

Data Mining

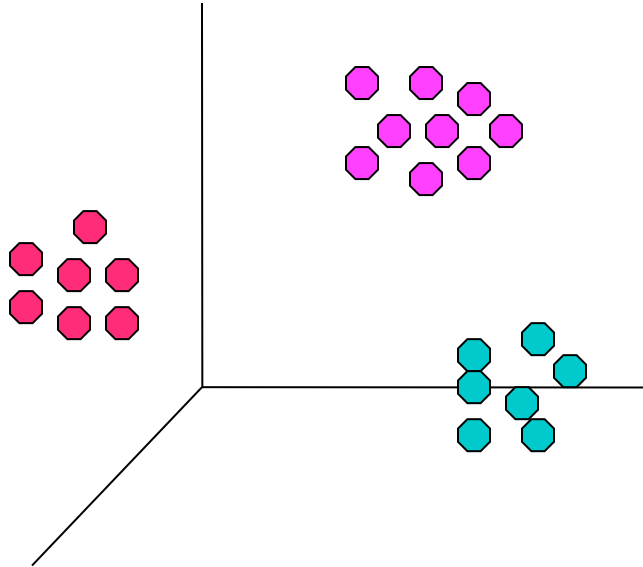
Introduction to Clustering

Mauro Sozio

some slides from Tan, Steinbach, Kumar, Introduction to Data Mining

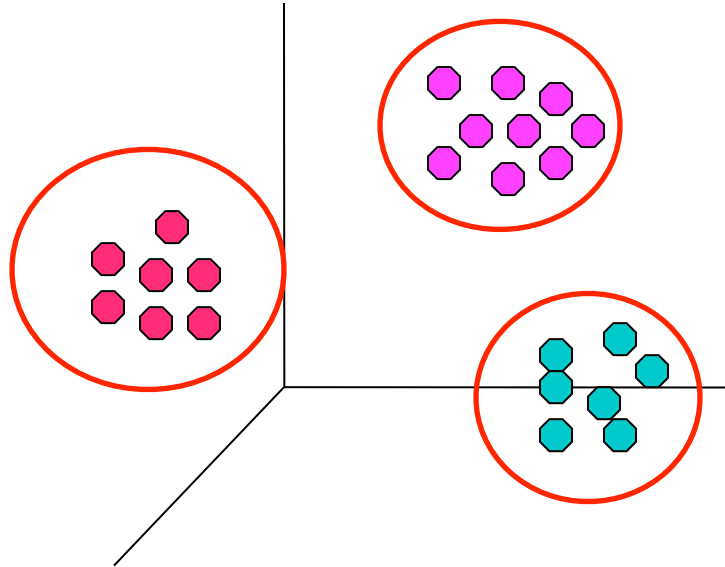
What is Cluster Analysis?

- Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups



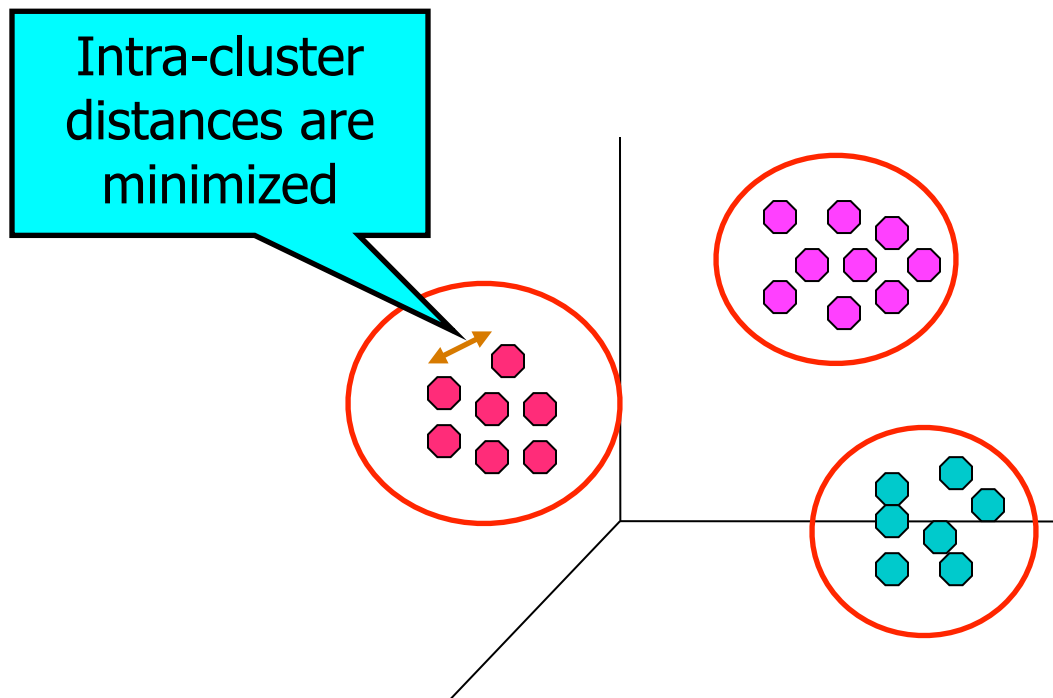
What is Cluster Analysis?

- Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups



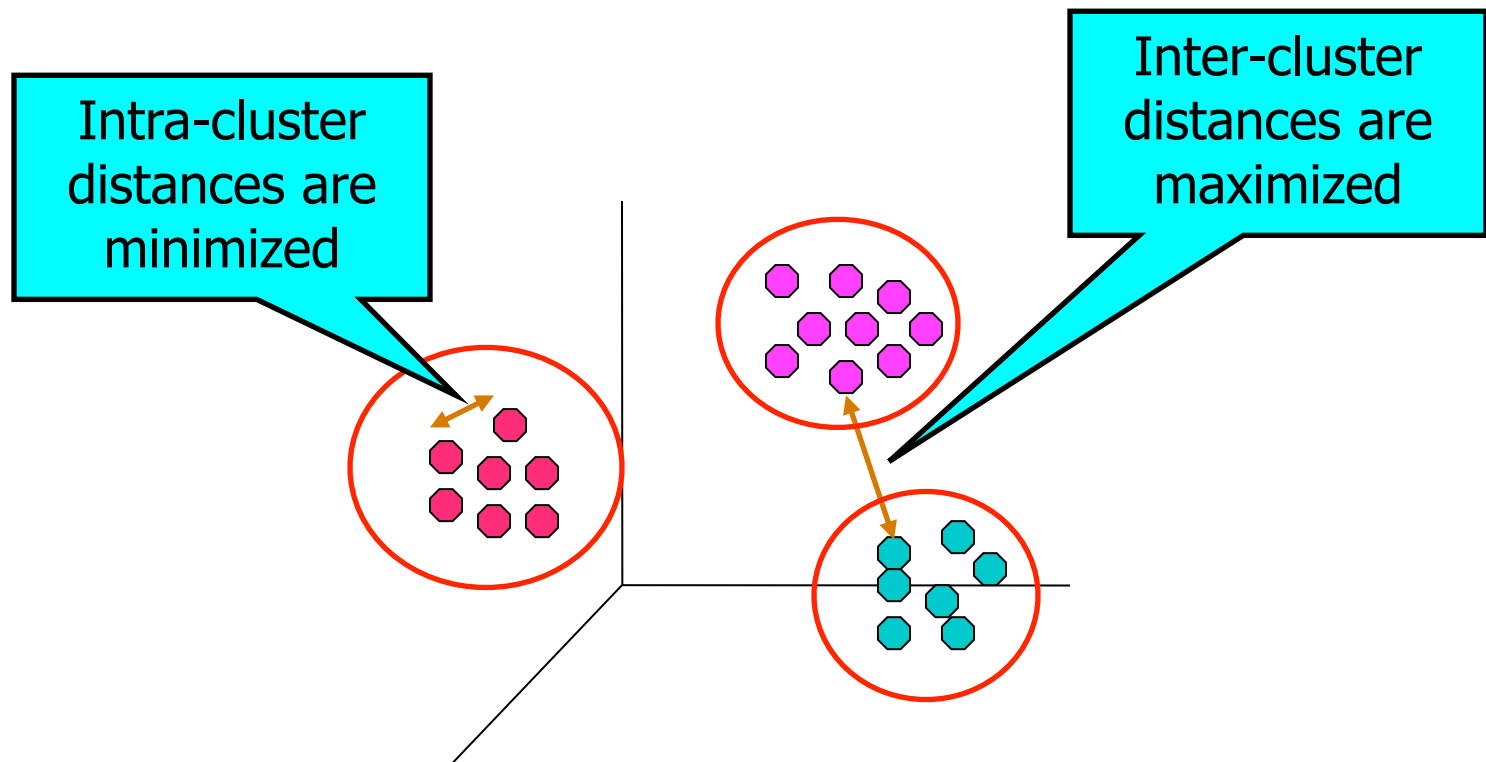
What is Cluster Analysis?

- Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups



What is Cluster Analysis?

- Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups



Applications of Cluster Analysis

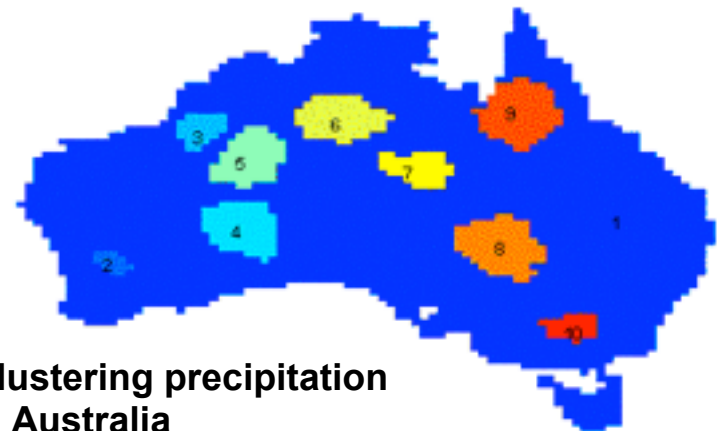
Understanding

- Group related documents for browsing, group genes and proteins that have similar functionality, or group stocks with similar price fluctuations

	<i>Discovered Clusters</i>	<i>Industry Group</i>
1	Applied-Matl-DOWN, Bay-Network-Down, 3-COM-DOWN, Cabletron-Sys-DOWN, CISCO-DOWN, HP-DOWN, DSC-Comm-DOWN, INTEL-DOWN, LSI-Logic-DOWN, Micron-Tech-DOWN, Texas-Inst-Down, Tellabs-Inc-Down, Natl-Semiconduct-DOWN, Oracle-DOWN, SGI-DOWN, Sun-DOWN	Technology1-DOWN
2	Apple-Comp-DOWN, Autodesk-DOWN, DEC-DOWN, ADV-Micro-Device-DOWN, Andrew-Corp-DOWN, Computer-Assoc-DOWN, Circuit-City-DOWN, Compaq-DOWN, EMC-Corp-DOWN, Gen-Inst-DOWN, Motorola-DOWN, Microsoft-DOWN, Scientific-Atl-DOWN	Technology2-DOWN
3	Fannie-Mae-DOWN, Fed-Home-Loan-DOWN, MBNA-Corp-DOWN, Morgan-Stanley-DOWN	Financial-DOWN
4	Baker-Hughes-UP, Dresser-Inds-UP, Halliburton-HLD-UP, Louisiana-Land-UP, Phillips-Petro-UP, Unocal-UP, Schlumberger-UP	Oil-UP

Summarization

- Reduce the size of large data sets



What is not Cluster Analysis?

- | Supervised classification
 - Have class label information
- | Simple segmentation
 - Dividing students into different registration groups alphabetically, by last name
- | Results of a query
 - Groupings are a result of an external specification
- | Graph partitioning
 - Some mutual relevance and synergy, but areas are not identical

Notion of a Cluster can be Ambiguous



How many clusters?

Notion of a Cluster can be Ambiguous

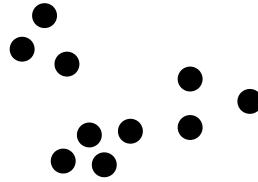
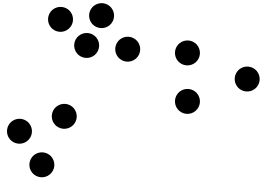


How many clusters?

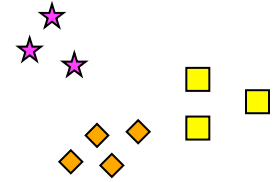
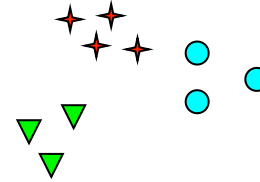


Two Clusters

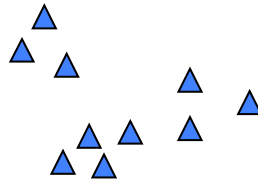
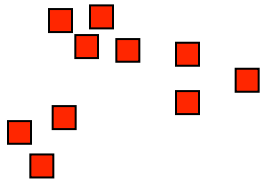
Notion of a Cluster can be Ambiguous



How many clusters?

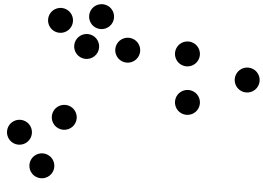


Six Clusters

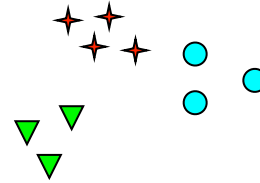
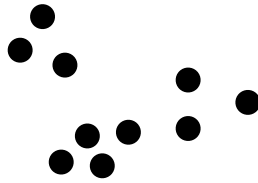


Two Clusters

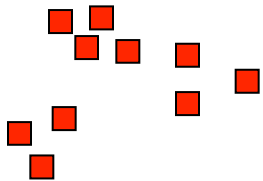
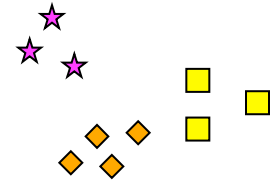
Notion of a Cluster can be Ambiguous



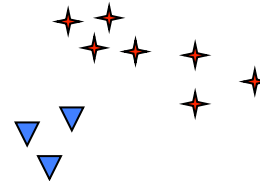
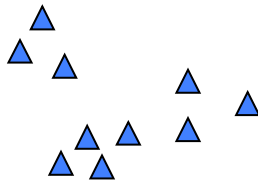
How many clusters?



