

Data Mining

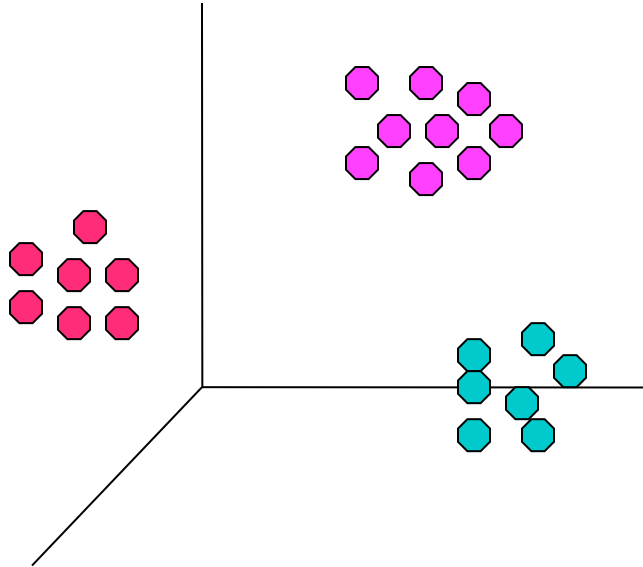
Introduction to Clustering

Mauro Sozio

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

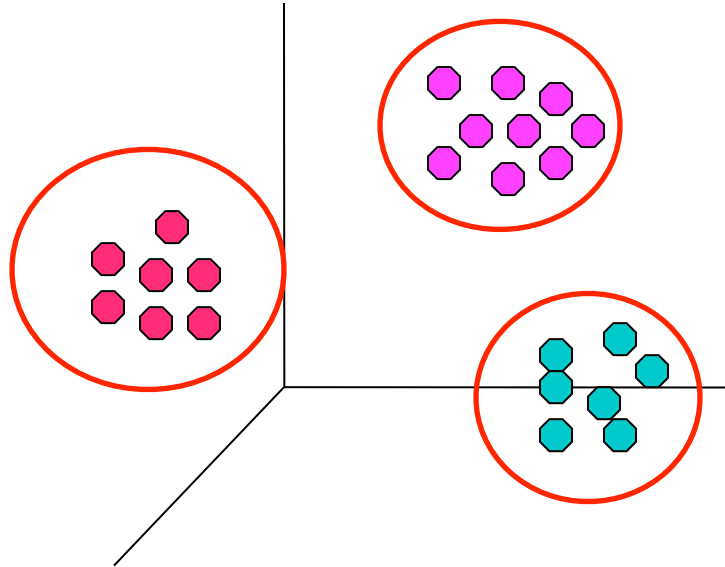
What is Cluster Analysis?

- 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



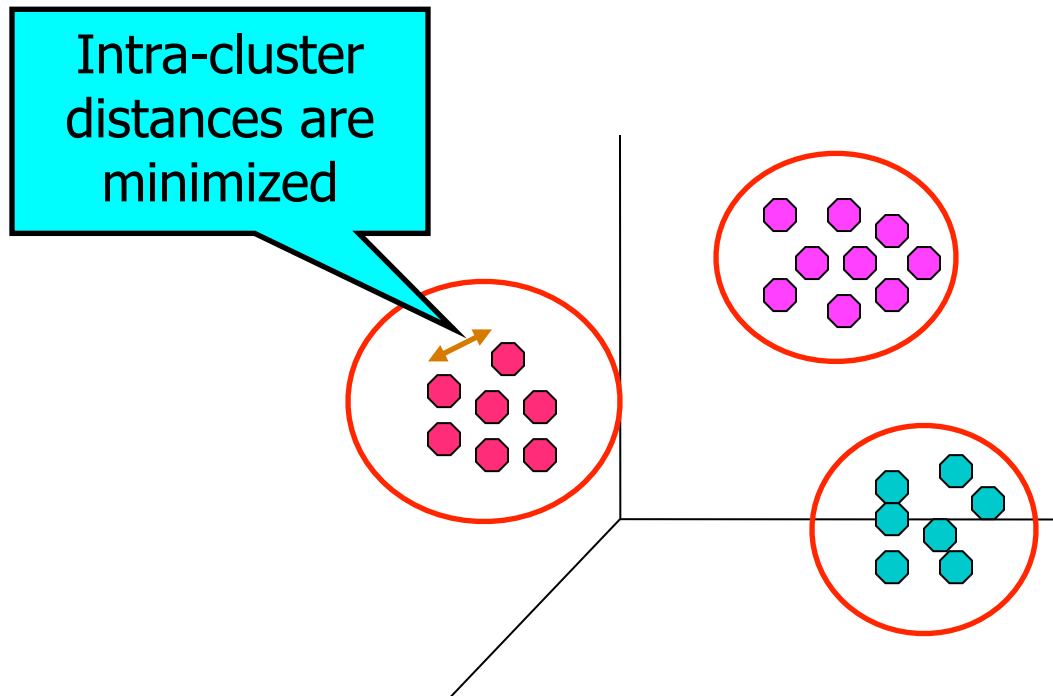
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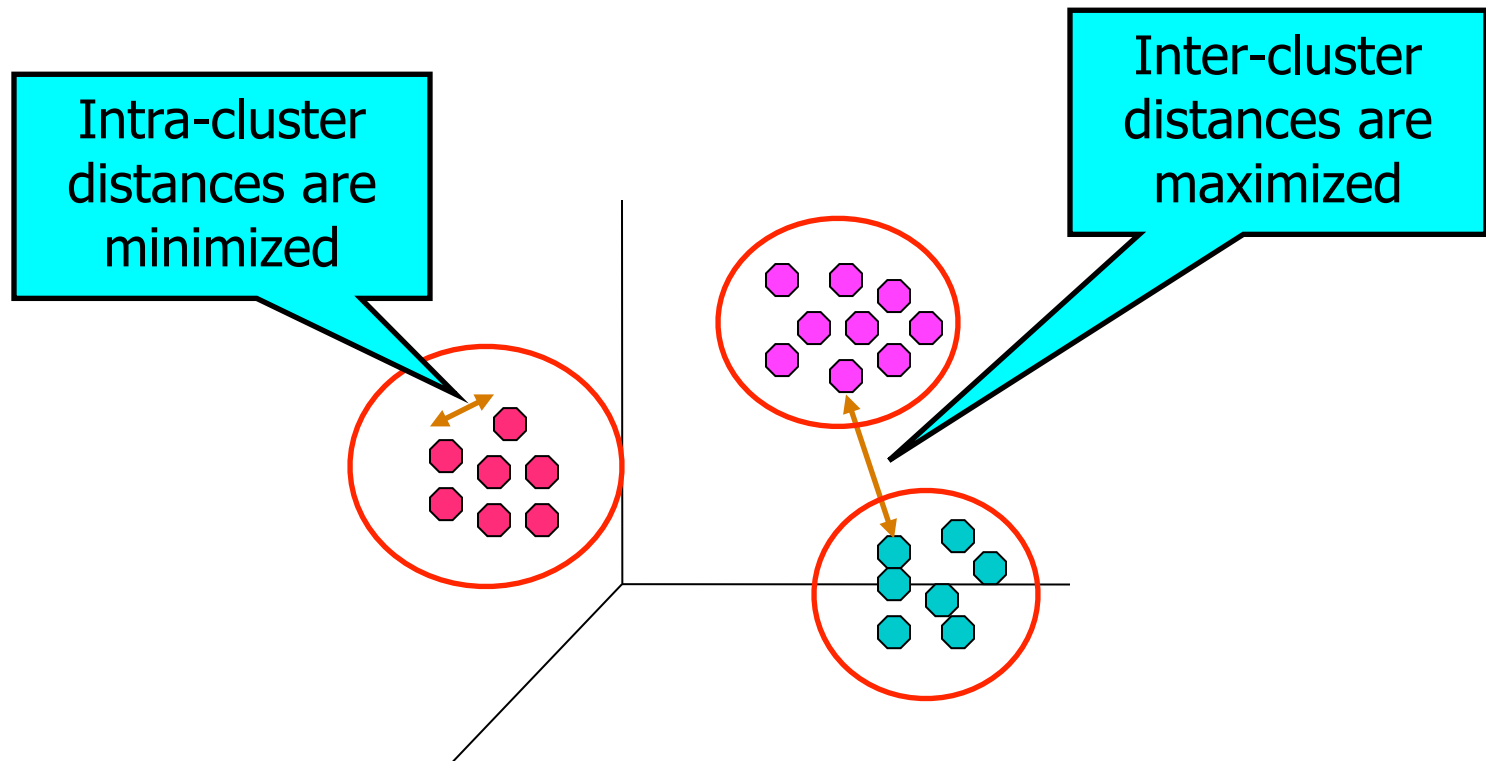
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Applications of Cluster Analysis

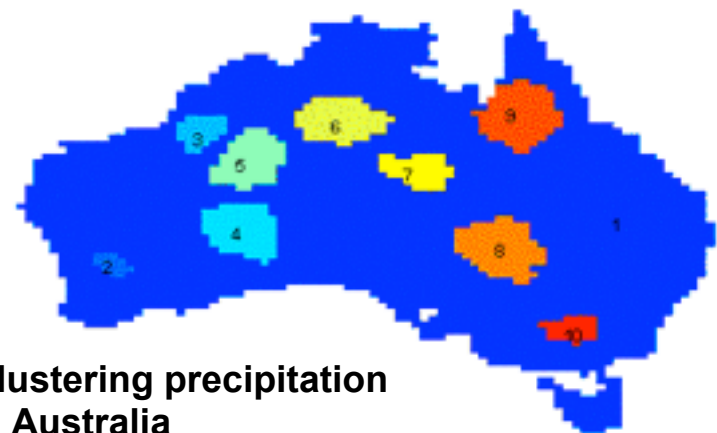
Understanding

- 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,OracI-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

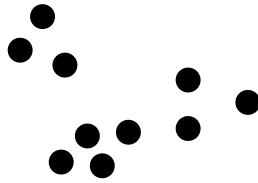
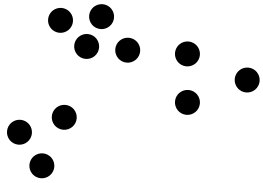


How many clusters?

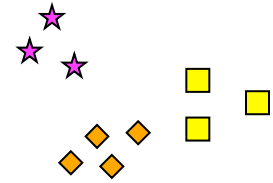
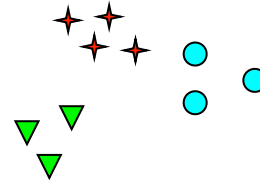


Two Clusters

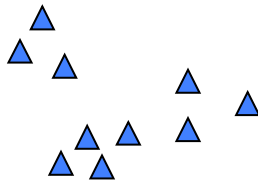
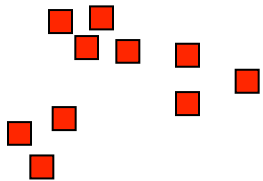
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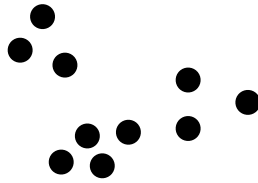
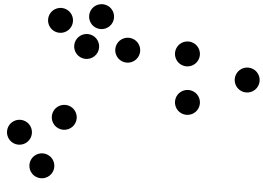


Six Clusters

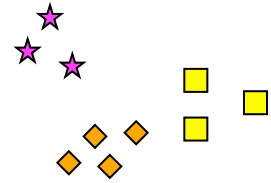
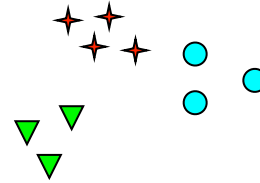


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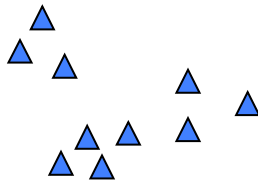
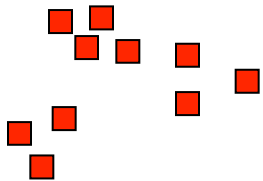
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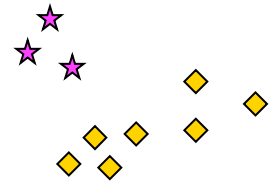
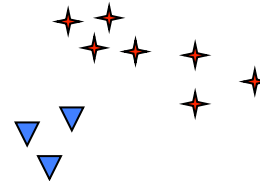
How many clusters?



