Cluster Validation

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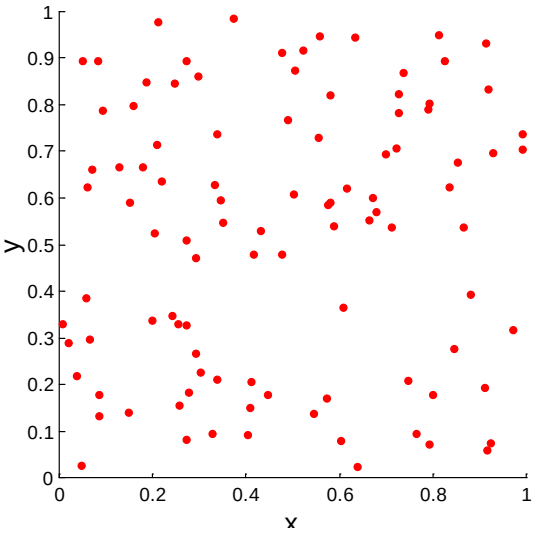
Cluster Validity

- 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



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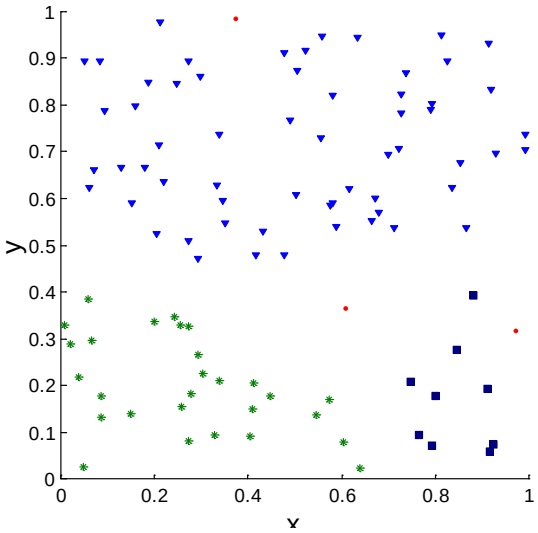
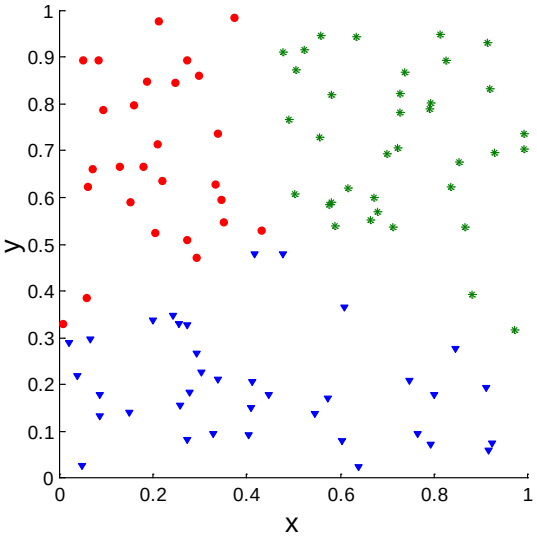


K-means



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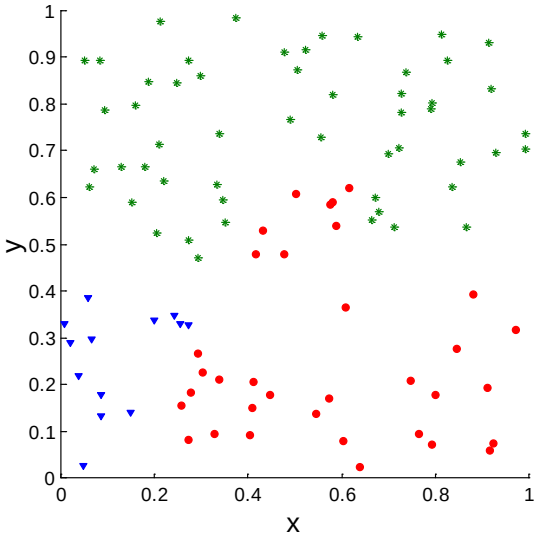


Different Aspects of Cluster Validation

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.

Supervised/External measures of Cluster Validation

- Classification Oriented
  - Entropy, Purity, Precision, Recall and F-measure
- Similarity Oriented
  - Involves comparison of two matrices
    - Ideal Cluster Similarity Matrix
    - Ideal Class Similarity Matrix

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 $purity = \sum_{i=1}^{K} \frac{m_i}{m} purity_j$.

Rand Index:Measures between pair decisions

Number of points	Same Cluster in clustering	Different Clusters in clustering
Same class in ground truth	20	24
Different classes in ground truth	20	72

$$RI = \frac{A + D}{A + B + C + D}$$

Compare with standard Precision and Recall:

$$P = \frac{A}{A + B} \qquad R = \frac{A}{A + C}$$

Unsupervised measures of Cluster Validation

- Measuring Cluster Validity via Correlation

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.

