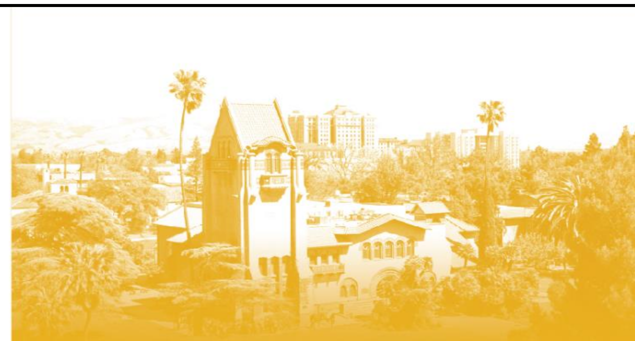

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Vector Data – Clustering

1

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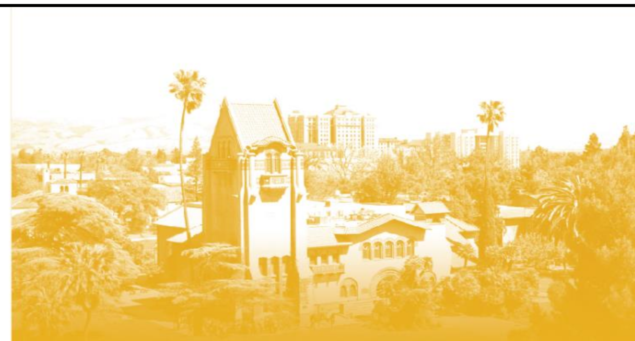
Agenda

- Review of Clustering Basics
- Partitioning methods: K-Means
- Hierarchical Methods
- Cluster Validity Evaluation

2



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Review of Clustering Basics

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Clustering

- Clustering refers to a very broad set of techniques for finding subgroups, or clusters, in a data set.
- We seek a partition of the data into distinct groups so that the observations within each group are quite similar to each other.
- To do so, we must define what it means for two or more observations to be similar or different (dissimilar).
- Very often a domain-specific consideration that must be made based on knowledge of the data being studied.

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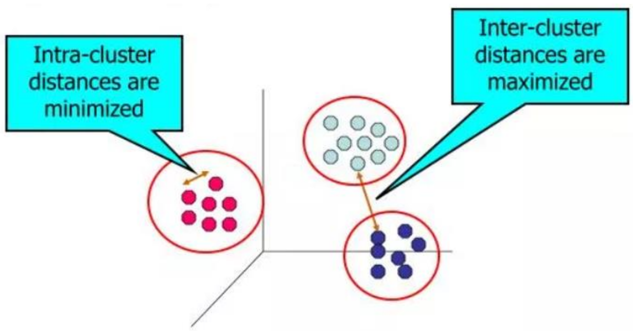
What is Cluster Analysis

- Cluster Analysis is a statistical method used to group "similar" items based on their characteristics.



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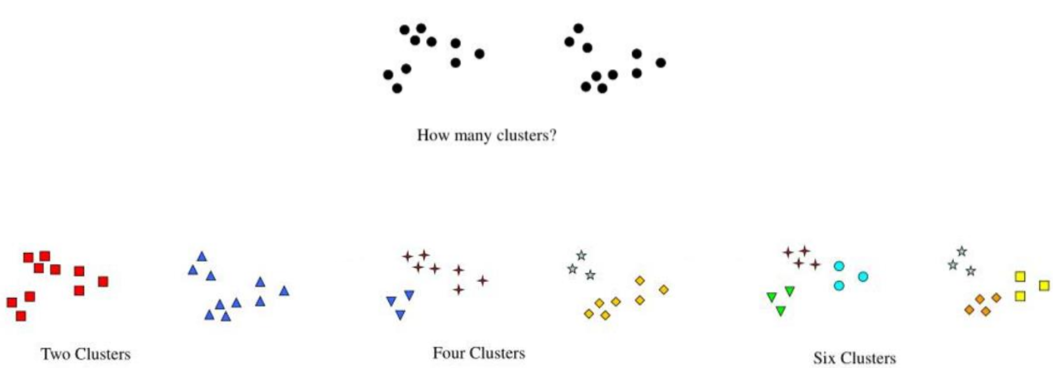
Clusters Can Be Ambiguous….



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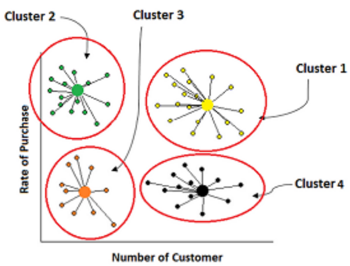
Types of Clustering Methods

Partitioning Methods

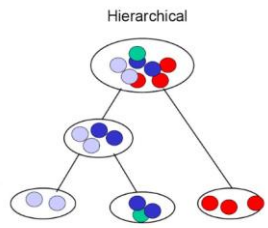
– split the data into distinct groups

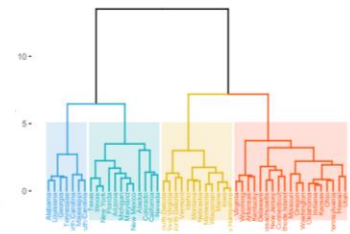


– K-Means, K-Medoids (PAM), CLARA

Hierarchical Methods

– Nested clusters organized as a hierarchical tree





– Agglomerative vs Divisive; Dendrograms

7

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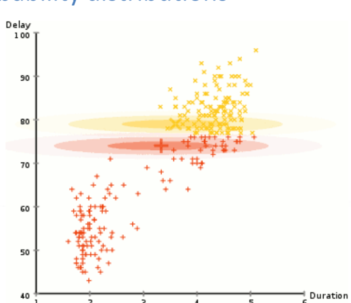
Types of Clustering Methods

Model-Based Methods

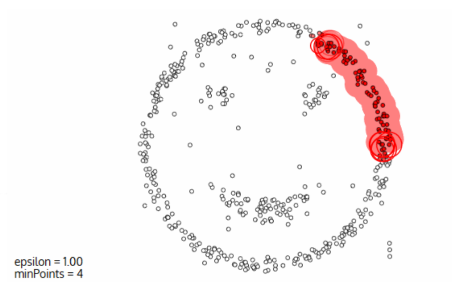
– assume data is based on a mixture of probability distributions



– Gaussian Mixture Models (GMMs), Bayesian Mixture Models, Expectation-Maximization

Density-Based Methods

– clusters based on density of data points



– Density-Based Spatial Clustering of Application with Noise (DBSCAN), OPTICS

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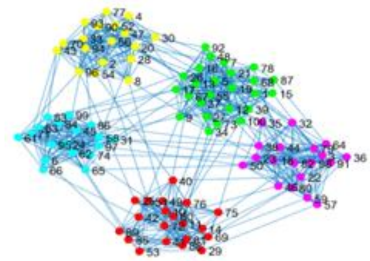
Types of Clustering Methods

Graph-Based Methods

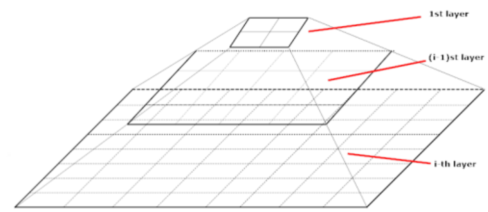
– data as graphs and clusters based on graph properties



