
Pattern Analysis and Machine Intelligence

Lecture Notes on Clustering (IV)
2013-2014

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Course Schedule [*Tentative*]

| Date | Topic |
|------------|--|
| 25/11/2013 | Clustering I: Introduction, K-means |
| 29/11/2013 | Clustering II: K-M alternatives, Hierarchical, SOM |
| 02/12/2013 | Clustering III: Mixture of Gaussians, DBSCAN, J-P |
| 13/12/2013 | Clustering IV: Spectral Clustering, cluster evaluation |

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Lecture outline

- Cluster Evaluation
 - Internal measures
 - External measures
- Finding the correct number of clusters
- Framework for cluster validity

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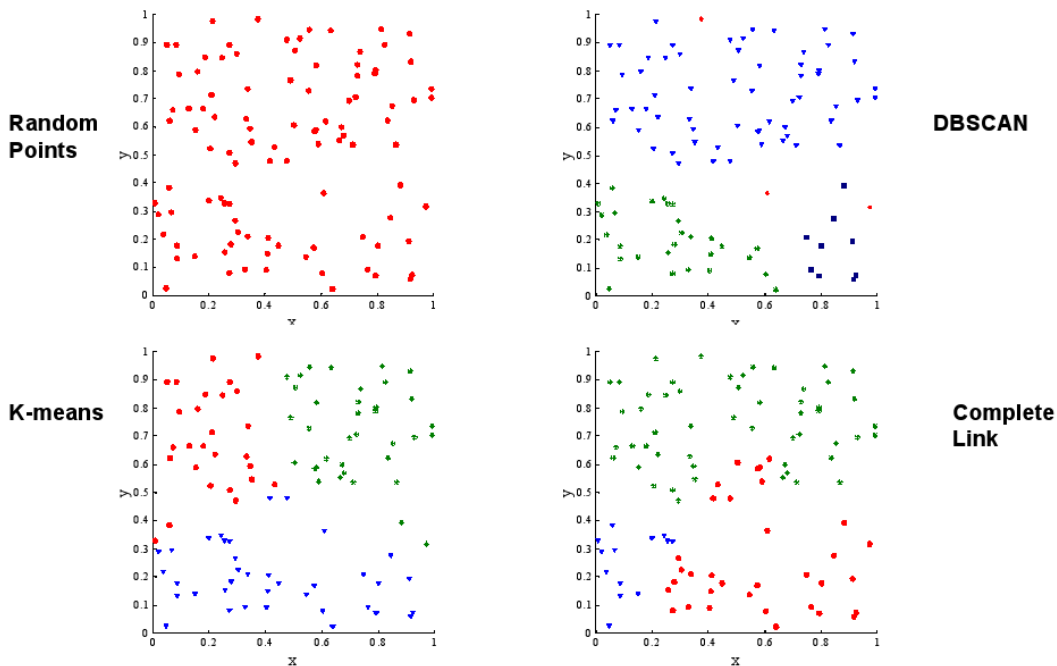
Cluster Evaluation

- Every algorithm has its pros and cons
 - (Not only about cluster quality: complexity, #clusters in advance, etc.)
- For what concerns cluster quality, we can *evaluate* (or, better, **validate**) clusters
- 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 can we evaluate the "goodness" of the resulting clusters?*
- But most of all... **why** should we evaluate it?

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Cluster found in random data

"Clusters are in the eye of the beholder"



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Why evaluate?

- To determine the **clustering tendency** of the dataset, that is distinguish whether non-random structure actually exists in the data
- To determine the **correct number of clusters**
- To evaluate how well the results of a cluster analysis fit the data *without* reference to external information
- To compare the results of a cluster analysis to externally known results, such as externally provided class labels
- To compare two sets of clusters to determine which is better

Note:

- the first three are *unsupervised techniques*, while the last two require external info
- the last three can be applied to the entire clustering or just to individual clusters

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Open challenges

Cluster evaluation has a number of challenges:

- a measure of cluster validity may be quite limited in the scope of its applicability
 - ie. dimensions of the problem: most work has been done only on 2- or 3-dimensional data
- we need a framework to interpret any measure
 - How good is "10"?
- if a measure is too complicated to apply or to understand, nobody will use it

