Chapter 14 – Cluster Analysis

Data Mining for Business Intelligence

Shmueli, Patel & Bruce

Clustering: The Main Idea

Goal: Form groups (clusters) of similar records

Used for **segmenting markets** into groups of similar customers

Example: Claritas segmented US neighborhoods based on demographics & income: “Furs & station wagons,” “Money & Brains”, …

Other Applications

- Periodic table of the elements
- Classification of species
- Grouping securities in portfolios
- Grouping firms for structural analysis of economy
- Army uniform sizes

Example: Public Utilities

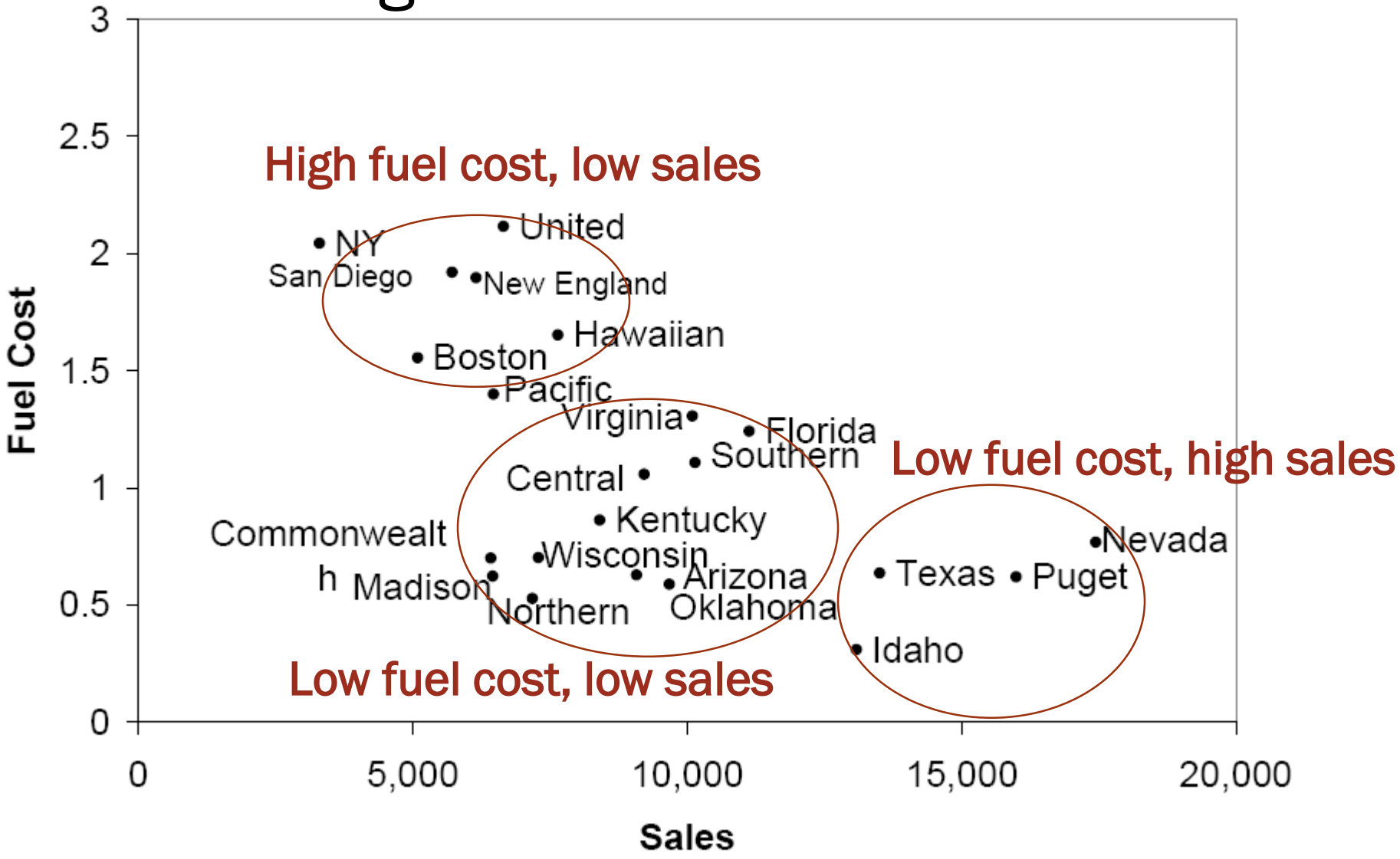
Goal: find clusters of similar utilities

Data: 22 firms, 8 variables

- Fixed-charge covering ratio
- Rate of return on capital
- Cost per kilowatt capacity
- Annual load factor
- Growth in peak demand
- Sales
- % nuclear
- Fuel costs per kwh

Company	Fixed_charge	RoR	Cost	Load	Δ Demand	Sales	Nuclear	Fuel_Cost
Arizona	1.06	9.2	151	54.4	1.6	9077	0	0.628
Boston	0.89	10.3	202	57.9	2.2	5088	25.3	1.555
Central	1.43	15.4	113	53	3.4	9212	0	1.058
Commonwealth	1.02	11.2	168	56	0.3	6423	34.3	0.7
Con Ed NY	1.49	8.8	192	51.2	1	3300	15.6	2.044
Florida	1.32	13.5	111	60	-2.2	11127	22.5	1.241
Hawaiian	1.22	12.2	175	67.6	2.2	7642	0	1.652
Idaho	1.1	9.2	245	57	3.3	13082	0	0.309
Kentucky	1.34	13	168	60.4	7.2	8406	0	0.862
Madison	1.12	12.4	197	53	2.7	6455	39.2	0.623
Nevada	0.75	7.5	173	51.5	6.5	17441	0	0.768
New England	1.13	10.9	178	62	3.7	6154	0	1.897
Northern	1.15	12.7	199	53.7	6.4	7179	50.2	0.527
Oklahoma	1.09	12	96	49.8	1.4	9673	0	0.588
Pacific	0.96	7.6	164	62.2	-0.1	6468	0.9	1.4
Puget	1.16	9.9	252	56	9.2	15991	0	0.62
San Diego	0.76	6.4	136	61.9	9	5714	8.3	1.92
Southern	1.05	12.6	150	56.7	2.7	10140	0	1.108
Texas	1.16	11.7	104	54	-2.1	13507	0	0.636
Wisconsin	1.2	11.8	148	59.9	3.5	7287	41.1	0.702
United	1.04	8.6	204	61	3.5	6650	0	2.116
Virginia	1.07	9.3	174	54.3	5.9	10093	26.6	1.306

Sales & Fuel Cost:
3 rough clusters can be seen



Clustering is Ambiguous

How many clusters?

Six Clusters

Two Clusters

Four Clusters

Extension to More Than 2 Dimensions

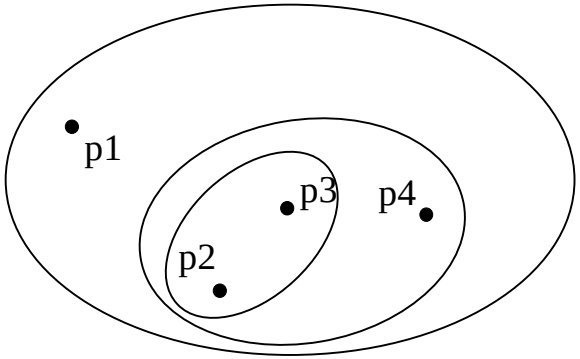
In prior example, clustering was done by eye

Multiple dimensions require formal algorithm with

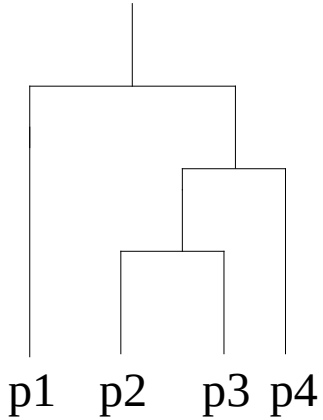
- A **distance measure**
- A way to use the distance measure in forming clusters

