人工智能

无监督(聚类)算法

Cluster Analysis

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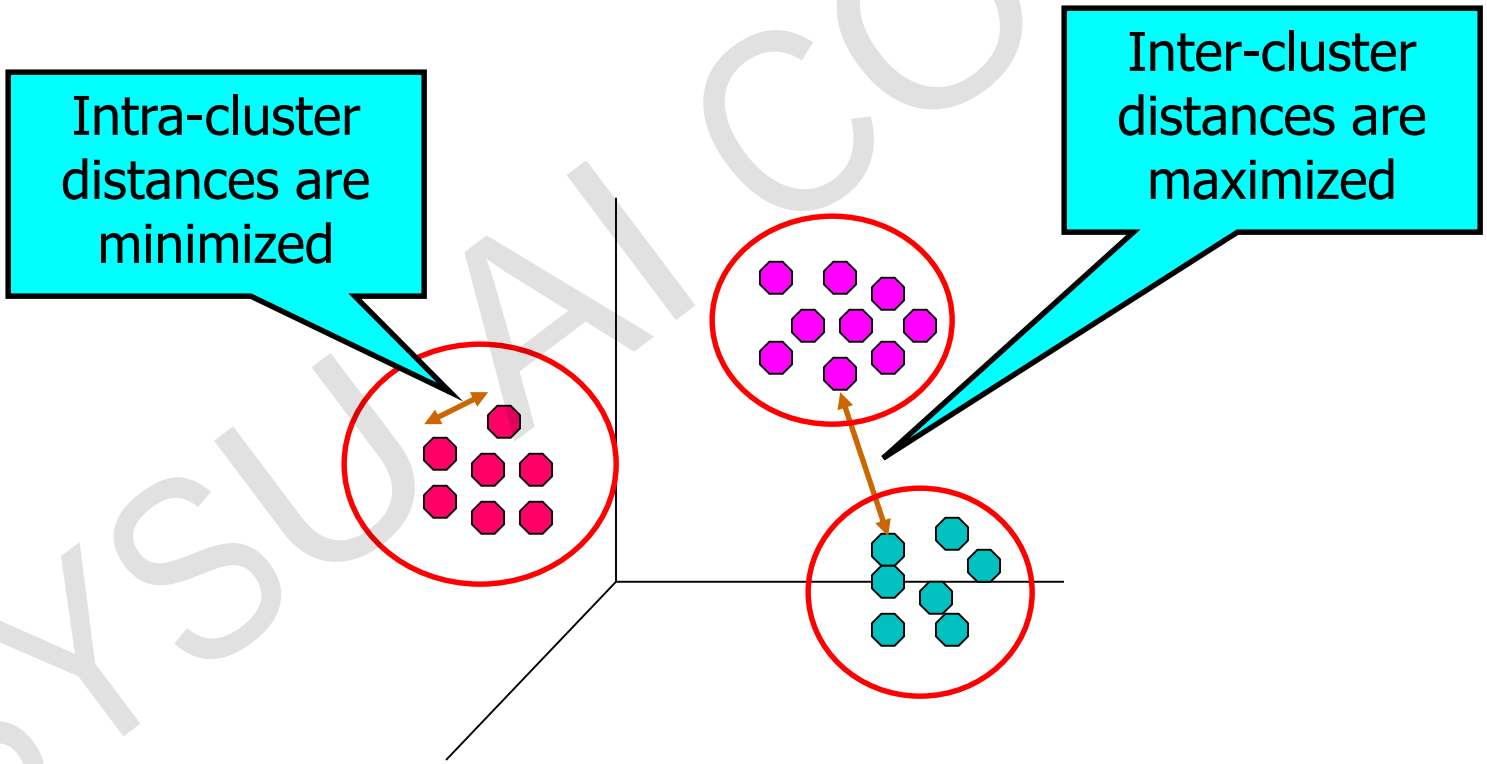
SUN YAT-SEN UNIVERSITY

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

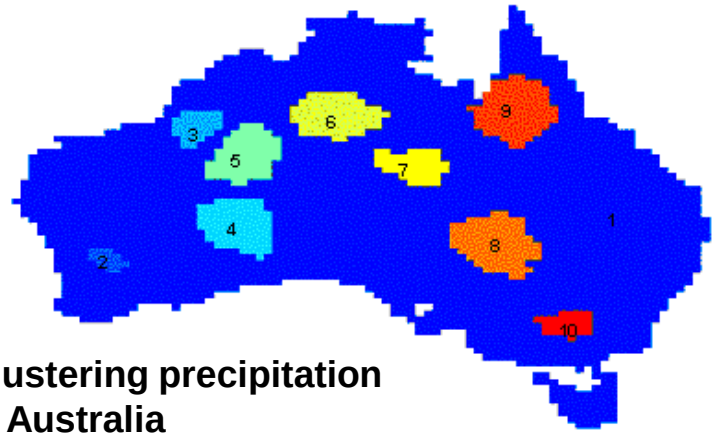
Understanding

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

	Discovered Clusters	*Industry Group*
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,Oracl-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

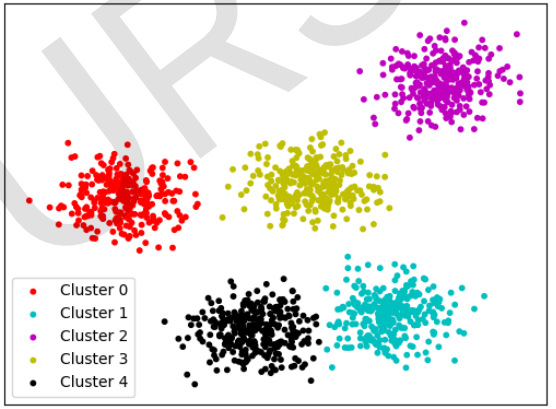
Summarization

- Reduce the size of large data sets

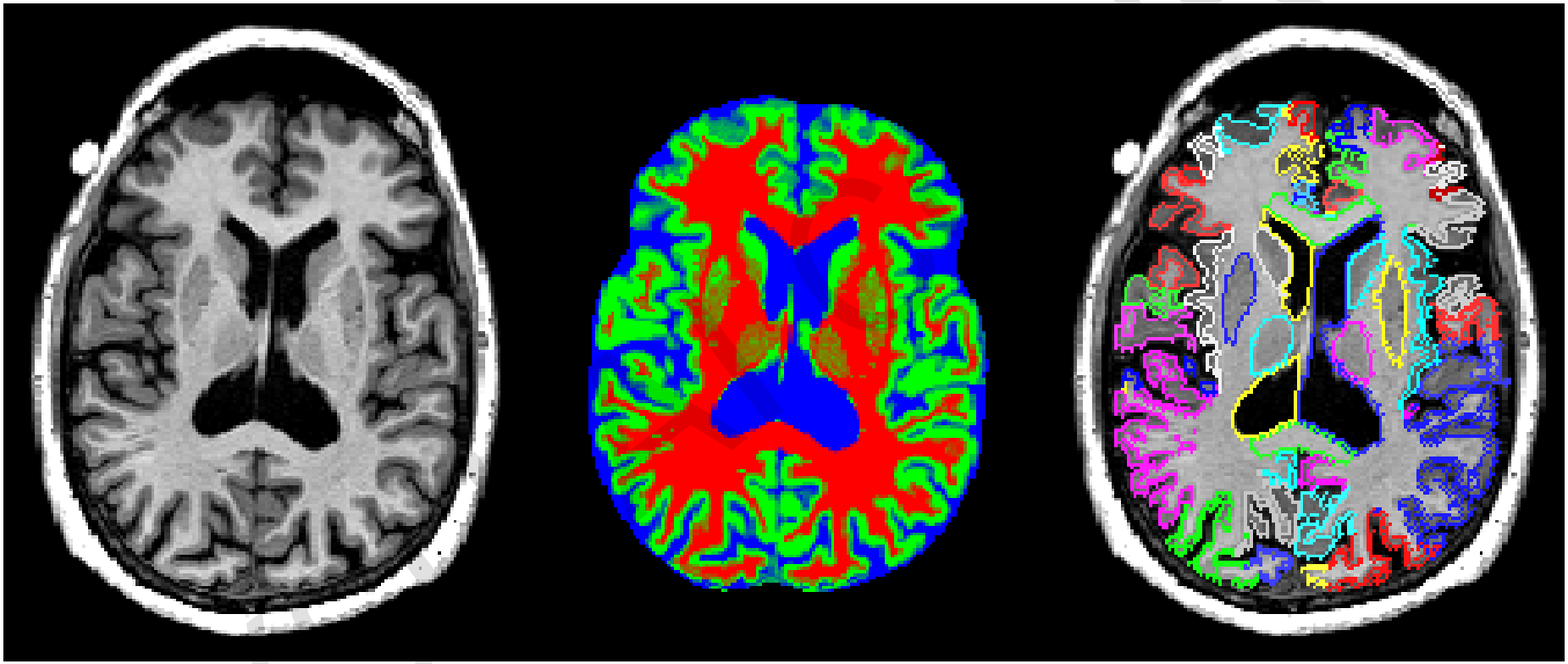


Clustering precipitation in Australia

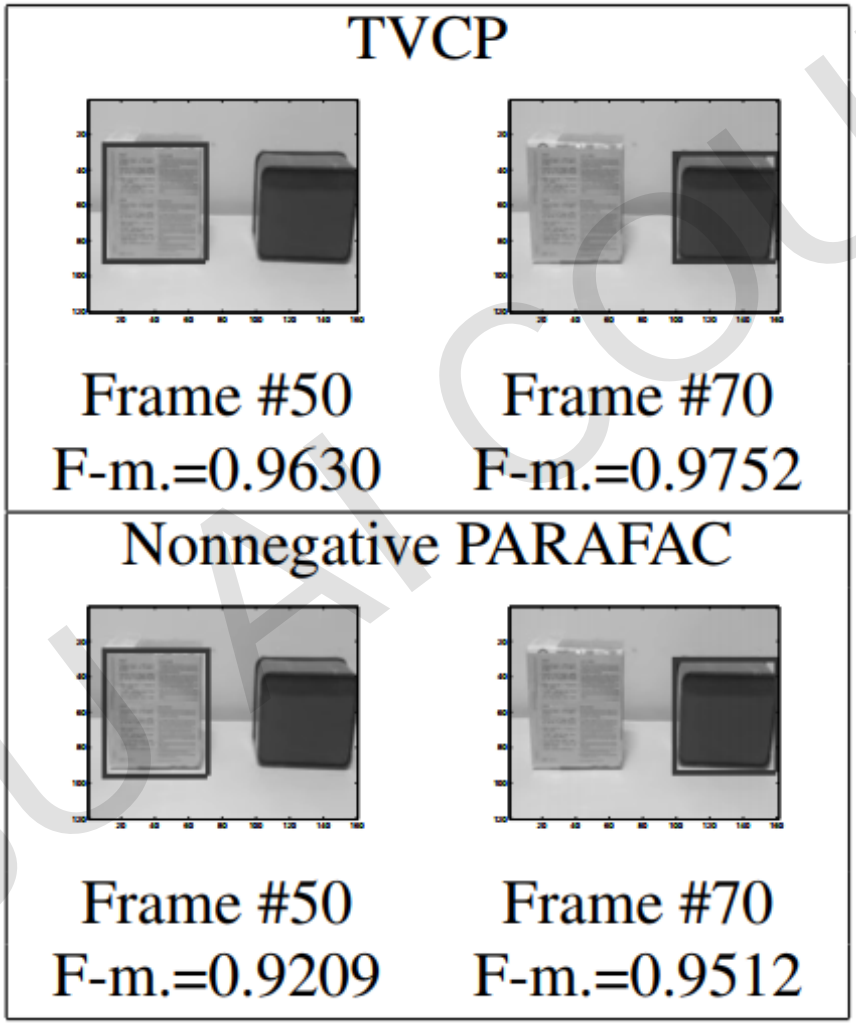
Clustering in Social Network



Clustering in Image Segmentation



Clustering in Video Detection



What is not Cluster Analysis?

Supervised classification

- Have class label information

Simple segmentation

- Dividing students into different registration groups alphabetically, by last name

Notion of a Cluster can be Ambiguous

How many clusters?

Six Clusters

Two Clusters

Four Clusters

Notion of a Cluster can be Ambiguous

What is a natural grouping among these objects?

Types of Clusterings

A clustering is a set of clusters

Important distinction between hierarchical and partitional sets of clusters

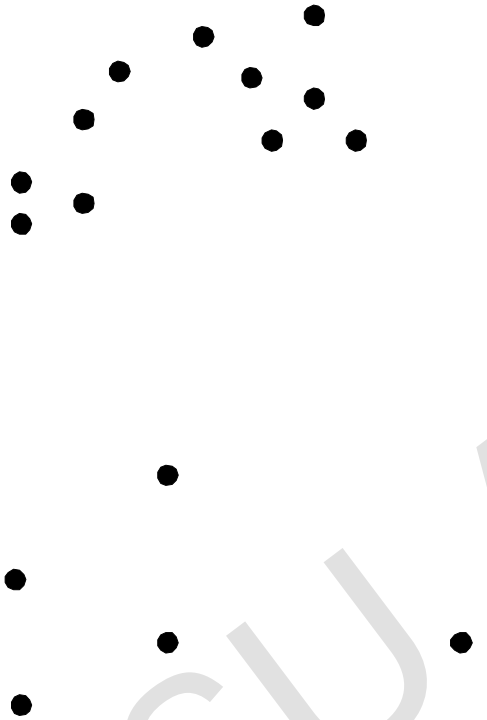
Partitional Clustering (分割式聚类)

- A division data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset
- # clusters is needed, kmeans….

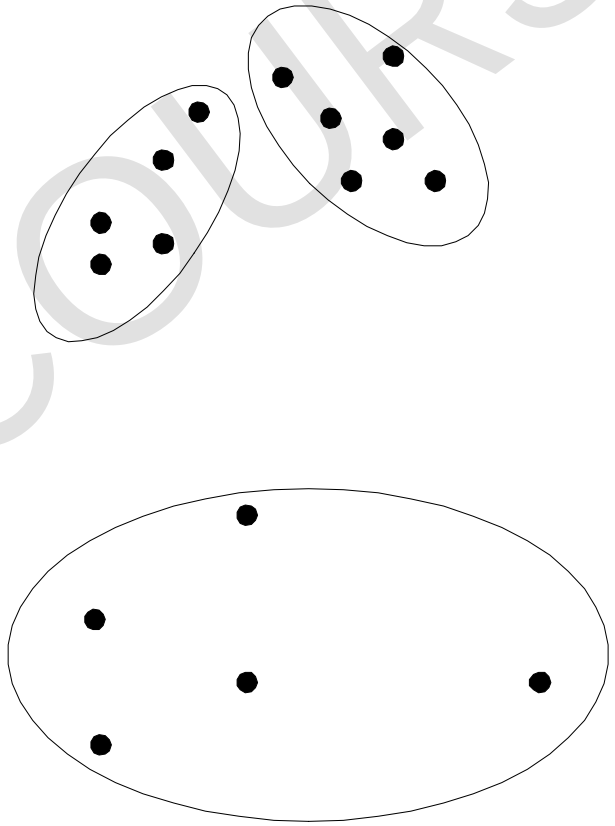
Hierarchical clustering (阶层式聚类)

- A set of nested clusters organized as a hierarchical tree
- # clusters is not needed

Partitional Clustering

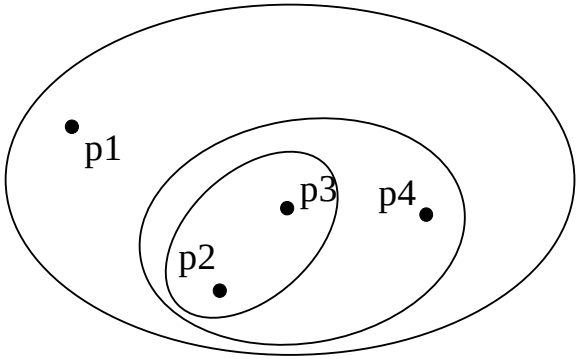


Original Points

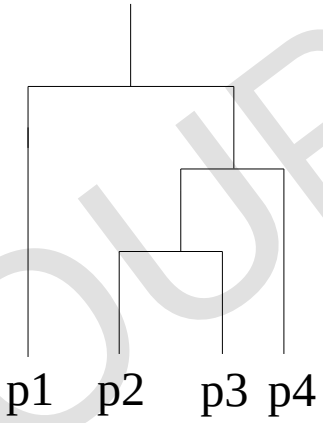


A Partitional Clustering

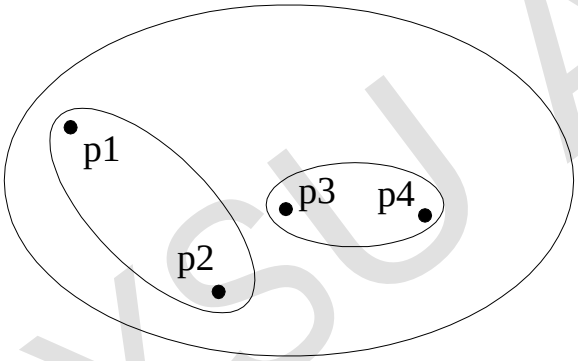
Hierarchical Clustering



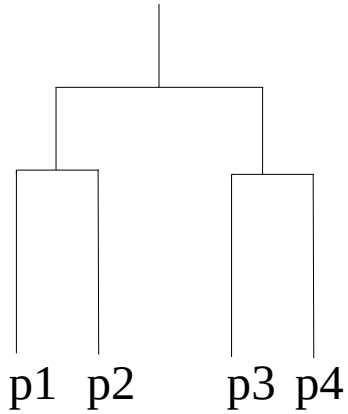
Traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Hierarchical Clustering



Non-traditional Dendrogram

Other Distinctions Between Sets of Clusters

Fuzzy versus non-fuzzy 模糊聚类

- 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 异质vs同质

- Cluster of widely different sizes, shapes, and densities

Types of Clusters

Well-separated clusters

Center-based clusters

Contiguous clusters

Density-based clusters

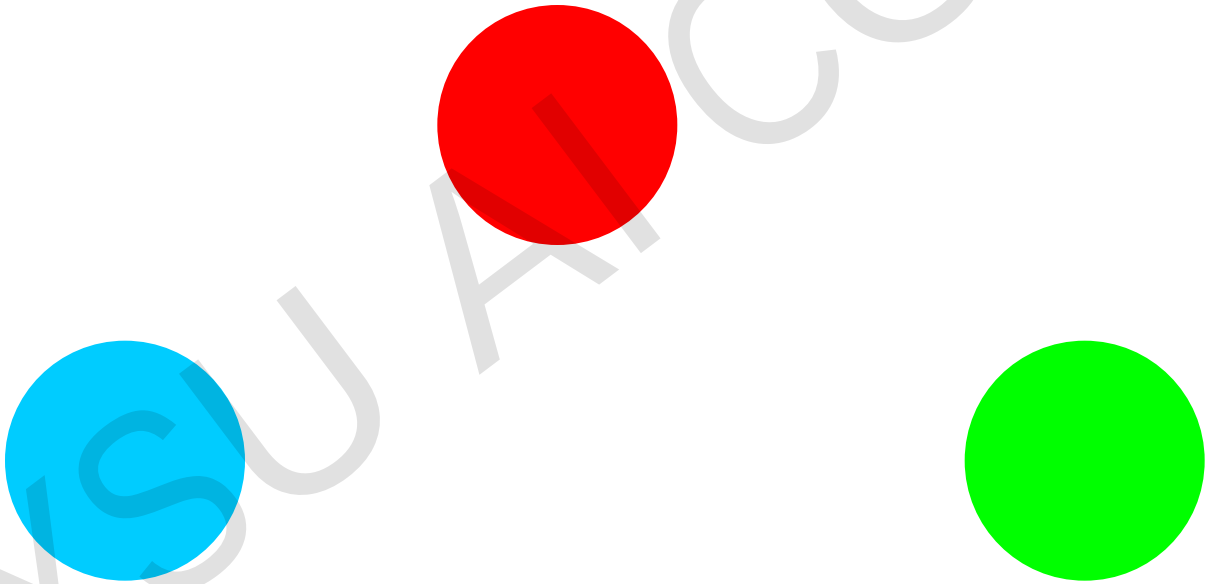
Property or Conceptual

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

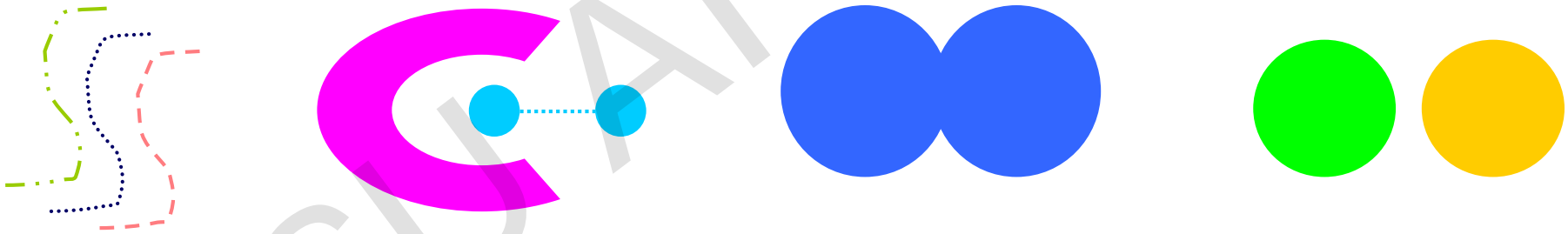
- A cluster is a set of objects such that an object in a cluster is closer (more similar) to the “center” of a cluster, than to the center of any other cluster
- The center of a cluster is often a centroid, the average of all the points in the cluster, or a medoid, the most “representative” point of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

4 center-based clusters

Types of Clusters: Contiguity(邻近)-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.

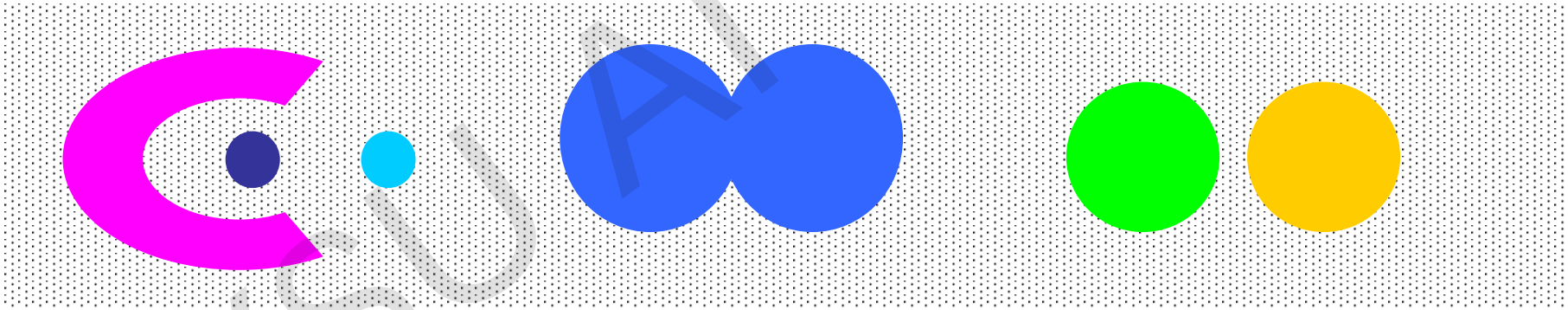


8 contiguous clusters

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(不规则or纠缠), and when noise and outliers are present.

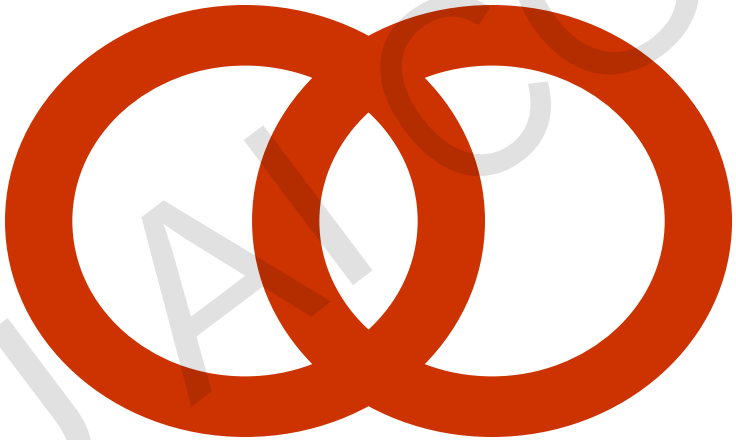


6 density-based clusters

Types of Clusters: Conceptual(概念) Clusters

Shared Property or Conceptual Clusters

- Finds clusters that share some common property or represent a particular concept.