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Measures of Cluster Validity

Numerical measures that are applied to judge various aspects of cluster validity are classified into the following three types:

- **Internal (unsupervised) Indices:** Used to measure the goodness of a clustering structure without respect to external information
 - cluster *cohesion* vs cluster *separation*
 - e.g. Sum of Squared Error (SSE)
- **External (supervised) Indices:** Used to measure the extent to which cluster labels match externally supplied class labels
 - e.g. entropy, purity, precision, ...
- **Relative Indices:** Used to compare two different clusterings or clusters
 - External or internal indices can be used, e.g. SSE or entropy

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External Measures

- Entropy
 - The degree to which each cluster consists of objects of a single class
 - For cluster i we compute p_{ij} , the probability that a member of **cluster** i belongs to **class** j , as $p_{ij} = m_{ij}/m_i$, where m_i is the number of objects in cluster i and m_{ij} is the number of objects of class j in cluster i
 - The **entropy** of each cluster i is $e_i = -\sum_{j=1}^L p_{ij} \log_2 p_{ij}$, where L is the number of classes
 - The **total entropy** is $e = \sum_{i=1}^K \frac{m_i}{m} e_i$, where K is the number of clusters and m is the total number of data points

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External Measures

- Purity
 - Another measure of the extent to which a cluster contains objects of a single class
 - Using the previous terminology, the **purity** of cluster i is $p_i = \max(p_{ij})$ for all the j
 - The **overall purity** is $purity = \sum_{i=1}^K \frac{m_i}{m} p_i$

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External Measures

- Precision
 - The fraction of a cluster that consists of objects of a specified class
 - The precision of cluster i with respect to class j is
 $precision(i, j) = p_{ij}$
- Recall
 - The extent to which a cluster contains all objects of a specified class
 - The recall of cluster i with respect to class j is
 $recall(i, j) = m_{ij}/m_j$, where m_j is the number of objects in class j

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External Measures

- F-measure
 - A combination of both precision and recall that measures the extent to which a cluster contains *only* objects of a particular class and *all* objects of that class
 - The F-measure of cluster i with respect to class j is
$$F(i, j) = \frac{2 \times precision(i, j) \times recall(i, j)}{precision(i, j) + recall(i, j)}$$

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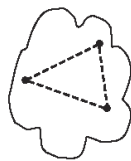
External Measures: example

Table 8.9. K-means clustering results for the *LA Times* document data set.

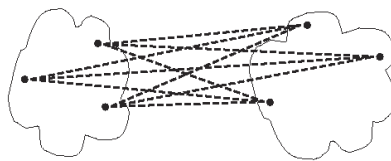
| Cluster | Entertainment | Financial | Foreign | Metro | National | Sports | Entropy | Purity |
|---------|---------------|-----------|---------|-------|----------|--------|---------|--------|
| 1 | 3 | 5 | 40 | 506 | 96 | 27 | 1.2270 | 0.7474 |
| 2 | 4 | 7 | 280 | 29 | 39 | 2 | 1.1472 | 0.7756 |
| 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 |

Internal measures: Cohesion and Separation

- Graph-based view



(a) Cohesion.

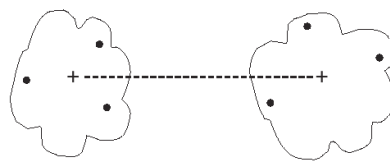


(b) Separation.

- Prototype-based view



(a) Cohesion.



(b) Separation.