– Spectral clustering

Grid-Based Methods

– use a multi-resolution grid data structure to process data



– Statistical Information Grid (STING), Clustering in Quest of the Interesting (CLIQUE)

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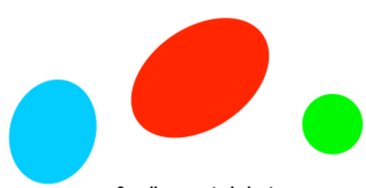
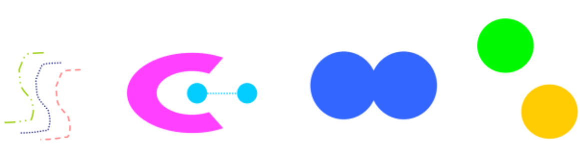
Types of Clusters

- Well-separated clusters
- Prototype-based clusters
- Contiguous clusters
- Density-based clusters

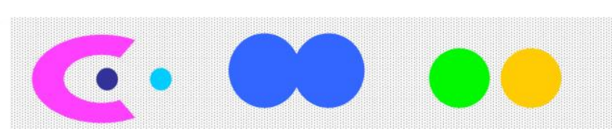


3 well-separated clusters

4 center-based clusters



8 contiguous clusters



6 density-based clusters

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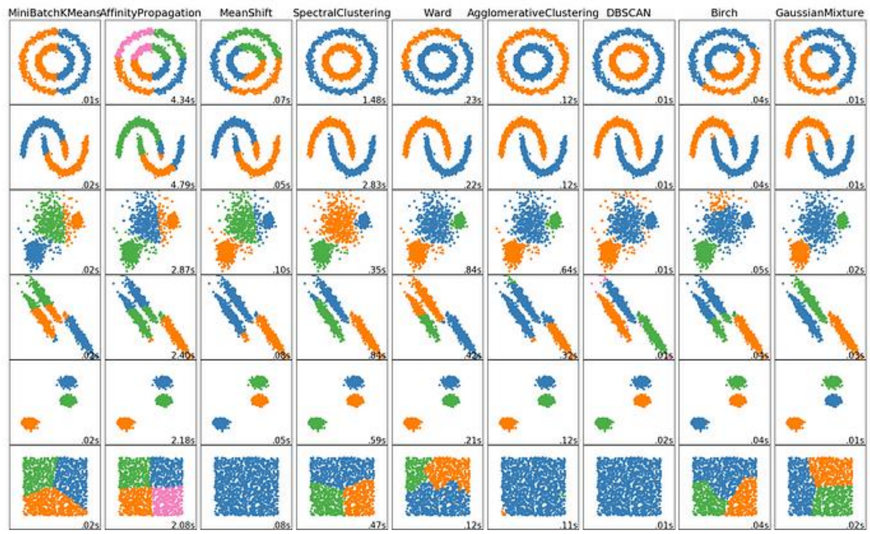

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Review of K-Means

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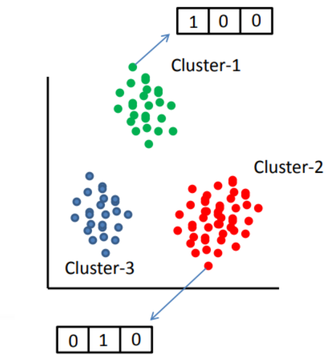
K-Means Clustering

- K-Means is one of the most popular clustering algorithms.
- Input:
  - Observations/data points (N): $x_i \quad \forall\, i \in \{1, \dots, N\}$
  - # of clusters: k
- Output:
  - Cluster Assignments: w_{ij}
  - Cluster Centroids: $c_j \quad \forall\, j \in \{1, \dots, k\}$



1-of-k representation for cluster assignment.

- Objective Function: It aims to minimize the within-cluster sum of squares (WCSS):

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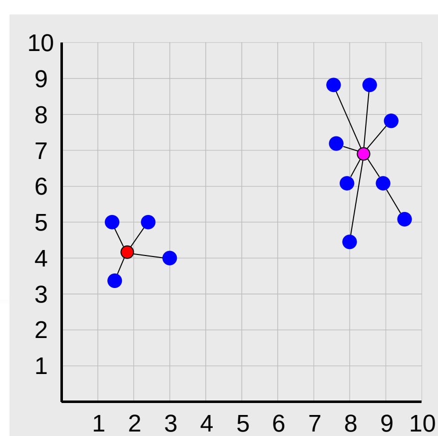
Squared Error

- Squared Error (SE):

$$SE_{C_j} = \sum_{x_i \in C_j}^{N} (x_i - c_j)^2 \qquad \text{for cluster } j$$

- Within-Cluster Sum of Squares (WCSS):

$$WCSS = \sum_{j=1}^{k} \sum_{x_i \in C_j} (x_i - c_j)^2 \qquad \text{sum over all clusters } 1, \dots, k$$



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K-Means Clustering

- K-Means is a minimization problem with the objective function:

$$J = \sum_{j=1}^{k} \sum_{x_i \in C_j} (x_i - c_j)^2 = \sum_{j=1}^{k} \sum_{i=1}^{N} w_{ij}(x_i - c_j)^2 \qquad w_{ij} = \begin{cases} 1 & if\ x_i \in C_{ij} \\ 0 & if\ x_i \notin C_j \end{cases}$$

- Find best assignments of w_{ij} and best cluster centroids c_j ➔ minimize J
- Differentiate wrt c_k and equate to 0:

$$c_k = \frac{\sum_{i=1}^{N} w_{ik} x_i}{\sum_{i=1}^{N} w_{ij}}$$

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K-Means Example & Algorithm

each object is randomly assigned to a cluster

cluster centroids are computed

each object is assigned to the nearest centroid

new cluster centroids are computed

results after 10 iterations

Iterative Algorithm For K-Means

- Initialize k centroids
- Repeat till convergence
  - Calculate w_{ij} ← Expectation Step (E-Step)
  - Update $c_j = \frac{\sum_{i=1}^{N} w_{ij} x_i}{\sum_{i=1}^{N} w_{ij}}$ ← Maximization Step (M-Step)

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Comments on the K-Means Method

- Strength:
  - Efficient: *O(tkn)*, where *n*: # objects, *k*: # clusters, and *t*:# iterations. Normally, *k*, *t*<< *n*.
  - Often terminates at a local optimal
- Weakness:
  - Applicable only when mean is defined, then what about categorical data?
  - Need to specify *k*, the # of clusters, in advance the best k
  - Unable to handle noisy data and outliers well
  - Not suitable to discover clusters with non-convex shapes

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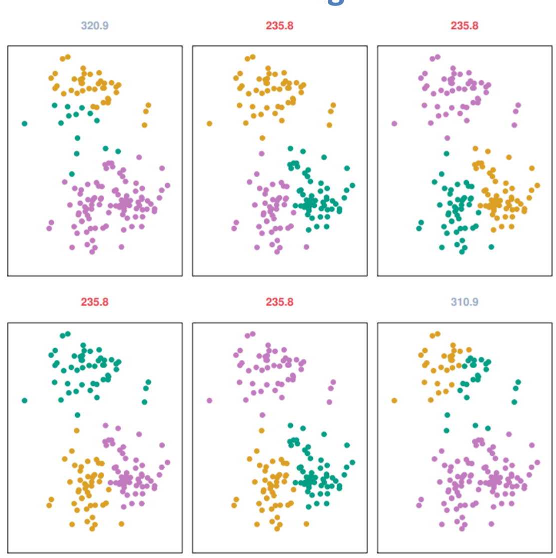
Different Starting Values…