We will consider two algorithms: **hierarchical** and **non-hierarchical**

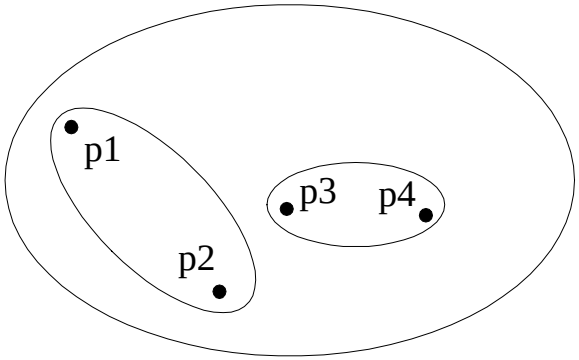
Hierarchical Clustering



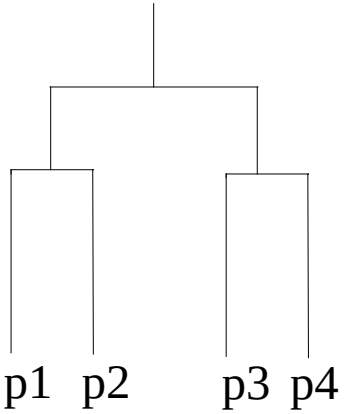
Traditional Hierarchical Clustering



Traditional Dendrogram

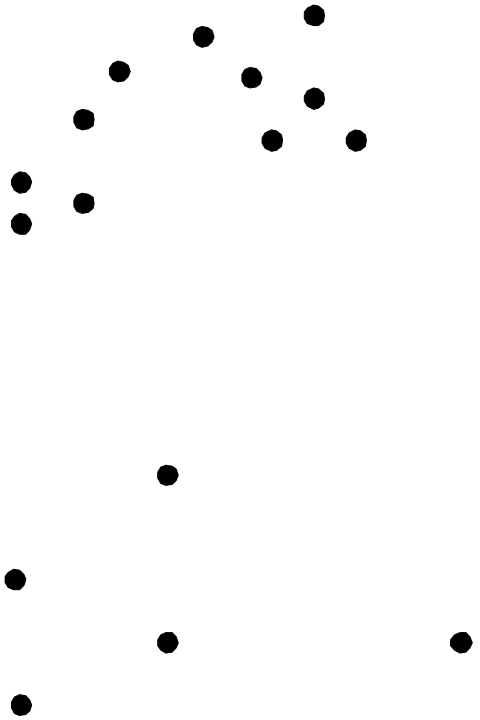


Non-traditional Hierarchical Clustering

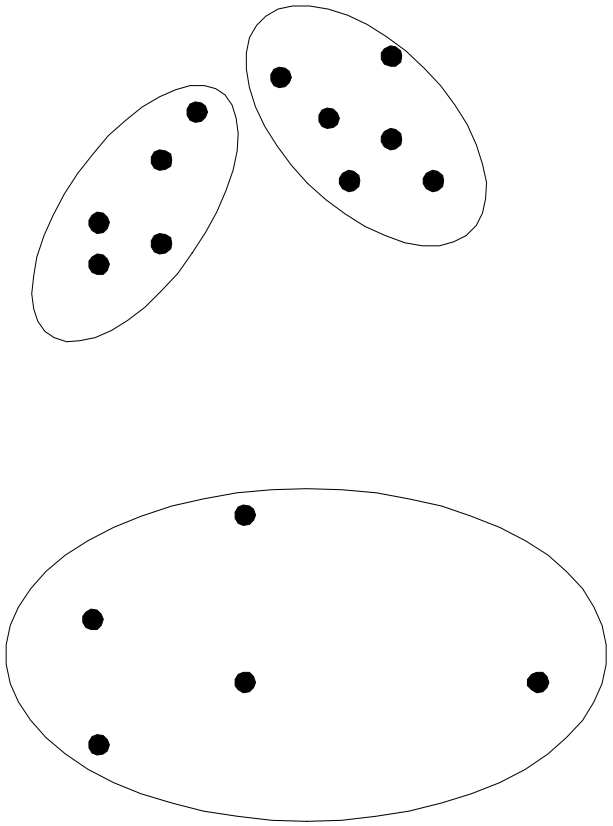


Non-traditional Dendrogram

Partitional Clustering



Original Points



A Partitional Clustering

Hierarchical Clustering

Hierarchical Methods

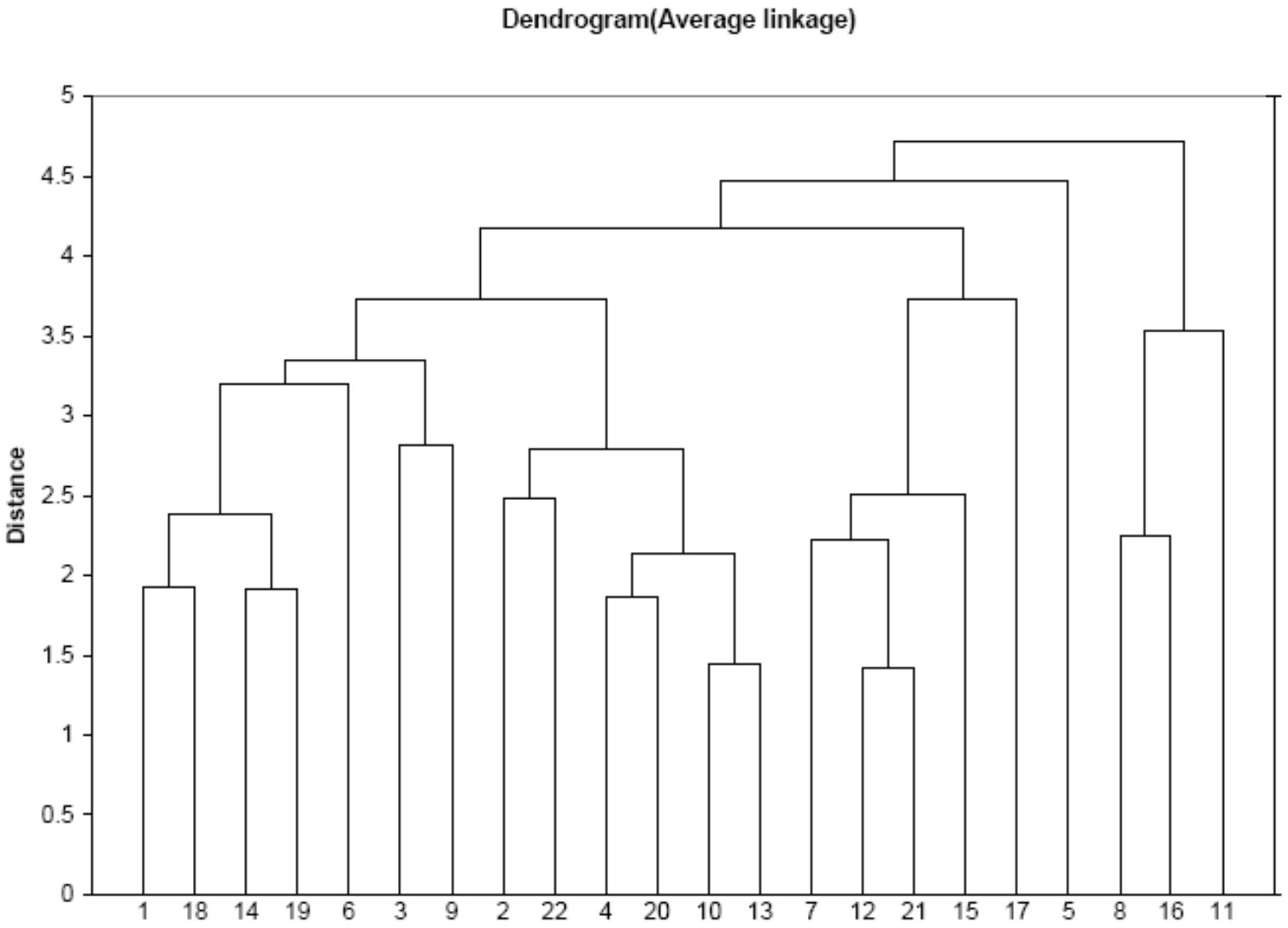
Agglomerative Methods

- Begin with n-clusters (each record its own cluster)
- Keep joining records into clusters until one cluster is left (the entire data set)
- Most popular

Divisive Methods

- Start with one all-inclusive cluster
- Repeatedly divide into smaller clusters

A **Dendrogram** shows the cluster hierarchy



Measuring Distance

Between records

Between clusters

Measuring Distance Between Records

Distance Between Two Records

Euclidean Distance is most popular:

$$d_{ij} = \sqrt{(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \cdots + (x_{ip} - x_{jp})^2}$$

Normalizing

Problem: Raw distance measures are highly influenced by scale of measurements

Solution: normalize (standardize) the data first

- Subtract mean, divide by std. deviation
- Also called **z-scores**

Example: Normalization

For 22 utilities:

Avg. sales = 8,914

Std. dev. = 3,550

Normalized score for Arizona sales:

(9,077-8,914)/3,550 = 0.046

For Categorical Data: **Similarity**

To measure the distance between records in terms of two 0/1 variables, create table with counts:

	0	1
0	a	b
1	c	d

Similarity metrics based on this table:

- Matching coef. = (a+d)/p
- Jaquard's coef. = d/(b+c+d)
  - Use in cases where a matching "1" is much greater evidence of similarity than matching "0" (e.g. "owns Corvette")

Other Distance Measures

- Correlation-based similarity
- Statistical distance (Mahalanobis)
- Manhattan distance (absolute differences)
- Maximum coordinate distance
- Gower's similarity (for mixed variable types: continuous & categorical)

Measuring Distance Between Clusters

Minimum Distance (Cluster A to Cluster B)

- Also called **single linkage**
- Distance between two clusters is the distance between the pair of records A_i and B_j that are closest

Maximum Distance (Cluster A to Cluster B)

- Also called **complete linkage**
- Distance between two clusters is the distance between the pair of records A_i and B_j that are farthest from each other

Average Distance

- Also called **average linkage**
- Distance between two clusters is the average of all possible pair-wise distances

Centroid Distance

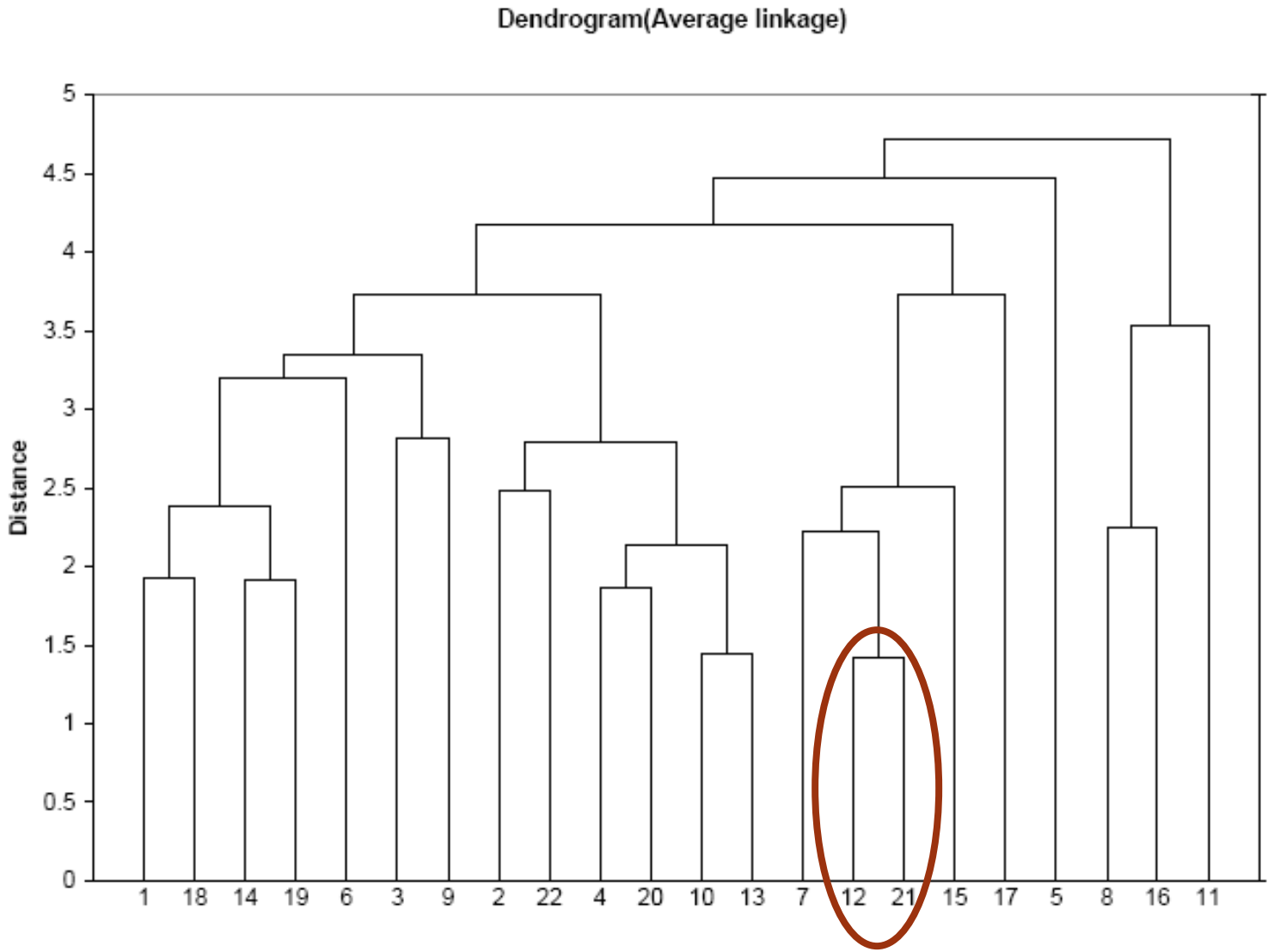
- Distance between two clusters is the distance between the two cluster centroids.
- Centroid is the vector of variable averages for all records in a cluster

The Hierarchical Clustering Steps (Using Agglomerative Method)

1. Start with *n* clusters (each record is its own cluster)
2. Merge two closest records into one cluster
3. At each successive step, the two clusters closest to each other are merged

