INTRODUCTION TO DATA ANALYTICS

Cluster Analysis

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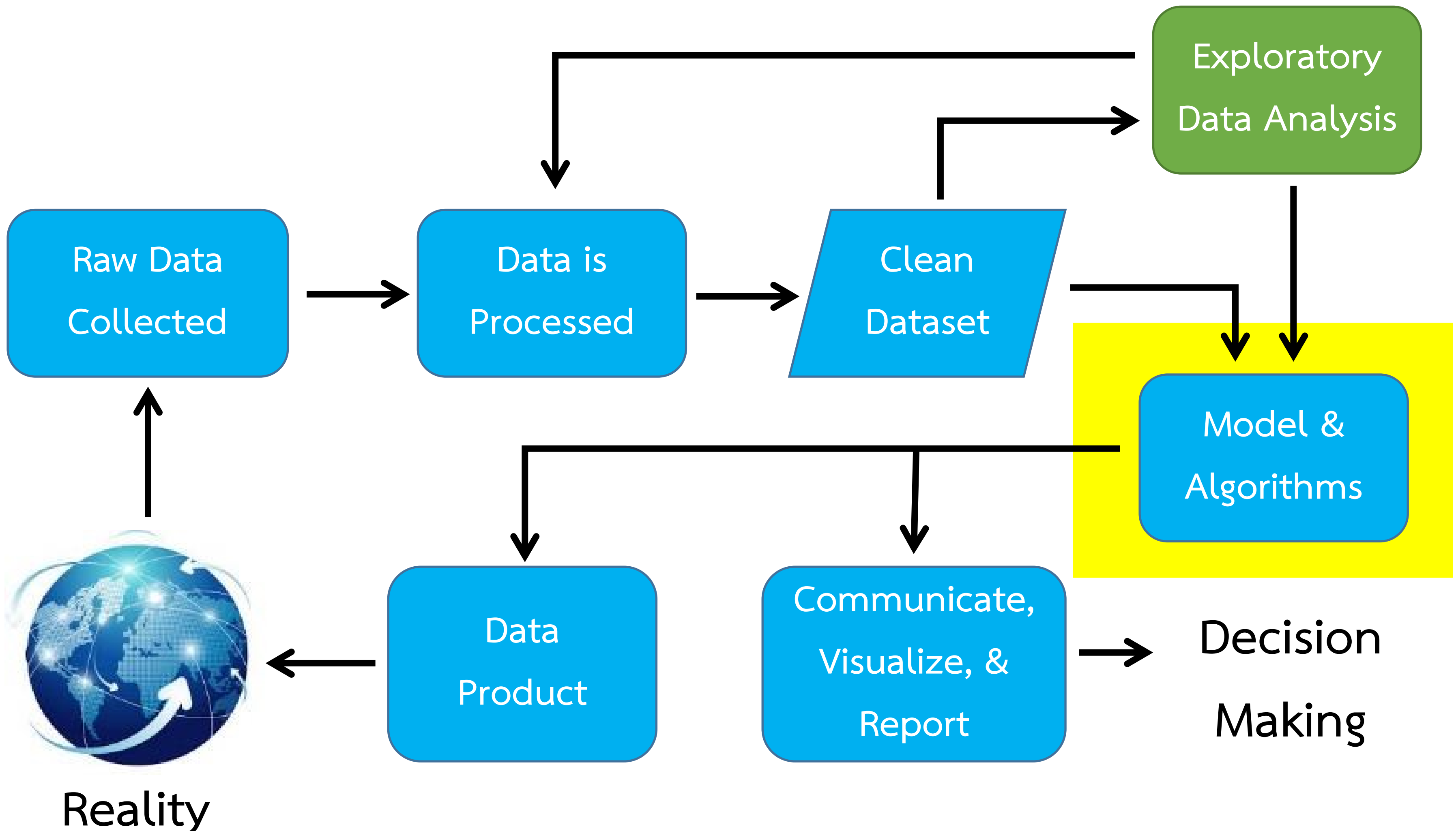
Agenda

- Clustering
- K-Means
- DBSCAN
- Cluster Validation
- Dimensionality Reduction

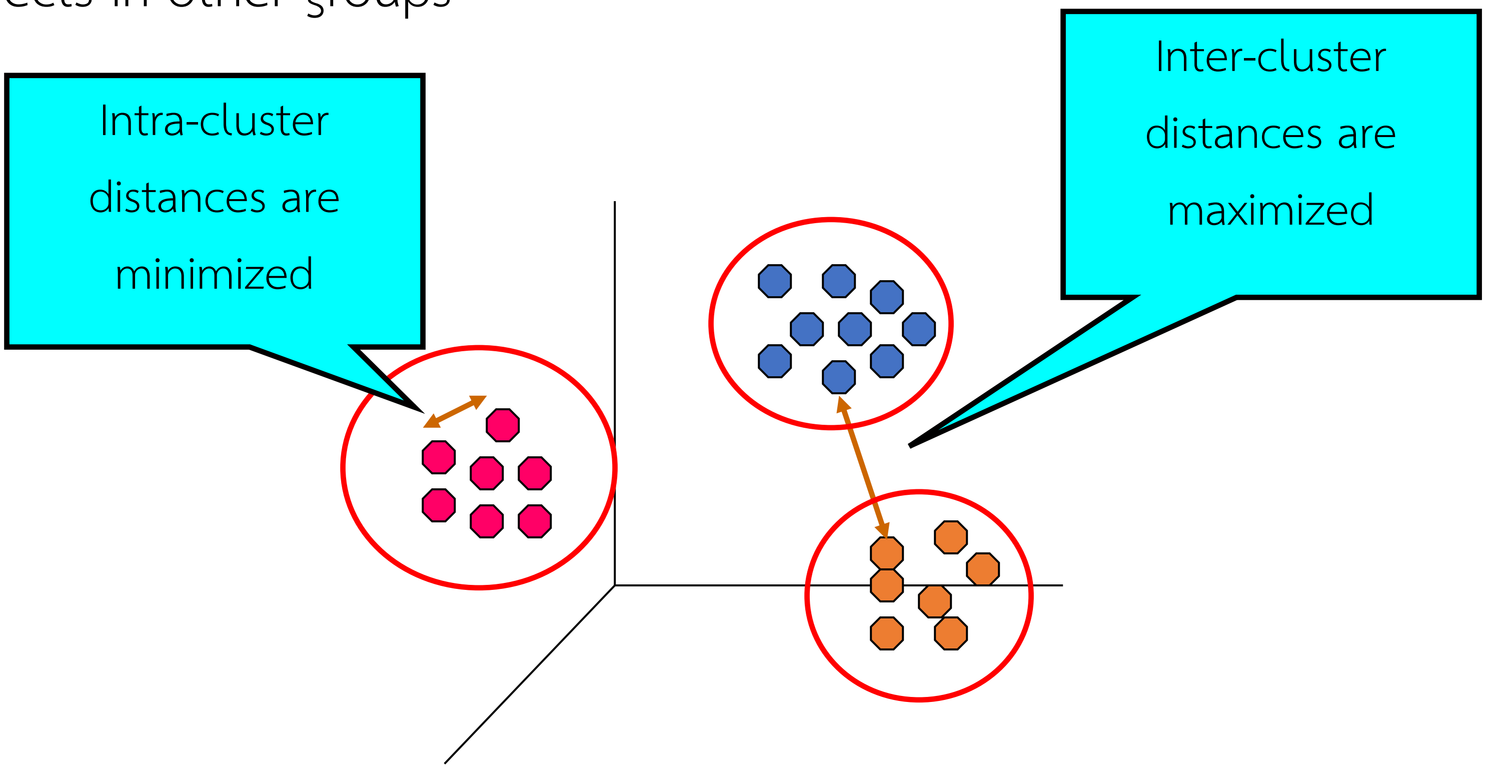
Data Science Process



Clustering

What is a Clustering?

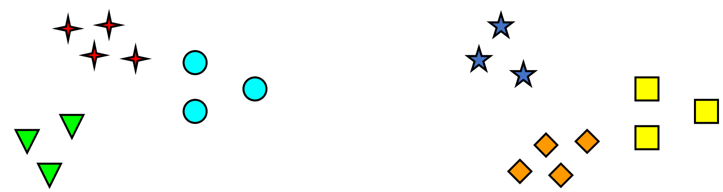
- In general a grouping of objects such that the objects in a group (cluster) are similar (or related) to one another and different from (or unrelated to) the objects in other groups



Ref: • Min-Hashing, “Locality Sensitive Hashing Clustering”

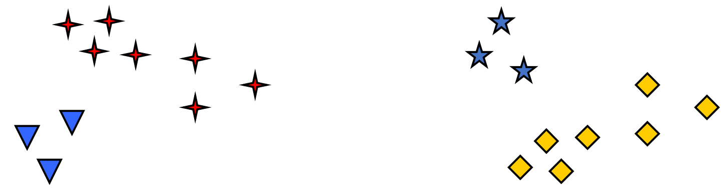
Notion of a Cluster can be Ambiguous

How many clusters?



