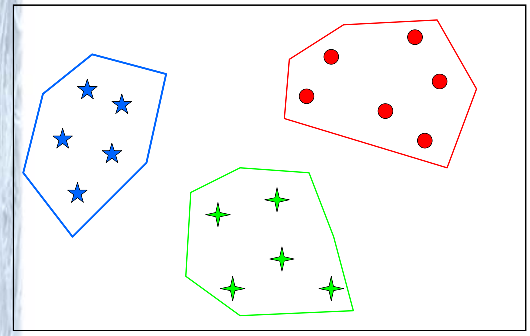
Clustering

- Unsupervised learning
- Generating “classes”
- Distance/similarity measures
- Agglomerative methods
- Divisive methods

What is Clustering?

- Form of *unsupervised* learning - no information from teacher
- The process of partitioning a set of data into a set of meaningful (hopefully) sub-classes, called *clusters*
- Cluster:
  - collection of data points that are “similar” to one another and collectively should be treated as group
  - as a collection, are sufficiently different from other groups

Clusters



Characterizing Cluster Methods

- Class - label applied by clustering algorithm
  - hard versus fuzzy:
    - hard - either is or is not a member of cluster
    - fuzzy - member of cluster with probability
- Distance (similarity) measure - value indicating how similar data points are
- Deterministic versus stochastic
  - deterministic - same clusters produced every time
  - stochastic - different clusters may result
- Hierarchical - points connected into clusters using a hierarchical structure

Basic Clustering Methodology

Two approaches:

Agglomerative: pairs of items/clusters are successively linked to produce larger clusters

Divisive (partitioning): items are initially placed in one cluster and successively divided into separate groups

Cluster Validity

- One difficult question: how *good* are the clusters produced by a particular algorithm?
- Difficult to develop an objective measure
- Some approaches:
  - external assessment: compare clustering to *a priori* clustering
  - internal assessment: determine if clustering intrinsically appropriate for data
  - relative assessment: compare one clustering methods results to another methods

Basic Questions

- Data preparation - getting/setting up data for clustering
  - extraction
  - normalization
- Similarity/Distance measure - how is the distance between points defined
- Use of domain knowledge (prior knowledge)
  - can influence preparation, Similarity/Distance measure
- Efficiency - how to construct clusters in a reasonable amount of time

Distance/Similarity Measures

- Key to grouping points

  distance = inverse of similarity
- Often based on representation of objects as feature vectors

An Employee DB

ID	Gender	Age	Salary
1	F	27	19,000
2	M	51	64,000
3	M	52	100,000
4	F	33	55,000
5	M	45	45,000

Term Frequencies for Documents

	T1	T2	T3	T4	T5	T6
Doc1	0	4	0	0	0	2
Doc2	3	1	4	3	1	2
Doc3	3	0	0	0	3	0
Doc4	0	1	0	3	0	0
Doc5	2	2	2	3	1	4

Which objects are more similar?

Distance/Similarity Measures

Properties of measures:

based on feature values $x_{instance\#,feature\#}$

for all objects x_i,B, dist(x_i, x_j) ≥ 0, dist(x_i, x_j)=dist(x_j, x_i)

for any object x_i, dist(x_i, x_i) = 0

dist(x_i, x_j) ≤ dist(x_i, x_k) + dist(x_k, x_j)

Manhattan distance: $\sum_{f=1}^{|features|} | x_{i,f} - x_{j,f} |$

Euclidean distance: $\sqrt{\sum_{f=1}^{|features|} (x_{i,f} - x_{j,f})^2}$

Distance/Similarity Measures

Minkowski distance (p): $\sqrt[p]{\sum_{f=1}^{|features|} (x_{i,f} - x_{j,f})^p}$

Mahalanobis distance: $(x_i - x_j)\nabla^{-1}(x_i - x_j)^T$

where ∇^{-1} is covariance matrix of the patterns

More complex measures:

Mutual Neighbor Distance (MND) - based on a count of number of neighbors

Distance (Similarity) Matrix

- Similarity (Distance) Matrix
  - based on the distance or similarity measure we can construct a symmetric matrix of distance (or similarity values)
  - (i, j) entry in the matrix is the distance (similarity) between items i and j

$$\begin{array}{c|cccc} & I_1 & I_2 & \cdots & I_n \\ \hline I_1 & \bullet & d_{12} & \cdots & d_{1n} \\ I_2 & d_{21} & \bullet & \cdots & d_{2n} \\ \vdots & \vdots & \vdots & \bullet & \vdots \\ I_n & d_{n1} & d_{n2} & \cdots & \bullet \end{array}$$

Note that $d_{ij} = d_{ji}$ (i.e., the matrix is symmetric). So, we only need the lower triangle part of the matrix.

The diagonal is all 1's (similarity) or all 0's (distance)

d_{ij} = similarity (or distance) of D_i to D_j

Employee Data Set

#	Age	Yrs	Salary	Sex	Group
1	45	9	50,000	M	Accnt
2	34	2	36,000	M	DBMS
3	54	22	45,000	M	Servc
4	41	15	53,000	F	DBMS
5	52	3	49,000	F	Accnt
6	23	1	26,000	M	Servc
7	22	1	26,000	F	Servc
8	61	30	98,000	F	Presd
9	51	18	39,000	M	Accnt

Calculating Distance

- Try to normalize (values fall in a range 0 to 1, approximately)

$$Dist_{x,y} = \frac{|Age_x - Age_y|}{50.0} + \frac{|Yrs_x - Yrs_y|}{50.0} + \frac{|Salary_x - Salary_y|}{100{,}000} + SexDiff + GroupDiff$$

- SexDiff is 0 if same Sex, 1 if different, GroupDiff is 0 if same group, 1 if different
- Example:

$$Dist1{,}2 = \frac{|45-34|}{50} + \frac{|9-2|}{50} + \frac{|50{,}000 - 36{,}000|}{100{,}000} + 0 + 1$$
$$= .22 + .14 + .14 + 0 + 1 = 1.50$$

Employee Distance Matrix

	1	2	3	4	5	6	7	8
2	1.50							
3	1.49	1.89						
4	2.23	1.57	2.48					
5	1.27	2.51	2.46	1.50				
6	1.84	1.34	1.23	2.91	2.85			
7	2.84	2.34	2.23	1.91	1.85	1.00		
8	3.22	3.72	2.83	2.15	2.21	4.06	3.06	
9	0.41	1.69	1.20	2.40	1.42	2.03	3.03	3.03

Employee Distance Matrix

	1	2	3	4	5	6	7	8
2	1.50							
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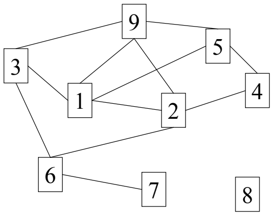
6	1.84	1.34	1.23	2.91	2.85			
7	2.84	2.34	2.23	1.91	1.85	1.00		
8	3.22	3.72	2.83	2.15	2.21	4.06	3.06	
9	0.41	1.69	1.20	2.40	1.42	2.03	3.03	3.03

Theshold, for example, keep links when distance <= 1.8

	1	2	3	4	5	6	7	8
2	1							
3	1	0						
4	0	1	0					
5	1	0	0	1				
6	0	1	1	0	0			
7	0	0	0	0	0	1		
8	0	0	0	0	0	0	0	
9	1	1	1	0	1	0	0	0

Visualizing Distance –Threshold Graph

	1	2	3	4	5	6	7	8
2	1							
3	1	0						
4	0	1	0					
5	1	0	0	1				
6	0	1	1	0	0			
7	0	0	0	0	0	1		
8	0	0	0	0	0	0	0	
9	1	1	1	0	1	0	0	0



Agglomerative Single-Link

- Single-link: connect all points together that are within a threshold distance
- Algorithm:

```
1. place all points in a cluster
2. pick a point to start a cluster
3. for each point in current cluster
      add all points within threshold not already in cluster
      repeat until no more items added to cluster
4. remove points in current cluster from graph
5. Repeat step 2 until no more points in graph
```

