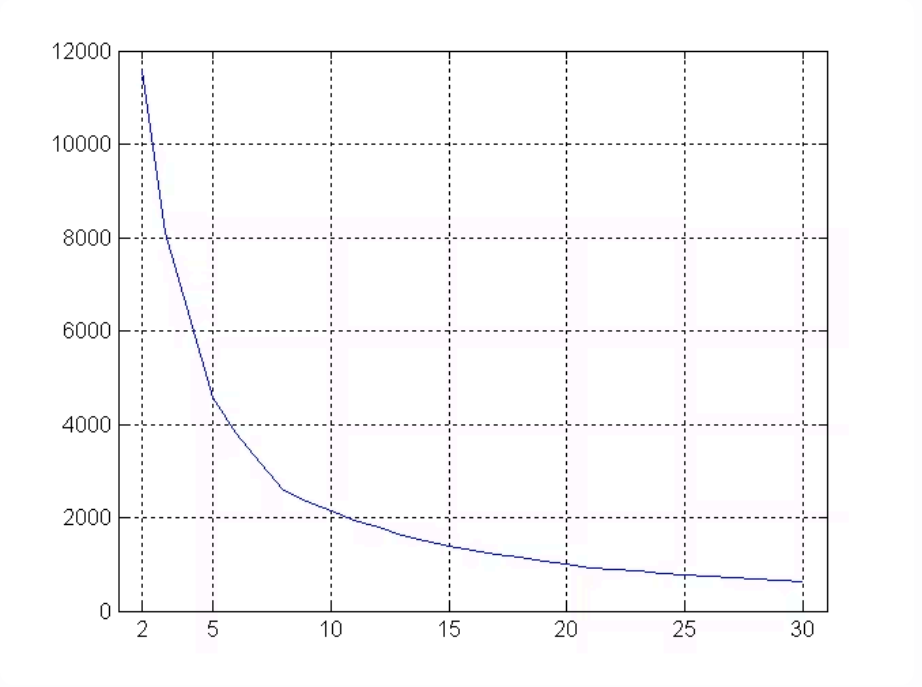




Internal Measures: SSE

- SSE curve for a more complicated data set





SSE of clusters found using K-means

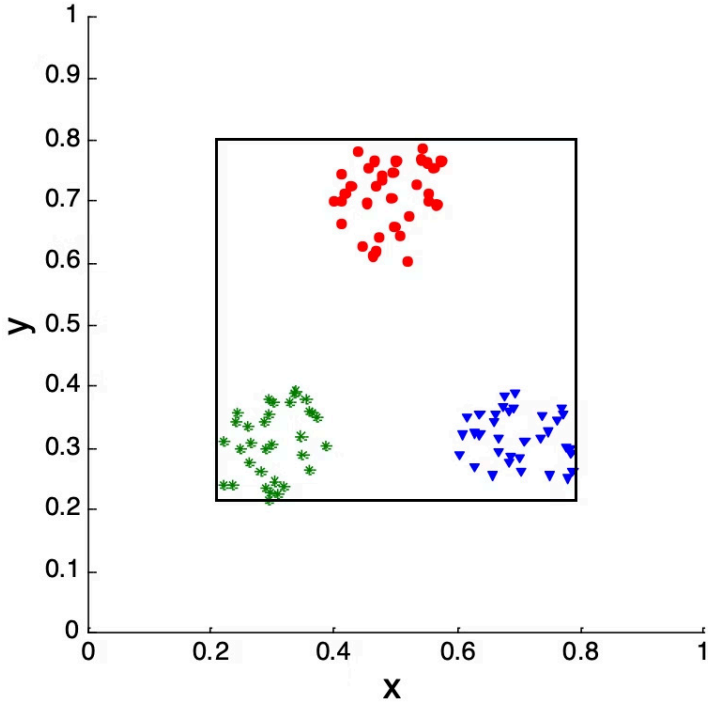
Framework for Cluster Validity

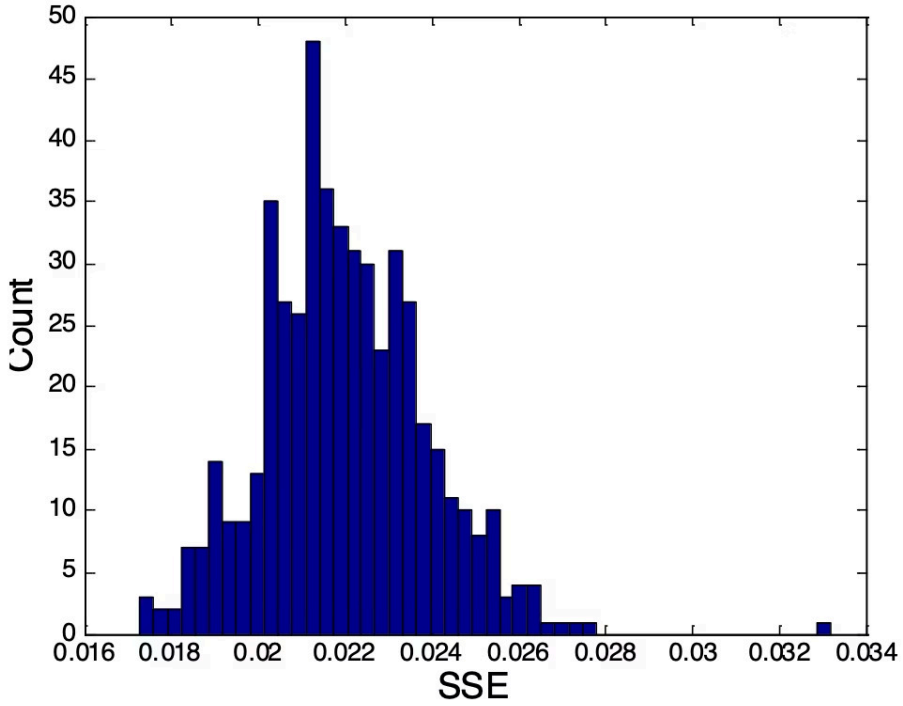
- Need a framework to interpret any measure.
  - For example, if our measure of evaluation has the value, 10, is that good, fair, or poor?
- Statistics provide a framework for cluster validity
  - The more "atypical" a clustering result is, the more likely it represents valid structure in the data