6 Clusters

2 Clusters



4 Clusters

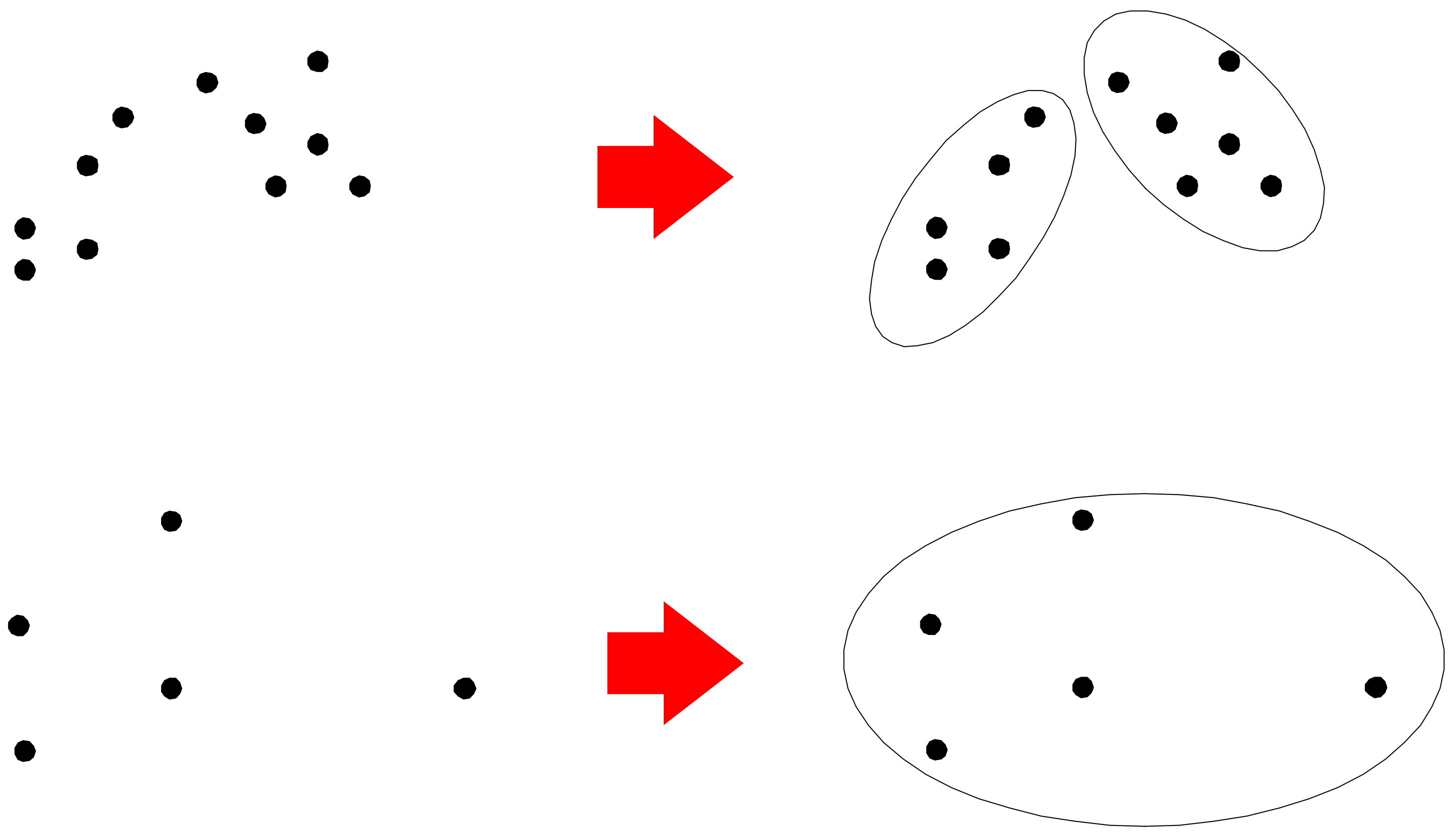
Ref: • Min-Hashing, “Locality Sensitive Hashing Clustering”

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 subsets (clusters) such that each data object is in exactly one subset
- Hierarchical clustering
  - A set of nested clusters organized as a hierarchical tree

Ref: • Min-Hashing, "Locality Sensitive Hashing Clustering"

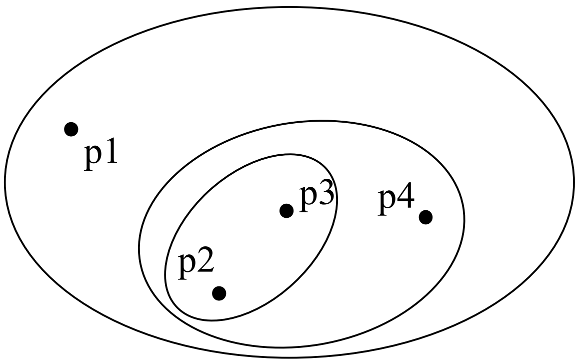
Partitional Clustering



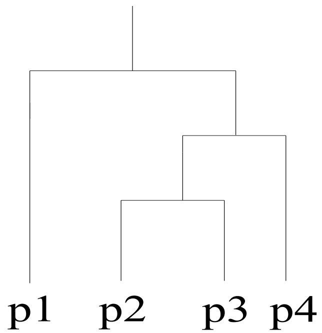
Original Points A Partitional Clustering

Ref: • Min-Hashing, "Locality Sensitive Hashing Clustering"

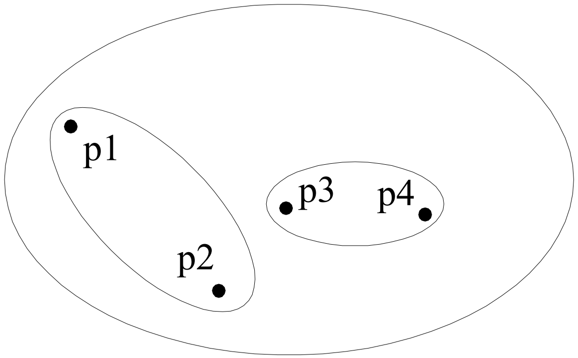
Hierarchical Clustering



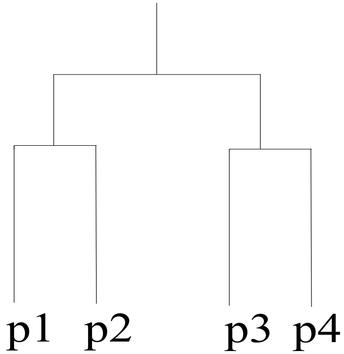
Traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Hierarchical Clustering



Non-traditional Dendrogram

Ref: • Min-Hashing, "Locality Sensitive Hashing Clustering"

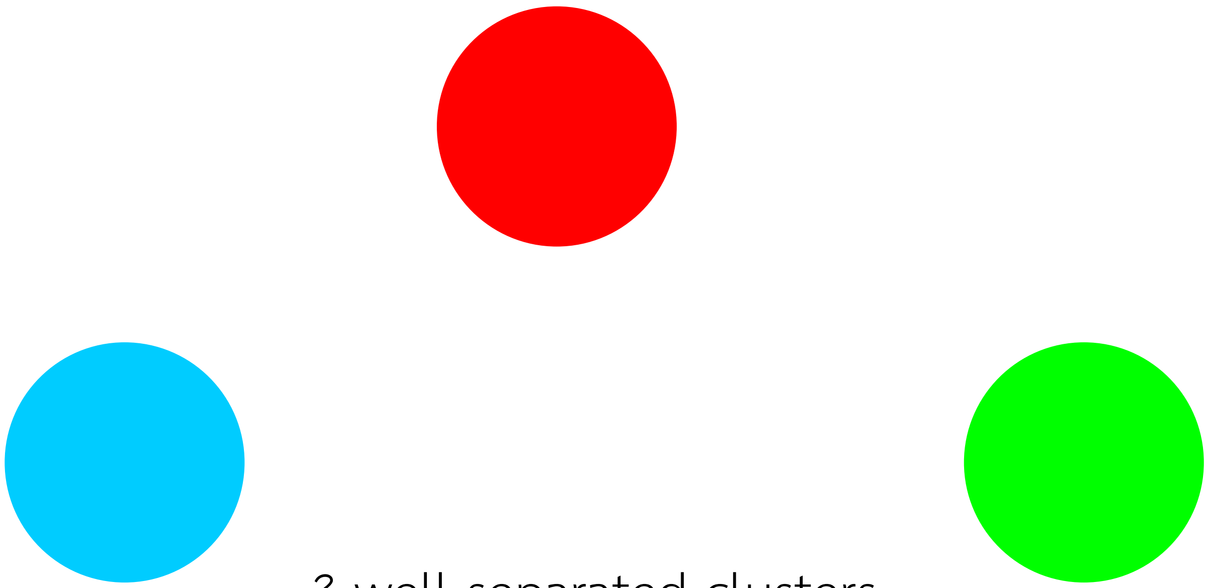
Other types of clustering

- **Exclusive** (or non-overlapping) versus **non-exclusive** (or overlapping)
  - In non-exclusive clusterings, points may belong to multiple clusters.
    - Points that belong to multiple classes, or ‘border’ points
- **Fuzzy** (or soft) versus **non-fuzzy** (or hard)
  - In fuzzy clustering, a point belongs to every cluster with some weight between 0 and 1
    - Weights usually must sum to 1 (often interpreted as probabilities)
- **Partial** versus **complete**
  - In some cases, we only want to cluster some of the data

Ref: • Min-Hashing, “Locality Sensitive Hashing Clustering”

Types of Clusters: Well-Separated

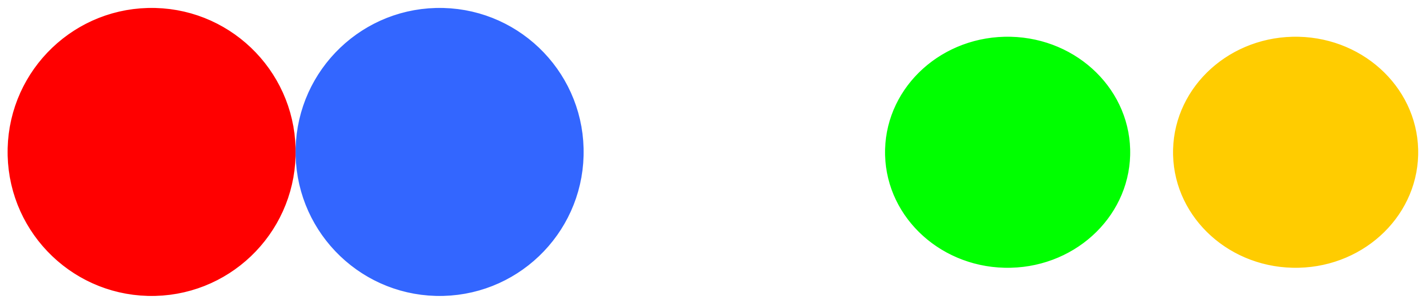
- Well-Separated Clusters:
  - A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.



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 minimizer of distances from all the points in the cluster, or a medoid, the most "representative" point of a cluster

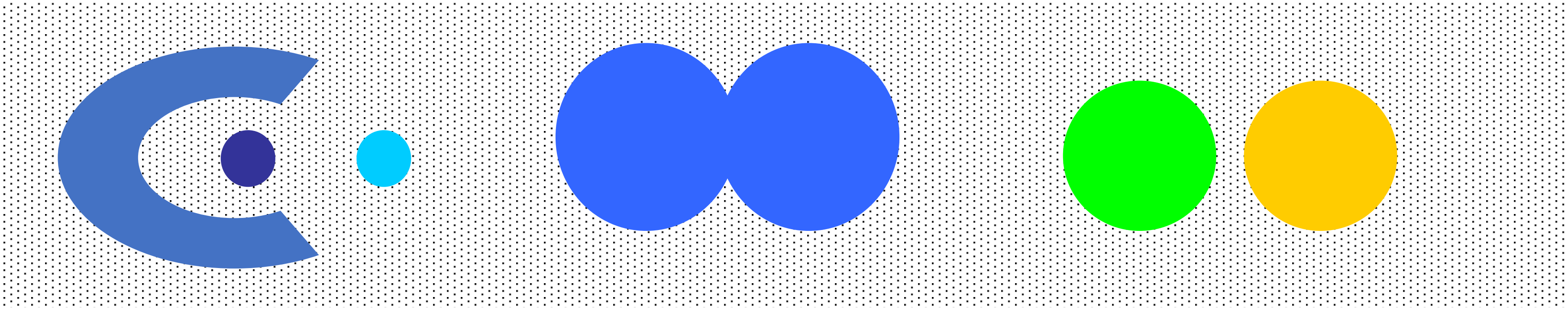


4 center-based clusters

Ref: • Min-Hashing, "Locality Sensitive Hashing Clustering"

