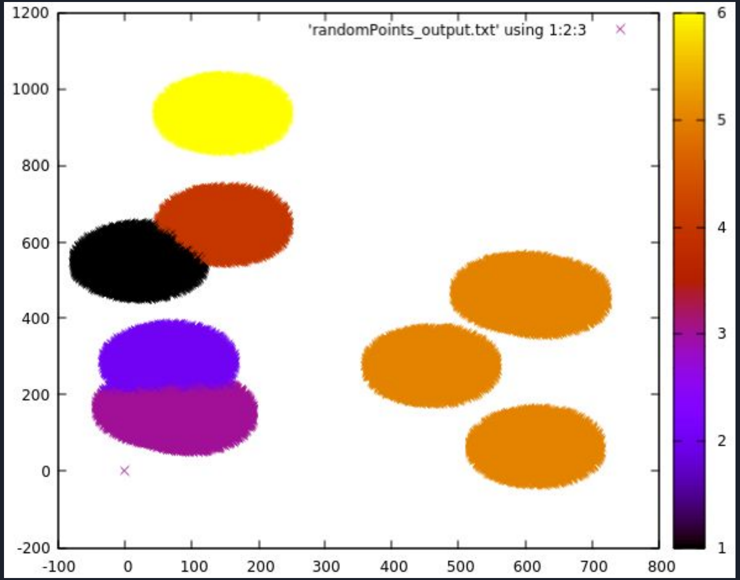
Cluster Validation

Knowing you got it right…

The Purpose of Clustering:

- “…clustering analyzes data objects without consulting class labels.” Data Mining: Concepts and Techniques.
- Associates unlabeled (unclassified) data into groups based on some distance measure.
- Distance, proximity, close-ness and similarity all measure roughly the same thing and there are many ways to measure distance.
- There are *many* decisions to make when clustering data.

Cluster Validity:



6-Means clustering of 100,000 points generated around 10 random centers.

- How can we tell that a clustering is “good”?
- Judgement is easy in low dimensional data but much harder when visualization is more difficult.
- Validation methods can either be external (which rely on external knowledge) or internal (which only relies on the distance measures within the data)

External Validation:

- Uses domain expertise to confirm good clustering.
- So to validate a clustering of students we might ask the Office of Admissions, or a clustering of animals we might ask a biologist.
- So the clustering from the previous page could be judged “bad” because I generated it with 10 centers and clustered it with 6.
- Most common but least “interesting”. Does not generate new information about data and can only validate assumptions that were already made.

Internal Validation:

- “Using this approach of cluster validity the goal is to evaluate the clustering result of an algorithm using only quantities and features inherited from the data set.” [1]
- Does not rely on any domain experts and can offer new insight into the data.
- Generally produce a numerical index which corresponds to the “goodness” of clustering.
- Methods to explore: Dunn Index, Hubert Gamma statistic, Davies-Bouldin

[1] “Cluster Validity Methods: Part 1”, Maria Halkidi, Yannis Batistakis, Michalis Vazirgiannia, SIGMOD 2002

Dunn Index:

- First proposed by JC Dunn in the Journal of Cybernetics in 1974.
- Indicates the ratio between the minimum distance between any two clusters and the the maximum of the mean distance between points in any cluster.
- High value indicates well separated clusters.
- Because it relies on a “max value in the denominator” it is very sensitive to one bad cluster.
- □(Ci, Cj) is the inter-cluster distance measure.
    - Center to center for this presentation.
- Δk is the max distance between 2 points is a cluster.
    - Can be other measures.

$$DI_m = \frac{\min\limits_{1 \leqslant i < j \leqslant m} \delta(C_i, C_j)}{\max\limits_{1 \leqslant k \leqslant m} \Delta_k}$$

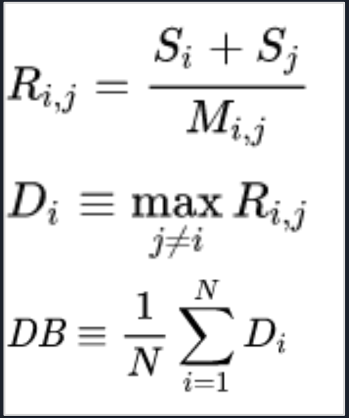
Hubert Gamma Statistic:

- Defined by S. Theodoridis and K. Koutroubas in *Pattern Recognition* in 1999.
- Indicates the sum of the products between point distances and cluster center distances.
- Value indicates compact clusters, but bigger isn’t necessarily better.
- P(i, j) is the distance between i and j.
- Q(i, j) is the distance between the centers of i’s and j’s clusters.
- M = (n*(n-1))/2

$$\Gamma = \left(1/M\right)\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} P(i, j)\cdot Q(i, j)$$

Davies-Bouldin Index:

- Defined by David Davies and Donald Bouldin in 1979 in *IEEE Transactions on Pattern Analysis and Machine Intelligence.*
- Represents a ratio between distances between points to centroids and centroids to centroids.
- Low values indicate strongly dissimilar clusters.
- S_i is the sum of all distances from a point to its own centroid i.
- $M_{i,j}$ is the distance between cluster i and j.
- N is the number of clusters.