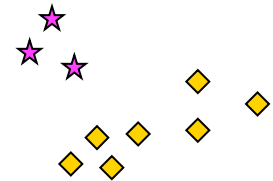
Six Clusters



Two Clusters



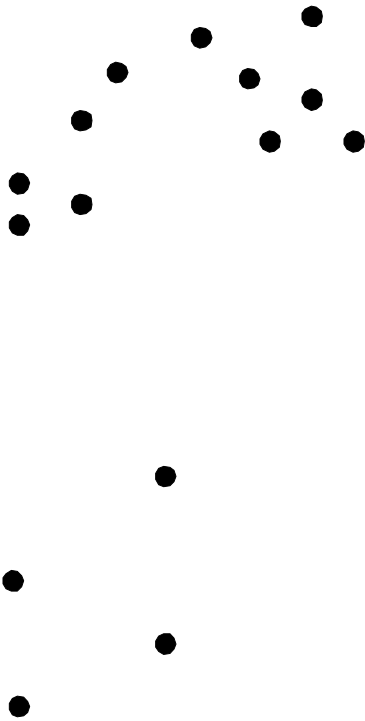
Four Clusters



Types of Clusterings

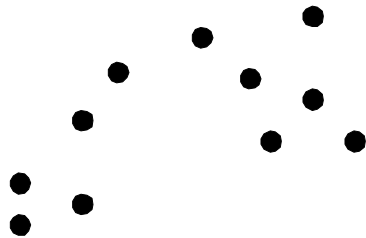
- | A **clustering** is a set of clusters
- | Important distinction between **hierarchical** and **partitional** sets of clusters
- | **Partitional Clustering**
 - A division data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset
- | **Hierarchical clustering**
 - A set of nested clusters organized as a hierarchical tree

Partitional Clustering

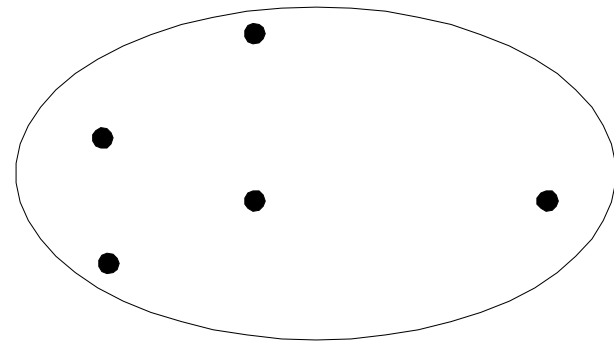
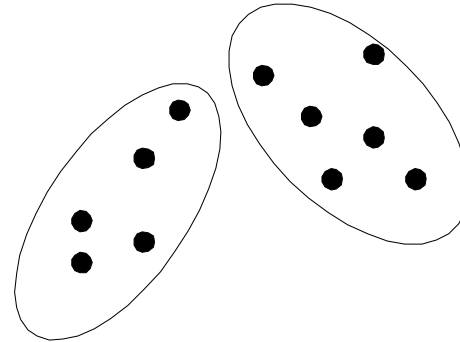


Original Points

Partitional Clustering

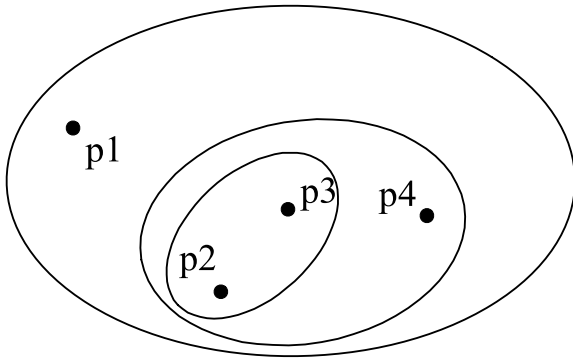


Original Points

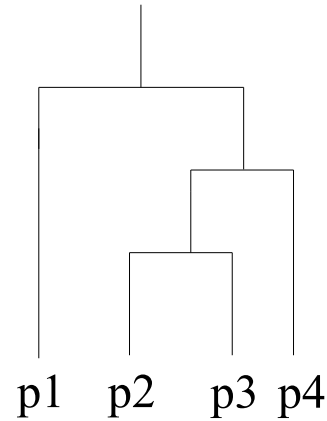


A Partitional Clustering

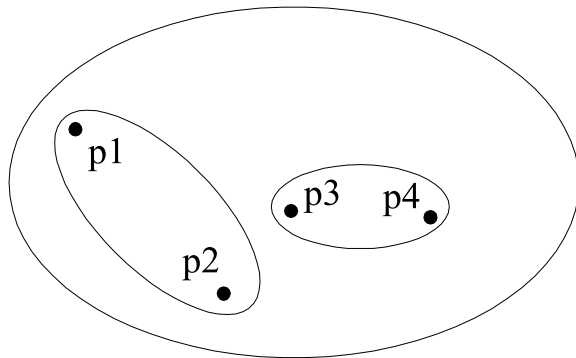
Hierarchical Clustering



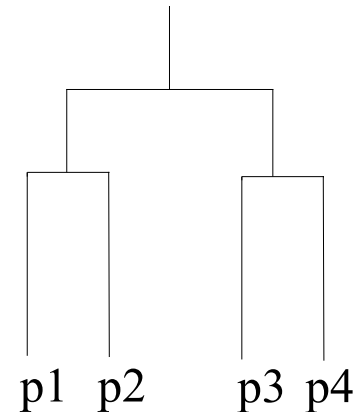
Traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Hierarchical Clustering



Non-traditional Dendrogram

Other Distinctions Between Sets of Clusters

| Exclusive versus non-exclusive

- In non-exclusive clusterings, points may belong to multiple clusters.
- Can represent multiple classes or ‘border’ points

| Fuzzy versus non-fuzzy

- In fuzzy clustering, a point belongs to every cluster with some weight between 0 and 1
- Weights must sum to 1
- Probabilistic clustering has similar characteristics

| Partial versus complete

- In some cases, we only want to cluster some of the data

| Heterogeneous versus homogeneous

- Cluster of widely different sizes, shapes, and densities

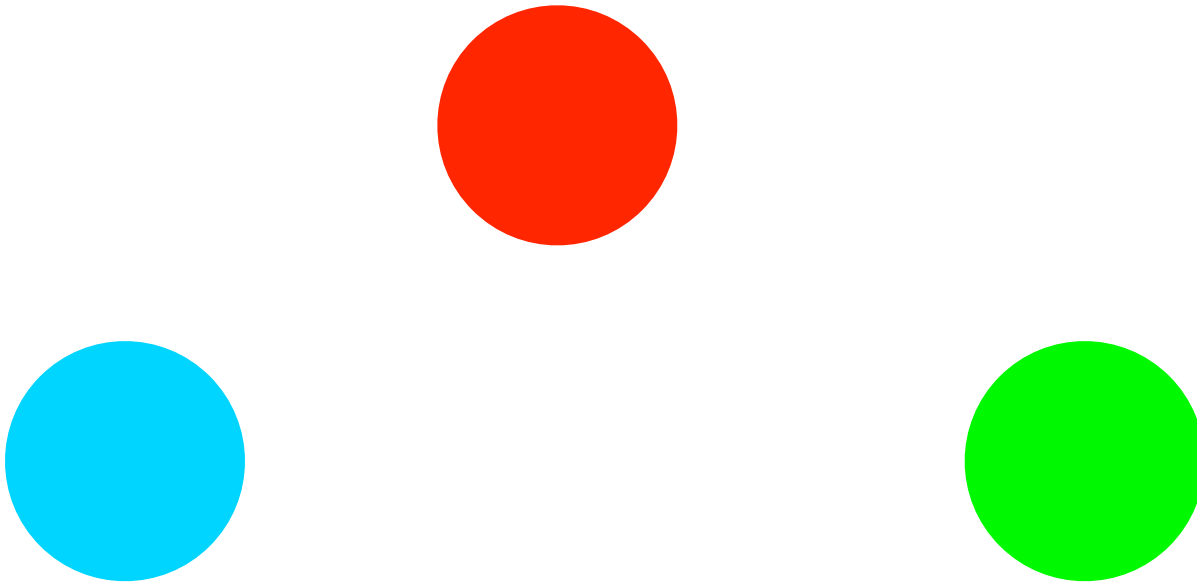
Types of Clusters

- | Well-separated clusters
- | Center-based clusters
- | Contiguous clusters
- | Density-based clusters
- | Property or Conceptual
- | Described by an Objective Function

Types of Clusters: Well-Separated

| Well-Separated Clusters:

- A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.



3 well-separated clusters

Types of Clusters: Center-Based

| Center-based

- A cluster is a set of objects such that an object in a cluster is closer (more similar) to the “center” of a cluster, than to the center of any other cluster
- The center of a cluster is often a **centroid**, the average of all the points in the cluster, or a **medoid**, the most “representative” point of a cluster



4 center-based clusters

Types of Clusters: Contiguity-Based

- | Contiguous Cluster (Nearest neighbor or Transitive)
 - A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.

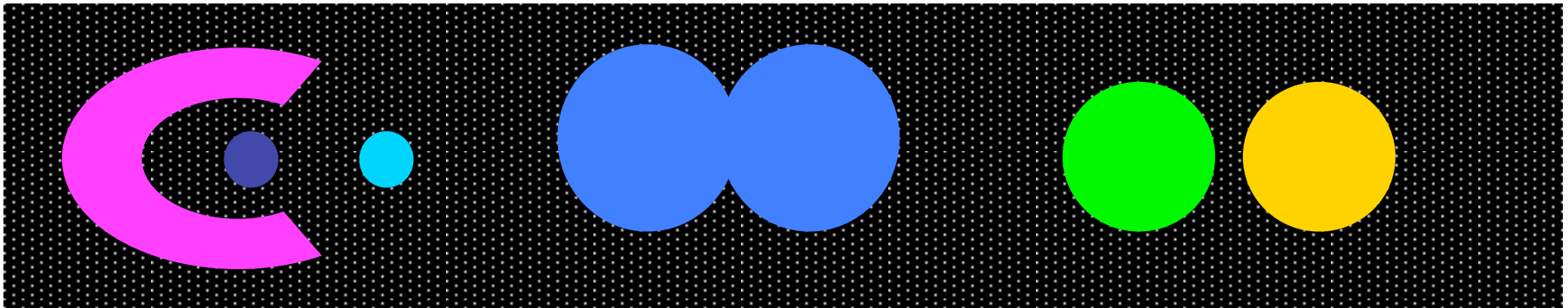


8 contiguous clusters

Types of Clusters: Density-Based

| Density-based

- A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
- Used when the clusters are irregular or intertwined, and when noise and outliers are present.

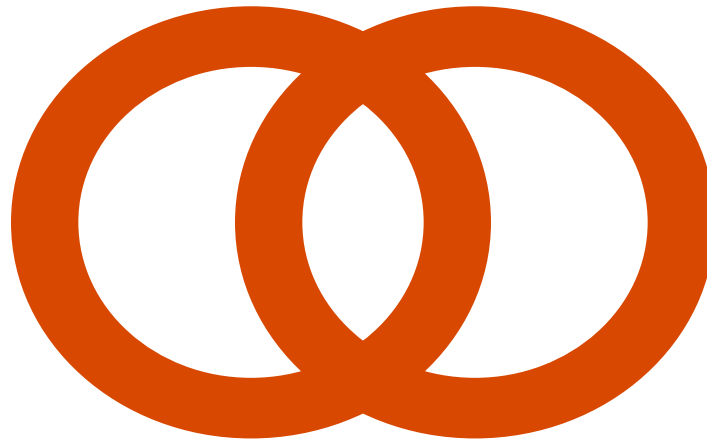


6 density-based clusters

Types of Clusters: Conceptual Clusters

- | Shared Property or Conceptual Clusters
 - Finds clusters that share some common property or represent a particular concept.

.



2 Overlapping Circles

Clustering Algorithms

- | K-means
- | K-means++
- | Hierarchical clustering

K-means Clustering

Input: integer $k > 0$, set S of points in the euclidean space

Output: A (partitional) clustering of S

1. Select k points in S as the initial centroids
2. Repeat until the centroids do not change
 - Form k clusters by assigning points to the closest centroids
 - For each cluster recompute its centroid

K-means Clustering

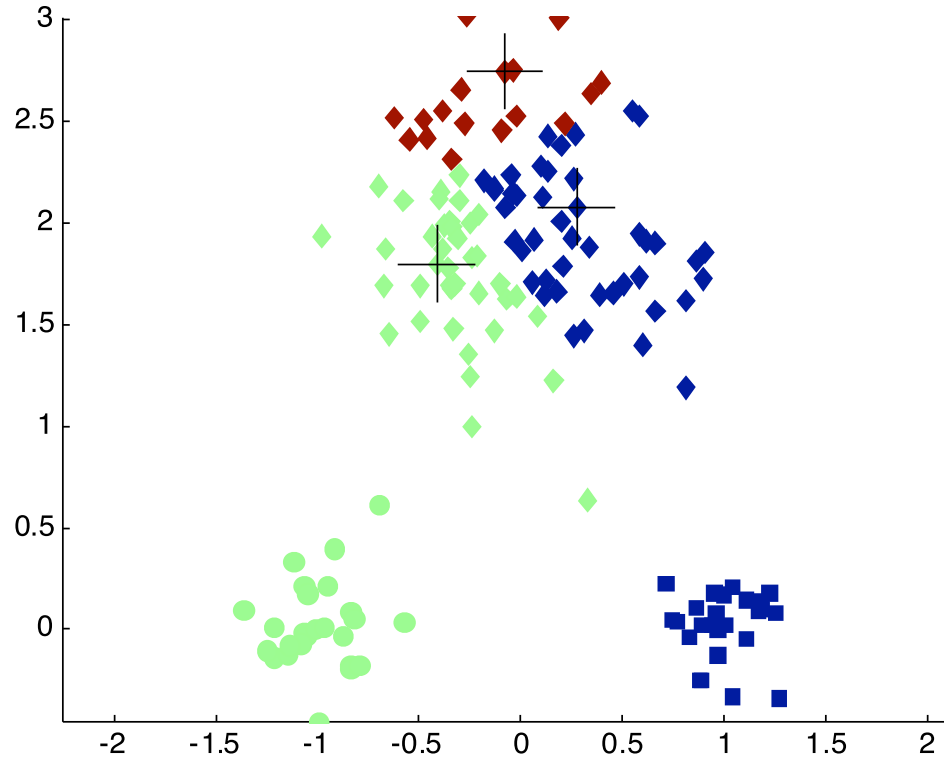
Input: integer $k > 0$, set S of points in the euclidean space