2 Overlapping Circles

Types of Clusters: Objective Function

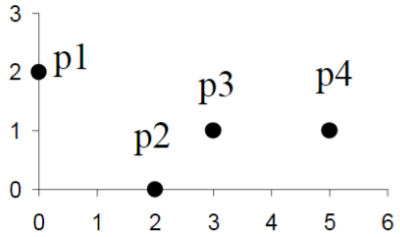
Clusters Defined by an Objective Function

- Finds clusters that minimize or maximize an objective function.
- **穷举法：** Enumerate all possible ways of dividing the points into clusters and evaluate the `goodness' of each potential set of clusters by using the given objective function. (NP Hard)
- Can have global or local objectives.
  - Hierarchical clustering algorithms typically have local objectives
  - Partitional algorithms typically have global objectives

Types of Clusters: Objective Function …

Map the clustering problem to a different domain and solve a related problem in that domain

- Proximity（亲近度） matrix defines a weighted graph, where the nodes are the data points, and the weighted edges represent the proximities (similarity or dissimilarity) between data points



point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1

	p1	p2	p3	p4
p1	0.000	2.828	3.162	5.099
p2	2.828	0.000	1.414	3.162
p3	3.162	1.414	0.000	2.000
p4	5.099	3.162	2.000	0.000

Figure Four points and their corresponding data and proximity (distance) matrices.

- Similarity? Dissimilarity?

Euclidean Distance / Manhattan Distance / Chebyshev Distance/

Cosine Similarity /…..

Similarity=1-Dissimilarity

Bonus: Some Distance Metrics

$$L_p(x_1, x_2) = \left(\sum_{l=1}^{n} \left| x_i^{(l)} - x_j^{(l)} \right|^p \right)^{\frac{1}{p}}$$

$$L_1(x_1, x_2) = \sum_{l=1}^{n} \left| x_i^{(l)} - x_j^{(l)} \right|$$ Manhattan Distance

$$L_2(x_1, x_2) = \sum_{l=1}^{n} \sqrt{\left(x_i^{(l)} - x_j^{(l)} \right)^2}$$ Euclidean Distance

$$L_\infty(x_1, x_2) = \sqrt[\infty]{\sum_{l=1}^{n} \left| x_i^{(l)} - x_j^{(l)} \right|^\infty} = max\left(\left| x_i - x_j \right| \right)$$

Chebyshev Distance

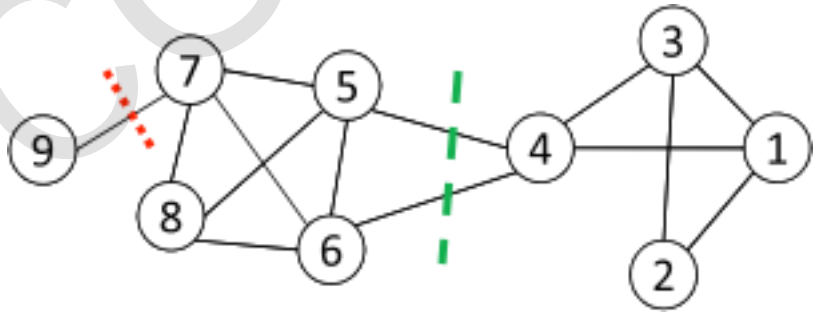
$$L_{-\infty}(x_1, x_2) = \sqrt[-\infty]{\sum_{l=1}^{n} \left| x_i^{(l)} - x_j^{(l)} \right|^{-\infty}} = min\left(\left| x_i - x_j \right| \right)$$

Cosine Distance: $D(x_1, x_2) = 1 - \cos(x_1, x_2) = 1 - \frac{x_1 \cdot x_2}{||x_1||_2 ||x_2||_2}$

Types of Clusters: Objective Function …

- Clustering is equivalent to breaking the graph into connected components, one for each cluster.

- Want to minimize the edge weight between clusters and maximize the edge weight within clusters



$$\text{Ratio Cut}(\pi) = \frac{1}{k}\sum_{i=1}^{k}\frac{cut(C_i, \bar{C}_i)}{|C_i|},$$

$$\text{Normalized Cut}(\pi) = \frac{1}{k}\sum_{i=1}^{k}\frac{cut(C_i, \bar{C}_i)}{vol(C_i)}$$

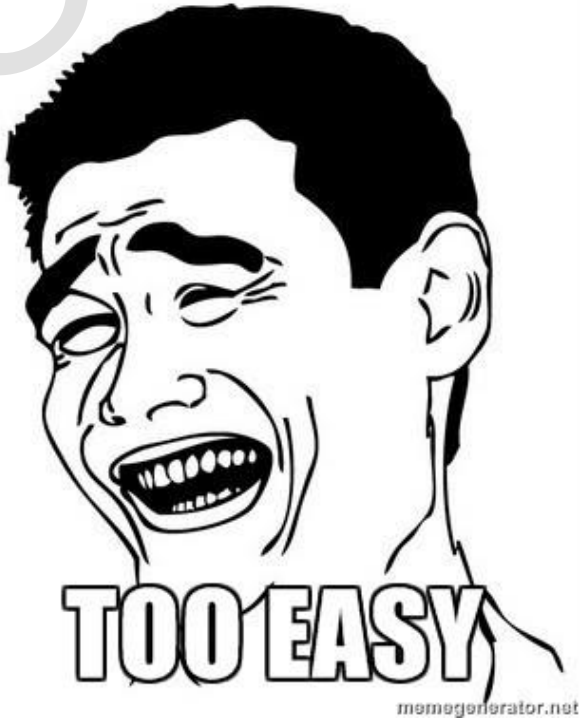
C_i: a community
$|C_i|$: # nodes in C_i
$vol(C_i)$: sum of degrees in C_i

Clustering Algorithms

Hierarchical clustering (Omit, because…)

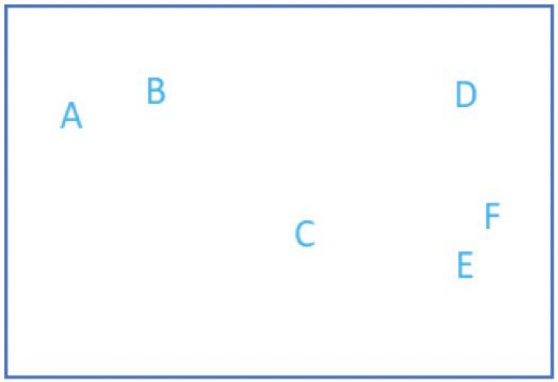
K-means and its variants

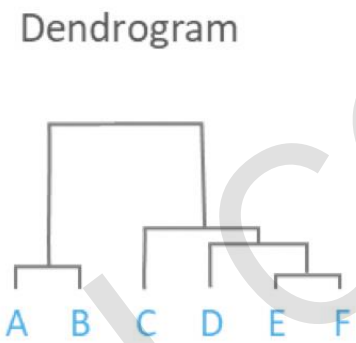
Density-based clustering



Clustering Algorithms

Hierarchical clustering

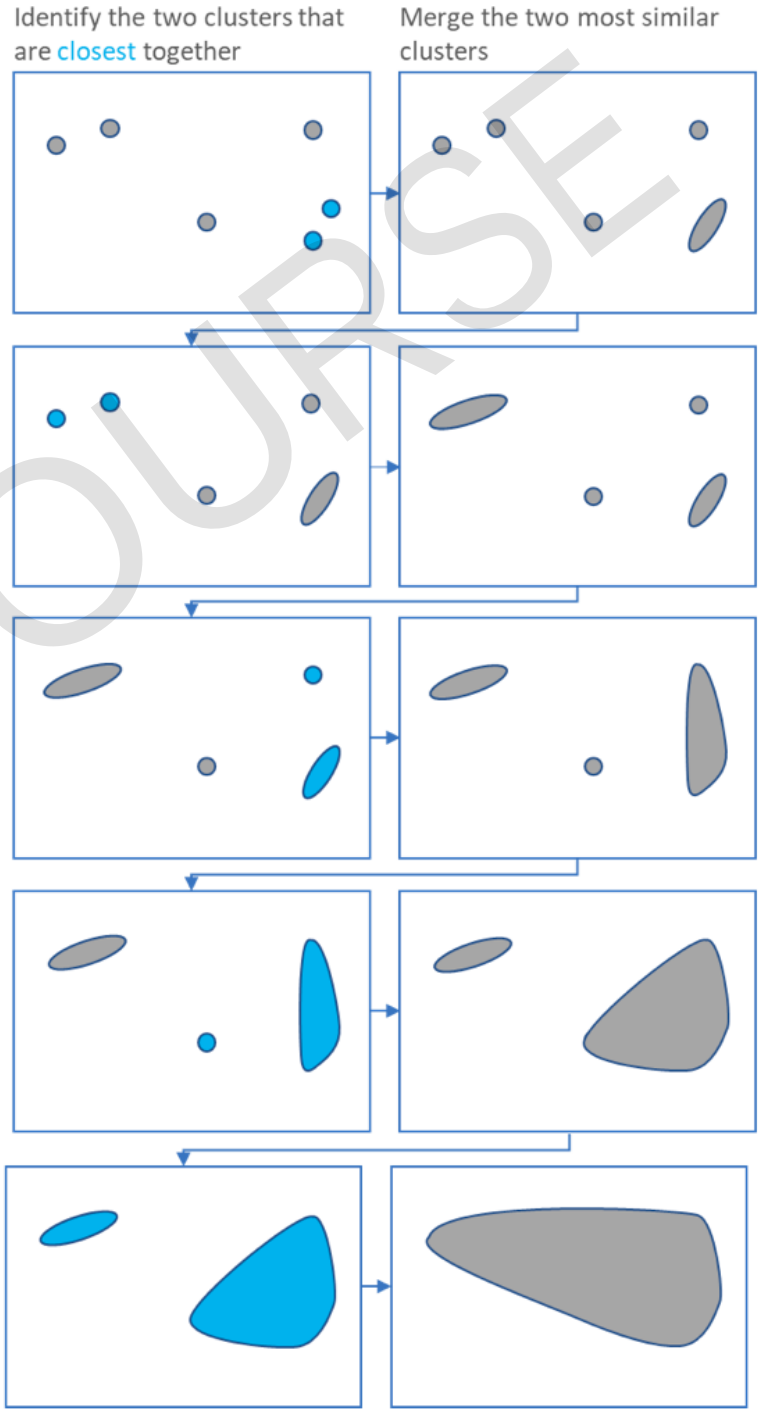




Hierarchical clustering starts by treating each observation as a separate cluster.

Then, it repeatedly executes the following two steps:
(1) identify the two clusters that are closest together,
(2) merge the two most similar clusters.

This iterative process continues until all the clusters are merged together.



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 basic algorithm is very simple

1: Select K points as the initial centroids.
2: **repeat**
3: Form K clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: **until** The centroids don't change

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https://www.naftaliharris.com/blog/visualizing-k-means-clustering/

K-means Clustering – Details

Initial centroids are often chosen randomly.

- Clusters produced vary from one run to another.

The centroid is (typically) the mean of the points in the cluster.

'Closeness' is measured by Euclidean distance, cosine similarity, correlation, etc.

K-means will converge for common similarity measures mentioned above.

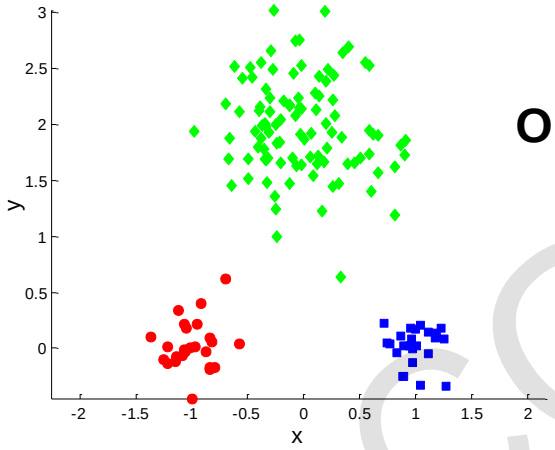
Most of the convergence happens in the first few iterations.

- Often the stopping condition is changed to 'Until relatively few points change clusters'

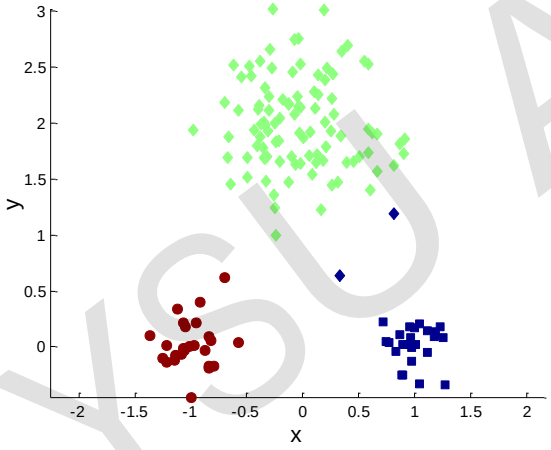
Complexity is O(n * K * I * d)

- n = number of points, K = number of clusters, I = number of iterations, d = number of attributes

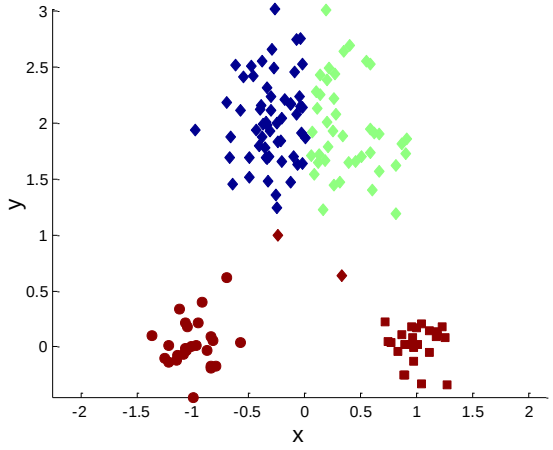
Two different K-means Clusterings



Original Points

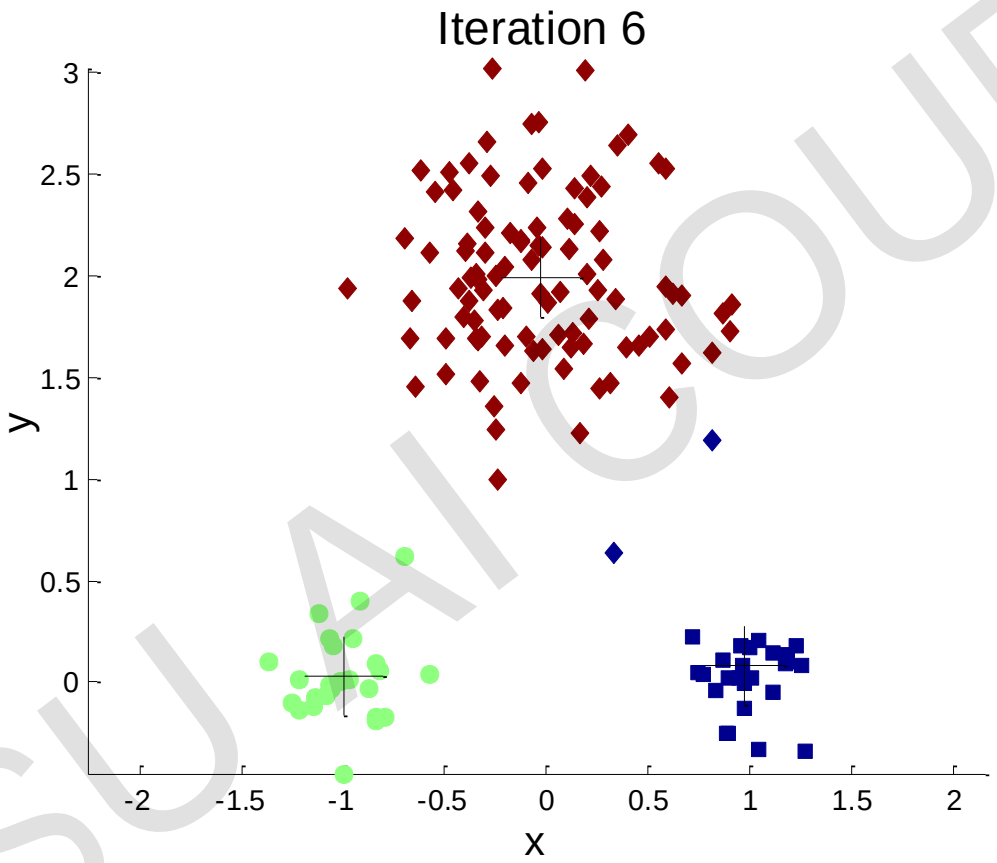


Optimal Clustering

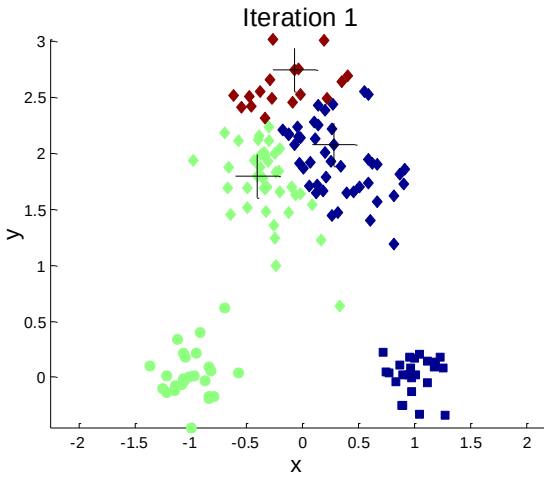


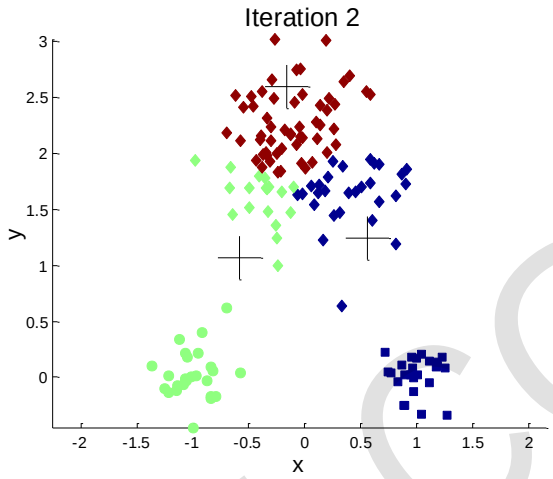
Sub-optimal Clustering

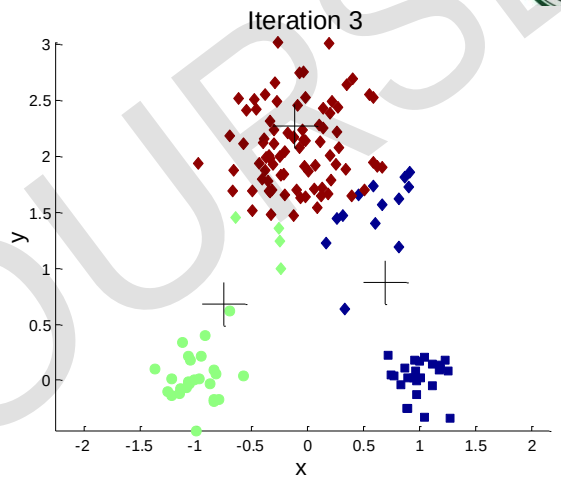
Importance of Choosing Initial Centroids

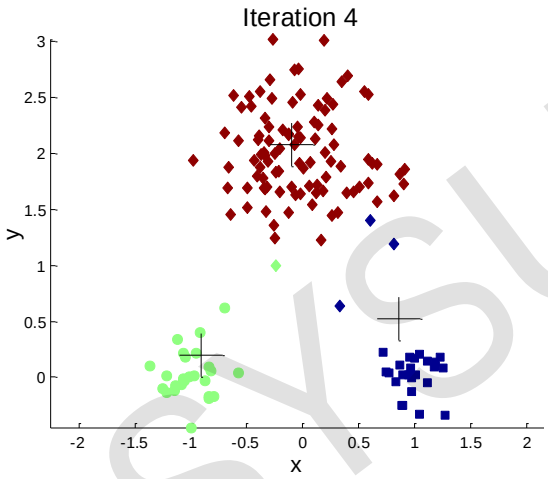


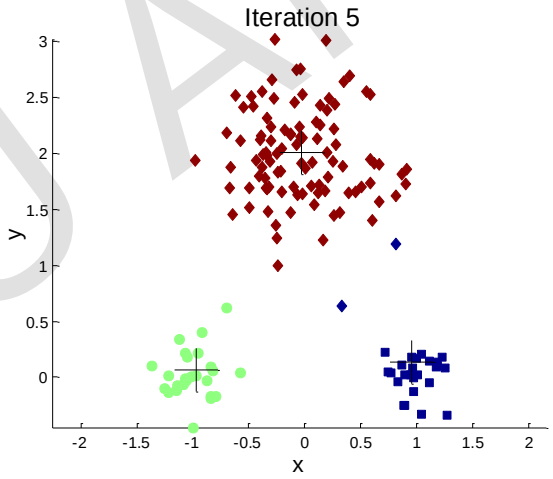
Importance of Choosing Initial Centroids

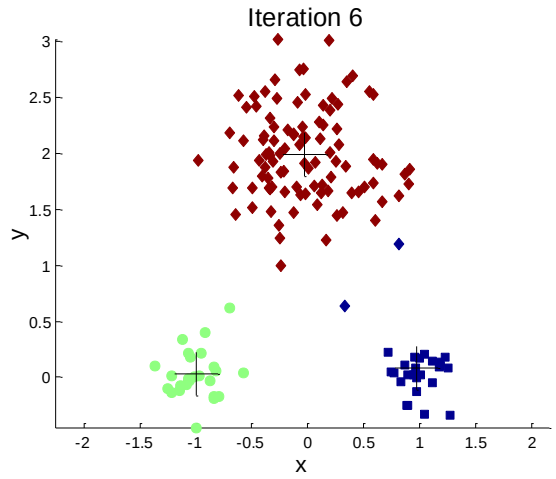












Evaluating K-means Clusters

Most common measure is Sum of Squared Error (SSE)

- For each point, the error is the distance to the nearest cluster
- To get SSE, we square these errors and sum them.

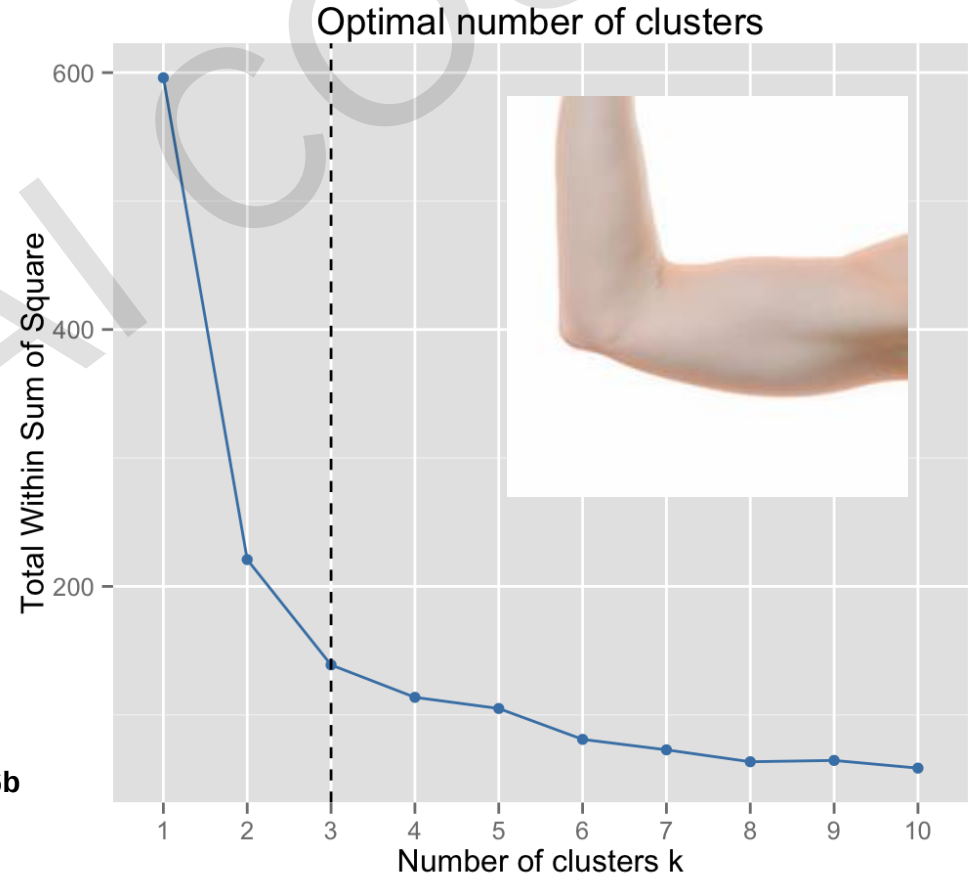
$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(m_i, x)$$

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

Bonus: how to choose a lovely “K”

- **Elbow method:** plot a line chart of the SSE for each value of k. If the line chart looks like an arm, then the "elbow" on the arm is the value of K that is the best.