Six Clusters



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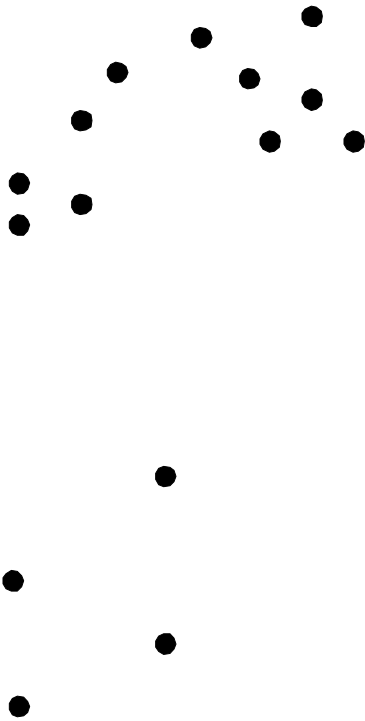


Four Clusters

Types of Clusterings

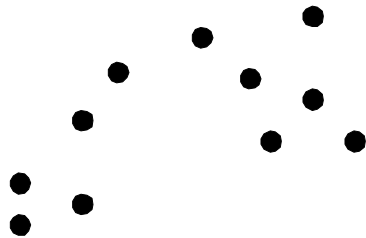
- | A **clustering** is a set of clusters
- | Important distinction between **hierarchical** and **partitional** sets of clusters
- | **Partitional Clustering**
 - A division data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset
- | **Hierarchical clustering**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

Partitional Clustering

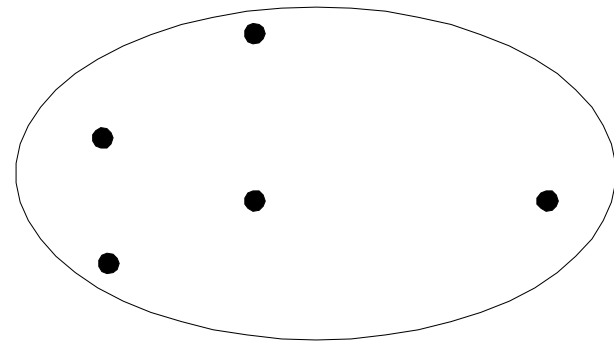
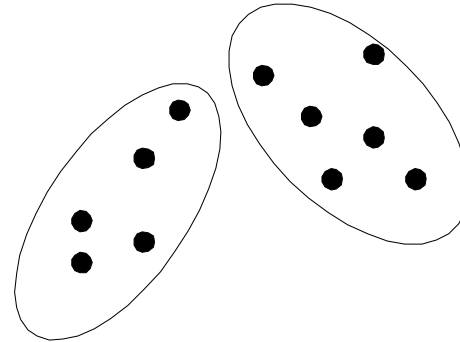


Original Points

Partitional Clustering

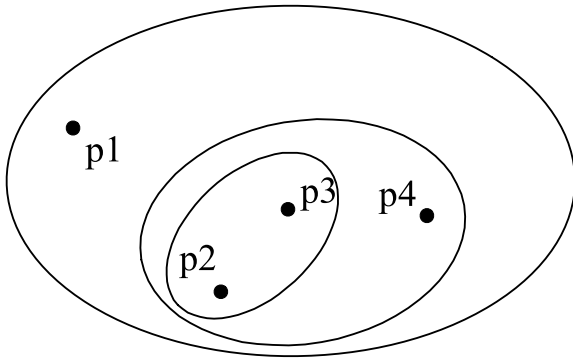


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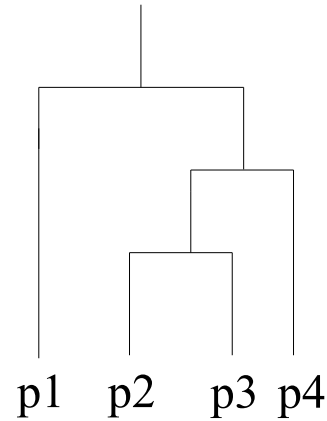


A Partitional Clustering

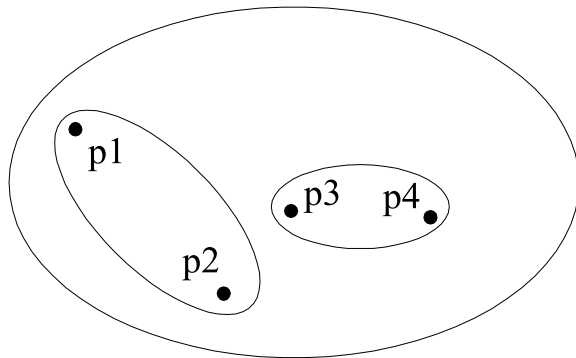
Hierarchical Clustering



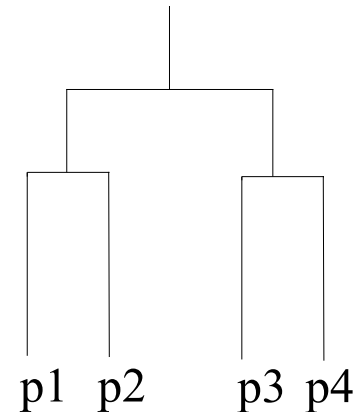
Traditional Hierarchical Clustering



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

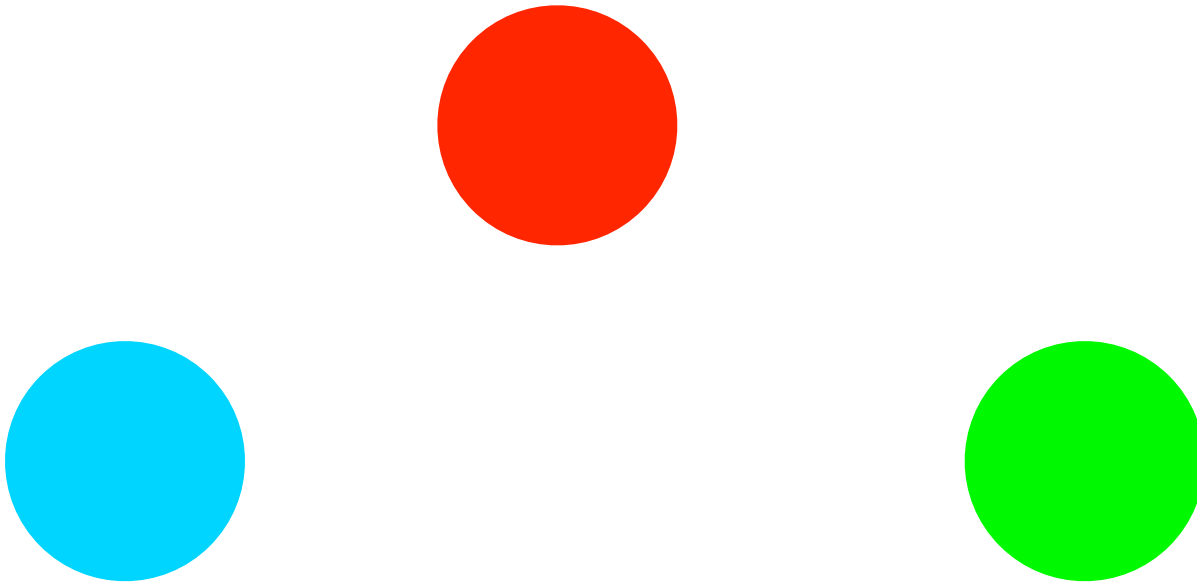
Types of Clusters

- | 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

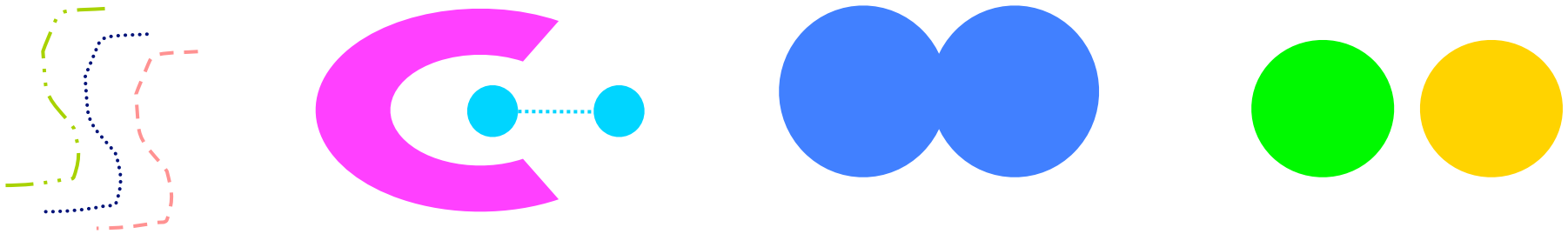
- A cluster is a set of objects such that an object in a cluster is closer (more similar) to the “center” of a cluster, than to the center of any other cluster
- The center of a cluster is often a **centroid**, the average of all the points in the cluster, or a **medoid**, the most “representative” point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

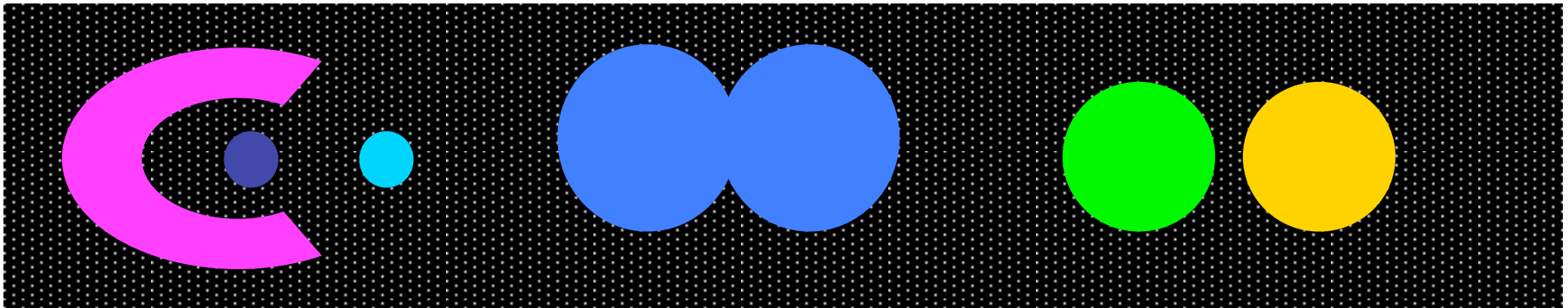


8 contiguous clusters

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.

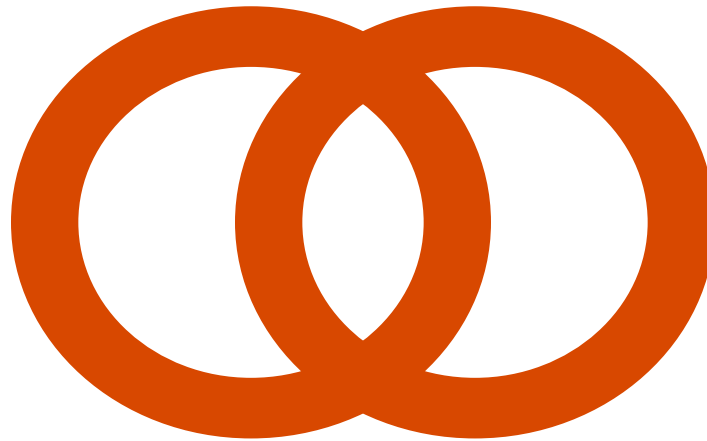


6 density-based clusters

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

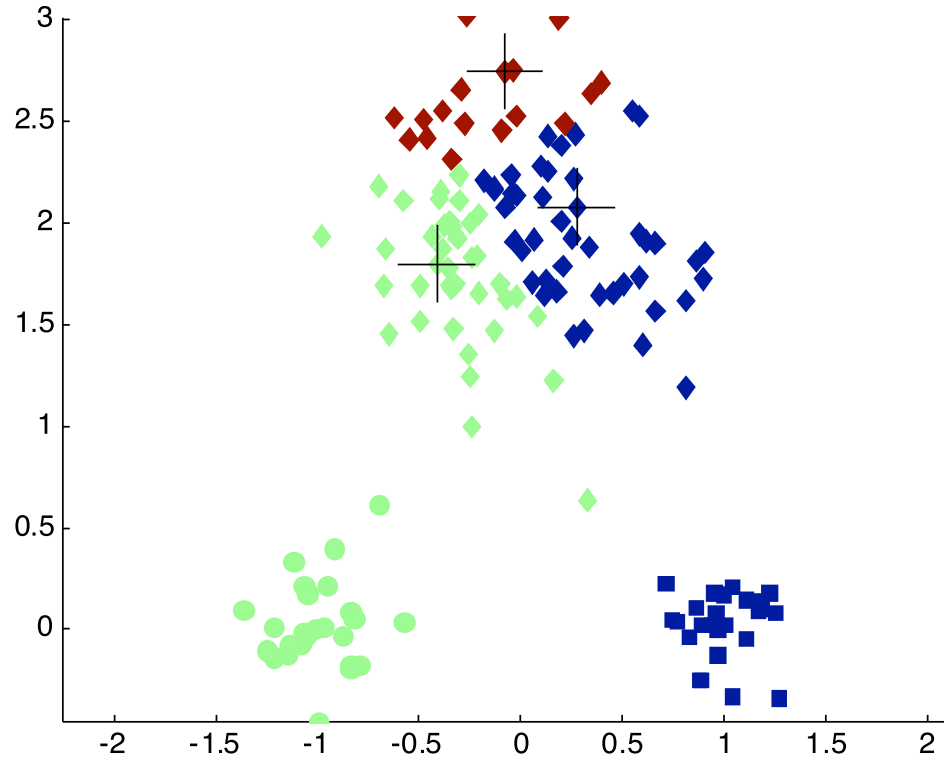
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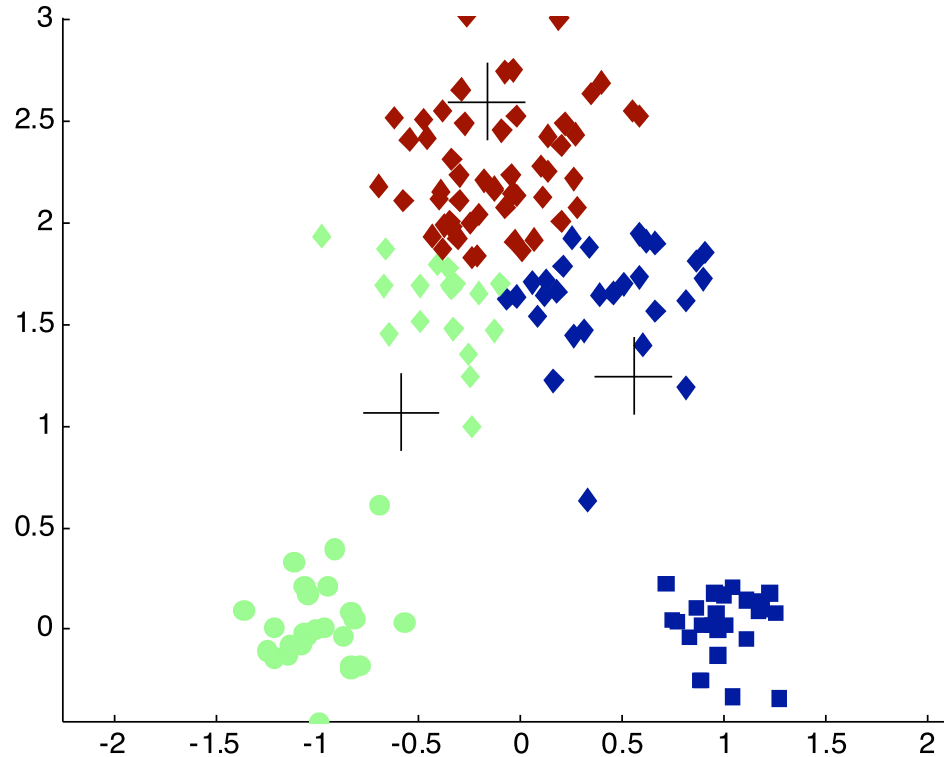
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- | Initial centroids are often chosen randomly.
- | Centroids are often the mean of the points in the cluster.
- | 'Closeness' is measured by Euclidean distance, cosine similarity, correlation, etc.

