Cluster Analysis

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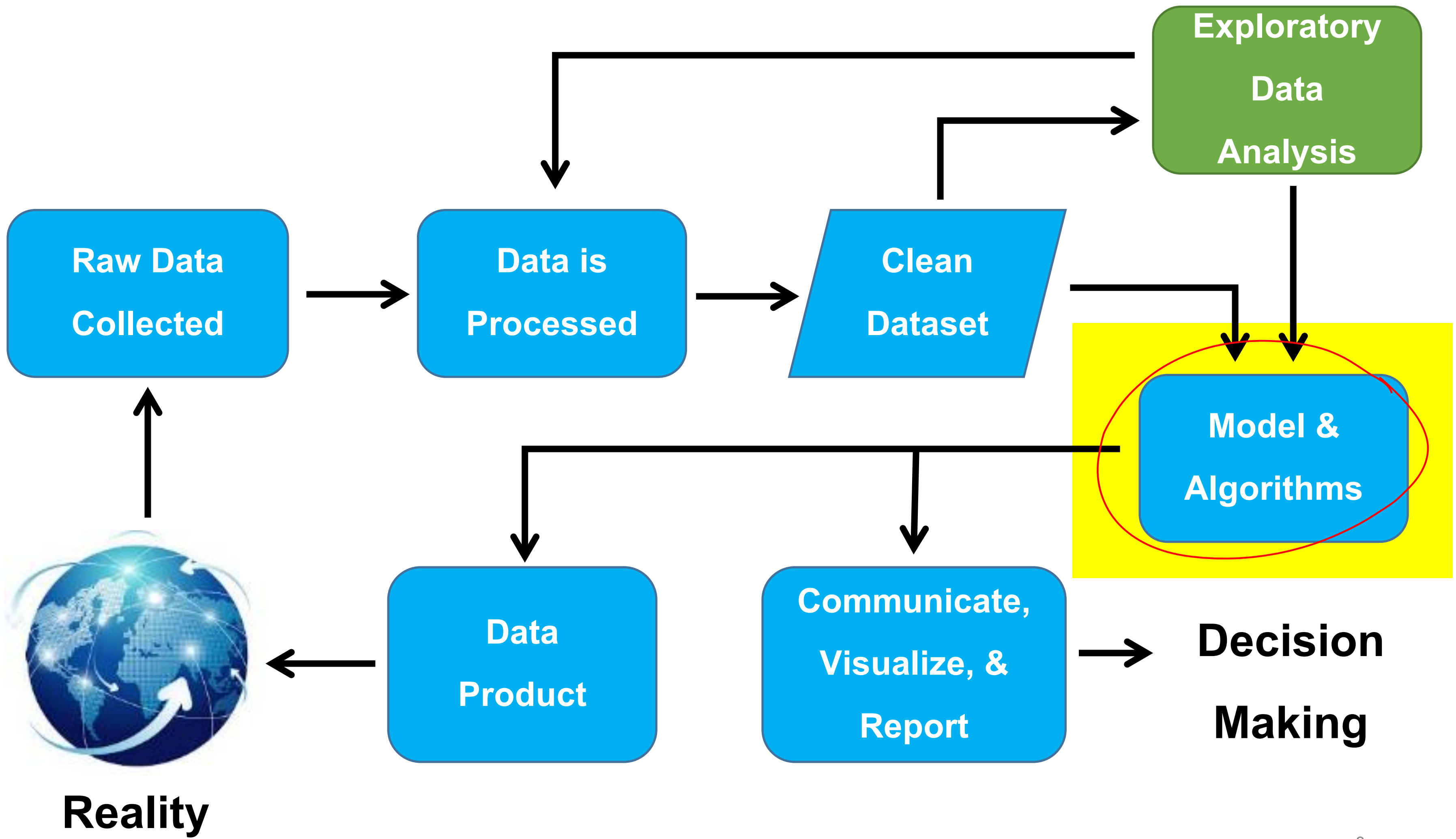
Agenda

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

Data Science Process



Machine Learning

Supervised Learning

Develop predictive model based on both input and output data

Regression

- Linear Regression
- Polynomial Regression

Classification

- Decision Tree
- Logistic Regression
- Neural Network
- etc.

Unsupervised Learning

รู้x ไม่รู้y อยากได้ y

Develop predictive model based on both input and output data

Clustering

- K-Means
- DB-SCAN
- etc.

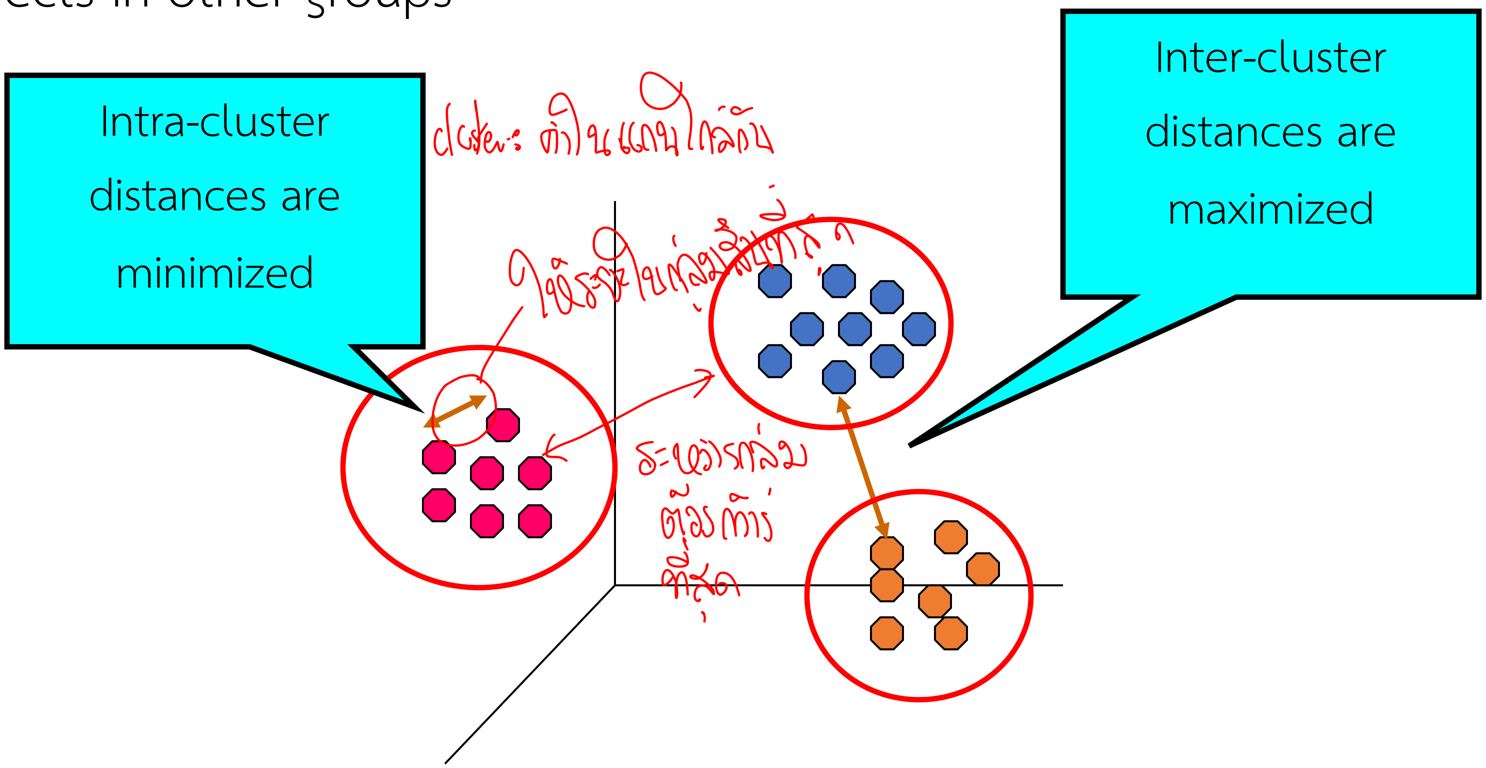
Clustering

การจัดกลุ่มโดยที่ไม่สนใจป้ายชื่อ

อะไรที่เหมือนกันจับมาอยู่ด้วยกัน

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

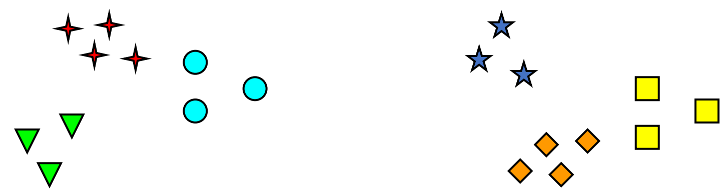


Notion of a Cluster can be Ambiguous

แล้วการจับกลุ่มของเดตาเป็นกี่กลุ่มหล่ะ?

แล้วแต่คนมอง

How many clusters?



6 Clusters

2 Clusters

4 Clusters

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

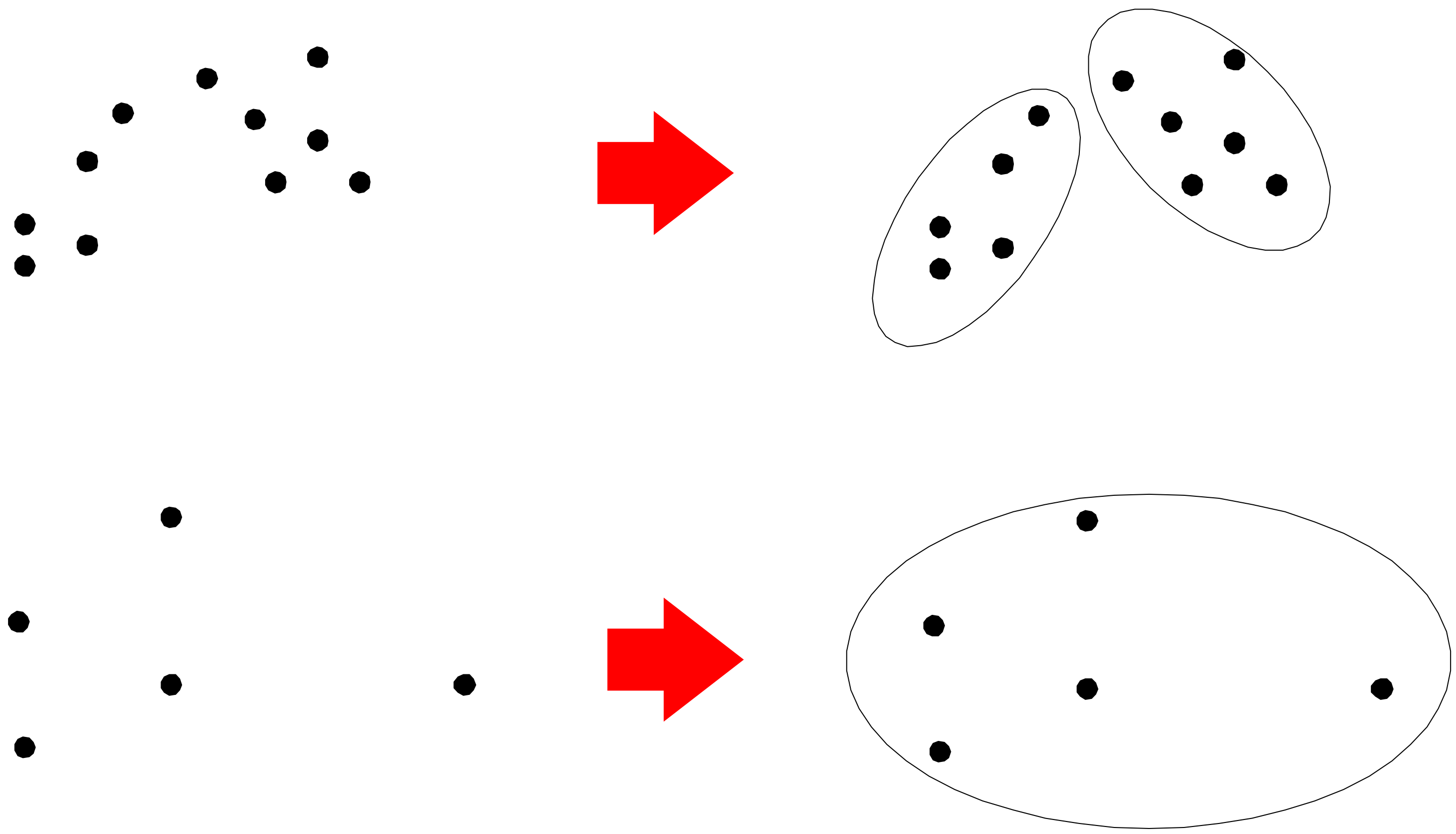
Types of Clusterings

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

สัตว์ กลุ่มใหญ่

กลุ่มย่อย

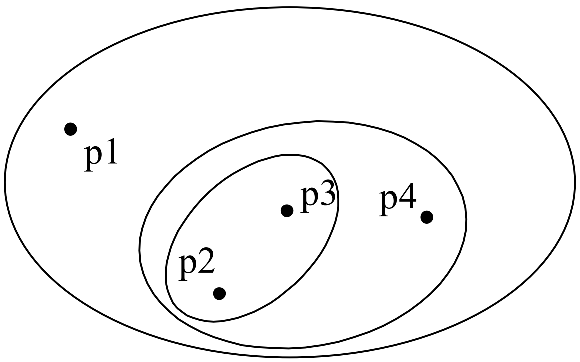
Partitional Clustering



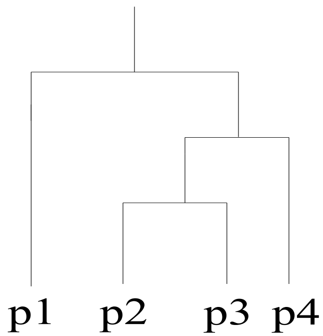
Original Points

A Partitional Clustering

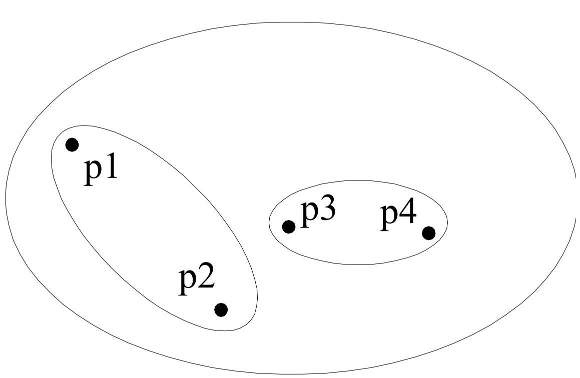
Hierarchical Clustering



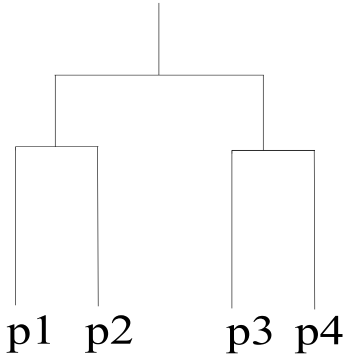
Traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Hierarchical Clustering



Non-traditional Dendrogram

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

Other types of clustering

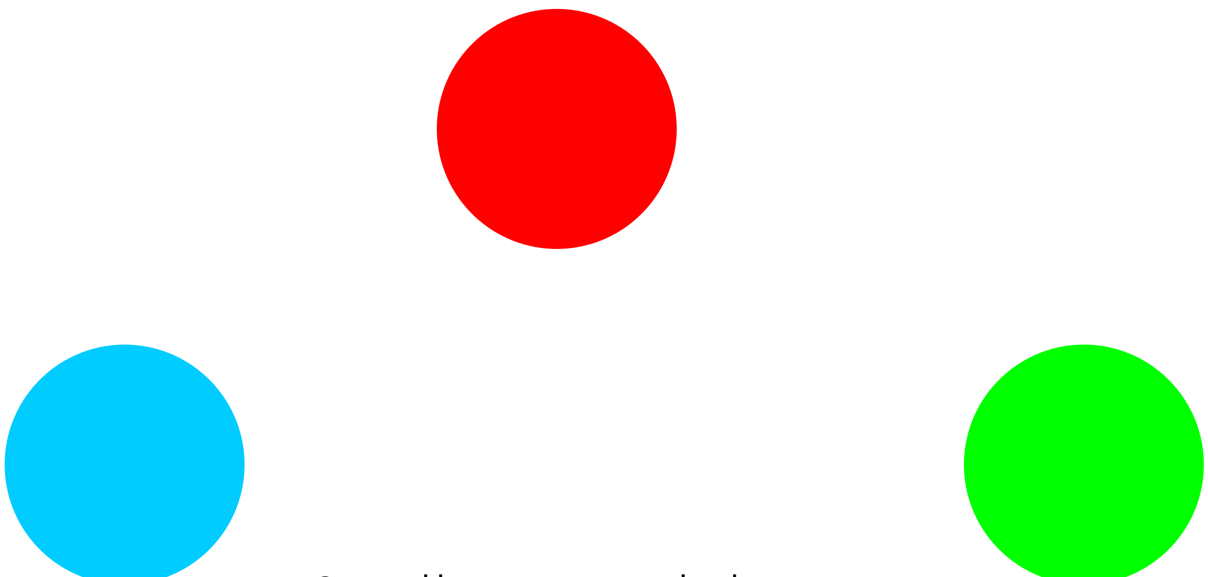
มีแบบอื่นมากมายๆ ไปศึกษาเพิ่มเอง

- **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: แยกกันอย่างชัดเจน
  - 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.