手臂曲线的肘关节



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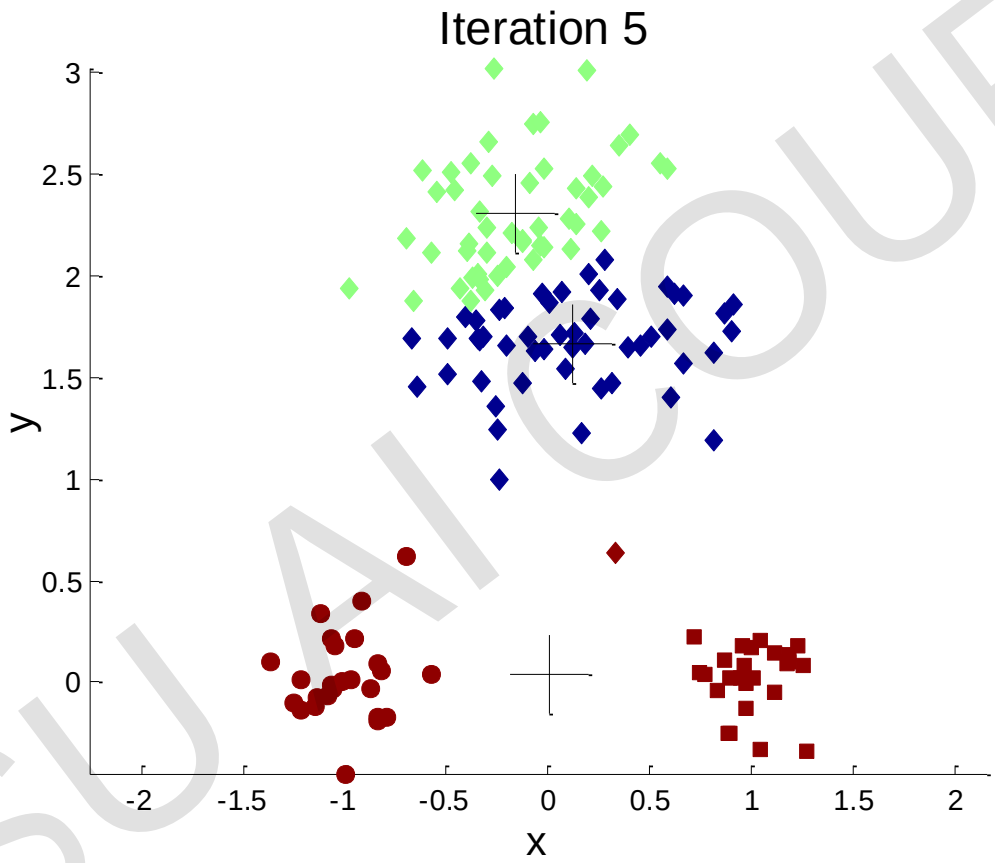
Importance of Choosing Initial Centroids ...



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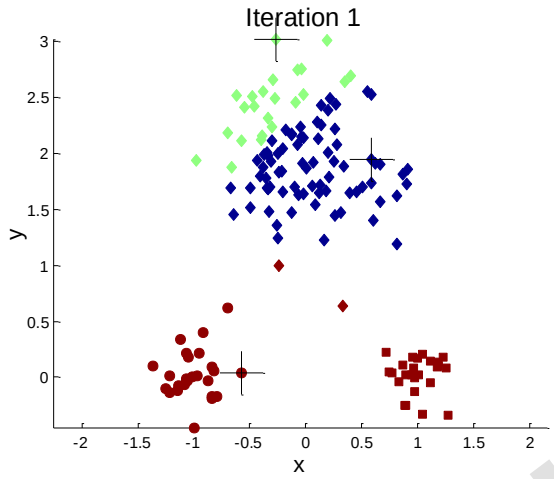
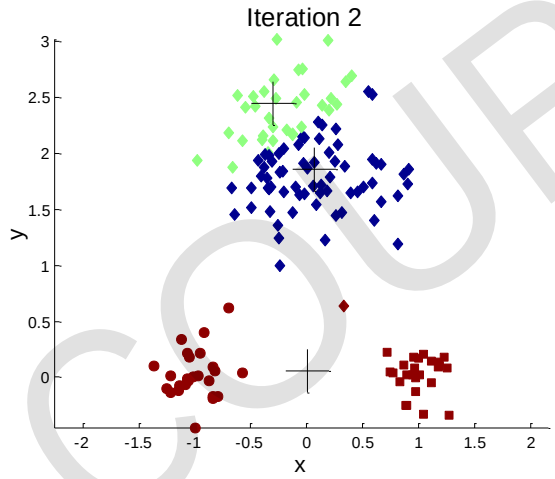
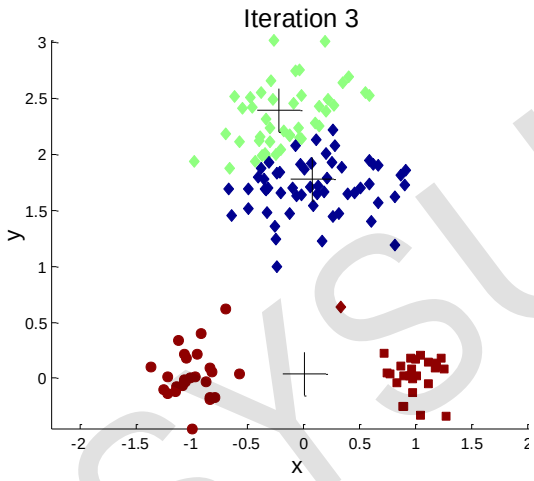
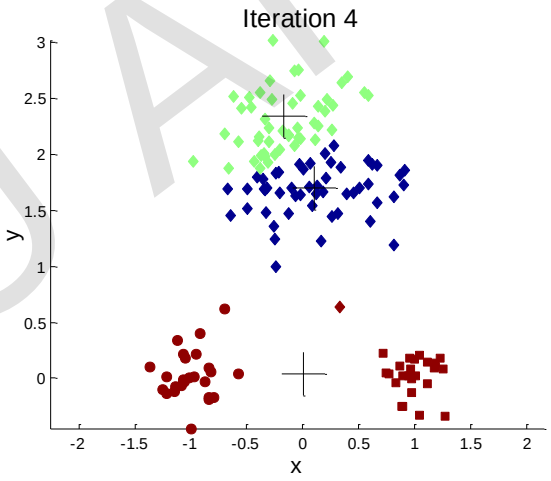
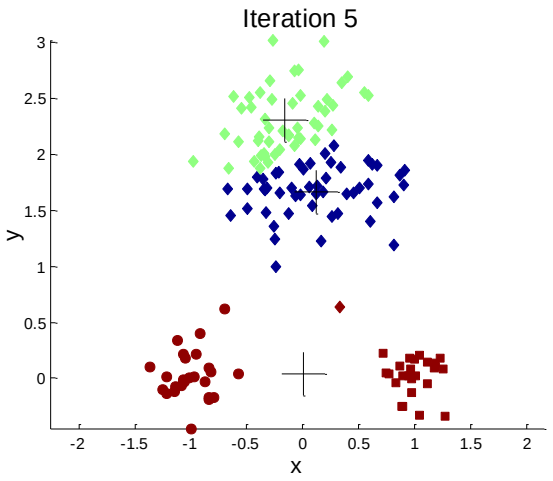


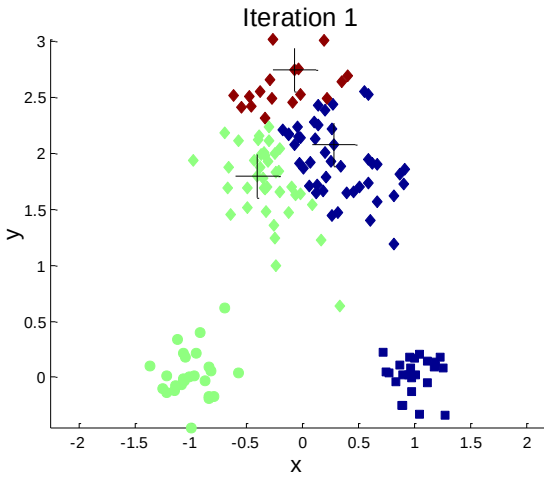


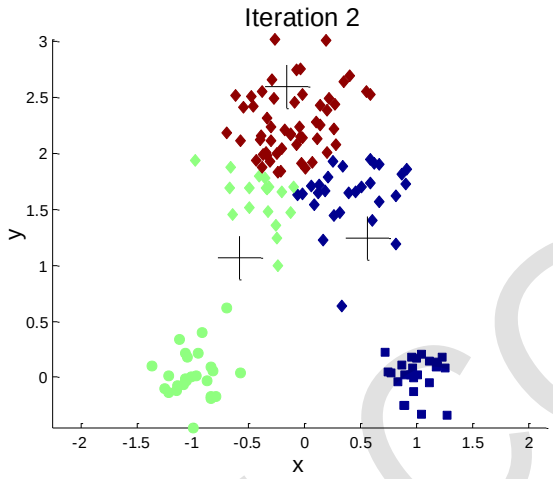


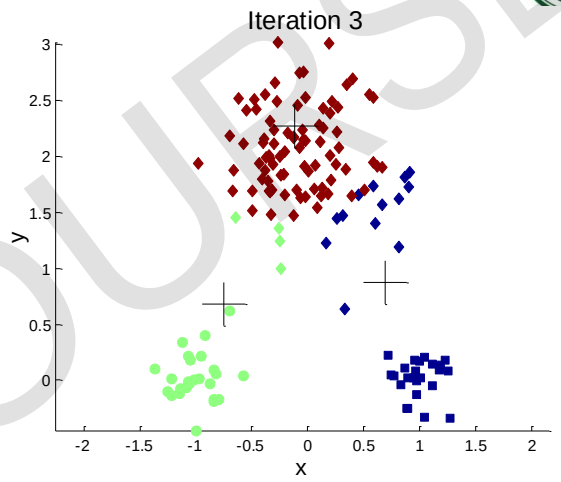


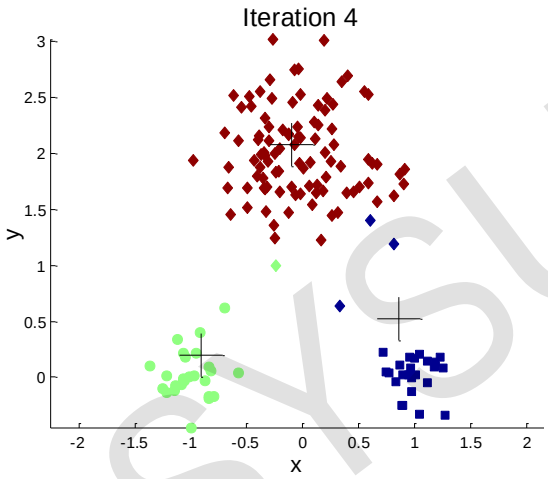


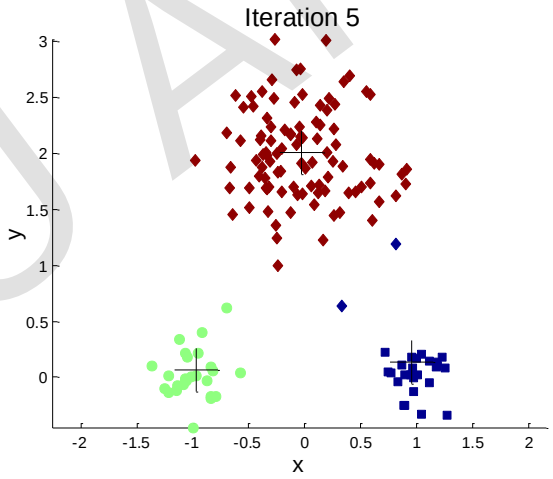
Importance of Choosing Initial Centroids

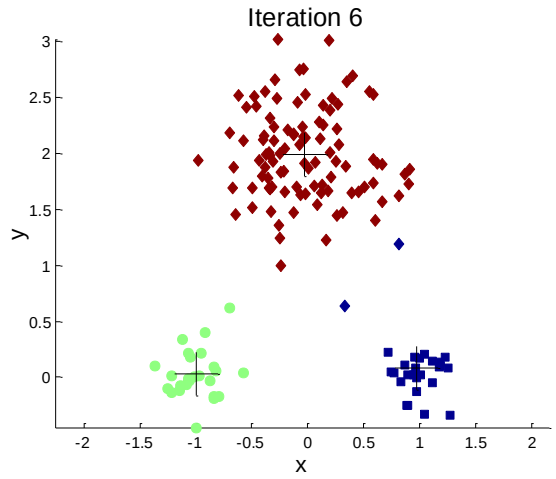












Problems with Selecting Initial Points

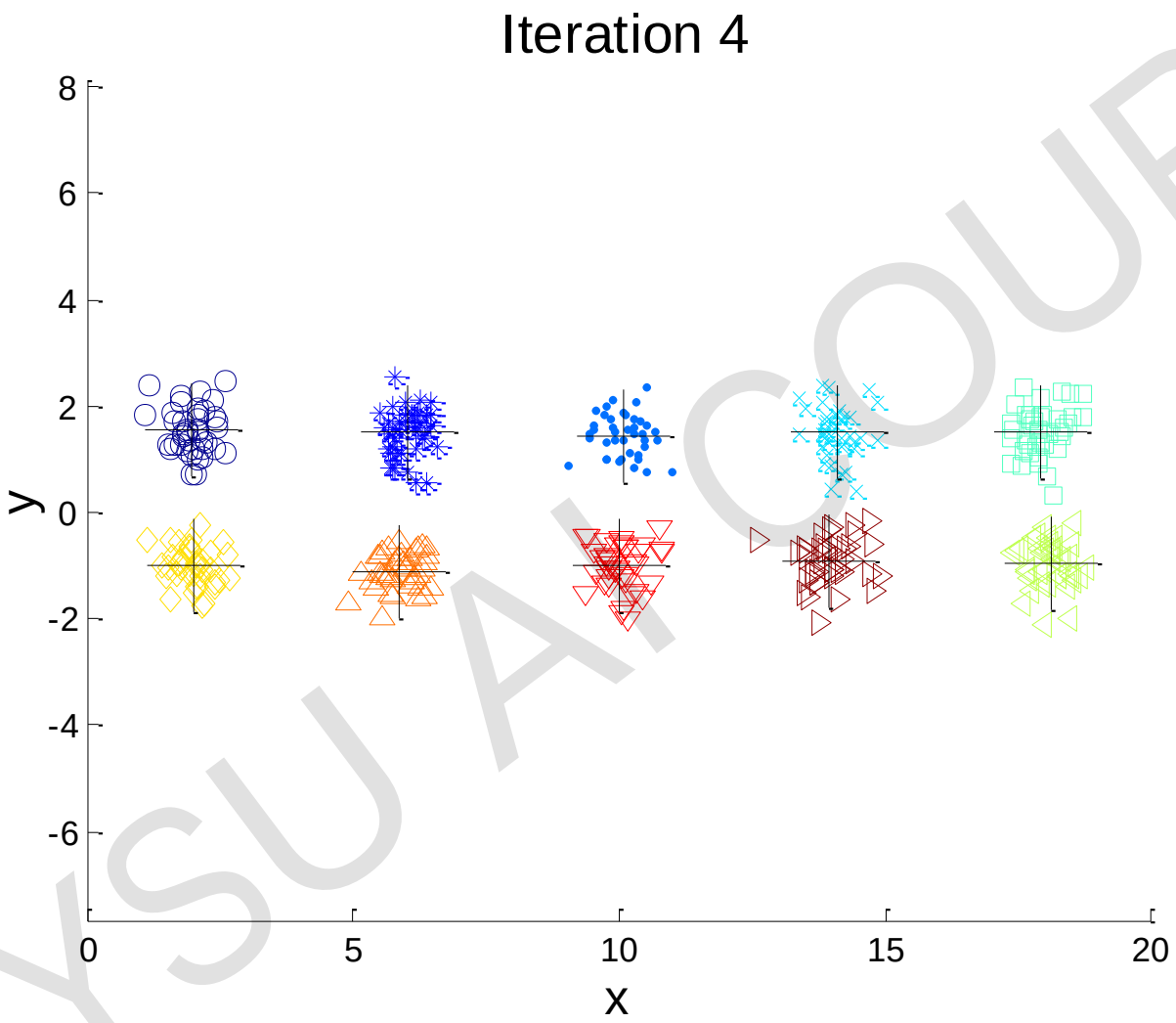
If there are K 'real' clusters then the chance of selecting one centroid from each cluster is small.

- Chance is relatively small when K is large
- If clusters are the same size, n, then

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

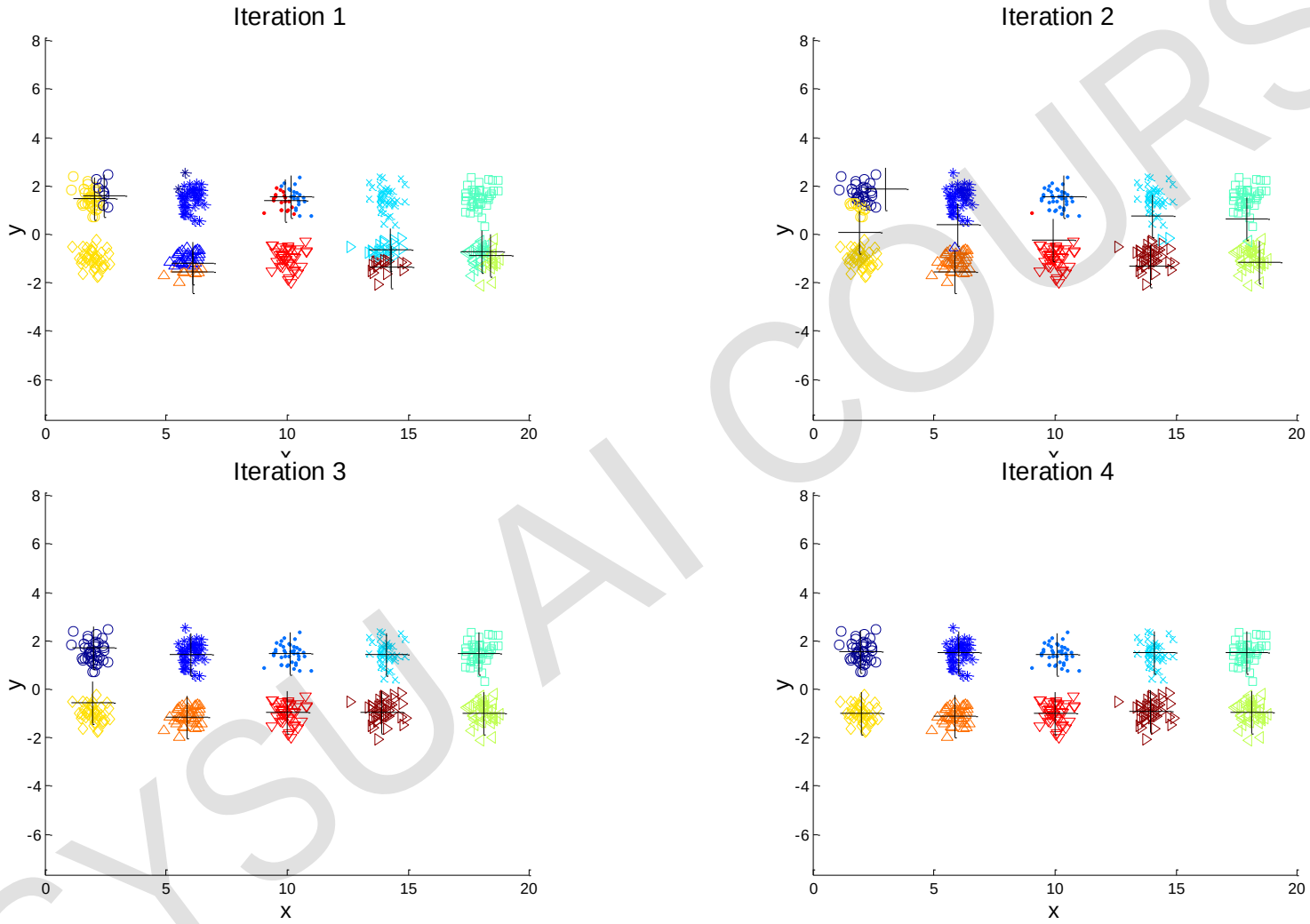
- For example, if K = 10, then probability = $10!/10^{10} = 0.00036$
- Sometimes the initial centroids will readjust themselves in 'right' way, and sometimes they don't
- Consider an example of five pairs of clusters

10 Clusters Example



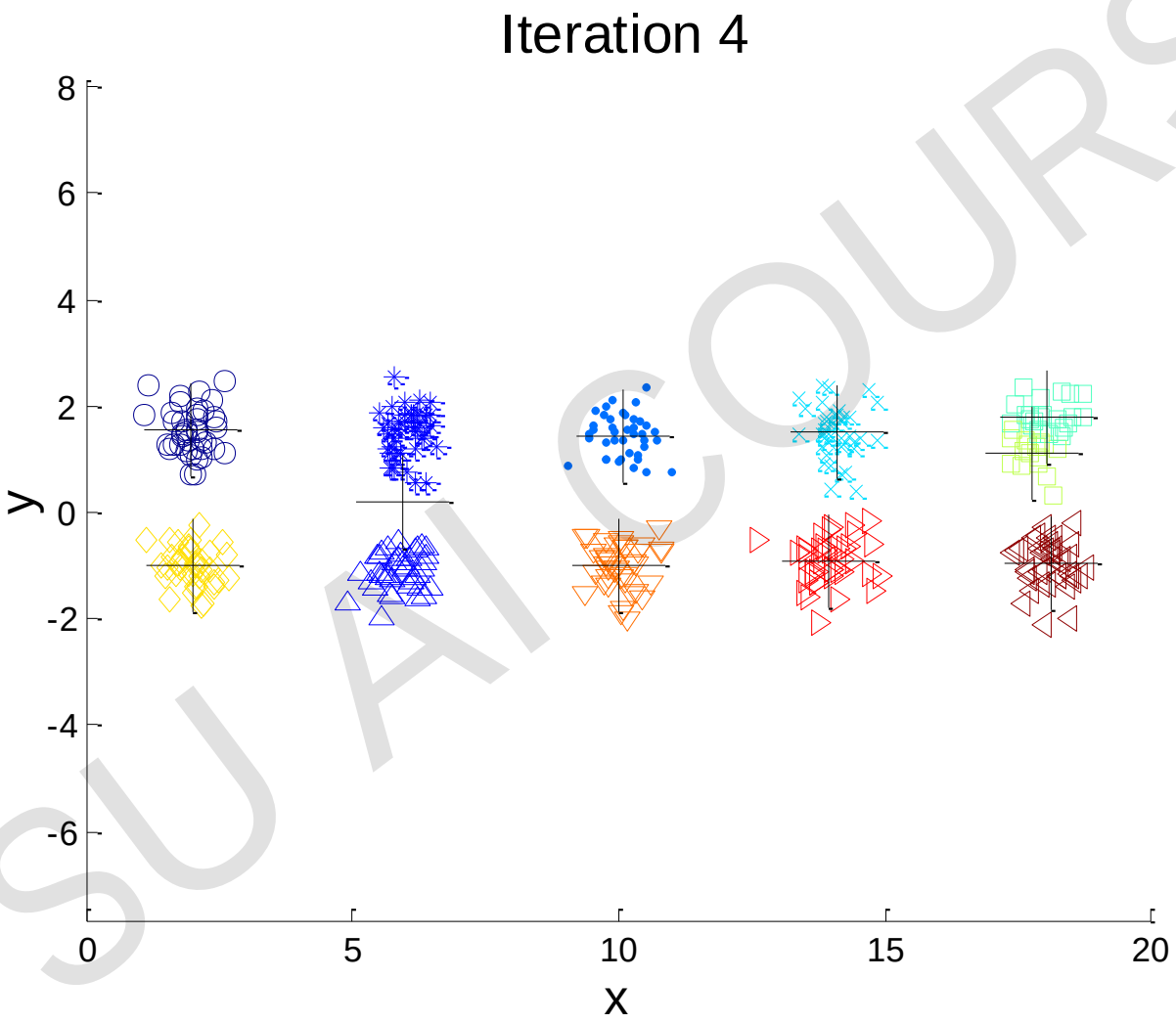
Starting with two initial centroids in one cluster of each pair of clusters