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

Ref: • Min-Hashing, “Locality Sensitive Hashing Clustering”

Clustering Algorithms

- K-Means
- DBSCAN
- Hierarchical clustering
- PAM, CLARANS: Solutions for the k-medoids problem
- BIRCH: Constructs a hierarchical tree that acts a summary of the data, and then clusters the leaves.
- MST: Clustering using the Minimum Spanning Tree.
- ROCK: clustering categorical data by neighbor and link analysis
- LIMBO, COOLCAT: Clustering categorical data using information theoretic tools.
- CURE: Hierarchical algorithm uses different representation of the cluster
- CHAMELEON: Hierarchical algorithm uses closeness and interconnectivity for merging

Ref: • Min-Hashing, “Locality Sensitive Hashing Clustering”

K-Means

K-means Clustering

- Partitional clustering approach
- Each cluster is associated with a centroid (center point)
- Each point is assigned to the cluster with the closest centroid
- Number of clusters, K, must be specified
- The objective is to minimize the sum of distances of the points to their respective centroid

Ref: • Min-Hashing, “Locality Sensitive Hashing Clustering”

K-means Clustering

- **Problem:** Given a set X of n points in a d-dimensional space and an integer K group the points into K clusters $C = \{C_1, C_2, \ldots, C_k\}$ such that

$$Cost(C) = \sum_{i=1}^{k} \sum_{x \in C_i} dist(x, c)$$

is minimized, where c_i is the centroid of the points in cluster C_i

Ref: • Min-Hashing, "Locality Sensitive Hashing Clustering"

K-means Algorithm

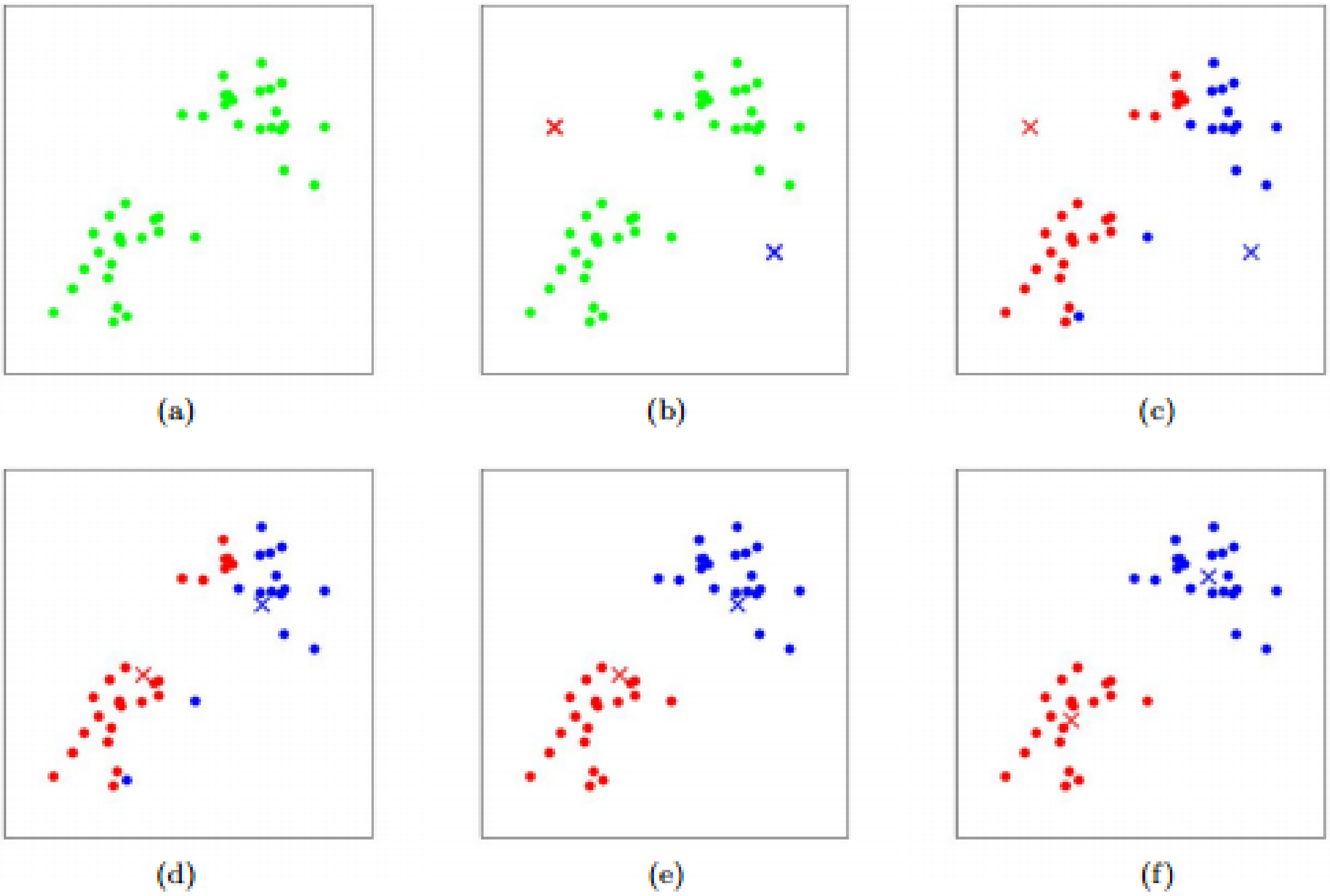
- Also known as Lloyd's algorithm.
- K-means is sometimes synonymous with this algorithm

```
Select K points as the initial centroids.
repeat
    Form K clusters by assigning all points to the closest centroid.
    Recompute the centroid of each cluster.
until The centroids don't change
```

- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.

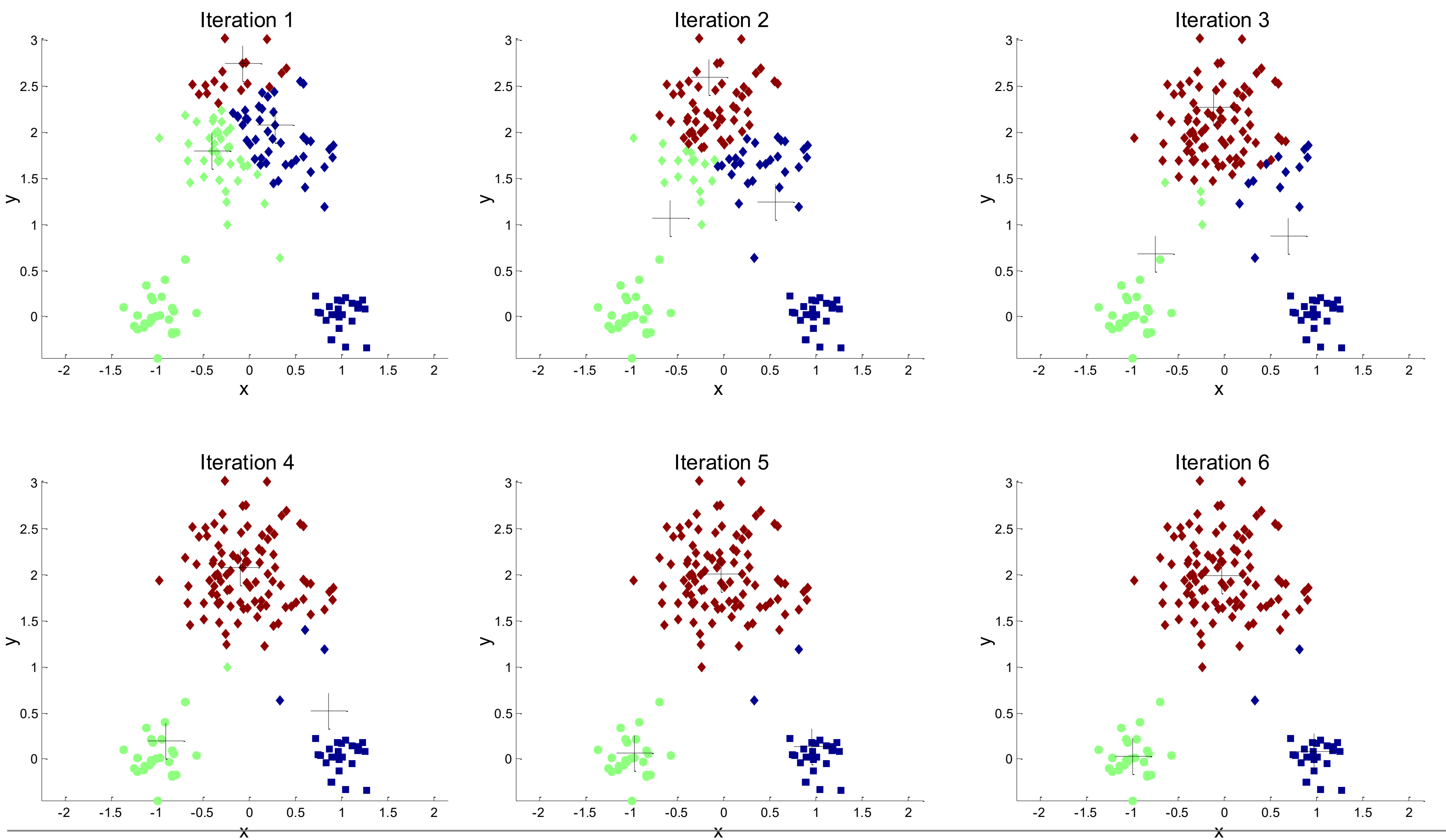
Ref: • Min-Hashing, "Locality Sensitive Hashing Clustering"