  - 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

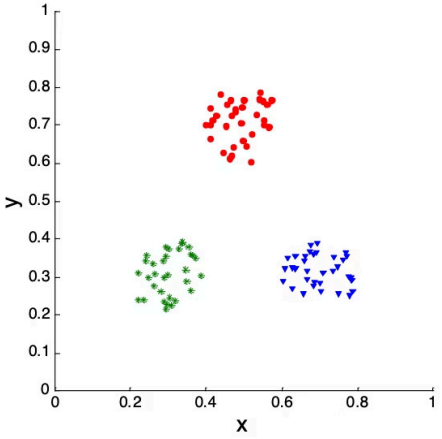
- Compare SSE of 0.005 against three clusters in random data
- Histogram shows SSE of three clusters in 500 sets of random data points of size 100 distributed over the range 0.2 – 0.8 for x and y values



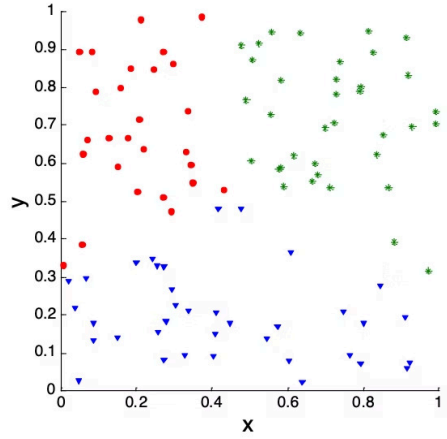


Statistical Framework for Correlation

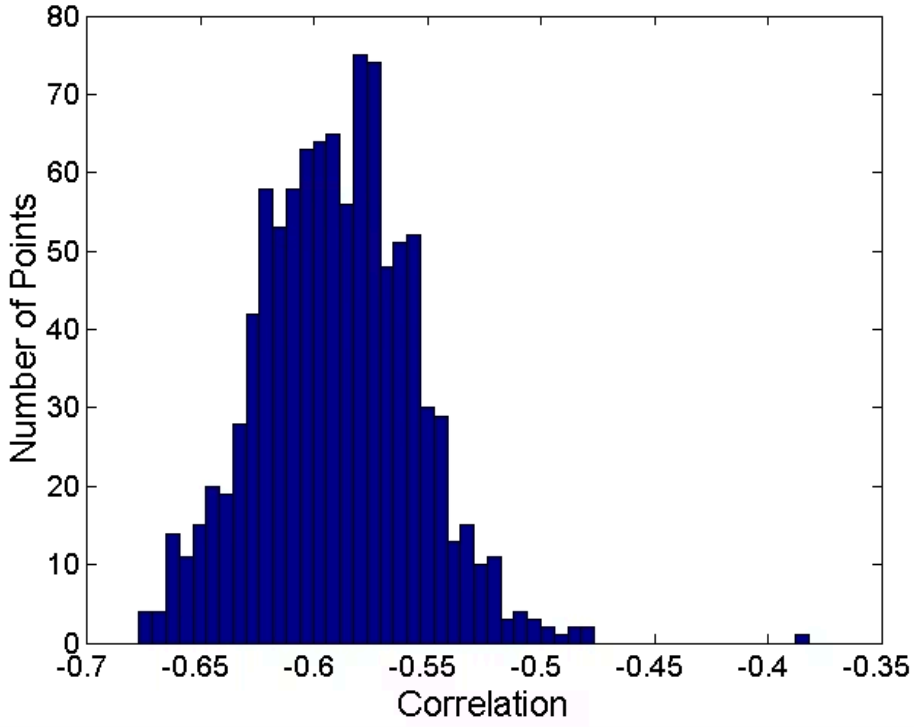
- Correlation of incidence and proximity matrices for the K-means clusterings of the following two data sets.