10 Clusters Example



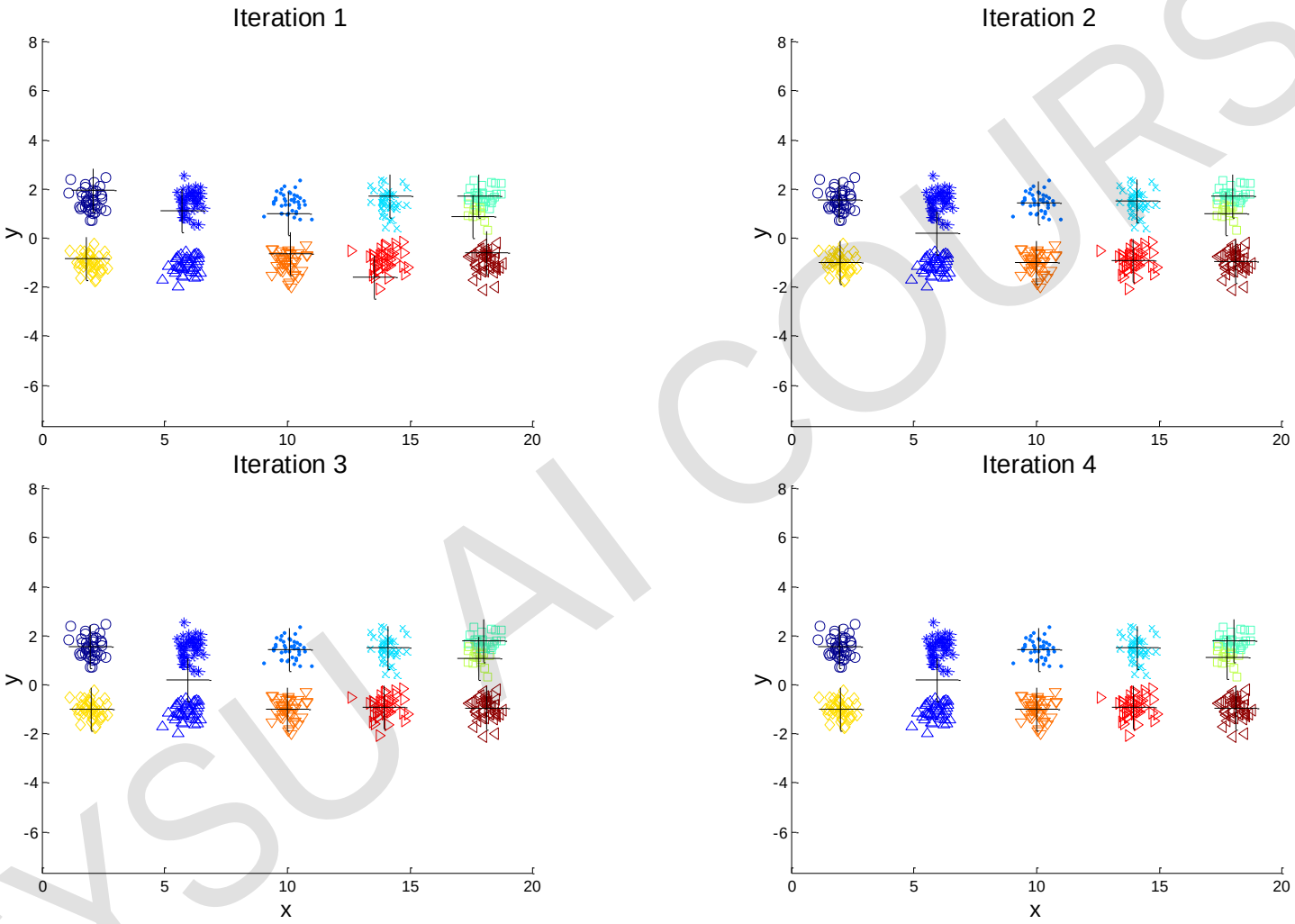
Starting with two initial centroids in one cluster of each pair of clusters

10 Clusters Example



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

10 Clusters Example



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

Solutions to Initial Centroids Problem

Multiple runs

- Helps, but probability is not on your side

Sample and use hierarchical clustering to determine initial centroids

Select more than k initial centroids and then select among these initial centroids

- Select most widely separated

Bisecting K-means

- Not as susceptible to initialization issues

Handling Empty Clusters

Basic K-means algorithm can yield empty clusters

Choose a replacement centroid, several strategies

- Choose the point that contributes most to SSE
- Choose a point from the cluster with the highest SSE
- If there are several empty clusters, the above can be repeated several times.

1: Select K points as the initial centroids.
2: **repeat**
3: Form K clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: **until** The centroids don't change

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

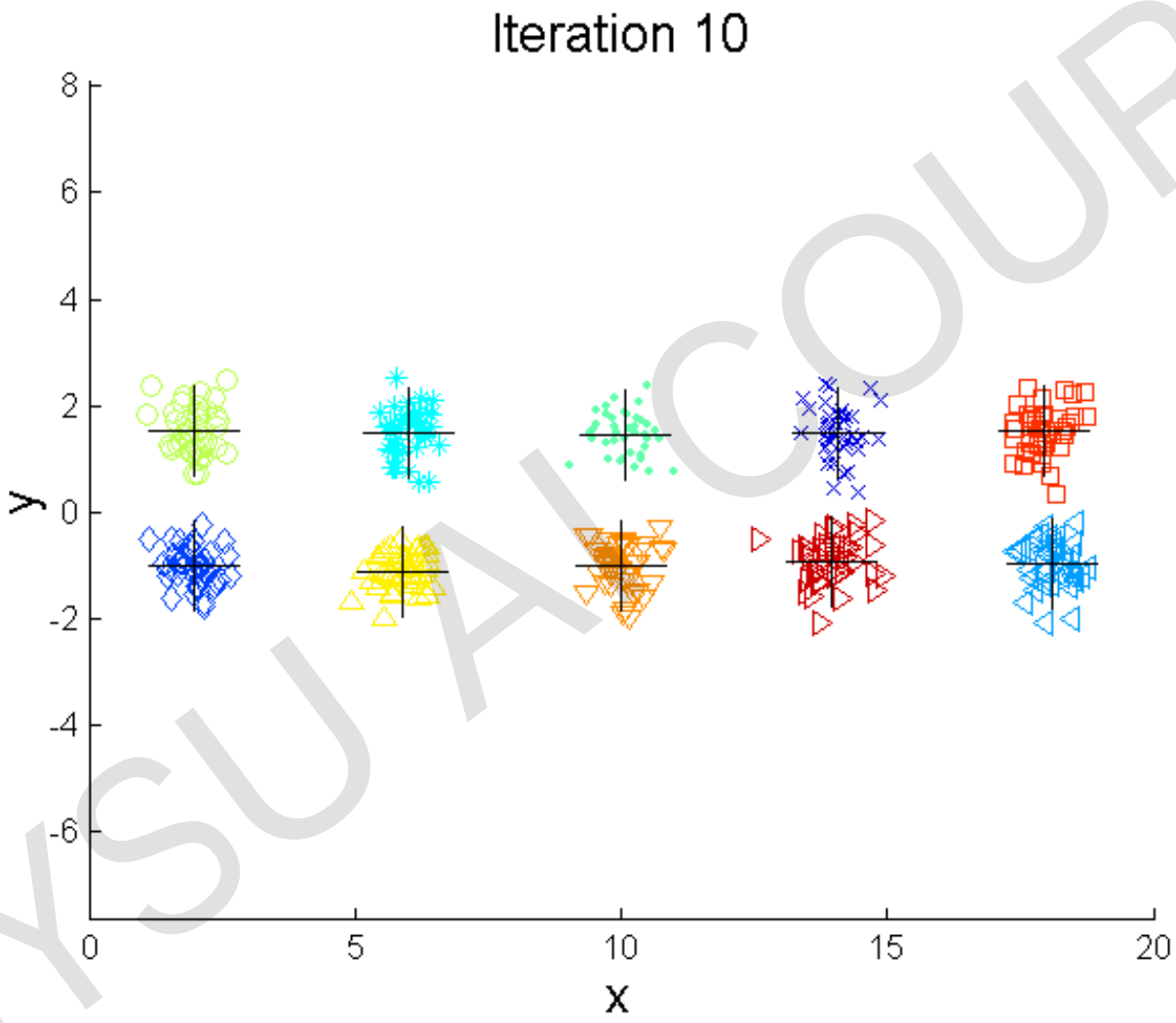
Bisecting K-means

Bisecting K-means algorithm

- Variant of K-means that can produce a partitional or a hierarchical clustering

1: Initialize the list of clusters to contain the cluster containing all points.
2: **repeat**
3: Select a cluster from the list of clusters
4: **for** $i = 1$ to *number_of_iterations* **do**
5: Bisect the selected cluster using basic K-means
6: **end for**
7: Add the two clusters from the bisection with the lowest SSE to the list of clusters.
8: **until** Until the list of clusters contains K clusters

Bisecting K-means Example



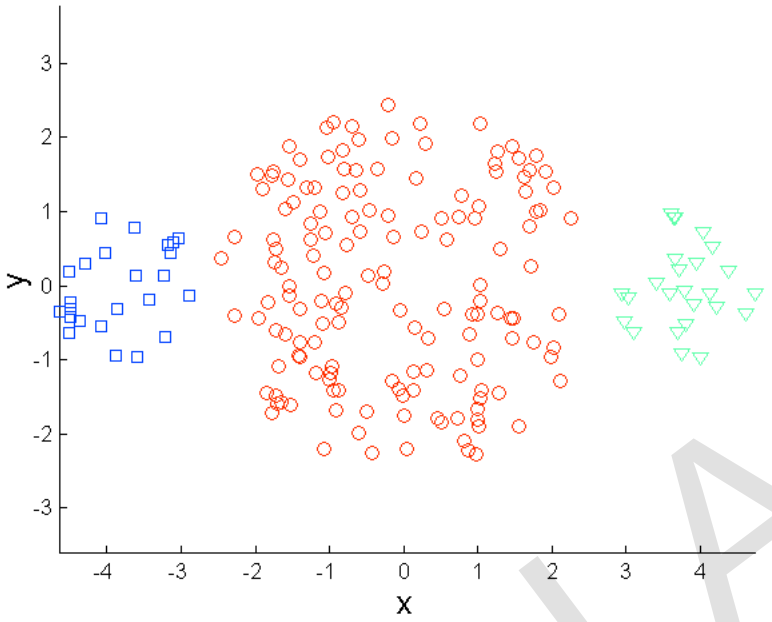
Limitations

K-means has problems when clusters are of differing

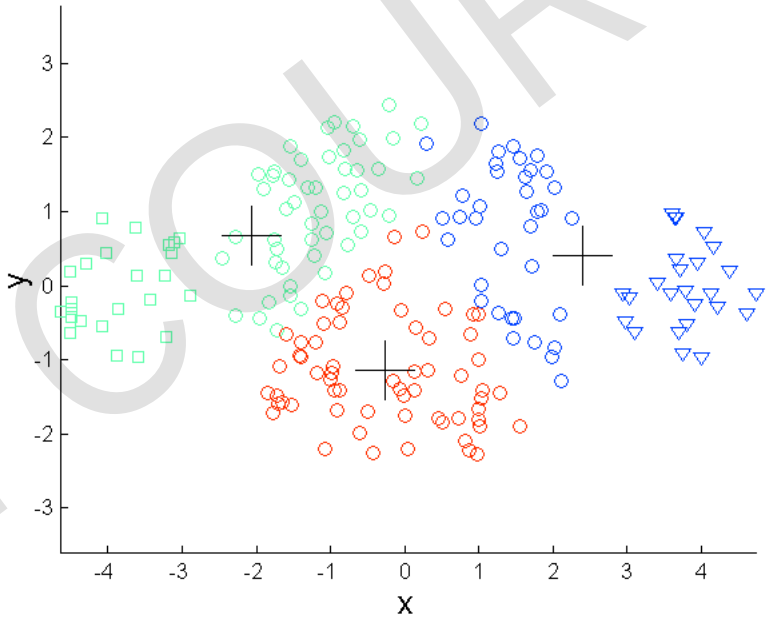
- Sizes
- Densities
- Non-globular shapes

K-means has problems when the data contains outliers.

Limitations of K-means: Differing Sizes

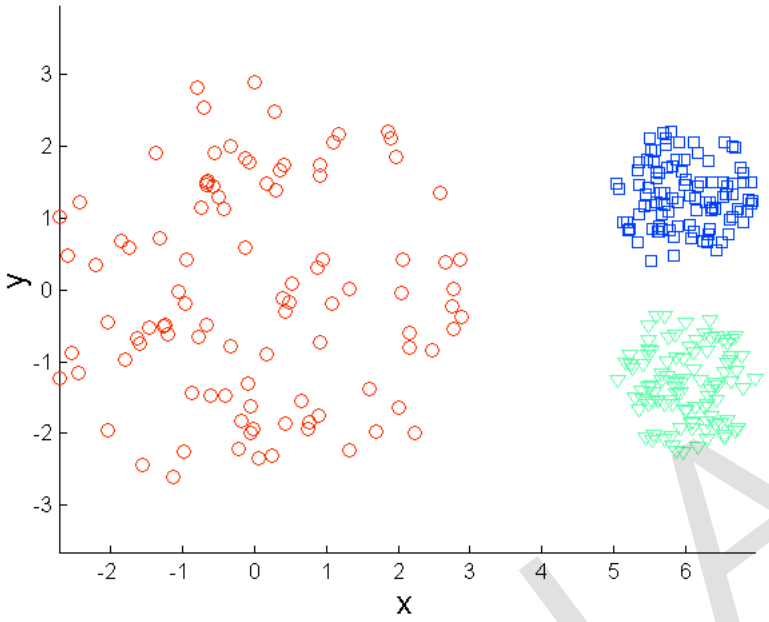


Original Points

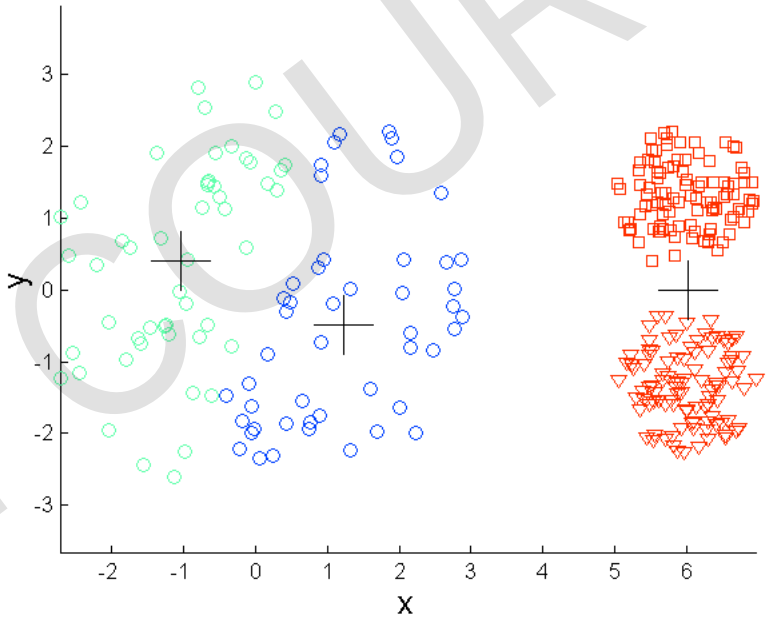


K-means (3 Clusters)

Limitations of K-means: Differing Density

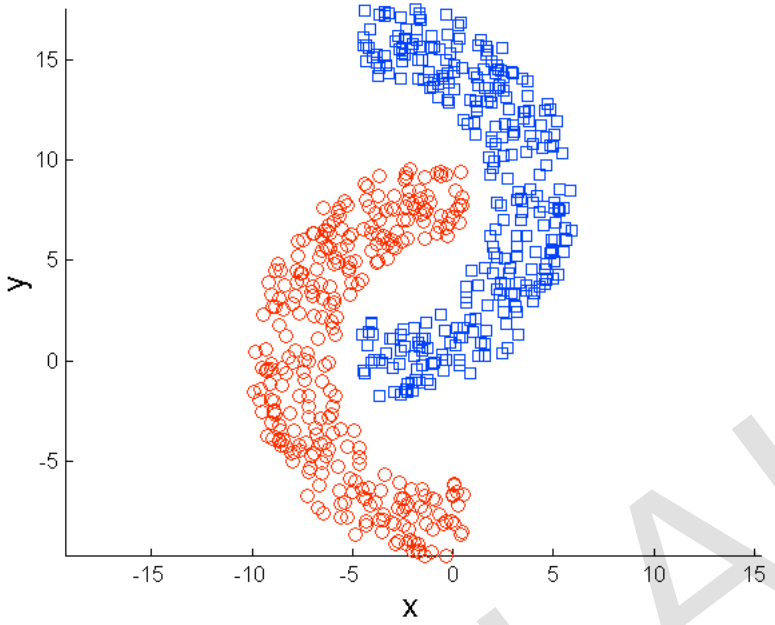


Original Points

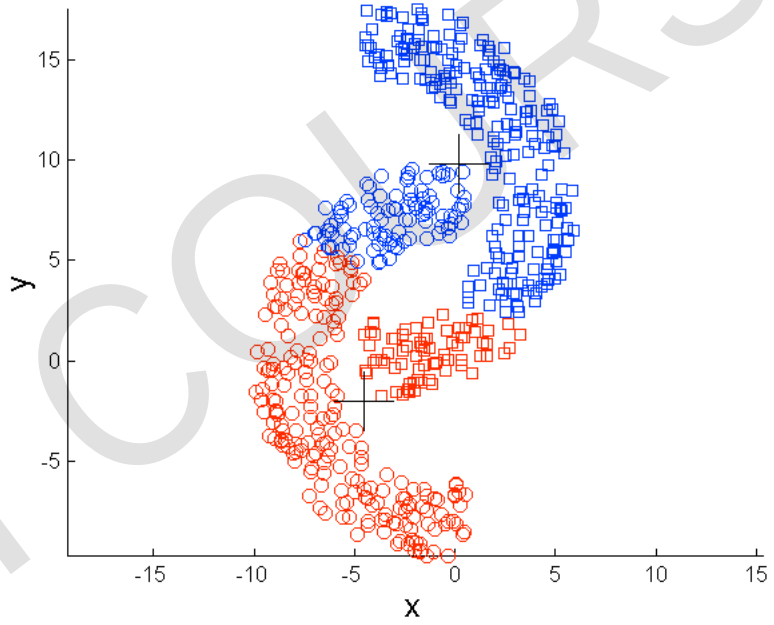


K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes

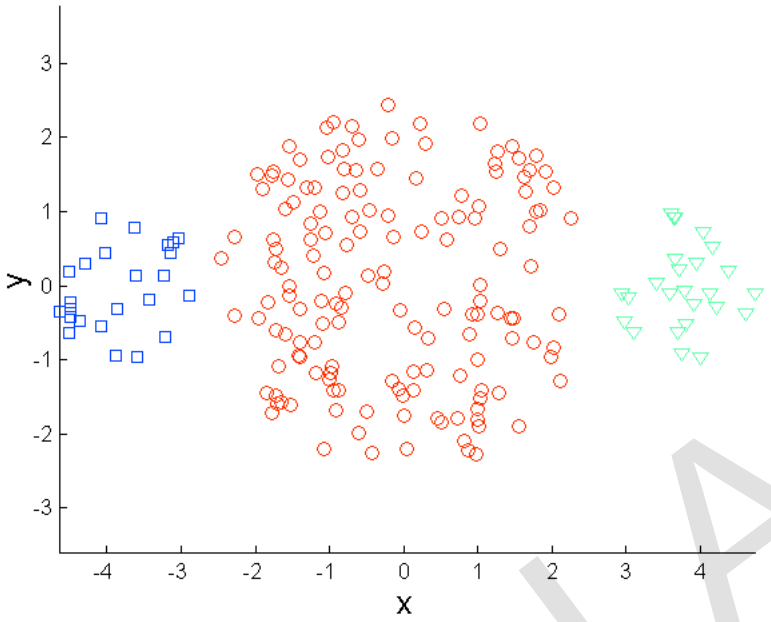


Original Points

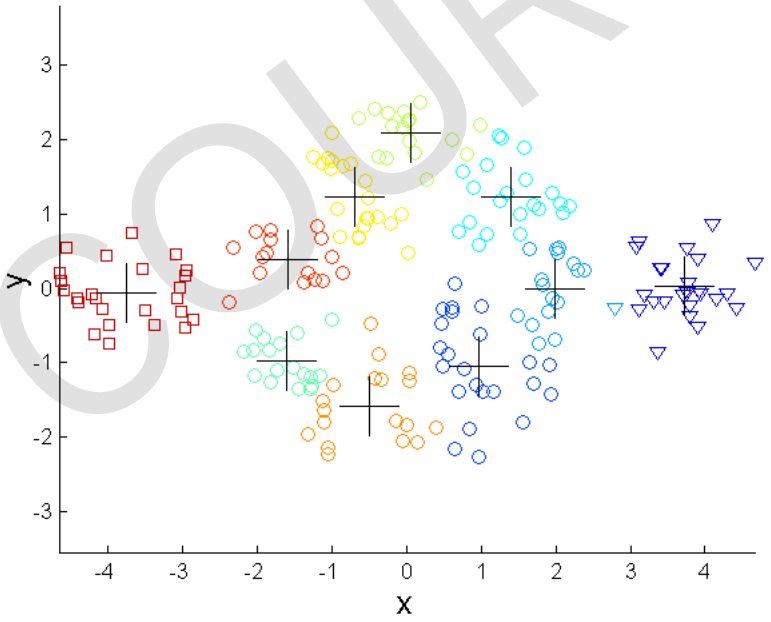


K-means (2 Clusters)

Overcoming K-means Limitations



Original Points

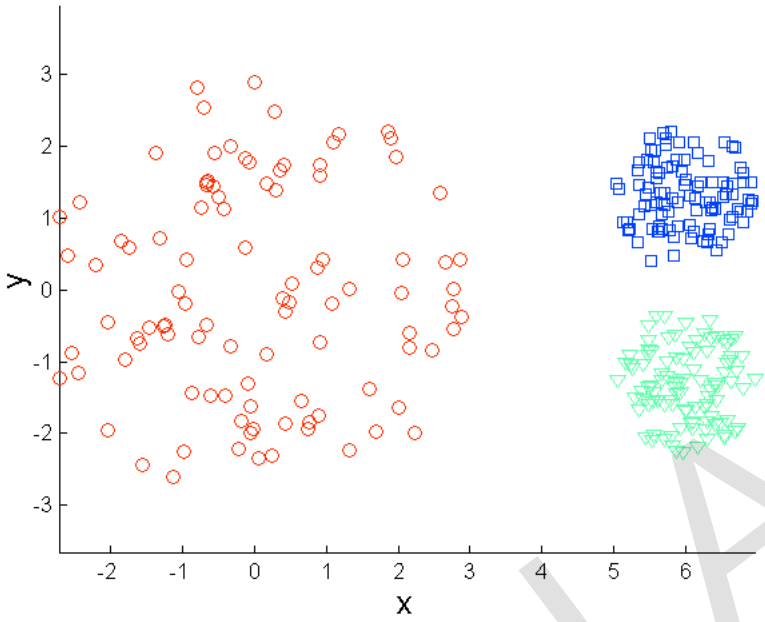


K-means Clusters

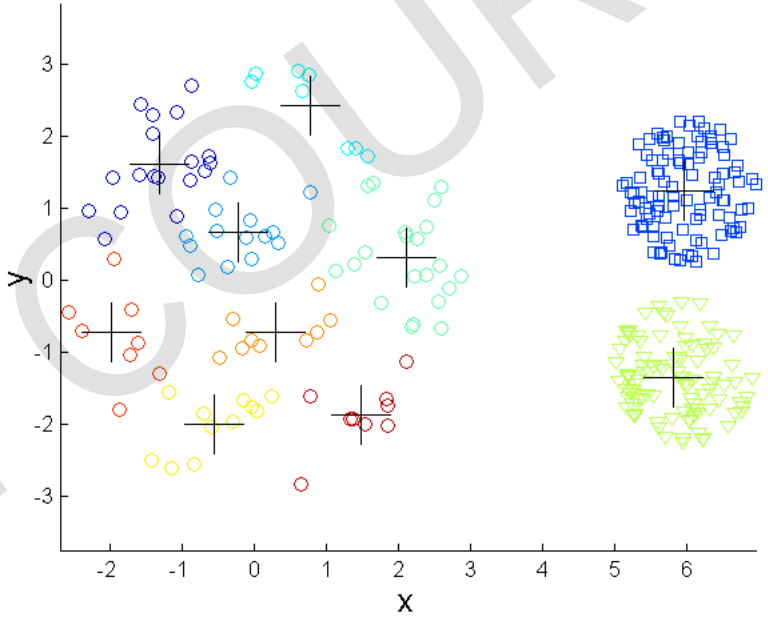
One solution is to use many clusters.