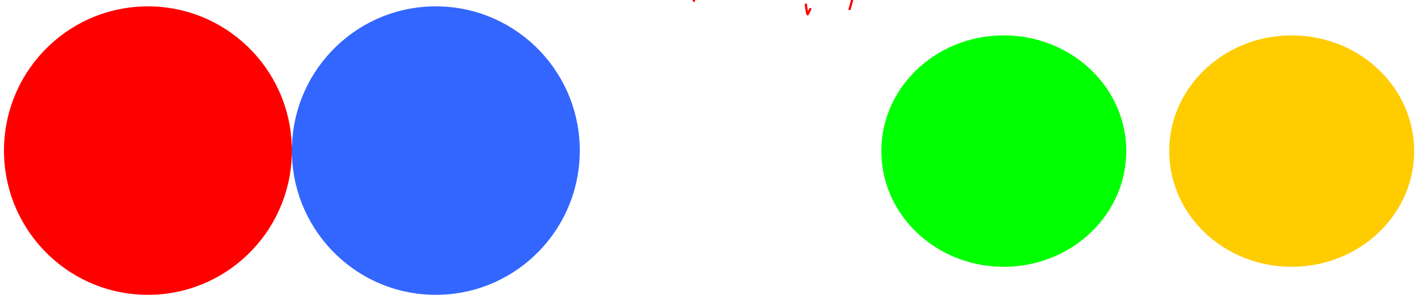


3 well-separated clusters

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

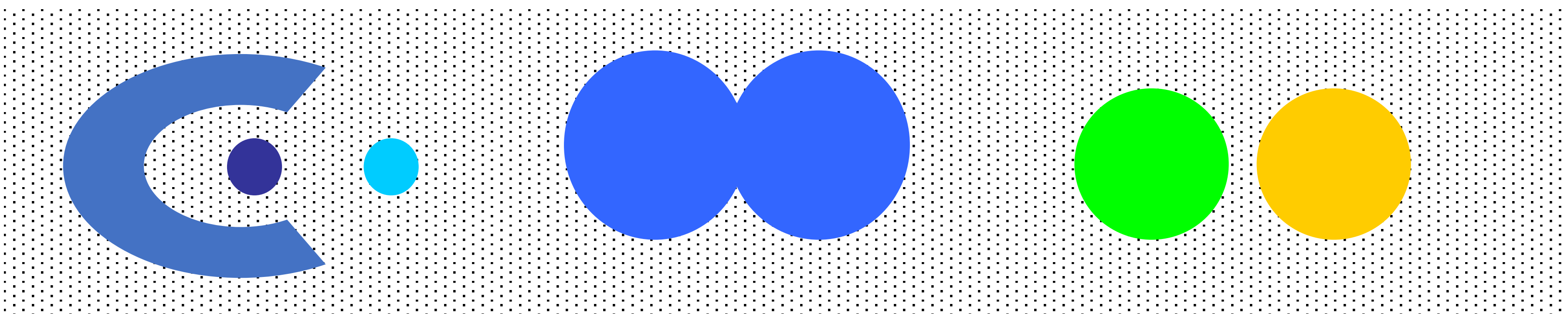
กลุ่มที่ใช้จุดศูนย์กลางร่วมกัน



4 center-based clusters

Types of Clusters: Density-Based

- Density-based อะไรอยู่ใกล้กันคือพวกเดียวกัน
  - 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 นอกนั้นไปหาเอาเอง
- 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