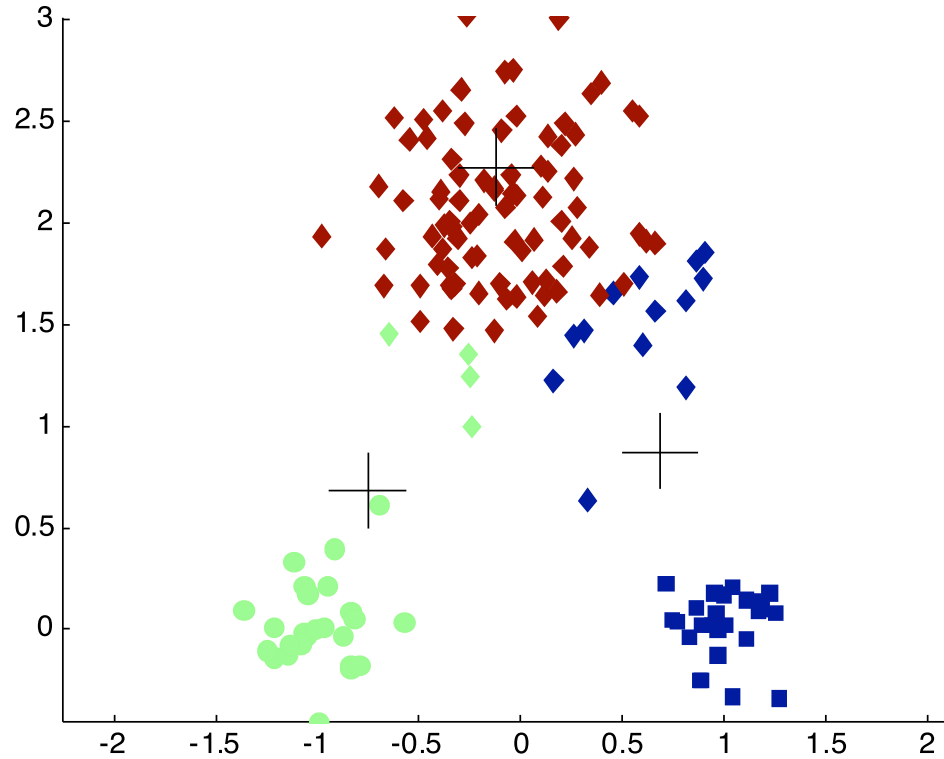
K-means: example



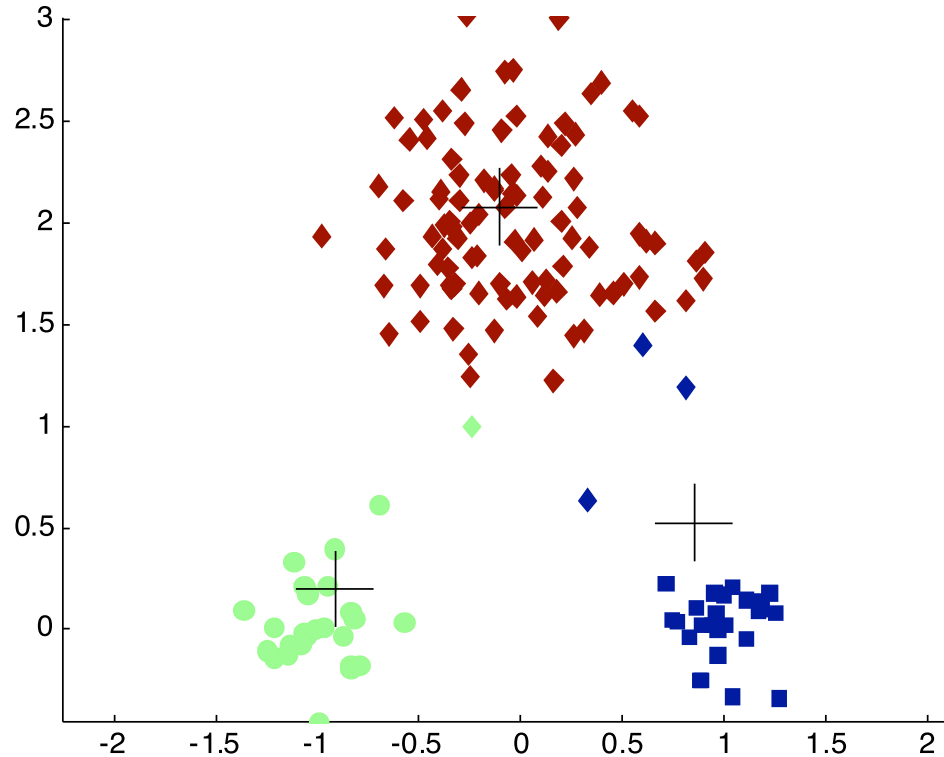
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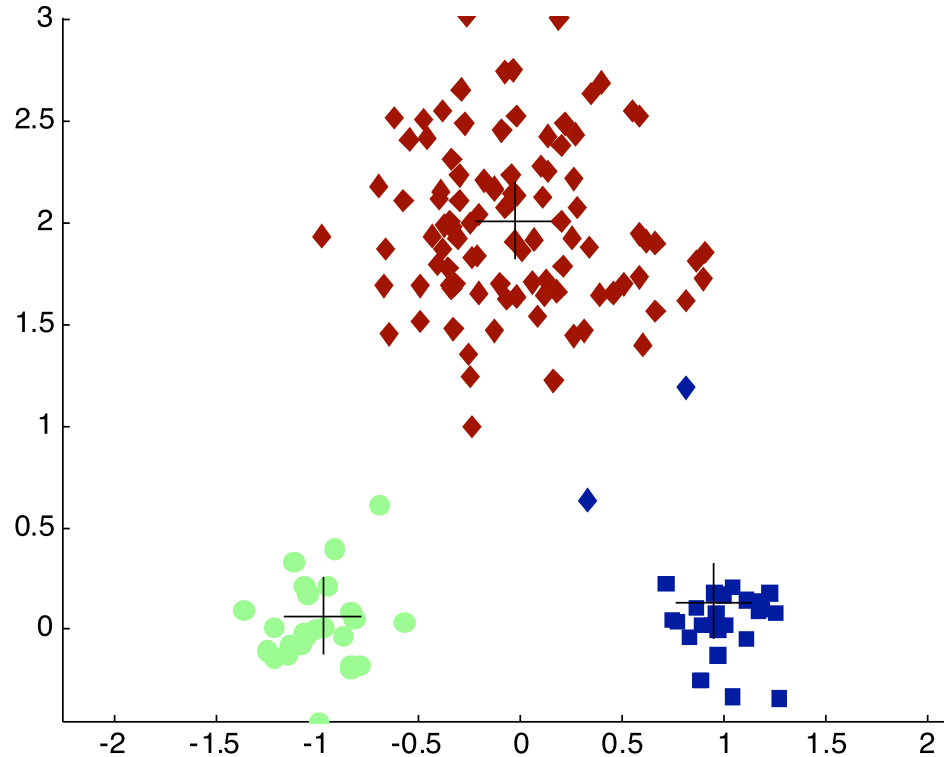
K-means: example