Dendrogram, from bottom up, illustrates the process

Records 12 & 21 are closest & form first cluster



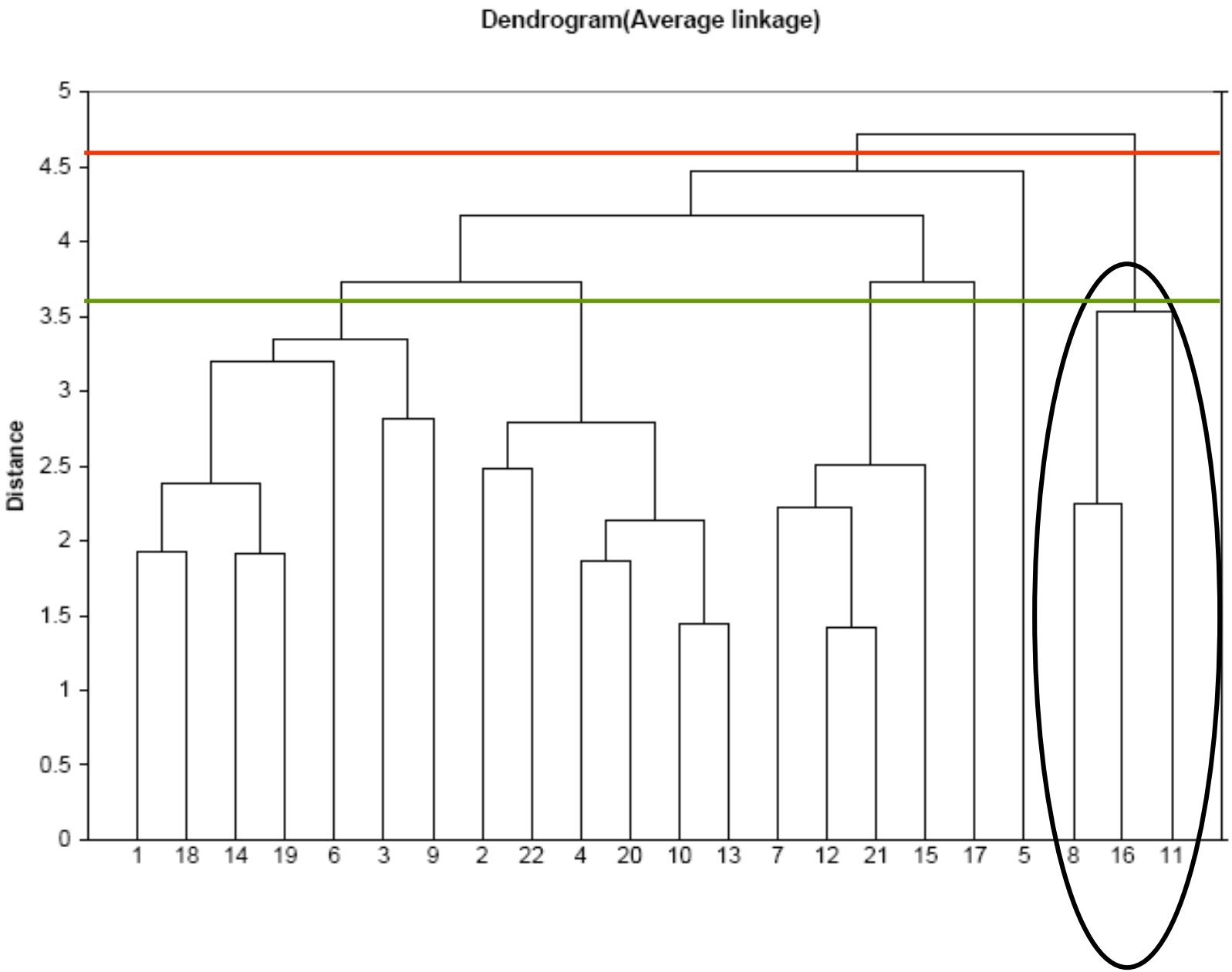
Reading the Dendrogram

See process of clustering: Lines connected lower down are merged earlier

- 10 and 13 will be merged next, after 12 & 21

Determining number of clusters: For a given "distance between clusters", a horizontal line intersects the clusters that are that far apart, to create clusters

- E.g., at distance of 4.6 (red line in next slide), data can be reduced to 2 clusters -- The smaller of the two is circled
- At distance of 3.6 (green line) data can be reduced to 6 clusters, including the circled cluster


Dendrogram(Average linkage)
Distance
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
1 18 14 19 6 3 9 2 22 4 20 10 13 7 12 21 15 17 5 8 16 11

Validating Clusters

Interpretation

Goal: obtain meaningful and useful clusters

Caveats:

(1) Random chance can often produce apparent clusters

(2) Different cluster methods produce different results

Solutions:

- Obtain summary statistics
- Also review clusters in terms of variables **not** used in clustering
- Label the cluster (e.g. clustering of financial firms in 2008 might yield label like “midsize, sub-prime loser”)

Desirable Cluster Features

Stability – are clusters and cluster assignments sensitive to slight changes in inputs? Are cluster assignments in partition B similar to partition A?

Separation – check ratio of between-cluster variation to within-cluster variation (higher is better)

Nonhierarchical Clustering: K-Means Clustering

K-Means Clustering Algorithm

1. Choose # of clusters desired, *k*
2. Start with a partition into k clusters

   Often based on random selection of k centroids
3. At each step, move each record to cluster with closest centroid
4. Recompute centroids, repeat step 3
5. Stop when moving records increases within-cluster dispersion

K-means Algorithm: Choosing k and Initial Partitioning

Choose *k* based on the how results will be used

- e.g., “How many market segments do we want?”

Also experiment with slightly different *k*’s

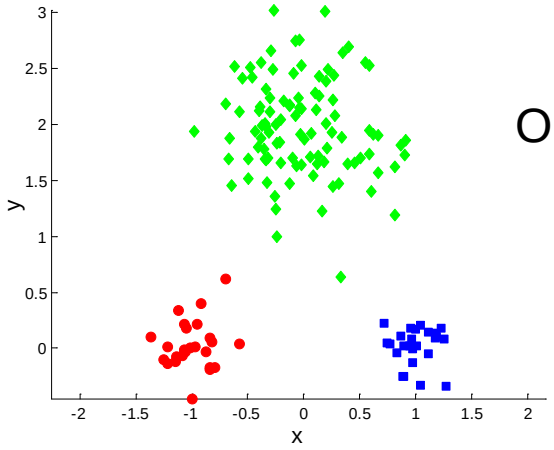
Initial partition into clusters can be random, or based on domain knowledge

- If random partition, repeat the process with different random partitions

K-means Clustering – Details

- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.
- The centroid is (typically) the mean of the points in the cluster.
- ‘Closeness’ is measured by Euclidean distance, cosine similarity, correlation, etc.
- K-means will converge for common similarity measures mentioned above.
- Most of the convergence happens in the first few iterations.
  - Often the stopping condition is changed to ‘Until relatively few points change clusters’
- Complexity is O(n * K * I * d)
  - n = number of points, K = number of clusters,
    I = number of iterations, d = number of attributes

Two different K-means Clusterings



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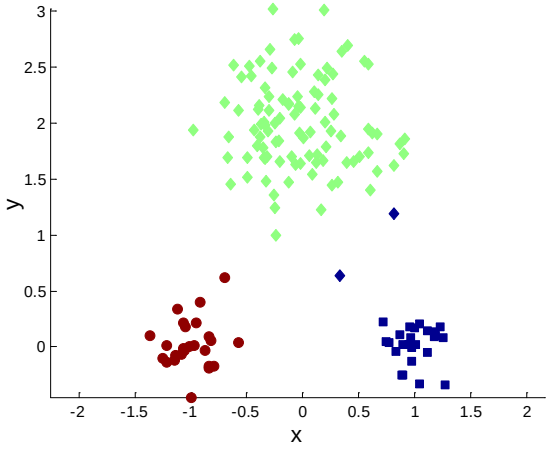
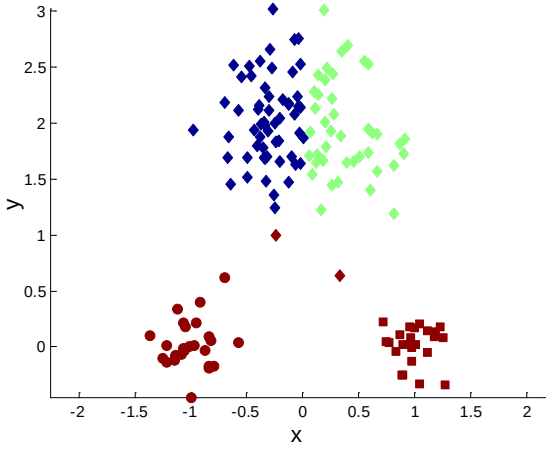
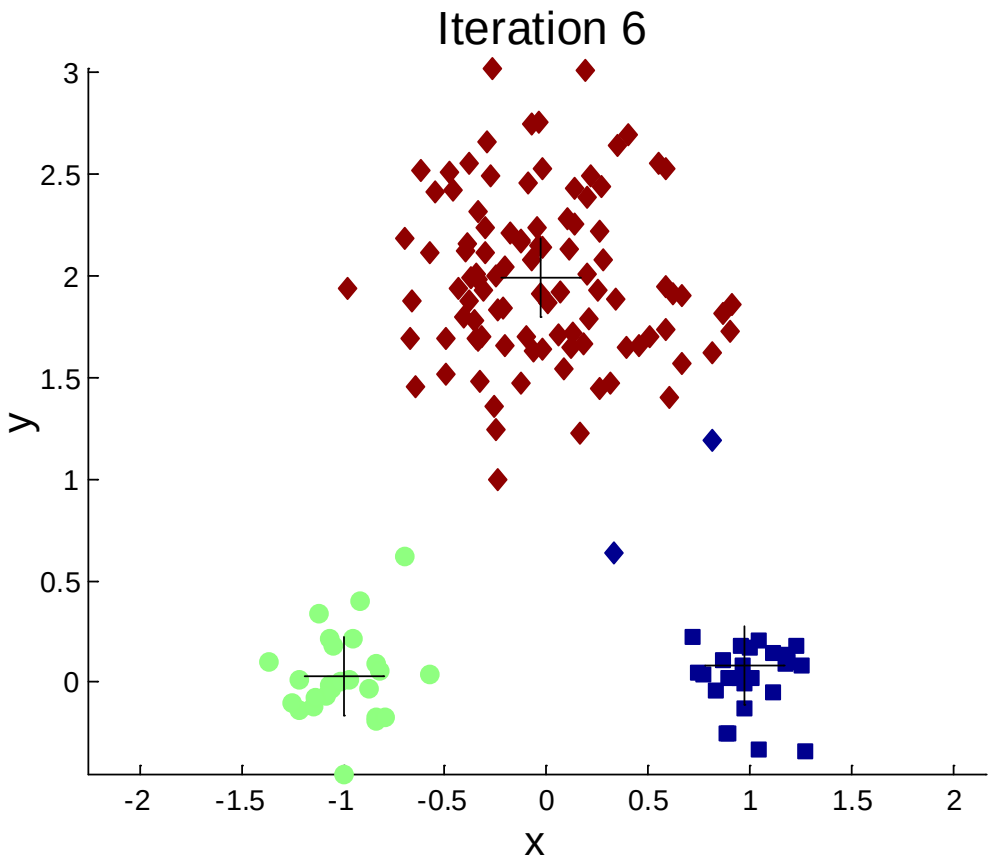