Correlation

- Correlation measures the linear relationship between objects
- To compute correlation, we standardize data objects, p and q, and then take their dot product

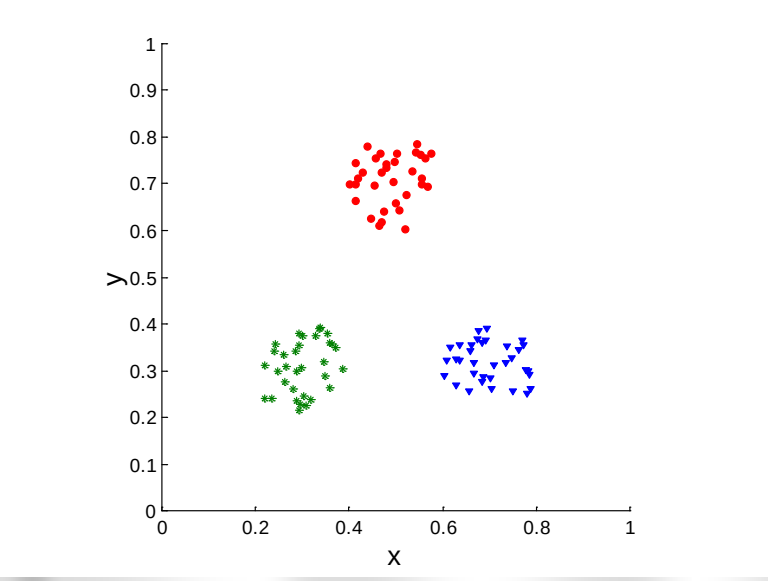
$$p'_k = (p_k - \boldsymbol{mean}(p)) / \boldsymbol{std}(p)$$