Corr = -0.9235



Corr = -0.5810



Internal Measures: Cohesion and Separation

Cluster Cohesion: Measures how closely related are objects in a cluster

Example: SSE

Cohesion is measured by the within cluster sum of squares (SSE)

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

Cluster Separation: Measure how distinct or well-separated a cluster is from other clusters

Example: Squared Error

Separation is measured by the between cluster sum of squares

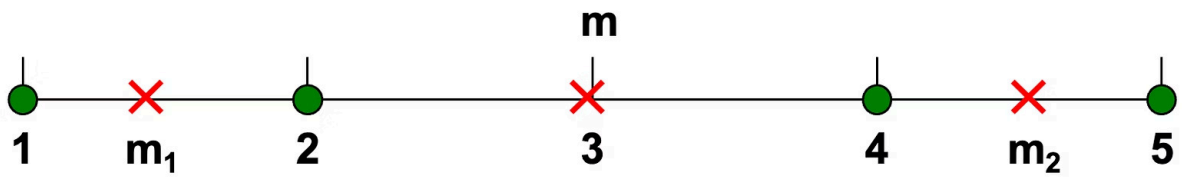
$$BSS = \sum_i |C_i| (m - m_i)^2$$

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

Internal Measures: Cohesion and Separation

lExample: SSE

–BSS + WSS = constant



K=1 cluster:

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

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

$$Total = 10 + 0 = 10$$

K=2 clusters:

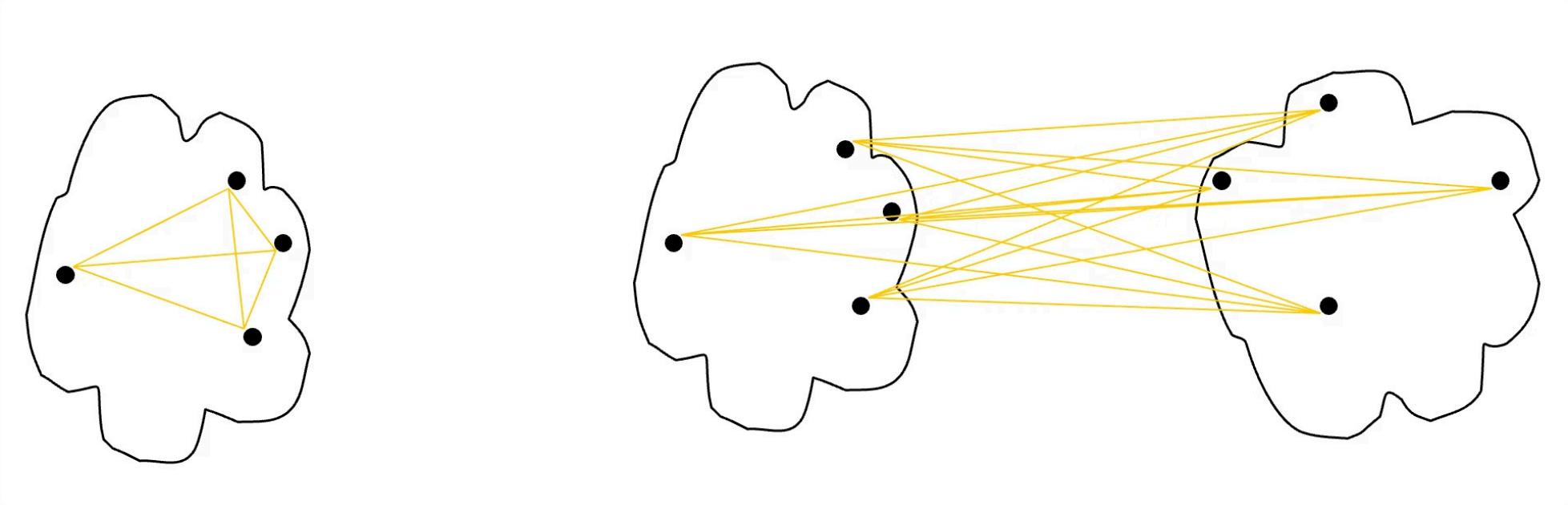
$$WSS = (1-1.5)^2 + (2-1.5)^2 + (4-4.5)^2 + (5-4.5)^2 = 1$$

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

$$Total = 1 + 9 = 10$$

Internal Measures: 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.

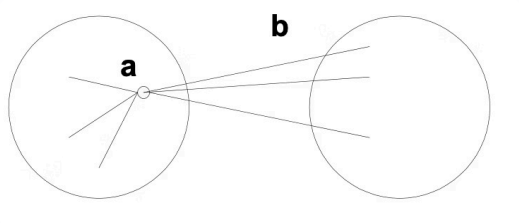


cohesion

separation

Internal Measures: Silhouette Coefficient

- Silhouette Coefficient combine 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 = 1 – a/b if a < b, (or s = b/a - 1 if a ≥ b, not the usual case)
  - Typically between 0 and 1.
  - The closer to 1 the better.
- Can calculate the Average Silhouette width 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$_j$ = $\Sigma_{i=1}^{L}$ p$_{ij}$ log2 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 = $\Sigma_{j=1}^{K}$ (m$_j$/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 = $\Sigma_{i=1}^{K}$ (m$_j$/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