Output: A (partitional) clustering of S

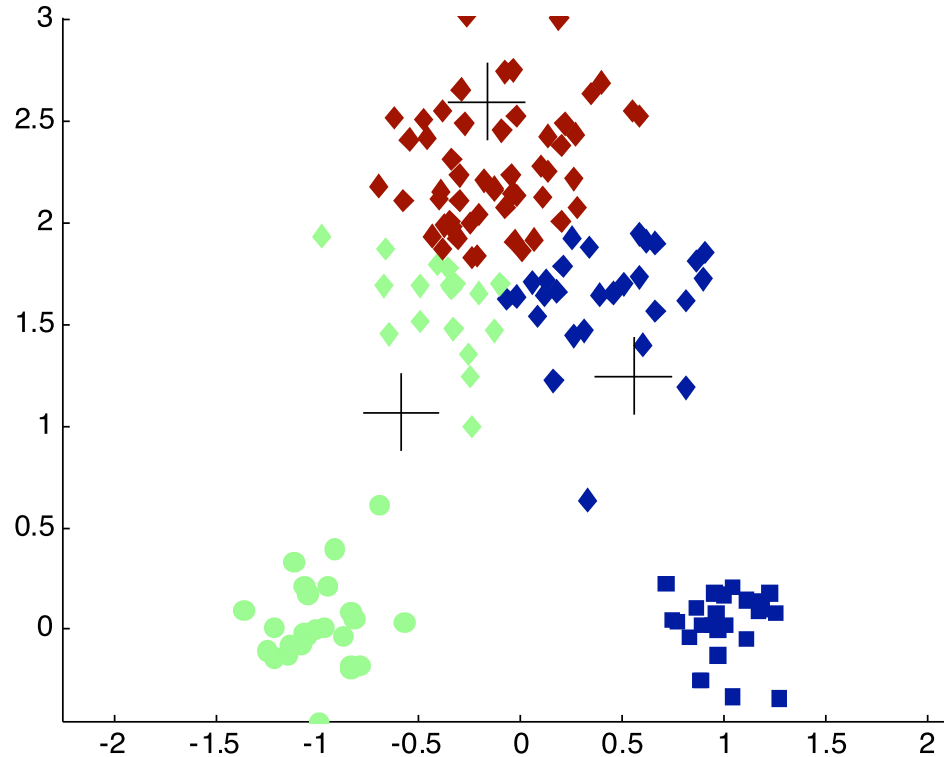
1. Select k points in S as the initial centroids
2. Repeat until the centroids do not change
 - Form k clusters by assigning points to the closest centroids
 - For each cluster recompute its centroid

- | Initial centroids are often chosen randomly.
- | Centroids are often the mean of the points in the cluster.
- | 'Closeness' is measured by Euclidean distance, cosine similarity, correlation, etc.