$$q'_k = (q_k - \boldsymbol{mean}(q)) / \boldsymbol{std}(q)$$

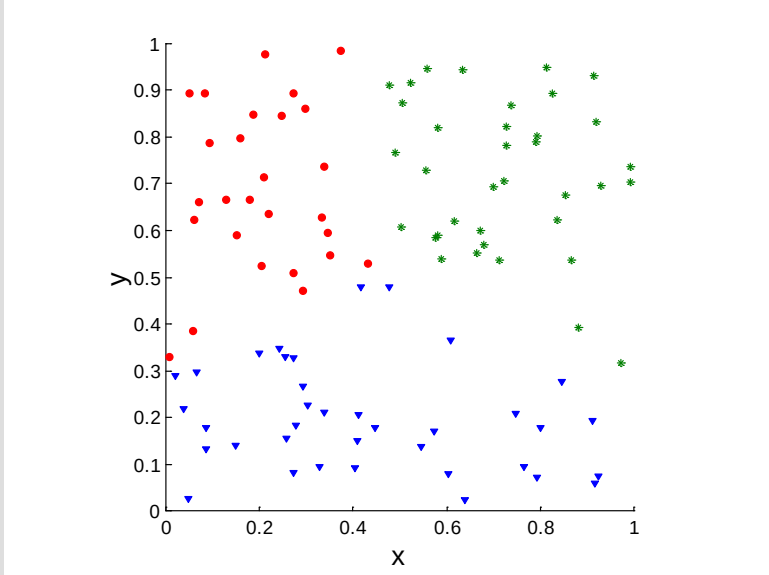
$$correlation(p, q) = p' \bullet q'$$

Measuring Cluster Validity Via Correlation

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



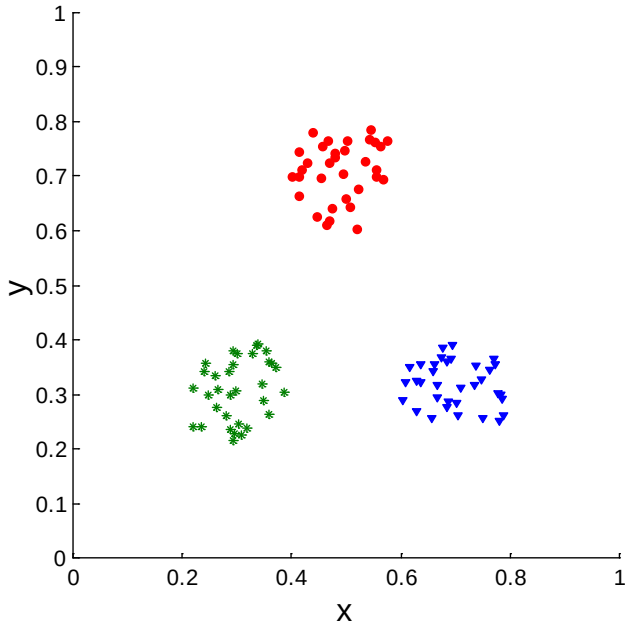
Corr = -0.9235

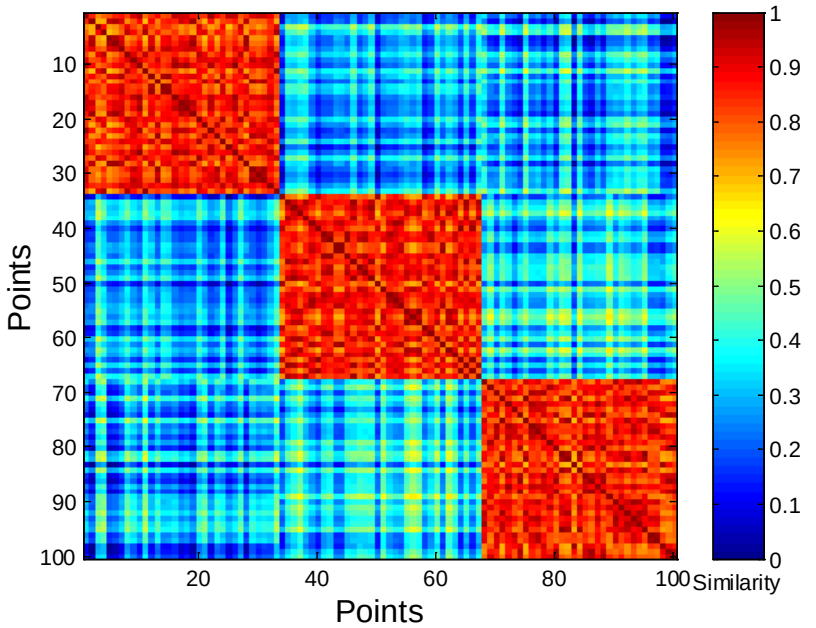


Corr = -0.5810

Using Similarity Matrix for Cluster Validation

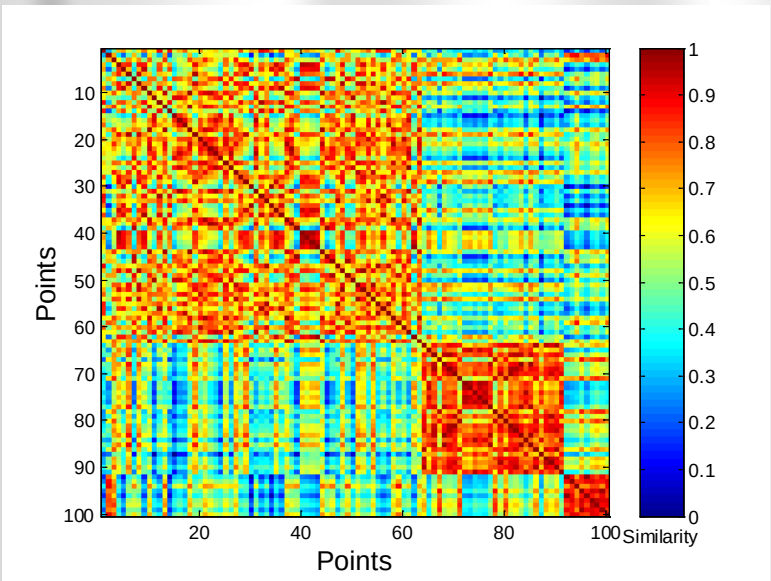
- Order the similarity matrix with respect to cluster labels and inspect visually.

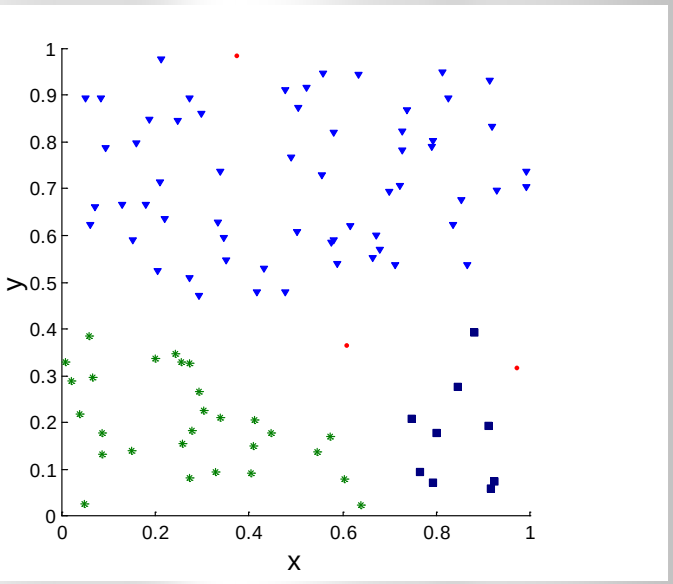




Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp





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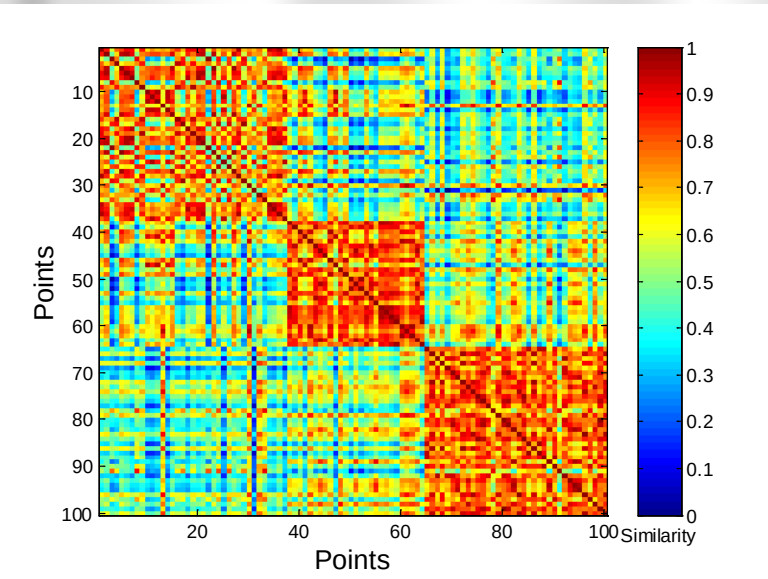
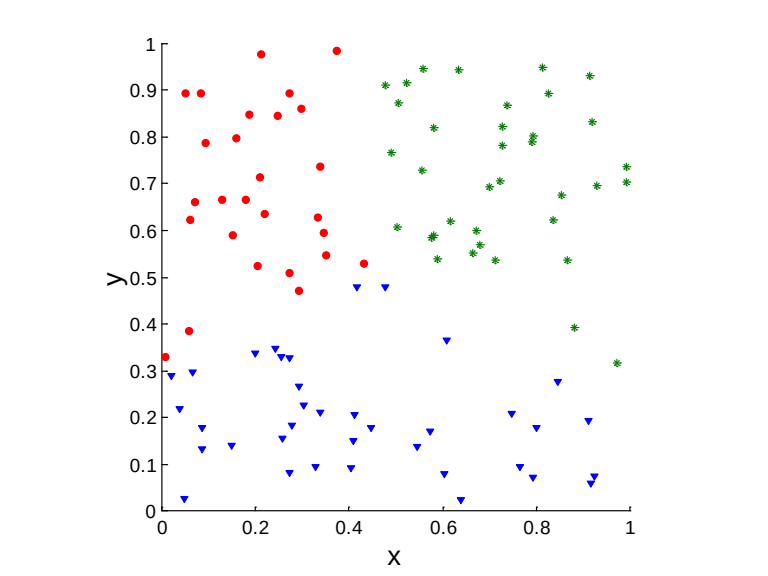
Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp

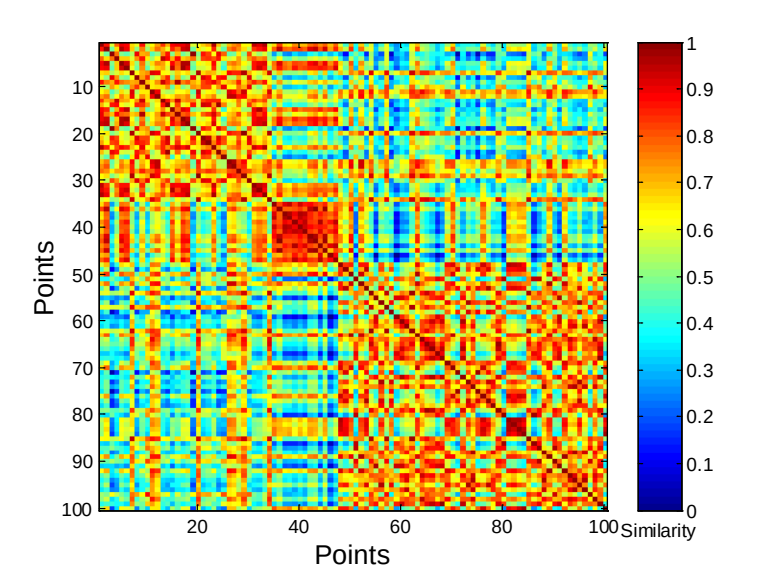


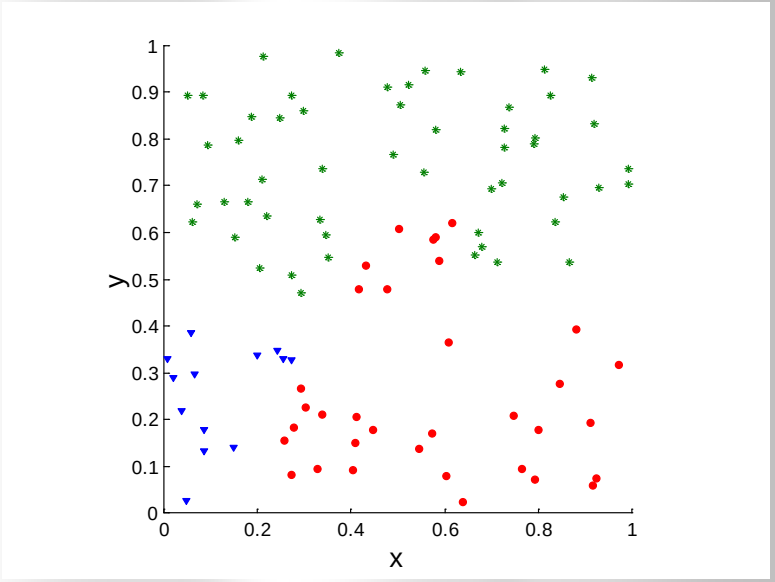


K-means

Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp





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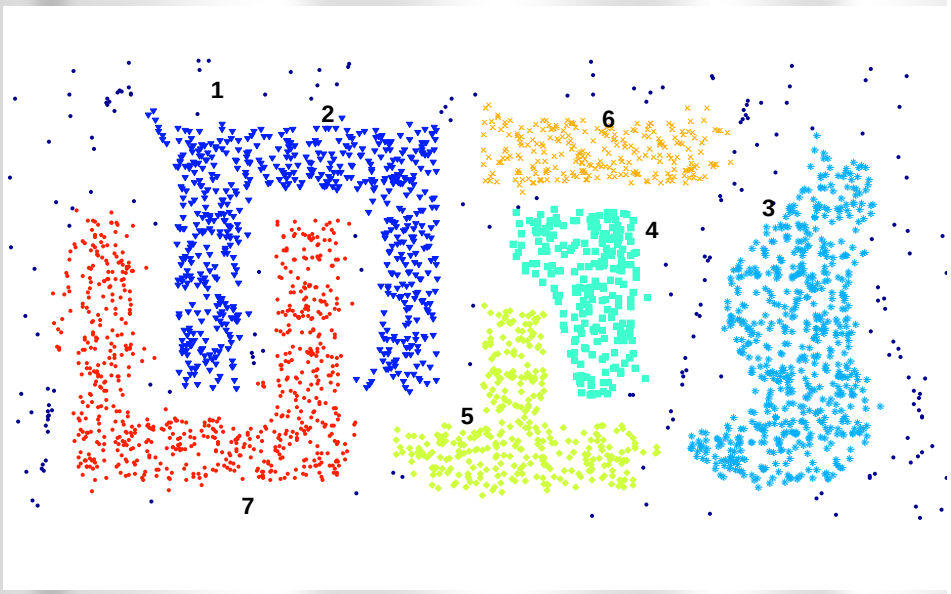
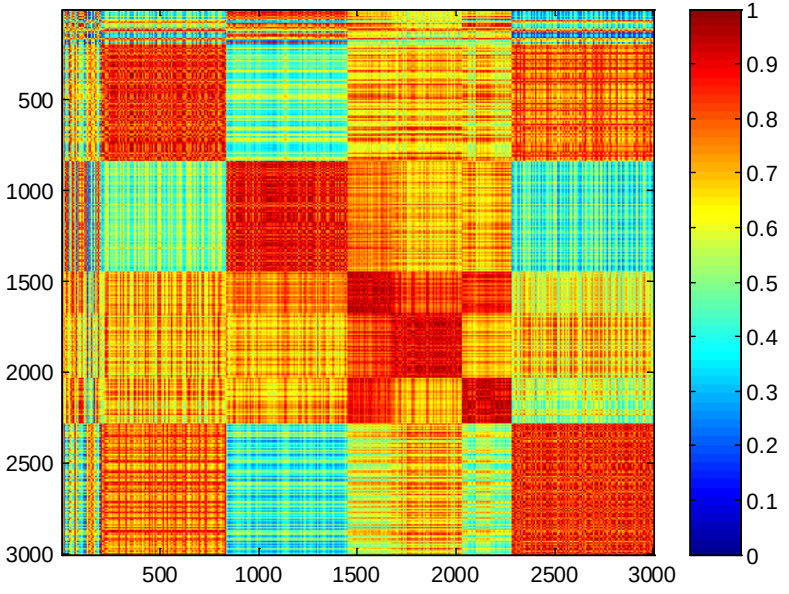
Using Similarity Matrix for Cluster Validation