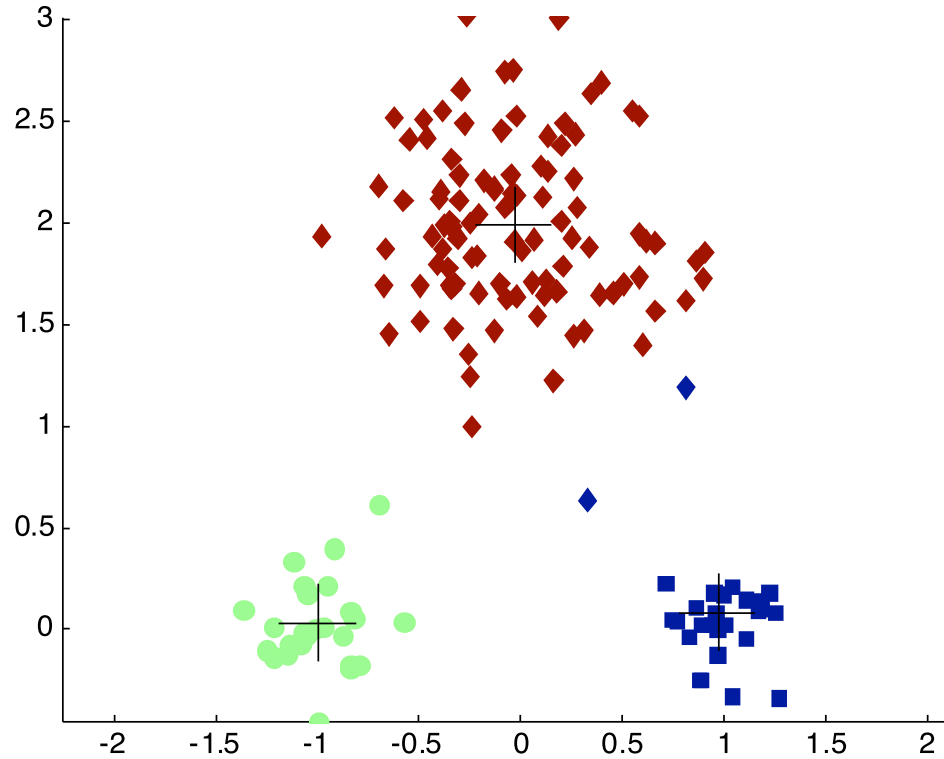
K-means: example



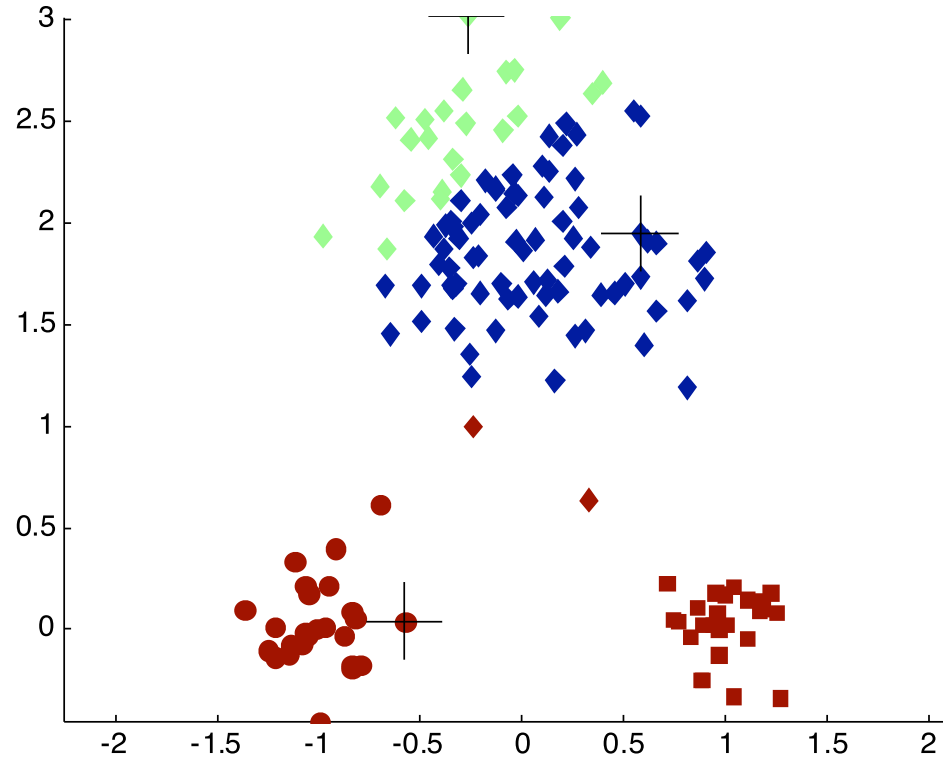
K-means: example



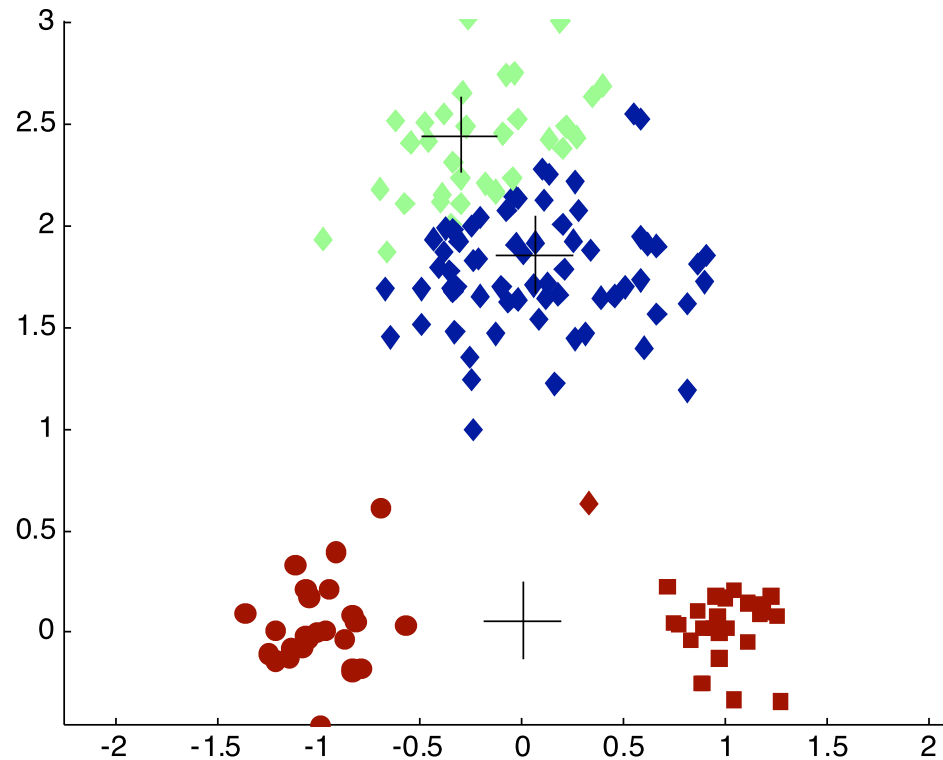
K-means: example



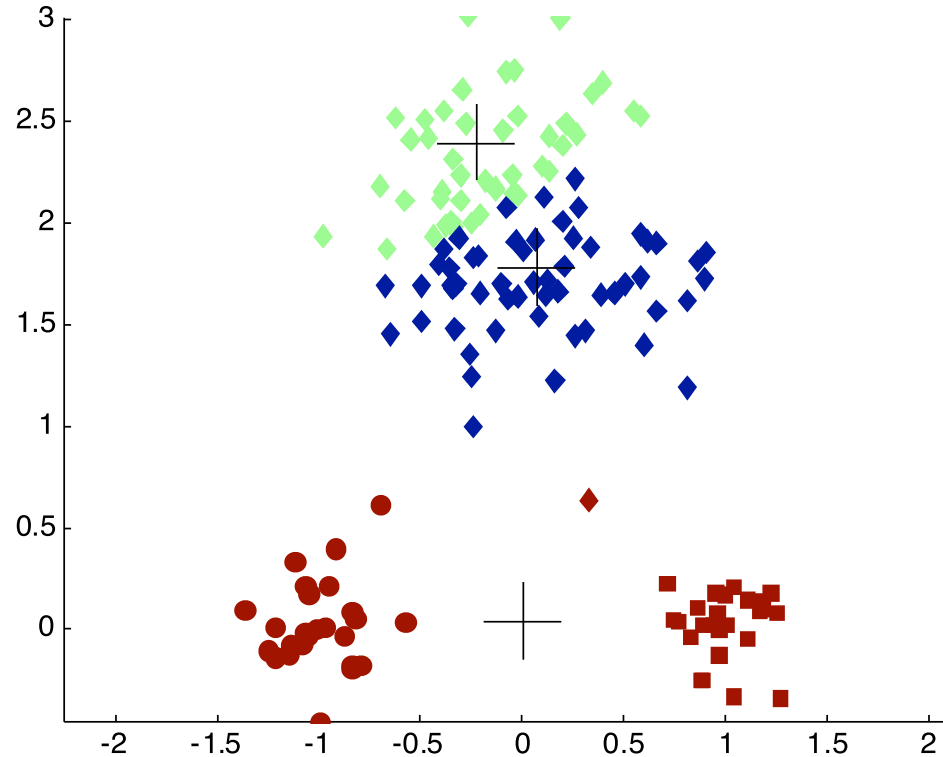
Importance of Choosing Initial Centroids ...



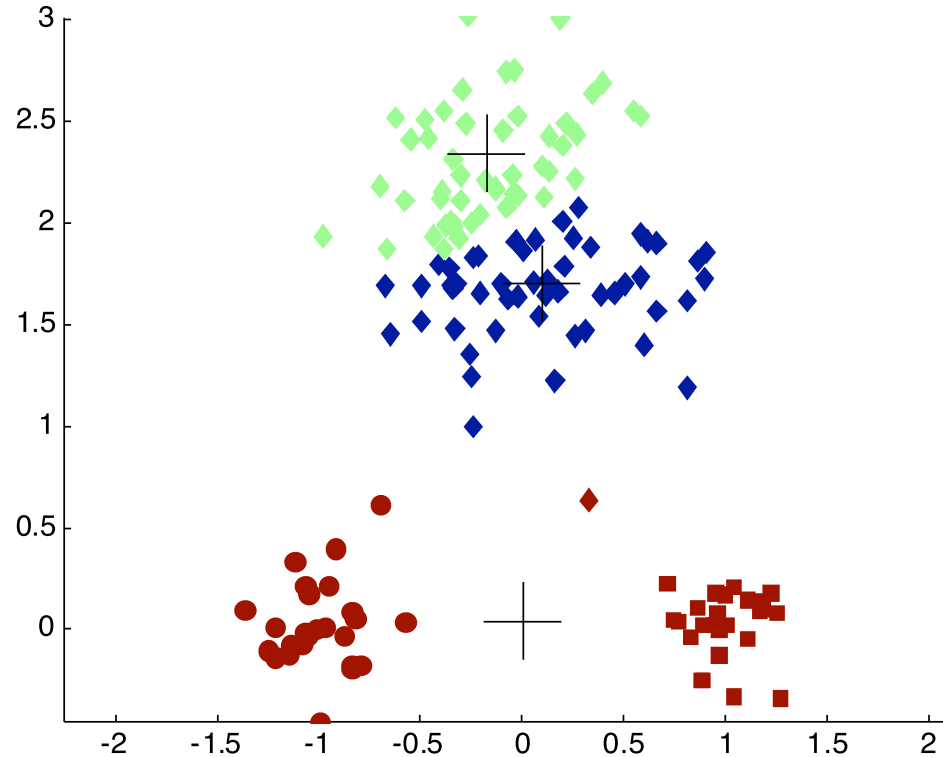
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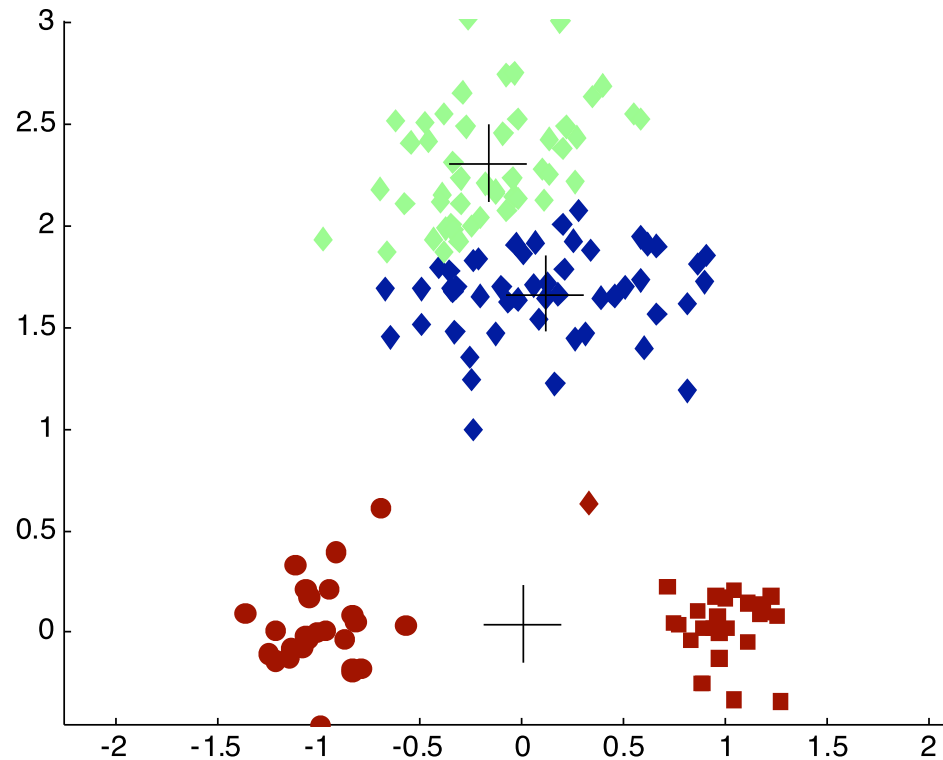
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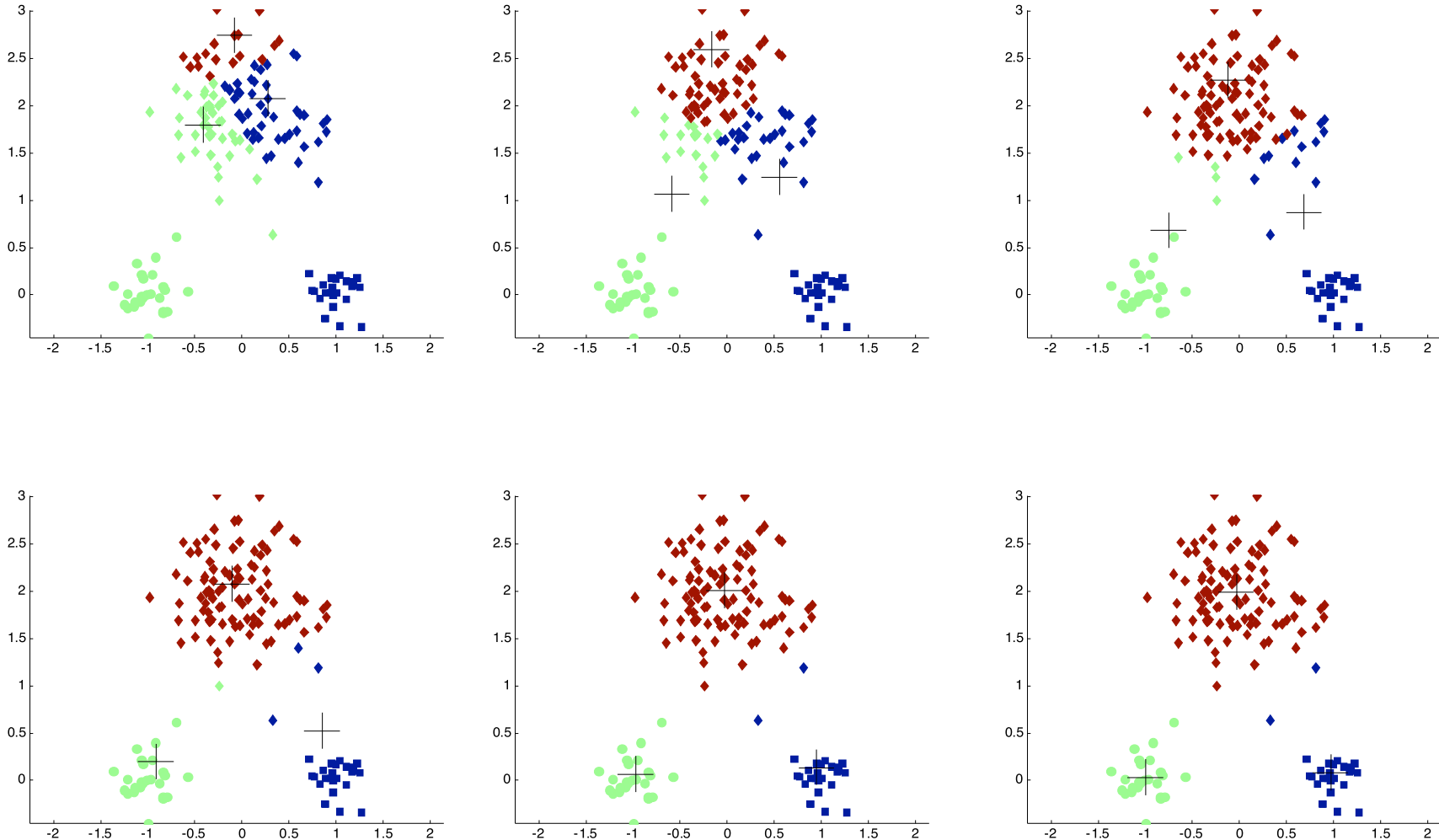
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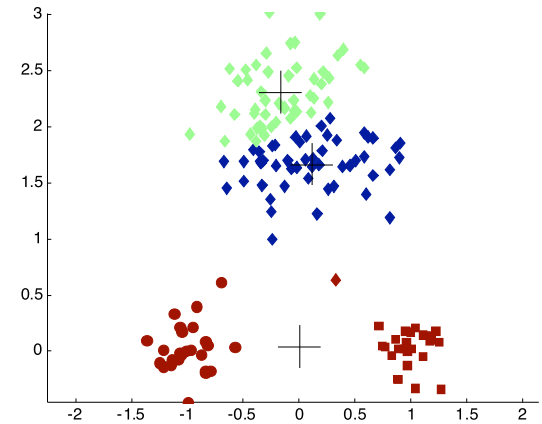
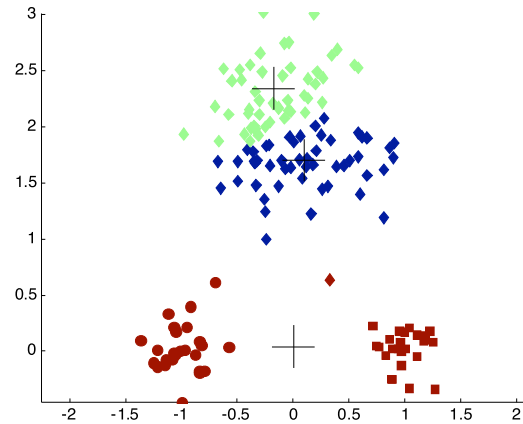
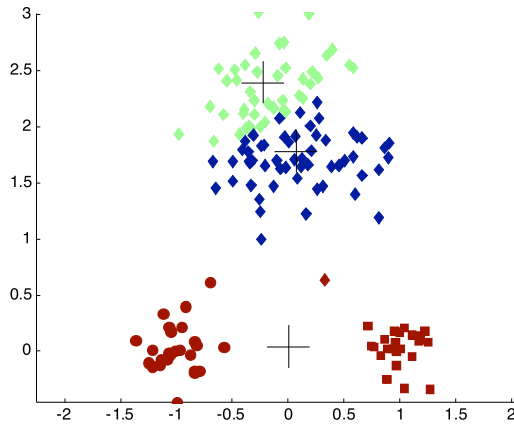
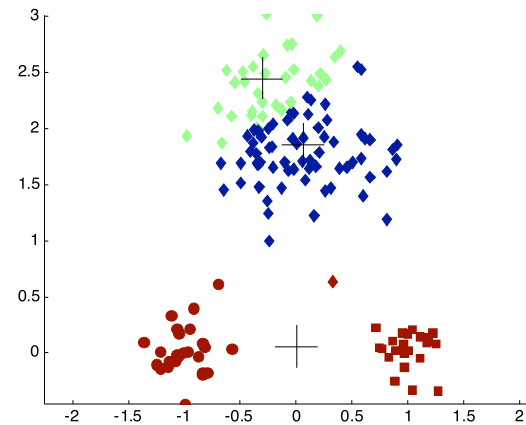
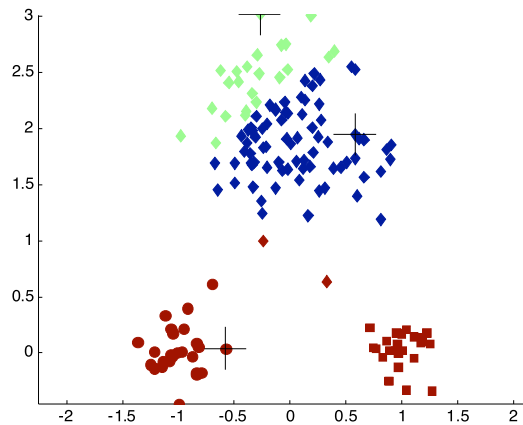
Importance of Choosing Initial Centroids ...