K-means: Steps



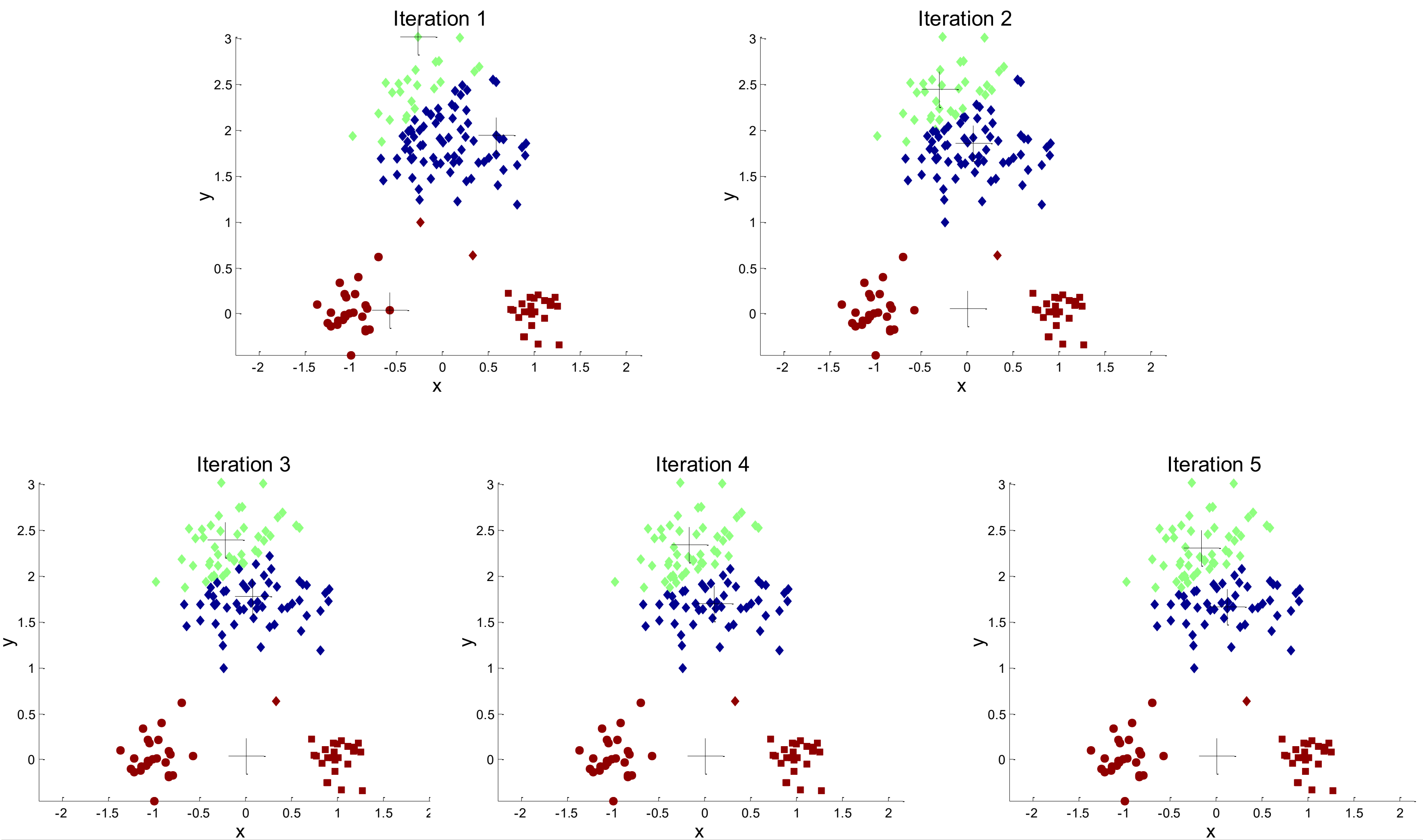
Ref: • http://stanford.edu/~cpiech/cs221/handouts/kmeans.html

Importance of Choosing Initial Centroids (A)



Ref: • Min-Hashing, “Locality Sensitive Hashing Clustering”

Importance of Choosing Initial Centroids (B)



Ref: • Min-Hashing, “Locality Sensitive Hashing Clustering”

Dealing with Initialization

- Do multiple runs and select the clustering with the smallest error
- Select original set of points by methods other than random . E.g., pick the most distant (from each other) points as cluster centers

Ref: • Min-Hashing, “Locality Sensitive Hashing Clustering”

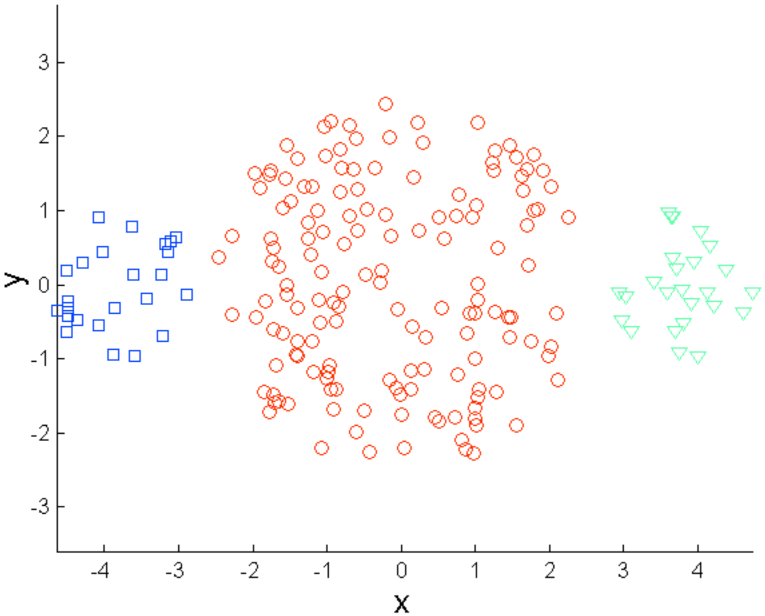
Limitations of K-means

- K-means has problems when clusters are of different
  - Sizes
  - Densities
  - Non-globular shapes

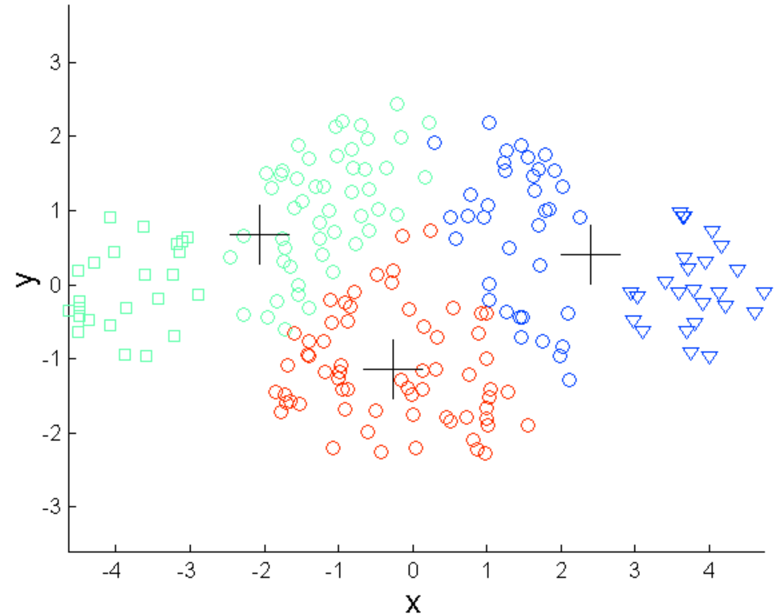
- K-means has problems when the data contains outliers.

Ref: • Min-Hashing, "Locality Sensitive Hashing Clustering"

Limitations of K-means: Differing Sizes



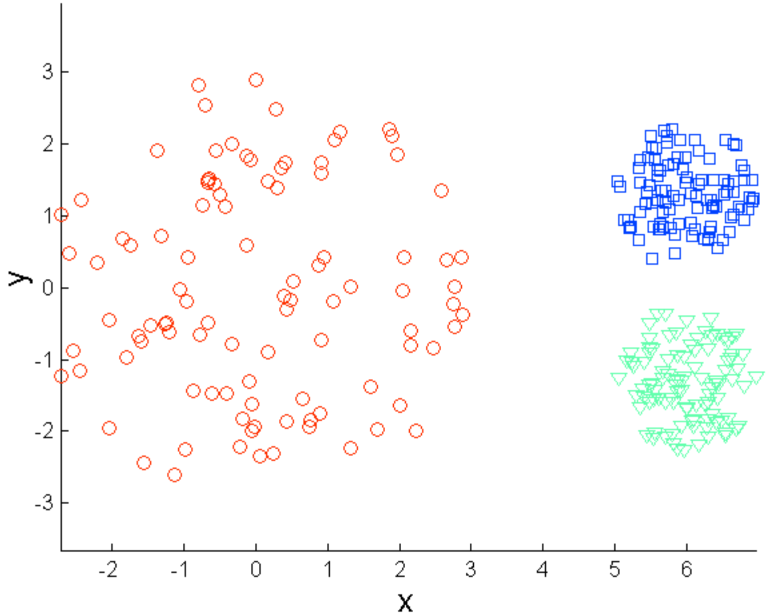
Original Points



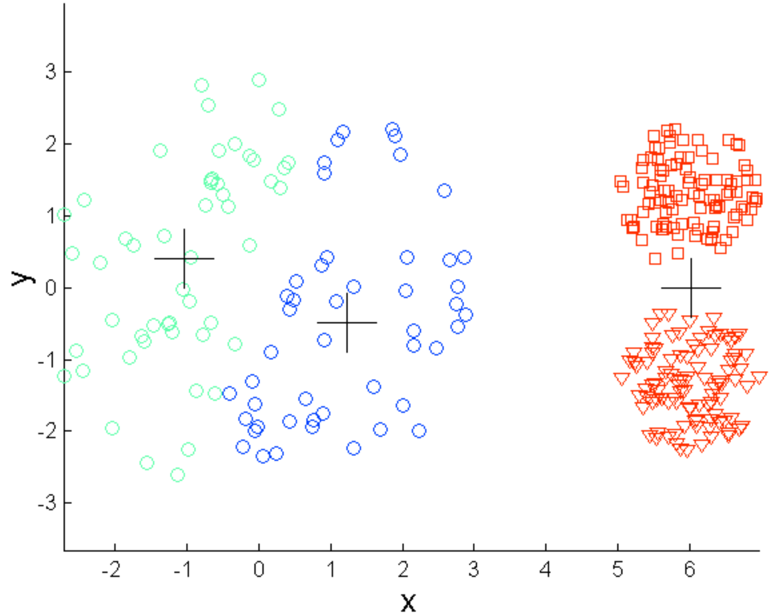
K-means (3 Clusters)

Ref: • Min-Hashing, "Locality Sensitive Hashing Clustering"