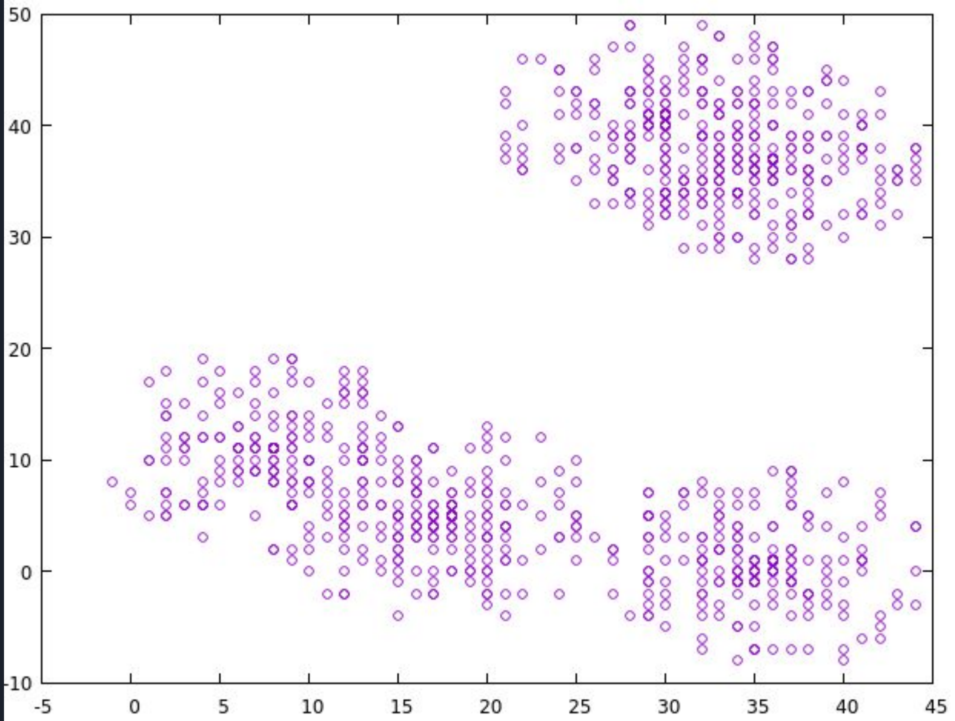


$$R_{i,j} = \frac{S_i + S_j}{M_{i,j}}$$

$$D_i \equiv \max_{j \neq i} R_{i,j}$$

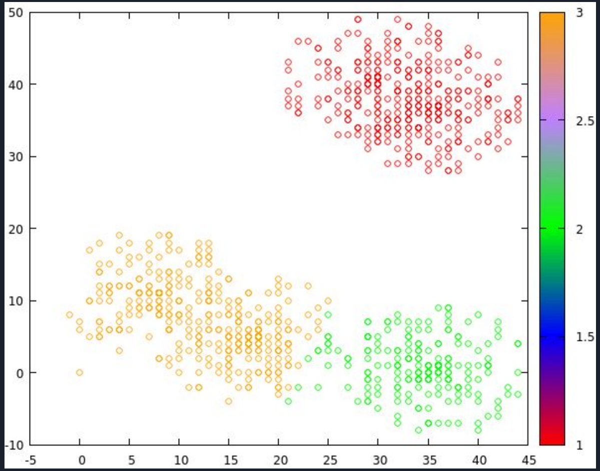
$$DB \equiv \frac{1}{N} \sum_{i=1}^{N} D_i$$

Test Data:

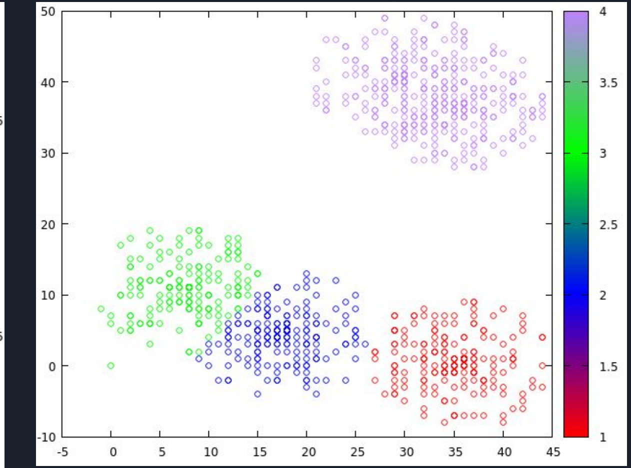


- 1000 points distributed equally at random around 5 randomly chosen centers.
- 2-dimensional
- Plotted using gnuplot