→ เรากำหนดค่า k เป็นจำนวนกลุ่มที่เราต้องการมีเท่าไหร่

↳ เริ่มสร้างตัวแทนกลุ่ม → ตัวแทนกลุ่มเดินไปมา

- 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

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

ผลระยะทางไปหา centriod

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

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
```

ตัวแทนกลุ่มเดินเข้าไปเรื่อยๆ

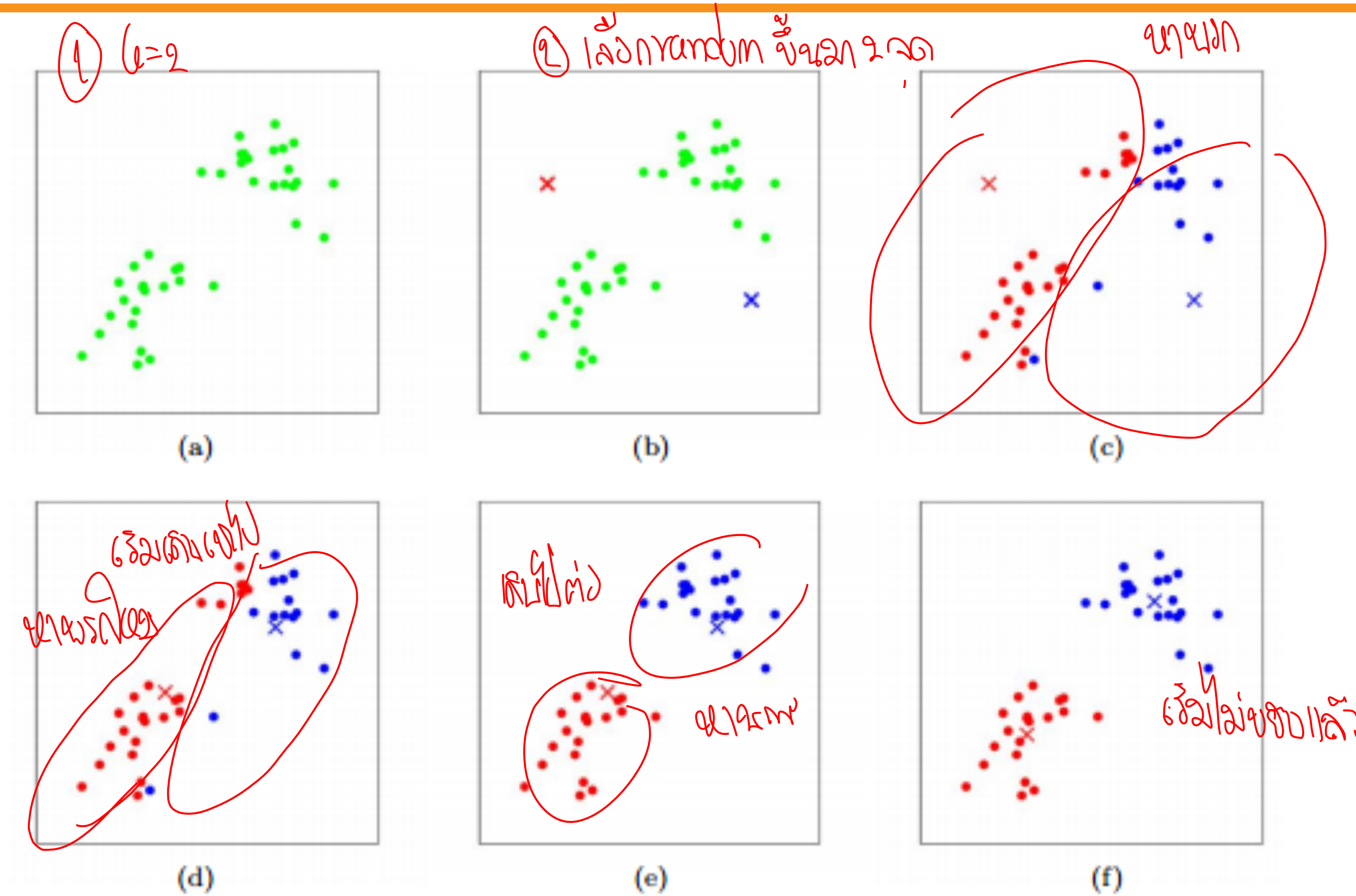
หาบอก

แล้วขยับ

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

K-means: Steps

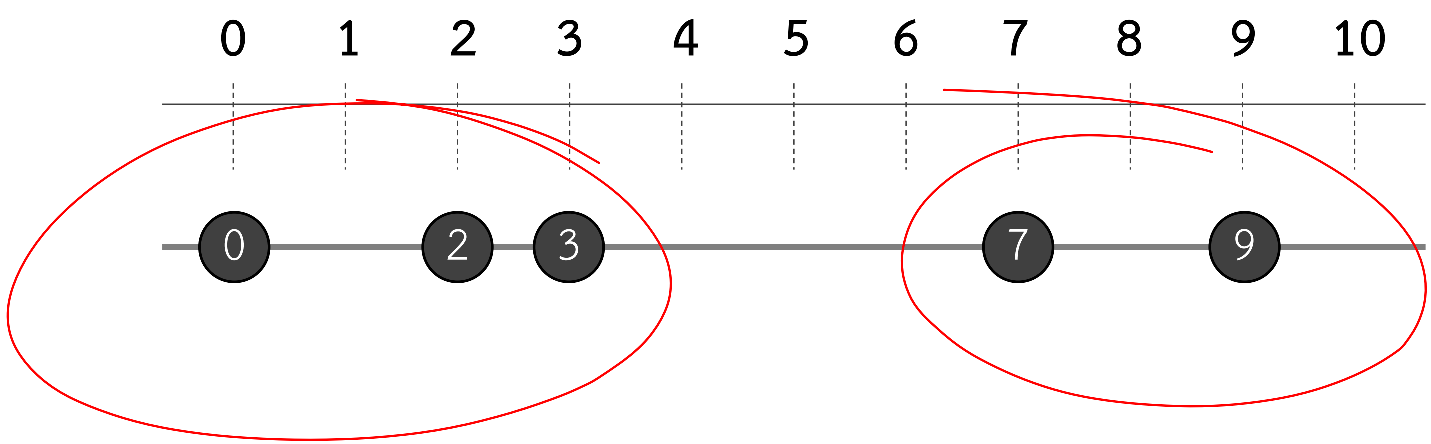
ตัวอย่างการทำงาน



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

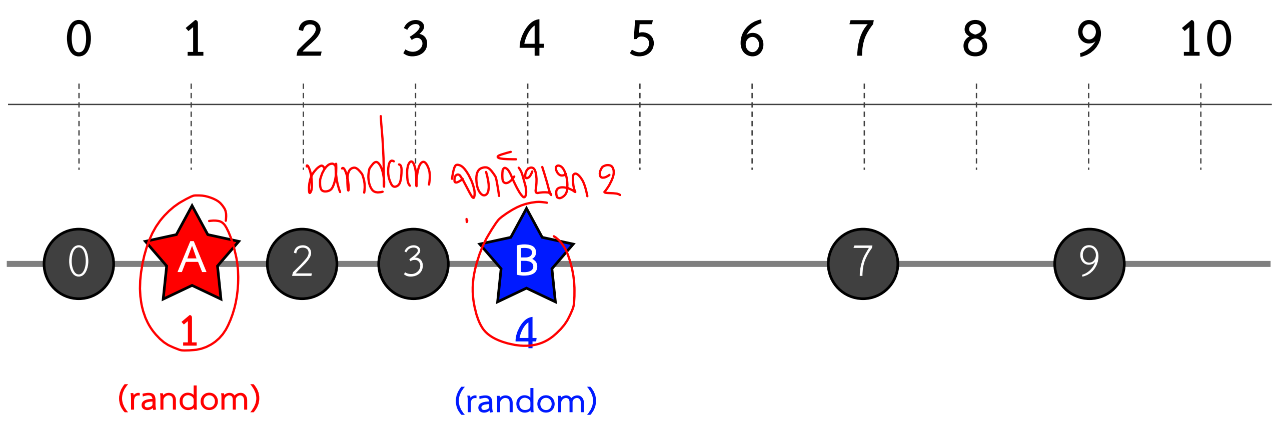
K-means: Example Steps (1 feature)

ดูด้วยตา #



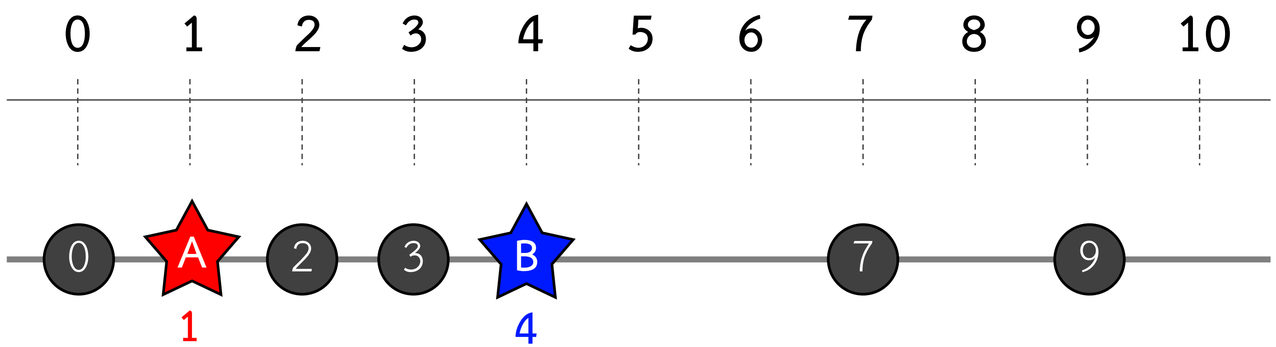
K-means: Example Steps (1 feature)

Round 0

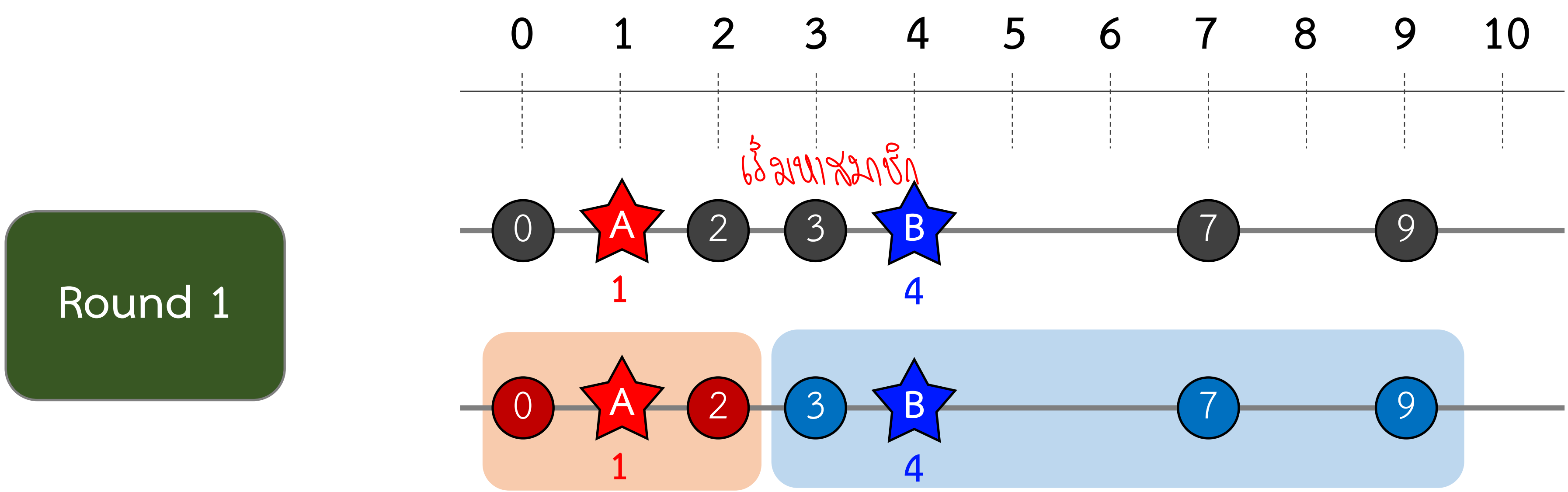


K-means: Example Steps (1 feature)

Round 1

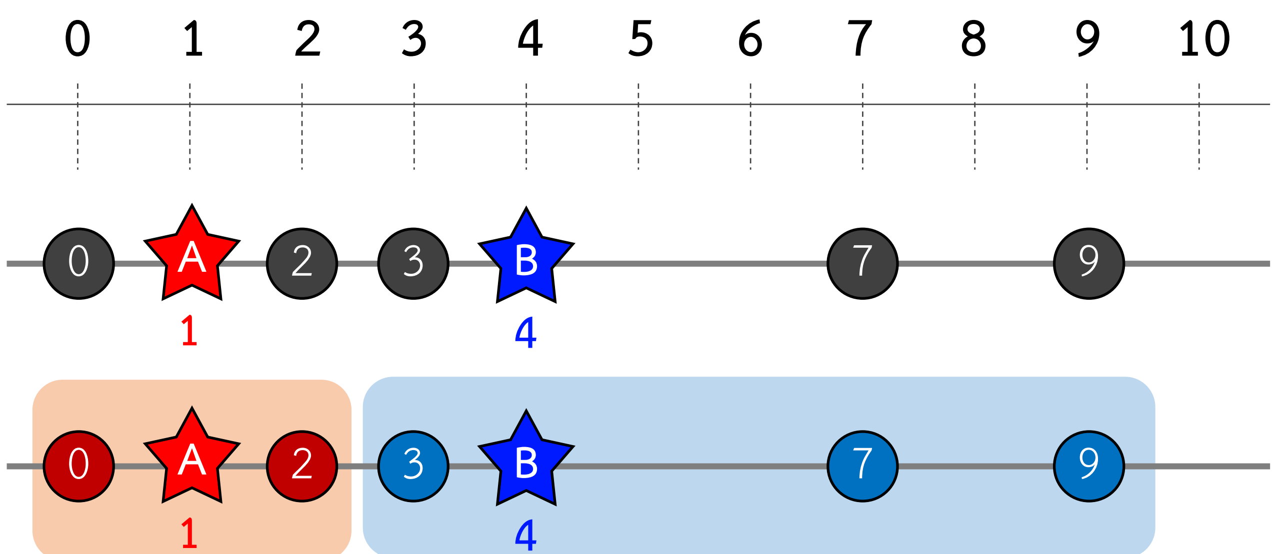


K-means: Example Steps (1 feature)



K-means: Example Steps (1 feature)

Round 1



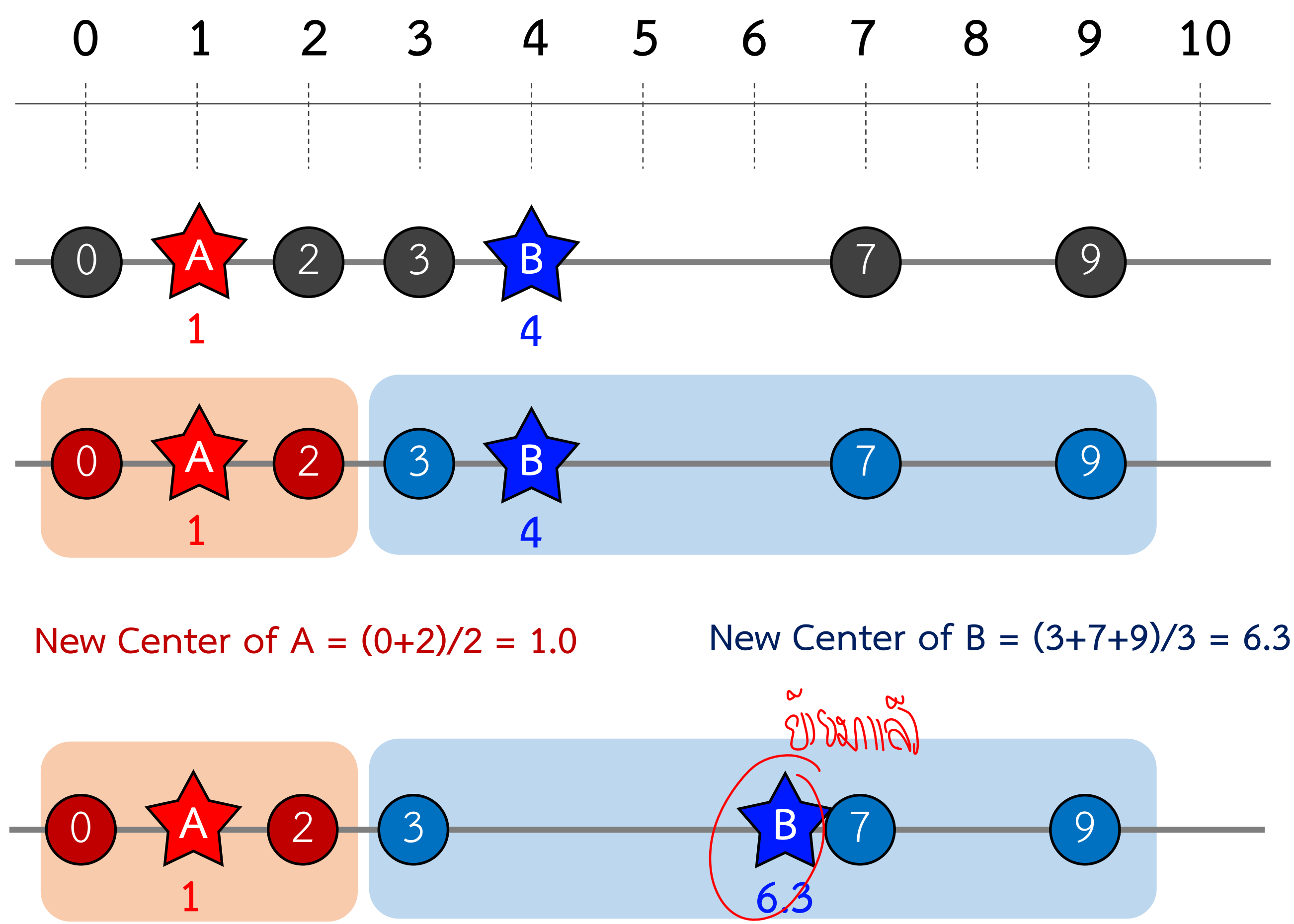
New Center of A = (0+2)/2 = 1.0

New Center of B = (3+7+9)/3 = 6.3

ค่าเซนเตอร์ใหม่

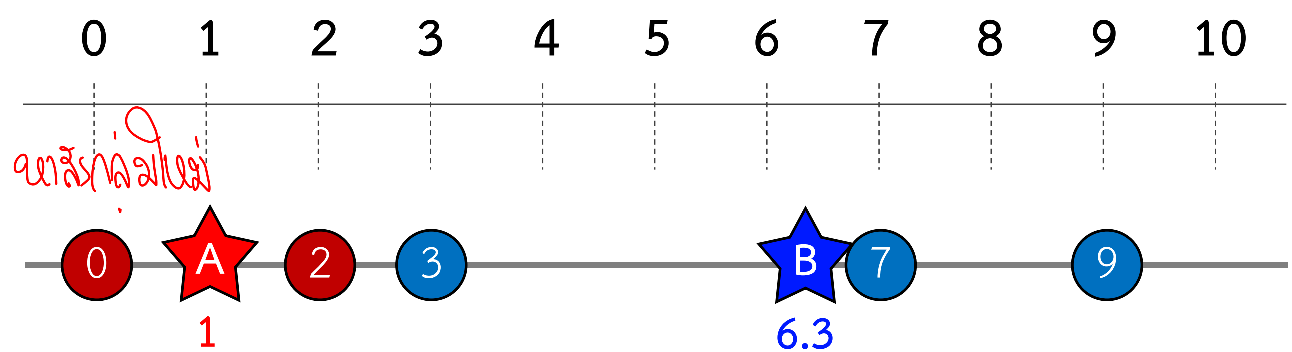
K-means: Example Steps (1 feature)