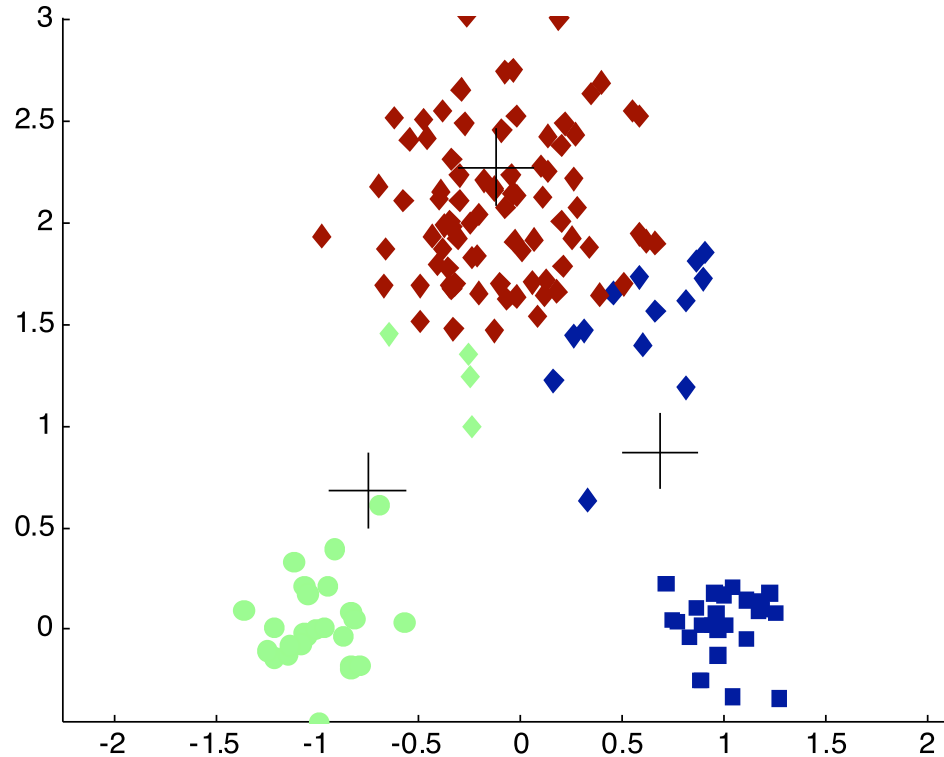
K-means: example



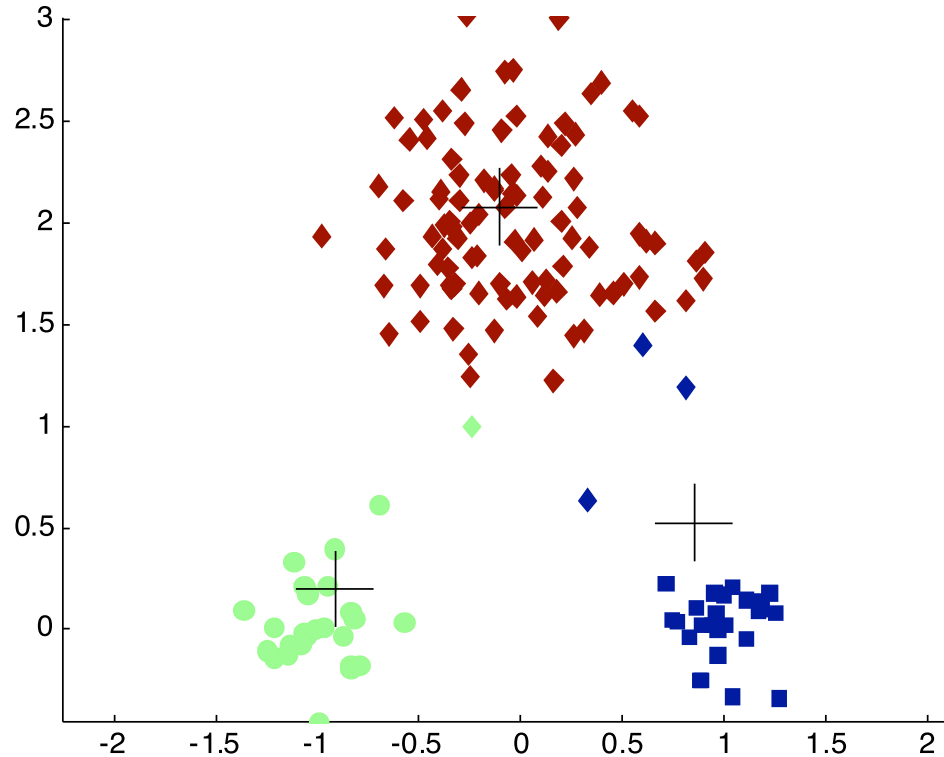
K-means: example



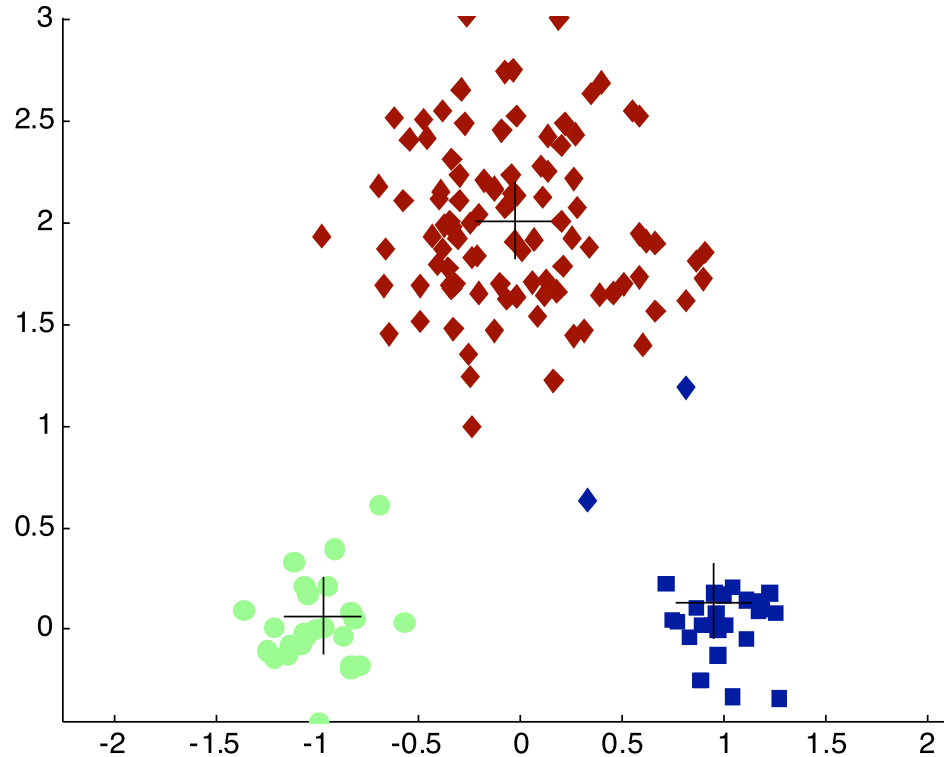
K-means: example



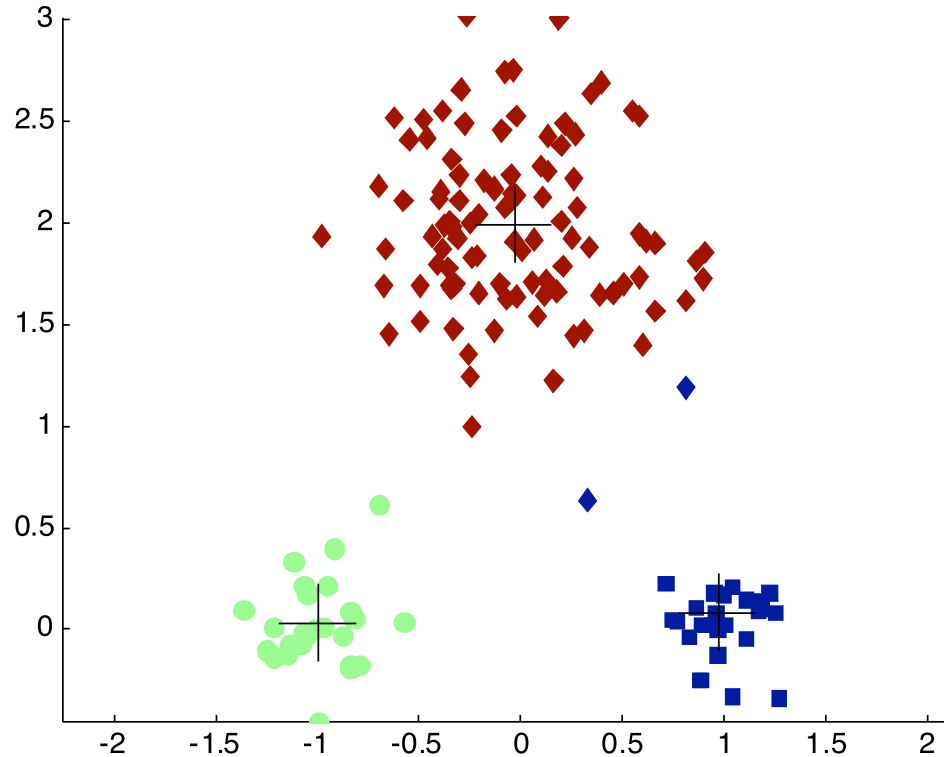
K-means: example



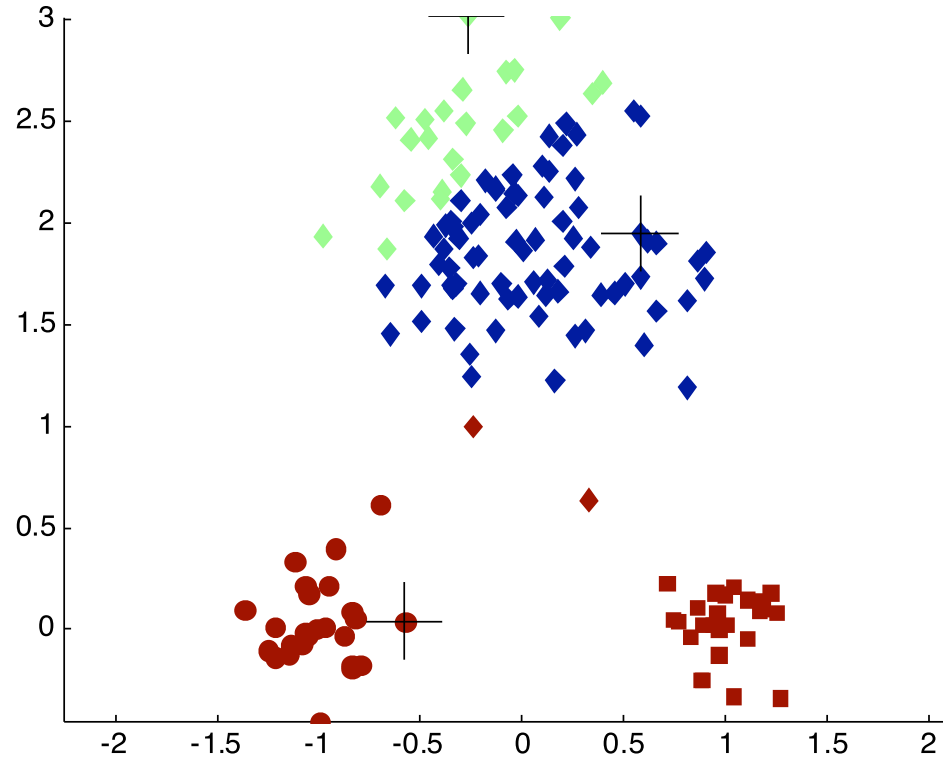
K-means: example



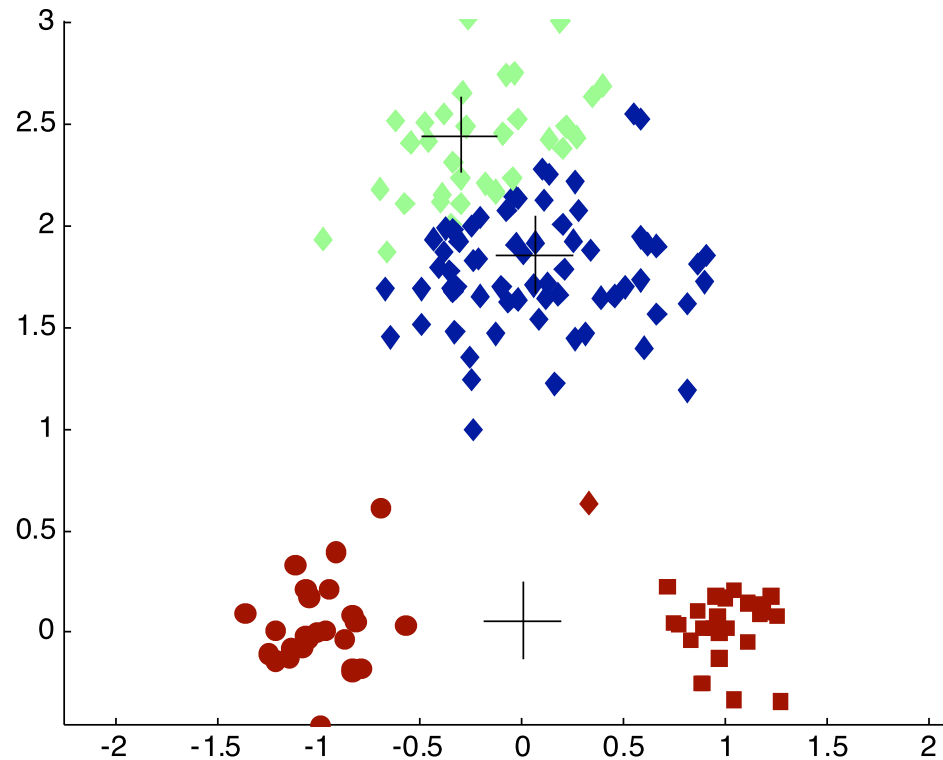
K-means: example



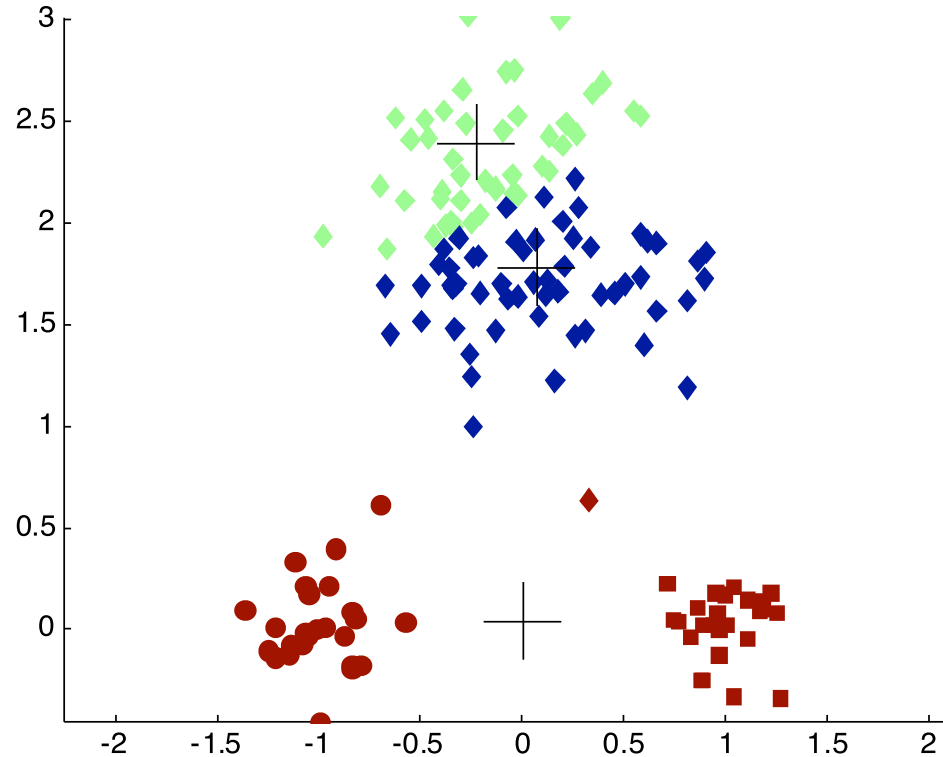
Importance of Choosing Initial Centroids ...



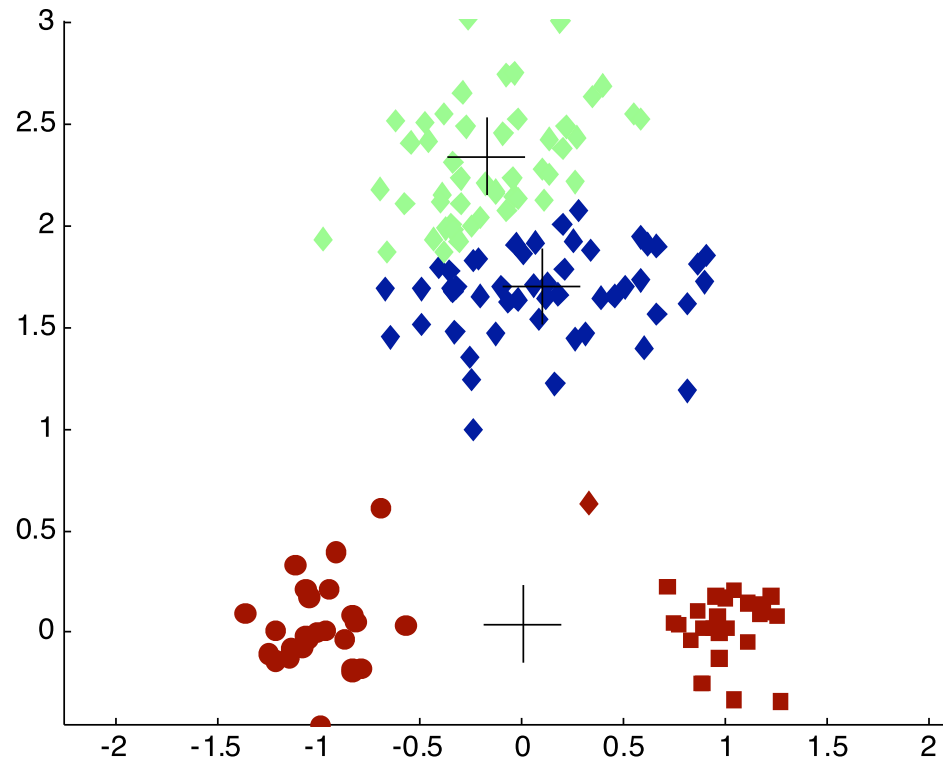
Importance of Choosing Initial Centroids ...



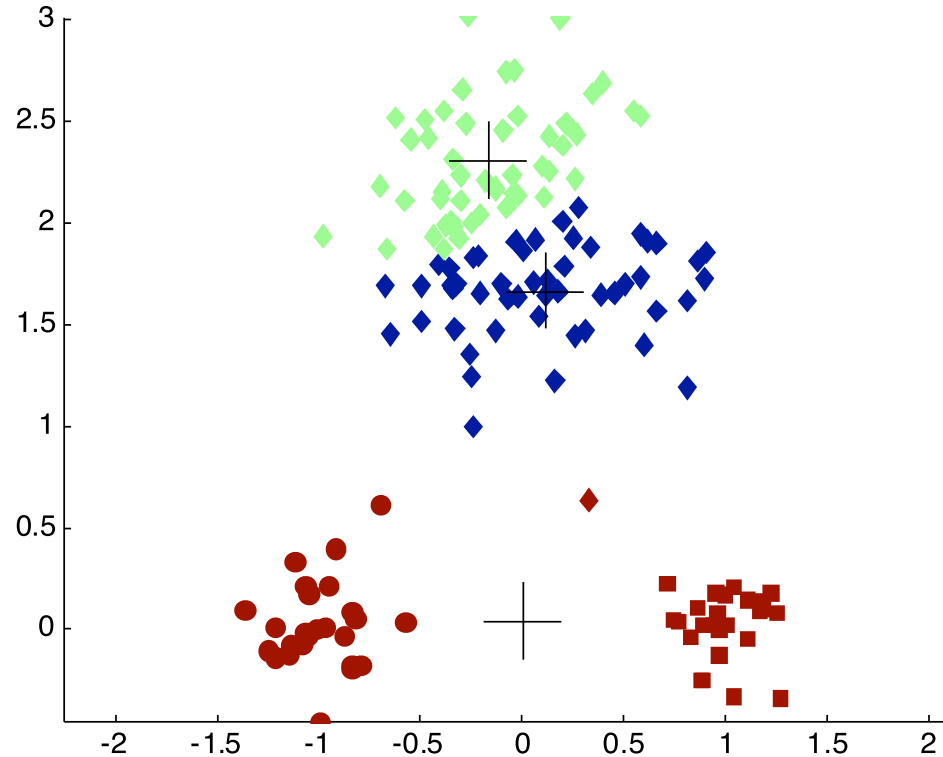
Importance of Choosing Initial Centroids ...



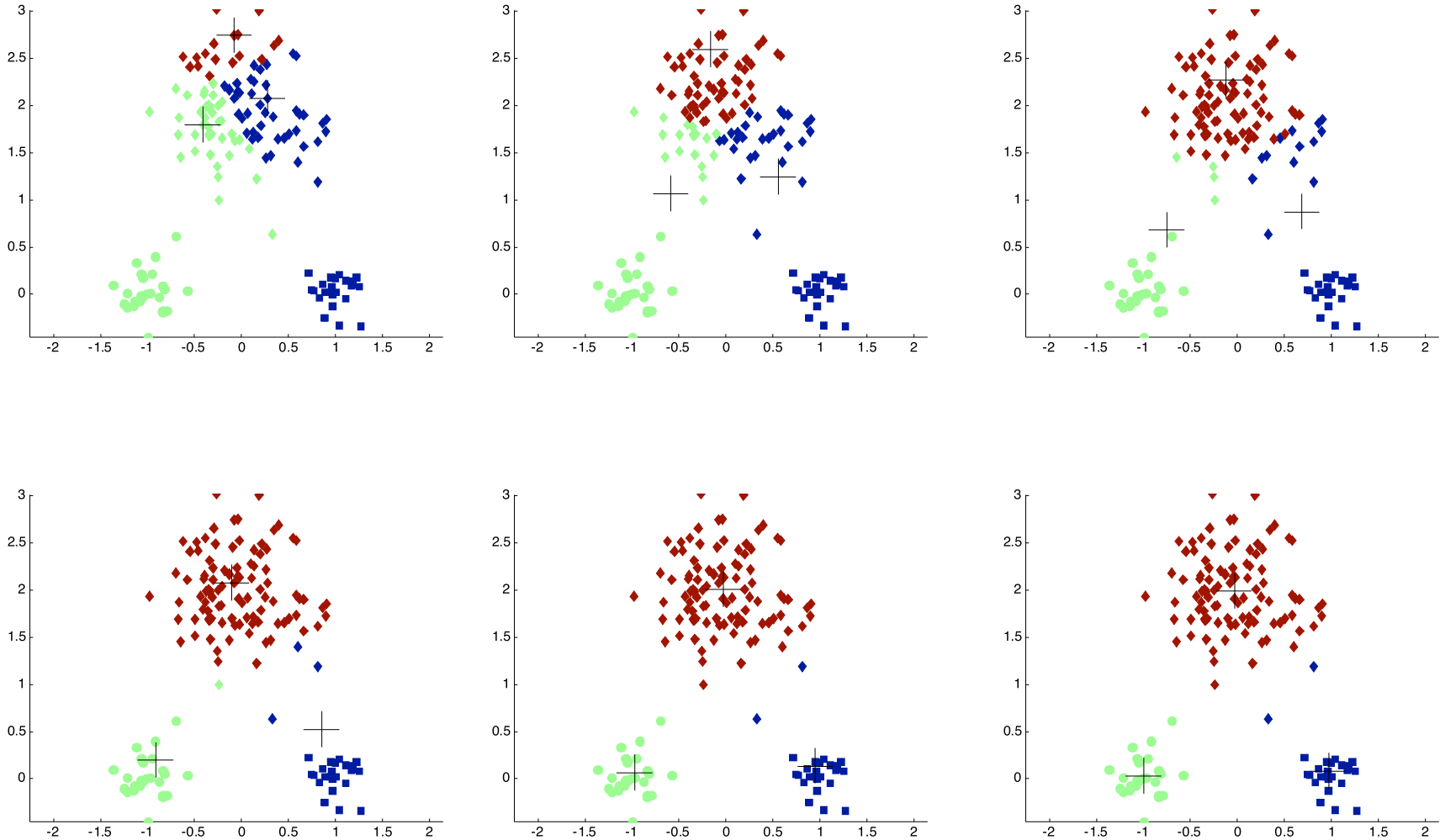
Importance of Choosing Initial Centroids ...