Find parts of clusters, but need to put together.

Overcoming K-means Limitations

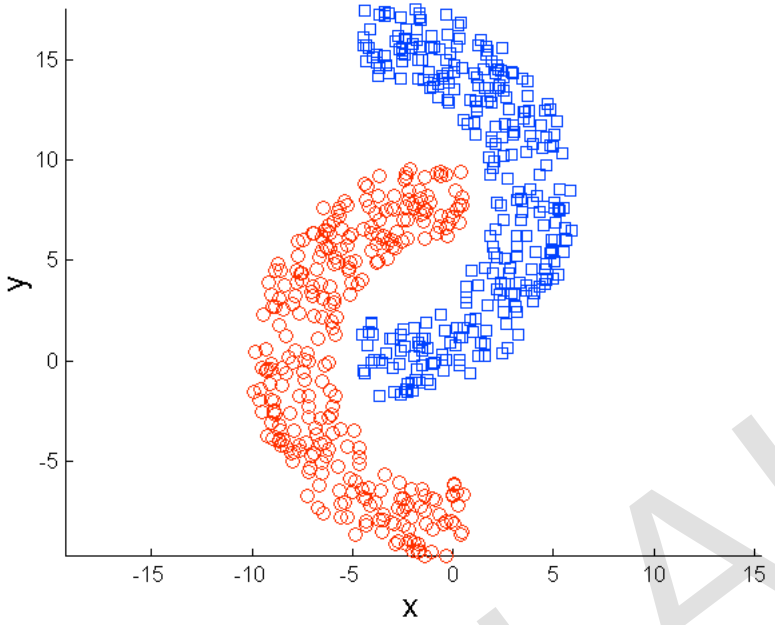


Original Points

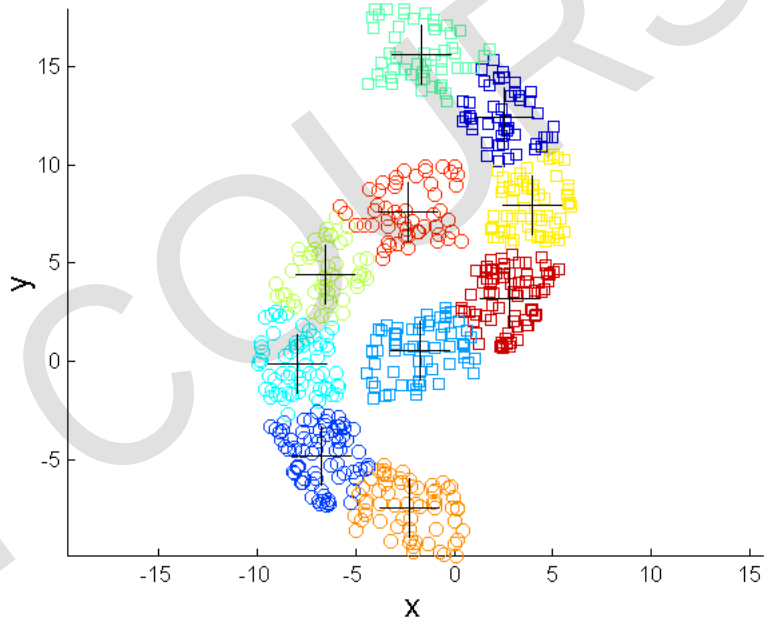


K-means Clusters

Overcoming K-means Limitations



Original Points



K-means Clusters

K-means++ [Arthur et al. '07]

Spreads out the centers

Choose first center, x1, uniformly at random from the data set

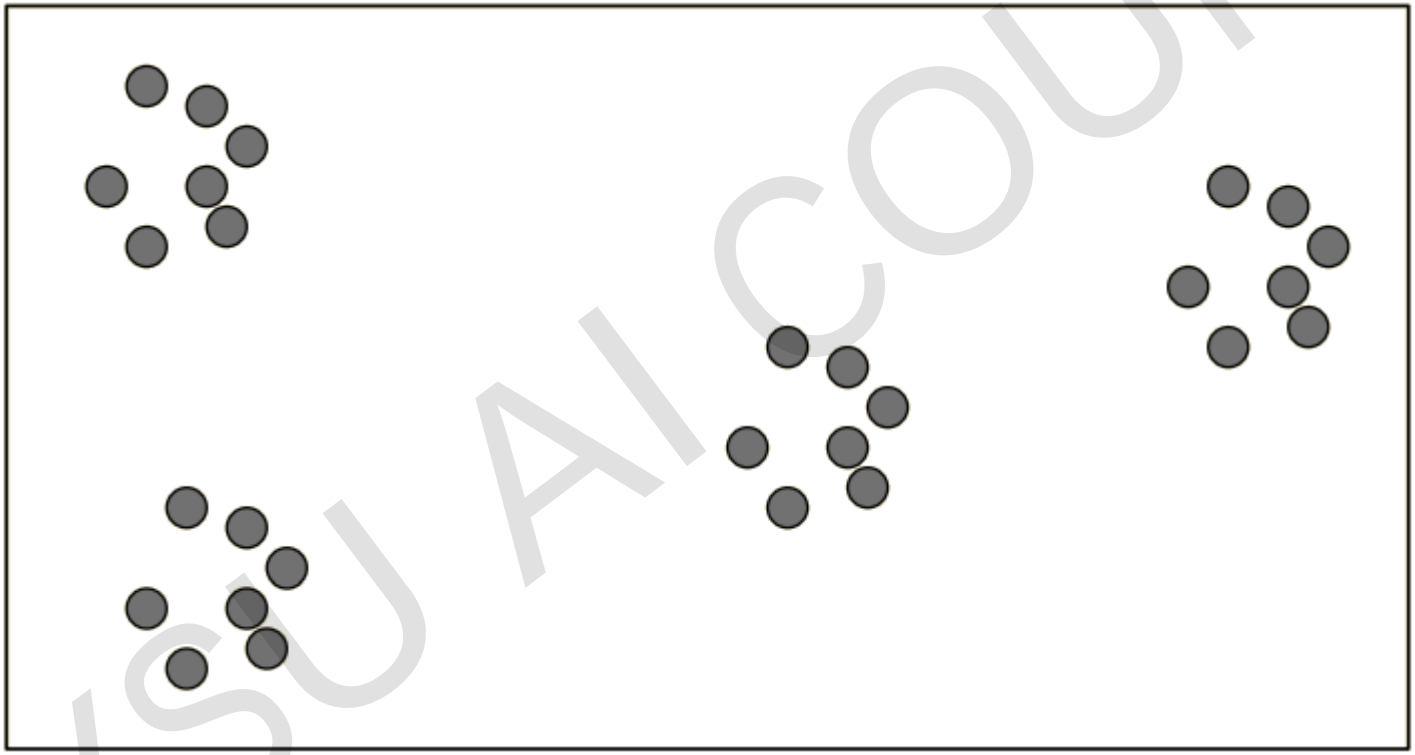
Repeat for 2 ≤ i ≤ k:

- Choose *x′* to be equal to a data point sampled from the distribution:

$$\frac{D(x')^2}{\sum_{x \in \mathcal{X}} D(x)^2}$$

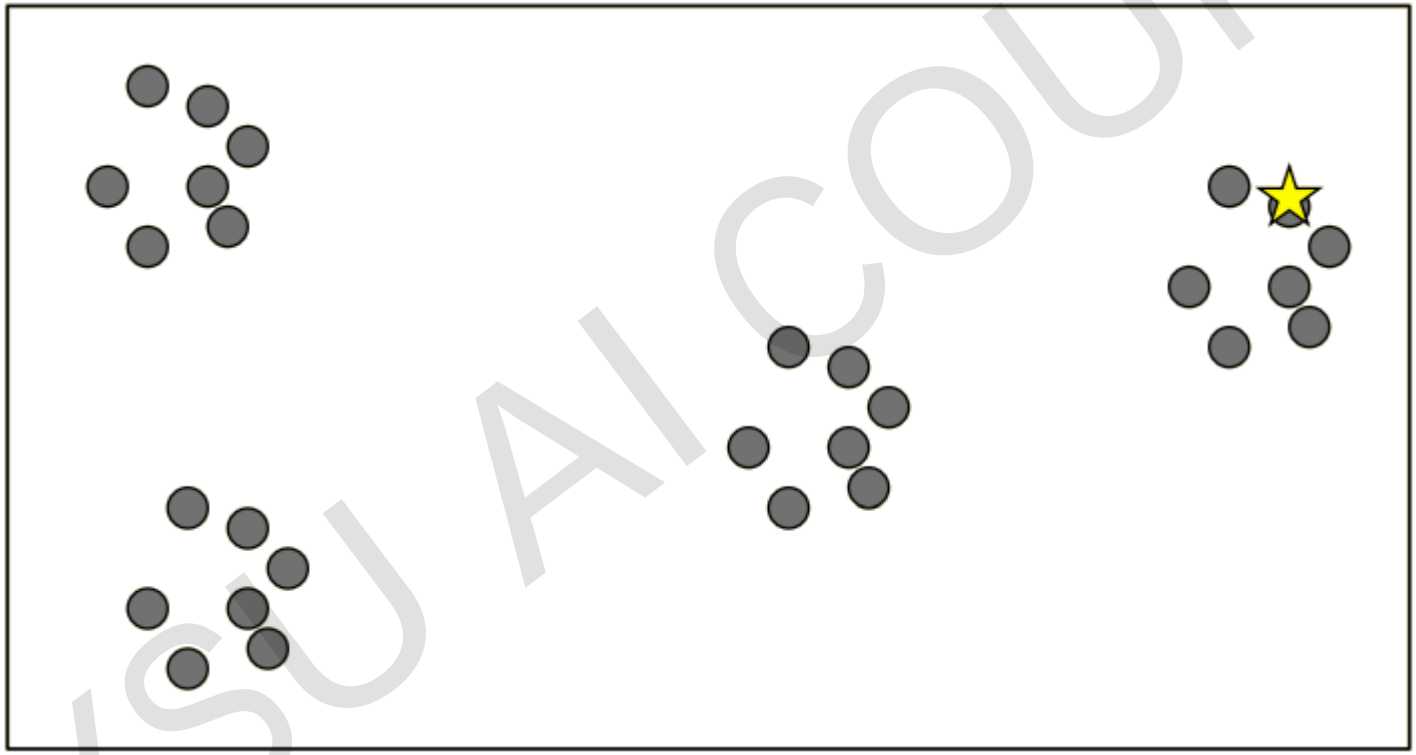
- *D(x)*: the shortest distance from a data point *x* to the closest center we have already chosen

K-means++ [Arthur et al. '07]



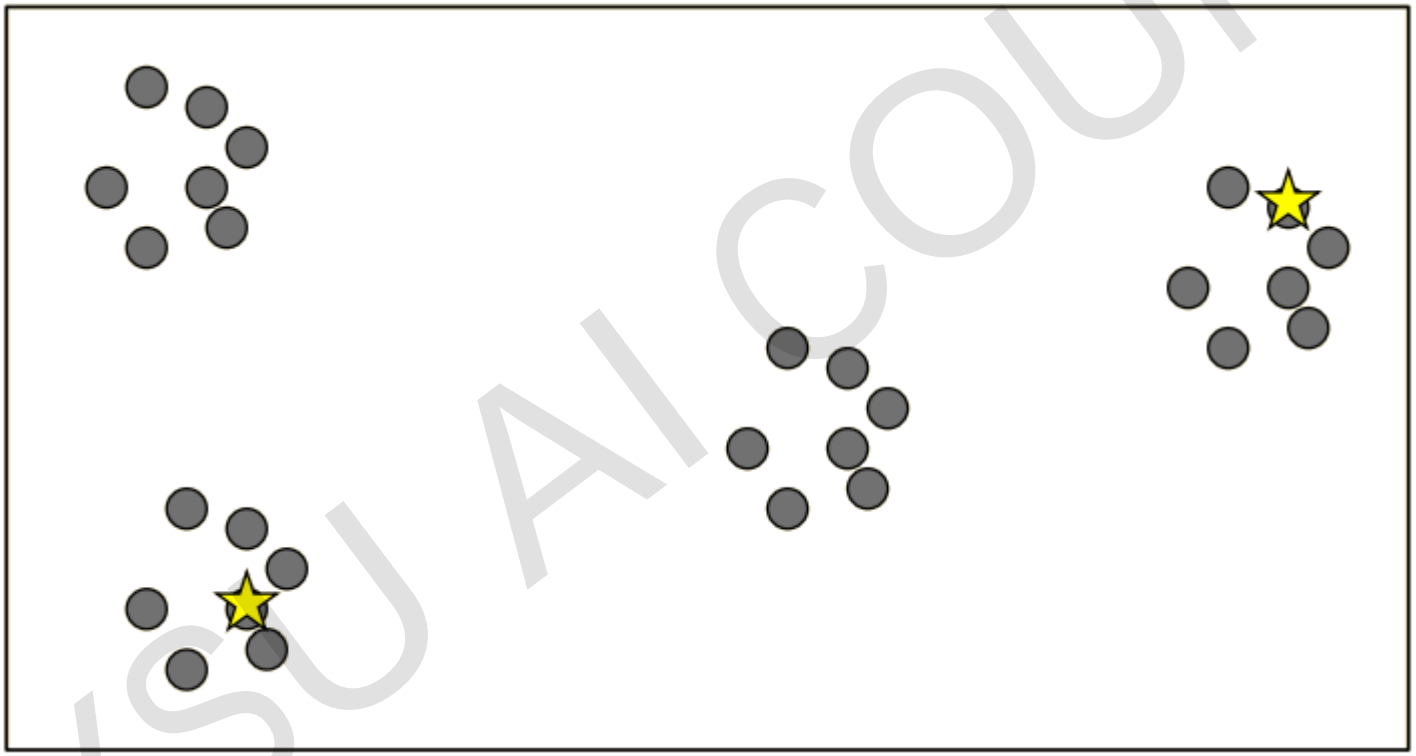
$$\frac{D(x')^2}{\sum_{x \in \mathcal{X}} D(x)^2}$$

K-means++ [Arthur et al. '07]



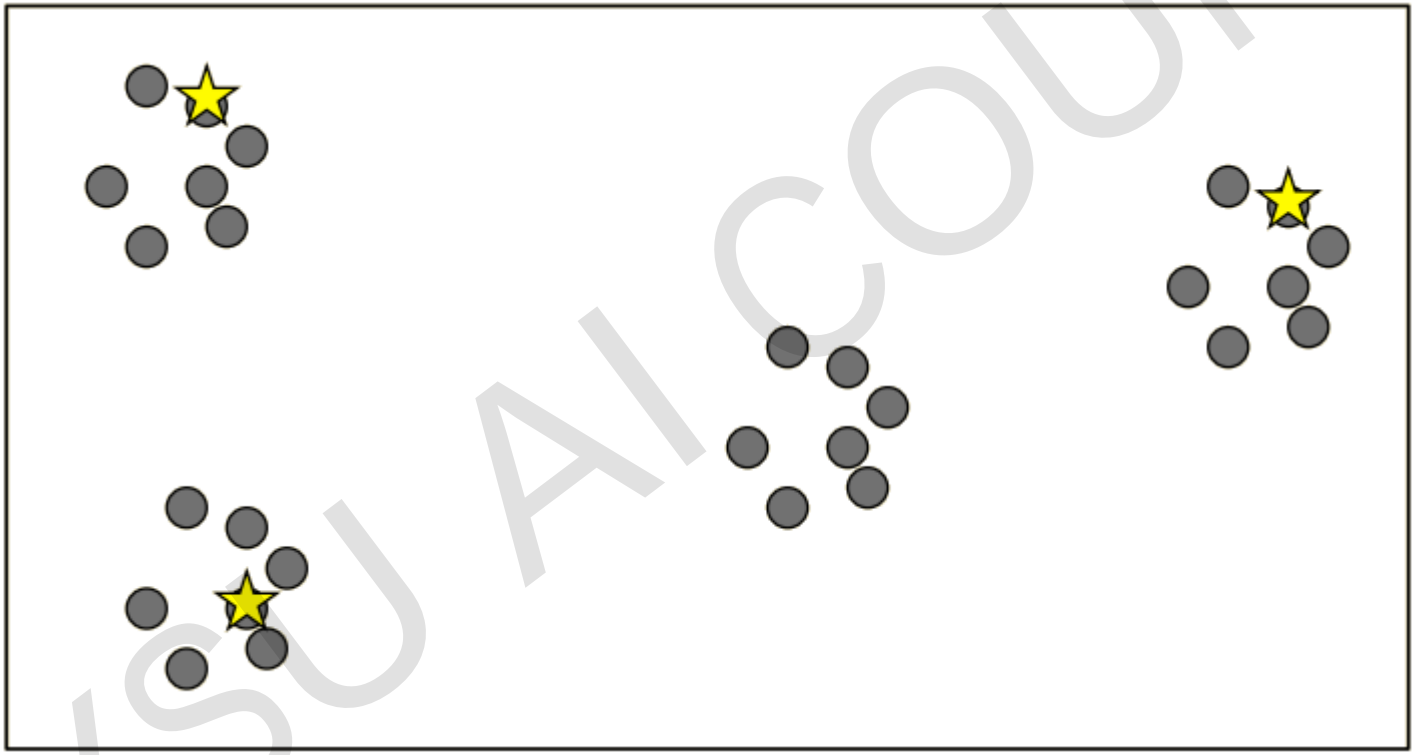
$$\frac{D(x')^2}{\sum_{x \in \mathcal{X}} D(x)^2}$$

K-means++ [Arthur et al. '07]



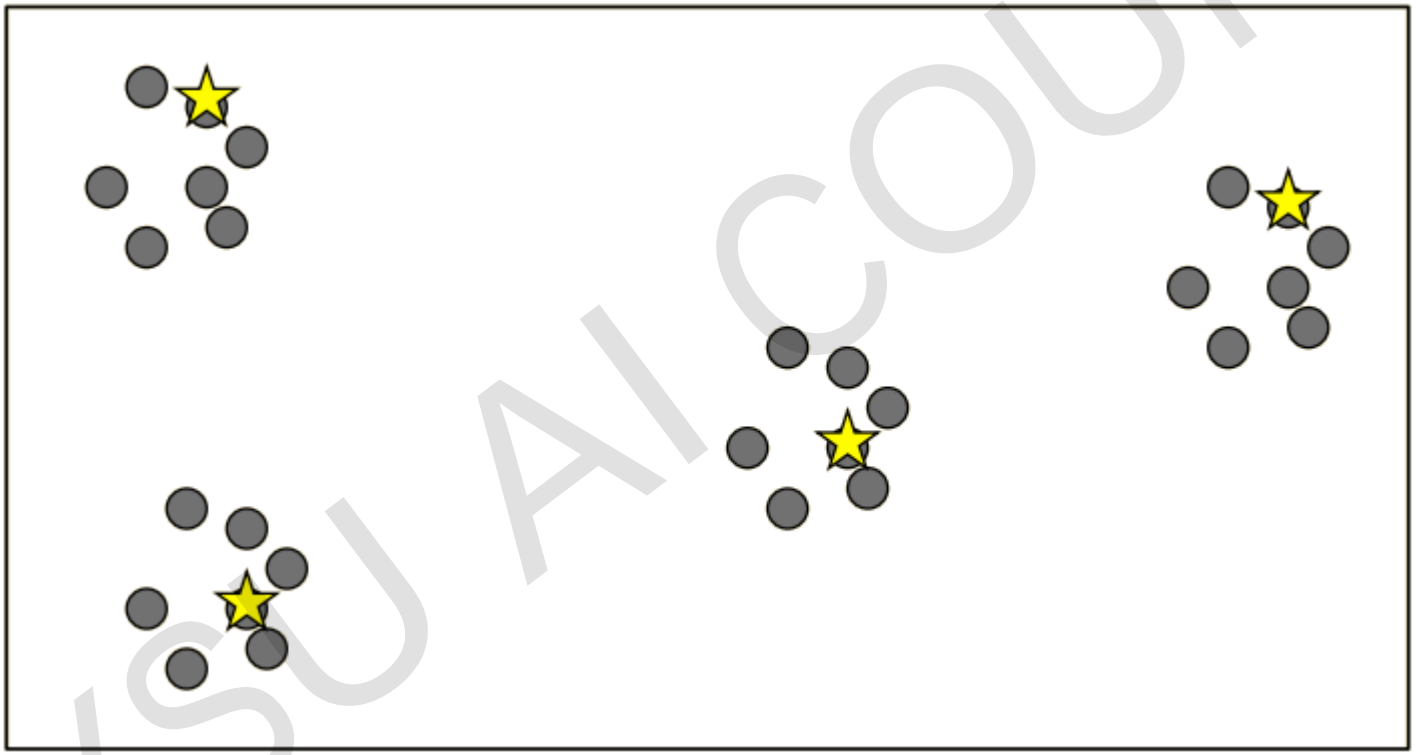
$$\frac{D(x')^2}{\sum_{x \in \mathcal{X}} D(x)^2}$$

K-means++ [Arthur et al. '07]



$$\frac{D(x')^2}{\sum_{x \in \mathcal{X}} D(x)^2}$$

K-means++ [Arthur et al. ’07]



$$\frac{D(x')^2}{\sum_{x \in \mathcal{X}} D(x)^2}$$

K-means++ [Arthur et al. '07]

What's **wrong** with K-means++?

- Needs K passes over the data
- In large data applications, not only the data is massive, but also K is typically large (e.g., easily 1000).
- Does not scale!