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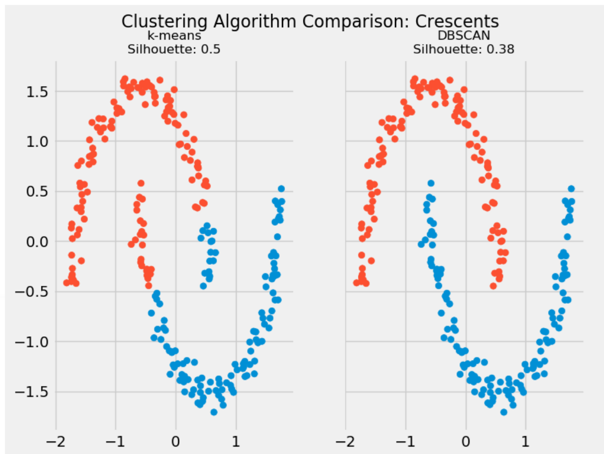
Problems with K-Means



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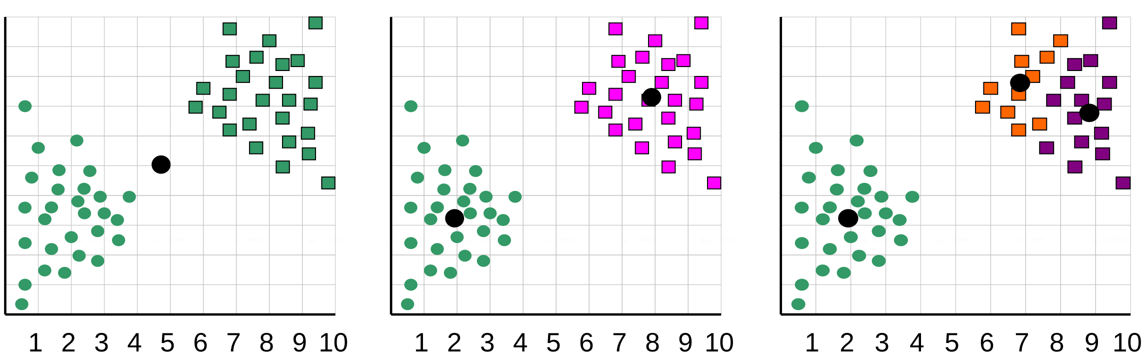
Example: Determine *k*

- SE can be used to determine the # of clusters needed



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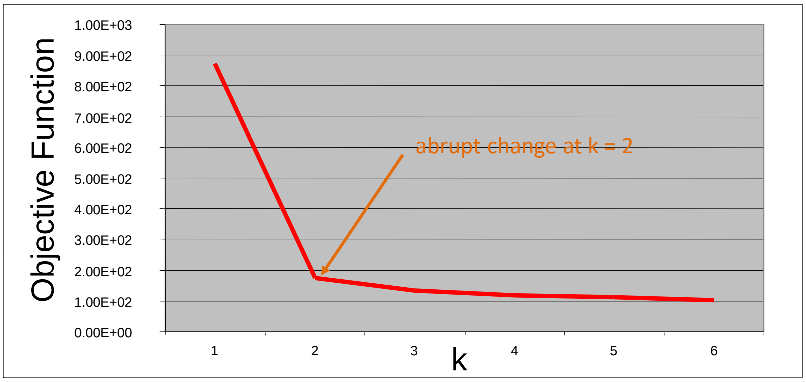
Example: Determine *k* (Knee Finding)

- Plot of Objective Function vs k



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Variations of K-Means Method

- Most of the variants of the k-means which differ in
  - Selection of the initial k-means
  - Dissimilarity calculations
  - Strategies to calculate cluster means

- Handling categorical data: k-modes
  - Replacing means of clusters with modes
  - Using new dissimilarity measures to deal with categorical objects
  - Using a frequency-based method to update modes of clusters
  - A mixture of categorical and numerical data: k-prototype method

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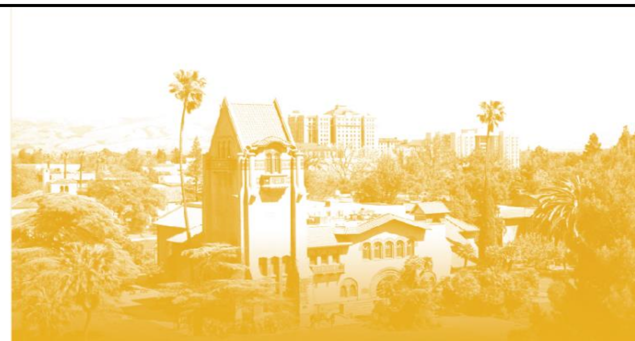
Hierarchical Clustering



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Hierarchical Clustering

- K-means clustering requires us to pre-specify the number of clusters k.
- Hierarchical Clustering is an alternative approach which does not require that we commit to a particular choice of k.

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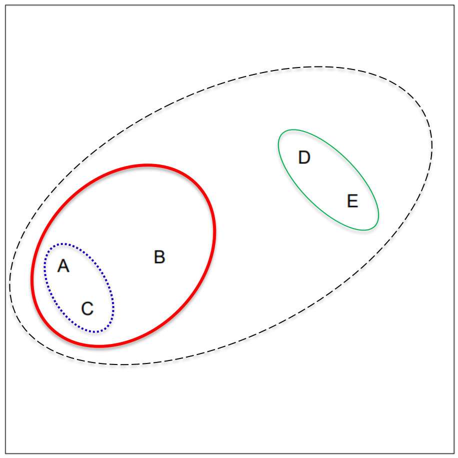
A Simple Hierarchical Clustering



- Start with each point in its own cluster.
- Identify the closest 2 clusters & merge them.
- Repeat.
- Ends when all points are in a single cluster.

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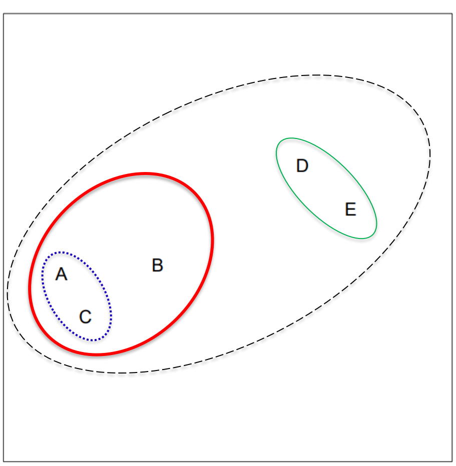
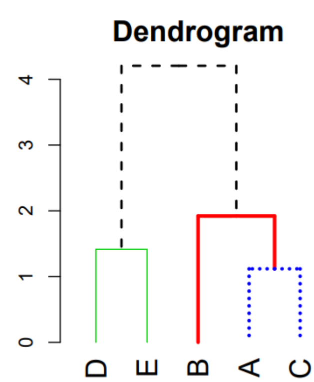
Hierarchical Clustering: Dendrogram





The similarity between two objects in a dendrogram is represented as the height of the lowest internal node they share.