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). **Exercise:** think why!

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 less than k clusters (so called 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

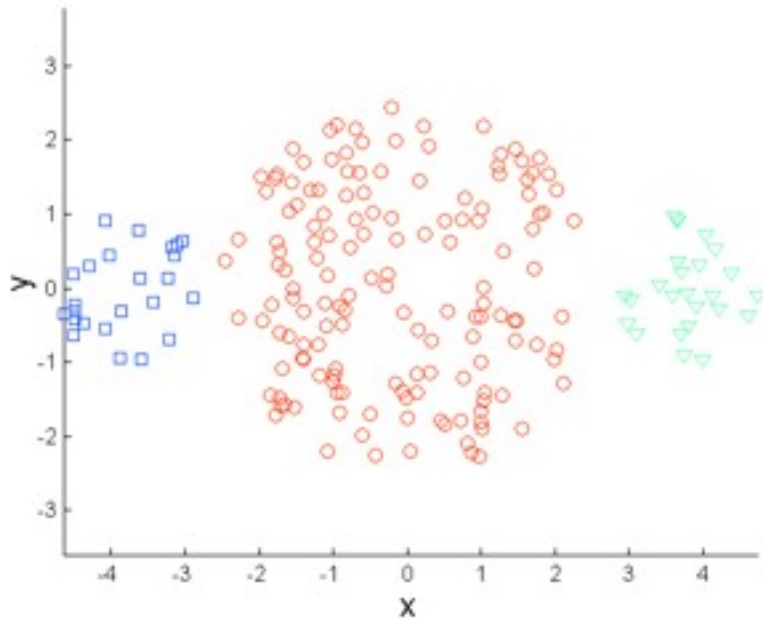
| Post-processing

- 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

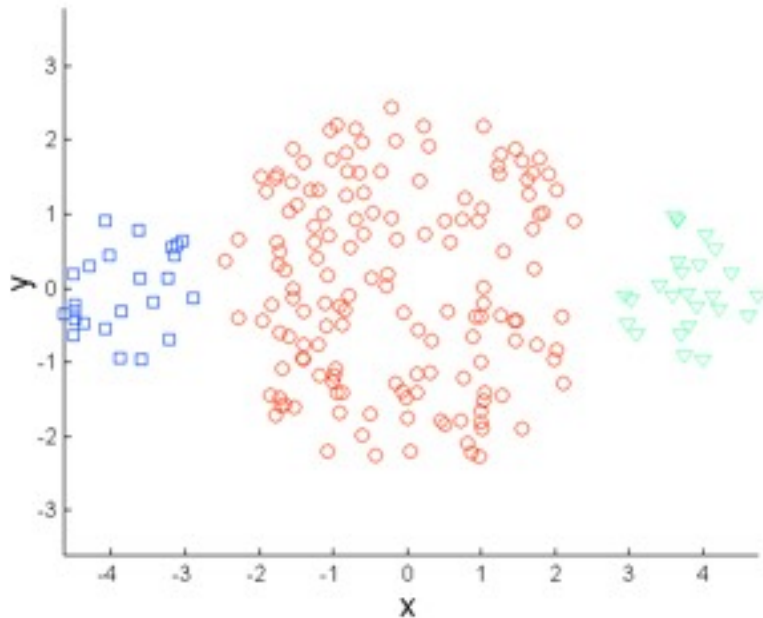
- | K-means has problems when clusters are of differing
 - Sizes
 - Densities
 - Non-globular shapes
- | K-means has problems when the data contains outliers.

Limitations of K-means: Differing Sizes



Original Points

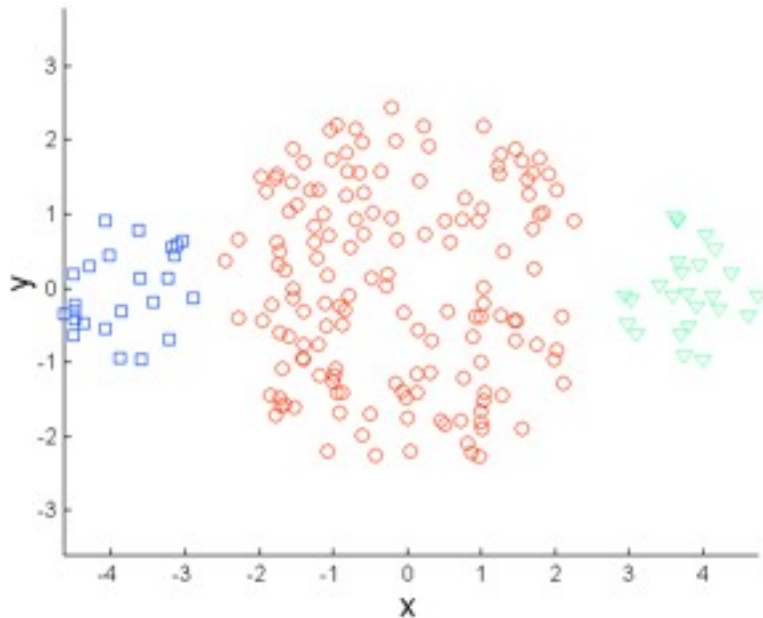
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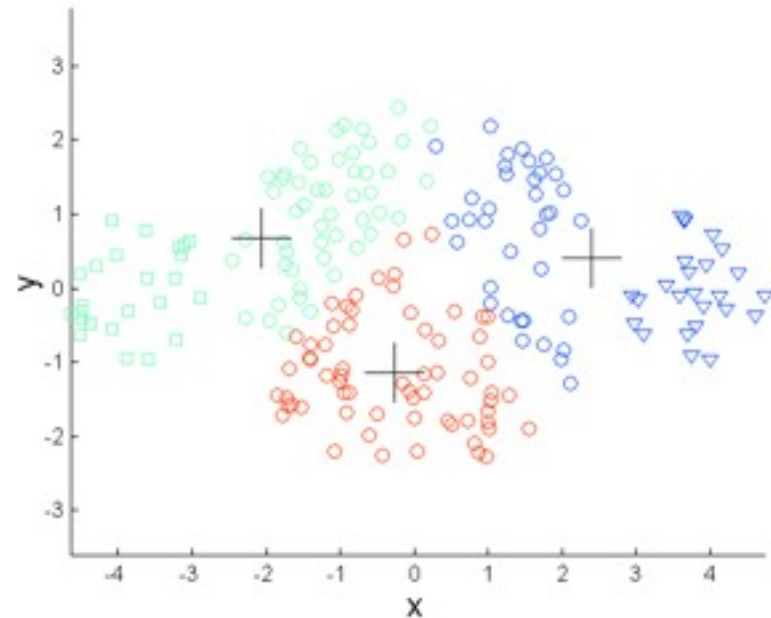
Original Points

K-means (3 Clusters)

Limitations of K-means: Differing Sizes

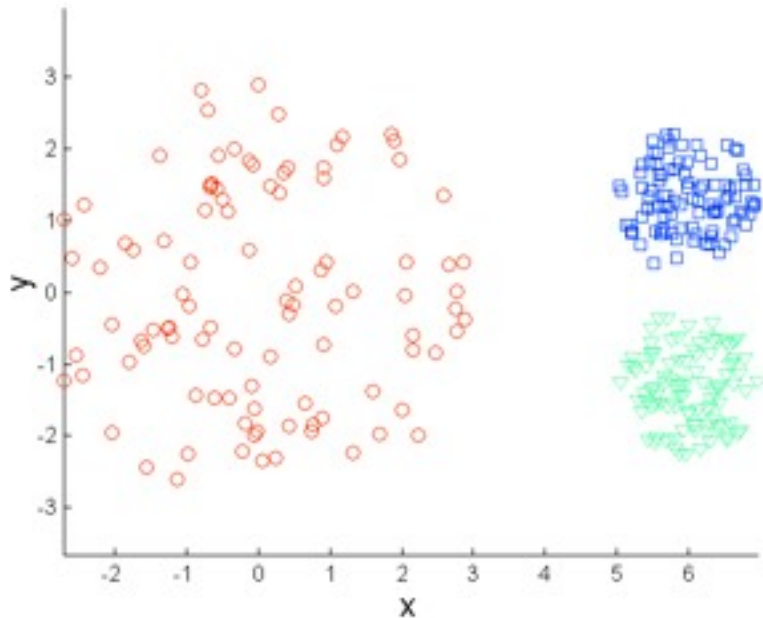


Original Points



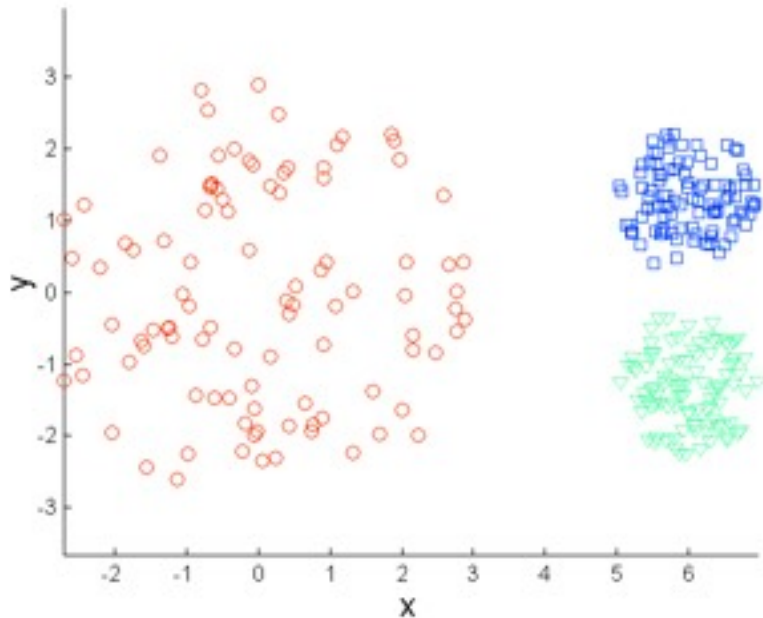
K-means (3 Clusters)