Scalable K-means: K-means||

Intuition of K-means||

- K-means++ samples one point per iteration and updates its distribution
- What if we **oversample** by sampling each point independently with a larger probability?
- Intuitively equivalent to updating the distribution much less frequently
- Coarser sampling
- Turns out to be sufficient: K-means||

Scalable K-means

主要思路在于改变每次遍历时的取样策略，并非按照 k-means++ 那样每次遍历只取样一个样本，而是每次遍历取样 O(k) 个样本，重复该取样过程大约 O(logn) 次，共得到 O(klogn) 个样本点组成的集合

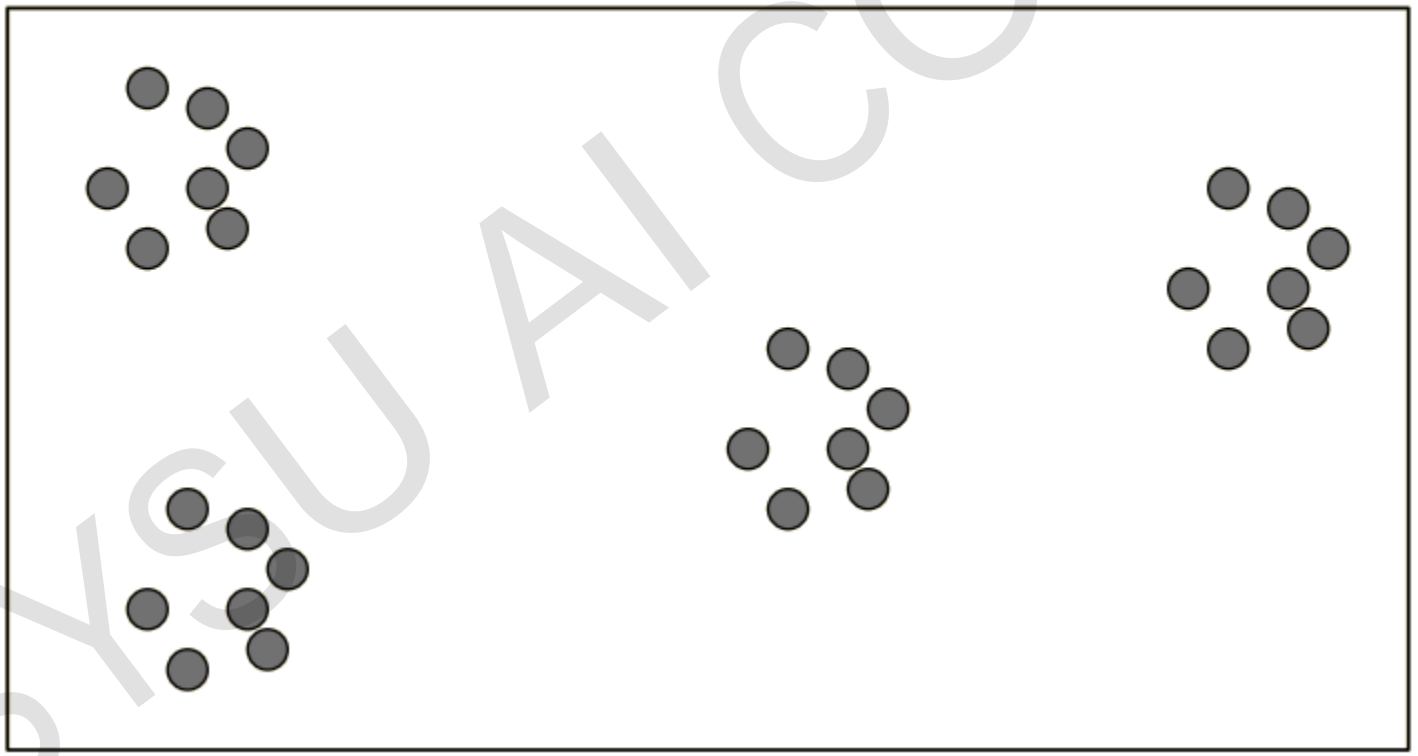
然后再聚类这 O(klogn) 个点成 k 个点，最后将这 k 个点作为初始聚类中心

实际实验证明 O(logn) 次重复取样是不需要的，一般5次重复取样就可以得到一个较好的聚类初始中心

Scalable K-means

K-means|| Initialization

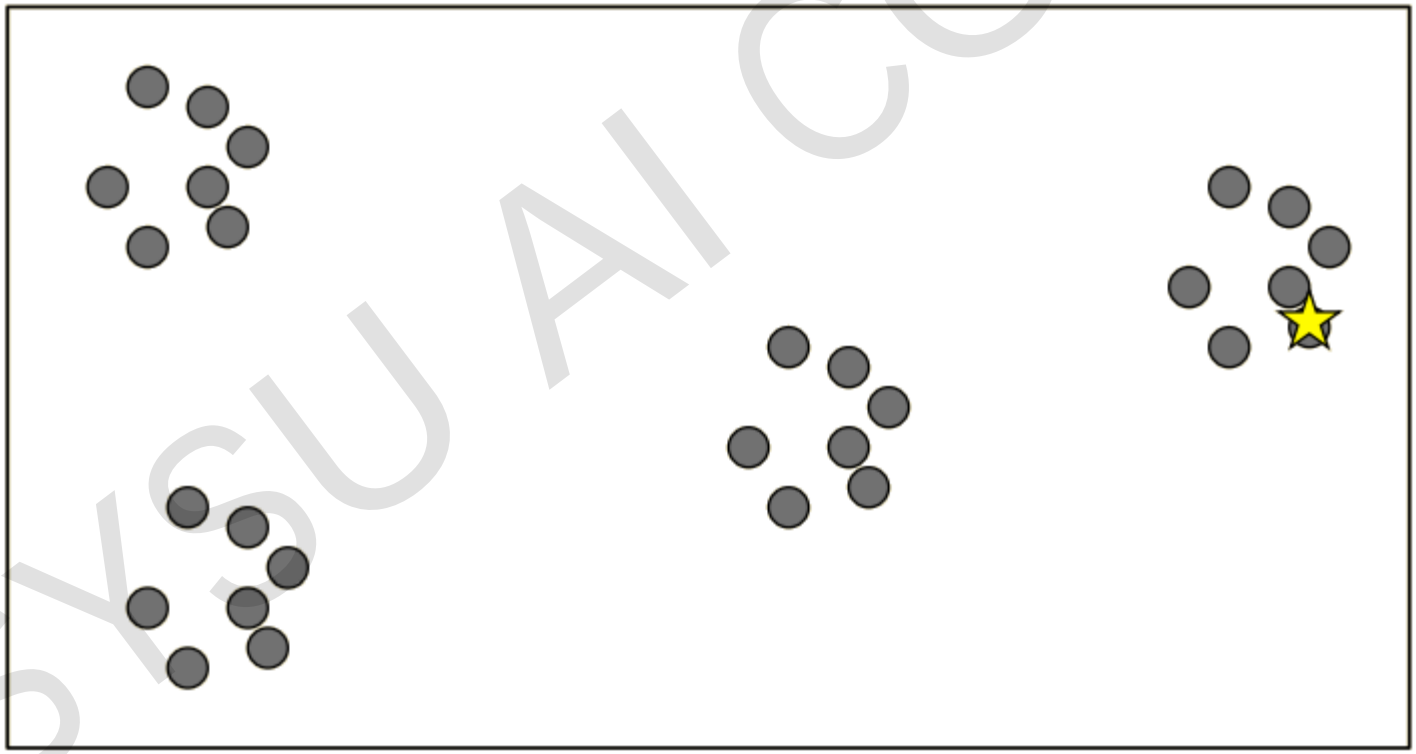
K=4,
Oversampling factor =3



Scalable K-means

K-means|| Initialization

K=4,
Oversampling factor =3

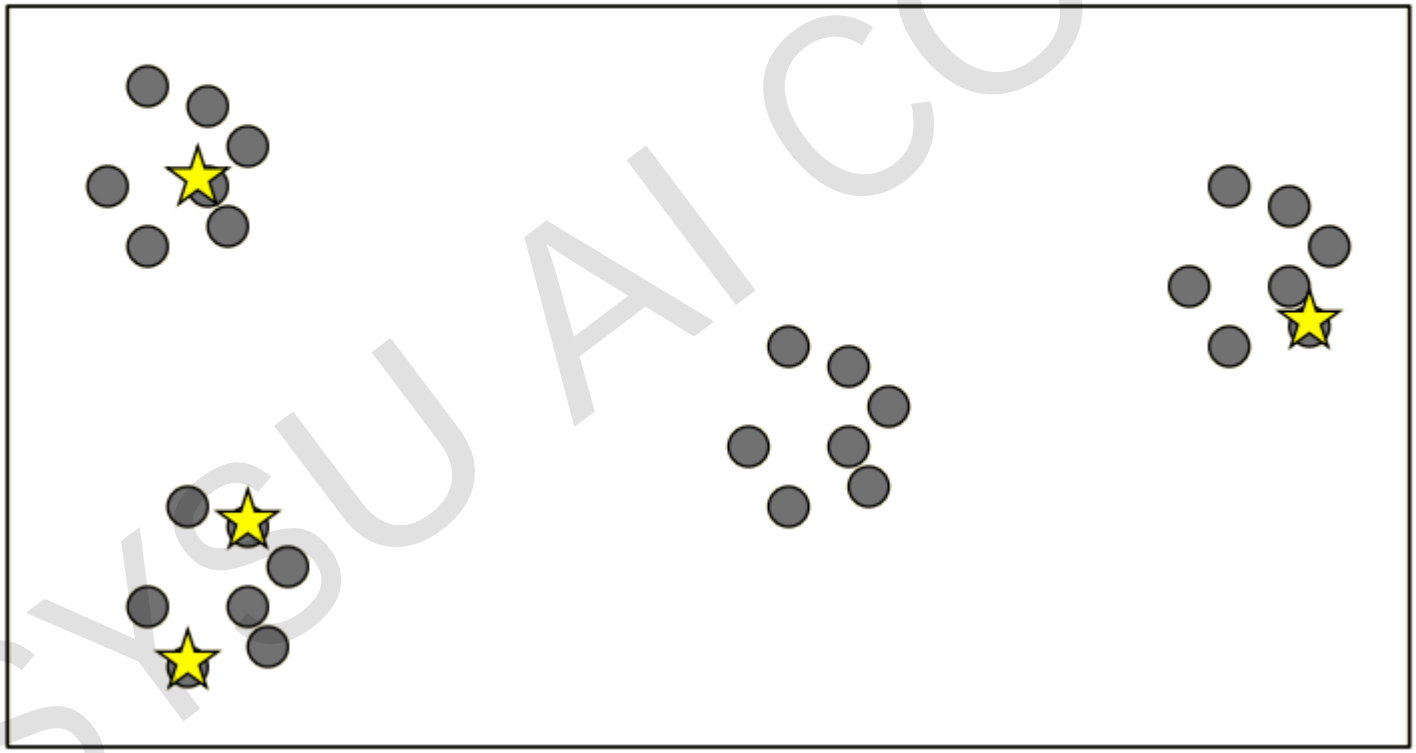


Scalable K-means

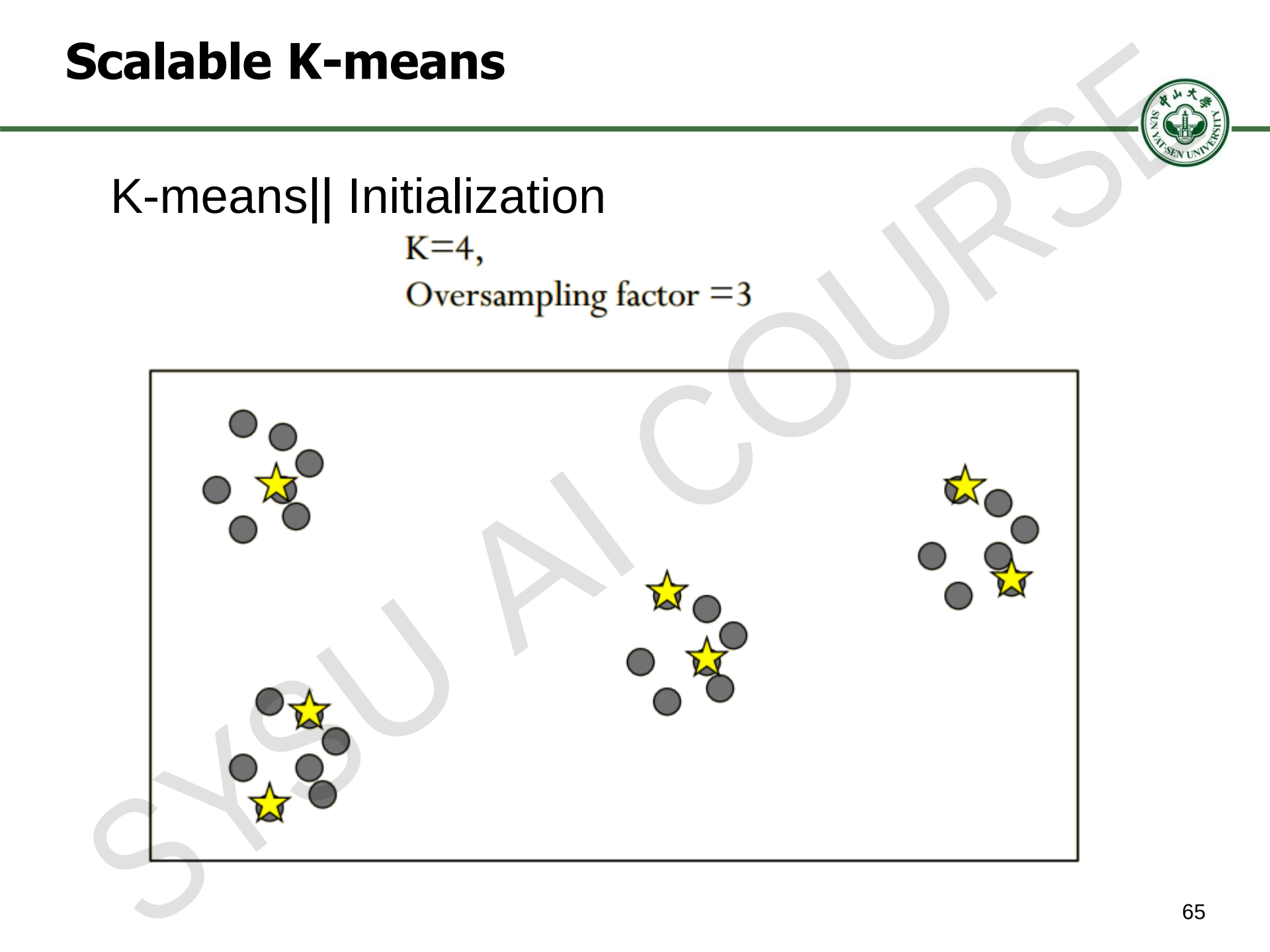
K-means|| Initialization

K=4,

Oversampling factor =3



Scalable K-means



K-means|| Initialization

K=4,

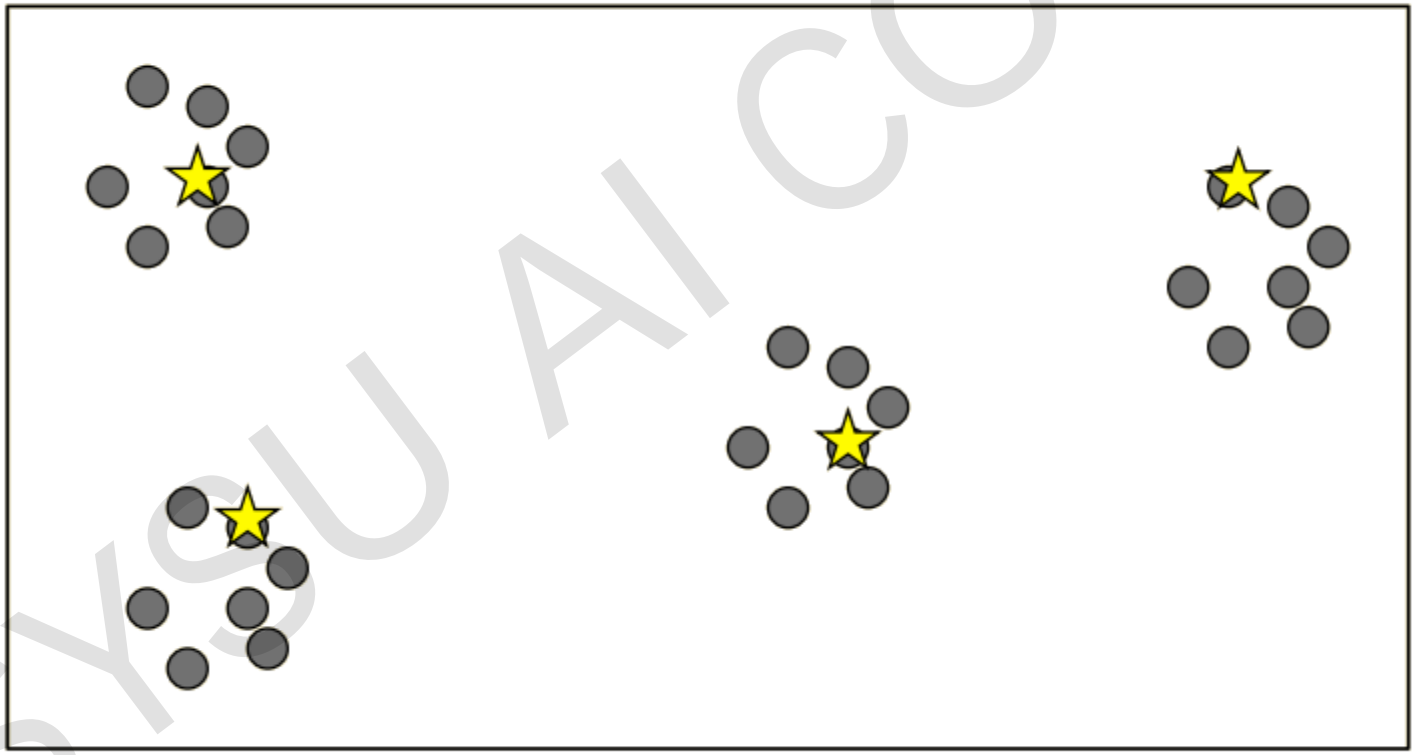
Oversampling factor =3

Scalable K-means

K-means|| Initialization

K=4,

Oversampling factor =3



Cluster the intermediate centers

Scalable K-means

K-means|| [Bahmani et al. '12]

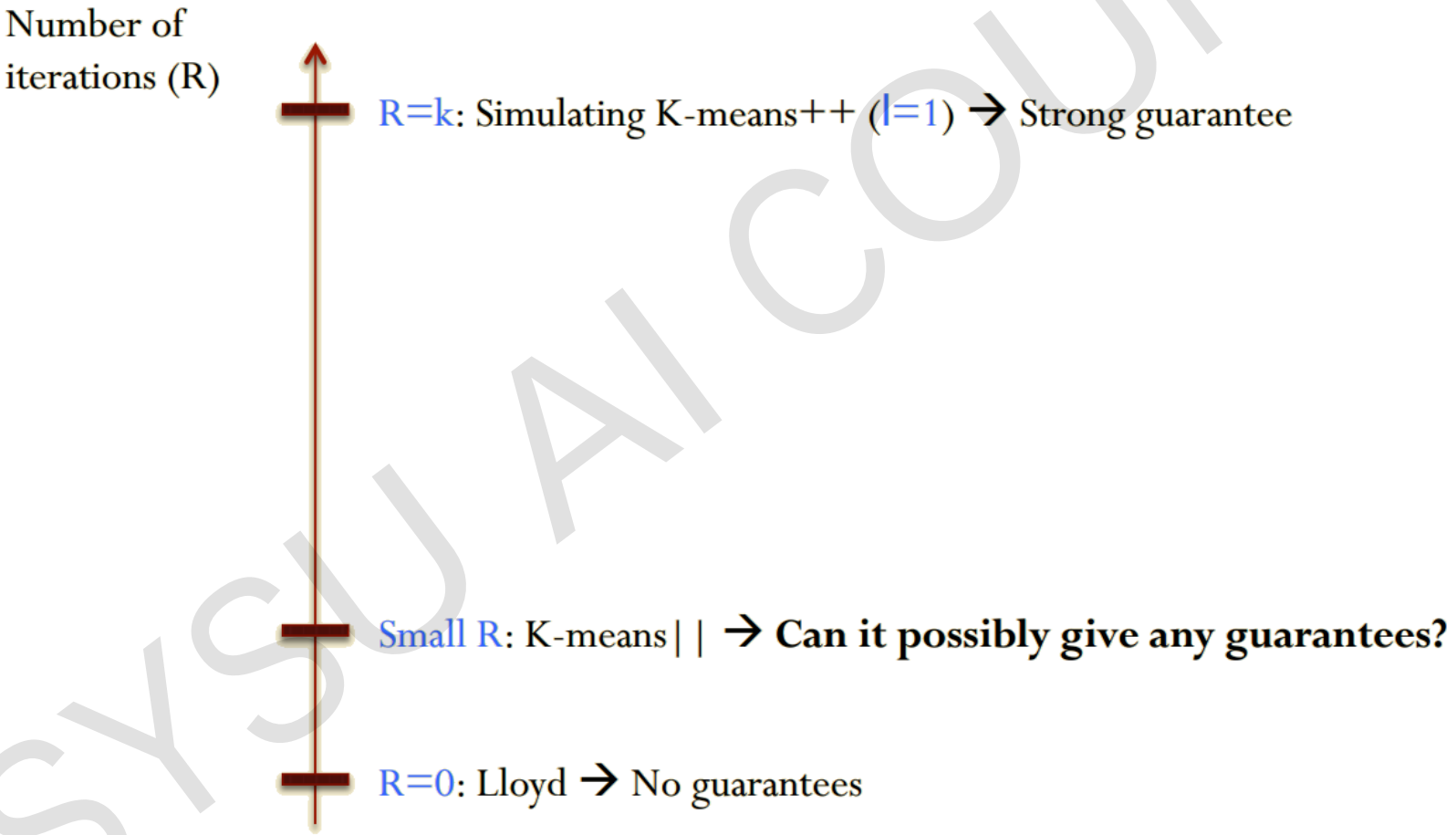
- Choose l>1 [Think l=Θ(k)]
- Initialize C to an arbitrary set of points
- For R iterations do:
- Sample l points, each point x in X independently with probability

$$p_x = l d^2(x, C) / \varphi_X(C).$$

- Add all the sampled points to C
- Cluster the (weighted) points in C to find the final k centers

Scalable K-means

K-means, K-means++, and K-means||



Scalable K-means

Theorem

- Optimal clustering： the sum of the squared distances between each point and its closest center is minimal
  - Solving this problem exactly is NP-hard
- Let ψ= cost of initial clustering, ψ'=cost of clustering after convergence, OPT=cost of the optimal clustering
- Using K-means++ for clustering the intermediate centers, the overall approximation factor = O(log k)
  - It means ψ' = O(log k)*OPT
  - **也就是说最终确定的质心能够使cost达到最优聚类的cost的O（log k）倍**
- K-means|| produces a constant-factor approximation to OPT, using only O(log (ψ/OPT)) iterations

Scalable K-means

Experimental Results: Quality

Let $C = \{c_1, \ldots, c_k\}$ be a set of points and let $Y \subseteq X$.
We define the *cost* of Y with respect to C as

$$\phi_Y(C) = \sum_{y \in Y} d^2(y, C) = \sum_{y \in Y} \min_{i=1,\ldots,k} \|y - c_i\|^2.$$

	Clustering Cost Right After Initialization	Clustering Cost After Convergence
Random	NA	22,000
K-means++	430	65
K-means||	16	14

GAUSSMIXTURE: 10,000 points in 15 dimensions
K=50
Costs scaled down by 10^4

Scalable K-means

Experimental Results: Convergence

- K-means|| reduces number of iterations even more than K-means++

	Iterations After Initialization
Random	167
K-means++	42
K-means||	28

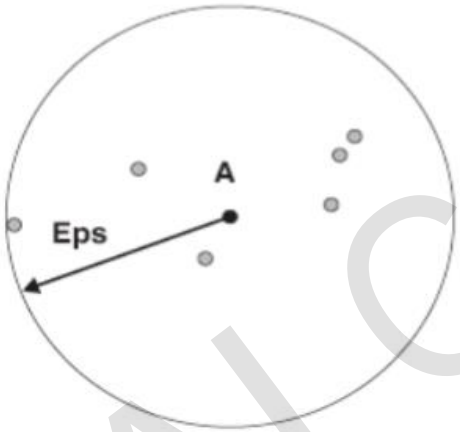
SPAM: 4,601 points in 58 dimensions
K=50

DBSCAN

DBSCAN is a density-based algorithm.

- Density = number of points within a specified radius (Eps)
- A point is a core point if it has more than a specified number of points (MinPts) within Eps
  - These are points that 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.

DBSCAN-Density



Density = 7 points

Figure 8.20. Center-based density.