Round 1



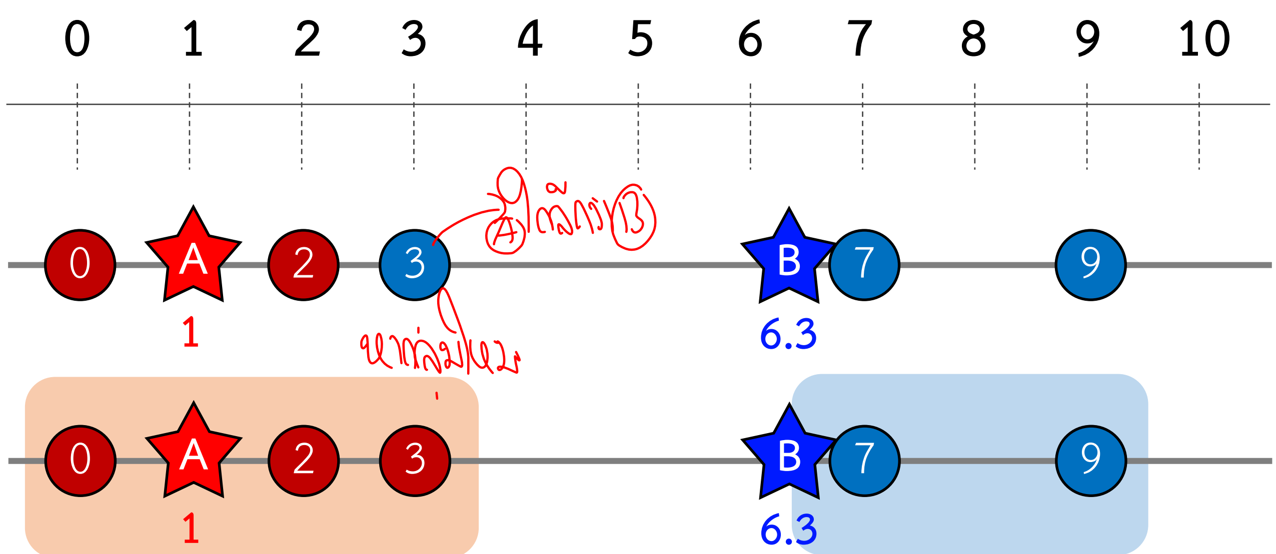
K-means: Example Steps (1 feature)

Round 2



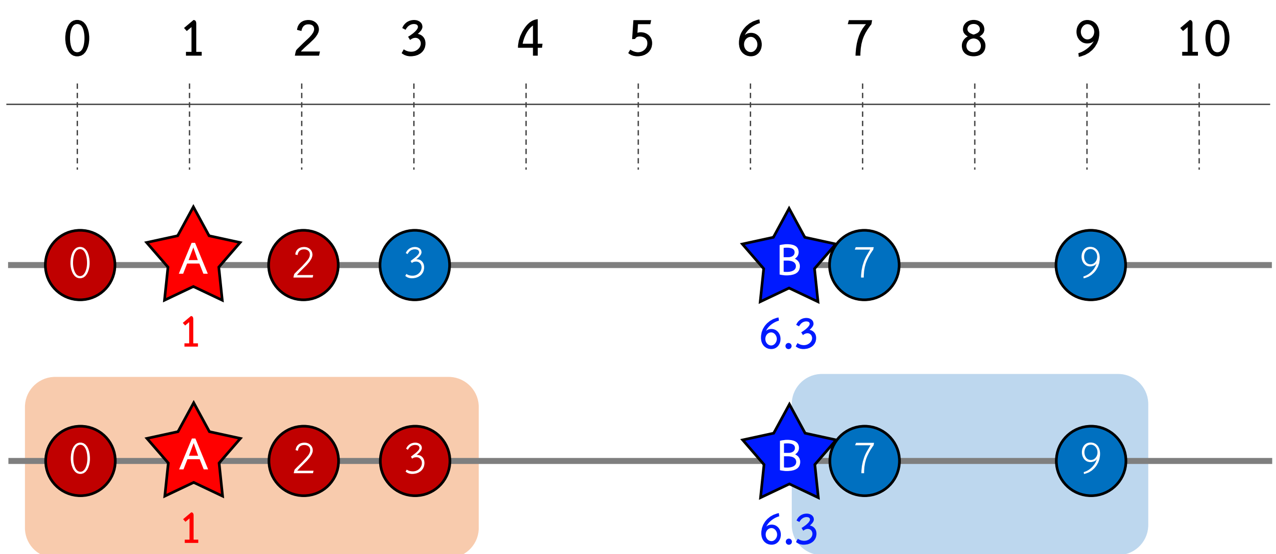
K-means: Example Steps (1 feature)

Round 2



K-means: Example Steps (1 feature)

Round 2



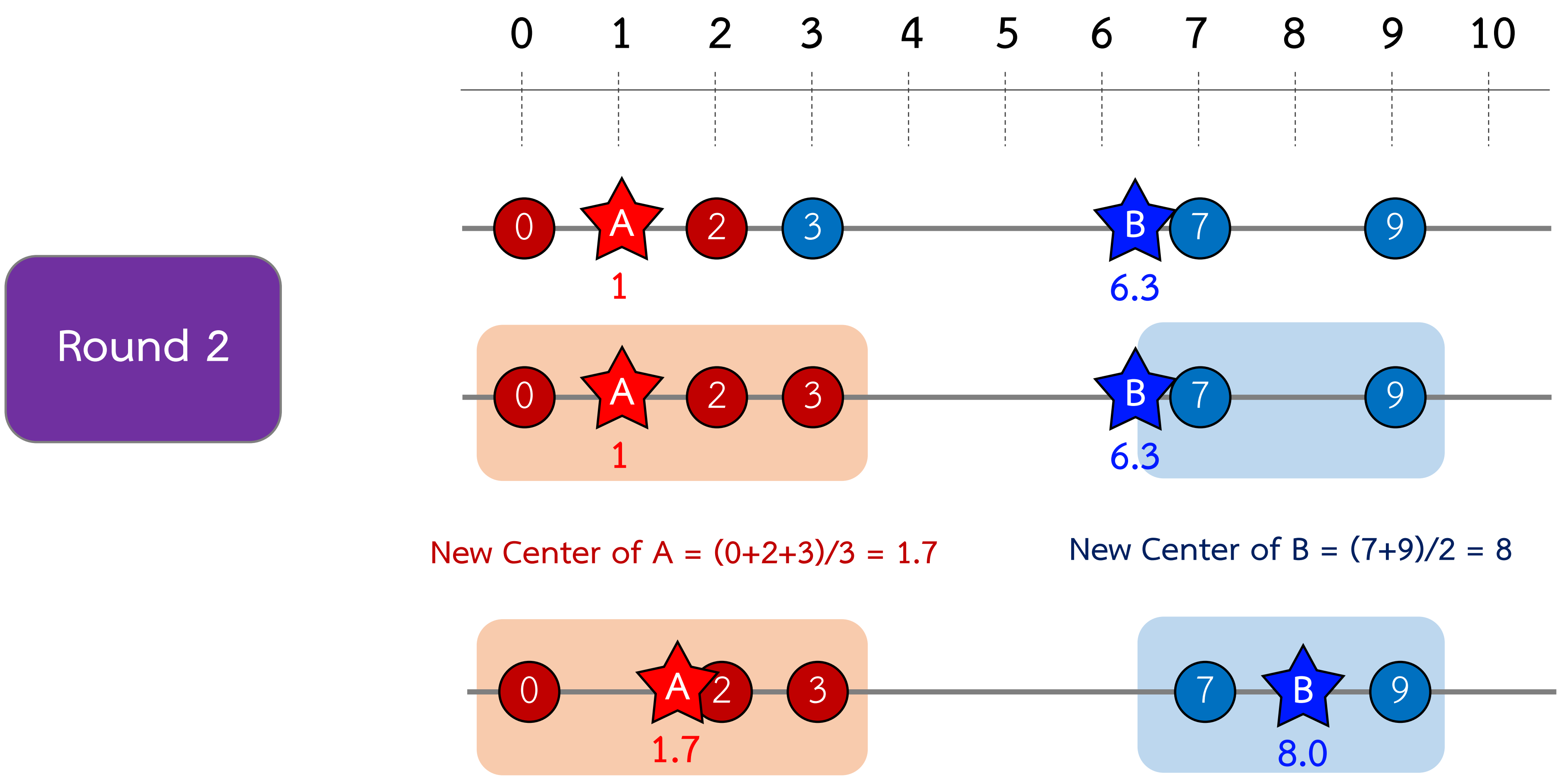
New Center of A = (0+2+3)/3 = 1.7

ได้ค่าเซนเตอร์ใหม่

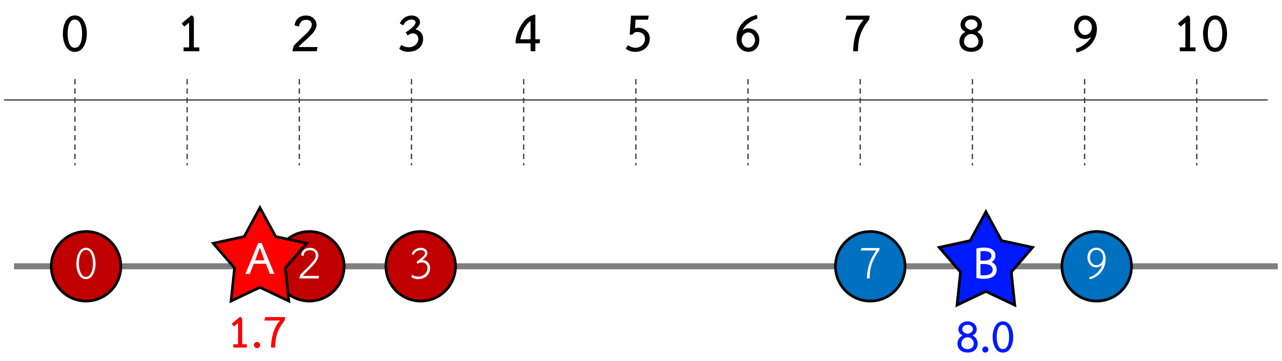
New Center of B = (7+9)/2 = 8

ขยับไปต่อ

K-means: Example Steps (1 feature)



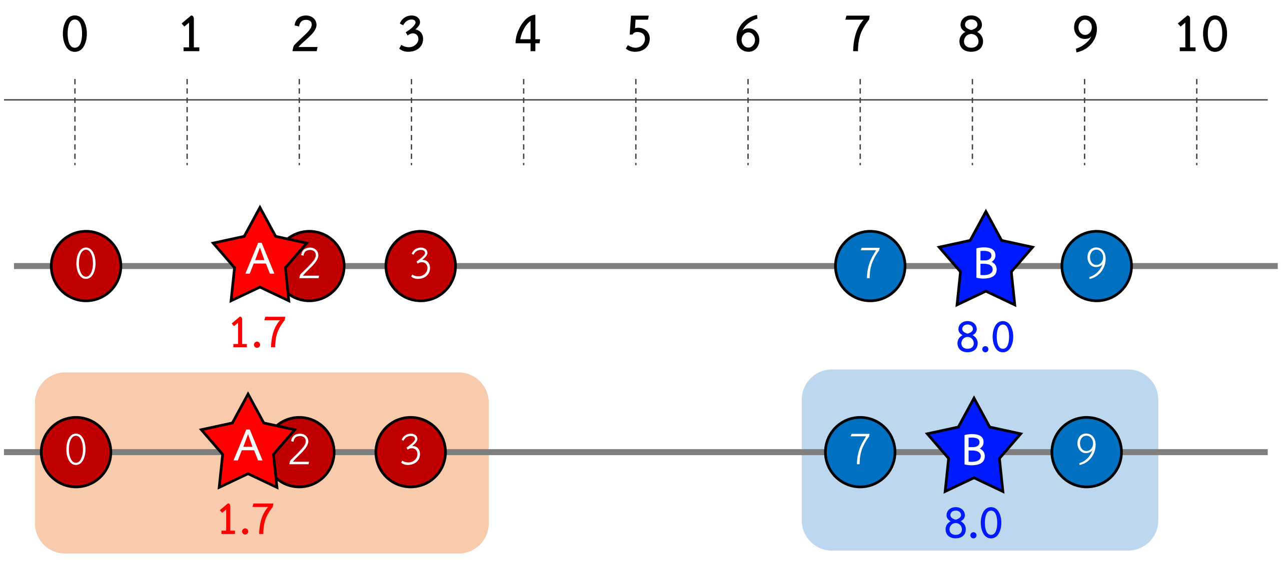
K-means: Example Steps (1 feature)



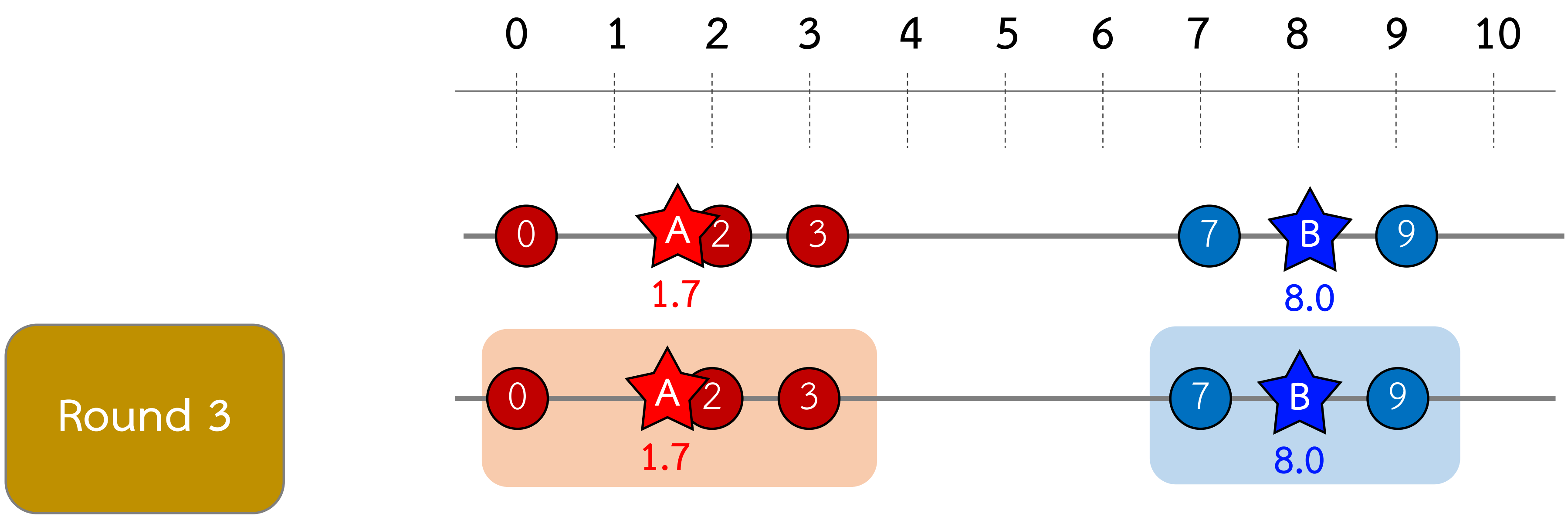
Round 3

K-means: Example Steps (1 feature)

Round 3



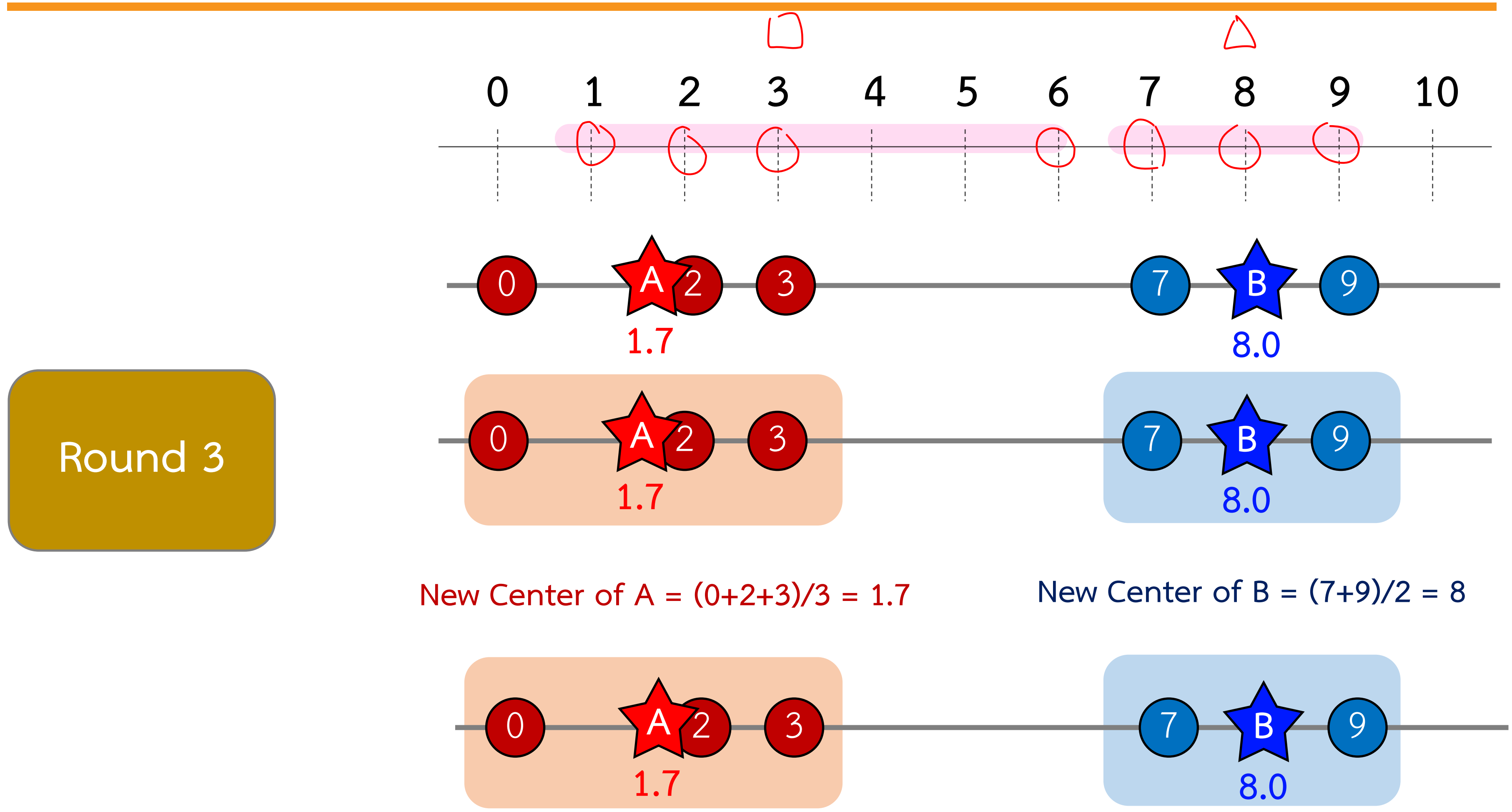
K-means: Example Steps (1 feature)



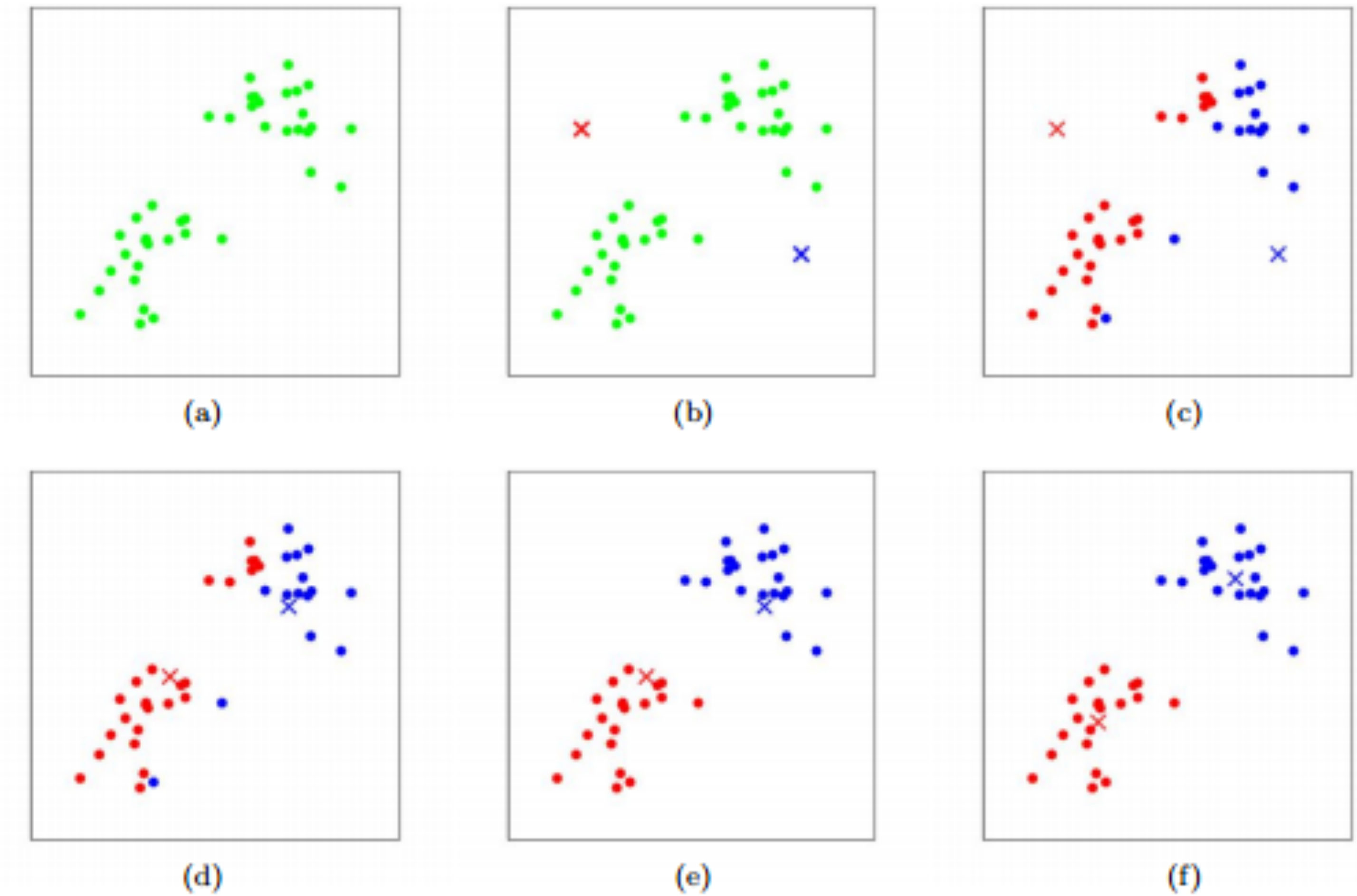
New Center of A = (0+2+3)/3 = 1.7

New Center of B = (7+9)/2 = 8

K-means: Example Steps (1 feature)



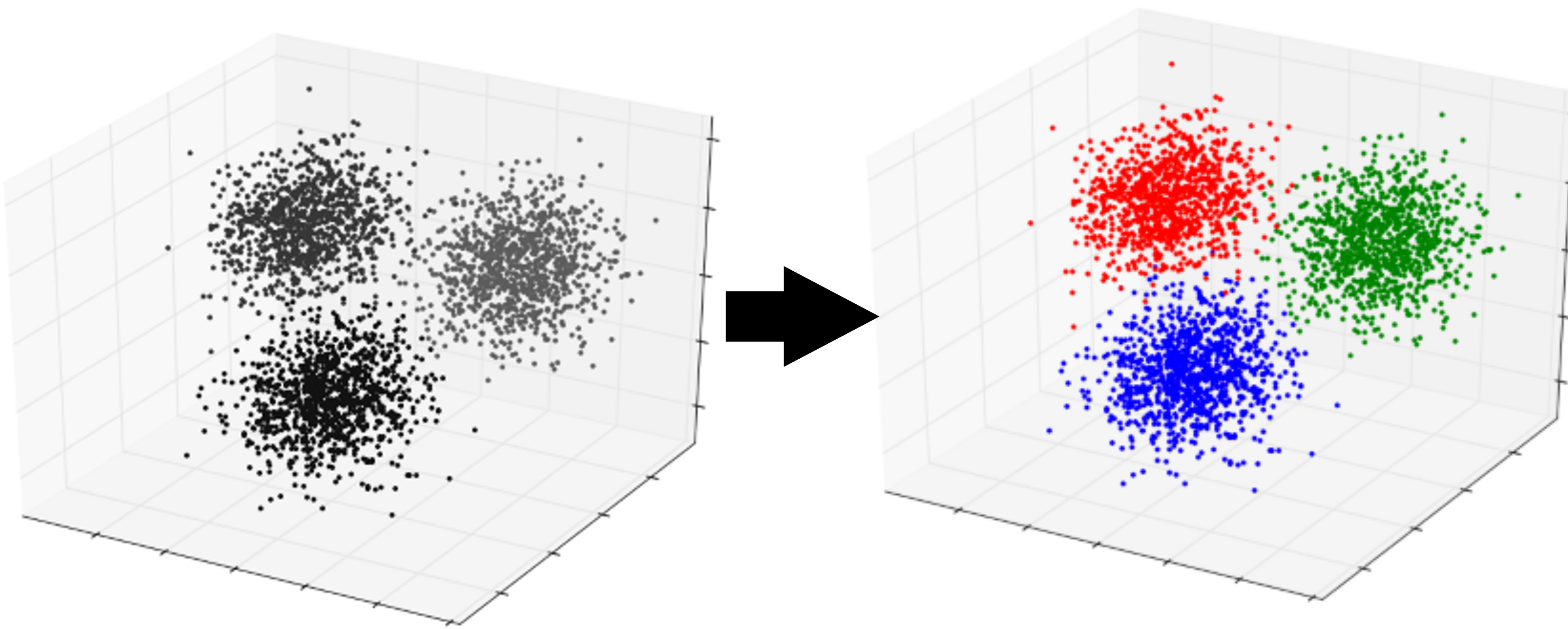
K-means: Example (2 features)



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

K-means: Example (3 features)

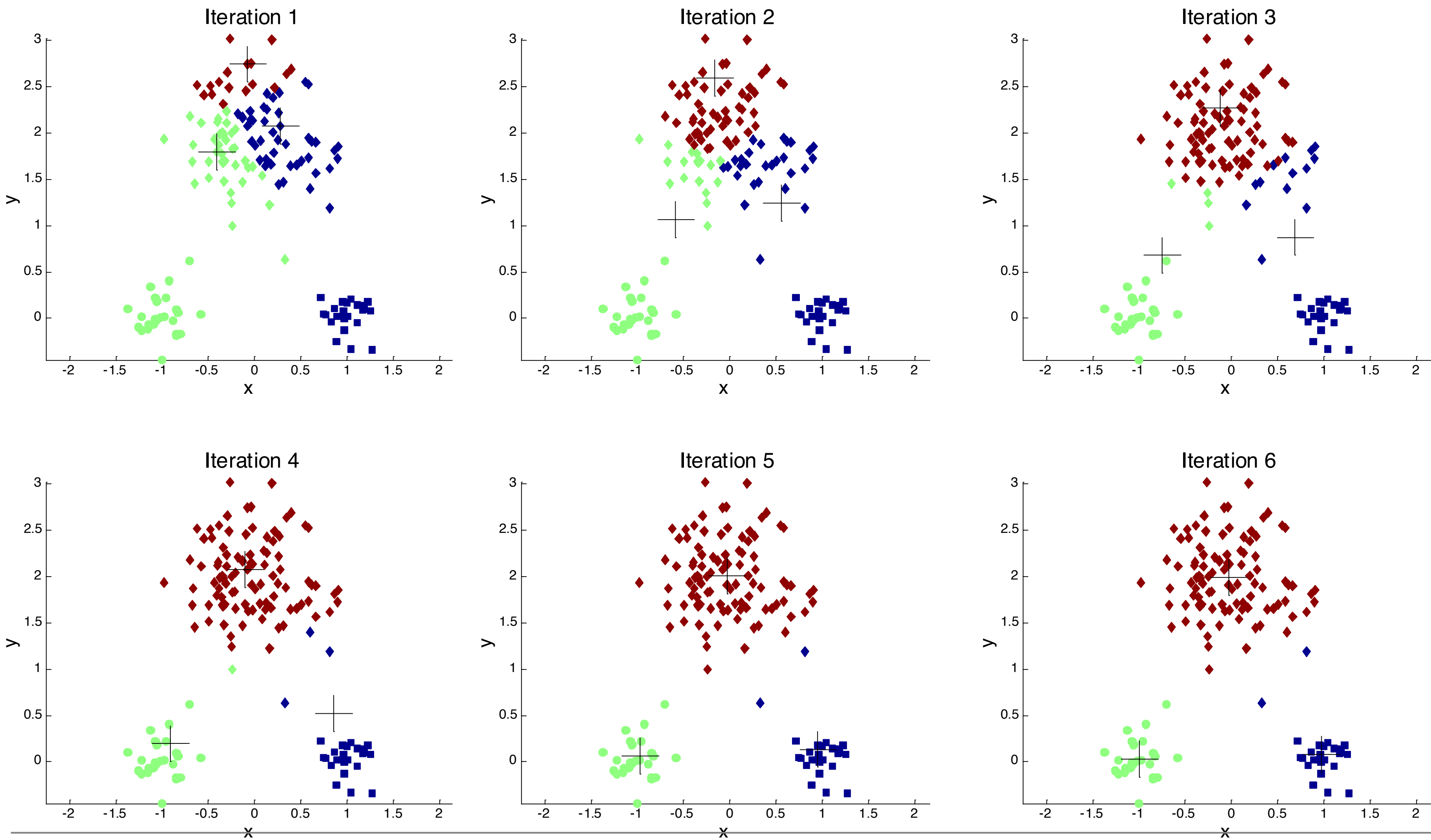
พอ feature มีเพิ่มๆ → visualize ยากแล้ว



Ref: • https://youneeq.ca/2014/12/04/adventures-data-analytics-visualizing-high-dimensional-data-2/

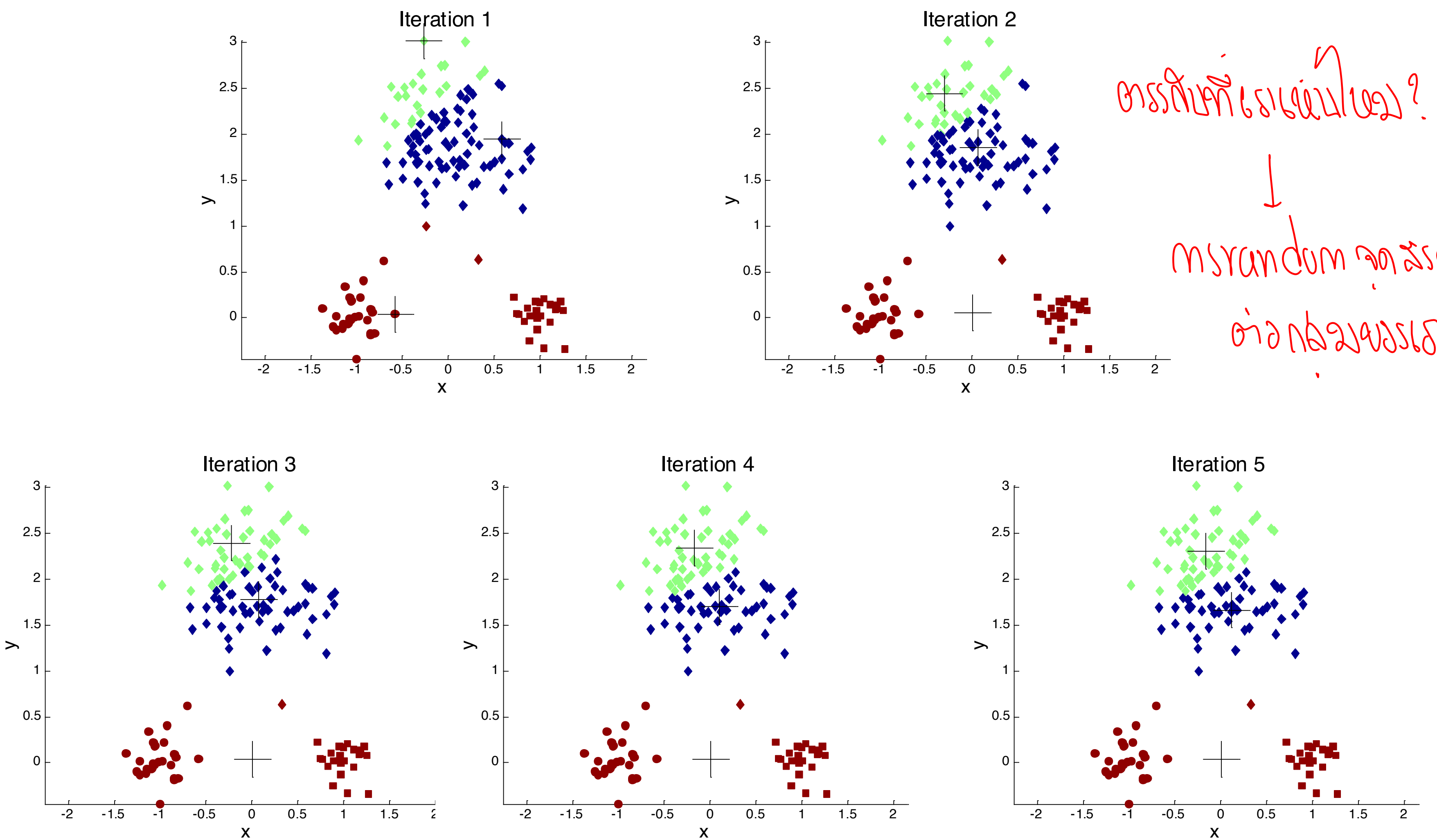
