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Lecture 4: Scalable k -means Clustering

COM6012: Scalable ML by Haiping Lu

YouTube Playlist: <https://www.youtube.com/c/HaipingLu/>

Week 4 Contents / Objectives

- Introduction to Cluster Analysis
- k -means Clustering
- Scalable k -means
- k -means in Spark & Limitations

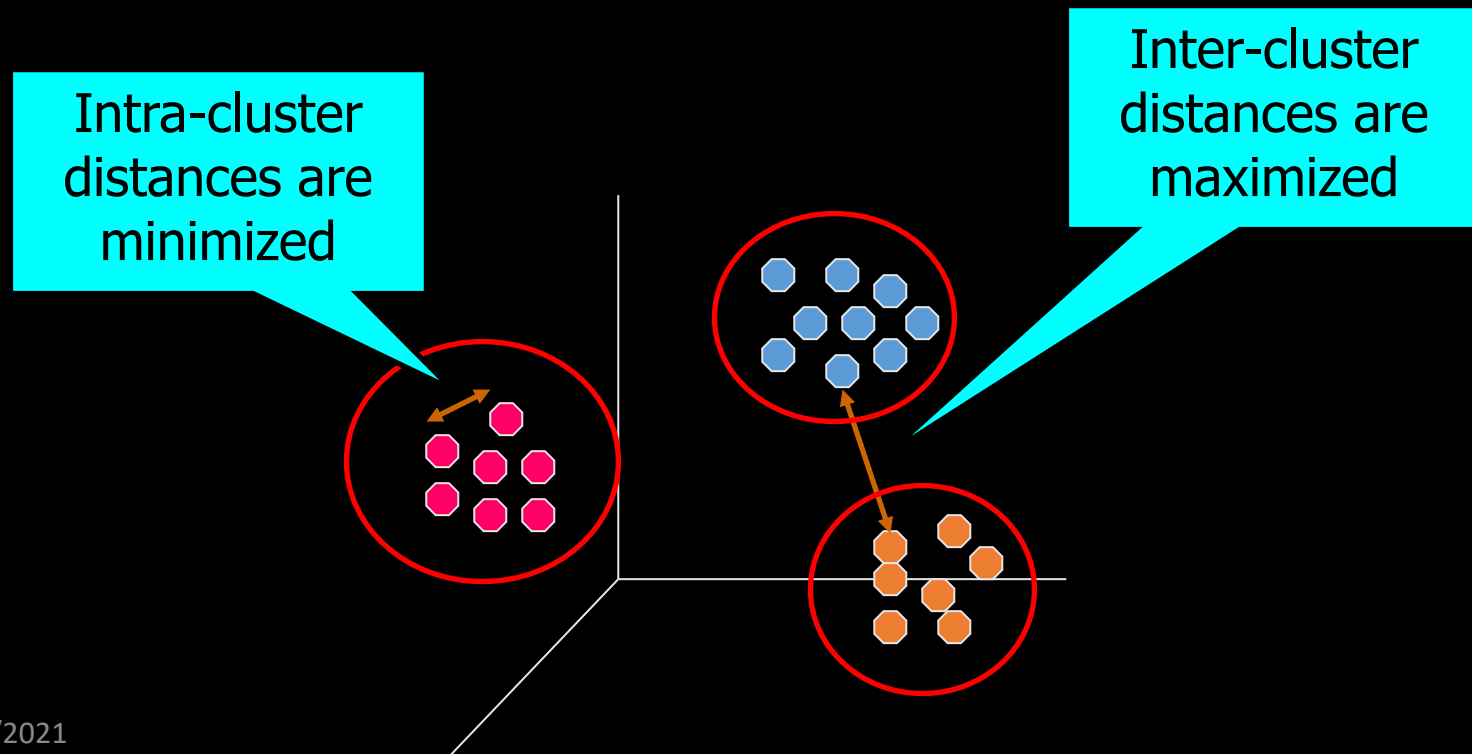
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Cluster Analysis

Output	Supervised	Unsupervised
Discrete	Classification	Clustering
Continuous	Regression	Dimensionality Reduction

- “Classification without labelled data”
- “Dimensionality reduction to 1 (cluster index)”



Cluster Analysis

- Divide data into clusters that are meaningful/useful
- Clusters: **pseudo**-classes
- Key for exploratory data analysis in many areas
 - Brain parcellation, social network analysis, customer segmentation, patient stratification, drug discovery, ...