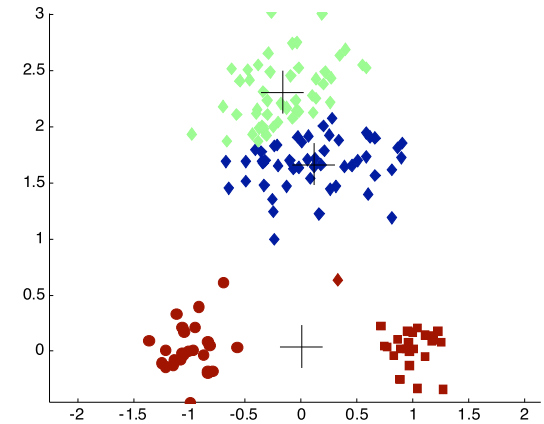
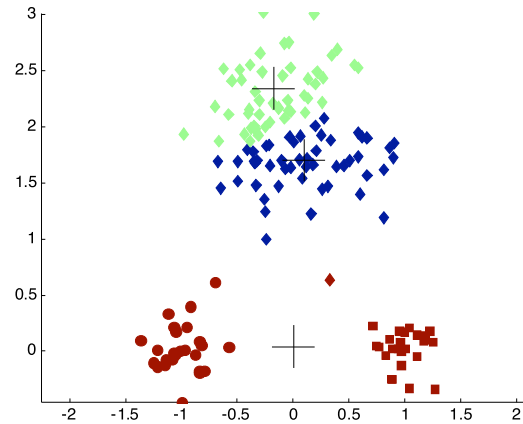
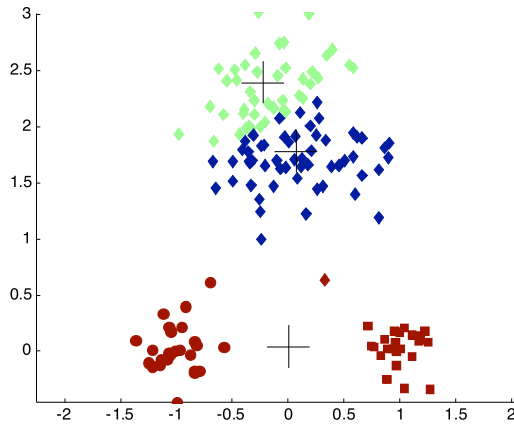
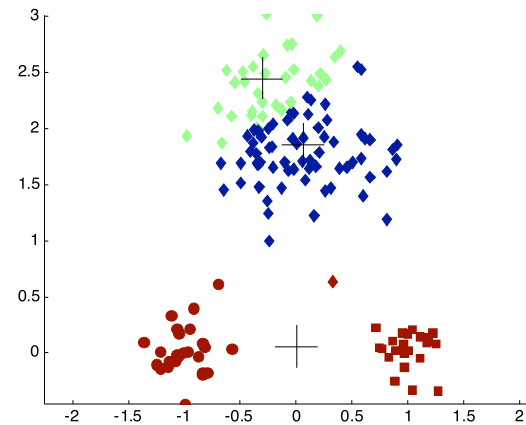
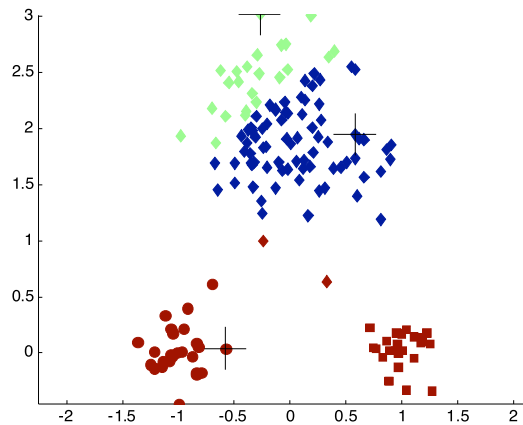
Importance of Choosing Initial Centroids ...



Importance of Choosing Initial Centroids



Importance of Choosing Initial Centroids ...



Problems with Selecting Initial Points

- | **Input:** k sets of points, n/k points per set.
- | Points in a same set are very close, while points in different sets are far apart.
- | If we don't select 1 point per set, doesn't work!

- | Prob. =
$$\frac{\left(\frac{n}{k}\right)^k}{\binom{n}{k}} \approx \frac{k!}{k^k}$$

For example, if $K = 10$, then probability = $10!/10^{10} = 0.00036$.

Evaluating K-means Clusterings

- | Most common measure is Sum of Squared Error (SSE):

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

- where x is a point in cluster C_i and m_i is the centroid of cluster C_i
- | Given two clusterings, we can choose the one with smallest error
- | Decreasing K might decrease SSE. However, good clusterings with small K might have a lower SSE than poor clusterings with higher K .

K-means always terminates

- | **Theorem:** K-means with euclidean distance as a measure of closeness always terminates.
- | **Proof (sketch):** 1) the number of possible clusterings is finite ($< n^k$) 2) it can be shown that SSE strictly decreases. From 2) it follows that we cannot yield twice the same clustering. Hence, in the worst case we produce all possible clusterings.
- | Observe that we need both 1) and 2).

Solutions to Initial Centroids Problem

- | Multiple runs (helps but low success probability)
- | Sample and use hierarchical clustering to determine initial centroids
- | Select more than k initial centroids and then select among these initial centroids
- | Postprocessing
- | K-Means++

Handling Empty Clusters

- | Basic K-means algorithm can yield empty clusters. (**Exercise**)
- | Several strategies:
 - Pick the points that contributes most to SSE and move them to empty cluster.
 - Pick the points from the cluster with the highest SSE
 - If there are several empty clusters, the above can be repeated several times.

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)
 - + Never get an empty cluster
 - - Introduces an order dependency
 - - More expensive

Pre-processing and Post-processing

| Pre-processing

- Normalize the data
- Eliminate outliers

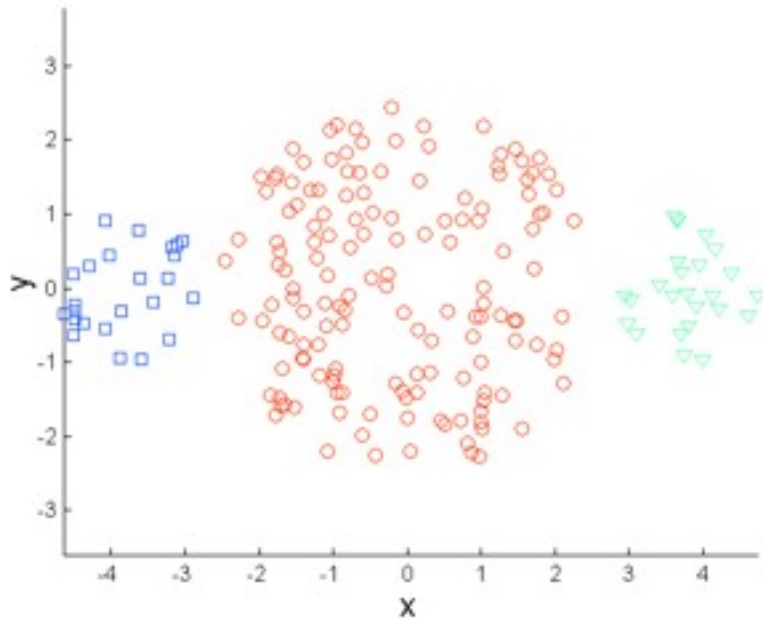
| Post-processing

- 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

Limitations of K-means

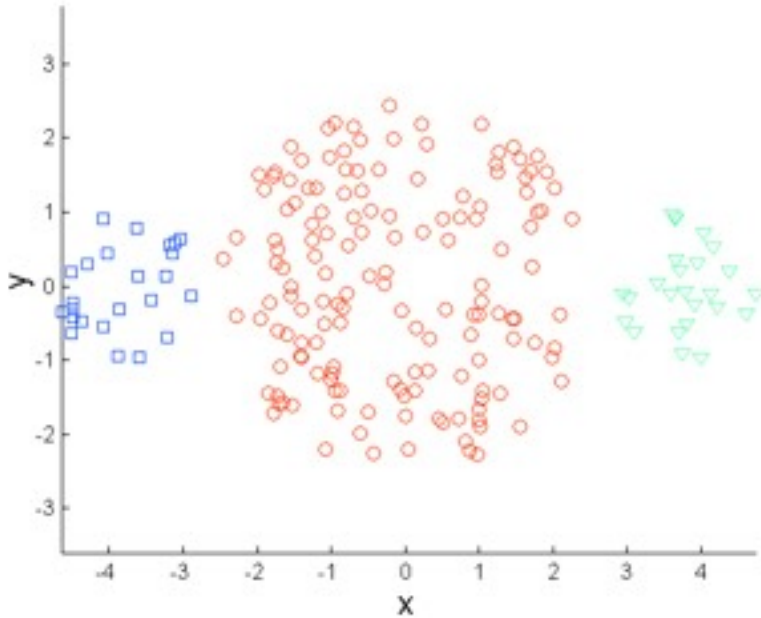
- | K-means has problems when clusters are of differing
 - Sizes
 - Densities
 - Non-globular shapes
- | K-means has problems when the data contains outliers.

Limitations of K-means: Differing Sizes



Original Points

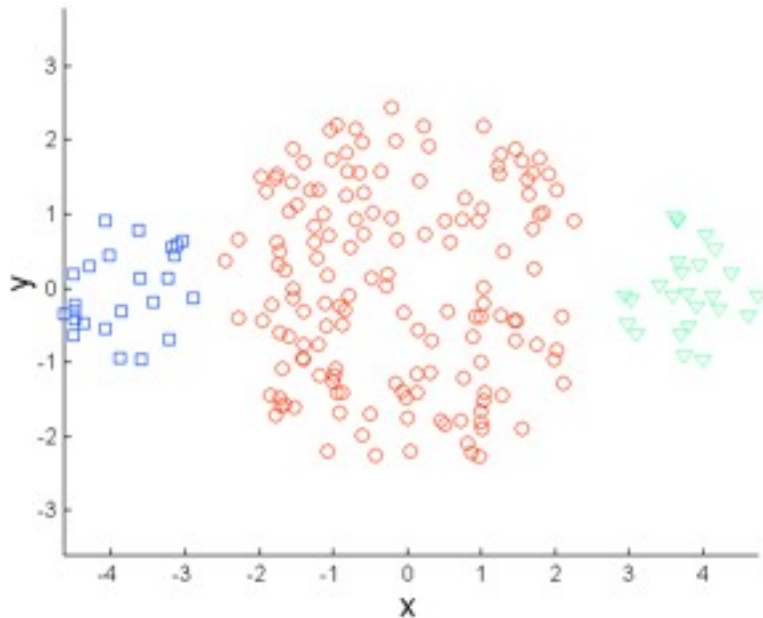
Limitations of K-means: Differing Sizes



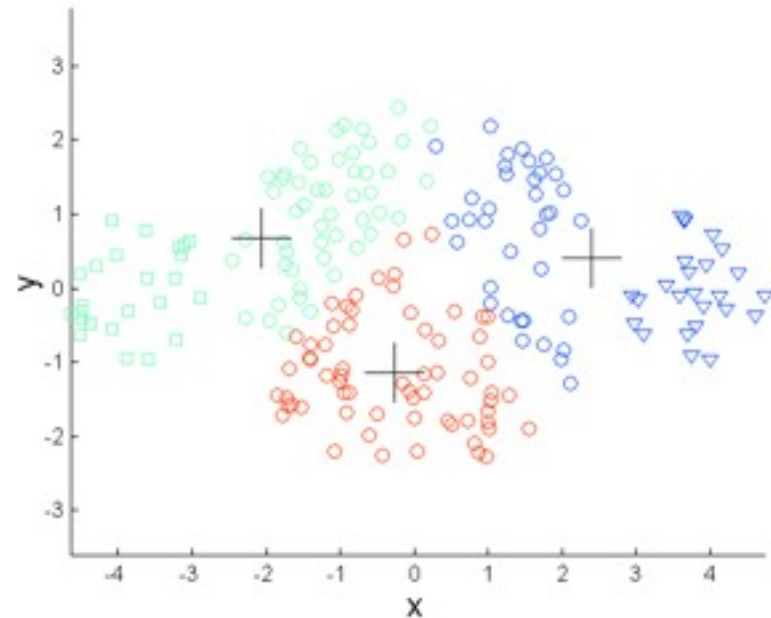
Original Points

K-means (3 Clusters)

Limitations of K-means: Differing Sizes

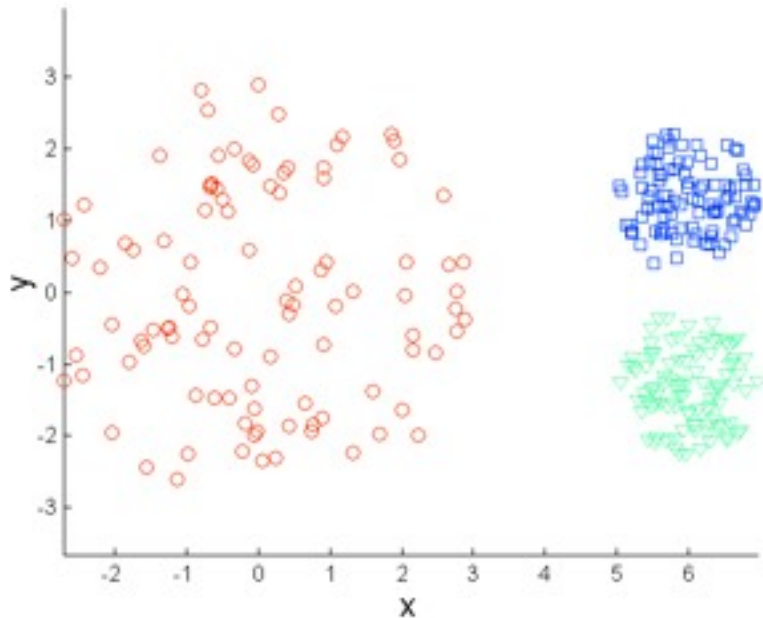


Original Points



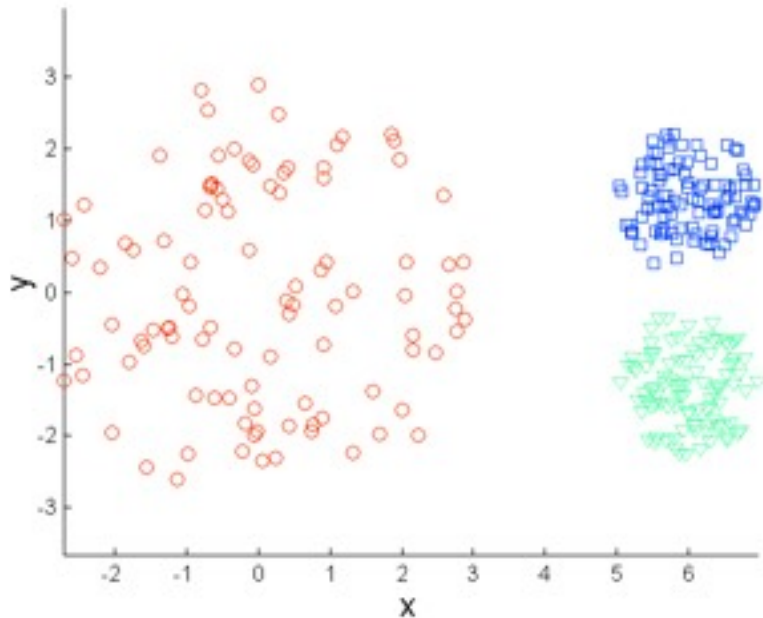
K-means (3 Clusters)