Importance of Choosing Initial Centroids (A)

ปัญหาของระบบคือ การ random กลุ่ม ณ ตอนแรก



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

Importance of Choosing Initial Centroids (B)



ตรรสินที่เราเน้นไหม?

↓

การrandom จุดส่งผล
ต่อกลุ่มของเรา

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

Dealing with Initialization

แก้ → (1) ทำหลายรอบ
(2) กำหนดจุดให้มันห่างๆ

- 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”

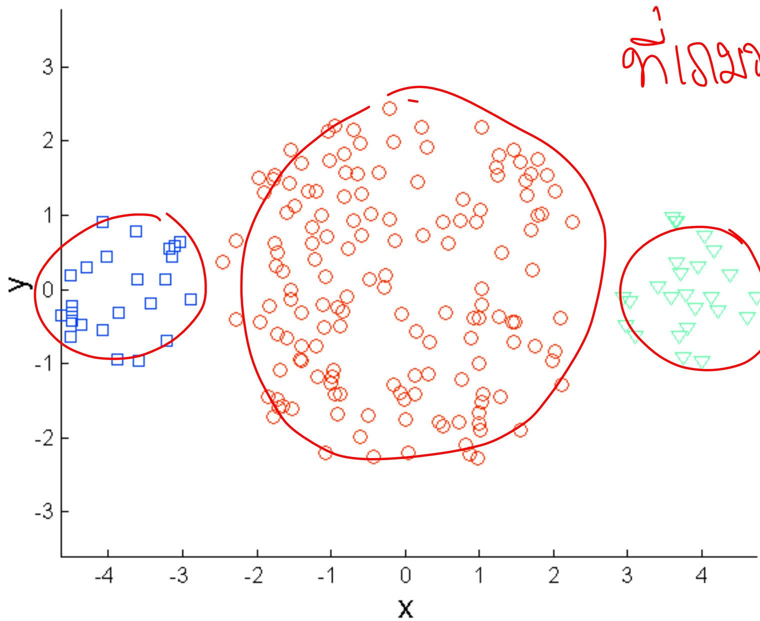
Limitations of K-means

- K-means has problems when clusters are of different
  - Sizes ขนาด
  - Densities ความหนาแน่น
  - Non-globular shapes ไม่มีรูปทรง
- K-means has problems when the data contains outliers.

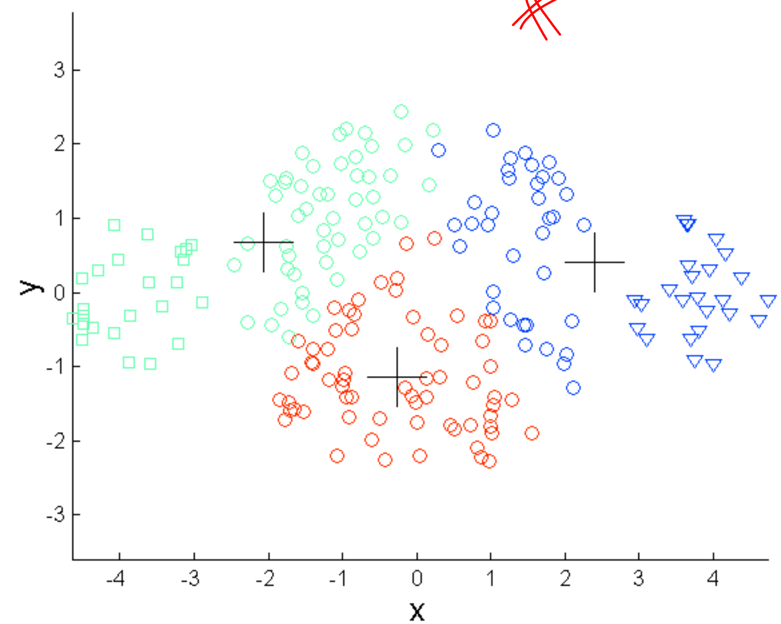
ทำกับ outlier ไม่ได้

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

Limitations of K-means: Differing Sizes



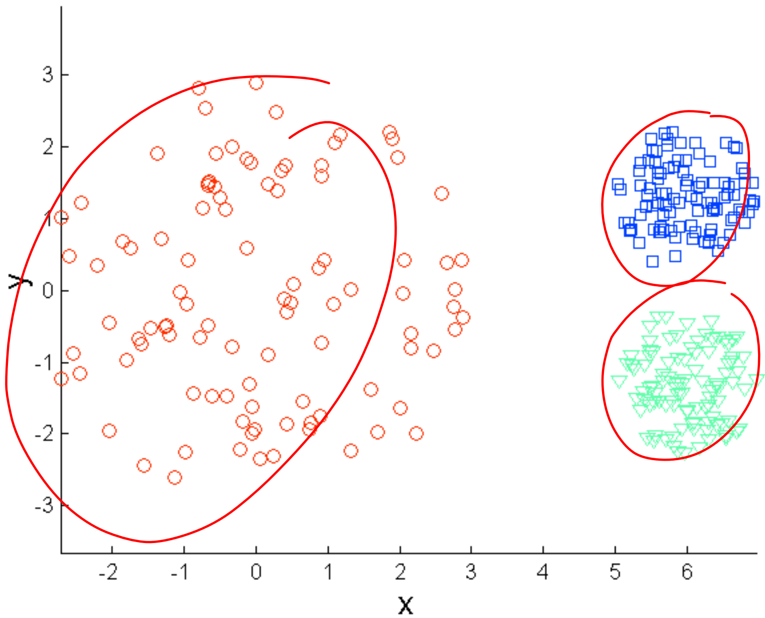
Original Points



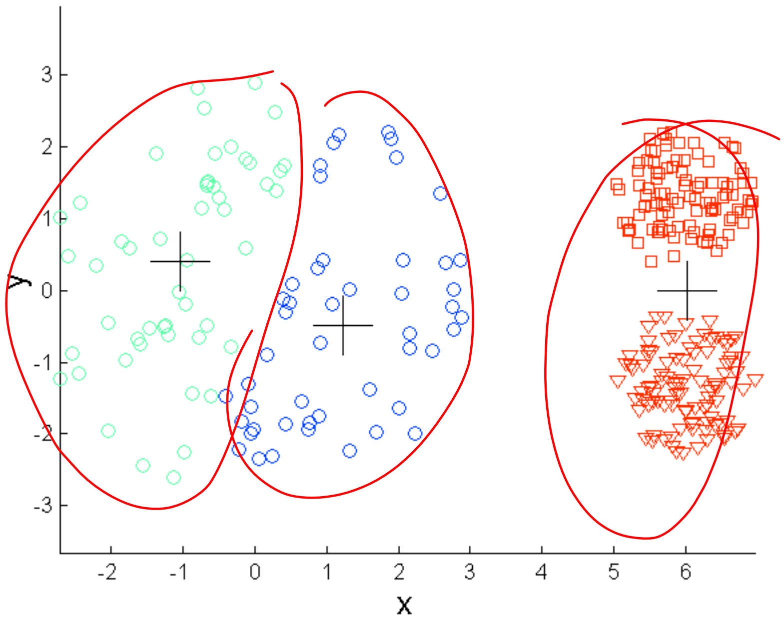
K-means (3 Clusters)

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

Limitations of K-means: Differing Density



Original Points

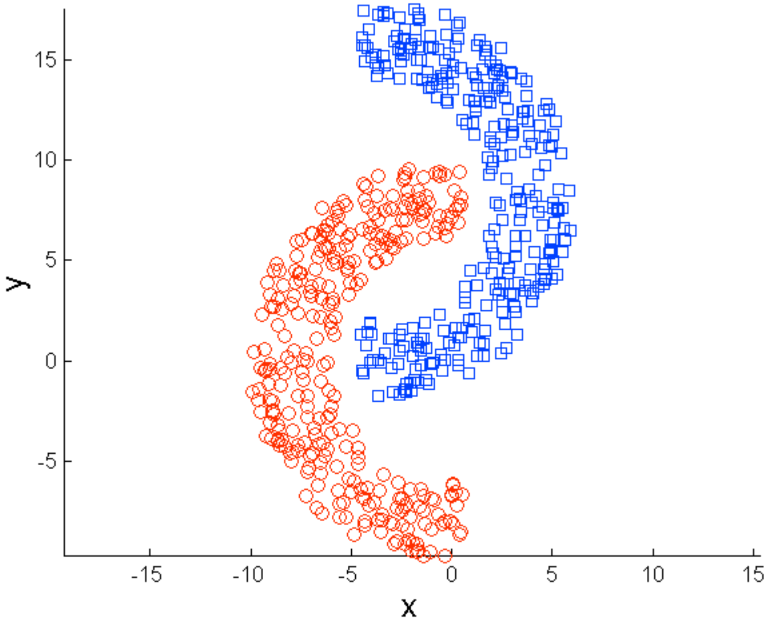


K-means (3 Clusters)

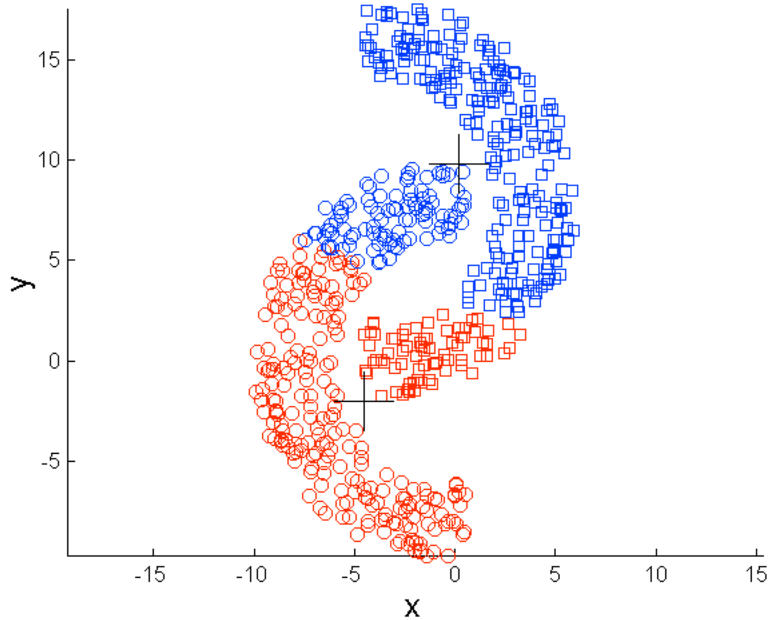