Limitations of K-means: Differing Density



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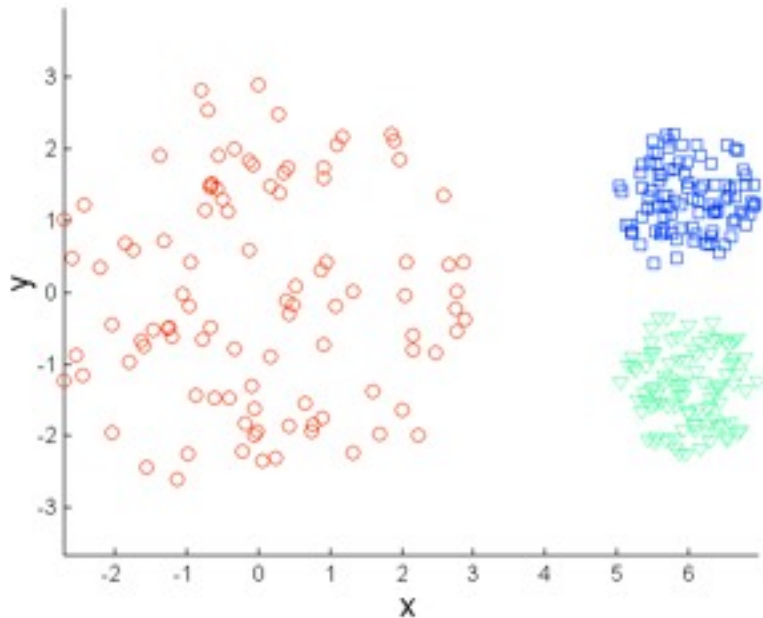
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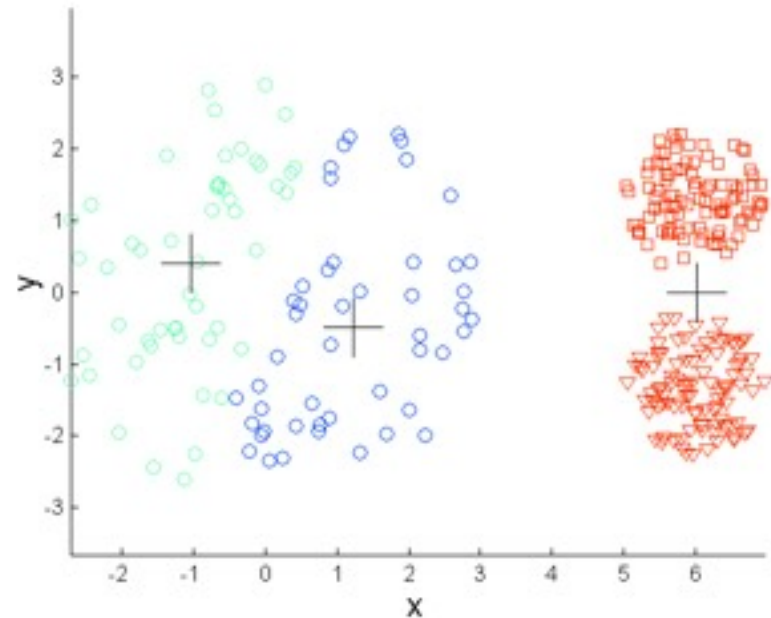
Original Points

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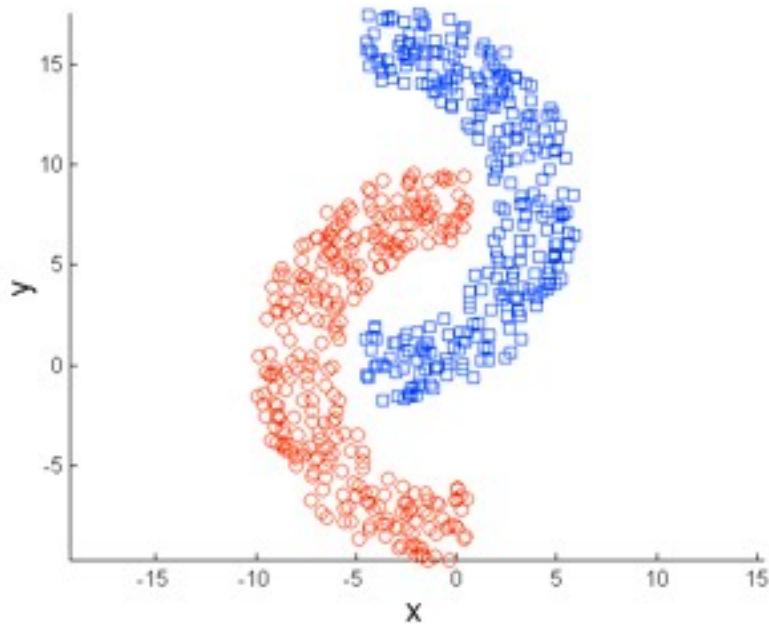


Original Points



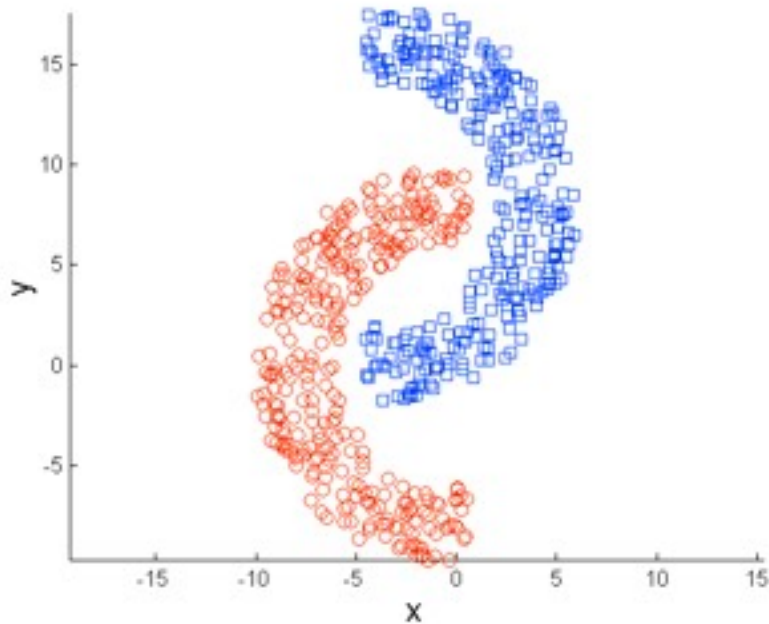
K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes



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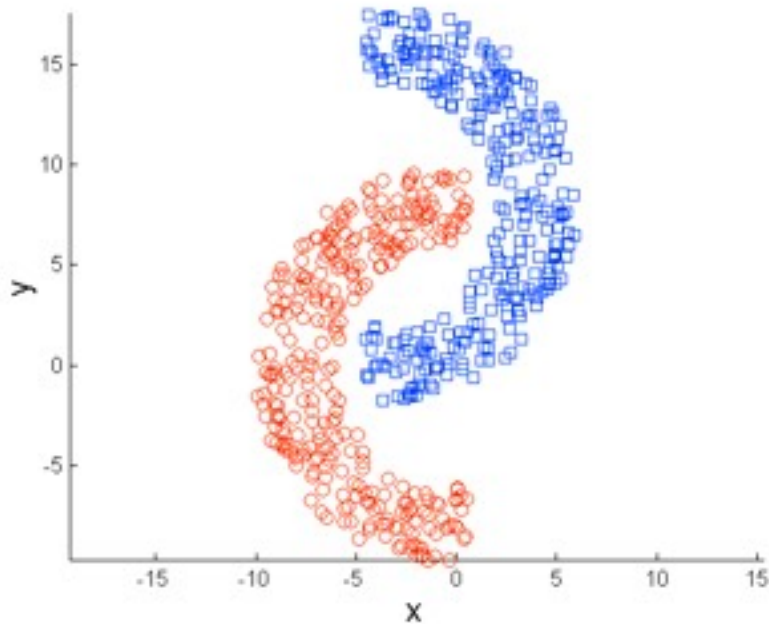
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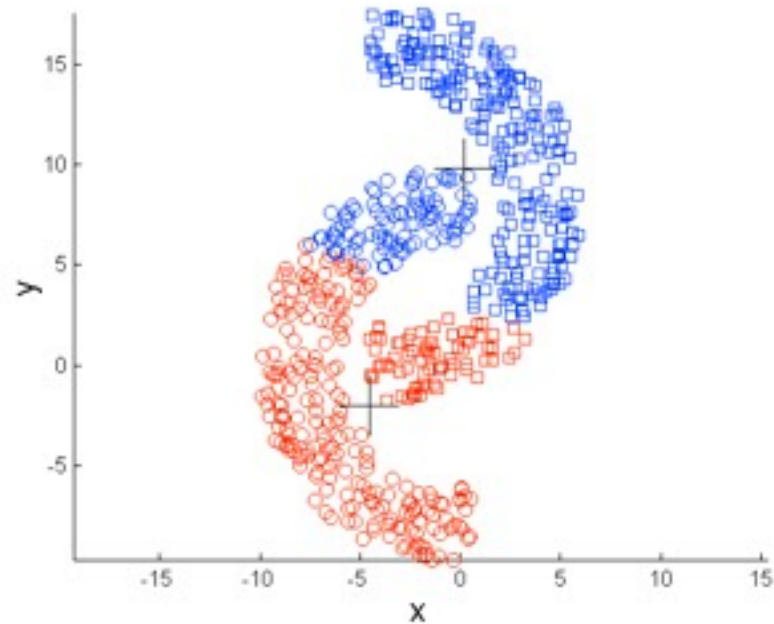
Original Points

K-means (2 Clusters)

Limitations of K-means: Non-globular Shapes

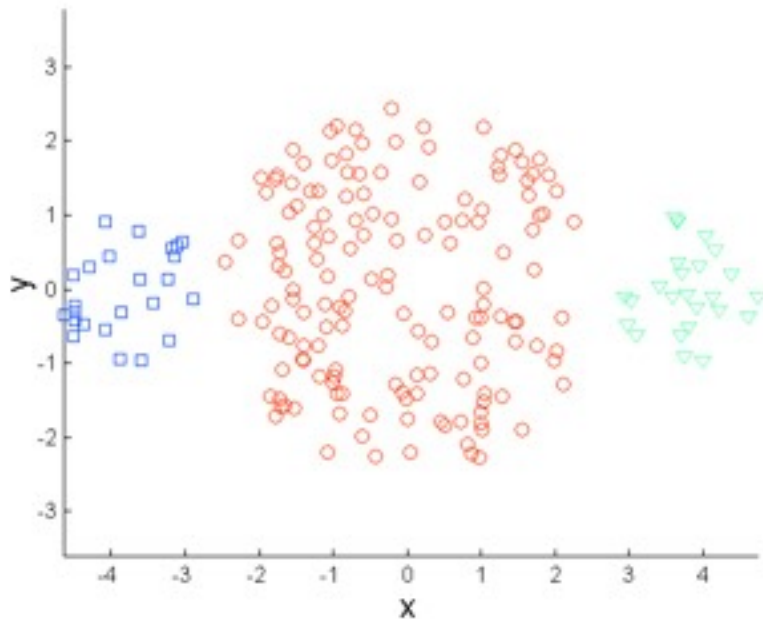


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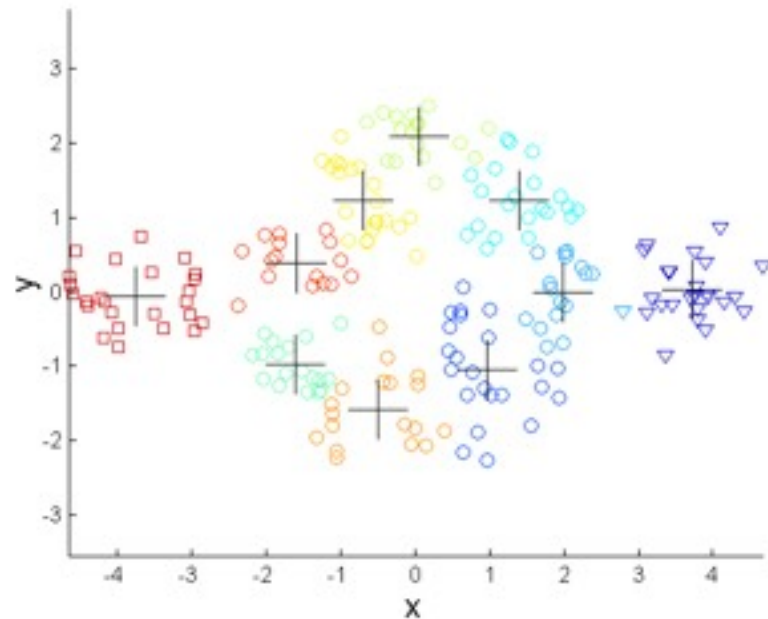


K-means (2 Clusters)