Limitations of K-means: Differing Density



Original Points

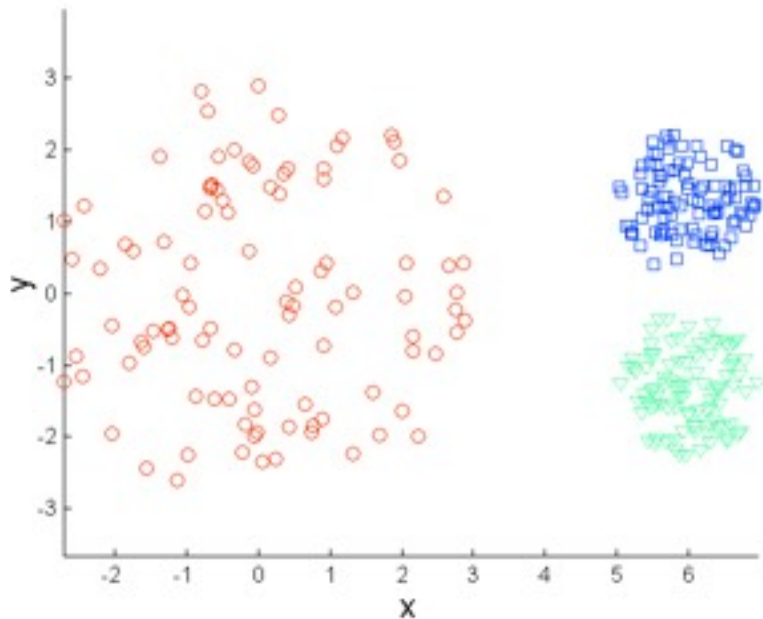
Limitations of K-means: Differing Density



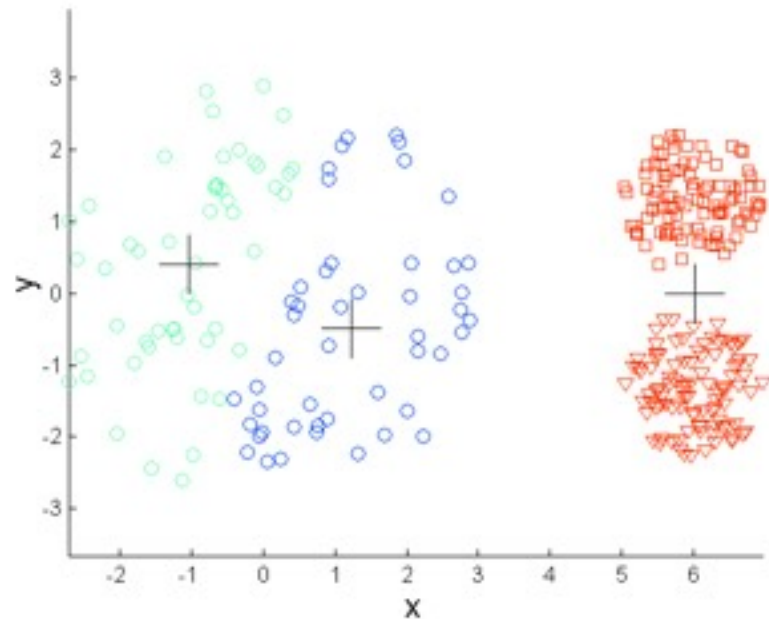
Original Points

K-means (3 Clusters)

Limitations of K-means: Differing Density

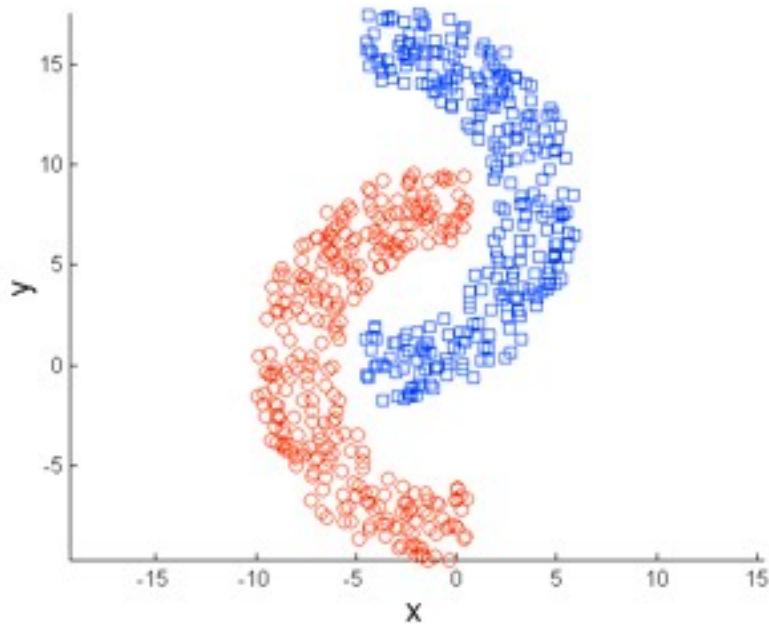


Original Points



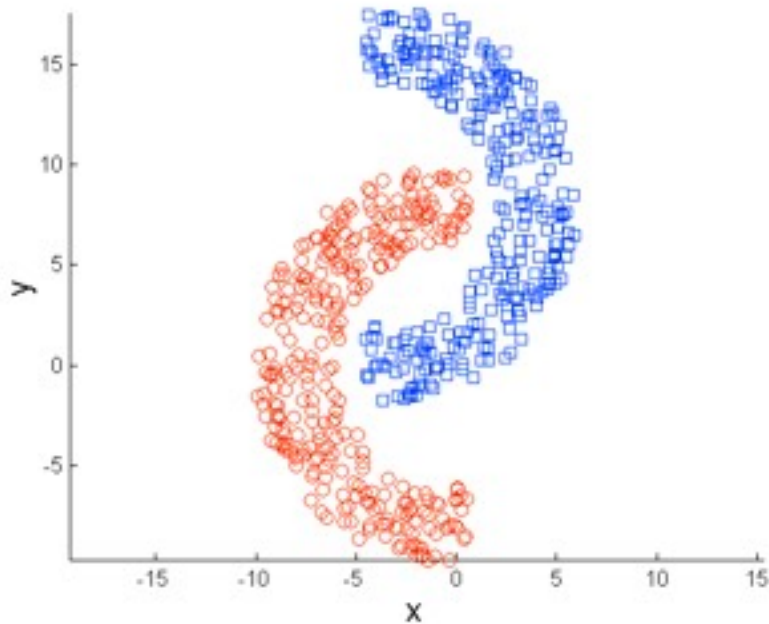
K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes



Original Points

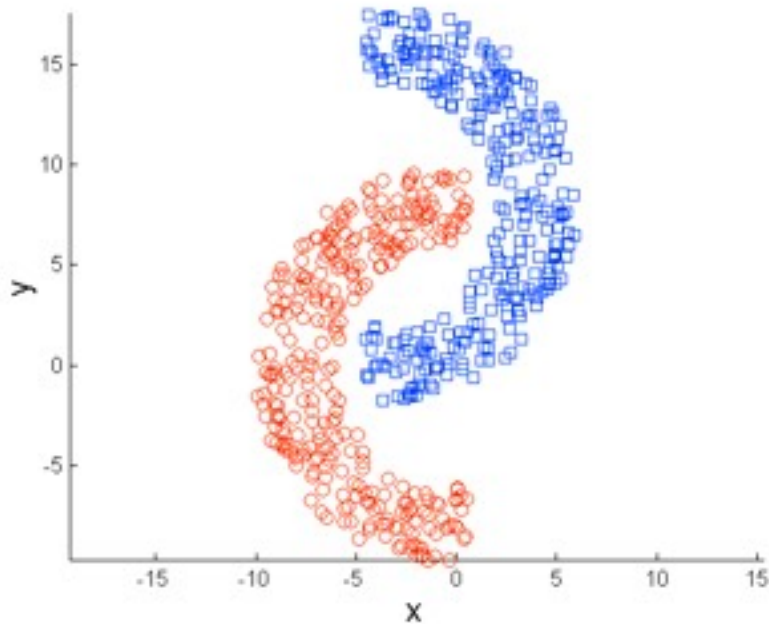
Limitations of K-means: Non-globular Shapes



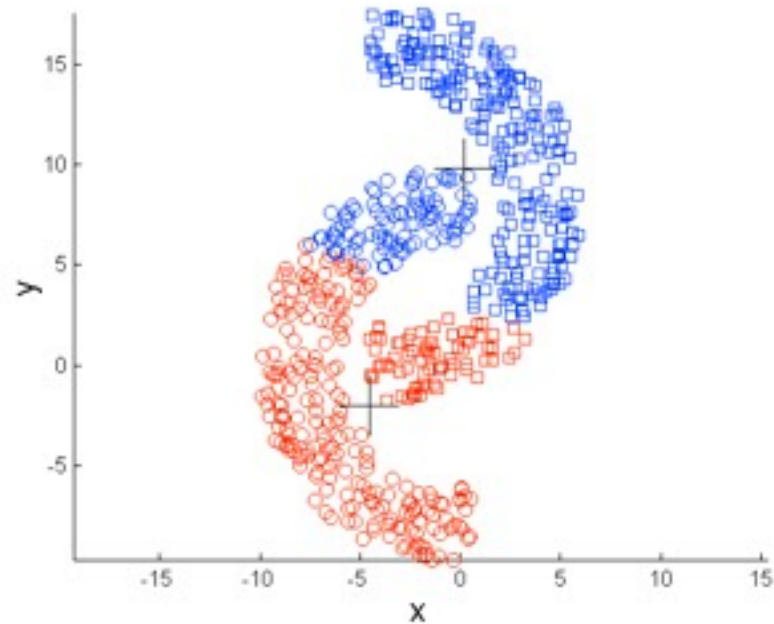
Original Points

K-means (2 Clusters)

Limitations of K-means: Non-globular Shapes

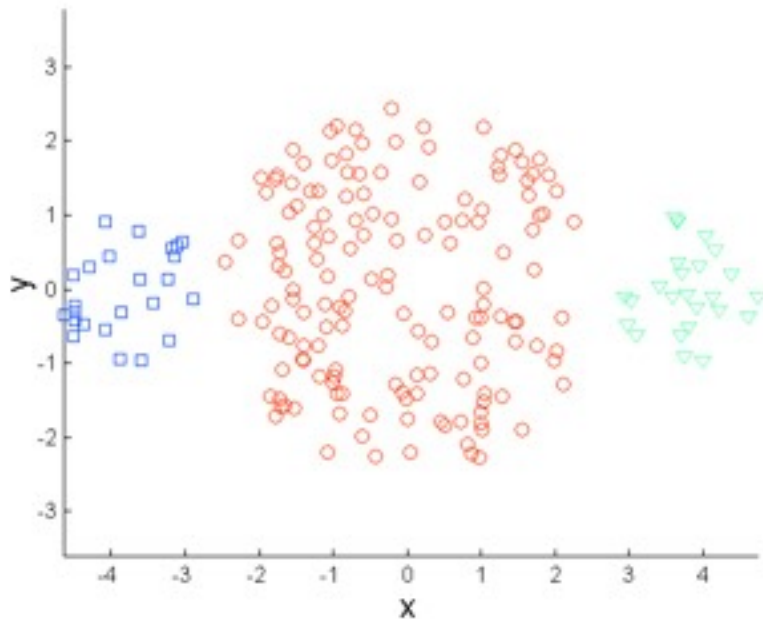


Original Points

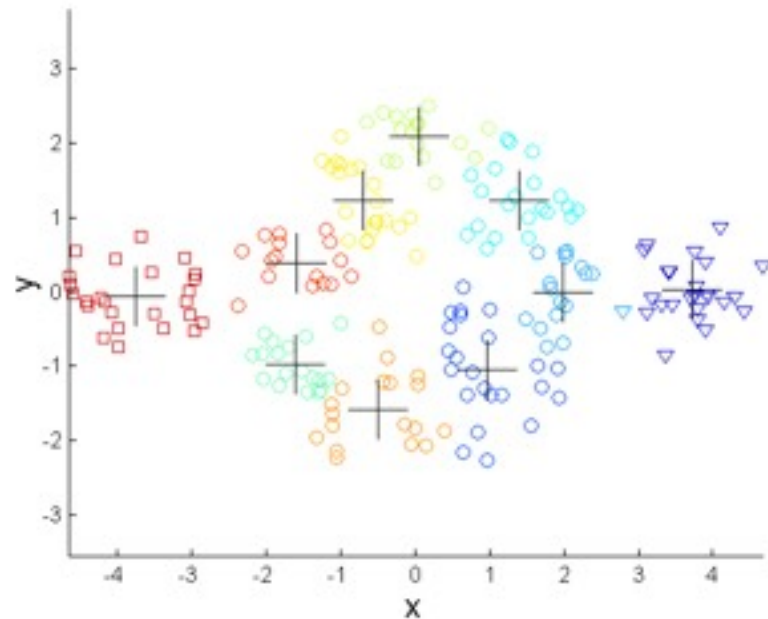


K-means (2 Clusters)

Overcoming K-means Limitations



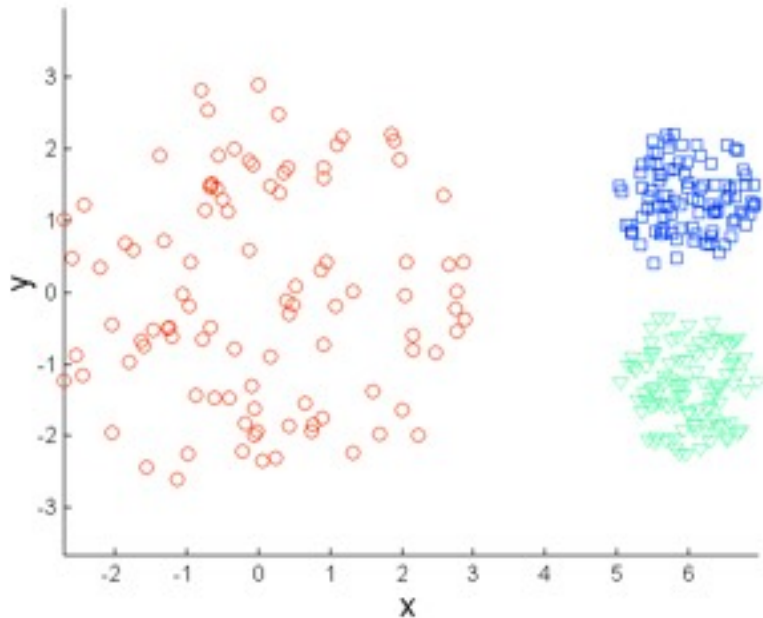
Original Points



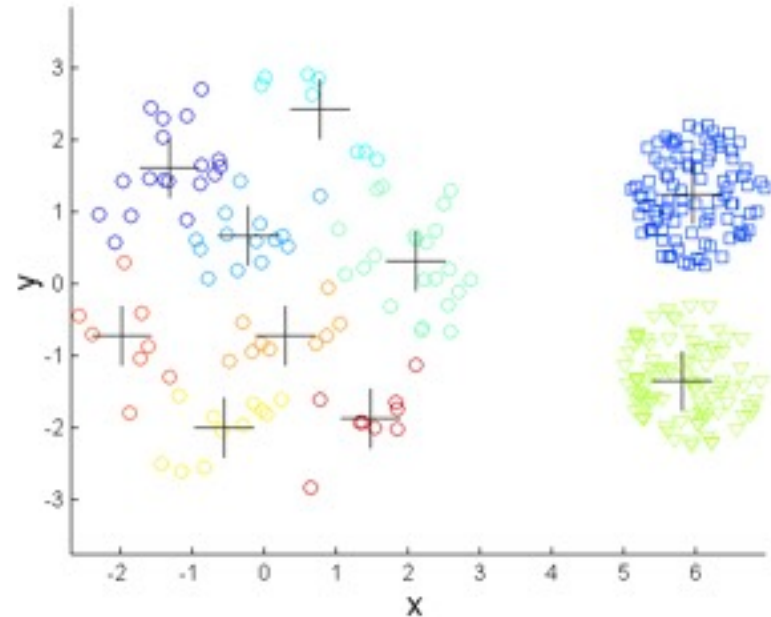
K-means Clusters

One solution is to use many clusters.
Find parts of clusters, but need to put together.