Ref: • Min-Hashing, “Locality Sensitive Hashing Clustering”

Limitations of K-means: Non-globular Shapes

ยึดติดจุดศูนย์กลาง (ความใกล้) มากเกินไป



Original Points

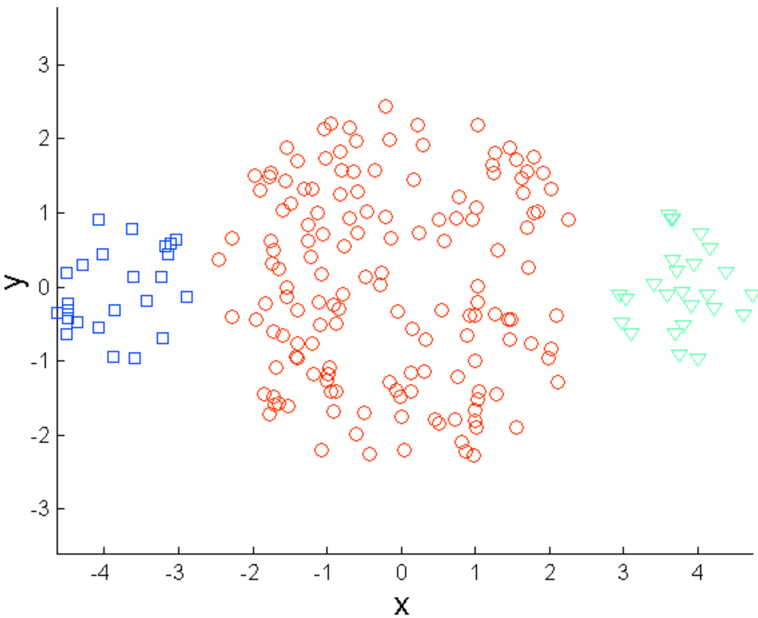


K-means (2 Clusters)

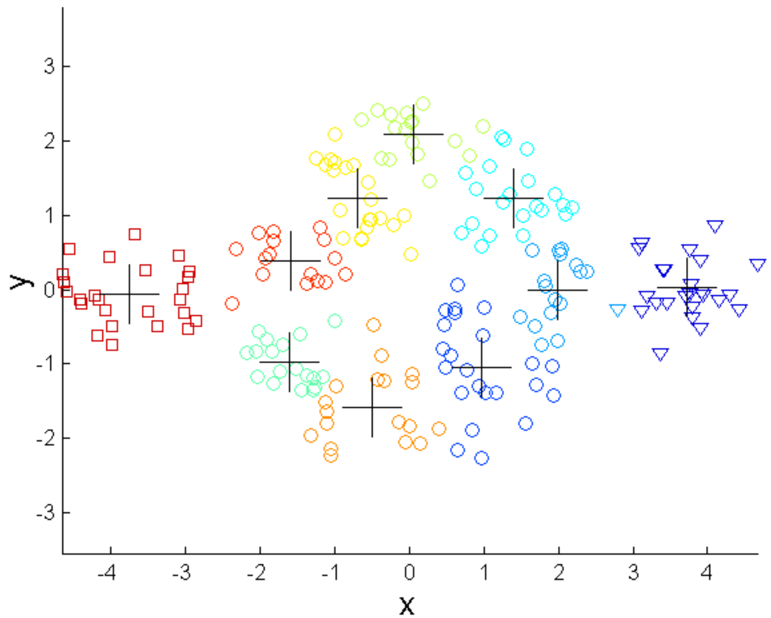
Ref: • Min-Hashing, “Locality Sensitive Hashing Clustering”

Overcoming K-means Limitations

set k เยอะไว้



Original Points



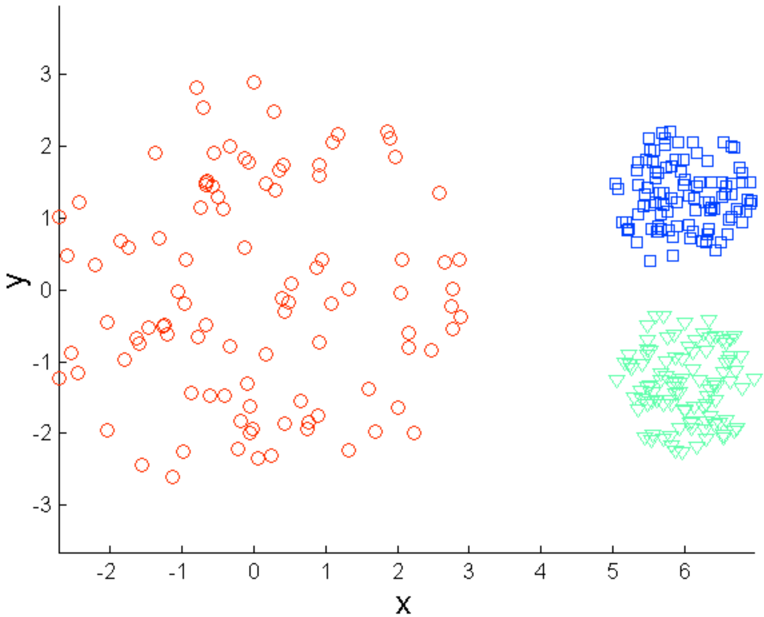
K-means Clusters

One solution is to use many clusters.

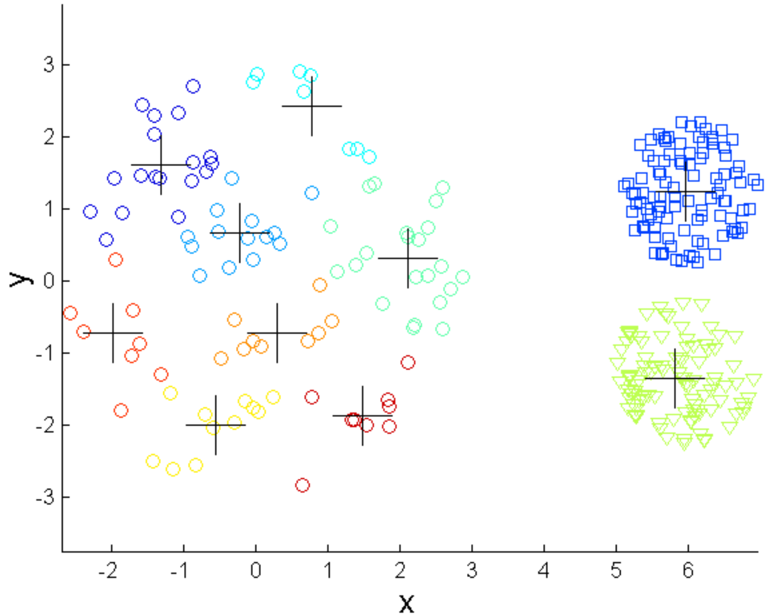
Find parts of clusters, but need to put together.

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

Overcoming K-means Limitations



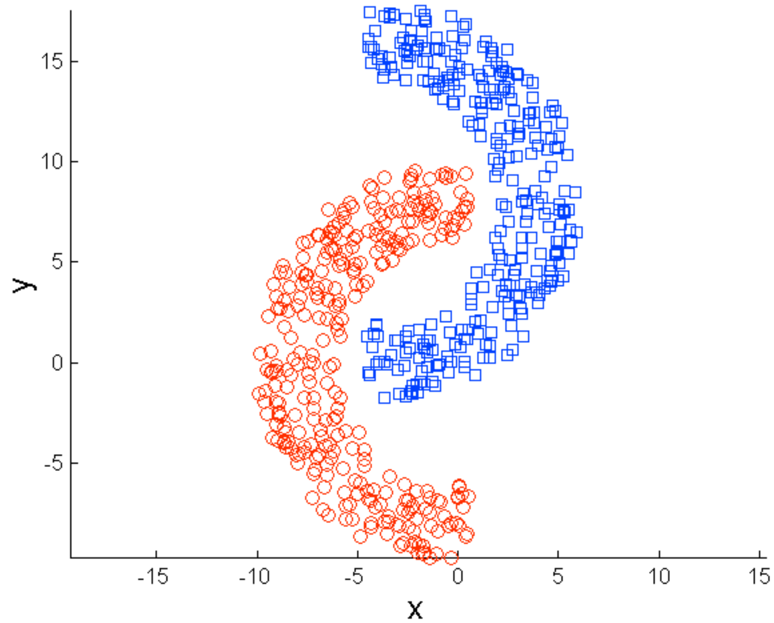
Original Points



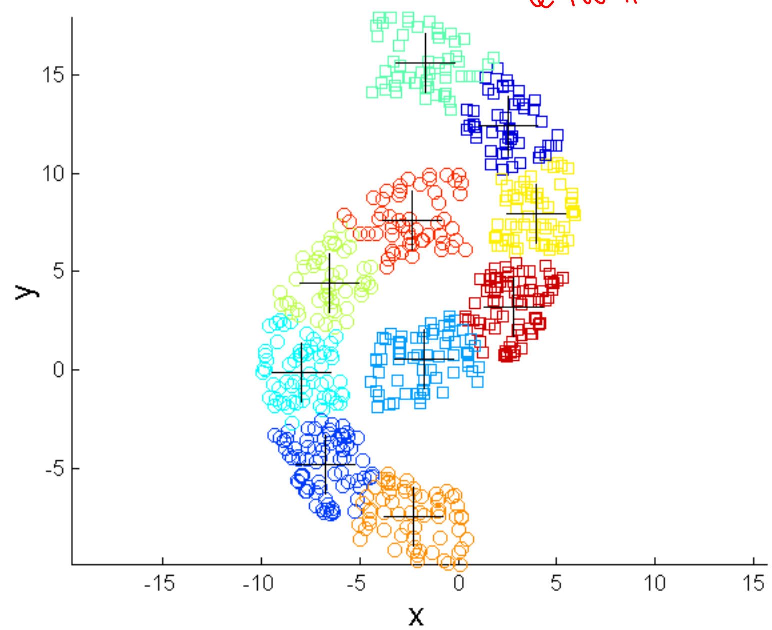
K-means Clusters

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

Overcoming K-means Limitations



Original Points



K-means Clusters

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

Variations

สมาชิก

การไม่ต้องเฉลี่ย

- **K-medoids** → เอาสมาชิกในกลุ่มเป็นตัวแทนเอง
  - 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** → ระยะทางที่ไกลสุด → จะลดสั้น
  - 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

ใช้ lib ที่มีอยู่เลยจ้า