Limitations of K-means: Differing Density



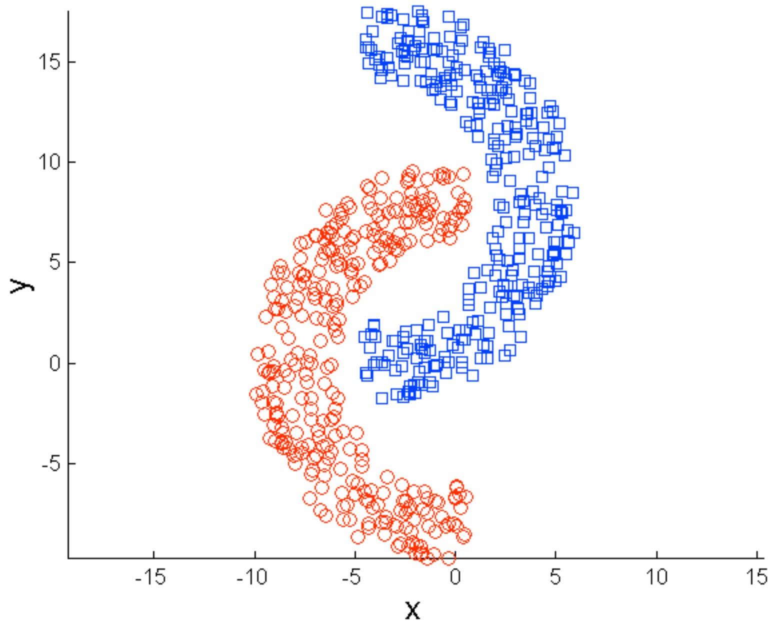
Original Points



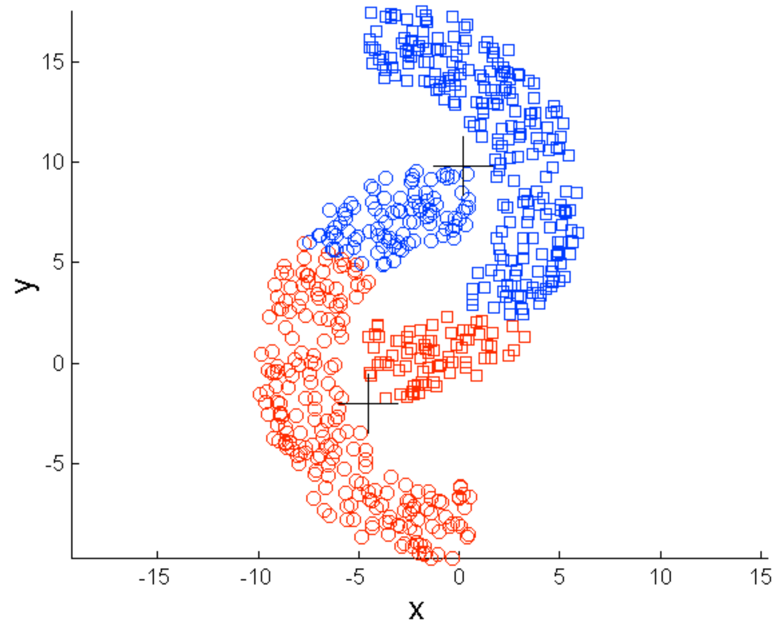
K-means (3 Clusters)

Ref: • Min-Hashing, "Locality Sensitive Hashing Clustering"

Limitations of K-means: Non-globular Shapes



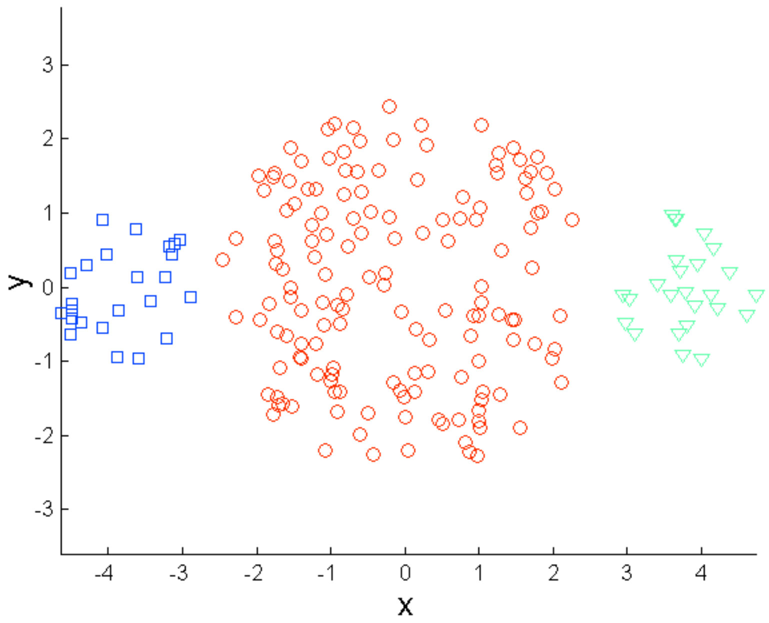
Original Points

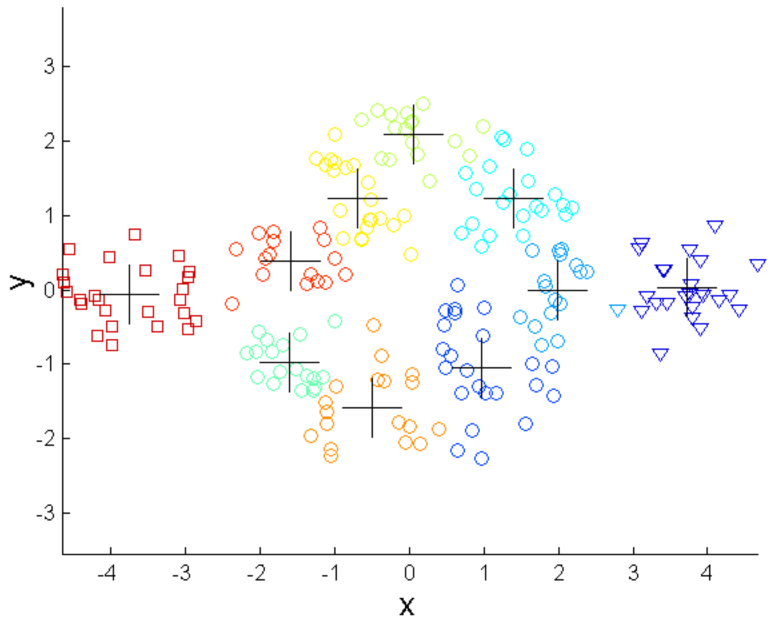


K-means (2 Clusters)

Ref: • Min-Hashing, "Locality Sensitive Hashing Clustering"

Overcoming K-means Limitations





Original Points

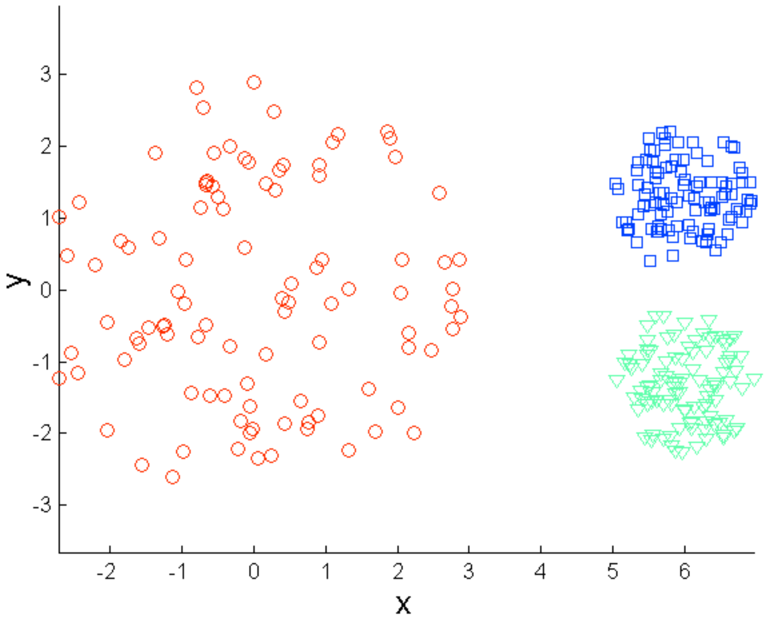
K-means Clusters

One solution is to use many clusters.

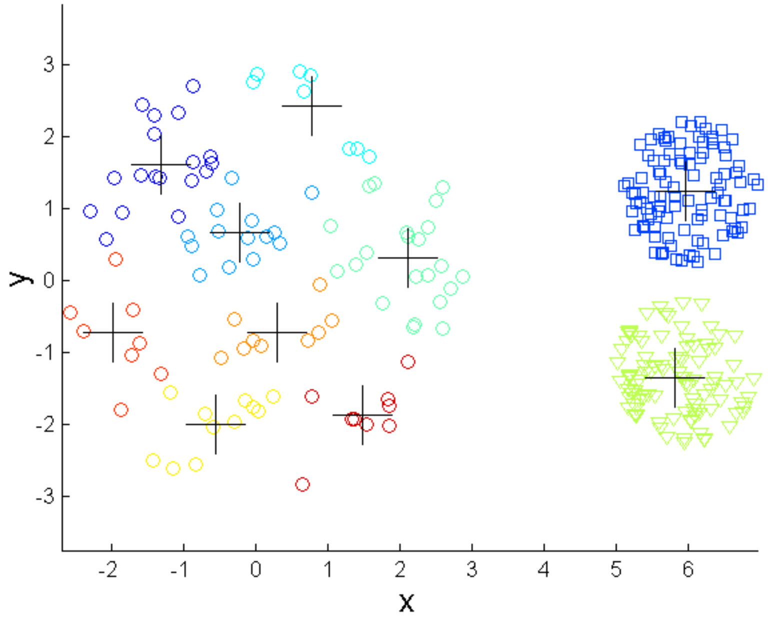
Find parts of clusters, but need to put together.

Ref: • Min-Hashing, "Locality Sensitive Hashing Clustering"

Overcoming K-means Limitations



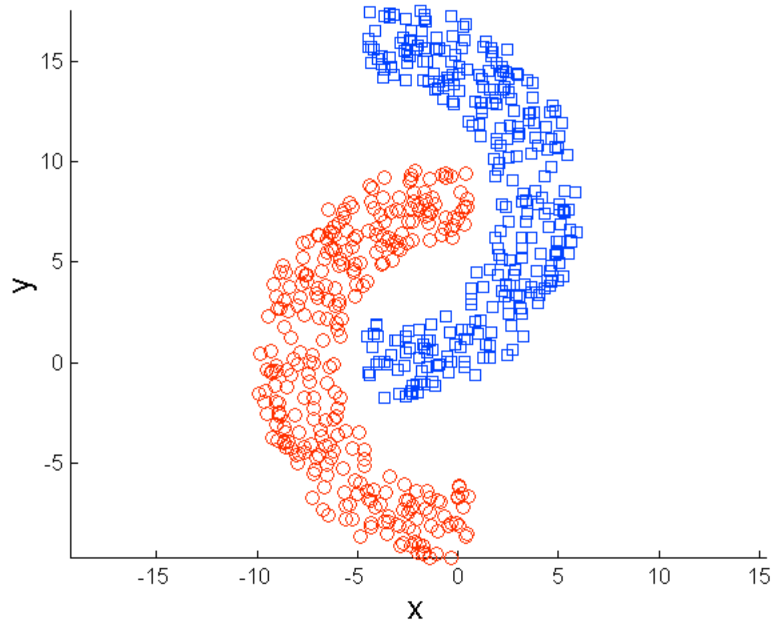
Original Points



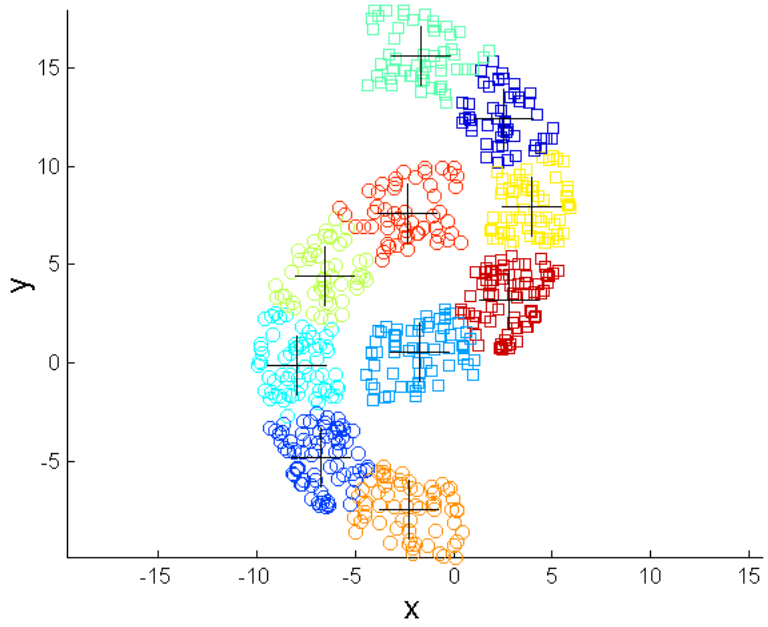
K-means Clusters

Ref: • Min-Hashing, "Locality Sensitive Hashing Clustering"

Overcoming K-means Limitations



Original Points



K-means Clusters

Ref: • Min-Hashing, "Locality Sensitive Hashing Clustering"

Variations

- K-medoids
  - Similar problem definition as in K-means, but the centroid of the cluster is defined to be one of the points in the cluster (the medoid).