Overcoming K-means Limitations



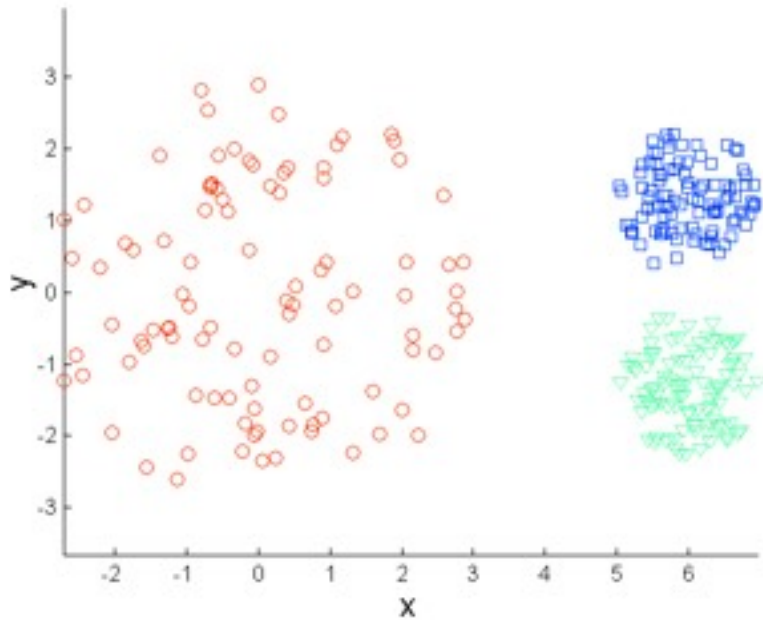
Original Points



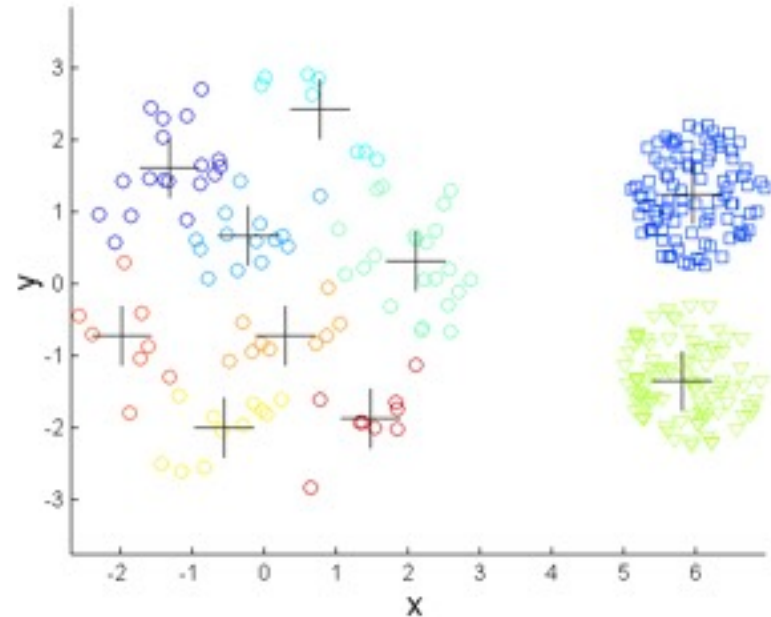
K-means Clusters

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

Overcoming K-means Limitations

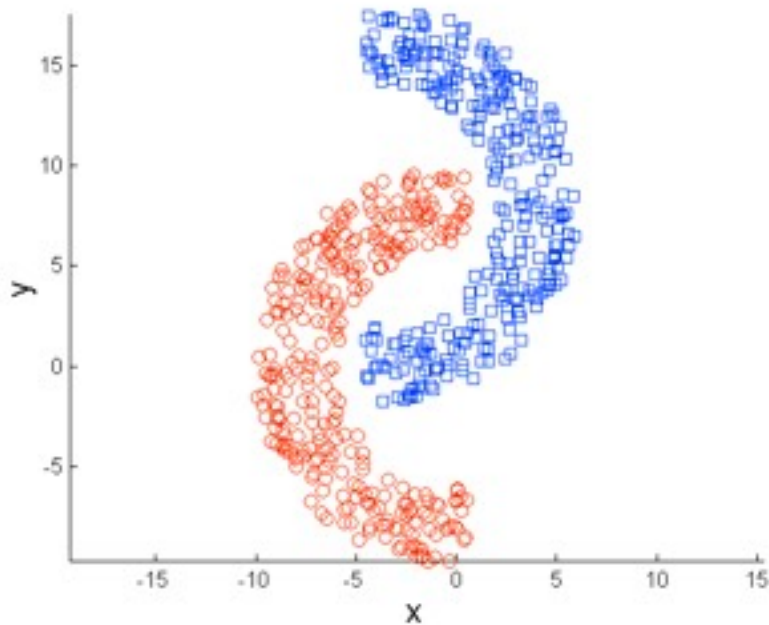


Original Points

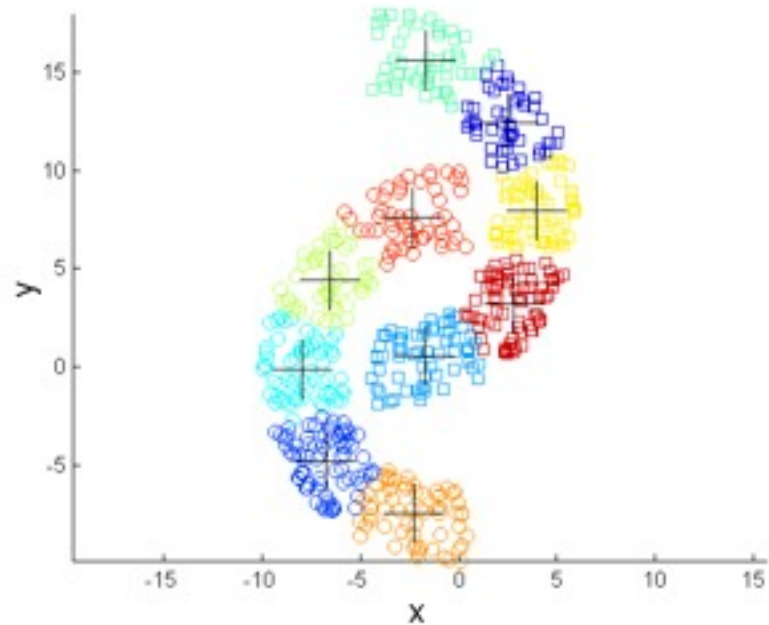


K-means Clusters

Overcoming K-means Limitations



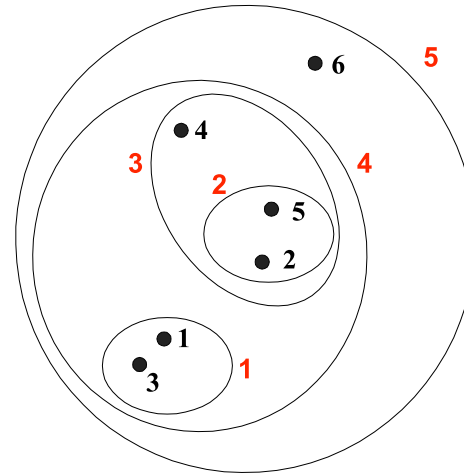
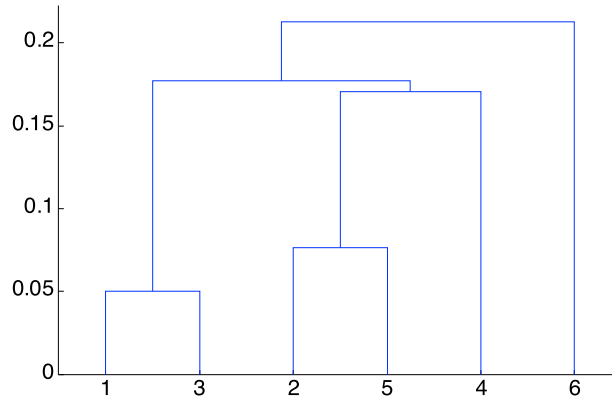
Original Points



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

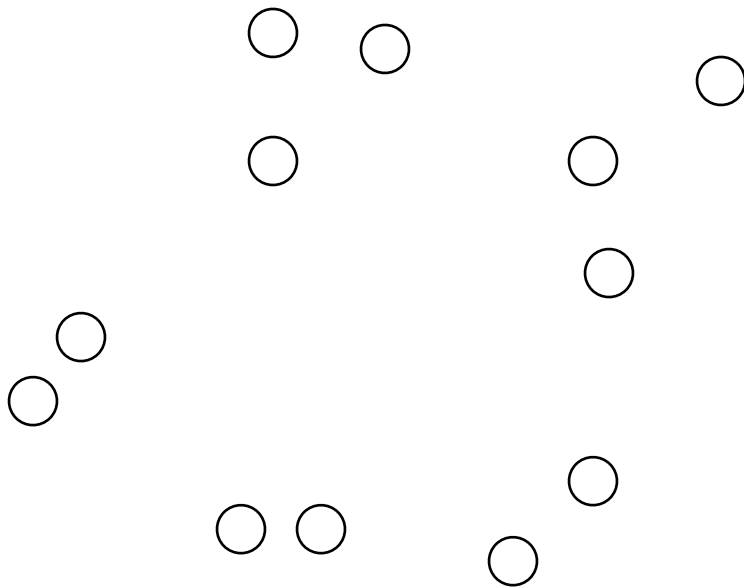
Agglomerative Clustering Algorithm

- | 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 $n \times n$

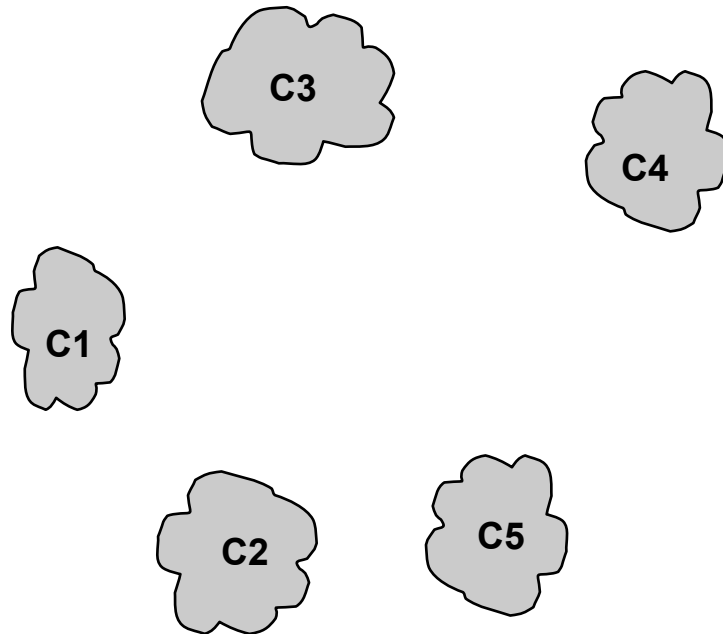


	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Distance Matrix

Intermediate Situation

- After some merging steps, we have some clusters



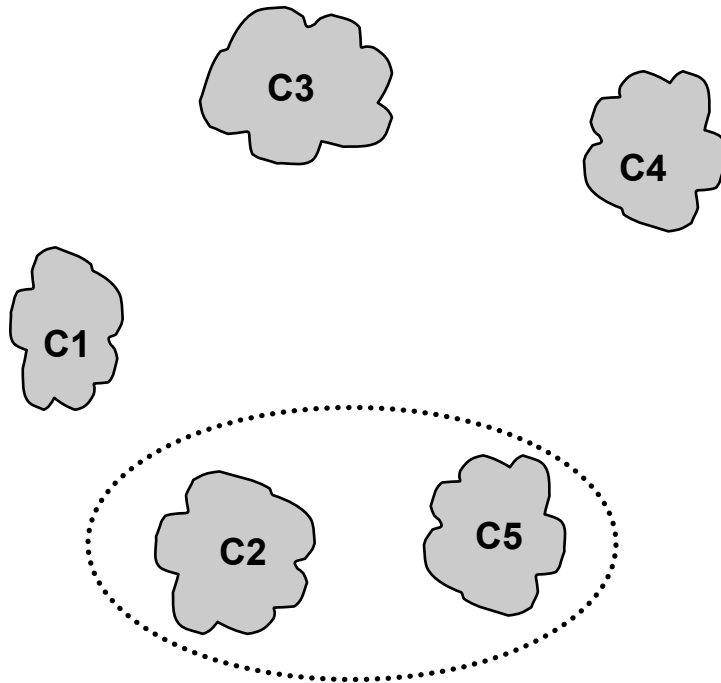
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Distance Matrix



Intermediate Situation

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

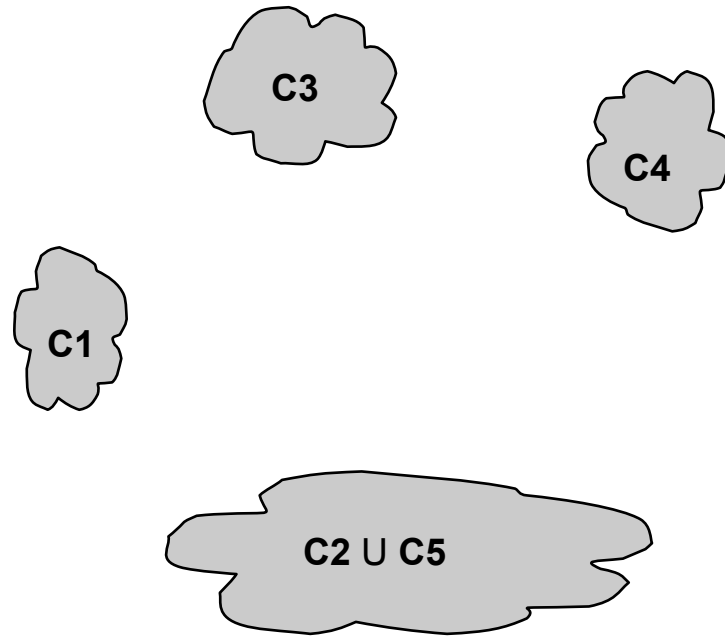


	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Distance Matrix

After Merging

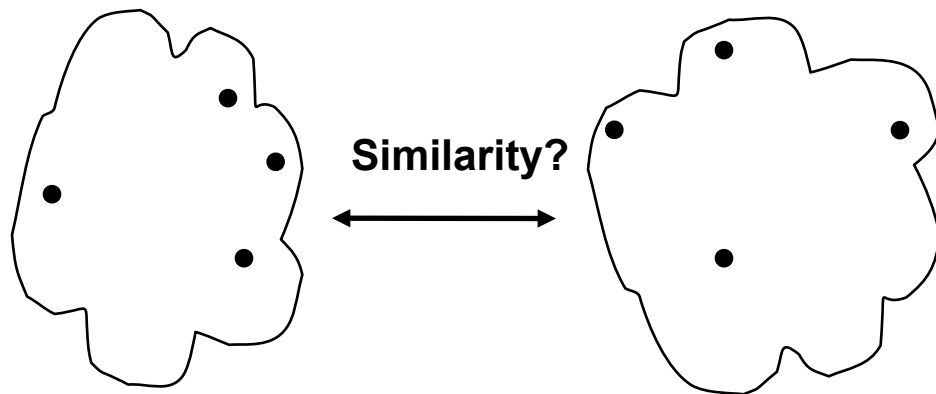
- The question is “How do we update the distance matrix?”