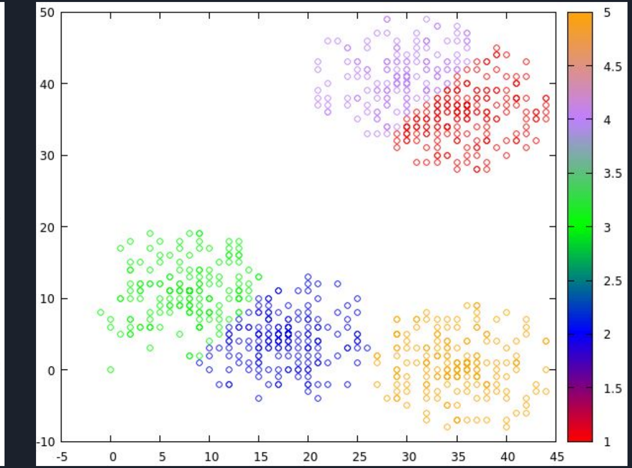
Test Clusters:



3-means

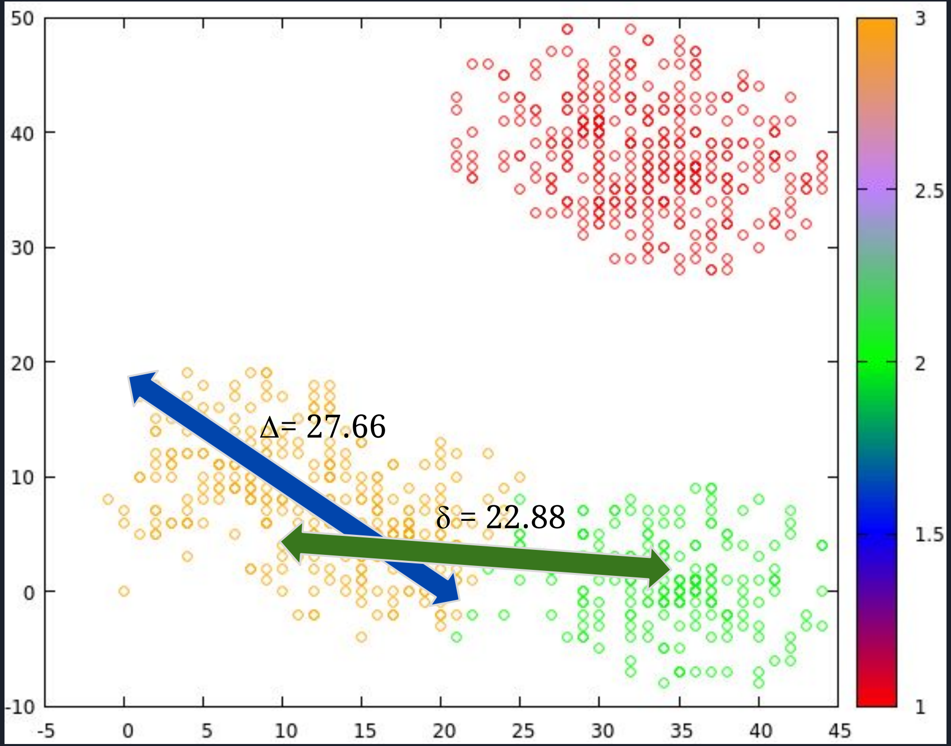


4-means



5-means

Dunn Index Results:



Largest Cluster:

27.66

Min Cluster Distance;