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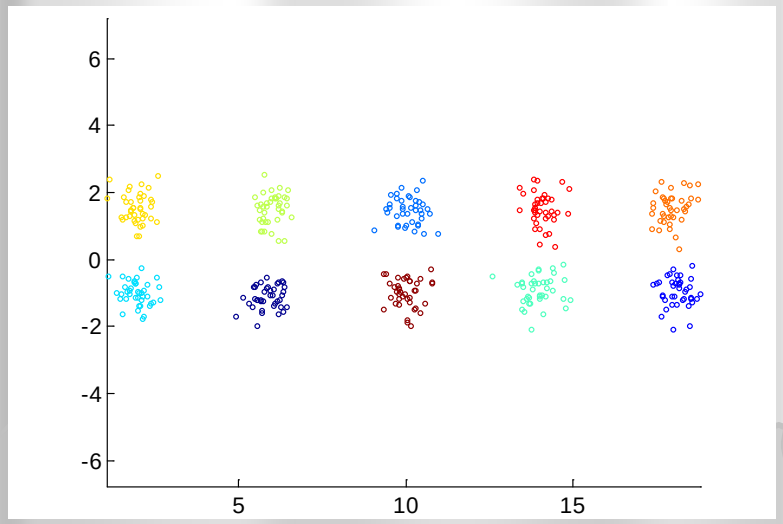
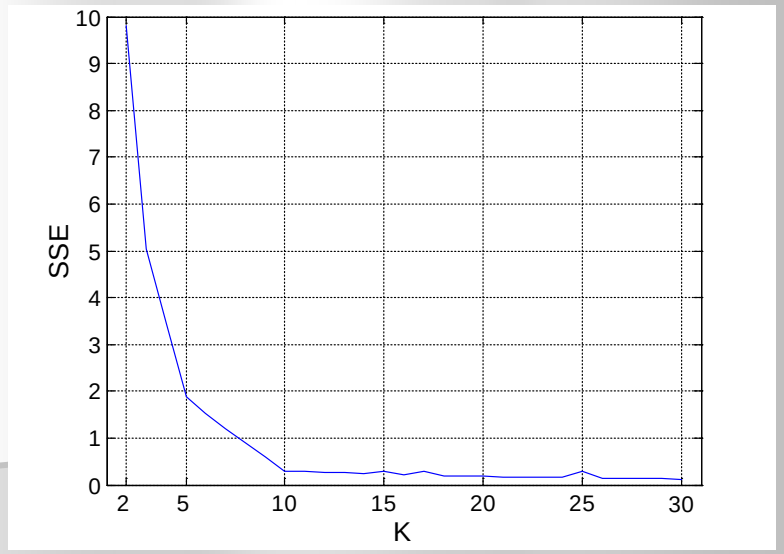
Internal Measures: SSE

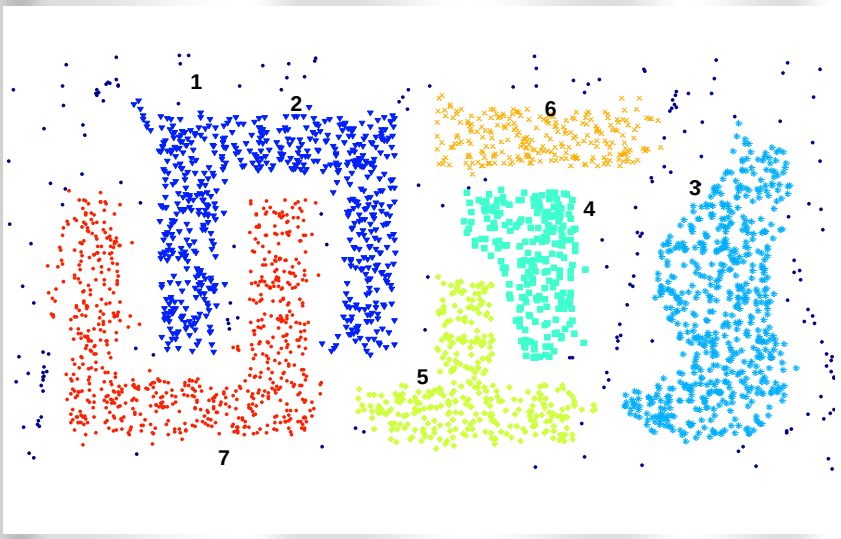
- Clusters in more complicated figures aren't well separated
- Internal Index: Used to measure the goodness of a clustering structure without respect to external information
  - SSE
- SSE is good for comparing two clusterings or two clusters (average SSE).
- Can also be used to estimate the number of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