```
>>> 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

เทคนิคต่อไป

DBSCAN

แก้ไขที่ k-mean ทำไม่ได้ → [illegible]

รูปทรงที่ไม่ใช่ทรงกลม

noise ของ data

CE-KMITL

DBSCAN: Density-Based Clustering

พยายามหาจุดที่อยู่ในก้อนเดียวกัน
และเชื่อมต่อกันได้

- 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:

  เราต้องกำหนด
  1
  - 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

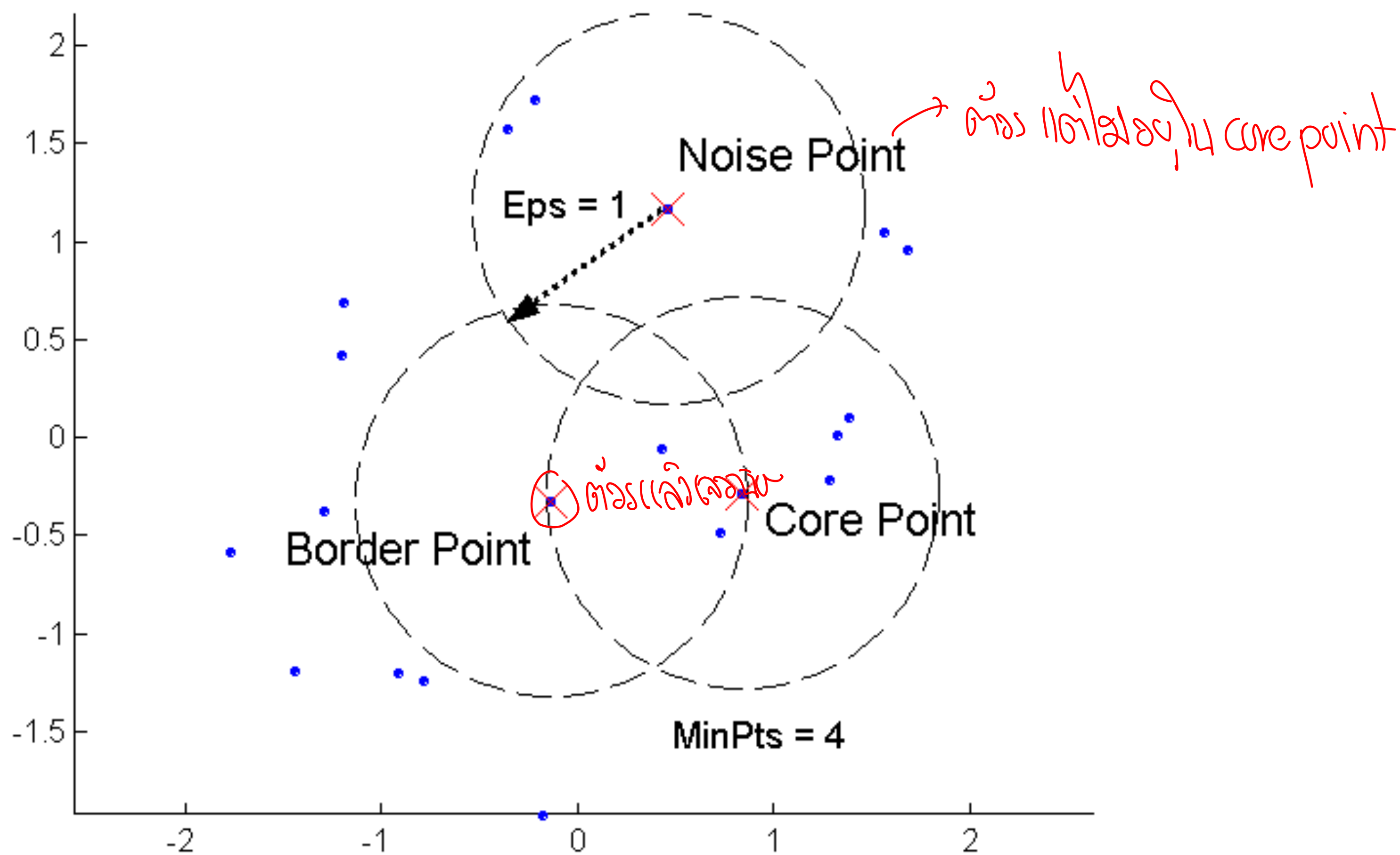
2 หลังจากต้องเลือก eps
แล้วต้องเลือก
เพื่อนับกี่จุด

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

DBSCAN

- Characterization of points ถ้าเราเริ่มต้นสร้างวง eps แล้วจะเกิดจุดทั้งหมด 3 แบบ
  - (1) เจอเพื่อนบ้าน ≥ min_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
  - (2) เจอเพื่อนบ้าน < min_point
  - 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. (3) ไม่เจออะไรเลย ⟶ ตัดทิ้งได้

DBSCAN: Core, Border, and Noise Points

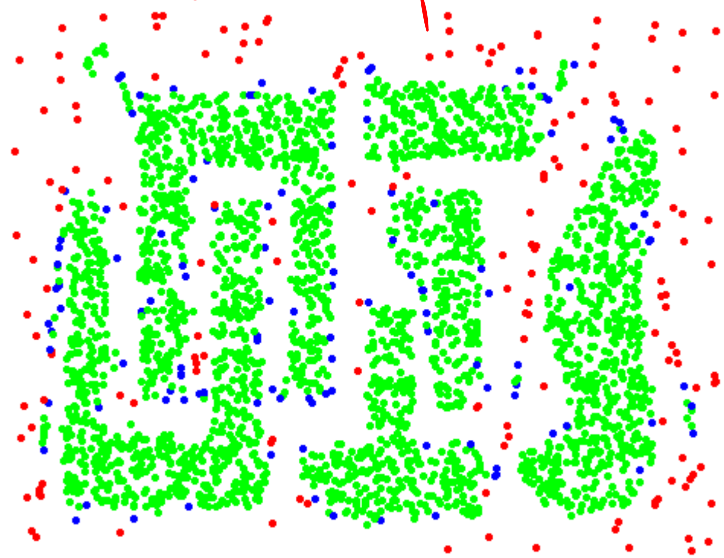


Ref: • Tan, Steinbach, Kumar, “Data Mining”

DBSCAN: Core, Border, and Noise Points

สีเขียวคือ core point

Original Points

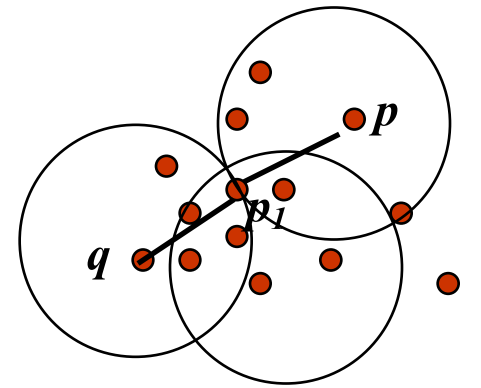


Point types: core, border and noise

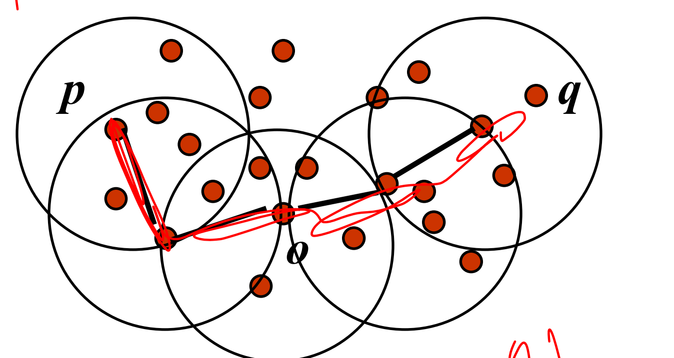
Eps = 10, MinPts = 4

Density-Connected points

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



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



วิ่งระหว่าง core point ไปเรื่อยๆ

DBSCAN Algorithm

(1) กำหนด label ให้ data

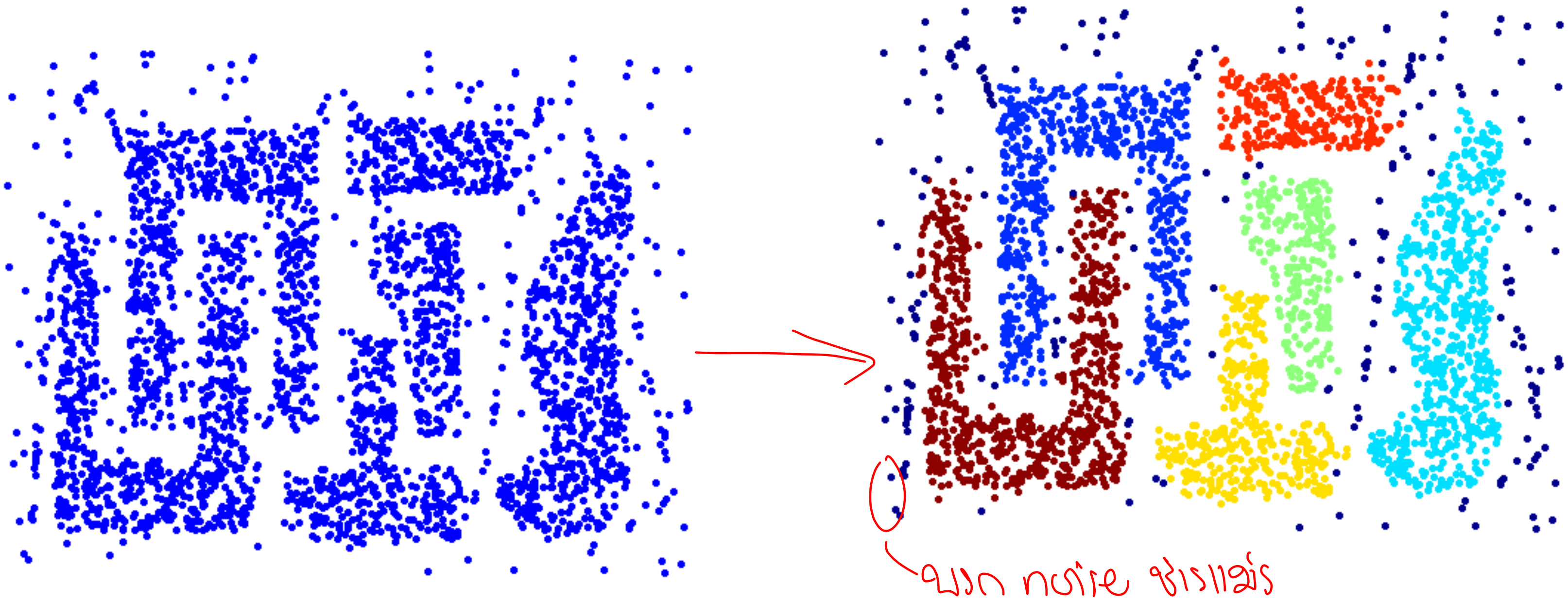
- Label points as core, border and noise
- Eliminate noise points (2) ลบทิ้ง
- For every core point p that has not been assigned to a cluster

  เอา core point ที่เชื่อมกันได้มาเป็น cluster เดียวกัน

  - 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

Cluster Validation

วัดความถูกต้องของ cluster

วัดว่าในกลุ่มเดียวกันต้องคล้าย

ต่างกัน ต้องไม่เหมือน

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. ตัวชี้วัด 3 แบบ
  - External Index: Used to measure the extent to which cluster labels match externally supplied class labels.
    การเปรียบเทียบกับกลุ่มที่มีเฉลยจัดอยู่แล้ว → entropy
    - Entropy
  - Internal Index: Used to measure the goodness of a clustering structure *without* respect to external information.
    วัดความเหมือนกันในกลุ่มตัวเอง → SSE
    - 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
      การเทียบกับเทคนิคอื่น ดูว่าอันไหน ใช้ค่า SSE, entropy ที่ดี
- 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.