- K-centers
  - Similar problem definition as in K-means, but the goal now is to minimize the maximum diameter of the clusters
    (diameter of a cluster is maximum distance between any two points in the cluster).

Ref: • Min-Hashing, "Locality Sensitive Hashing Clustering"

Python

```
>>> from sklearn.cluster import KMeans
>>> import numpy as np
>>> X = np.array([[1, 2], [1, 4], [1, 0],
...                [4, 2], [4, 4], [4, 0]])
>>> kmeans = KMeans(n_clusters=2, random_state=0).fit(X)
>>> kmeans.labels_
array([0, 0, 0, 1, 1, 1], dtype=int32)
>>> kmeans.predict([[0, 0], [4, 4]])
array([0, 1], dtype=int32)
>>> kmeans.cluster_centers_
array([[ 1.,  2.],
       [ 4.,  2.]])
```

Ref: • http://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html

DBSCAN

DBSCAN: Density-Based Clustering

- DBSCAN is a Density-Based Clustering algorithm
- Reminder: In density based clustering we partition points into dense regions separated by not-so-dense regions.
- Important Questions:
  - How do we measure density?
  - What is a dense region?
- DBSCAN:
  - Density at point p: number of points within a circle of radius Eps
  - Dense Region: A circle of radius Eps that contains at least MinPts points

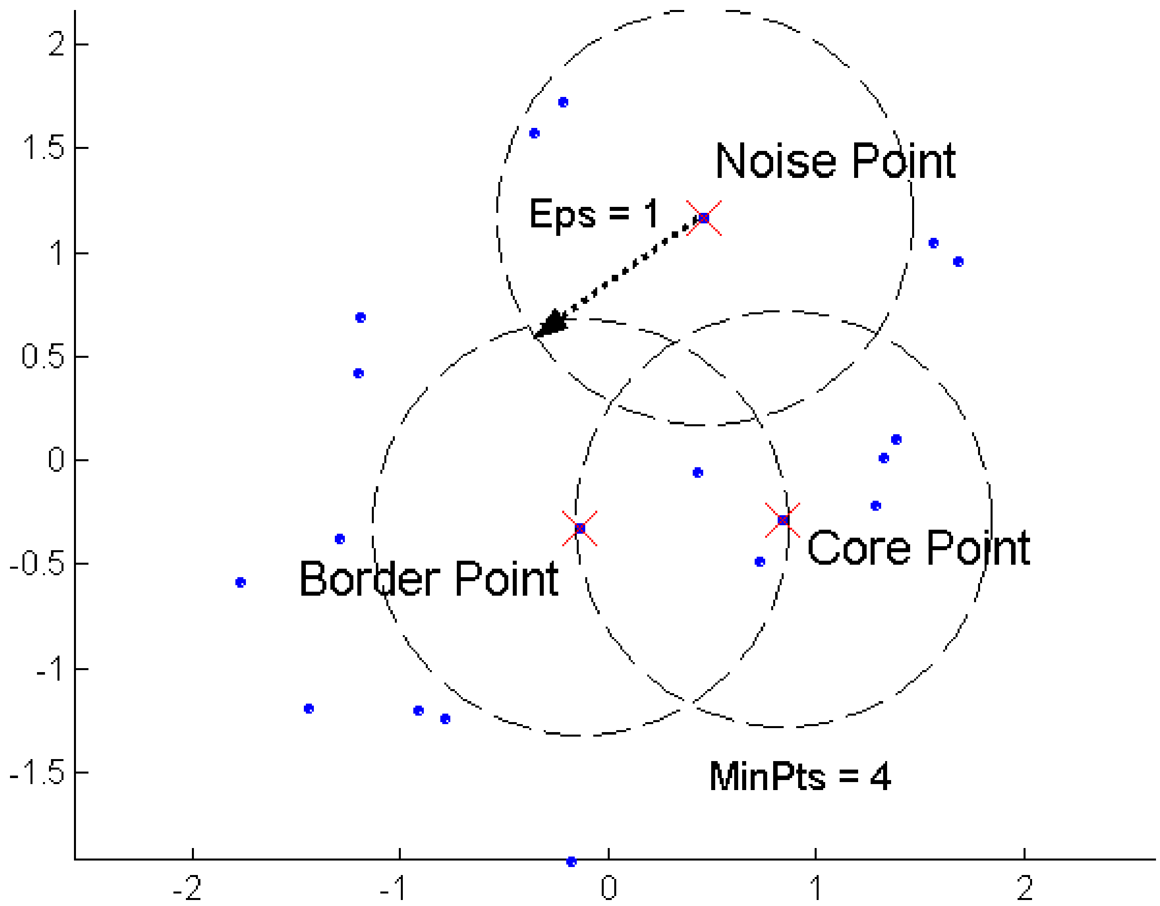
Ref: • Tan, Steinbach, Kumar, “Data Mining”

DBSCAN

- Characterization of points
  - A point is a core point if it has more than a specified number of points (MinPts) within Eps
    - These points belong in a dense region and are at the interior of a cluster
  - A border point has fewer than MinPts within Eps, but is in the neighborhood of a core point.
  - A noise point is any point that is not a core point or a border point.

Ref: • Tan, Steinbach, Kumar, "Data Mining"

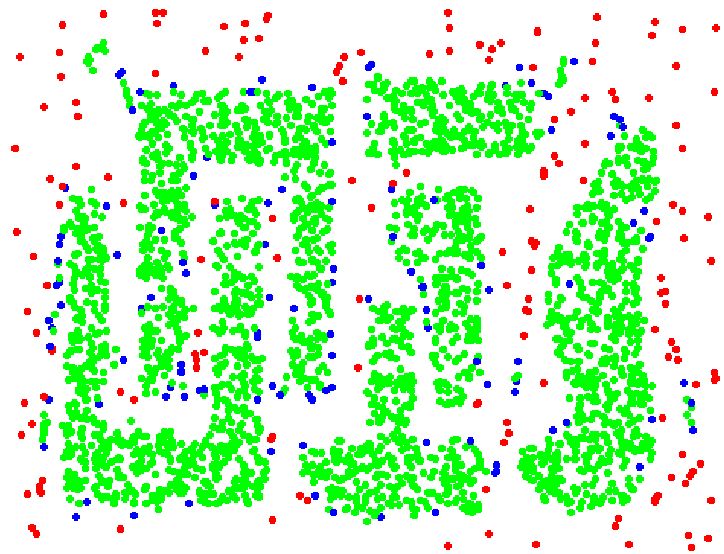
DBSCAN: Core, Border, and Noise Points



Ref: • Tan, Steinbach, Kumar, “Data Mining”

DBSCAN: Core, Border, and Noise Points

Original Points



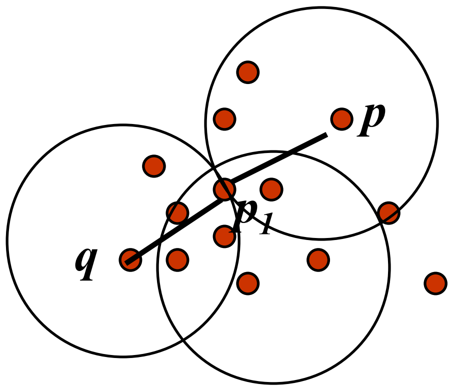
Point types: core, border and noise

Eps = 10, MinPts = 4

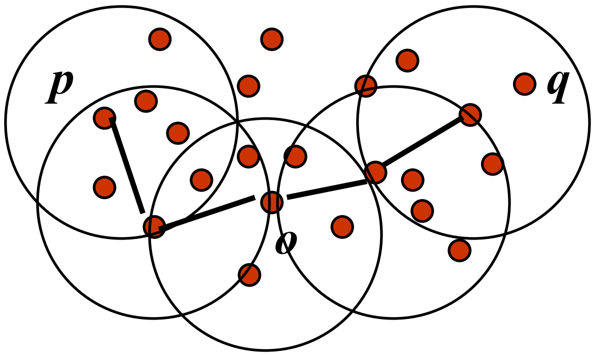
Ref: • Tan, Steinbach, Kumar, “Data Mining”

Density-Connected points

- Density edge
  - We place an edge between two core points q and p if they are within distance Eps.



- Density-connected
  - A point p is density-connected to a point q if there is a path of edges from p to q



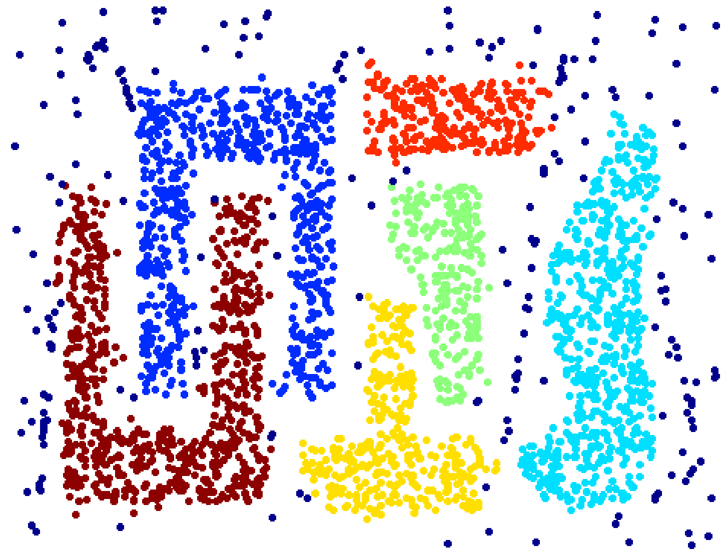
DBSCAN Algorithm

- Label points as core, border and noise
- Eliminate noise points
- For every core point p that has not been assigned to a cluster
  - Create a new cluster with the point p and all the points that are density-connected to p.
- Assign border points to the cluster of the closest core point.

