CS685: Data Mining
Clustering

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Clustering

- A dataset of n objects $O_i, i = 1, \ldots, n$
- Partitioning of the dataset into k clusters or groups
- Can be
  - Crisp: Each object belongs to one and only one cluster
  - Fuzzy: An object belongs to a cluster with a probability; such probabilities add up to 1
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- Five main types
  - Partitioning-based
  - Hierarchical
    - *Agglomerative* or bottom-up
    - *Divisive* or top-down
  - Density-based
  - Grid-based
  - Model-based

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  - Images
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- Noise
  - Detection of outliers
  - Noise objects as separate cluster

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- When no "ground" truth is available, i.e, the actual clusters are not known, use silhouette coefficient
- These are called intrinsic methods or *unsupervised* methods

Neighboring Cluster of an Object

- Suppose object O_i is in cluster A, i.e., $O_i \in A$
- Define a_i as the *average* distance of O_i to A

$$a_i = \frac{\sum_{p \in A} d(o_i, p)}{|A|}$$

- Similarly, define $d_i(C)$ to be the *average* distance of O_i to any other cluster C

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- In a sense, cluster B is the "neighbor" of O_i
- O_i could have been in cluster B instead of A

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    - If $s_i \rightarrow +1$, $b_i \gg a_i$ and O_i is in a good cluster
    - If $s_i \approx 0$, $b_i \approx a_i$ and O_i could have been in B as well
    - If $s_i < 0$, $b_i < a_i$ and O_i is better in B than current cluster

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- Different ranges of silhouette index
  - > 0.75: strong clustering
  - $0.5 - 0.75$: reasonable clustering
  - $0.25 - 0.5$: weak clustering
  - < 0.25: no structure

BCubed Measures

- C is a clustering on D
- Labels $l(O_i)$ are given as ideal (ground truth) for each $O_i \in D$
- For points O_i and O_j, correctness is agreement in ground truth

$$correctness(O_i, O_j) = \begin{cases} 1 & \text{if } l(O_i) = l(O_j) \Leftrightarrow C(O_i) = C(O_j) \\ 0 & \text{otherwise} \end{cases}$$

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- BCubed precision measures fraction of same-cluster points that agree in ground truth

$$bcprecision = \frac{1}{n} \sum_{i=1}^{n} \frac{\sum_{O_j, i \neq j, C(O_i) = C(O_j)} correctness(O_i, O_j)}{|\{O_j, i \neq j, C(O_i) = C(O_j)\}|}$$

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- BCubed recall measures fraction of same-ground truth points that agree in clustering

$$bcrecall = \frac{1}{n} \sum_{i=1}^{n} \frac{\sum_{O_j, i \neq j, l(O_i) = l(O_j)} correctness(O_i, O_j)}{|\{O_j, i \neq j, l(O_i) = l(O_j)\}|}$$

- Can define BCubed F-measure using these

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- Suppose (ideal) clustering is $I = I_1, \dots, I_m$ where I_i are partitions
- Cluster to be measured is $C = C_1, \dots, C_k$
- Consider pairs of objects
  - a: Number of object pairs that are in the same cluster in both I and C
  - b: Number of object pairs that are in different clusters in both I and C
  - c: Number of object pairs that are in the same cluster in I but not in C
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- RAND Index is

$$R = \frac{a+b}{a+b+c+d} = \frac{a+b}{\binom{n}{2}} = \frac{TP+TN}{D}$$

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- Contingency table of common objects

Clusters	C_1	$\cdots$	C_k	Total
I_1	n_{11}	$\cdots$	n_{1k}	i_1
$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
I_m	n_{m1}	$\cdots$	n_{mk}	i_m
Total	c_1	$\cdots$	c_k	n

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- Expected number of pair matches assuming the same total distribution is

$$E\left[\sum_{i,j} \binom{n_{ij}}{2}\right] = \left[\sum_i \binom{n_{i\cdot}}{2} \cdot \sum_j \binom{n_{\cdot j}}{2}\right] \Big/ \binom{n}{2}$$

Adjusted RAND Index

- ARI can be written as

$$ARI = \frac{\sum_{i,j}\binom{n_{ij}}{2} - \left[\sum_i \binom{n_{i\cdot}}{2} \cdot \sum_j \binom{n_{\cdot j}}{2}\right] / \binom{n}{2}}{\frac{1}{2}\left[\sum_i \binom{n_{i\cdot}}{2} + \sum_j \binom{n_{\cdot j}}{2}\right] - \left[\sum_i \binom{n_{i\cdot}}{2} \cdot \sum_j \binom{n_{\cdot j}}{2}\right] / \binom{n}{2}}$$