Optimal Clustering



Sub-optimal Clustering

Importance of Choosing Initial Centroids



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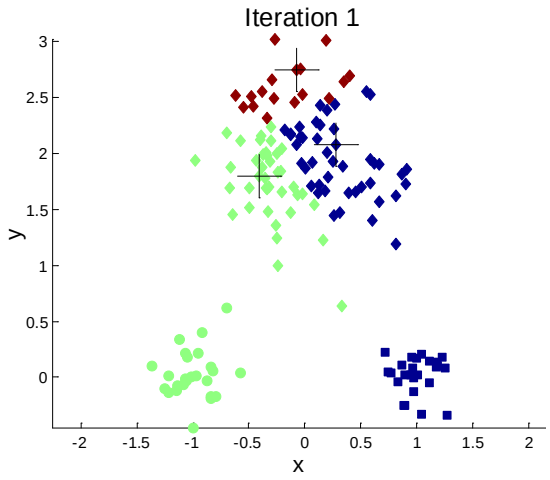
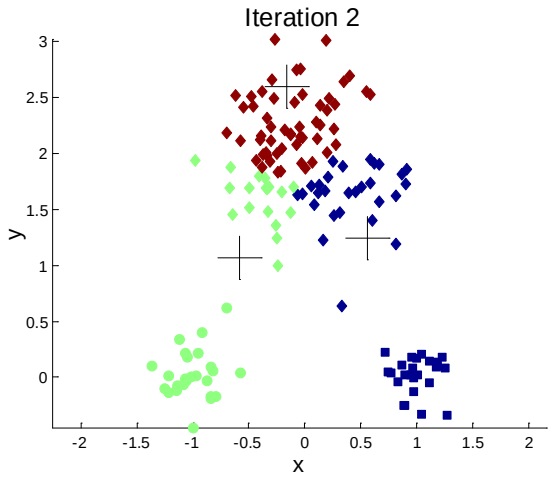
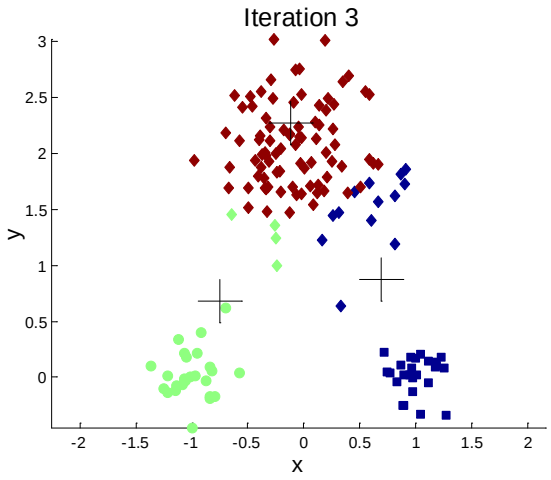
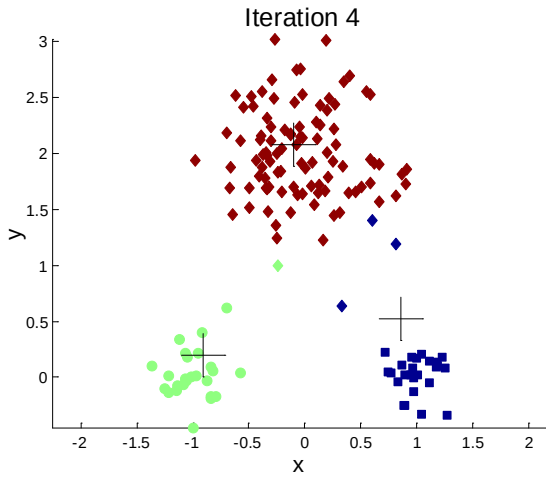
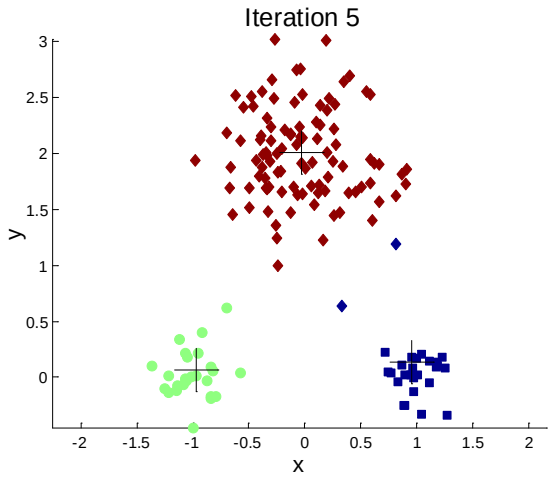
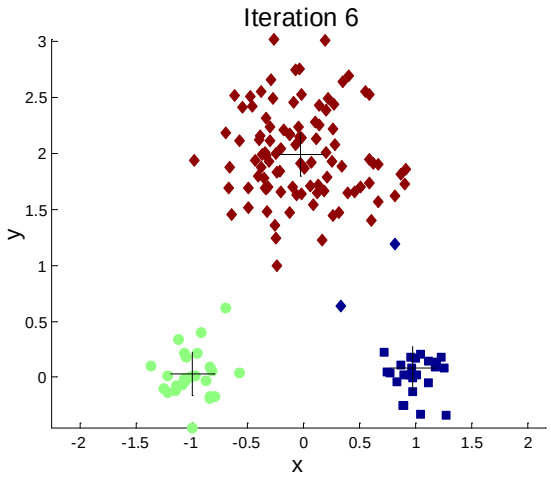












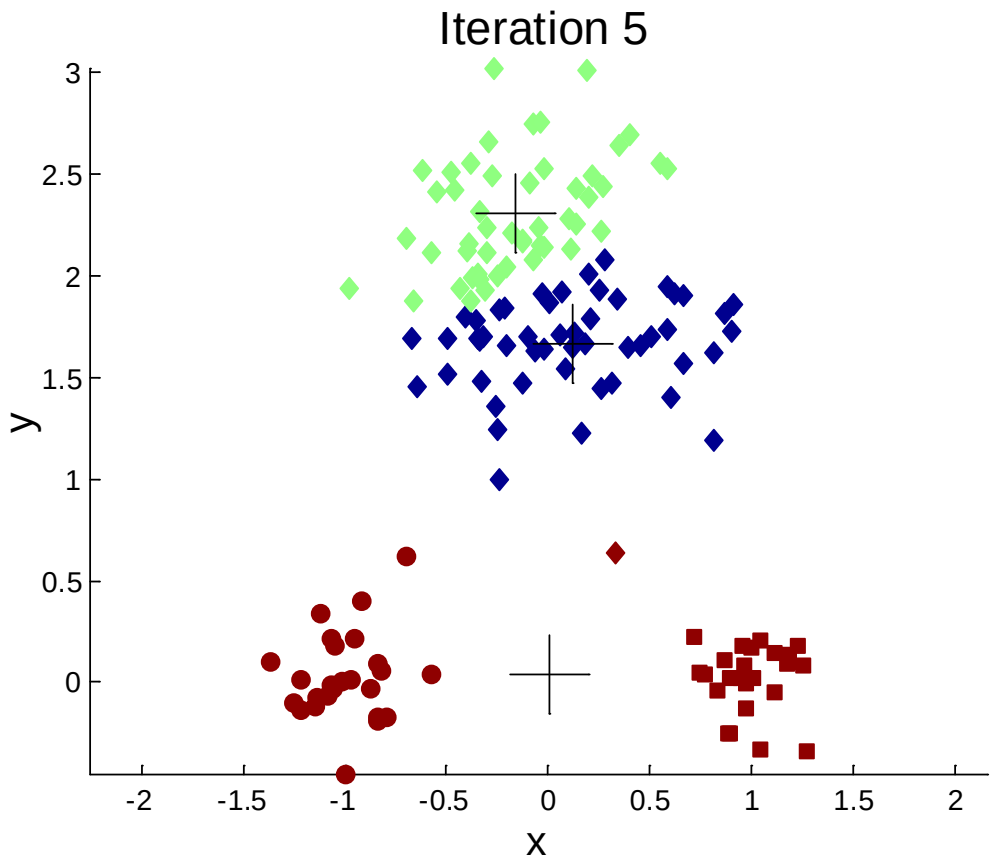
Evaluating K-means Clusters

- Most common measure is Sum of Squared Error (SSE)
  - For each point, the error is the distance to the nearest cluster
  - To get SSE, we square these errors and sum them.

$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(m_i, x)$$

  - x is a data point in cluster C_i and m_i is the representative point for cluster C_i
    - can show that m_i corresponds to the center (mean) of the cluster
  - Given two clusters, we can choose the one with the smallest error
  - One easy way to reduce SSE is to increase K, the number of clusters
    - A good clustering with smaller K can have a lower SSE than a poor clustering with higher K