Internal measures: Cohesion and Separation

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

$$cohesion(C_i) = \sum_{x \in C_i, y \in C_i} proximity(x, y)$$

$$cohesion(C_i) = \sum_{x \in C_i} proximity(x, c_i)$$

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

$$separation(C_i, C_j) = \sum_{x \in C_i, y \in C_j} proximity(x, y)$$

$$separation(C_i, C_j) = proximity(c_i, c_j)$$

$$separation(C_i) = proximity(c_i, c)$$

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Cohesion and separation example

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

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

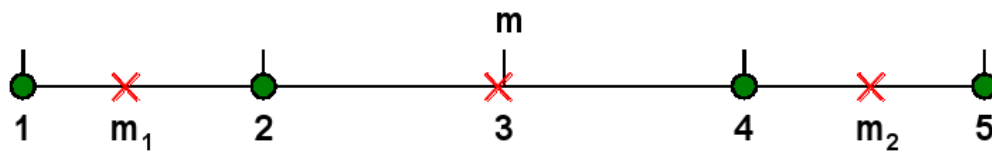
- Separation is measured by the between cluster sum of squares

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

where $|C_i|$ is the size of cluster i

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Cohesion and separation example



- 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:

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

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

$$Total = 1 + 9 = 10$$

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Evaluating individual clusters and Objects

- So far, we have focused on evaluation of a group of clusters
- Many of these measures, however, can also be used to evaluate individual clusters and objects
 - For example, a cluster with a high cohesion may be considered better than a cluster with a lower one
- This information can often be used to improve the quality of the clustering
 - Split not very cohesive clusters
 - Merge not very separated ones
- We can also evaluate the objects within a cluster in terms of their contribution to the overall cohesion or separation of the cluster

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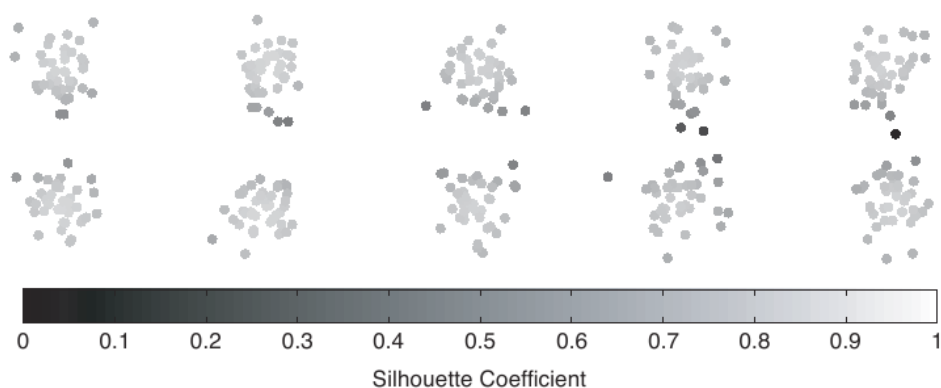
The Silhouette Coefficient

- 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_i = average distance of i to the points in its cluster
 - Calculate b_i = min (average distance of i to points in another cluster)
 - The silhouette coefficient for a point is then given by $s_i = (b_i - a_i) / \max(a_i, b_i)$

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The Silhouette Coefficient

- Silhouette Coefficient combine ideas of both cohesion and separation, but for individual points, as well as clusters and clusterings



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Measuring Cluster Validity via Correlation

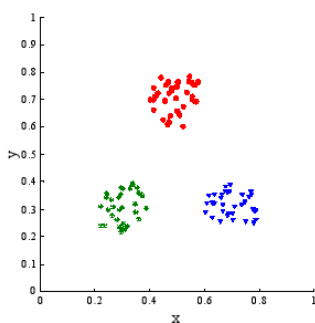
If we are given the similarity matrix for a data set and the cluster labels from a cluster analysis of the data set, then we can evaluate the "goodness" of the clustering by looking at the **correlation** between the similarity matrix and an ideal version of the similarity matrix based on the cluster labels

- Similarity/Proximity Matrix
- Ideal Matrix
 - One row and one column for each data point
 - An entry is 1 if the associated pair of points belongs to the same cluster
 - An entry is 0 if the associated pair of points belongs to different clusters

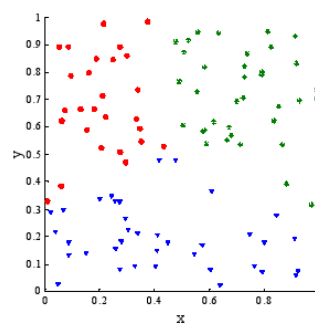
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Measuring Cluster Validity via Correlation