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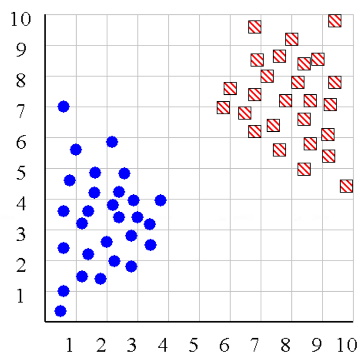
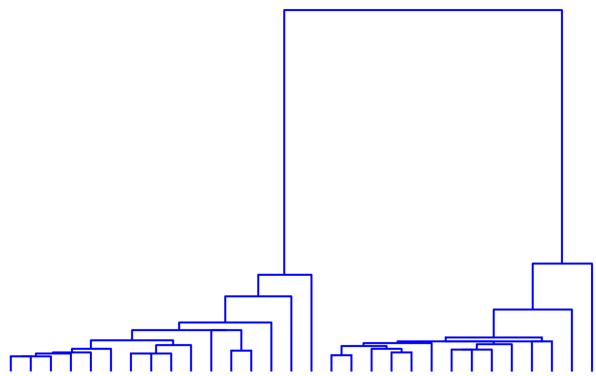
Hierarchical Clustering: Dendrogram

- Dendrogram can be used to determine the “correct” number of clusters:





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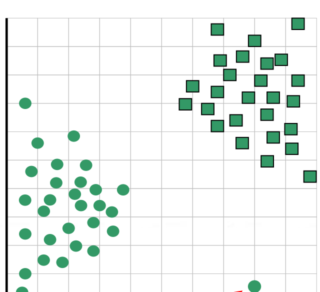
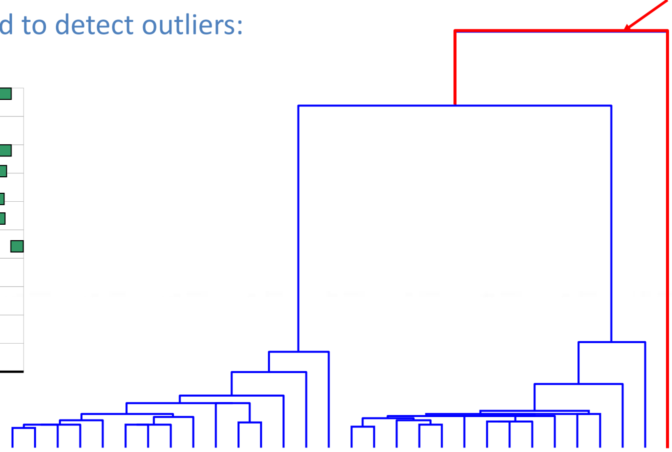
Hierarchical Clustering: Dendrogram

This single isolated branch indicates that the data point that is very different to all others

- Dendrogram can also be used to detect outliers:



Outlier



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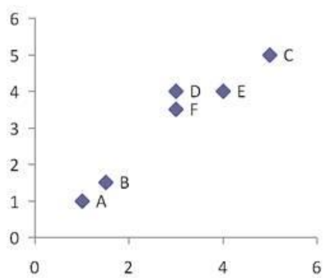
Hierarchical Clustering: Distance Matrix

- Distance matrix is used as clustering criteria. It does not require the number of clusters k as an input, but needs a termination condition
- Different distance or dissimilarity metrics can be used (Euclidean etc):



	X1	X2
A	1	1
B	1.5	1.5
C	5	5
D	3	4
E	4	4
F	3	3.5

Dist	A	B	C	D	E	F
A	0.00	0.71	5.66	3.61	4.24	3.20
B	0.71	0.00	4.95	2.92	3.54	2.50
C	5.66	4.95	0.00	2.24	1.41	2.50
D	3.61	2.92	2.24	0.00	1.00	0.50
E	4.24	3.54	1.41	1.00	0.00	1.12
F	3.20	2.50	2.50	0.50	1.12	0.00

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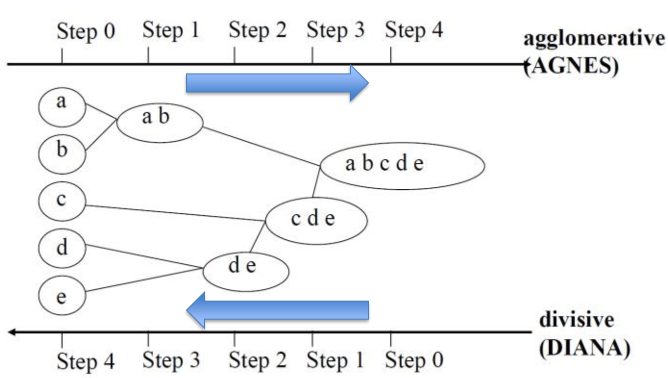
Hierarchical Clustering

- Distance matrix is used as clustering criteria. It does not require the number of clusters k as an input, but needs a termination condition



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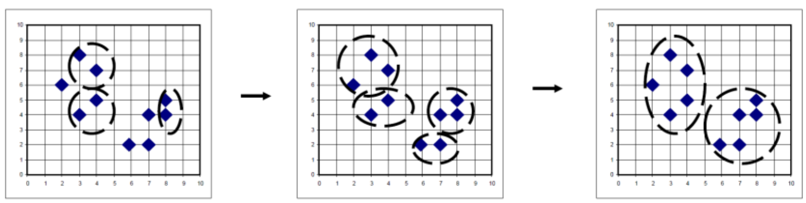
AGNES (Agglomerative Nesting)

- Introduced in Kaufmann and Rousseeuw (1990)
- Use the single-link method and the dissimilarity matrix
- Merge nodes that have the least dissimilarity
- Go on in a non-descending fashion
- Eventually all nodes belong to the same cluster



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Hierarchical Clustering: Linkage

Linkage is used to "measure" the distance between an object and a cluster. Here are some options:

- Single Linkage (nearest neighbor)
- Complete Linkage (furthest neighbor)
- Group Average Linkage
- Distance Between Centroids
- Ward's Method

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Linkage Criteria – Single Linkage

Single or Minimum Linkage (nearest neighbors)

- Measures the distance between the closest points of 2 clusters: $D(c_1, c_2) = \min_{x_1 \in c_1, x_2 \in c_2} D(x_1, x_2)$
- Can handle elongated shapes well

can handle non-elliptical shapes

sensitive to noise

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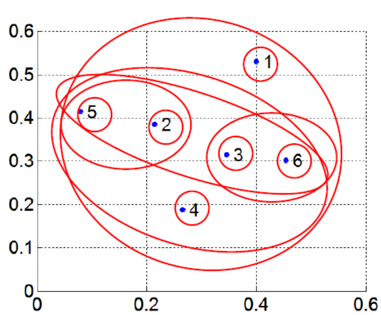
Single or MIN Link

- Proximity of two clusters is based on the two closest points in the different clusters



Distance Matrix:

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

- D({3,6} , {2,5}) = min(D(3,2), D((6,2) , D(3,5), D(6,5)) = min(0.15, 0.25, 0.28, 0.39) = 0.15
- D({3,6} , {1 }) = min(D(3,1), D(6,1)) = min(0.22, 0.23) = 0.22
- D({3,6} , {4 }) = min(D(3,4), D(6,4)) = min(0.15, 0.22) = 0.15
- D({2,5} , {1 }) = min(D(2,1), D(5,1)) = min(0.24, 0.34) = 0.24
- D({2,5} , {4 }) = min(D(2,4), D(5,4)) = min(0.20, 0.29) = 0.20

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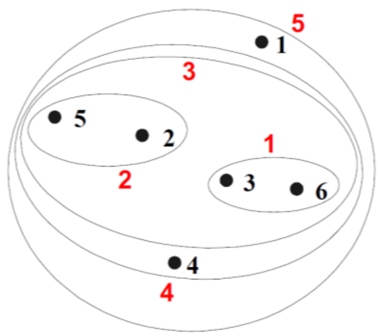
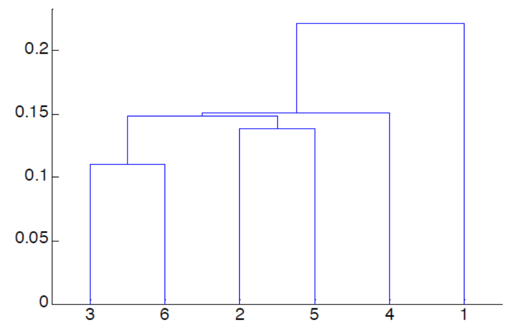
Single or MIN Link



Nested Clusters



Dendrogram

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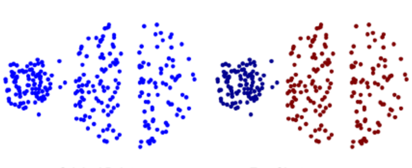
Linkage Criteria – Complete Link

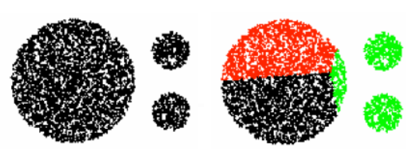
Complete or Maximum Linkage

- Measures the distance between the furthest points of 2 clusters.
- Tends to produce compact and spherical clusters.

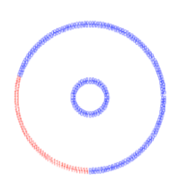
$$D(c_1, c_2) = \max_{x_1 \in c_1, x_2 \in c_2} D(x_1, x_2)$$



less susceptible to noise



tends to break large clusters



biased towards globular clusters

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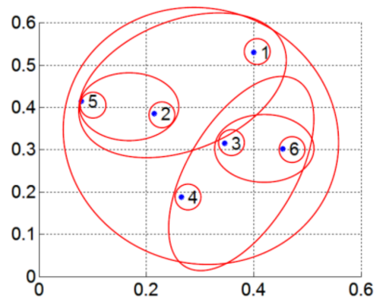
Complete or MAX Link

- Proximity of two clusters is based on the two furthest points in the different clusters



Distance Matrix:

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

- D({3,6} , {2,5}) = max($D(3,2)$, $D((6,2)$, D(3,5), D(6,5)) = max(0.15, 0.25, 0.28, 0.39) = 0.39
- D({3,6} , {1 }) = max($D(3,1)$, $D(6,1)$) = max(0.22, 0.23) = 0.23
- D({3,6} , {4 }) = max($D(3,4)$, $D(6,4)$) = max(0.15, 0.22) = 0.22

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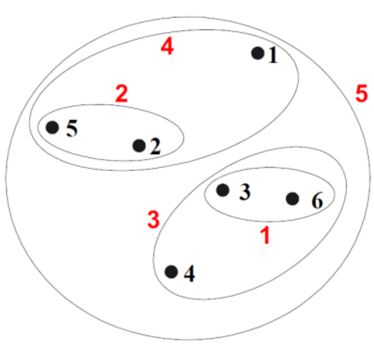
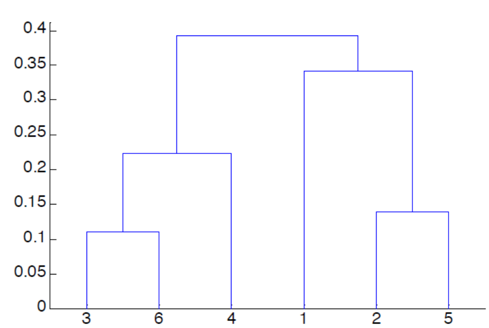
Complete or MAX Link



Nested Clusters



Dendrogram

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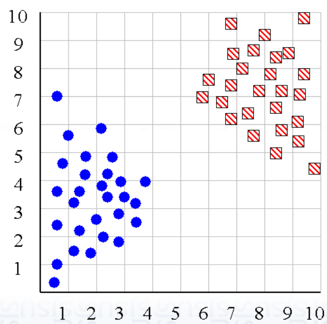
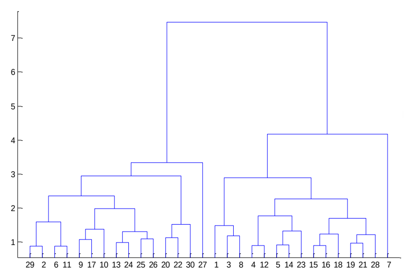
Linkage Criteria: Group Average

Group Average or Mean Linkage

- Measures the **average distance** between all points of 2 clusters.
- Balances between single and complete linkage.

$$D(c_1, c_2) = \frac{1}{|C_1|}\frac{1}{|c_2|}\sum_{x_1 \in c_1}\sum_{x_2 \in c_2} D(x_1, x_2)$$





Average linkage

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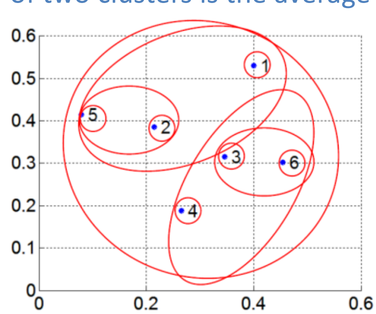
Group Average Link

- Proximity of two clusters is the average of pairwise proximity betweenin the different clusters



Distance Matrix:

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

- D({3,6} , {2,5}) = $(D(3,2) + D((6,2) + D(3,5) + D(6,5))/2x2 = (0.15 + 0.25 + 0.28 + 0.39)/4 = 0.2675$
- D({3,6} , {1 }) $= (D(3,1) + D(6,1))/2x1 = (0.22 + 0.23)/2 = 0.225$
- D({3,6} , {4 }) $= (D(3,4) + D(6,4))/2x1 = (0.15 + 0.22)/2 = 0.185$

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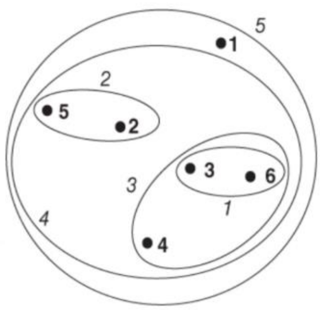
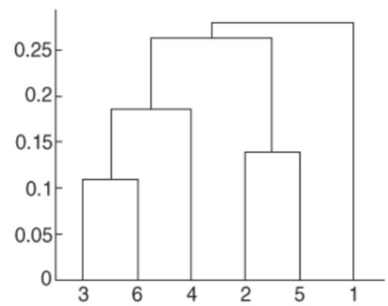
Group Average Link