- **Density** = number of points within a specified radius (Eps)

Core, border, noise points

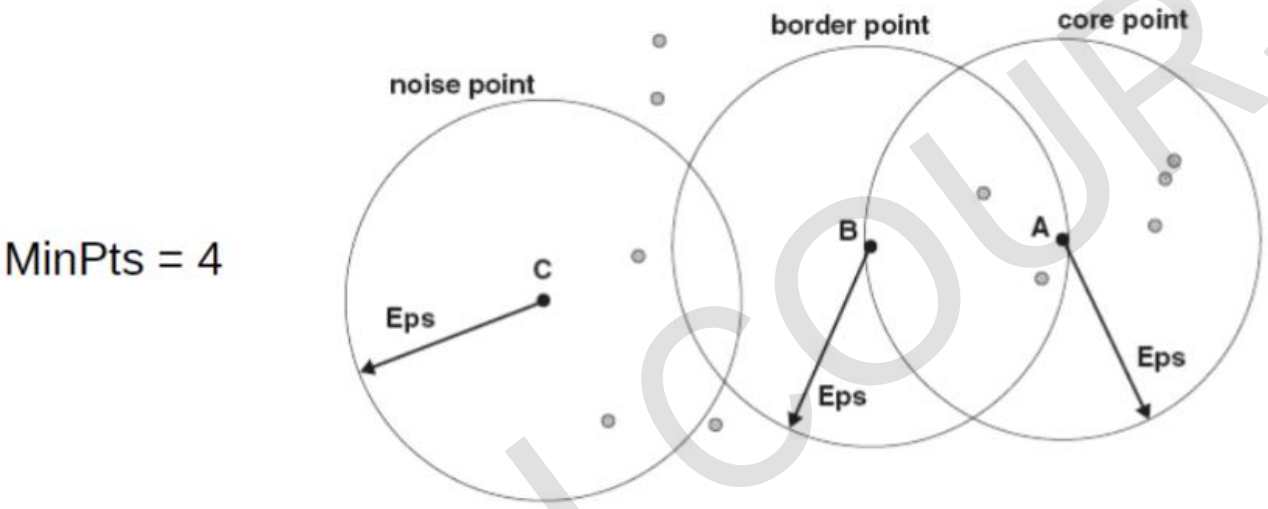
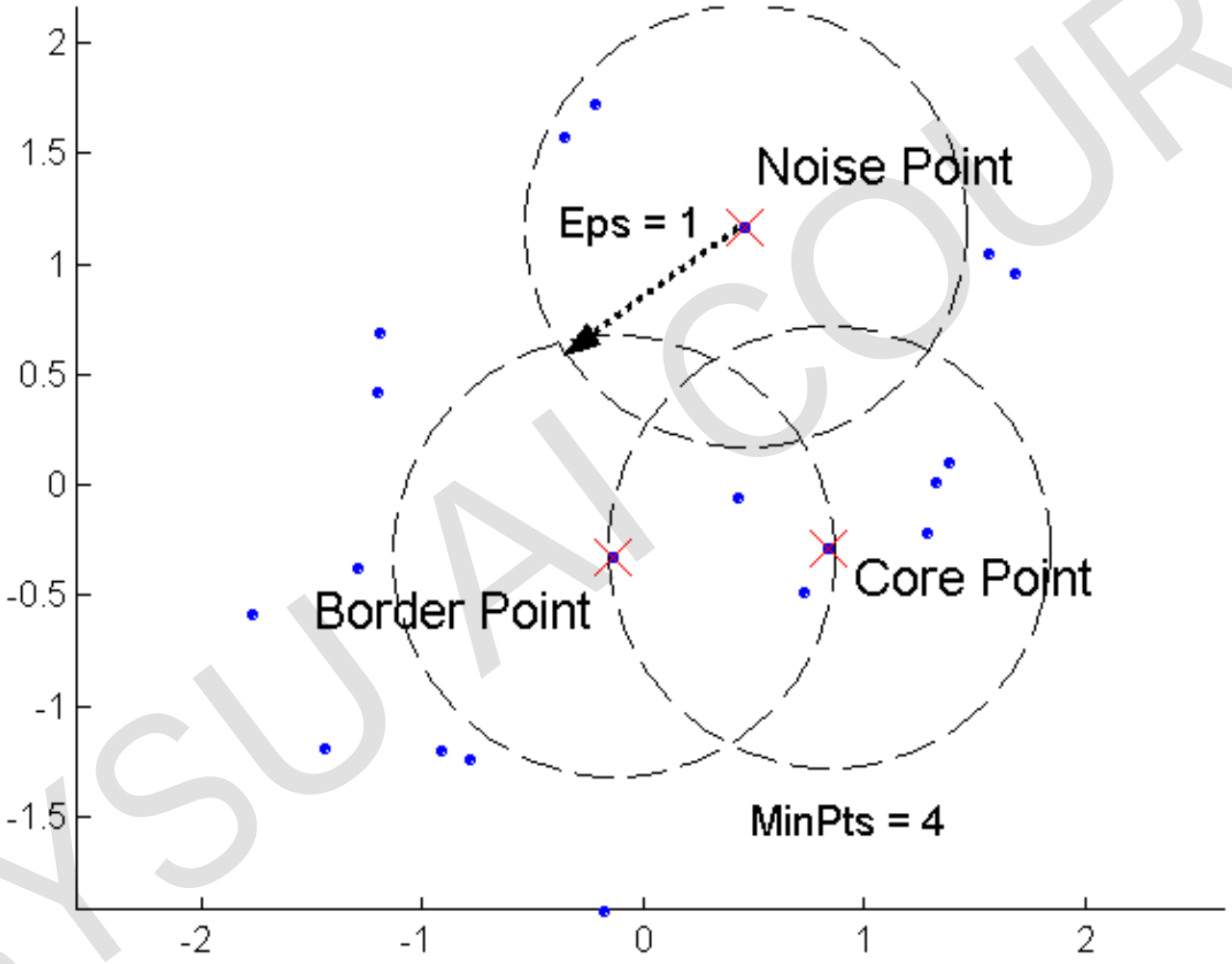


Figure 8.21. Core, border, and noise points.

- A point is a **core point** if it has more than a specified number of points (MinPts) within Eps. These are points that 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.

DBSCAN: Core, Border, and Noise Points



DBSCAN Algorithm

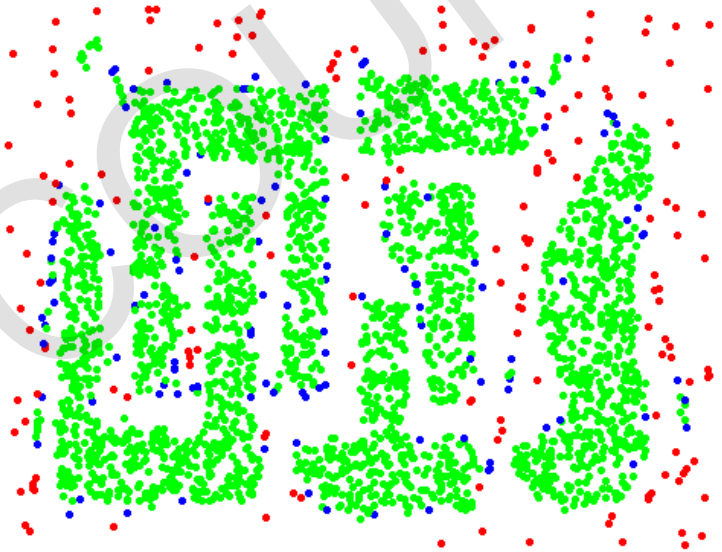
Center-based approach

Algorithm 8.4 DBSCAN algorithm.

1: Label all points as core, border, or noise points.
2: Eliminate noise points.
3: Put an edge between all core points that are within *Eps* of each other.
4: Make each group of connected core points into a separate cluster.
5: Assign each border point to one of the clusters of its associated core points.

DBSCAN: Core, Border and Noise Points

Original Points

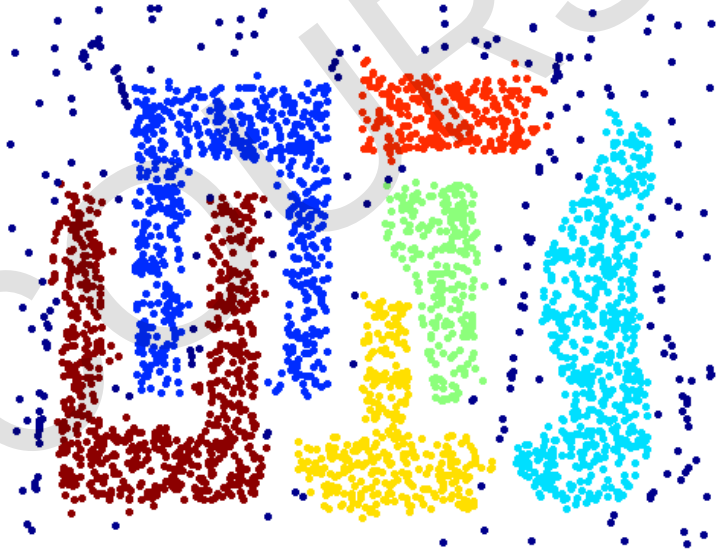


Point types: core, border and noise

Eps = 10, MinPts = 4

When DBSCAN Works Well

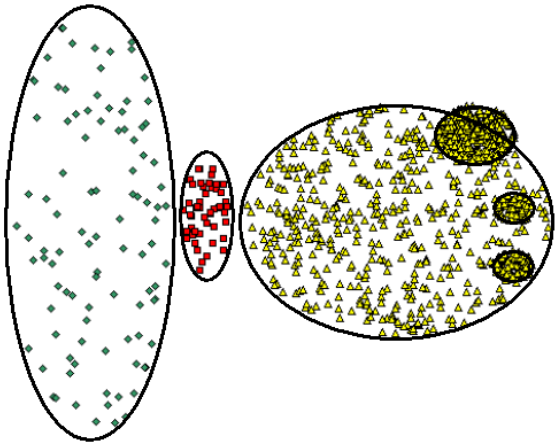
Original Points



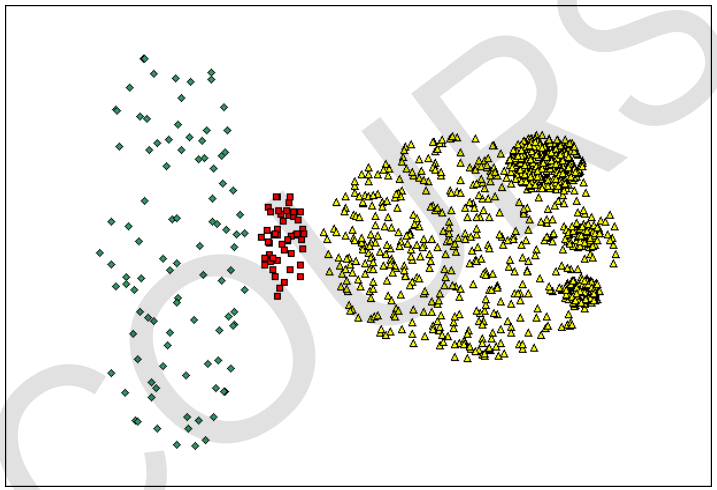
Clusters

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

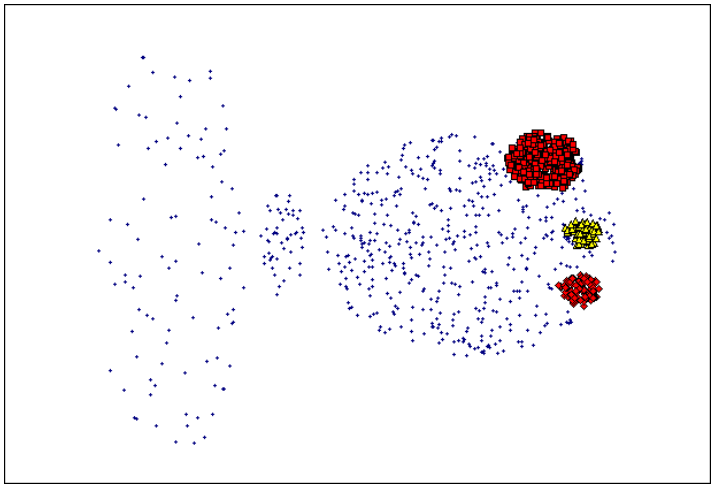
When DBSCAN Does NOT Work Well



Original Points



(MinPts=4, Eps=9.75).



(MinPts=4, Eps=9.92)

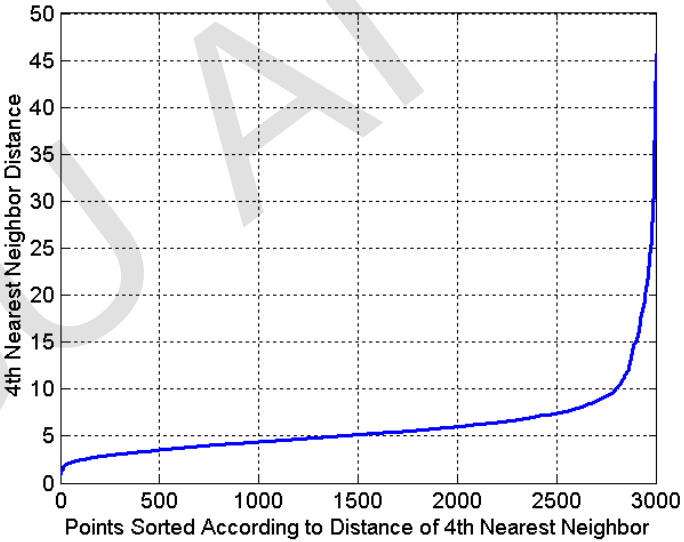
- **Varying densities**
- **High-dimensional data**

DBSCAN: Determining EPS and MinPts

Idea is that for points in a cluster, their k^{th} nearest neighbors are at roughly the same distance

Noise points have the k^{th} nearest neighbor at farther distance

So, plot sorted distance of every point to its k^{th} nearest neighbor



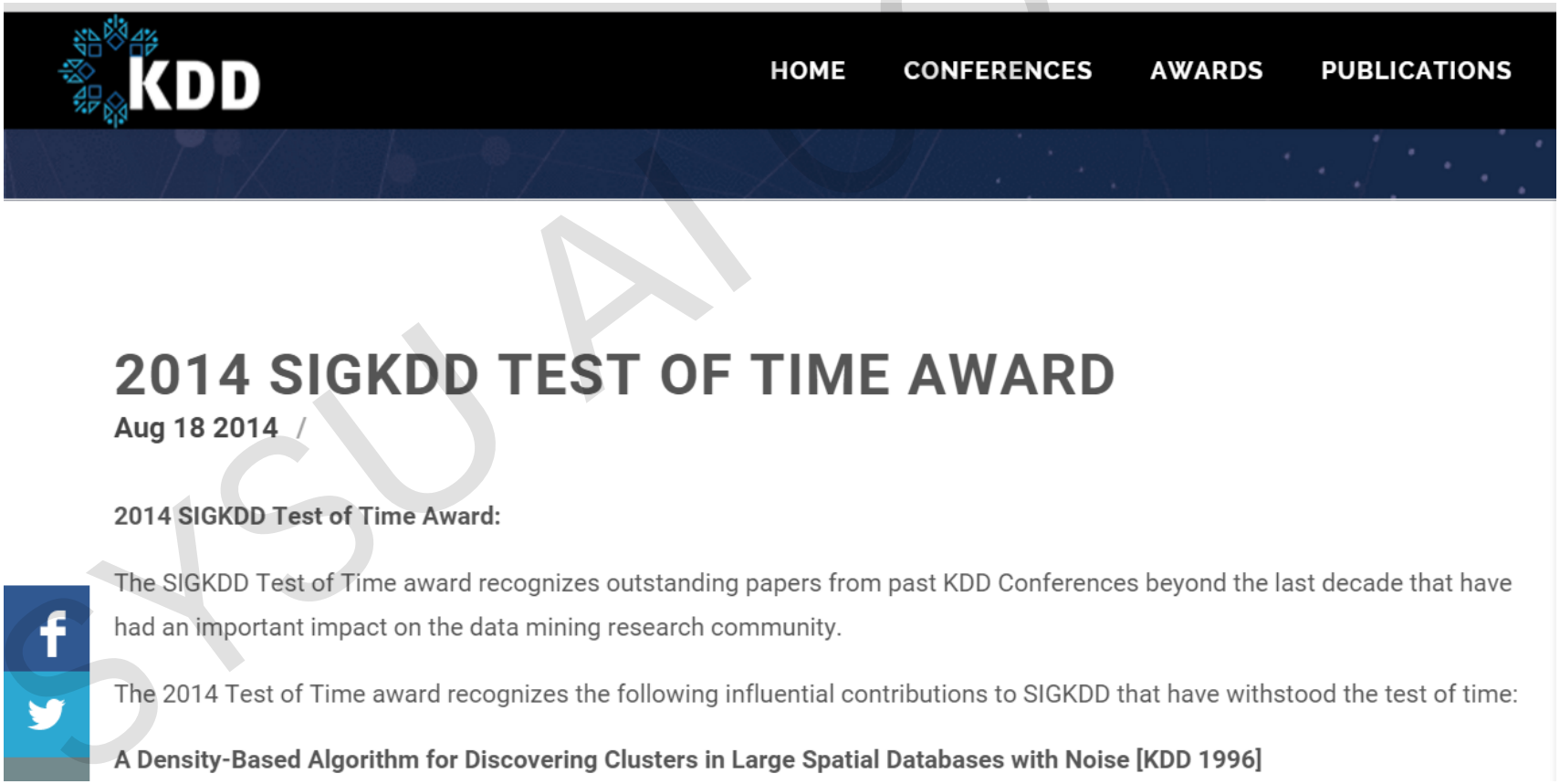
Time and Space Complexity

Time and Space Complexity

The basic time complexity of the DBSCAN algorithm is $O(m \times$ time to find points in the Eps-neighborhood), where m is the number of points. In the worst case, this complexity is $O(m^2)$. However, in low-dimensional spaces, there are data structures, such as kd-trees, that allow efficient retrieval of all points within a given distance of a specified point, and the time complexity can be as low as $O(m \log m)$. The space requirement of DBSCAN, even for high-dimensional data, is $O(m)$ because it is only necessary to keep a small amount of data for each point, i.e., the cluster label and the identification of each point as a core, border, or noise point.

2014 KDD TEST OF TIME AWARD

A Density-Based Algorithm for Discovering Clusters in Large Spatial Databases with Noise [KDD 1996]



2014 KDD TEST OF TIME AWARD

A Density-Based Algorithm for Discovering Clusters in Large Spatial Databases with Noise [KDD 1996]

- Proposed the now well-known clustering algorithm DBSCAN
- 10000+ citations

[PDF] A density-based algorithm for discovering clusters in large spatial databases with noise.
M Ester, HP Kriegel, J Sander, X Xu - Kdd, 1996 - aaai.org
Abstract Clustering algorithms are attractive for the task of class identification in spatial databases. However, the application to large spatial databases rises the following requirements for clustering algorithms: minimal requirements of domain knowledge to determine the input parameters, discovery of clusters with arbitrary shape and good efficiency on large databases. The well-known clustering algorithms offer no solution to ...
被引用次数：10010 相关文章 所有 75 个版本 引用 保存 更多

2014 KDD TEST OF TIME AWARD

A Density-Based Algorithm for Discovering Clusters in Large Spatial Databases with Noise [KDD 1996]

- Claimed that the average run time complexity of DBSCAN is O(n*logn)
- Follow papers mis-claimed that the complexity of DBSCAN is O(n*logn)

2015 SIGMOD Best Paper Award

DBSCAN Revisited: Mis-Claim, Un-Fixability, and Approximation.

SIGMOD Best Paper Award

Recipients of the award are the following:

2015	DBSCAN Revisited: Mis-Claim, Un-Fixability, and Approximation. Yufei Tao, Junhao Gan
2014	Materialization Optimizations for Feature Selection Workloads. Ce Zhang, Arun Kumar, Christopher Ré
2013	Massive Graph Triangulation. Xiaocheng Hu, Yufei Tao, Chin-Wan Chung
2012	High-Pe[2013 SIGMOD Best Paper Award]rocessing over XML Streams. Barzan Mozafari, Kai Zeng, Carlo Zaniolo
2011	Entangled Queries: Enabling Declarative Data-Driven Coordination. Nitin Gupta, Lucja Kot, Sudip Roy, Gabriel Bender, Johannes Gehrke, Christoph Koch
2010	FAST: Fast Architecture Sensitive Tree Search on Modern CPUs and GPUs. Changkyu Kim, Jatin Chhugani, Nadathur Satish, Eric Sedlar, Anthony Nguyen, Tim Kaldewey, Victor Lee, Scott Brandt, and Pradeep Dubey [award citation]

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2015 SIGMOD Best Paper Award

- DBSCAN Revisited: Mis-Claim, Un-Fixability, and Approximation.
  - For d ≥ 3, DBSCAN can't have O(n*logn) time complexity.
  - Prove that the DBSCAN problem requires $\Omega(n^{4/3})$ time to solve in d ≥ 3.
  - Introduce a new concept called ρ-*approximate DBSCAN* as an alternative to DBSCAN on large datasets of d ≥ 3.

2015 SIGMOD Best Paper Award

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Publications and Google Scholar

General

Short Bio

Yufei Tao joined as a Professor the School of Information Technology and Electrical Engineering, the University of Queensland (UQ) in Jan 2016. He obtained his PhD degree from Hong Kong University of Science and Technology (HKUST) in 2002, proudly under the supervision of Prof. Dimitris Papadias. He was a Visiting Scientist at the Carnegie Mellon University during 2002-2003, and then an Assistant Professor at the City University of Hong Kong during 2003-2006, after which he worked till Jan 2016 at the Chinese University of Hong Kong (CUHK), where he was promoted to Professor in 2009. From 2011 to 2013, he was simultaneously a Visiting Professor, under the World Class University program of the Korean government, in the Korea Advanced Institute of Science and Technology (KAIST), Korea. Currently, he also holds an honorary position of Adjunct Professor in the Department of Computer Science and Engineering, CUHK.

He served as an associate editor of *ACM Transactions on Database Systems* (*TODS*) from 2008 to 2015, and of *IEEE Transactions on Knowledge and Data Engineering* (*TKDE*) from 2012 to 2014. He served as a PC co-chair of *International Conference on Data Engineering* (*ICDE*) 2014, and of *International Symposium on Spatial and Temporal Databases* (*SSTD*) 2011. He gave a keynote speech at *International Conference on Database Theory* (*ICDT*) 2016.

Major Awards

SIGMOD Best Paper Award 2015
SIGMOD Best Paper Award 2013
Hong Kong Young Scientist Award 2002

DBSCAN Revisited

怀疑的精神

善于思考，善于发现问题

科学研究的发展是在曲折中不断前进的！

Reference

Ester, Martin, et al. "A density-based algorithm for discovering clusters in large spatial databases with noise." *Kdd*. Vol. 96. No. 34. 1996.

Gan, Junhao, and Yufei Tao. "DBSCAN Revisited: Mis-Claim, Un-Fixability, and Approximation." *Proceedings of the 2015 ACM SIGMOD International Conference on Management of Data*. ACM, 2015.

如何评价 SIGMOD 2015 最佳论文《DBSCAN Revisited》？
http://www.zhihu.com/question/31845624

Comparing K-means and DBSCAN

Both are partitional clustering that assign each object to a single cluster

- K-means: all object
- DBSCAN: discard noise

Type

- K-means: prototype-based notion
- DBSCAN: density-based notion

Both perform poorly with widely differing densities

- K-means: has difficult with non-globular cluster and clusters with different size
- DBSCAN: can handle clusters of different size and shapes, not affected by nosie

Comparing K-means and DBSCAN

Definition requirement

- K-means: need well-defined centroid
- DBSCAN: need definition of density

Sparse, high-dimensional data

- K-means: work well, such as document data
- DBSCAN: performs poorly for Euclidean definition of density

Distribution of data

- K-means: spherical Gaussian distributions
- DBSCAN: no assumption

Comparing K-means and DBSCAN

Both using all attributes

Overlap

- K-means: can find clusters
- DBSCAN: merge clusters that overlap

Determination

- K-means: no
- DBSCAN: yes

Comparing K-means and DBSCAN

Number of clusters

- K-means: user define
- DBSCAN: automatically,

  Two parameters: Eps and Minpts

Cluster Validity

For supervised classification we have a variety of measures to evaluate how good our model is

- Accuracy, precision, recall

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

Different Aspects of Cluster Validation 簇评估

1. Determining the **clustering tendency聚类趋势** of a set of data, i.e., distinguishing whether non-random structure actually exists in the data **聚类的前提需要数据是非均匀分布的**
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.

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 熵
- 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. 实际上不是一个单独的簇评估类型，而是度量的具体使用
  - 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.

Measuring Cluster Validity Via Correlation

Two matrices

- Proximity Matrix (Similarity/Dissimilarity Matrix)
- "Incidence" 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

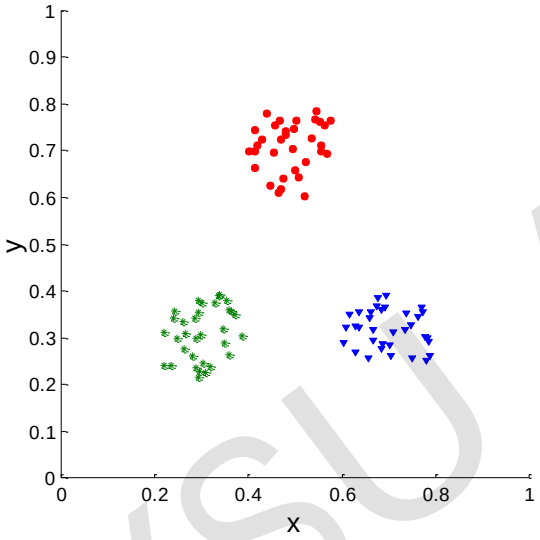
- Since the matrices are symmetric, only the correlation between n(n-1) / 2 entries needs to be calculated.