- 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



Corr = -0.9235

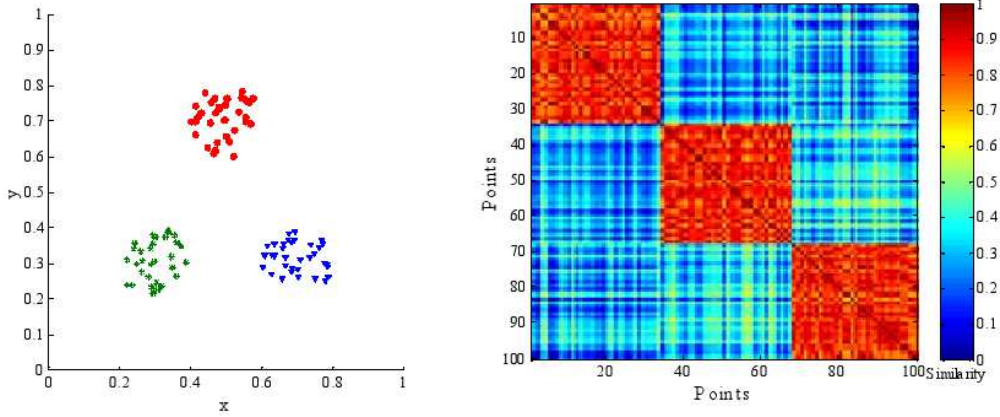


Corr = -0.5810

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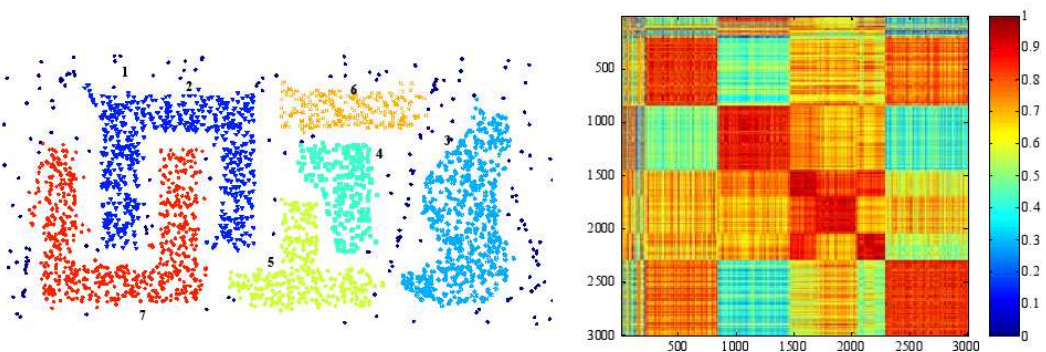
Using Similarity Matrix for Cluster Validation

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



Using Similarity Matrix for Cluster Validation

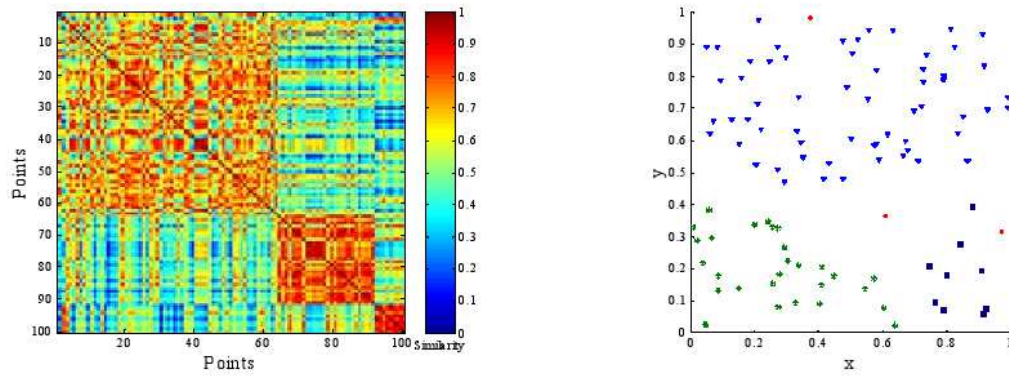
- Order the similarity matrix with respect to cluster labels and inspect visually