Importance of Choosing Initial Centroids …



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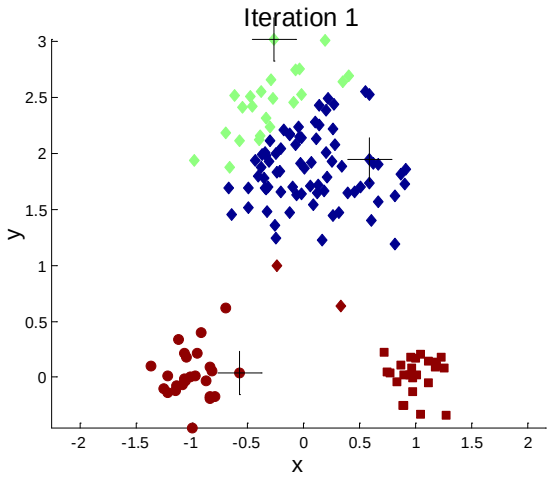
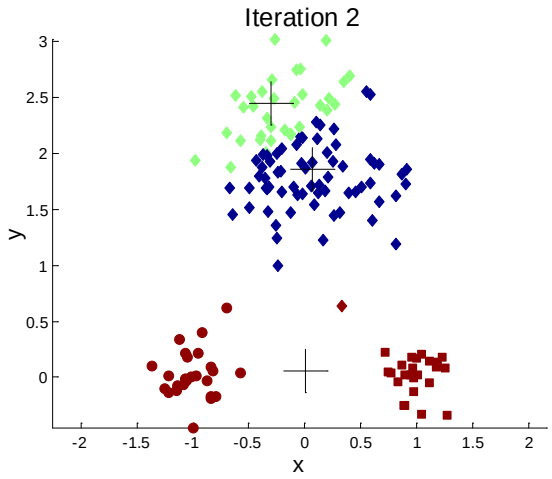
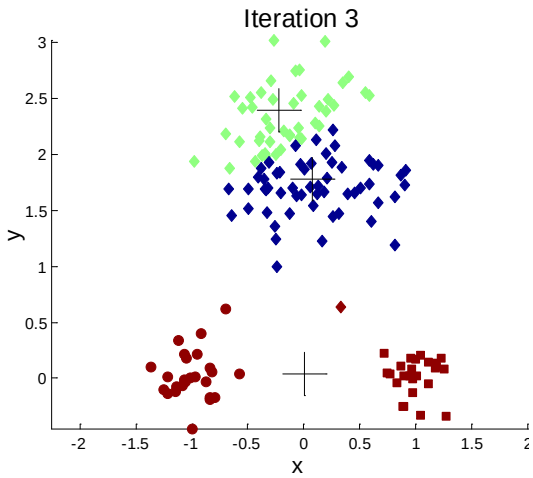
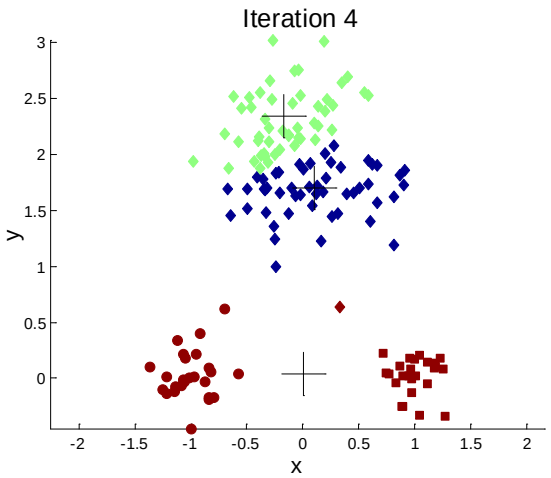
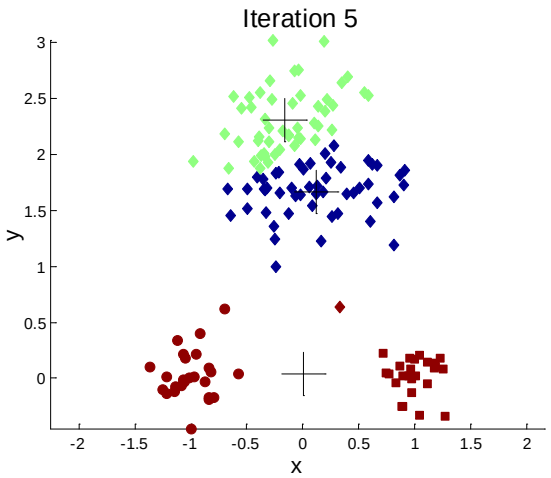










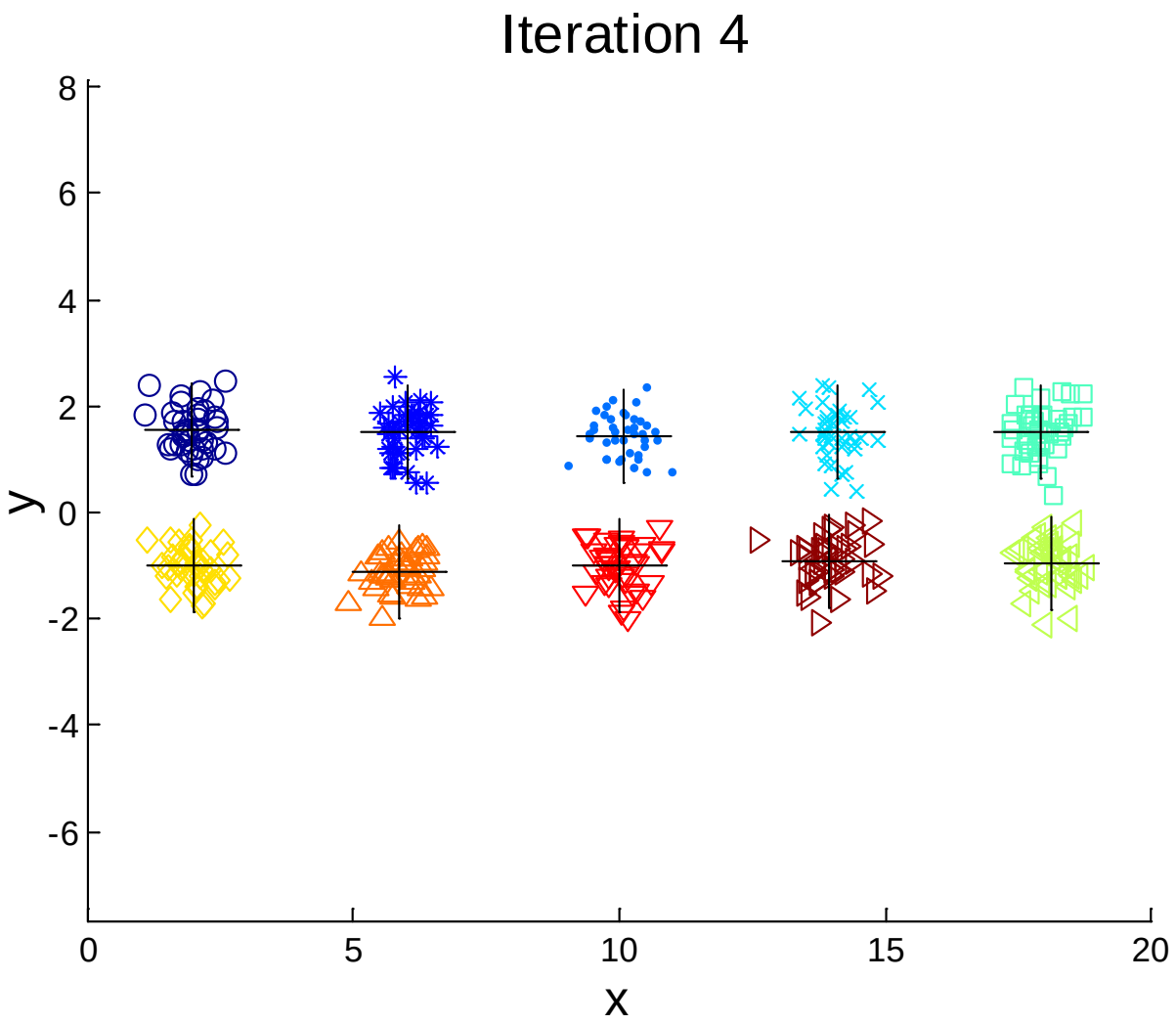
Problems with Selecting Initial Points

- If there are K 'real' clusters then the chance of selecting one centroid from each cluster is small.
  - Chance is relatively small when K is large
  - If clusters are the same size, n, then

$$P = \frac{\text{number of ways to select one centroid from each cluster}}{\text{number of ways to select } K \text{ centroids}} = \frac{K!n^K}{(Kn)^K} = \frac{K!}{K^K}$$

  - For example, if K = 10, then probability = $10!/10^{10} = 0.00036$
  - Sometimes the initial centroids will readjust themselves in 'right' way, and sometimes they don't
  - Consider an example of five pairs of clusters

10 Clusters Example



Starting with two initial centroids in one cluster of each pair of clusters

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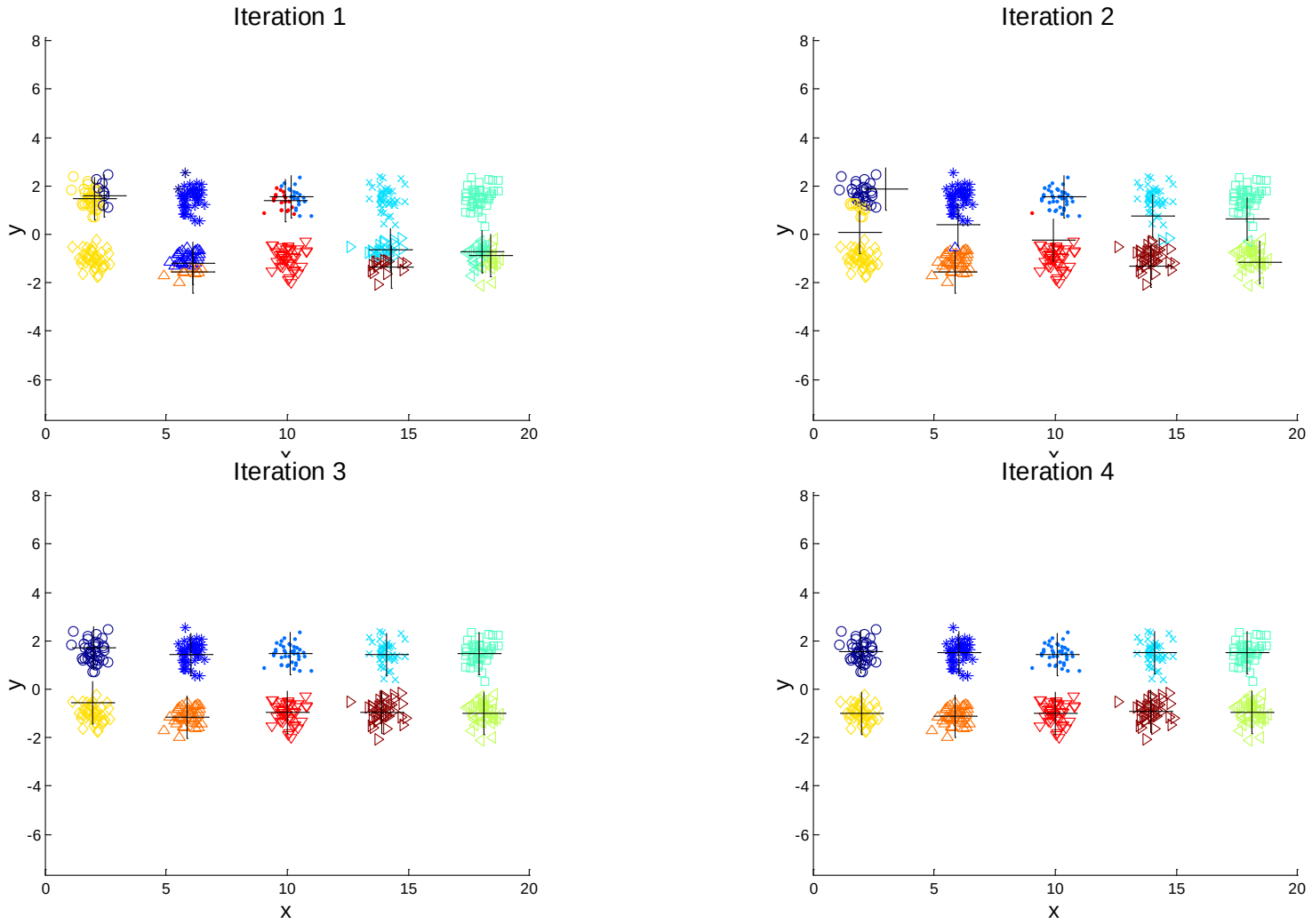