High correlation indicates that points that belong to the same cluster are close to each other.

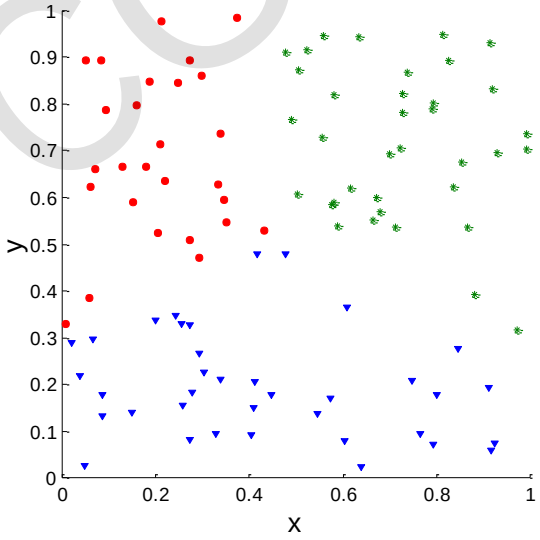
Not a good measure for some density or contiguity based clusters.

Measuring Cluster Validity Via Correlation

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



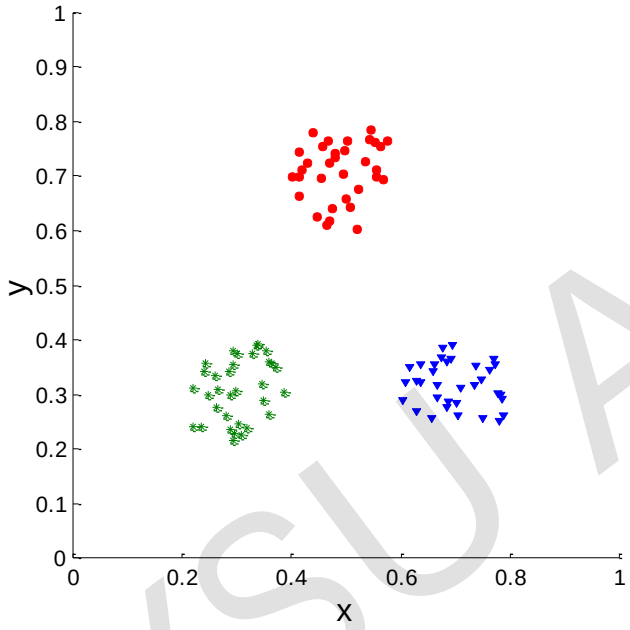
Corr = 0.9235

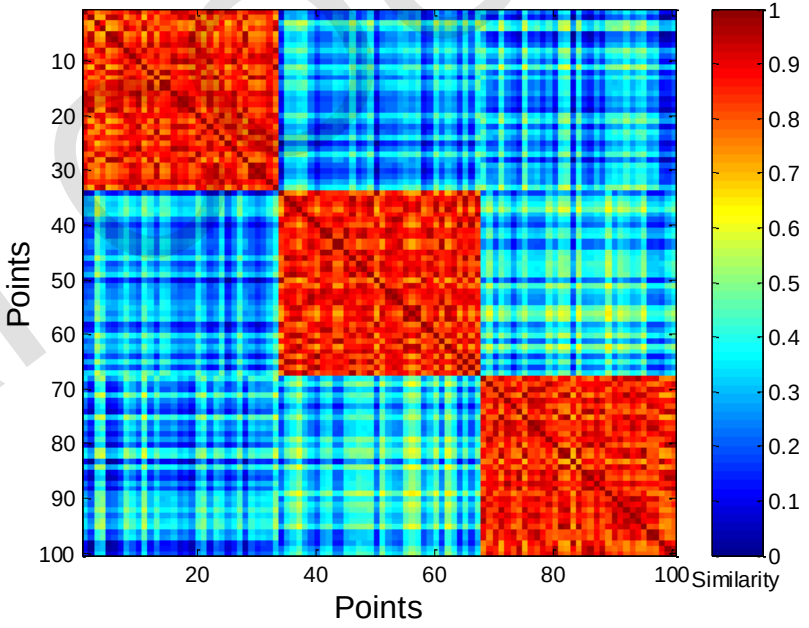


Corr = 0.5810

Using Similarity Matrix for Cluster Validation

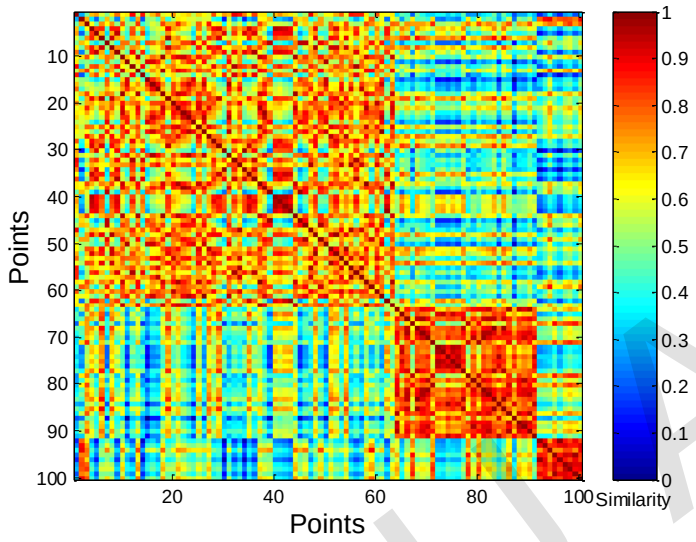
Order the similarity matrix with respect to cluster labels and inspect visually.

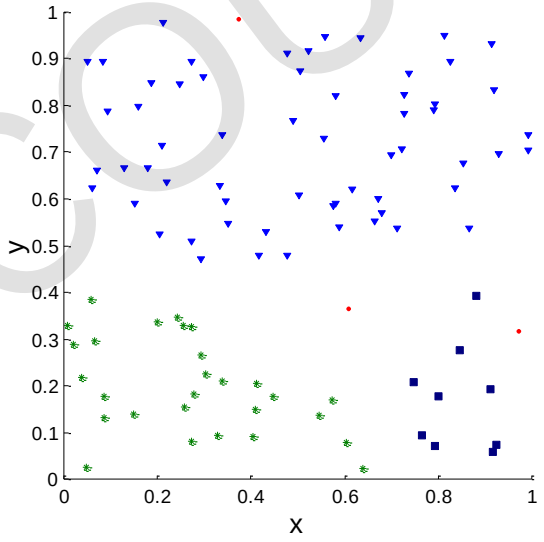




Using Similarity Matrix for Cluster Validation

Clusters in random data are not so crisp

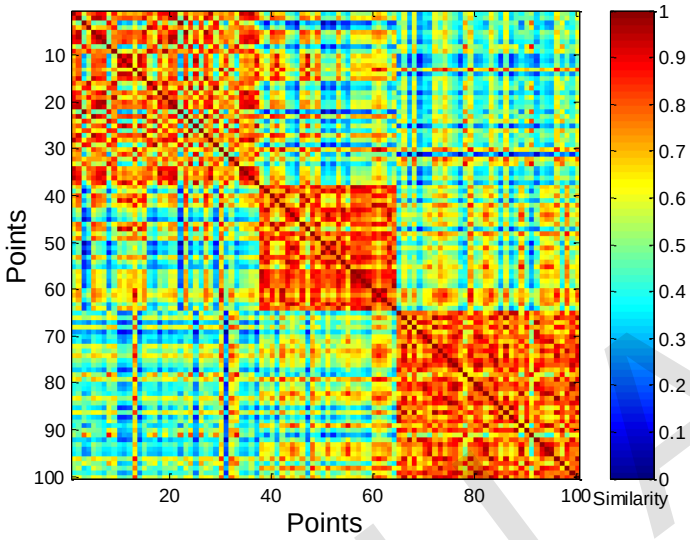


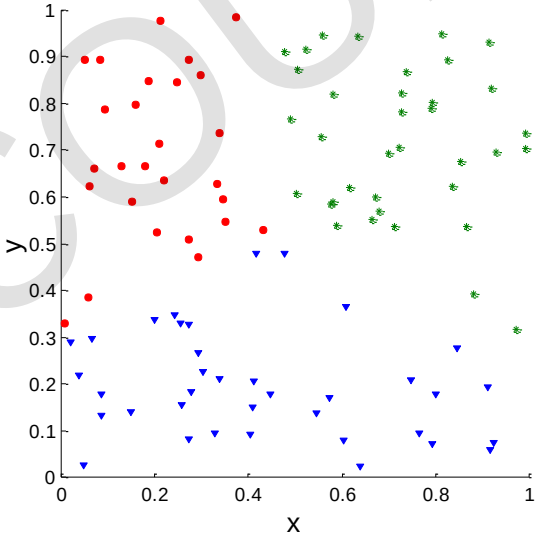


DBSCAN

Using Similarity Matrix for Cluster Validation

Clusters in random data are not so crisp

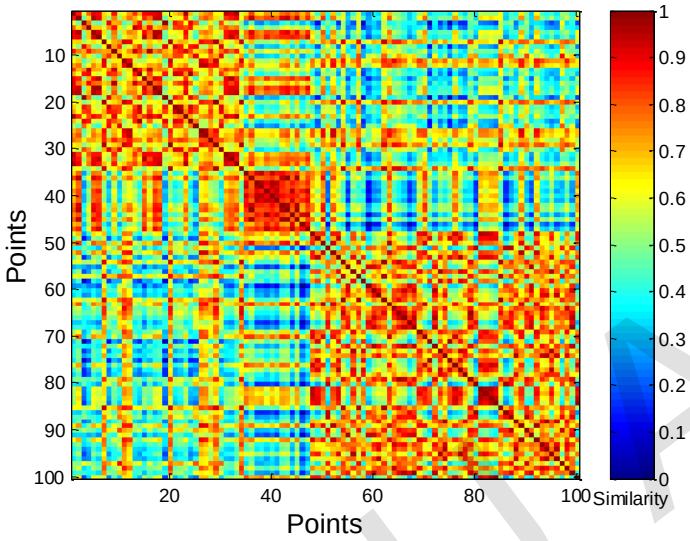


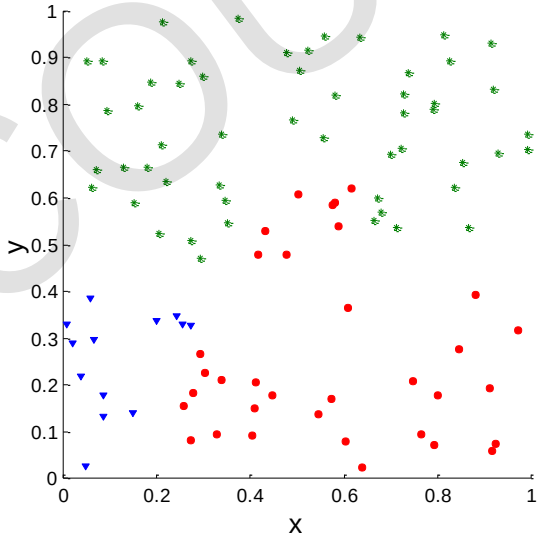


K-means

Using Similarity Matrix for Cluster Validation

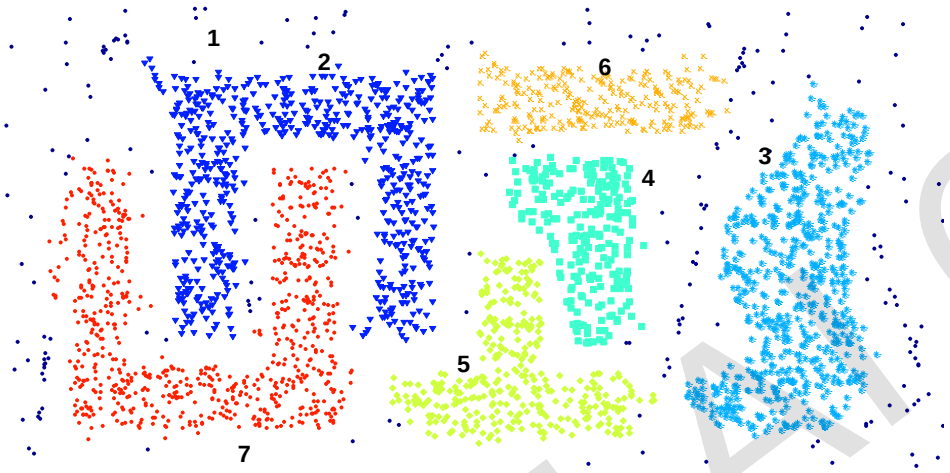
Clusters in random data are not so crisp

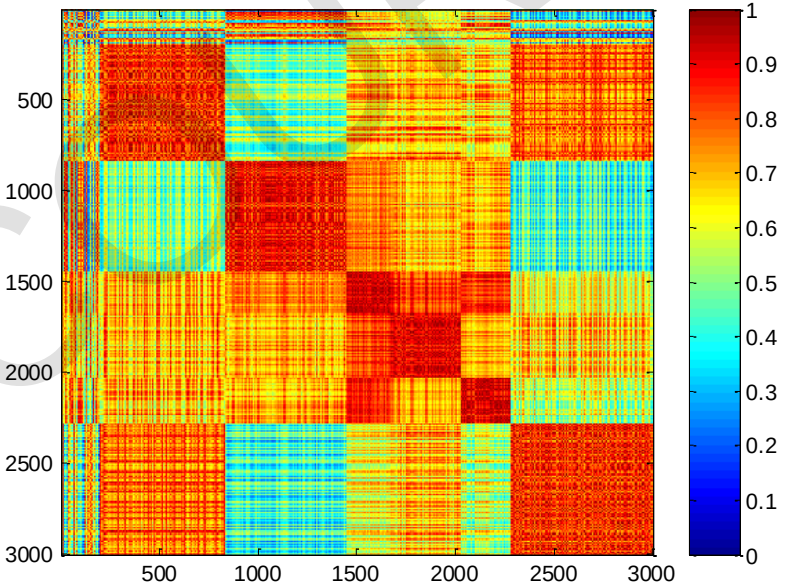




Complete linkage hierarchical clustering

Using Similarity Matrix for Cluster Validation





DBSCAN

Internal Measures: SSE

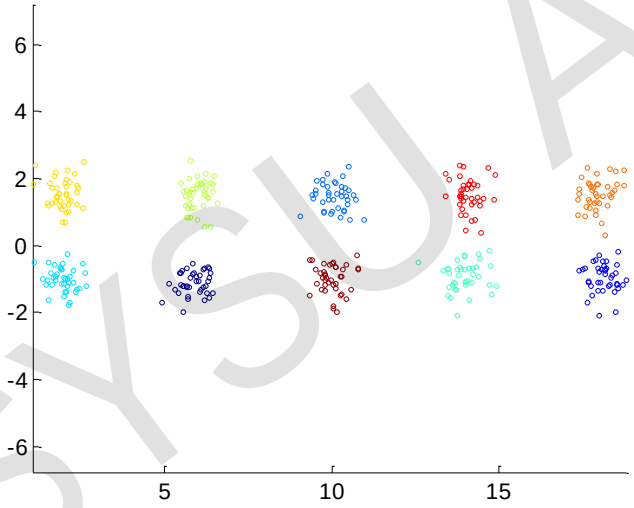
Clusters in more complicated figures aren't well separated

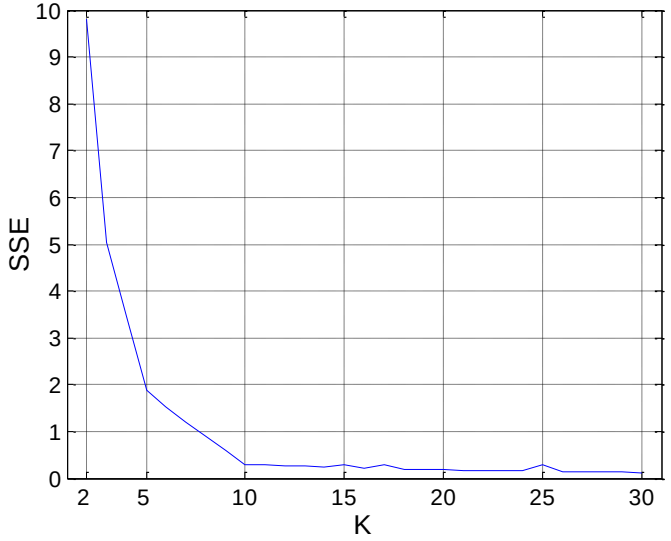
Internal Index: Used to measure the goodness of a clustering structure without respect to external information

- SSE

SSE is good for comparing two clusterings or two clusters (average SSE).

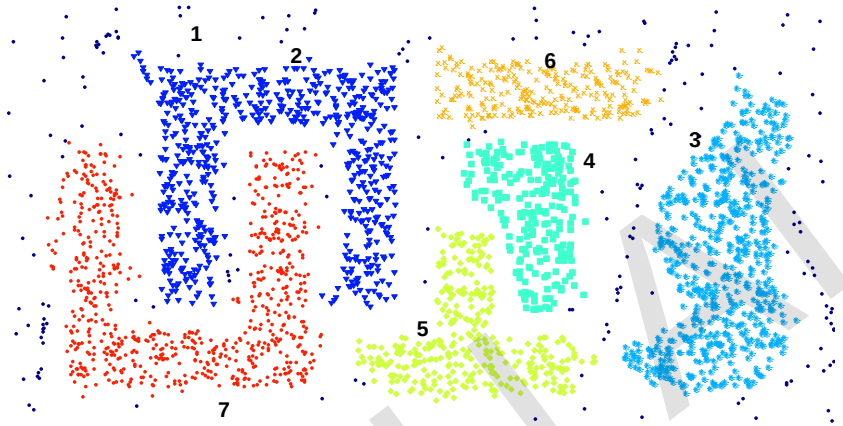
Can also be used to estimate the number of clusters

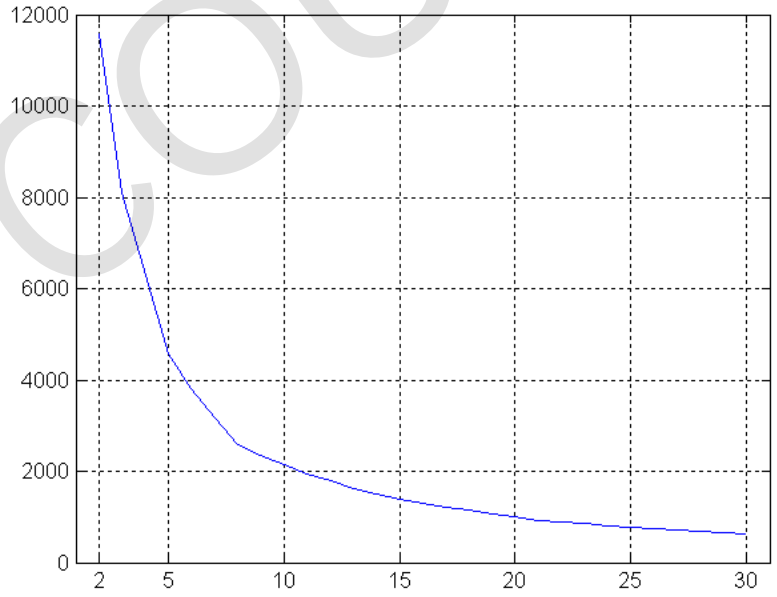




Internal Measures: SSE

SSE curve for a more complicated data set





SSE of clusters found using K-means

Internal Measures: Cohesion and Separation

Cluster Cohesion 凝聚度: Measures how closely related are objects in a cluster

- Example: SSE

Cluster Separation 分离度: Measure how distinct or well-separated a cluster is from other clusters

Example: Squared Error

- Cohesion is measured by the within cluster sum of squares (SSE)

$$SSE = \sum_{i} \sum_{x \in C_i} (x - m_i)^2$$

- Separation is measured by the between cluster sum of squares

$$SSB = \sum_{i} |C_i| (m - m_i)^2$$

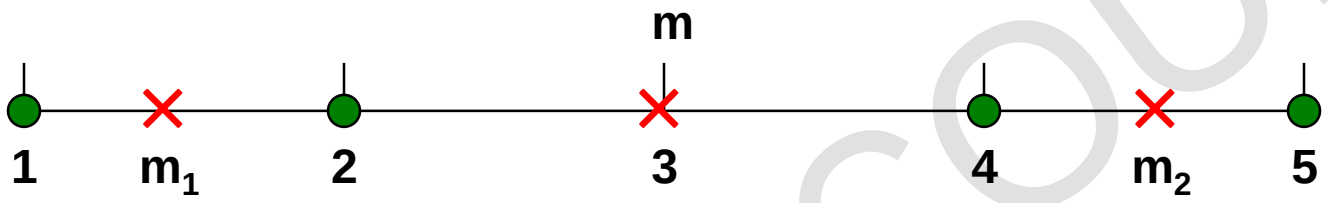
- Where $|C_i|$ is the size of cluster i

Internal Measures: Cohesion and Separation

Example:

$$TSS = \sum_{x} (x - m)^2$$

SSE+SSB=TSS **constant**



K=1 cluster:

$$SSE = (1-3)^2 + (2-3)^2 + (4-3)^2 + (5-3)^2 = 10$$

$$SSB = 4 \times (3-3)^2 = 0$$

$$Total = 10 + 0 = 10$$

K=2 clusters:

$$SSE = (1-1.5)^2 + (2-1.5)^2 + (4-4.5)^2 + (5-4.5)^2 = 1$$

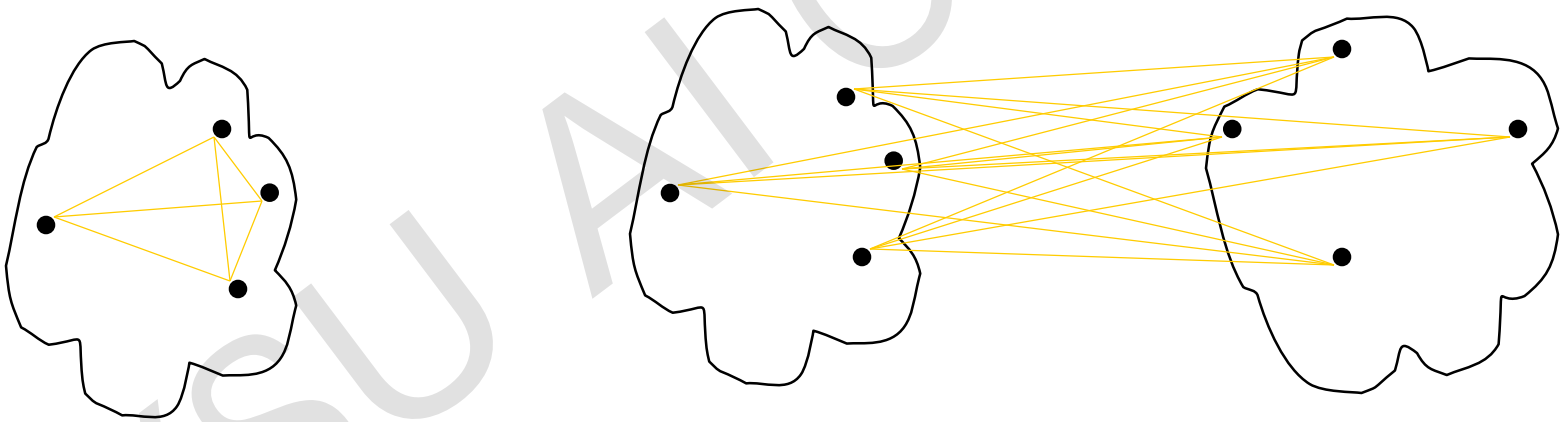
$$SSB = 2 \times (3-1.5)^2 + 2 \times (4.5-3)^2 = 9$$

$$Total = 1 + 9 = 10$$

Internal Measures: Cohesion and Separation

A proximity graph based approach can also be used for cohesion and separation.

- Cluster cohesion is the sum of the weight of all links within a cluster.
- Cluster separation is the sum of the weights between nodes in the cluster and nodes outside the cluster.



cohesion

separation

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