DBSCAN

Using Similarity Matrix for Cluster Validation

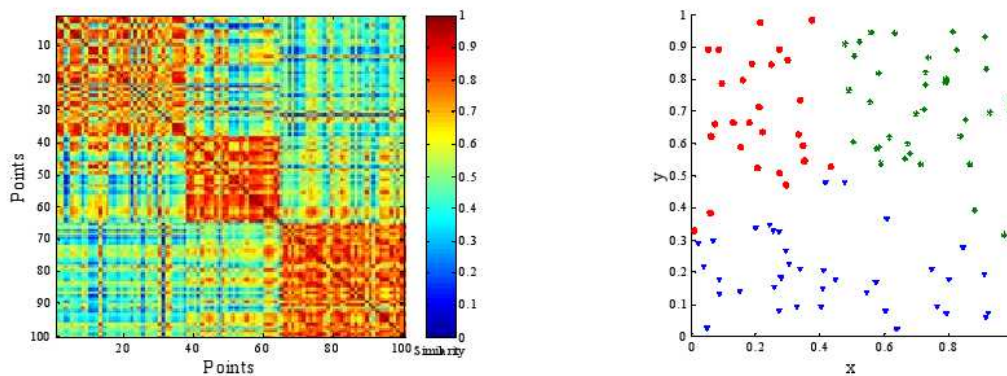
- Clusters in random data are not so crisp



DBSCAN

Using Similarity Matrix for Cluster Validation

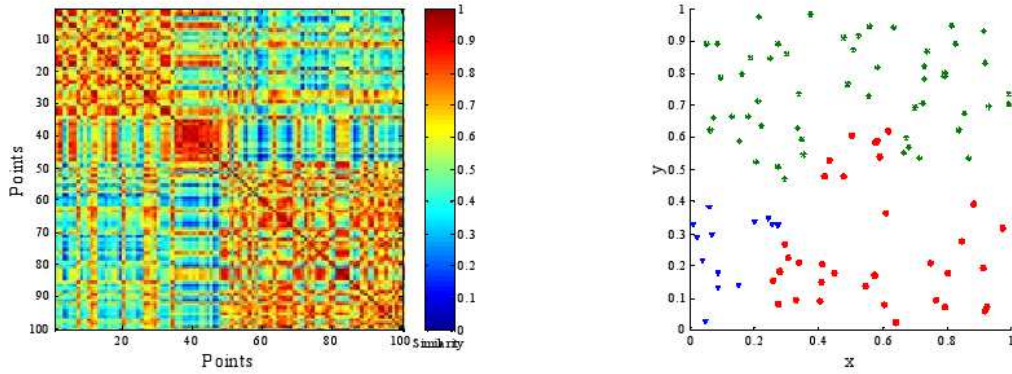
- Clusters in random data are not so crisp



K-means

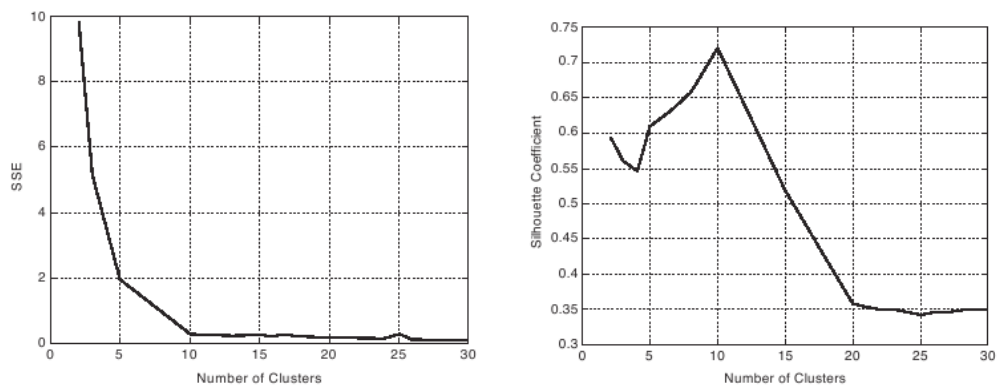
Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp



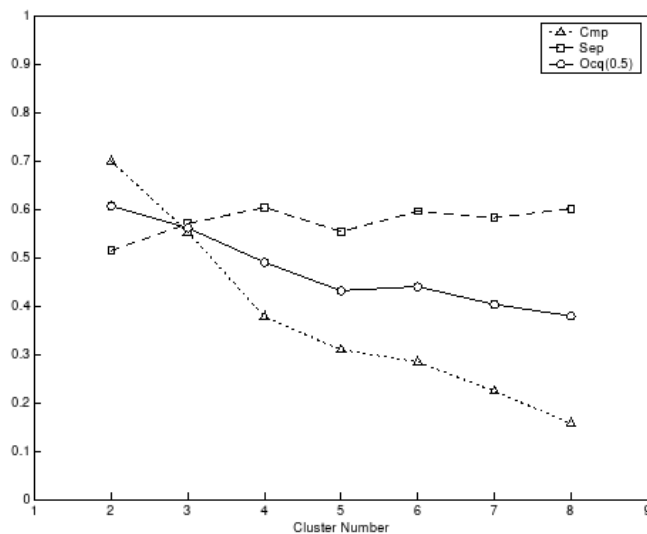
Complete Link

Finding the Correct Number of Clusters



- Look for the number of clusters for which there is a knee, peak, or dip in the plot of the evaluation measure when it is plotted against the number of clusters

Finding the Correct Number of Clusters



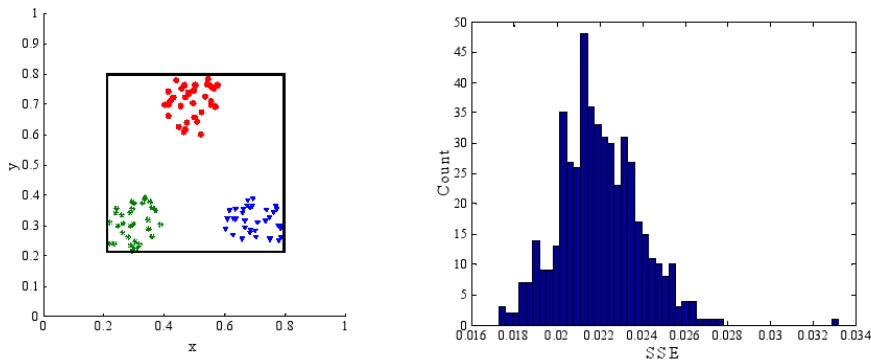
- Of course, this isn't always easy...

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

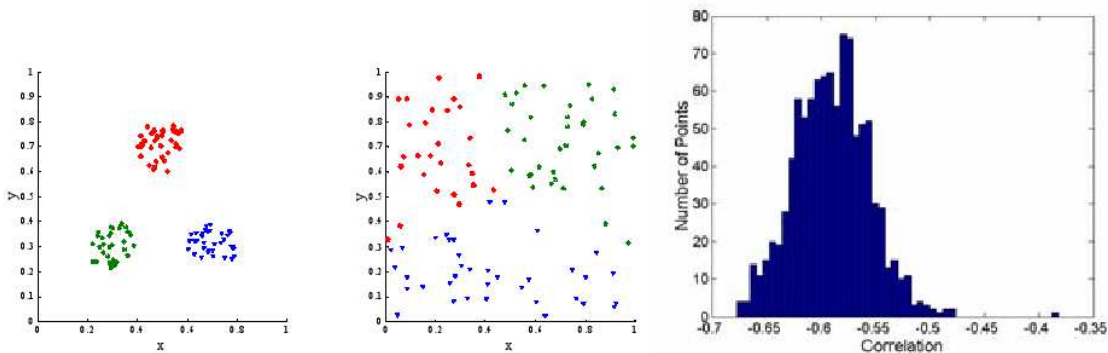
Statistical Framework for SSE

- 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

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

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Bibliography

- Slides about clustering for the Data Mining course
prof. Salvatore Orlando ([link](#))
- Tan, Steinbach, Kumar: "Introduction to Data Mining", Ch. 8
<http://www-users.cs.umn.edu/kumar/dmbook/index.php>

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