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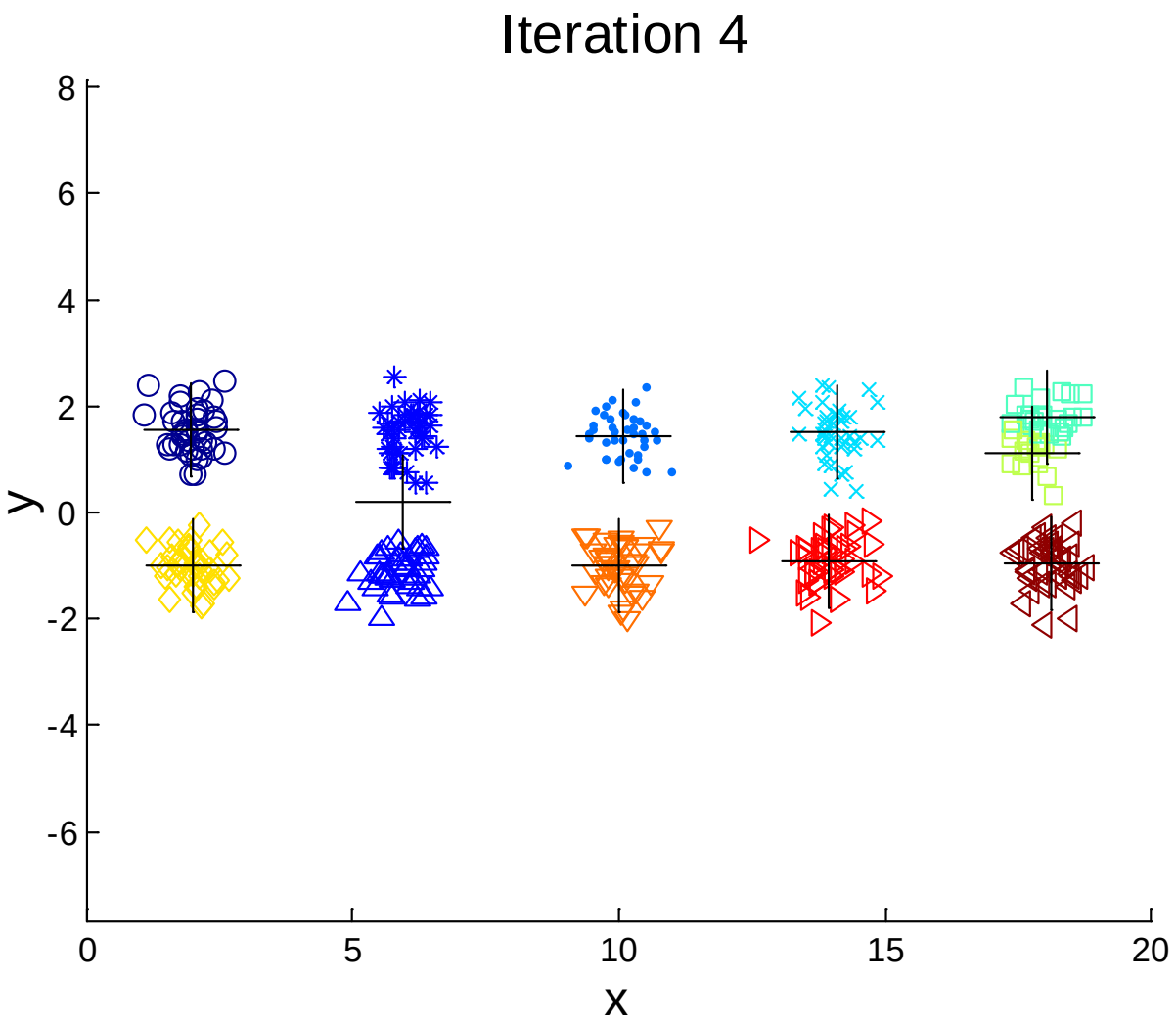

Starting with some pairs of clusters having three initial centroids, while other have only one.

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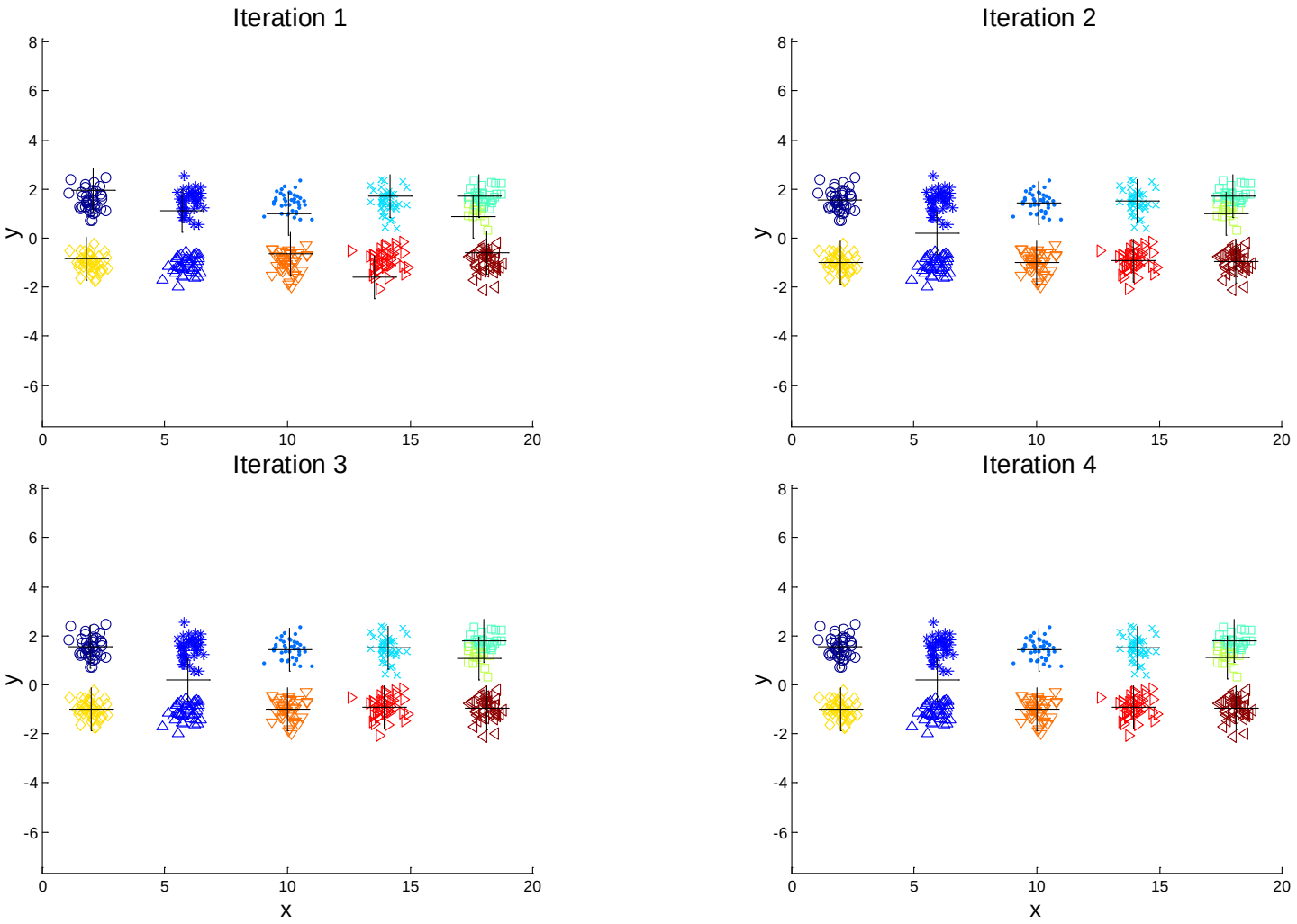


Starting with some pairs of clusters having three initial centroids, while other have only one.

Solutions to Initial Centroids Problem

- Multiple runs
  - Helps, but probability is not on your side
- Sample and use hierarchical clustering to determine initial centroids
- Select more than k initial centroids and then select among these initial centroids
  - Select most widely separated
- Postprocessing
- Bisecting K-means
  - Not as susceptible to initialization issues

Updating Centers Incrementally

- In the basic K-means algorithm, centroids are updated after all points are assigned to a centroid

- An alternative is to update the centroids after each assignment (incremental approach)
  - Each assignment updates zero or two centroids
  - More expensive
  - Introduces an order dependency
  - Never get an empty cluster
  - Can use “weights” to change the impact
  - A simpler version of Self Organizing Map neural network

Pre-processing and Post-processing

- Pre-processing
  - Normalize the data
  - Eliminate outliers
- Post-processing
  - Eliminate small clusters that may represent outliers
  - Split ‘loose’ clusters, i.e., clusters with relatively high SSE
  - Merge clusters that are ‘close’ and that have relatively low SSE
  - Can use these steps during the clustering process
    - ISODATA

XLMiner Output: Cluster Centroids

Cluster	Fixed_charge	RoR	Cost	Load_factor
Cluster-1	0.89	10.3	202	57.9
Cluster-2	1.43	15.4	113	53
Cluster-3	1.06	9.2	151	54.4

We chose $k = 3$

4 of the 8 variables are shown

Distance Between Clusters

Distance between	Cluster-1	Cluster-2	Cluster-3
Cluster-1	0	5.03216253	3.16901457
Cluster-2	5.03216253	0	3.76581196
Cluster-3	3.16901457	3.76581196	0

Clusters 1 and 2 are relatively well-separated from each other, while cluster 3 not as much

Within-Cluster Dispersion

Data summary (In Original coordinates)

Cluster	#Obs	Average distance in cluster
Cluster-1	12	1748.348058
Cluster-2	3	907.6919822
Cluster-3	7	3625.242085
Overall	22	2230.906692

Clusters 1 and 2 are relatively tight, cluster 3 very loose

Conclusion: Clusters 1 & 2 well defined, not so for cluster 3

Next step: try again with k=2 or k=4

silouette

a graphical way of finding the “optimal” K

Peter J. Rousseeuw in 1986

- For each datum, *i*
- let *a*(*i*) be the average dissimilarity of *i* with all other data within the same cluster.
- We can interpret *a*(*i*) as how well matched *i* is to the cluster it is assigned (the smaller the value, the better the matching).

- Then find the average dissimilarity of *i* with the data of another single cluster.
- Repeat this for every cluster of which *i* is not a member.
- Denote the lowest average dissimilarity to *i* of any such cluster by $b(i)$.

- The cluster with this average dissimilarity is said to be the "neighbouring cluster" of *i* as it is, aside from the cluster *i* is assigned, the cluster in which *i* fits best. We now define:

$$s(i) = \frac{b(i) - a(i)}{max\{a(i), b(i)\}}$$

which can be written as:

$$s(i) = \begin{cases} 1 - a(i)/b(i), & \text{if } a(i) < b(i) \\ 0, & \text{if } a(i) = b(i) \\ b(i)/a(i) - 1, & \text{if } a(i) > b(i) \end{cases}$$

From the above definition it is clear that

$$-1 \leq s(i) \leq 1$$

- For s(i) to be close to 1 we require $a(i) << b(i)$.
- As $a(i)$ is a measure of how dissimilar i is to its own cluster, a small value means it is well matched.
- a large $b(i)$ implies that i is badly matched to its neighboring cluster.