Agglomerative Single-Link Example

	1	2	3	4	5	6	7	8
2	1.50							
3	1.49	1.89						
4	2.23	1.57	2.48					
5	1.27	2.51	2.46	1.50				
6	1.84	1.34	1.23	2.91	2.85			
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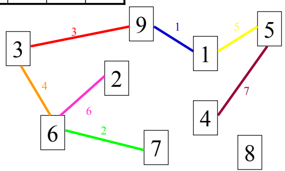
After all but 8 is connected

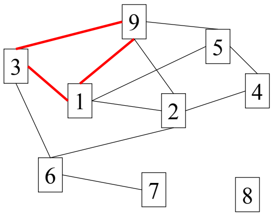


Agglomerative Complete-Link (Clique)

- Complete-link (clique): all of the points in a cluster must be within the threshold distance
- In the threshold distance matrix, a clique is a complete graph
- Algorithms based on finding maximal cliques (once a point is chosen, pick the largest clique it is part of)
  - not an easy problem

Complete Link – Clique Search

	1	2	3	4	5	6	7	8
2	1							
3	1	0						
4	0	1	0					
5	1	0	0	1				
6	0	1	1	0	0			
7	0	0	0	0	0	1		
8	0	0	0	0	0	0	0	
9	1	1	1	0	1	0	0	0



Look for all maximal cliques:
{1,3,9}
{1,2,9}
??

Hierarchical Clustering

	1	2	3	4	5	6	7	8
2	1.50							
3	1.49	1.89						
4	2.23	1.57	2.48					
5	1.27	2.51	2.46	1.50				
6	1.84	1.34	1.23	2.91	2.85			
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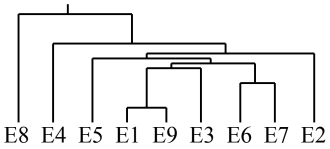
8	3.22	3.72	2.83	2.15	2.21	4.06	3.06	
9	0.41	1.69	1.20	2.40	1.42	2.03	3.03	3.03

- Based on some method of representing hierarchy of data points
- One idea: hierarchical dendogram (connects points based on similarity)



Hierarchical Agglomerative

- Compute distance matrix
- Put each data point in its own cluster
- Find most similar pair of clusters
  - merge pairs of clusters (show merger in dendogram)
  - update proximity matrix
  - repeat until all patterns in one cluster

Partitional Methods

- Divide data points into a number of clusters
- Difficult questions
  - how many clusters?
  - how to divide the points?
  - how to represent cluster?
- Representing cluster: often done in terms of centroid for cluster
  - centroid of cluster minimizes squared distance between the centroid and all points in cluster

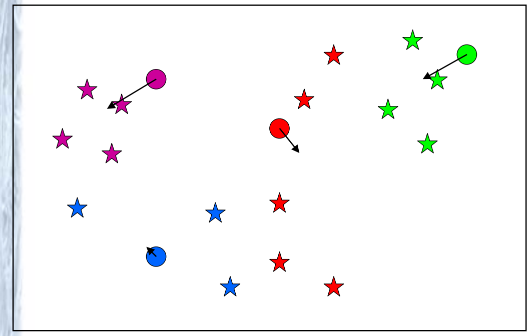
k-Means Clustering

1. Choose *k* cluster centers (randomly pick k data points as center, or randomly distribute in space)
2. Assign each pattern to the closest cluster center
3. Recompute the cluster centers using the current cluster memberships (moving centers may change memberships)
4. If a convergence criterion is not met, goto step 2

Convergence criterion:

- no reassignment of patterns
- minimal change in cluster center

k-Means Clustering



k-Means Variations

- What if too many/not enough clusters?
- After some convergence:
  – any cluster with too large a distance between members is split
  – any clusters too close together are combined
  – any cluster not corresponding to any points is moved
  – thresholds decided empirically

An Incremental Clustering Algorithm

1. Assign first data point to a cluster
2. Consider next data point. Either assign data point to an existing cluster or create a new cluster. Assignment to cluster based on threshold
3. Repeat step 2 until all points are clustered

Useful for efficient clustering