Overcoming K-means Limitations

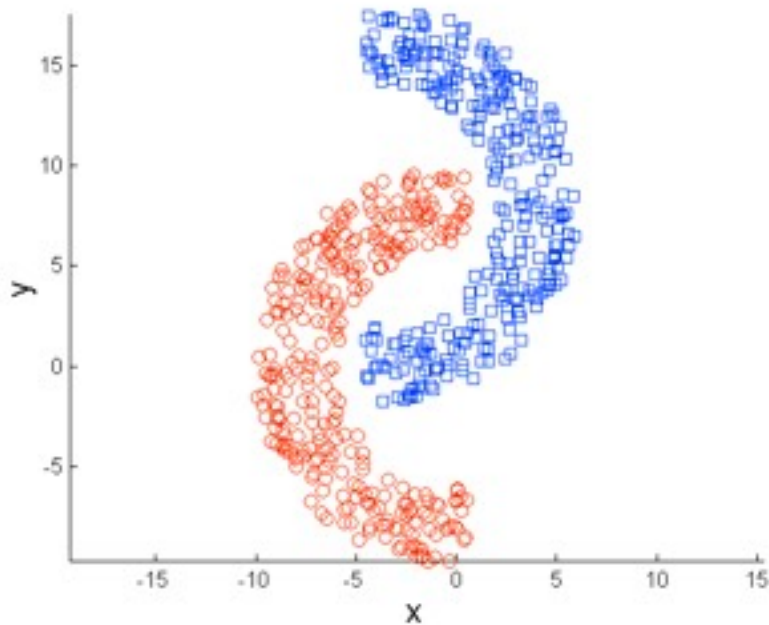


Original Points

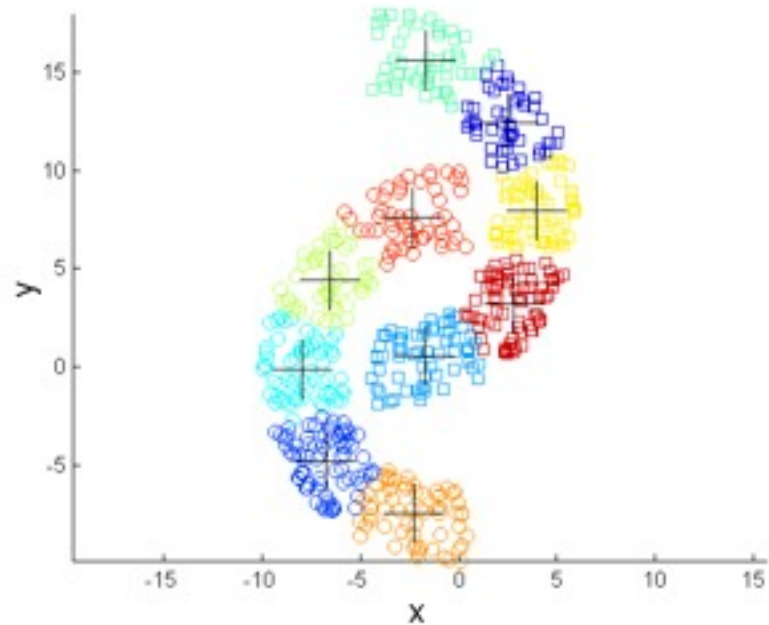


K-means Clusters

Overcoming K-means Limitations



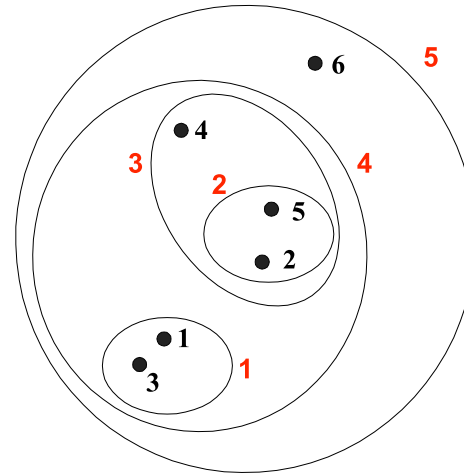
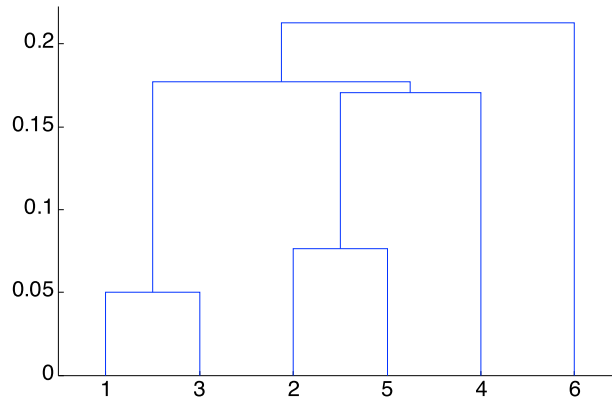
Original Points



K-means Clusters

Hierarchical Clustering

- | Produces a set of nested clusters organized as a hierarchical tree
- | Can be visualized as a dendrogram
 - A tree like diagram that records the sequences of merges or splits



Strengths of Hierarchical Clustering

- | Do not have to assume any particular number of clusters
 - Any desired number of clusters can be obtained by 'cutting' the dendrogram at the proper level
- | They may correspond to meaningful taxonomies
 - Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, ...)

Hierarchical Clustering

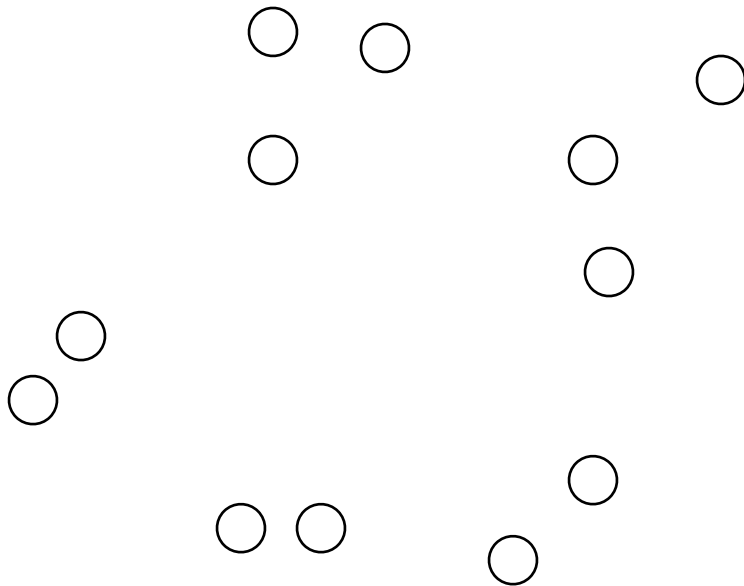
- | Two main types of hierarchical clustering
 - Agglomerative:
 - ◆ Start with the points as individual clusters
 - ◆ At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
 - Divisive:
 - ◆ Start with one, all-inclusive cluster
 - ◆ At each step, split a cluster until each cluster contains a point (or there are k clusters)
- | Traditional hierarchical algorithms use a similarity or distance matrix
 - Merge or split one cluster at a time

Agglomerative Clustering Algorithm

- | Most popular hierarchical clustering technique
- | Algorithm:
 1. Let each data point be a cluster
 1. Compute the distance matrix $n \times n$
 2. Repeat
 3. Merge the two closest clusters
 4. Update distance matrix
 5. **Until** only a single cluster remains

Starting Situation

- Start with clusters of individual points and a distance matrix $n \times n$



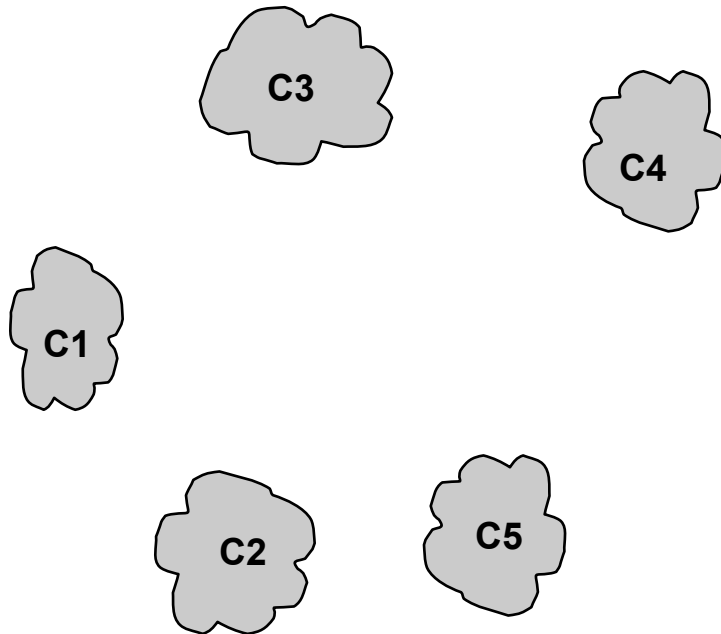
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Distance Matrix



Intermediate Situation

- After some merging steps, we have some clusters

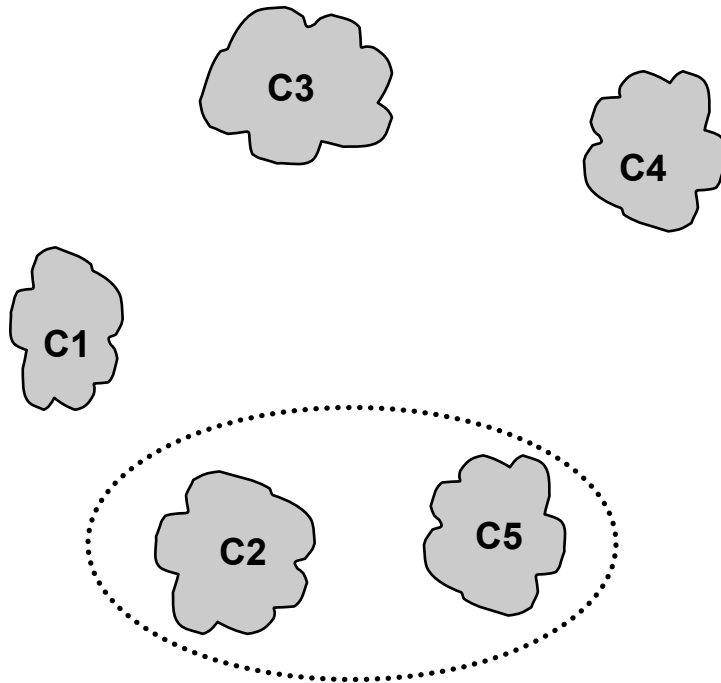


	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Distance Matrix

Intermediate Situation

- We want to merge the two closest clusters (C2 and C5) and update the distance matrix.



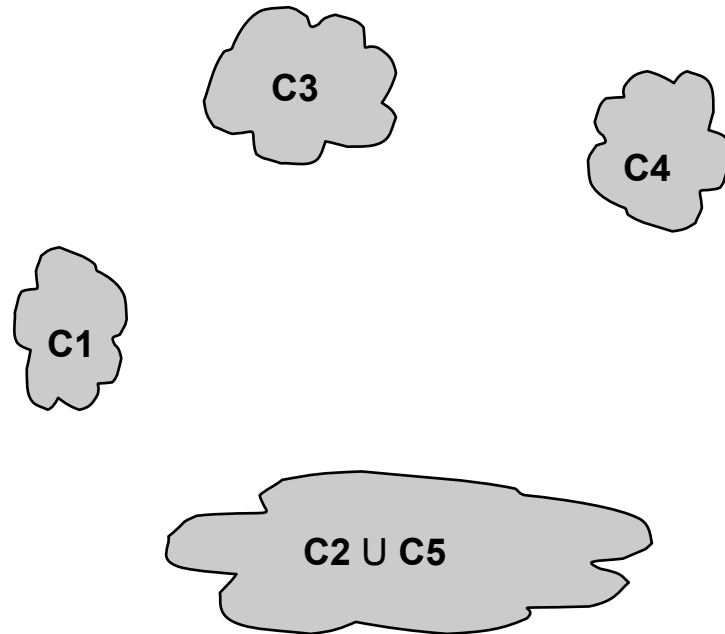
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Distance Matrix



After Merging

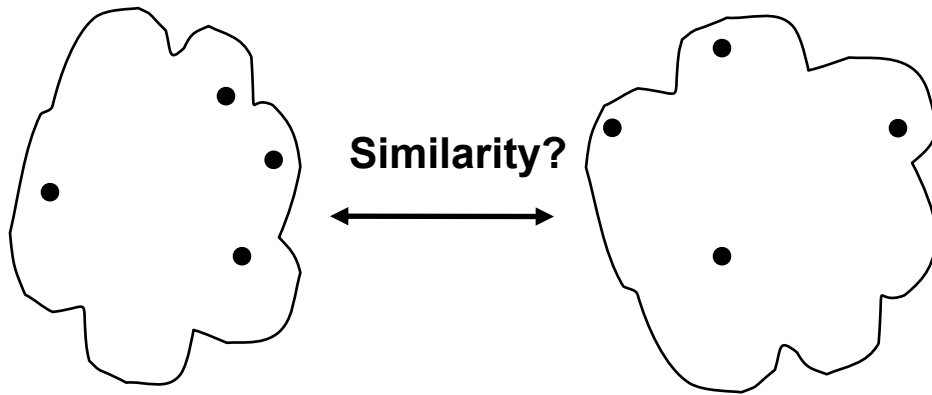
- The question is “How do we update the distance matrix?”