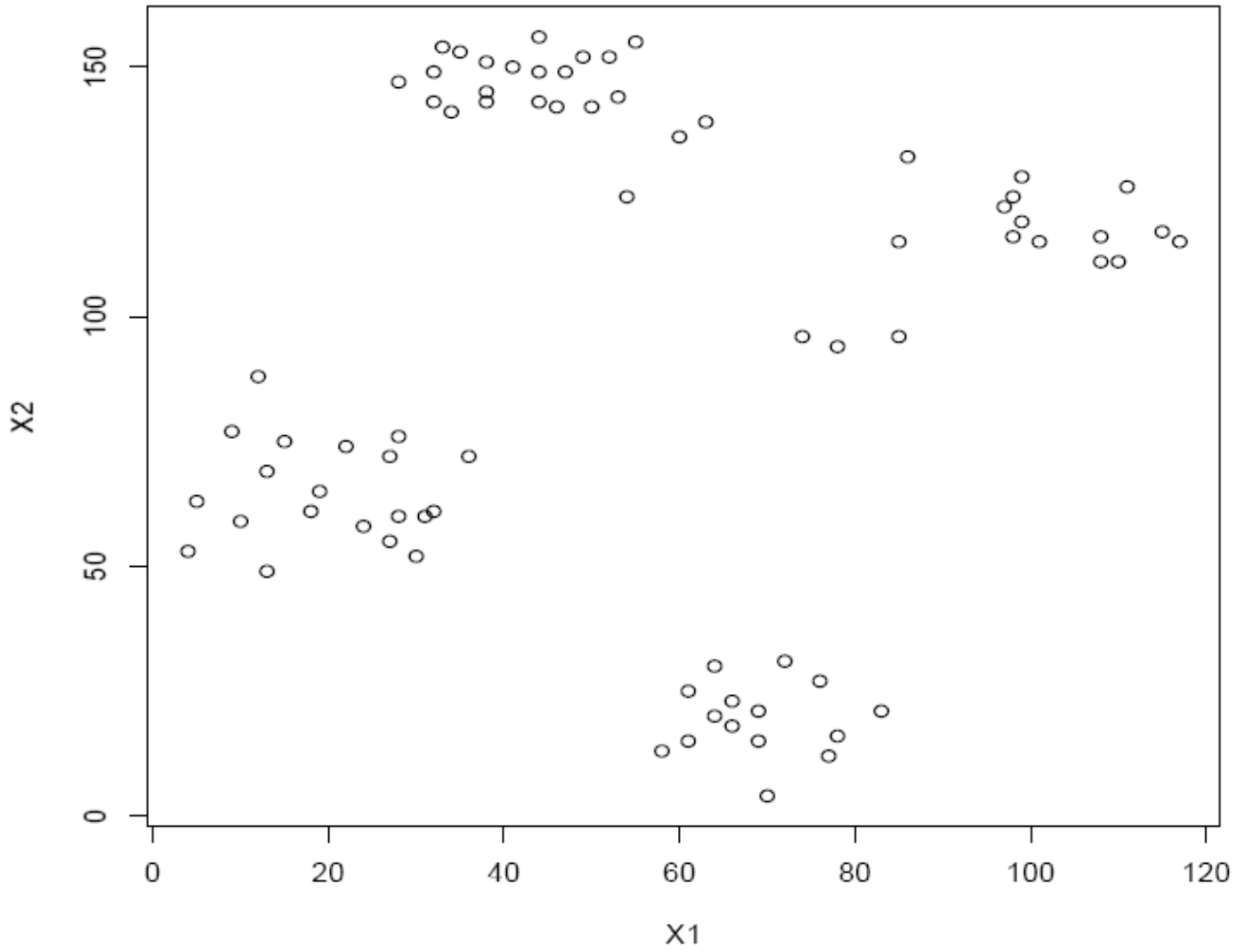
- an $s(i)$ close to one means that the datum is appropriately clustered.
- If $s(i)$ is close to negative one, then by the same logic we see that i would be more appropriate if it was clustered in its neighboring cluster.
- An $s(i)$ near zero mean that the datum is on the border of two natural clusters.

- The average $s(i)$ of a cluster is a measure of how tightly grouped all the data in the cluster are.
- Thus the average $s(i)$ of the entire dataset is a measure of how appropriately the data has been clustered.

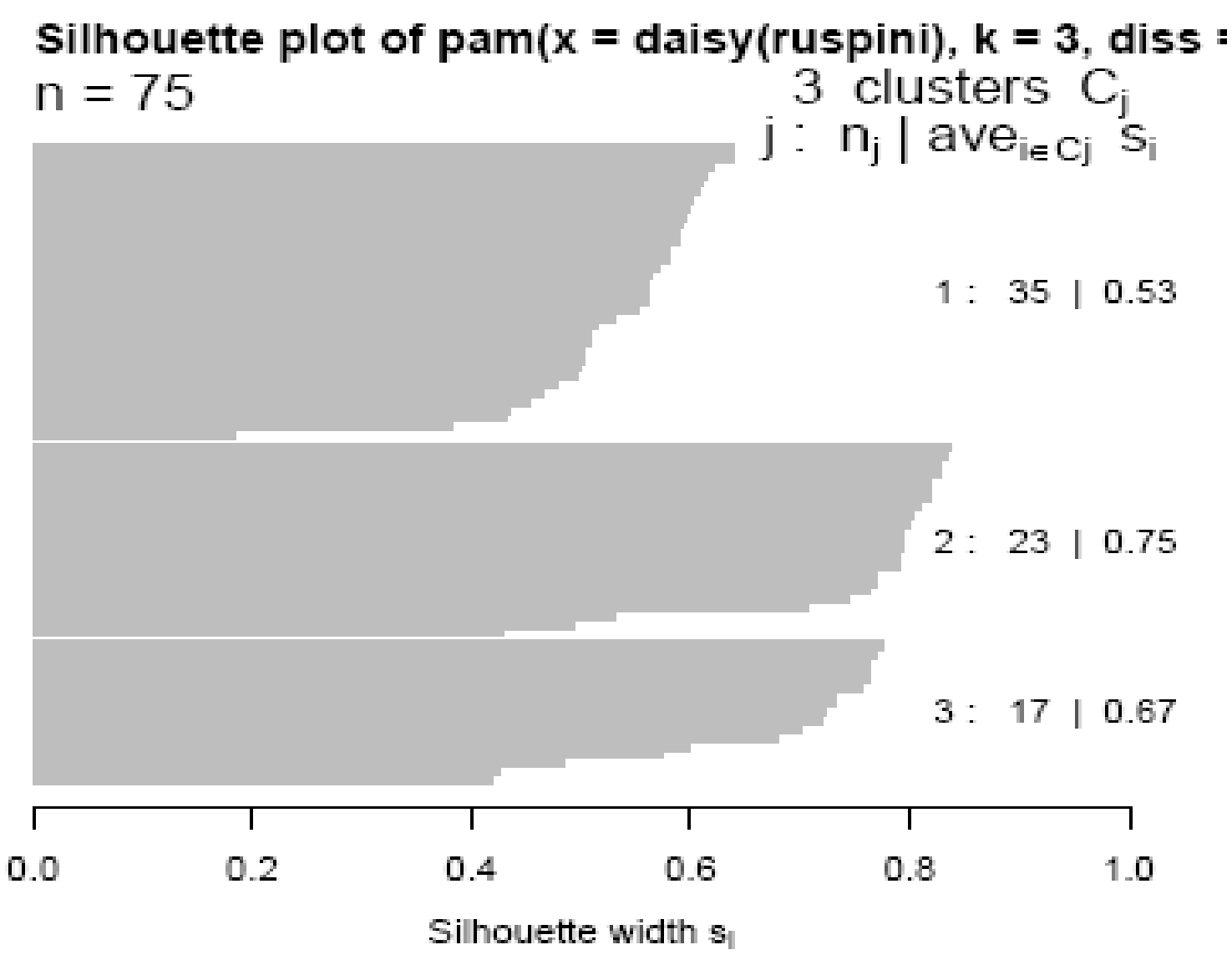
- If there are too many or too few clusters, as may occur when a poor choice of *k* is used in the k-means algorithm, some of the clusters will typically display much narrower silhouettes than the rest.
- Thus silhouette plots and averages may be used to determine the natural number of clusters within a dataset.

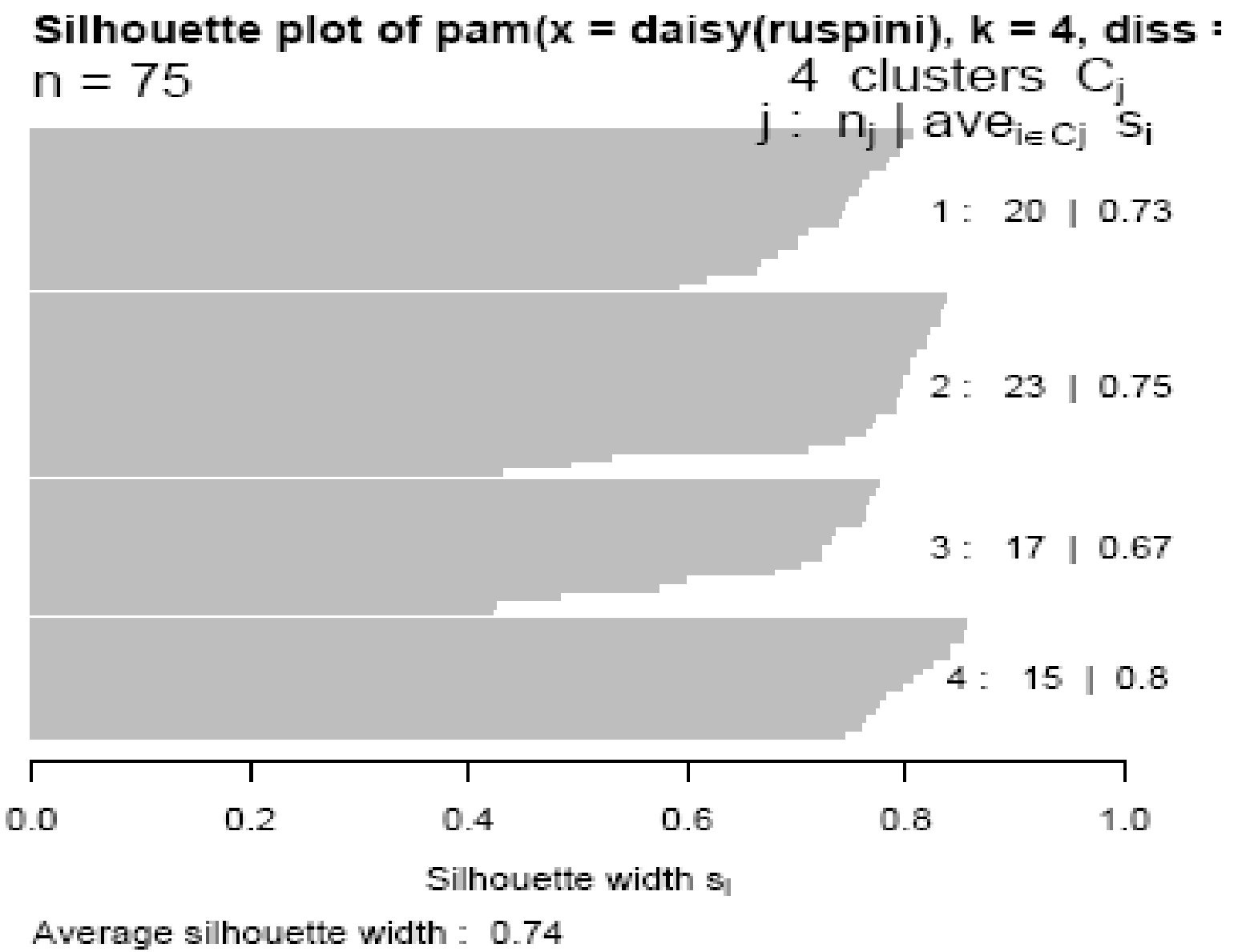
- Let’s consider an artificial 2D data set shown below. A K-medoid clustering was applied with different K values.