Nested Clusters



Dendrogram

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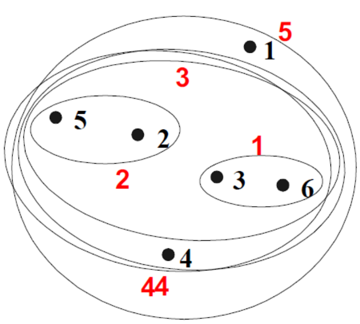
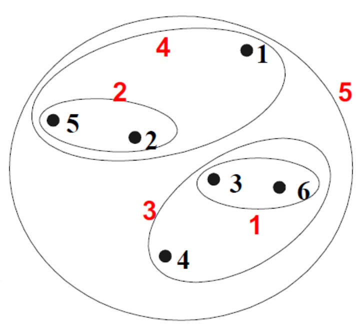
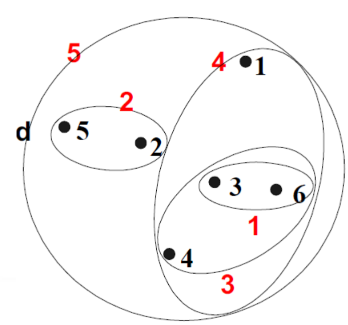
Linkage Comparison



MIN



MAX



Group Average

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Hierarchical Clustering: Problems and Limitations

- Computationally heavy with large datasets.
- Once a decision is made to merge or split two clusters, it cannot be undone.
- No global objective function is directly minimized.
- Different schemes have problems with one or more of the following:
  - Sensitivity to noise (MIN)
  - Difficulty handling clusters of different sizes and non-globular shapes (MAX, Group Average)
  - Breaking large clusters(MAX)

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Evaluation of Clustering

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Measures of Cluster Validity

- Measures of cluster validity can be classified as follows.
  - External Index: Measure the extent to which cluster labels match externally supplied class labels ➔ Entropy, Purity
  - Internal index: Measure the goodness of a clustering structure without respect to external information ➔ 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 scaled dot product
- Both supervised or unsupervised measures can be used to compare clusters

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Unsupervised Measures: Cohesion and Separation

- Cluster Cohesion (within-cluster sum of squares, WCSS): Measure how closely data points in a cluster are to each other.
  - Lower values indicate that the points within the cluster are tightly packed.

$$WCSS = \sum_{j=1}^{k} \sum_{x_i \in C_j} (x_i - c_j)^2 \quad \text{sum over all clusters } 1, \dots, k$$

- Cluster Separation (between-clusters sum of squares, BCSS): Measure how distinct or well-separated a cluster is from other clusters.
  - Higher values indicate that the clusters are well-separated from each other

$$BCSS = \sum_{j=1}^{k} |size(C_j)| (c - c_j)^2 \quad \text{sum over all clusters } 1, \dots, k$$

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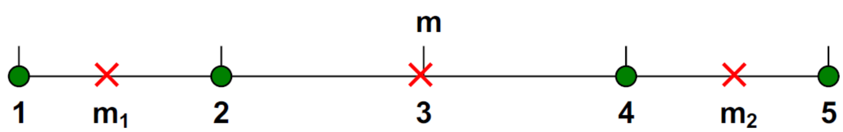
Example: Cluster Cohesion and Separation



K=1 cluster:

$$SSE = (1-3)^2 + (2-3)^2 + (4-3)^2 + (5-3)^2 = 10$$
$$SSB = 4\times(3-3)^2 = 0$$

K=2 clusters:

$$SSE = (1-1.5)^2 + (2-1.5)^2 + (4-4.5)^2 + (5-4.5)^2 = 1$$
$$SSB = 2\times(3-1.5)^2 + 2\times(4.5-3)^2 = 9$$

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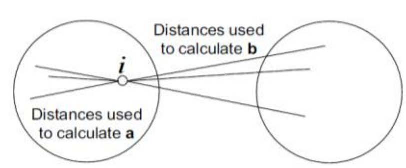
Unsupervised Measures: Silhouette Coefficient

- Silhouette coefficient combines ideas of both cohesion and separation, but for individual points, as well as clusters and clustering
- 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

$$s_i = \frac{(b_i - a_i)}{\max(a_i, b_i)}$$



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

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Cluster Validity Using Correlation

- Proximity Matrix
  - D_{ij} is the similarity between object O_i and O_j
- 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

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Cluster Validity Using Correlation

- Compute the correlation between the two matrices
  - Given proximity Matrix $D = \{d_{11}, d_{12}, \ldots, d_{nn}\}$ and Incidence Matrix $C = \{c_{11}, c_{12}, \ldots, c_{nn}\}$

$$r = \frac{\sum_{i=1,j=1}^{n}(d_{ij}-\bar{d})(c_{ij}-\bar{c})}{\sqrt{\sum_{i=1,j=1}^{n}(d_{ij}-\bar{d})^2}\sqrt{\sum_{i=1,j=1}^{n}(c_{ij}-\bar{c})^2}}$$

- High magnitude of correlation indicates that points that belong to the same cluster are close to each other

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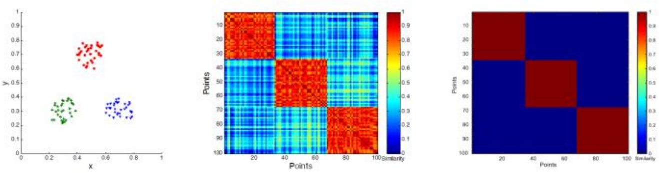
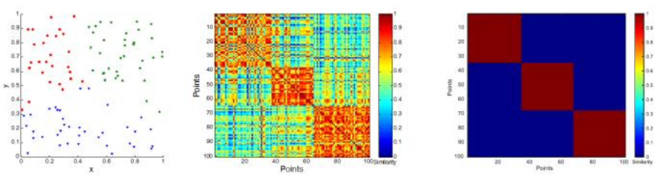
Example: Cluster Validity Using Correlation

- Correlation for a well-clustered data set:



Corr = 0.9235

- Correlation for a random data set:



K-means

Corr = 0.5810

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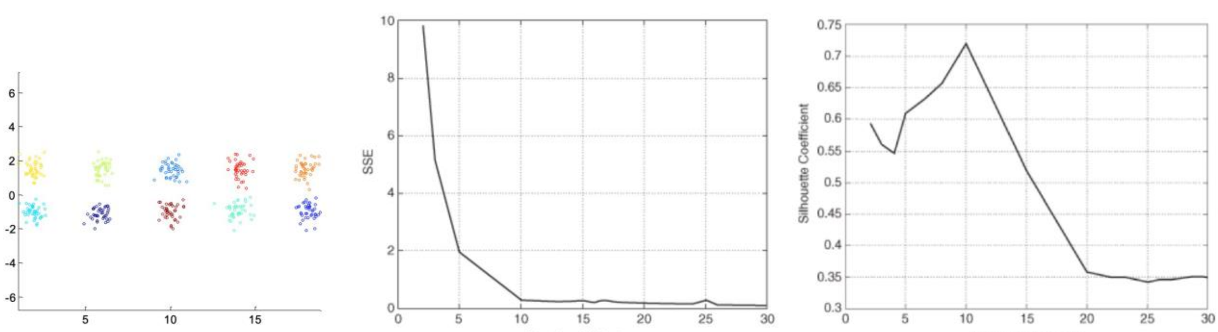
Determining the Number of Clusters

- From SSE and silhouette coefficient, you can determine the (optimal?) # of clusters needed.