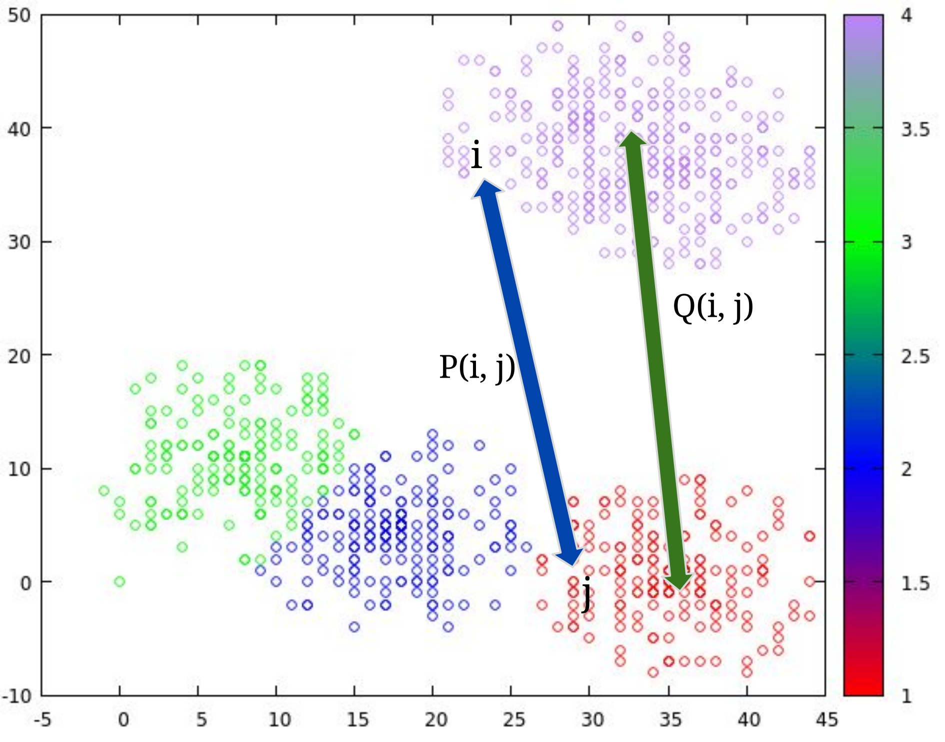
22.88

3 Clusters: 0.827

4 Cluster: 0.478

5 Clusters: 0.462

Hubert Gamma Results:



P -> point to point distance

Q -> center to center distance

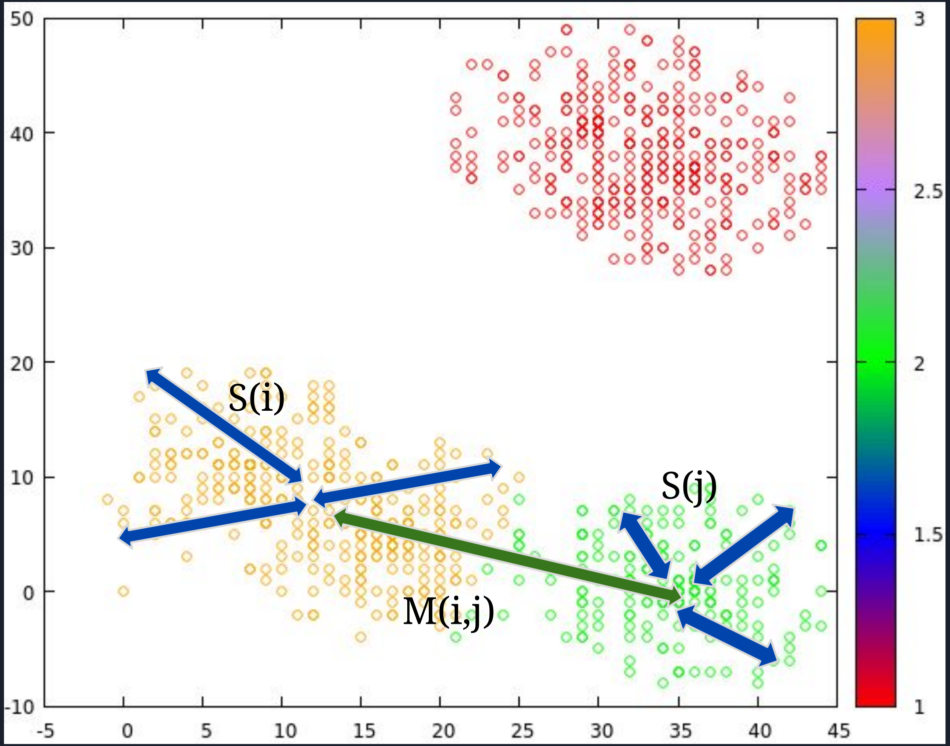
Bigger or smaller values do not necessarily indicate anything, rather we look for a “knee”.

3 clusters: 604.7

4 clusters: 620.3

5 clusters: 708.7

Davies-Bouldin Results:



S -> the distance from points to center

M -> the distance from center to center

R = (Si + Sj) / M = the similarity of two clusters

DB = the average of each cluster max R. So a smaller DB value is “better”.

3 Clusters: 0.288

4 Clusters: 0.359

5 Clusters: 0.432

Collected Results:

	3 Clusters	**4 Clusters**	**5 Clusters**
Dunn	0.827	0.478	0.462
Hubert Gamma	604.7	620.4	708.7
Davies-Bouldin	0.287	0.359	0.432
	Best separation, Most dissimilar	Best compactness	

Based on these measures, 3 clusters is our best choice.

Questions or Comments?

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Code and test data available at: https://github.com/gentry-atkinson/cs7312_assignments