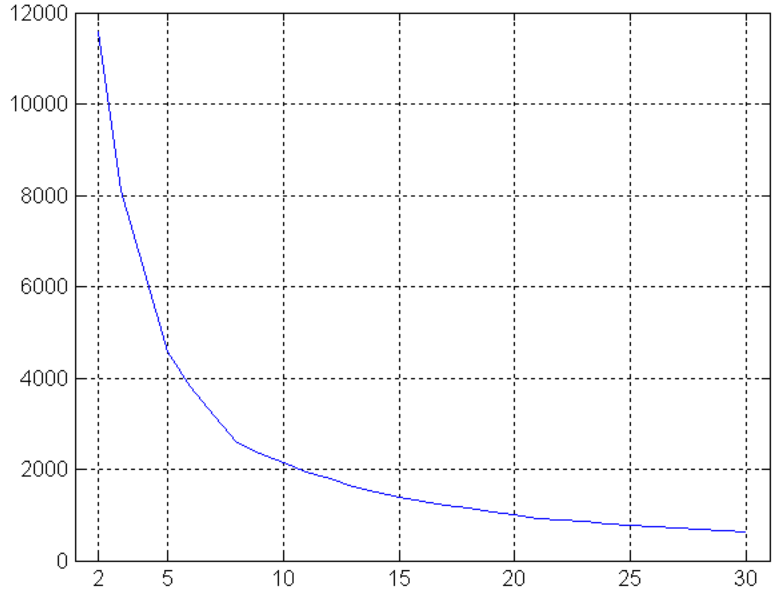




Internal Measures: SSE

- SSE curve for a more complicated data set

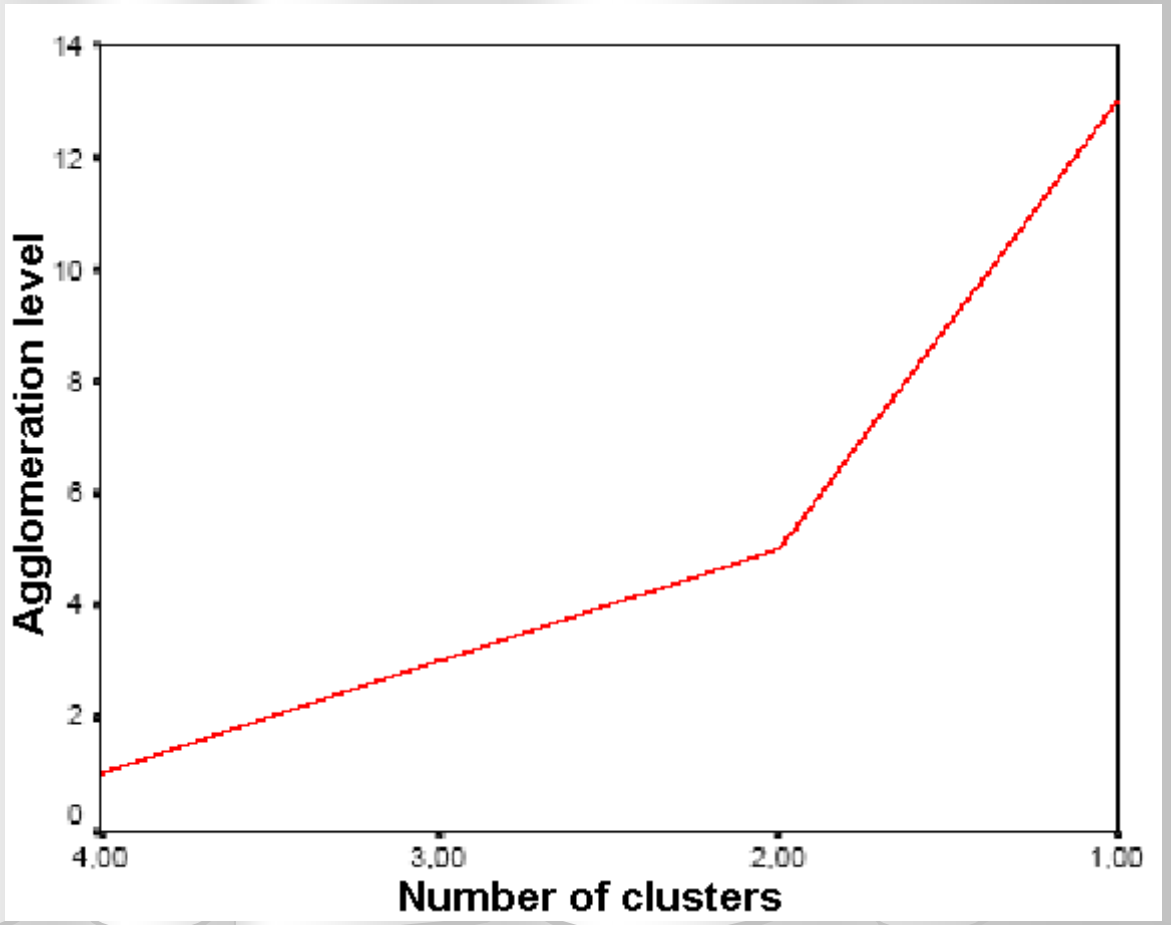




SSE of clusters found using K-means

Inverse Scree Test

- It is a plot with number of clusters on x-axis and agglomeration level on y-axis
- Look for sharp increase – elbow knick



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)

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

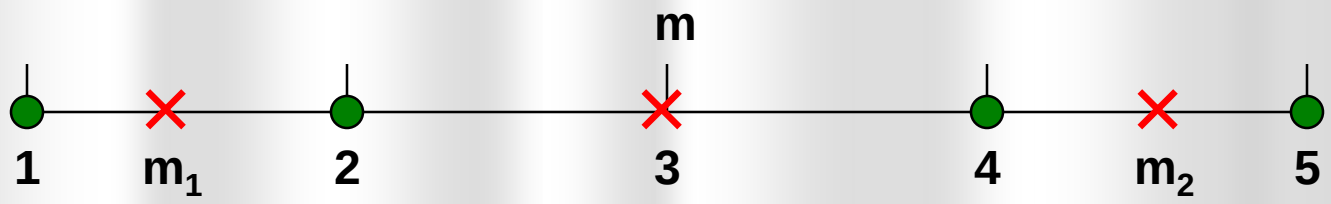
  - Separation is measured by the between cluster sum of squares