- RAND Index is always between 0 and 1
- ARI is between -1 and $+1$
- ARI is negative when clustering is worse than random

Example

Clusters	C_1	C_2	C_3	Total
l_1	1	1	0	2
l_2	1	2	1	4
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Total	2	3	5	10

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- Therefore, number of pairs not agreeing, i.e., $b = \binom{10}{2} - 7 - 6 - 7 = 45 - 20 = 25$

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- RAND Index is $\frac{7+25}{45} = 0.71$
- ARI is $\frac{7-(13\times14)/45}{(13+14)/2-(13\times14)/45} = 0.31$

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- If $H \to 0$, then data is clustered
- If $H \to 1$, then data is regular or sparse

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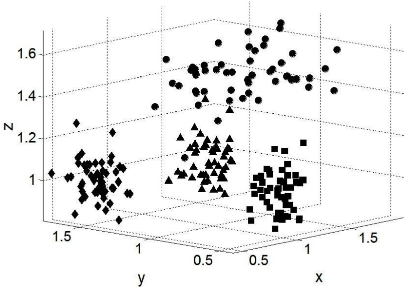
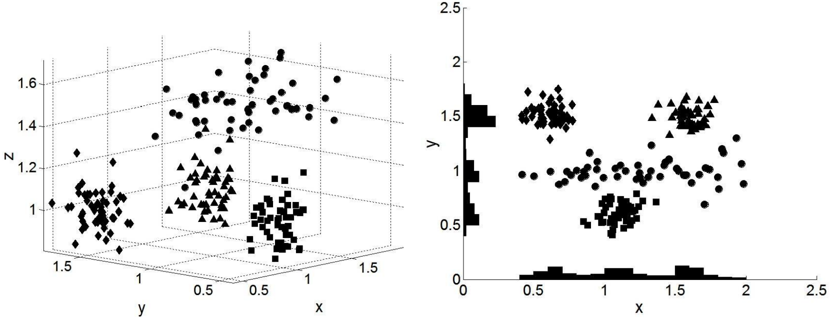
- $\bigcirc$ points weakly cluster



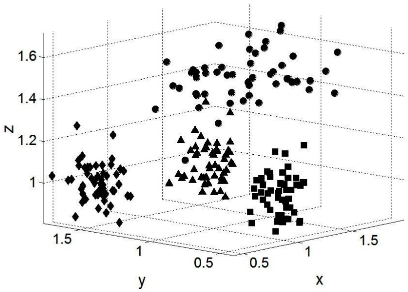
Clusters in xy Subspace

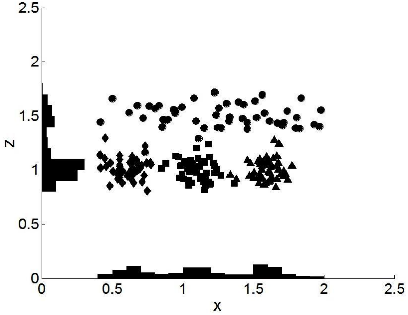
- In x space: $\diamond$, $\square$ and $\triangle$ points cluster but $\bigcirc$ acts as noise
- In y space: $\square$ separate, $\bigcirc$ separate, $\diamond$ and $\triangle$ together
- In xy space: $\diamond$, $\square$ and $\triangle$ points cluster and $\bigcirc$ points weakly cluster



Clusters in xz Subspace

- In x space: $\diamond$, $\square$ and $\triangle$ points cluster but $\bigcirc$ acts as noise
- In z space: $\bigcirc$ separate, $\square$, $\diamond$ and $\triangle$ together
- In xz space: $\diamond$, $\square$ and $\triangle$ points cluster and $\bigcirc$ points weakly cluster





Clusters in yz Subspace

- In y space: $\bigcirc$ separate, $\square$ separate, $\diamond$ and $\triangle$ together
- In z space: $\bigcirc$ separate, $\square$, $\diamond$ and $\triangle$ together
- In yz space: $\bigcirc$ separate, $\square$ separate, $\diamond$ and $\triangle$ together