Supervised Measure of Cluster Validity

- Measure the degree of correspondence between the cluster labels and the class labels.
- Classification-oriented: measures from classification, such as entropy, purity, and the F-measure. These measures evaluate the extent to which a cluster contains objects of a single class.
- Similarity-oriented: measure the extent to which two objects that are in the same class are in the same cluster and vice versa

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Classification-Oriented Measures of Cluster Validity (Entropy)

Entropy: The degree of impurity within clusters or how mixed the cluster is.

- For each cluster i, compute the class distribution of the data:

$$p_{ij} = \frac{m_{ij}}{m_i}$$

m_i # objects in cluster i,
m_{ij} # of objects of class j in cluster i.

- Calculate entropy of each cluster i:

$$e_i = -\sum_{j=1}^{L} p_{ij} \log_2 p_{ij}$$

L = # of classes

- Calculate total entropy for a set of clusters:

$$e = \sum_{i=1}^{k} \frac{m_i}{m} e_i$$

k: # of clusters, m: total # of data points

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Classification-Oriented Measures of Cluster Validity (Purity)

Purity: The degree to which each cluster consists of objects of a single class.

- For each cluster i, compute the class distribution of the data:

$$p_{ij} = \frac{m_{ij}}{m_i}$$

m_i # objects in cluster i,
m_{ij} # of objects of class j in cluster i.

- Calculate the purity of each cluster i

$$purity(i) = \max_j p_{ij}$$

- Calculate the overall purity:

$$purity(total) = \sum_{i=1}^{k} \frac{m_i}{m} purity(i)$$

k: # of clusters, m: total # of data points

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Classification-Oriented Measures of Cluster Validity (F-measure)

- 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

$$Precision(i,j) = \frac{m_{ij}}{m_i}$$

m_i # objects in cluster i,
m_{ij} # of objects of class j in cluster i.

- 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:

$$Recall(i,j) = \frac{m_{ij}}{m_j}$$

m_j # objects in cluster j,
m_{ij} # of objects of class j in cluster i.

- 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

$$F(i,j) = 2 \times \frac{Precision(i,j) \times Recall(i,j)}{Precision(i,j) + Recall(i,j)}$$

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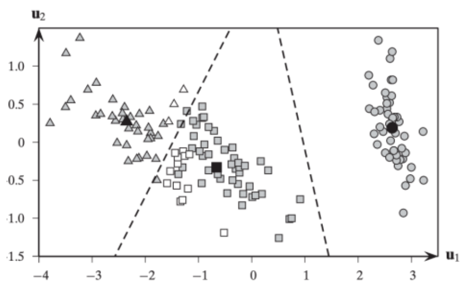
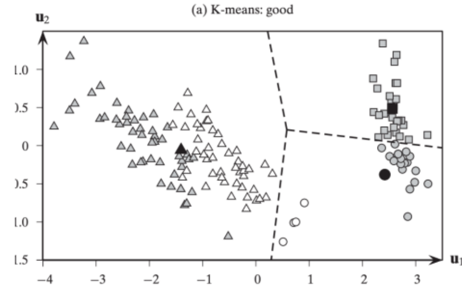
Example: Classification-Oriented Evaluation Measures



(a) K-means: good

(a) K-means: good



(b) K-means: bad

	iris-setosa T_1	iris-versicolor T_2	iris-virginica T_3	n_i
C_1(squares)	0	47	14	61
C_2(circles)	50	0	0	50
C_3(triangles)	0	3	36	39
m_j	50	50	50	$n = 100$

	iris-setosa T_1	iris-versicolor T_2	iris-virginica T_3	n_i
C_1	30	0	0	30
C_2	20	4	0	24
C_3	0	46	50	96
m_j	50	50	50	$n = 150$

Example: Classification-Oriented Evaluation Measures

	iris-setosa T_1	iris-versicolor T_2	iris-virginica T_3	n_i
C_1(squares)	0	47	14	61
C_2(circles)	50	0	0	50
C_3(triangles)	0	3	36	39
m_j	50	50	50	$n = 100$

$$e_i = -\Sigma_{j=1}^{L} p_{ij} \log_2 p_{ij} \qquad purity(i) = \max_j p_{ij}$$

$$e = -\Sigma_{i=1}^{k} \frac{m_i}{m} e_i \qquad purity(total) = \sum_{i=1}^{k} \frac{m_i}{m} purity(i)$$

$$e(C_1) = -(p_{11}\log_2 p_{11} + p_{12}\log_2 p_{12} + p_{13}\log_2 p_{13}) = -\left(\frac{0}{61}\log_2\frac{0}{61} + \frac{47}{61}\log_2\frac{47}{61} + \frac{14}{61}\log_2\frac{14}{61}\right) = 0.75$$

$$e(C_2) = -(p_{21}\log_2 p_{21} + p_{22}\log_2 p_{22} + p_{23}\log_2 p_{23}) = -\left(\frac{50}{50}\log_2\frac{50}{50} + \frac{0}{50}\log_2\frac{0}{50} + \frac{0}{50}\log_2\frac{0}{50}\right) = 0$$

$$e(C_3) = -(p_{31}\log_2 p_{31} + p_{32}\log_2 p_{32} + p_{33}\log_2 p_{33}) = -\left(\frac{0}{39}\log_2\frac{0}{39} + \frac{3}{39}\log_2\frac{3}{39} + \frac{36}{39}\log_2\frac{36}{39}\right) = 0.39$$

$$Purity(C_1) = max(p_{11}, p_{12}, p_{13}) = max\left(\frac{47}{61}, \frac{14}{61}, 0\right) = \frac{47}{61}$$

$$Purity(C_1) = max(p_{21}, p_{22}, p_{23}) = max\left(\frac{50}{50}, 0, 0\right) = 1$$

$$Purity(C_1) = max(p_{31}, p_{32}, p_{33}) = max\left(0, \frac{3}{39}, \frac{36}{39}\right) = \frac{36}{39}$$

$$Entropy(total) = -\left(\frac{61}{150} \times 0.75 + \frac{39}{150} \times 0.39\right) = 0.40$$

$$Purity(total) = \frac{61}{150} \times \frac{47}{61} + \frac{50}{150} \times 1 + \frac{39}{150} \times \frac{36}{39} = 0.89$$