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

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

Internal Measures: Cohesion and Separation

- Example: SSE
  - BSS + WSS = constant



K=1 cluster:

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

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

$$Total = 10 + 0 = 10$$

K=2 clusters:

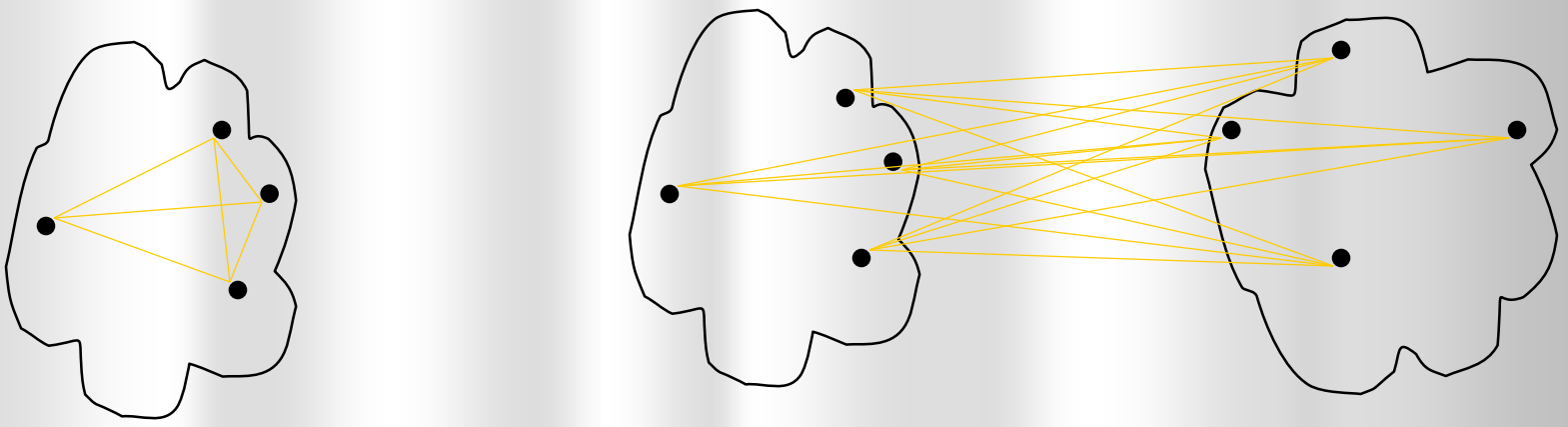
$$WSS = (1-1.5)^2 + (2-1.5)^2 + (4-4.5)^2 + (5-4.5)^2 = 1$$

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

$$Total = 1 + 9 = 10$$

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.

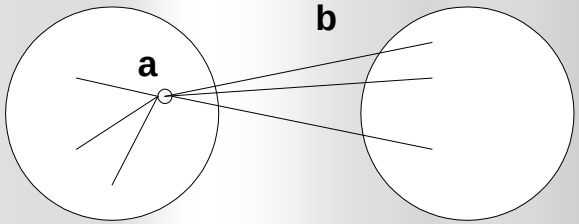


cohesion

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 $a \geq b$, 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

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

Anomaly/Outlier Detection

- What are anomalies/outliers?
  - The set of data points that are considerably different than the remainder of the data
- Variants of Anomaly/Outlier Detection Problems
  - Given a database D, find all the data points $\mathbf{x} \in D$ with anomaly scores greater than some threshold t
  - Given a database D, find all the data points $\mathbf{x} \in D$ having the top-n largest anomaly scores f($\mathbf{x}$)
  - Given a database D, containing mostly normal (but unlabeled) data points, and a test point $\mathbf{x}$, compute the anomaly score of $\mathbf{x}$ with respect to D
- Applications:
  - Credit card fraud detection, telecommunication fraud detection, network intrusion detection, fault detection{

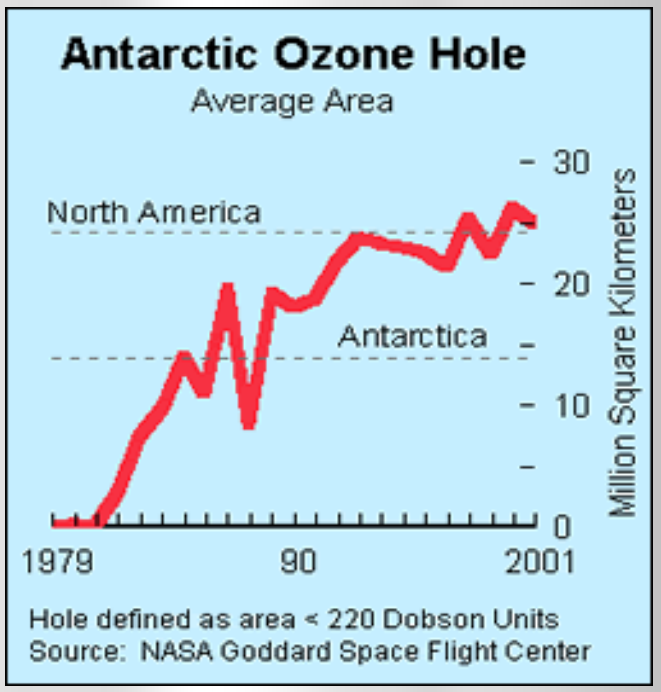
Importance of Anomaly Detection

Ozone Depletion History

- In 1985 three researchers (Farman, Gardinar and Shanklin) were puzzled by data gathered by the British Antarctic Survey showing that ozone levels for Antarctica had dropped 10% below normal levels

- Why did the Nimbus 7 satellite, which had instruments aboard for recording ozone levels, not record similarly low ozone concentrations?

- The ozone concentrations recorded by the satellite were so low they were being treated as outliers by a computer program and discarded!