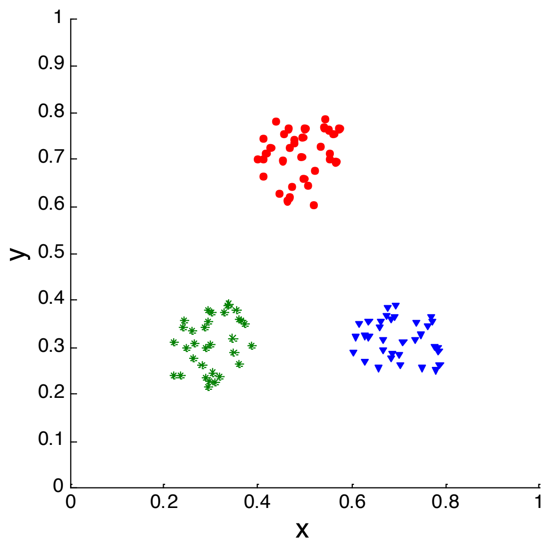
Ref: • Tan, Steinbach, Karpatne, Kumar, “Introduction to Data Mining (Second Edition)”

Measuring Cluster Validity Via Correlation

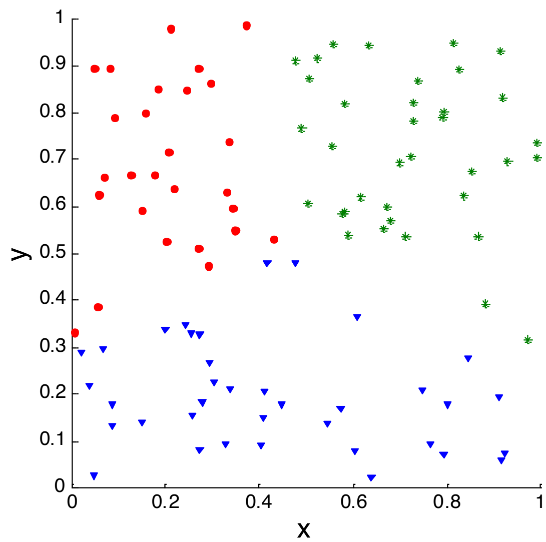
- Two matrices
  - Proximity Matrix
  - Ideal Similarity Matrix
    - One row and one column for each data point
    - An entry is 1 if the associated pair of points belong to the same cluster
    - An entry is 0 if the associated pair of points belongs to different clusters
- Compute the correlation 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

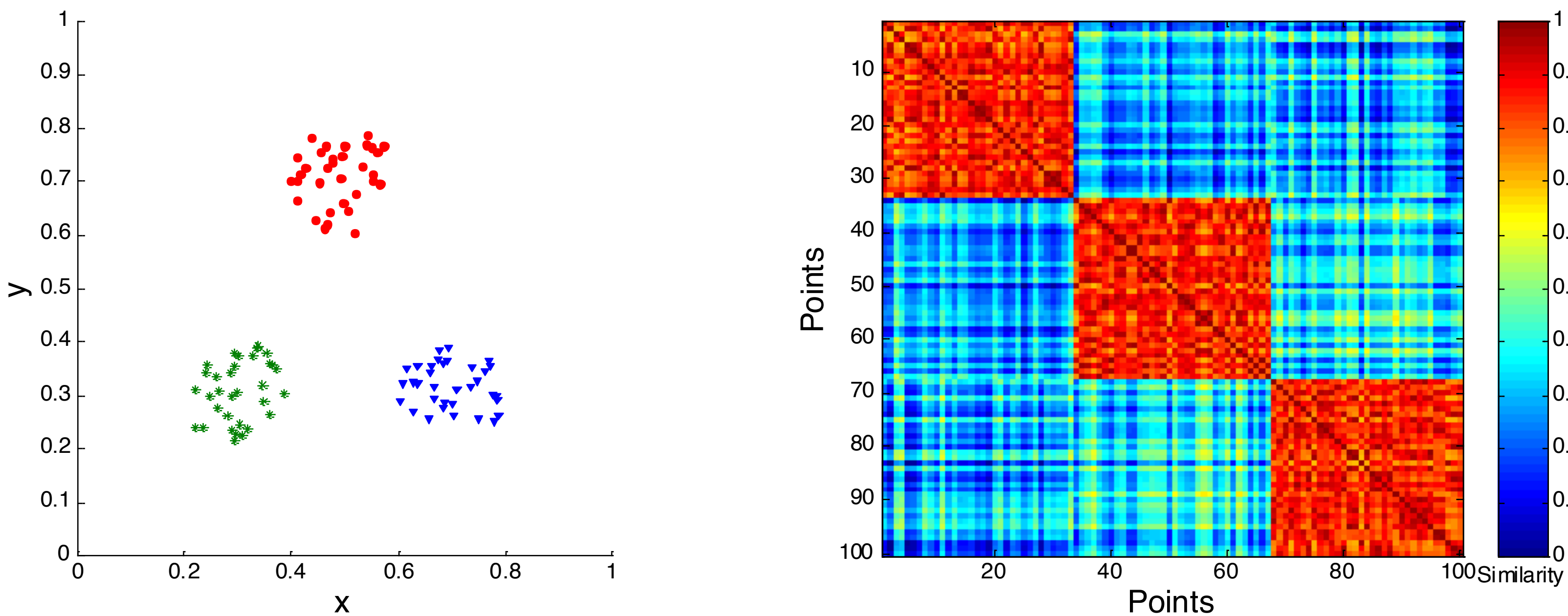


Corr = -0.5810

Using Similarity Matrix for Cluster Validation

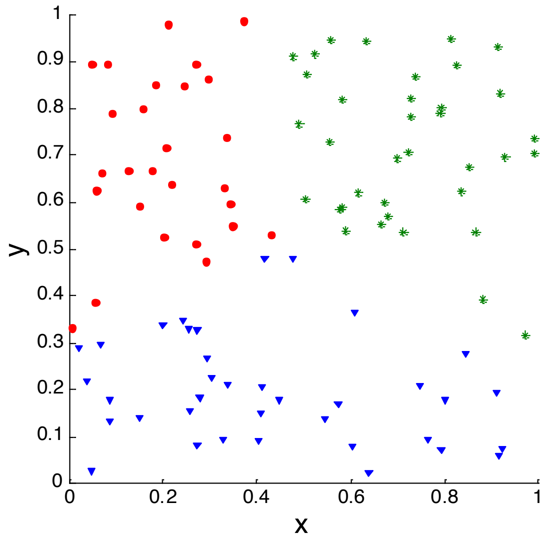
- Order the similarity matrix with respect to cluster labels and inspect visually.

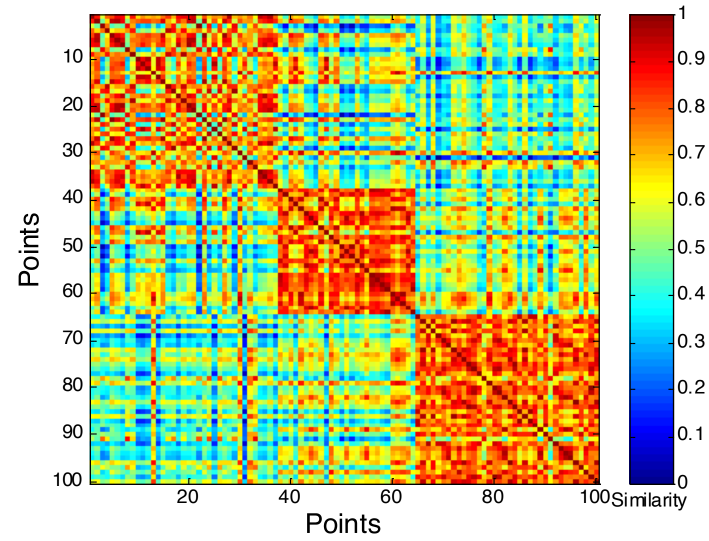
หาความหนาแน่นของจุด



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

Using Similarity Matrix for Cluster Validation

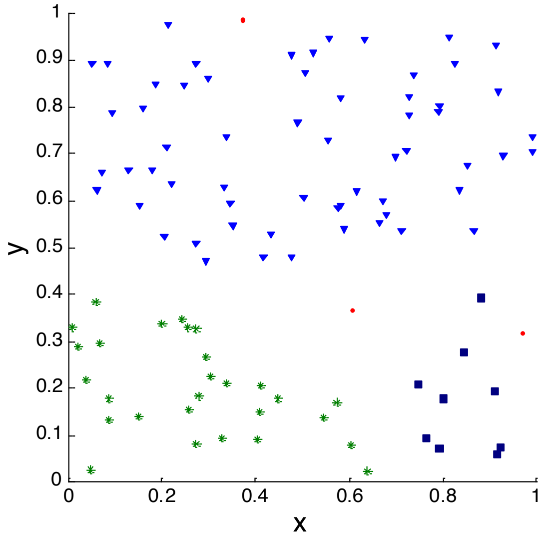


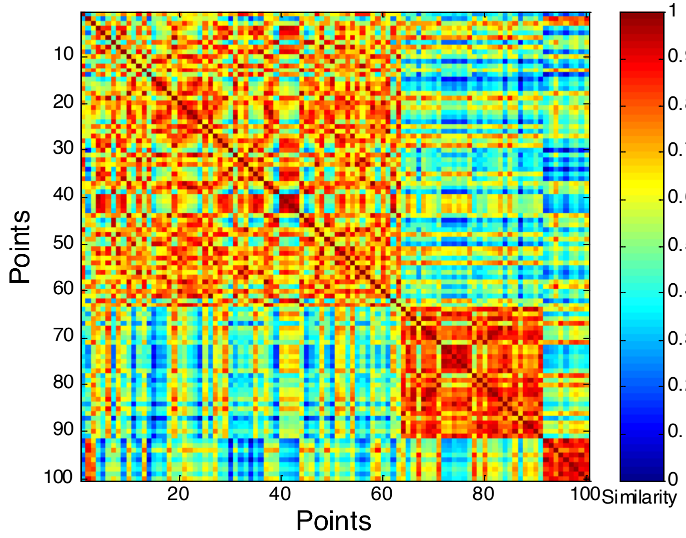


K-means

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

Using Similarity Matrix for Cluster Validation





DBSCAN

Dimensionality Reduction

เมื่อเกิน feature มากๆ

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 ens
  - 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.

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

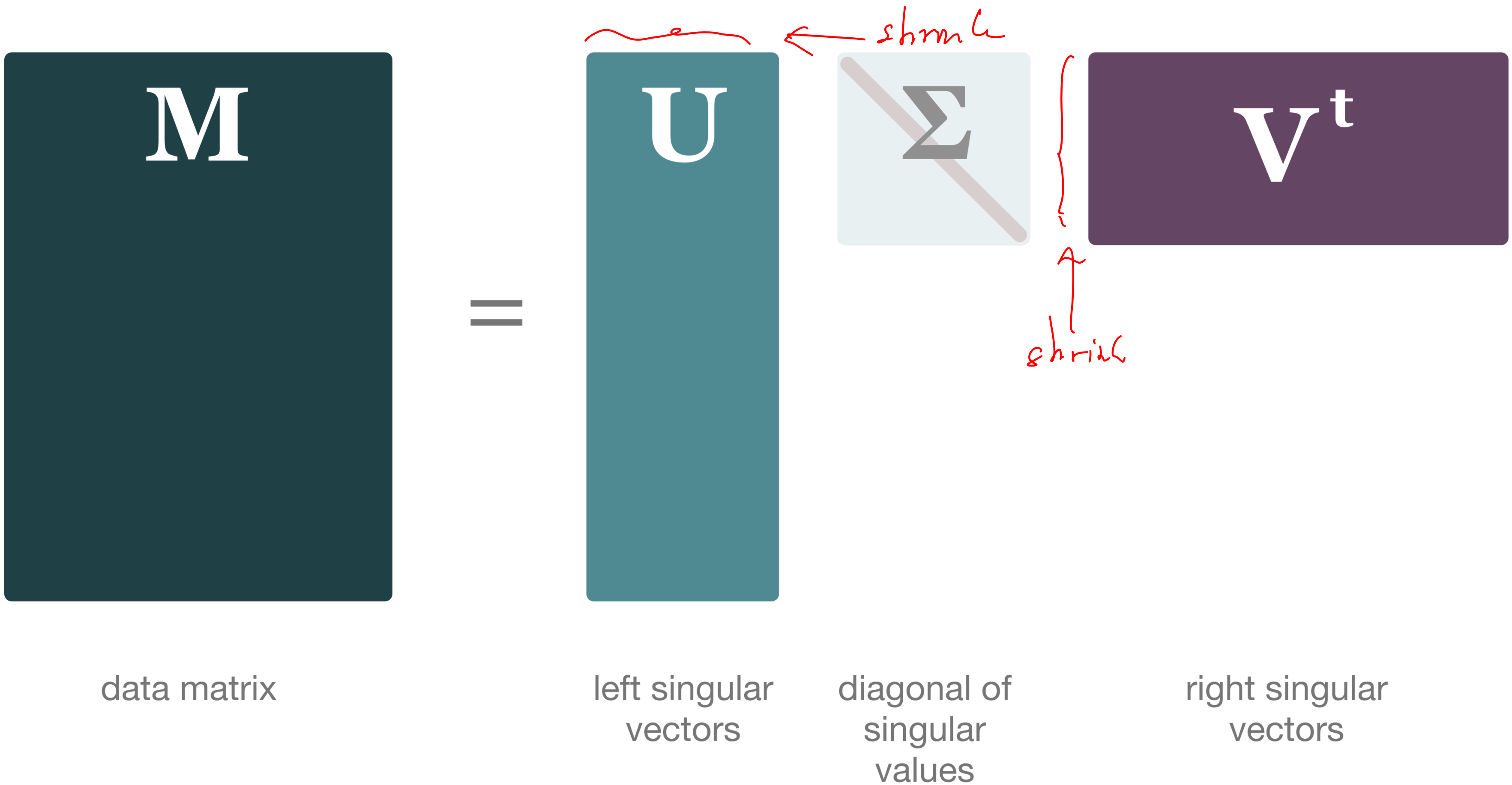
Ref: • Tan, Steinbach, Karpatne, Kumar, "Introduction to Data Mining (Second Edition)"

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).

SVD (Singular Value Decomposition)

ได้ matrix ใหม่มา 3 อัน



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

SVD

- Example

นำไป cluster ต่อได้เลย

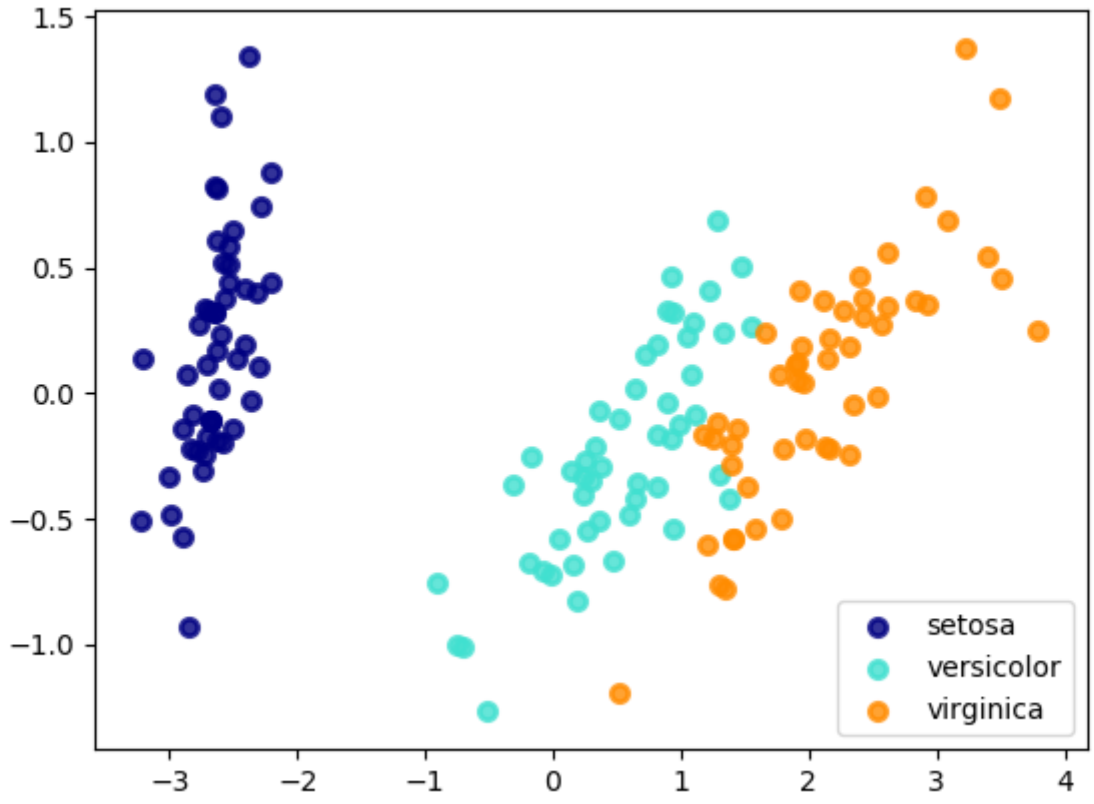
เหลือมิติที่<u>น้อยลง</u>

ไวขึ้น

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

Plot

- Dimensionality Reduction of the Iris Dataset



Python

ที่จารย์ให้ไปดูเมื่อเทอมก่อน เขียนแยกไว้แล้ว

```
>>> 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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