Ref: • Tan, Steinbach, Kumar, "Data Mining"

When DBSCAN Works Well

Original Points



Clusters

- Resistant to Noise
- Can handle clusters of different shapes and sizes

Ref: • Tan, Steinbach, Kumar, "Data Mining"

Cluster Validation

Different Aspects of Cluster Validation

1. Determining the clustering tendency of a set of data, i.e., distinguishing whether non-random structure actually exists in the data.
2. Comparing the results of a cluster analysis to externally known results, e.g., to externally given class labels.
3. Evaluating how well the results of a cluster analysis fit the data *without* reference to external information.
   - Use only the data
4. Comparing the results of two different sets of cluster analyses to determine which is better.
5. Determining the 'correct' number of clusters.

For 2, 3, and 4, we can further distinguish whether we want to evaluate the entire clustering or just individual clusters.

Ref: • Tan, Steinbach, Karpatne, Kumar, "Introduction to Data Mining (Second Edition)"

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: Used to compare two different clusterings or clusters.
    - Often 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
  - However, sometimes criterion is the general strategy and index is the numerical measure that implements the criterion.

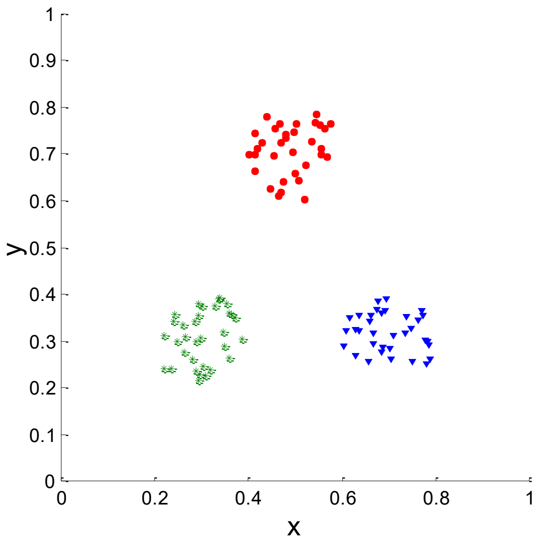
Ref: • Tan, Steinbach, Karpatne, Kumar, "Introduction to Data Mining (Second Edition)"

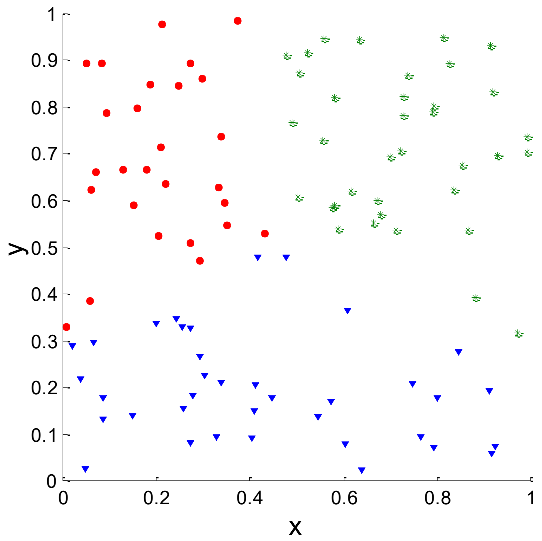
Measuring Cluster Validity Via Correlation

- Two matrices
  - Proximity Matrix
  - Ideal Similarity Matrix
    - One row and one column for each data point
    - An entry is 1 if the associated pair of points belong to the same cluster
    - An entry is 0 if the associated pair of points belongs to different clusters
- Compute the correlation between the two matrices
  - Since the matrices are symmetric, only the correlation between n(n-1) / 2 entries needs to be calculated.
- High correlation indicates that points that belong to the same cluster are close to each other.
- Not a good measure for some density or contiguity based clusters.

Measuring Cluster Validity Via Correlation

- Correlation of ideal similarity and proximity matrices for the K-means clusterings of the following two data sets.



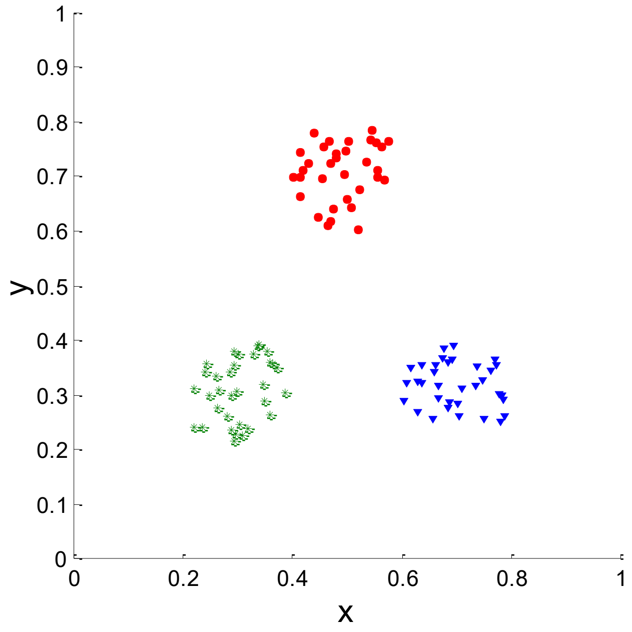


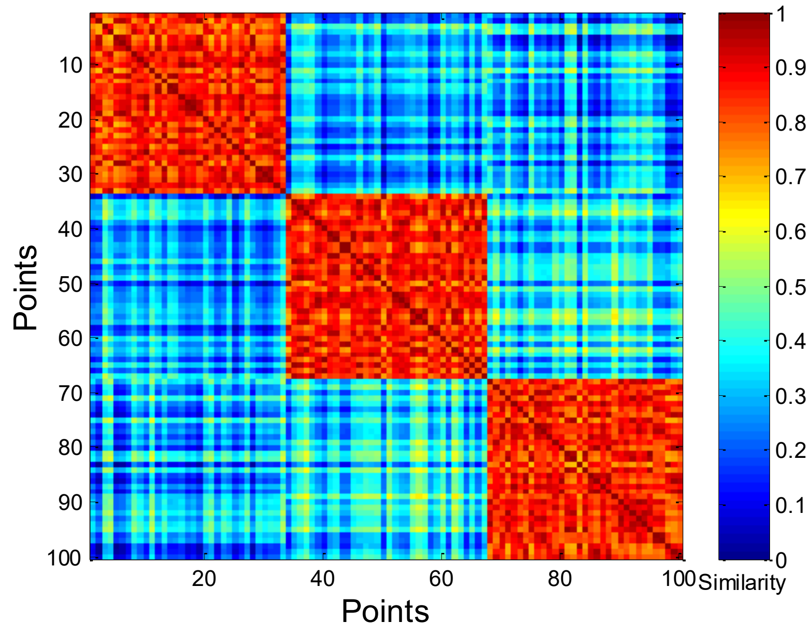
Corr = -0.9235

Corr = -0.5810

Using Similarity Matrix for Cluster Validation

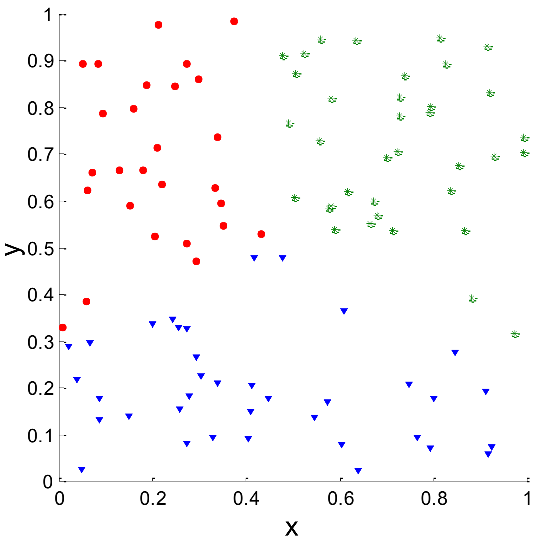
- Order the similarity matrix with respect to cluster labels and inspect visually.

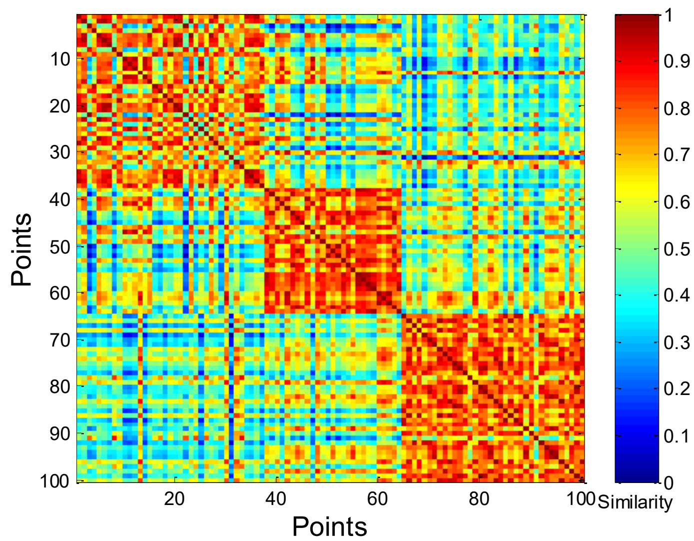




Ref: • Tan, Steinbach, Karpatne, Kumar, "Introduction to Data Mining (Second Edition)"