		$C2 \cup C5$			
		C1	C5	C3	C4
$C2 \cup C5$	C1		?		
	C5	?	?	?	?
	C3		?		
	C4		?		

Distance Matrix

How to Define Inter-Cluster Similarity

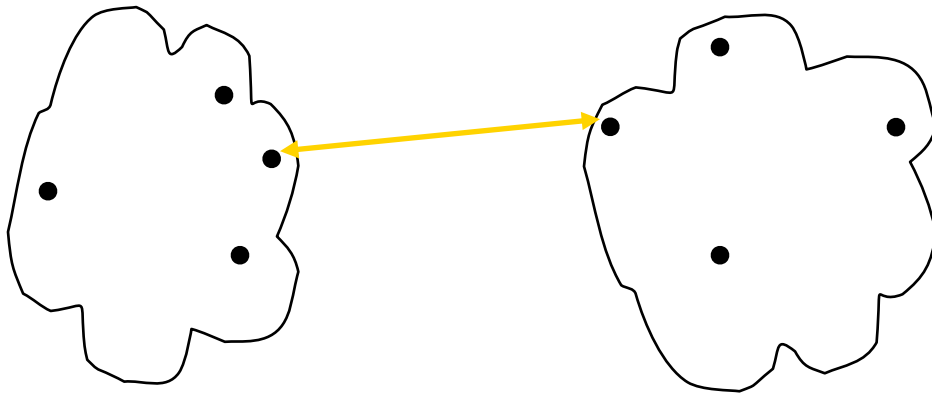


- | MIN
- | MAX
- | Group Average
- | Distance Between Centroids
- | Other methods driven by an objective function
 - Ward's Method uses squared error

	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Distance Matrix

How to Define Inter-Cluster Similarity

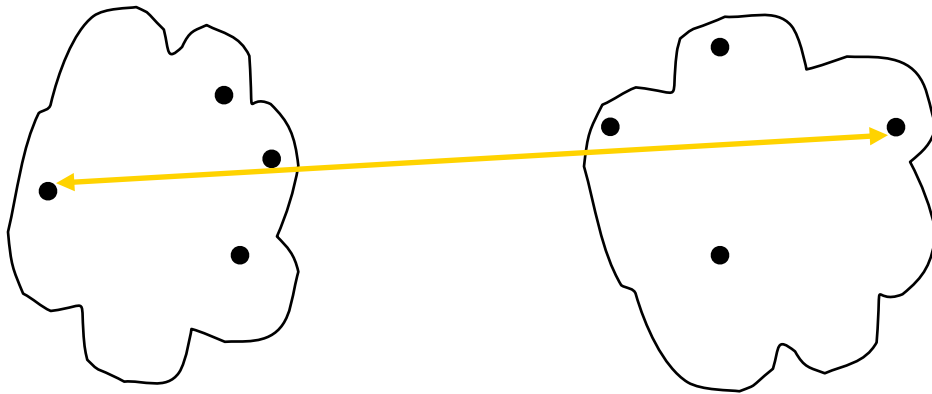


- | MIN
- | MAX
- | Group Average
- | Distance Between Centroids
- | Other methods driven by an objective function
 - Ward's Method uses squared error

	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
.						

Distance Matrix

How to Define Inter-Cluster Similarity

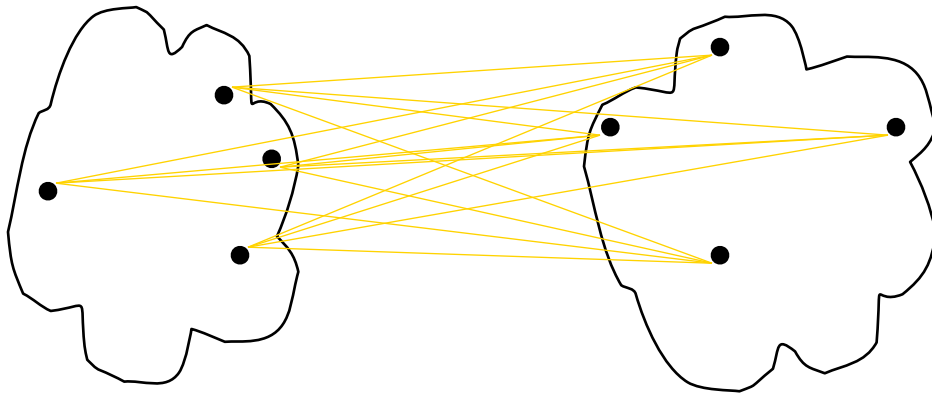


- | MIN
- | **MAX**
- | Group Average
- | Distance Between Centroids
- | Other methods driven by an objective function
 - Ward's Method uses squared error

	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
.						

Distance Matrix

How to Define Inter-Cluster Similarity

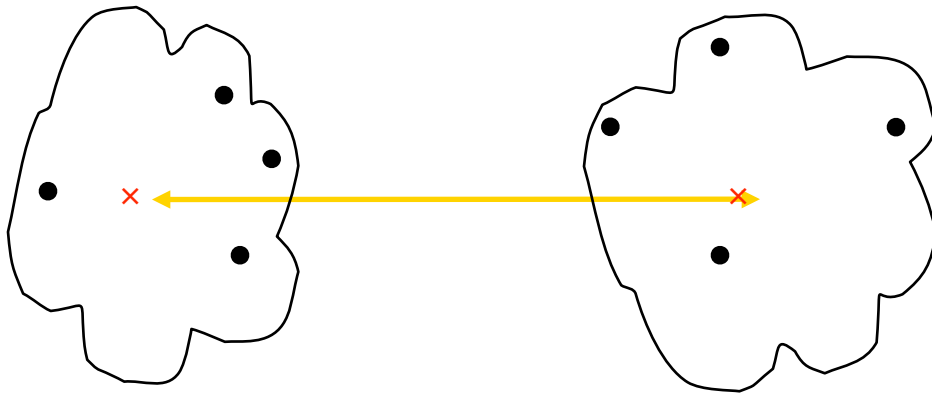


- | MIN
- | MAX
- | **Group Average**
- | Distance Between Centroids
- | Other methods driven by an objective function
 - Ward's Method uses squared error

	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
.						

Distance Matrix

How to Define Inter-Cluster Similarity



- | MIN
- | MAX
- | Group Average
- | **Distance Between Centroids**
- | Other methods driven by an objective function
 - Ward's Method uses squared error

	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Distance Matrix

Hierarchical Clustering: Problems and Limitations

- | Once a decision is made to combine two clusters, it cannot be undone
- | No objective function is directly minimized
- | Different schemes have problems with one or more of the following:
 - Sensitivity to noise and outliers
 - Difficulty handling different sized clusters and convex shapes
 - Breaking large clusters

Cluster Validity

- | For cluster analysis, the analogous question is how to evaluate the “goodness” of the resulting clusters?
- | But “clusters are in the eye of the beholder”!
- | Then why do we want to evaluate them?
 - To avoid finding patterns in noise
 - To compare clustering algorithms
 - To compare two sets of clusters
 - To compare two clusters

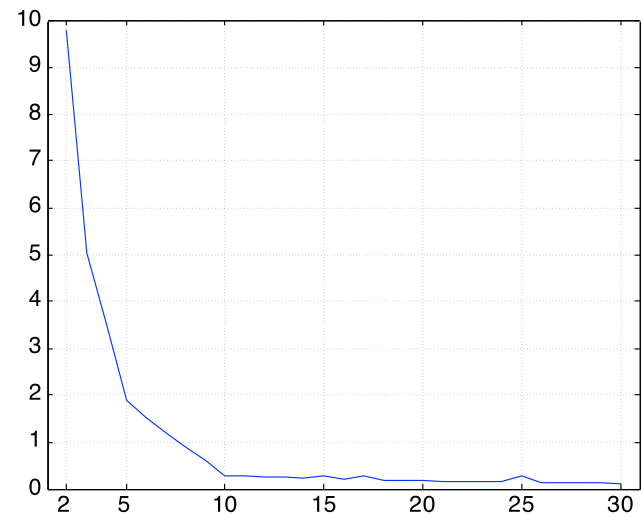
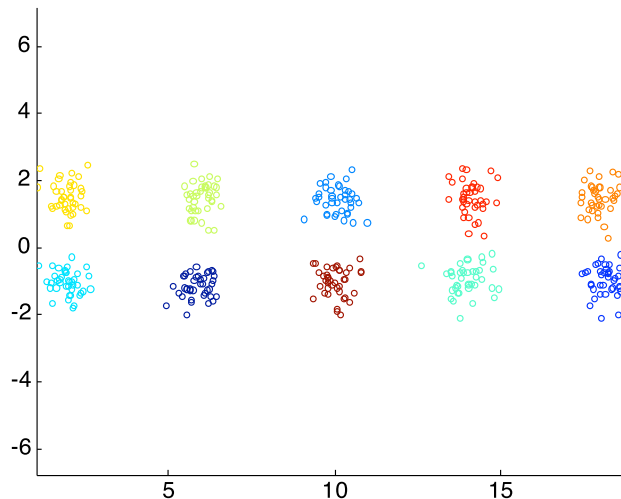
Measures of Cluster Validity

- | Numerical measures that are applied to judge various aspects of cluster validity, are classified into the following three types.
 - **External Index:** Used to measure the extent to which cluster labels match externally supplied class labels.
 - ◆ Entropy
 - **Internal Index:** Used to measure the goodness of a clustering structure *without* respect to external information.
 - ◆ Sum of Squared Error (SSE)
 - **Relative Index:** To compare two different clusterings or clusters.
 - ◆ An external or internal index is used for this function, e.g., SSE or entropy

- | Sometimes these are referred to as **criteria** instead of **indices**

Internal Measures: SSE

- | Clusters in more complicated figures aren't well separated
- | Internal Index: Used to measure the goodness of a clustering structure without respect to external information
 - SSE
- | SSE is good for comparing two clusterings or two clusters (average SSE).
- | Can also be used to estimate the number of clusters



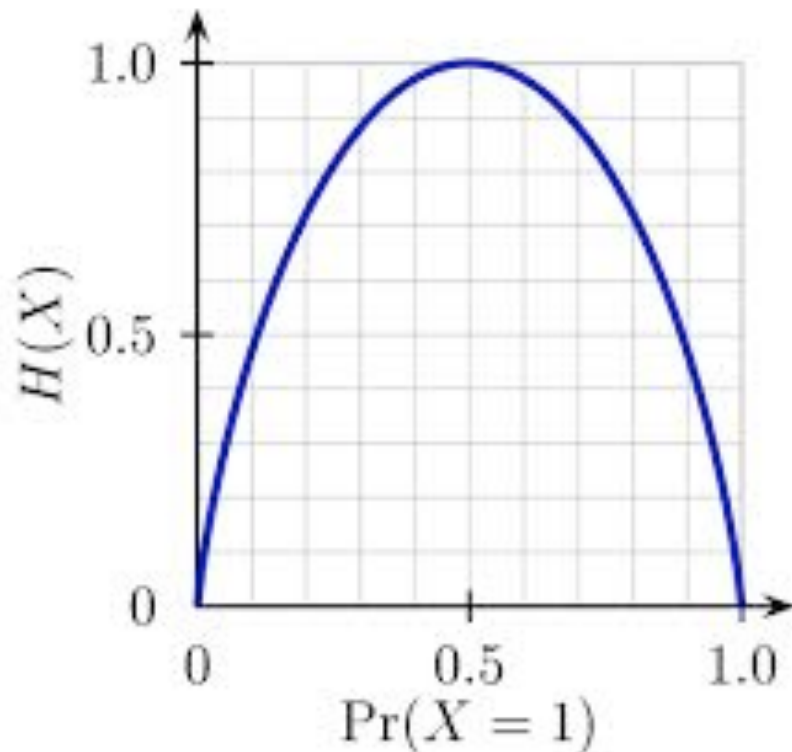
Entropy: definition

- | Given a discrete random variable X with possible value $\{1, \dots, n\}$ entropy is defined as

$$H(X) = - \sum_{i=1}^n P(X = i) \log_2 P(X = i)$$

- | Entropy measure how **uncertain** is an event, the larger the entropy the more uncertain is the event

Entropy: intuition



Entropy of a binary variable.

Examples:

1. entropy of unbiased coin vs biased coin?
2. entropy of a dice roll?
3. Probability distribution:
 $P(X=c_i)$ = probability of finding character c_i in a text document.
Easier to compress a document when entropy is high or low?

External Measures of Cluster Validity: Entropy

Table 5.9. K-means Clustering Results for LA Document Data Set

Cluster	Entertainment	Financial	Foreign	Metro	National	Sports	Entropy	Purity
1	3	5	40	506	96	27	1.2270	0.7474
2	4	7	280	29	39	2	1.1472	0.7756
3	1	1	1	7	4	671	0.1813	0.9796
4	10	162	3	119	73	2	1.7487	0.4390
5	331	22	5	70	13	23	1.3976	0.7134
6	5	358	12	212	48	13	1.5523	0.5525
Total	354	555	341	943	273	738	1.1450	0.7203

Topics = {Entertainment, Financial, Metro, ...} = {1, 2, 3, ..., k}

p_{ij} = Probability that an element of cluster j belongs to topic i .

E.g. $p_{13} = 1/685$

For a cluster j better to have higher or lower entropy?

External Measures of Cluster Validity: Entropy

Table 5.9. K-means Clustering Results for LA Document Data Set

Cluster	Entertainment	Financial	Foreign	Metro	National	Sports	Entropy	Purity
1	3	5	40	506	96	27	1.2270	0.7474
2	4	7	280	29	39	2	1.1472	0.7756
3	1	1	1	7	4	671	0.1813	0.9796
4	10	162	3	119	73	2	1.7487	0.4390
5	331	22	5	70	13	23	1.3976	0.7134
6	5	358	12	212	48	13	1.5523	0.5525
Total	354	555	341	943	273	738	1.1450	0.7203

m_j = size of cluster j , m = number of docs.

Entropy and purity of a cluster

$$e_j = - \sum_{i=1}^K p_{ij} \log p_{ij} \quad \text{purity}_j = \max_i p_{ij}$$

Entropy and purity of a clustering:

$$\sum_j \frac{m_j}{m} e_j \quad \sum_j \frac{m_j}{m} \text{purity}_j$$