		C2 U C5			
		C1	C5	C3	C4
C2 U C5	C1		?		
	C5	?	?	?	?
	C3		?		
	C4		?		

Distance Matrix

How to Define Inter-Cluster Similarity

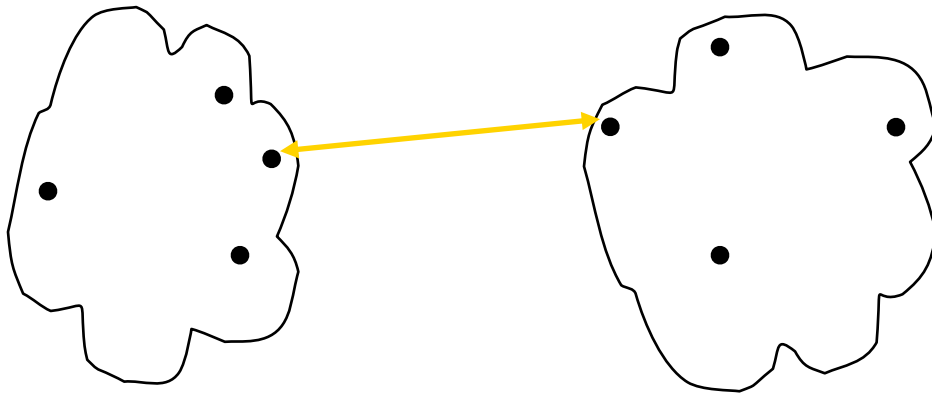


- | MIN
- | MAX
- | Group Average
- | Distance Between Centroids
- | Other methods driven by an objective function
 - Ward's Method uses squared error

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

Distance Matrix

How to Define Inter-Cluster Similarity

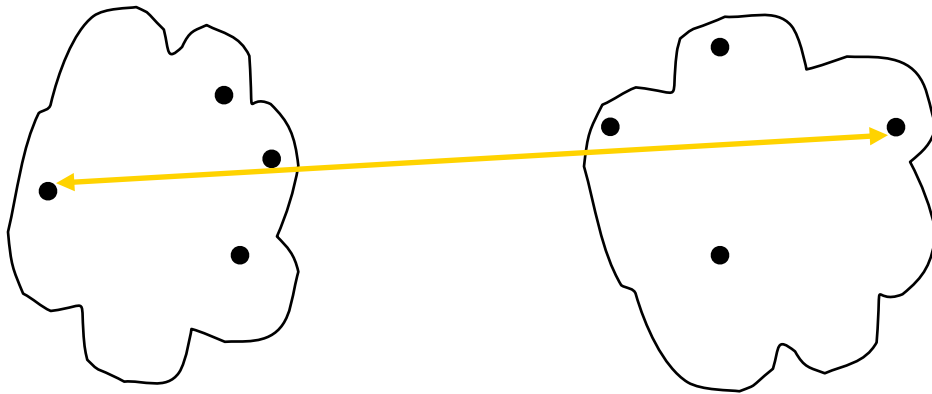


- | MIN
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	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Distance Matrix

How to Define Inter-Cluster Similarity

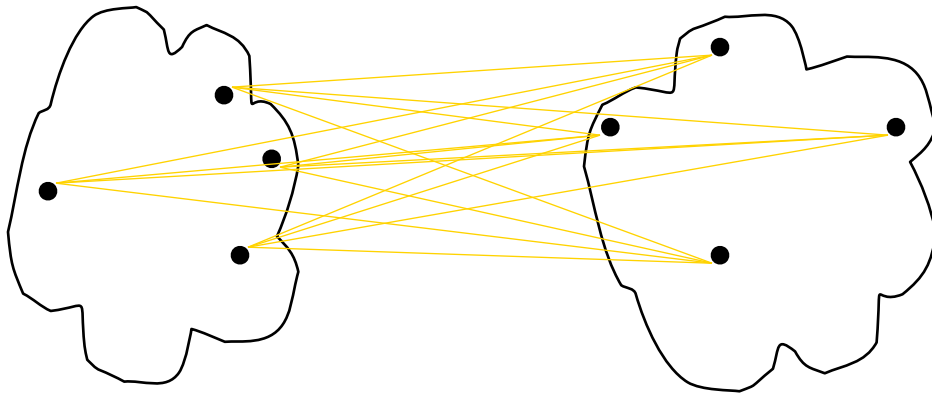


- | MIN
- | MAX
- | Group Average
- | Distance Between Centroids
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 - Ward's Method uses squared error

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

Distance Matrix

How to Define Inter-Cluster Similarity

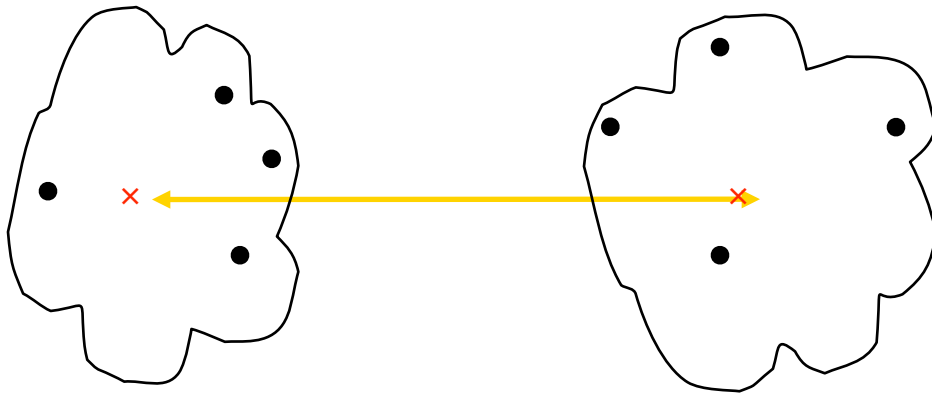


- | MIN
- | MAX
- | **Group Average**
- | Distance Between Centroids
- | Other methods driven by an objective function
 - Ward's Method uses squared error

	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
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	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

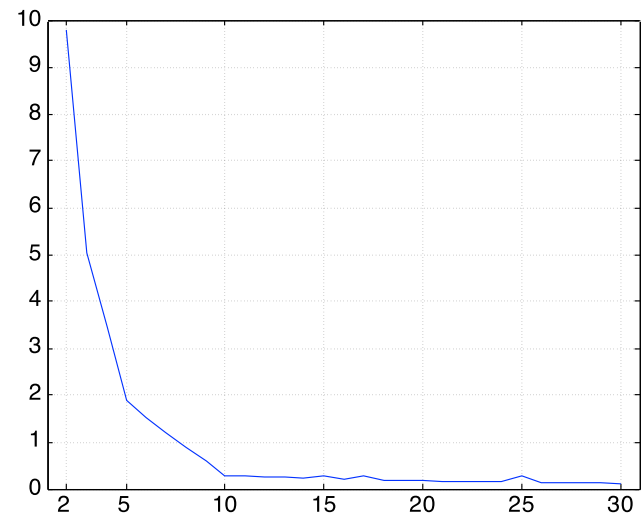
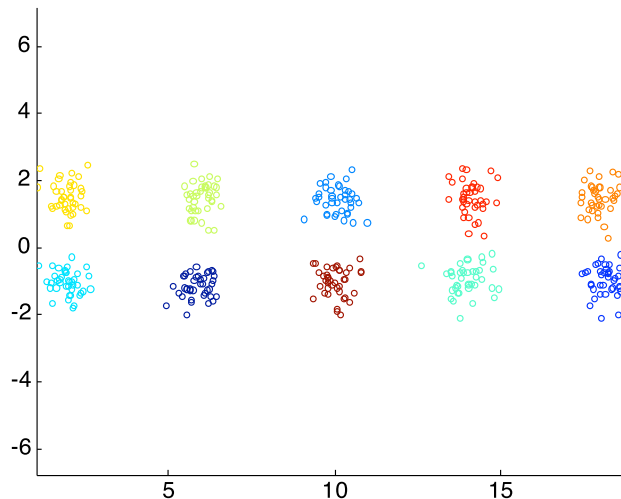
Measures of Cluster Validity

- | 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



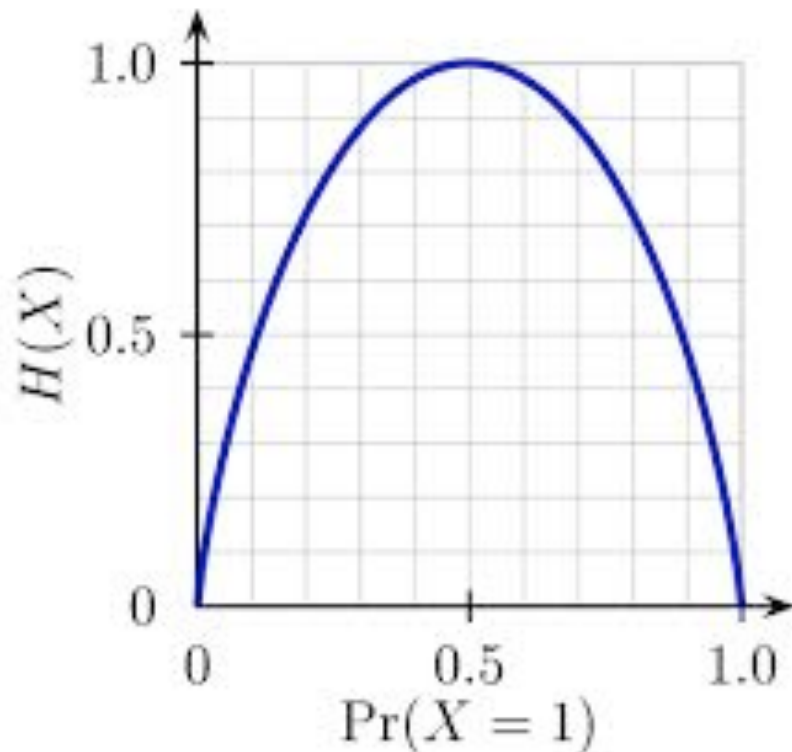
Entropy: definition

- | 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

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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:

$$\sum_j \frac{m_j}{m} e_j$$

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

Final Comment on Cluster Validity

“The validation of clustering structures is the most difficult and frustrating part of cluster analysis. Without a strong effort in this direction, cluster analysis will remain a black art accessible only to those true believers who have experience and great courage.”

Algorithms for Clustering Data, Jain and Dubes

k-means++

Algorithm 1 *k*-means++(*k*) initialization.

- 1: $\mathcal{C} \leftarrow$ sample a point uniformly at random from X
 - 2: **while** $|\mathcal{C}| < k$ **do**
 - 3: Sample $x \in X$ with probability $\frac{d^2(x, \mathcal{C})}{\Phi_X(\mathcal{C})}$
 - 4: $\mathcal{C} \leftarrow \mathcal{C} \cup \{x\}$
 - 5: **end while**
-

where:

$$d(x, \mathcal{C}) = \min_{c \in \mathcal{C}} d(x, c), \quad \Phi_X(\mathcal{C}) = \sum_{x \in X} d^2(x, \mathcal{C})$$

$d^2(x, \mathcal{C})$ measures how “good” is the clustering for point x .
Points that are *relatively* far away from “their” centroids will be selected with higher probability.

K-means ++

- | K-means++:
 - Initialize the centroids as in Algorithm 1
 - Run K-means algorithm to improve the clustering.
- | **Theorem:** Let $C_{\text{KM++}}$ be the clustering produced by the K-means++ algorithm, let C_{opt} be an optimal clustering (with minimum SSE among all possible clusterings). Then, $\text{SSE}(C_{\text{KM++}}) \leq 8 \cdot (\ln k + 2) \cdot \text{SSE}(C_{\text{opt}})$, on expectation (average).
- | **Exercise:** give an example where k-means computes an approximation “worse” than k-means++.

Algorithms

- K-means:
 - ◆ no guarantees on the quality of the solution
 - ◆ it always terminates
 - ◆ running time could be exponential but it is OK in practice
- K-means++
 - ◆ it always terminates
 - ◆ $O(\log k)$ -approximation on the quality of the solution.
 - ◆ In practice the advantage is noticeable for large k