Sources:
http://exploringdata.cqu.edu.au/ozone.html
http://www.epa.gov/ozone/science/hole/size.html

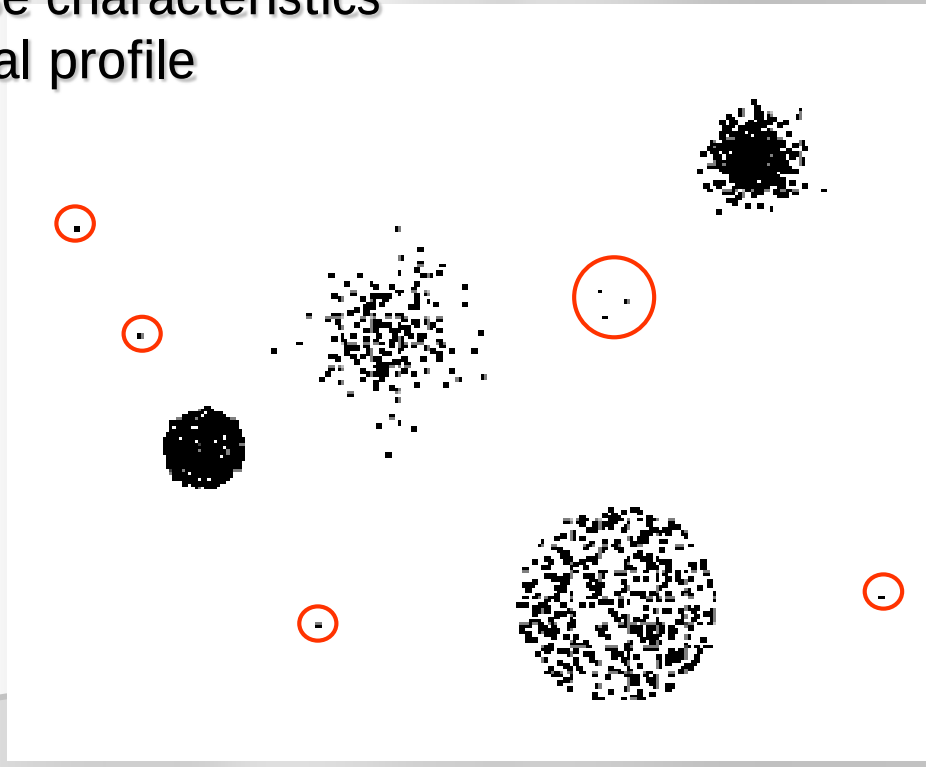
Anomaly Detection

- Challenges
  - How many outliers are there in the data?
  - Method is unsupervised
    - Validation can be quite challenging (just like for clustering)
- Working assumption:
  - There are considerably more “normal” observations than “abnormal” observations (outliers/anomalies) in the data

Anomaly Detection Schemes

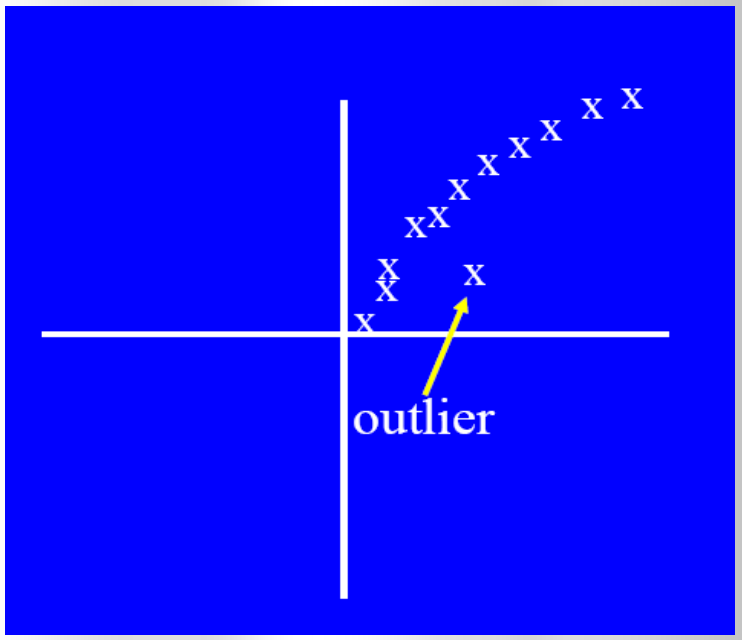
- General Steps
  - Build a profile of the “normal” behavior
    - Profile can be patterns or summary statistics for the overall population
  - Use the “normal” profile to detect anomalies
    - Anomalies are observations whose characteristics differ significantly from the normal profile

- Types of anomaly detection schemes
  - Graphical & Statistical-based
  - Distance-based
  - Model-based



Graphical Approaches

- Boxplot (1-D), Scatter plot (2-D), Spin plot (3-D)
- Limitations
  - Time consuming



Limitations of Statistical Approaches

- Most of the tests are for a single attribute
- In many cases, data distribution may not be known
- For high dimensional data, it may be difficult to estimate the true distribution

Distance-based Approaches

- Data is represented as a vector of features
- Three major approaches
  - Nearest-neighbor based
  - Density based
  - Clustering based

Nearest-Neighbor Based Approach

- Approach:
  - Compute the distance between every pair of data points
  - There are various ways to define outliers:
    - Data points for which there are fewer than *p* neighboring points within a distance *D*
    - The top n data points whose distance to the kth nearest neighbor is greatest
    - The top n data points whose average distance to the k nearest neighbors is greatest

Clustering-Based

- Basic idea:
  - Cluster the data into groups of different density
  - Choose points in small cluster as candidate outliers
  - Compute the distance between candidate points and non-candidate clusters.
    - If candidate points are far from all other non-candidate points, they are outliers