Figure 1: Ruspini data, n = 75



- For each cluster, data points i are sorted according to s(i) and displayed as a horizontal line whose length is s(i). First is a silhouette plot of K=3 clusters of 35, 23 and 17 data points. Each cluster's average silhouette value is 0.53, 0.75 and 0.67, respectively. One can judge that clusters 2 and 3 are more pronounced than cluster 1.


Silhouette plot of pam(x = daisy(ruspini), k = 3, diss :
n = 75
3 clusters C_j
j : n_j | $ave_{i \in Cj}$ s_i
1 : 35 | 0.53
2 : 23 | 0.75
3 : 17 | 0.67
0.0
0.2
0.4
0.6
0.8
1.0
Silhouette width s_i
Average silhouette width : 0.63


Silhouette plot of pam(x = daisy(ruspini), k = 4, diss :
n = 75
4 clusters C_j
j : n_j | $ave_{i \in Cj}$ s_i
1 : 20 | 0.73
2 : 23 | 0.75
3 : 17 | 0.67
4 : 15 | 0.8
0.0
0.2
0.4
0.6
0.8
1.0
Silhouette width s_i
Average silhouette width : 0.74

- The plot from K=5 clusters are not as good as that from K=4 with a slightly smaller average silhouette value.

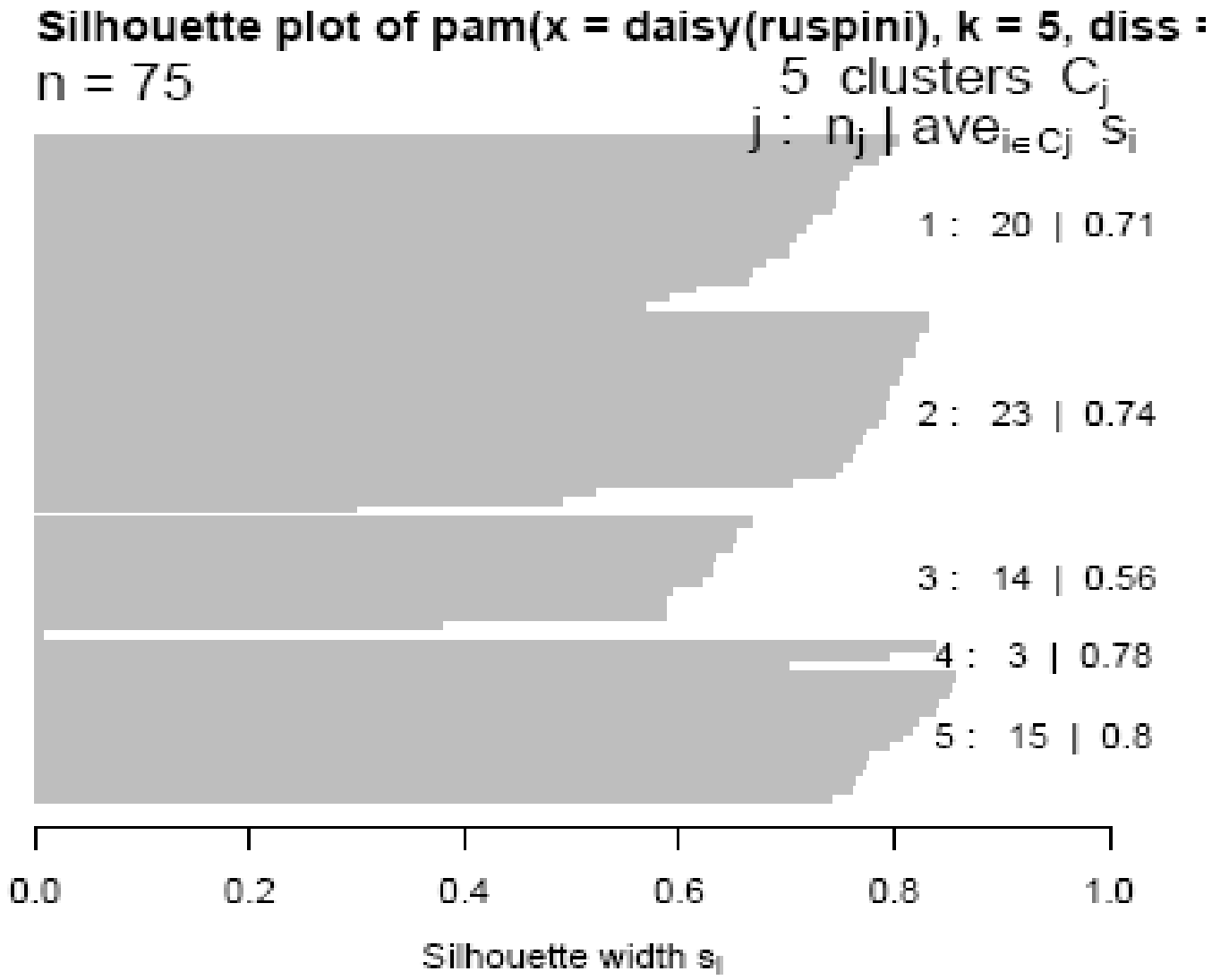
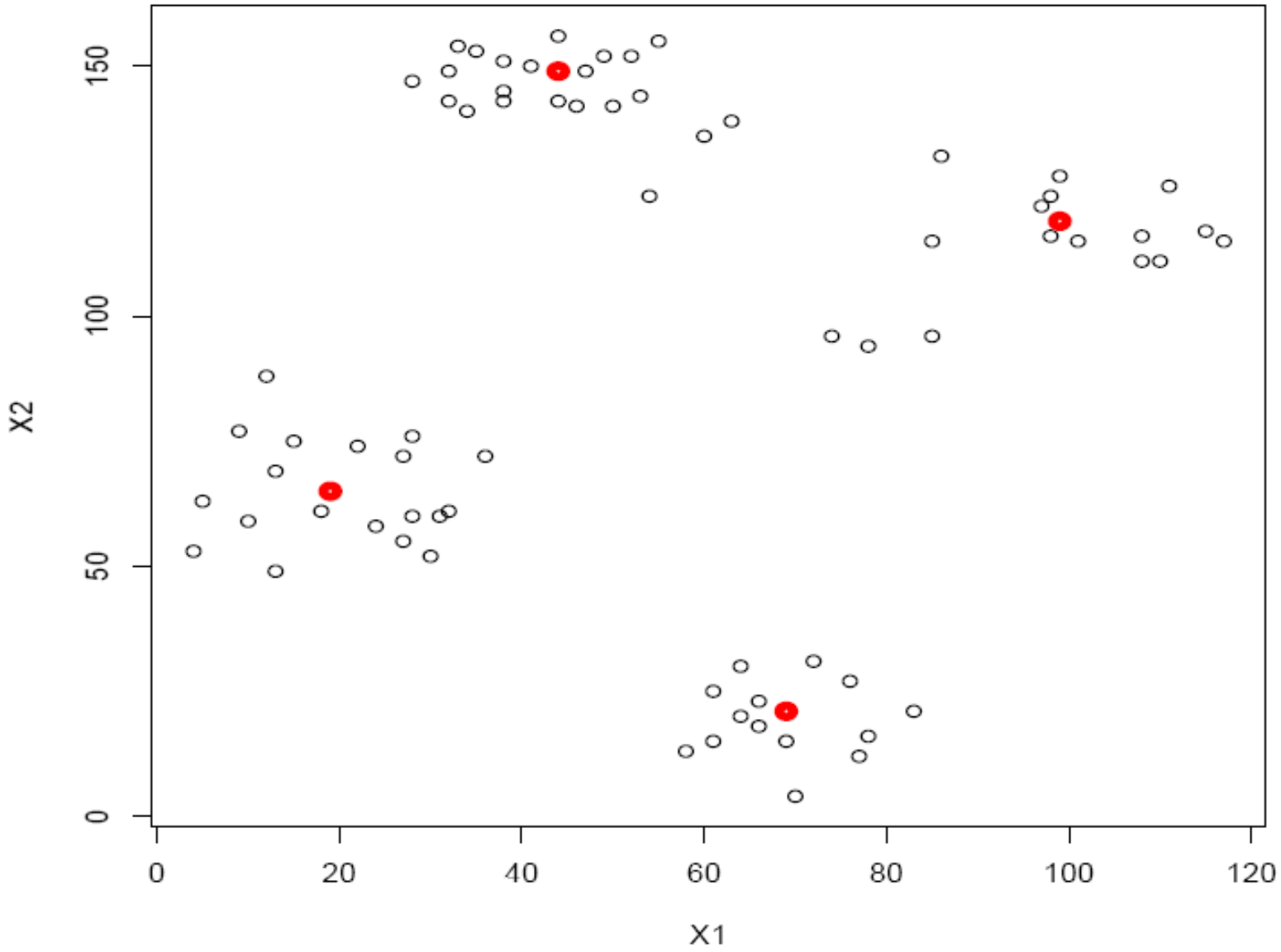

Silhouette plot of pam(x = daisy(ruspini), k = 5, diss =
n = 75
5 clusters C_j
j : n_j | $ave_{i \in Cj}$ s_i
1 : 20 | 0.71
2 : 23 | 0.74
3 : 14 | 0.56
4 : 3 | 0.78
5 : 15 | 0.8
0.0
0.2
0.4
0.6
0.8
1.0
Silhouette width s_i
Average silhouette width : 0.71

Figure 3: Ruspini data with 4 medoids marked in red



Applications

- Data Exploration and Understanding
- Data Compression: codebook
- Market Segmentation
- Multiple Regression / Classification models
- Characterization of Normality in Novelty Detection

Summary

- Cluster analysis is an exploratory tool. Useful only when it produces **meaningful** clusters
- **Hierarchical** clustering gives visual representation of different levels of clustering
  - On other hand, due to non-iterative nature, it can be unstable, can vary highly depending on settings, and is computationally expensive
- **Non-hierarchical** is computationally cheap and more stable; requires user to set *k*
- Can use both methods
- Be wary of chance results; data may not have definitive “real” clusters