Using Similarity Matrix for Cluster Validation

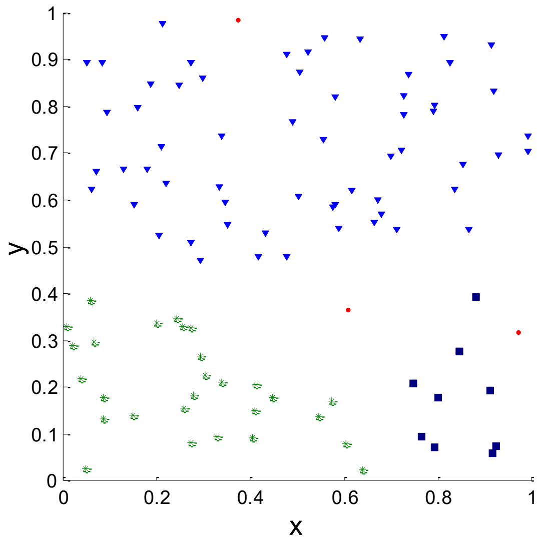


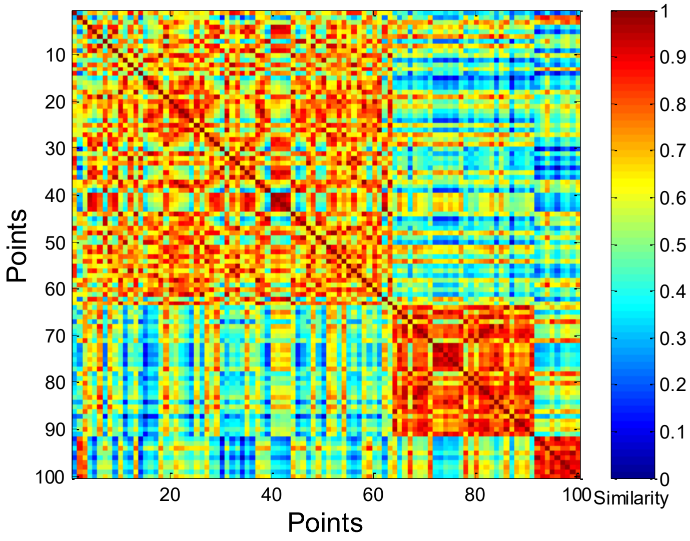


K-means

Ref: • Tan, Steinbach, Karpatne, Kumar, “Introduction to Data Mining (Second Edition)”

Using Similarity Matrix for Cluster Validation





DBSCAN

Ref: • Tan, Steinbach, Karpatne, Kumar, "Introduction to Data Mining (Second Edition)"

Dimensionality Reduction

The curse of dimensionality

- Real data usually have thousands, or millions of dimensions
  - E.g., web documents, where the dimensionality is the vocabulary of words
  - Facebook graph, where the dimensionality is the number of users
- Huge number of dimensions causes problems
  - Data becomes very sparse, some algorithms become meaningless (e.g. density based clustering)
  - The complexity of several algorithms depends on the dimensionality and they become infeasible.

Ref: • Tan, Steinbach, Karpatne, Kumar, “Introduction to Data Mining (Second Edition)”

Dimensionality Reduction

- Usually the data can be described with fewer dimensions, without losing much of the meaning of the data.
  - The data reside in a space of lower dimensionality

- Essentially, we assume that some of the data is noise, and we can approximate the useful part with a lower dimensionality space.
  - Dimensionality reduction does not just reduce the amount of data, it often brings out the useful part of the data

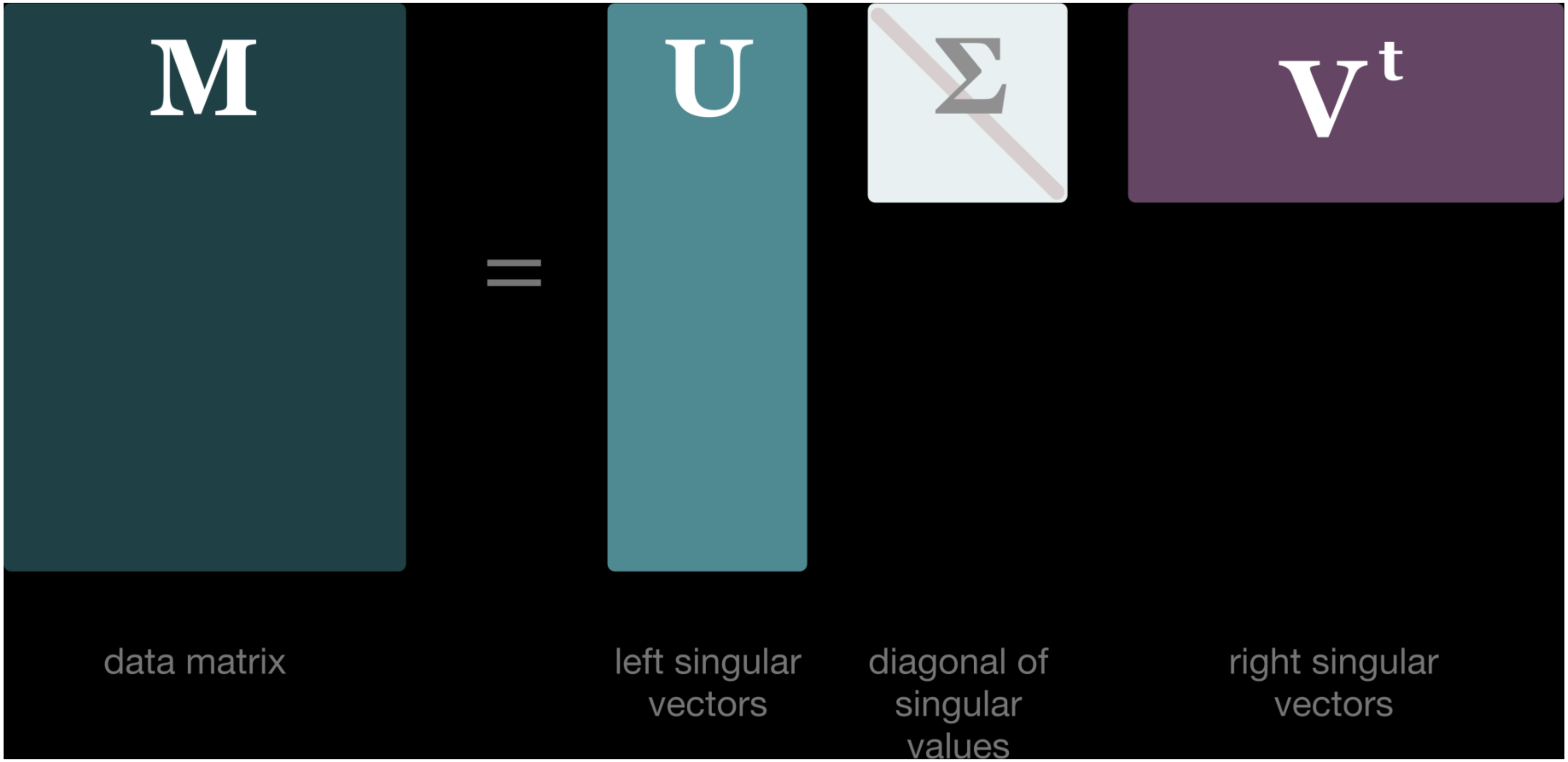
Ref: • Tan, Steinbach, Karpatne, Kumar, "Introduction to Data Mining (Second Edition)"

Latent factor model

- Rows (columns) are linear combinations of k latent factors
  - E.g., in our extreme document example there are two factors
- Some noise is added to this rank-k matrix resulting in higher rank
- SVD retrieves the latent factors (hopefully).

Ref: • Tan, Steinbach, Karpatne, Kumar, “Introduction to Data Mining (Second Edition)”

SVD (Singular Value Decomposition)



Ref: • (image) https://dsc-spidal.github.io/harp/docs/harpdaal/svd/

SVD

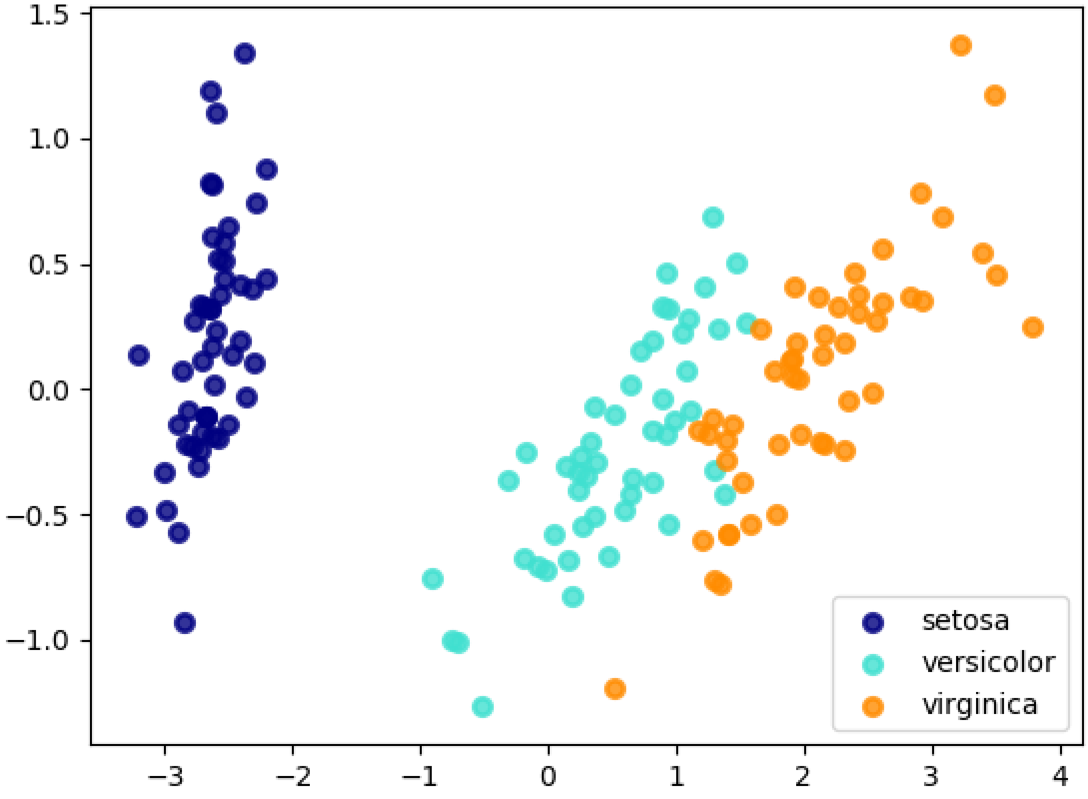
- Example

$$
\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \mathbf{x} \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \mathbf{x} \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ 0 & 0 & 0 & 0.71 & 0.71 \end{bmatrix}
$$

Ref: • (image) http://people.seas.harvard.edu/~babis/kdd09.html

Plot

- Dimensionality Reduction of the Iris Dataset



Ref: • Tan, Steinbach, Karpatne, Kumar, “Introduction to Data Mining (Second Edition)”

Python

```
>>> import numpy as np
>>> from sklearn.decomposition import PCA
>>> X = np.array([[-1, -1], [-2, -1], [-3, -2], [1, 1], [2, 1], [3, 2]])
>>> pca = PCA(n_components=2)
>>> pca.fit(X)
PCA(copy=True, iterated_power='auto', n_components=2, random_state=None,
  svd_solver='auto', tol=0.0, whiten=False)
>>> print(pca.explained_variance_ratio_)
[ 0.99244...  0.00755...]
>>> print(pca.singular_values_)
[ 6.30061...  0.54980...]
```

Ref: • http://scikit-learn.org/stable/modules/generated/sklearn.decomposition.PCA.html

Thanks to big data, machines can now be programmed to the next thing right.
But only humans can do the next right thing.

Dov Seidman

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