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Example: Classification-Oriented Evaluation Measures

	iris-setosa T_1	iris-versicolor T_2	iris-virginica T_3	n_i
C_1	30	0	0	30
C_2	20	4	0	24
C_3	0	46	50	96
m_j	50	50	50	$n = 150$

$$e_i = -\Sigma_{j=1}^{L} p_{ij} \log_2 p_{ij}$$

$$e = -\Sigma_{i=1}^{k} \frac{m_i}{m} e_i$$

$$purity(i) = \max_j p_{ij}$$

$$purity(total) = \sum_{i=1}^{k} \frac{m_i}{m} purity(i)$$

$$e(C_1) = -(p_{11}\log_2 p_{11} + p_{12}\log_2 p_{12} + p_{13}\log_2 p_{13}) = -\left(\frac{30}{30}\log_2\frac{30}{30} + \frac{0}{30}\log_2\frac{0}{30} + \frac{0}{30}\log_2\frac{0}{30}\right) = 0$$

$$e(C_2) = -(p_{21}\log_2 p_{21} + p_{22}\log_2 p_{22} + p_{23}\log_2 p_{23}) = -\left(\frac{20}{24}\log_2\frac{20}{24} + \frac{4}{24}\log_2\frac{4}{24} + \frac{0}{24}\log_2\frac{0}{24}\right) = 0.65$$

$$e(C_3) = -(p_{31}\log_2 p_{31} + p_{32}\log_2 p_{32} + p_{33}\log_2 p_{33}) = -\left(\frac{0}{96}\log_2\frac{0}{96} + \frac{46}{96}\log_2\frac{46}{96} + \frac{50}{96}\log_2\frac{50}{96}\right) = 1$$

$$Purity(C_1) = max(p_{11}, p_{12}, p_{13}) = max\left(\frac{30}{30}, 0, 0\right) = 1$$

$$Purity(C_1) = max(p_{21}, p_{22}, p_{23}) = max\left(\frac{20}{24}, \frac{4}{24}, 0\right) = \frac{20}{24}$$

$$Purity(C_1) = max(p_{31}, p_{32}, p_{33}) = max\left(\frac{0}{96}, \frac{46}{96}, \frac{50}{96}\right) = \frac{50}{96}$$

$$Entropy(total) = -\left(\frac{46}{96} \times 0.65 + \frac{50}{96} \times 1\right) = 0.74$$

$$Purity(total) = \frac{30}{150} \times 1 + \frac{24}{150} \times \frac{20}{24} + \frac{96}{150} \times \frac{50}{96} = 0.66$$

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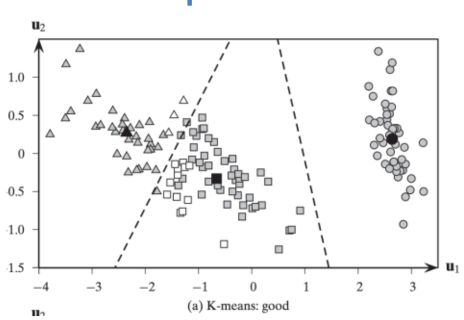
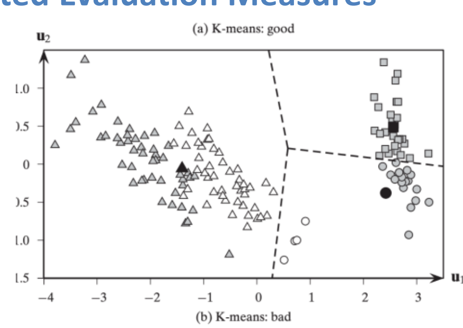
Example: Classification-Oriented Evaluation Measures





	iris-setosa T_1	iris-versicolor T_2	iris-virginica T_3	n_i
C_1(squares)	0	47	14	61
C_2(circles)	50	0	0	50
C_3(triangles)	0	3	36	39
m_j	50	50	50	$n = 100$

$Entropy(total) = 0.40$
$Purity(total) = 0.89$
$F\ Measure = 0.88$

	iris-setosa T_1	iris-versicolor T_2	iris-virginica T_3	n_i
C_1	30	0	0	30
C_2	20	4	0	24
C_3	0	46	50	96
m_j	50	50	50	$n = 150$

$Entropy(total) = 0.74$
$Purity(total) = 0.66$
$F\ Measure = 0.65$

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Supervised Similarity-Oriented Evaluation Measure

Ideal cluster similarity matrix

- $C_{ij} = 1$ if O_i and O_j belong to the same cluster, $C_{ij} = 0$ otherwise

Class similarity matrix

- $C_{ij} = 1$ if O_i and O_j belong to the same class, $C_{ij} = 0$ otherwise

- Calculate correlation of these two matrices as the measure of cluster validity.

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Supervised Similarity-Oriented Evaluation measure

- Five data points, p_1, p_2, p_3, p_4, p_5, two clusters, $C_1 = \{p_1, p_2, p_3\}$ and $C_2 = \{p_4, p_5\}$, and two classes, $L_1 = \{p_1, p_2\}$ *and* $L_2 = \{p_3, p_4, p_5\}$.

Point	p_1	p_2	p_3	p_4	p_5
p_1	1	1	1	0	0
p_2	1	1	1	0	0
p_3	1	1	1	0	0
p_4	0	0	0	1	1
p_5	0	0	0	1	1

Ideal cluster similarity matrix

Point	p_1	p_2	p_3	p_4	p_5
p_1	1	1	0	0	0
p_2	1	1	0	0	0
p_3	0	0	1	1	1
p_4	0	0	1	1	1
p_5	0	0	1	1	1

Class similarity matrix

Correlation = 0.359

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Supervised Similarity-Oriented Evaluation Measure

- Five data points, p_1, p_2, p_3, p_4, p_5, two clusters, $C_1 = \{p_1, p_2, p_3\}$ and $C_2 = \{p_4, p_5\}$, and two classes, $L_1 = \{p_1, p_2\}$ *and* $L_2 = \{p_3, p_4, p_5\}$.

	Same Cluster	Different Cluster
Same Class	f11	f10
Different Class	f01	f00

f_{00} = number of pairs of objects having a different class and a different cluster
f_{01} = number of pairs of objects having a different class and the same cluster
f_{10} = number of pairs of objects having the same class and a different cluster
f_{11} = number of pairs of objects having the same class and the same cluster

$$\text{Rand statistic} = \frac{f_{00} + f_{11}}{f_{00} + f_{01} + f_{10} + f_{11}}$$

$$\text{Jaccard coefficient} = \frac{f_{11}}{f_{01} + f_{10} + f_{11}}$$

f_{00}: $\{p_1, p_4\},\{p_1, p_5\},\{p_2, p_4\}, \{p_2, p_5\} = 4$
f_{01}: $\{p_3, p_4\},\{p_3, p_5\} = 2$
f_{10}: $\{p_3, p_4\},\{p_3, p_5\} = 2$
f_{11}: $\{p_1, p'\},\{p_4, p_5\} = 2$

Rand statistic = (2 + 4)/10 = 0.6

Jaccard Coefficient = 2/6 = 0.66

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Assessing the Significance of Cluster Validity Measures

- How to interpret a single number provided by validity measures?
- Using minimum and Maximum value:

  e.g., a purity of 0 is bad, while a purity of 1 is good Likewise, an entropy of 0 is good, as is an SSE of 0

- Use absolute standard:

  e.g., clustering for utility, we are often willing to tolerate only a certain level of error in the approximation of our points by a cluster centroid.

- Interpreting the value of our validity measure in statistical terms.

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Interpreting Validity Measure in Statistical Terms

- Judging how likely it is that our observed value was achieved by random chance.
  - The value is good if it is unusual; i.e., if it is unlikely to be the result of random chance.
- The motivation is that we are interested only in clusters that reflect non-random structure in the data
- Such structures should generate unusually high values of our cluster validity measures, at least if the validity measures are designed to reflect the presence of strong cluster structure.

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