[brain-video2.jpg \(1014×570\) \(wp.com\)](#)

n



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[segmentation3.png \(586×236\) \(visionedgemarketing.com\)](#)

Anomaly/Outlier Detection

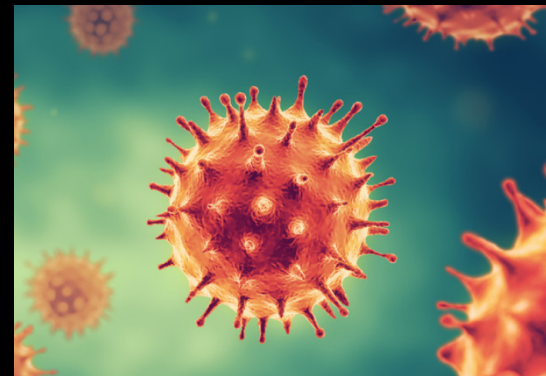
- Anomalies: data points very different from others
- Applications: credit card fraud, network intrusion, unknow virus, eco disturbance, unusual symptom, ...



[financial protection credit card fraud img1.jpg \(512×347\) \(traderdefenseadvisory.com\)](#)



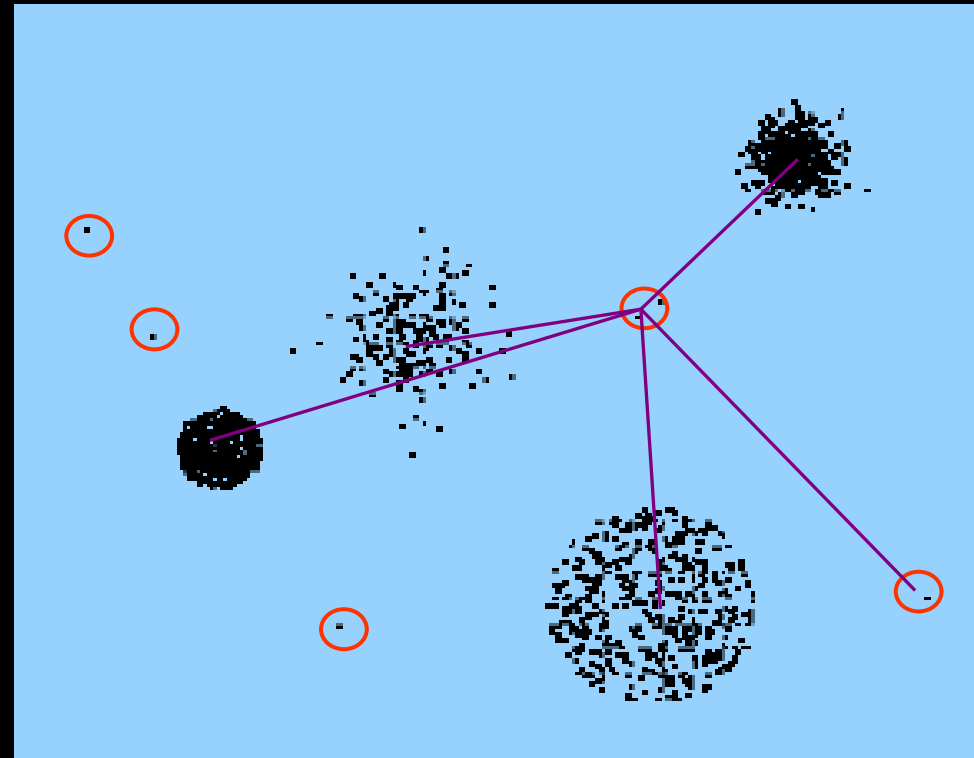
[Network-Intrusion-Detection-and-Prevention-.jpg \(1600×962\) \(wp.com\)](#)



[newseventsimage_1613554577167_mainnews2012_x1.jpg \(700×484\) \(imperial.ac.uk\)](#)

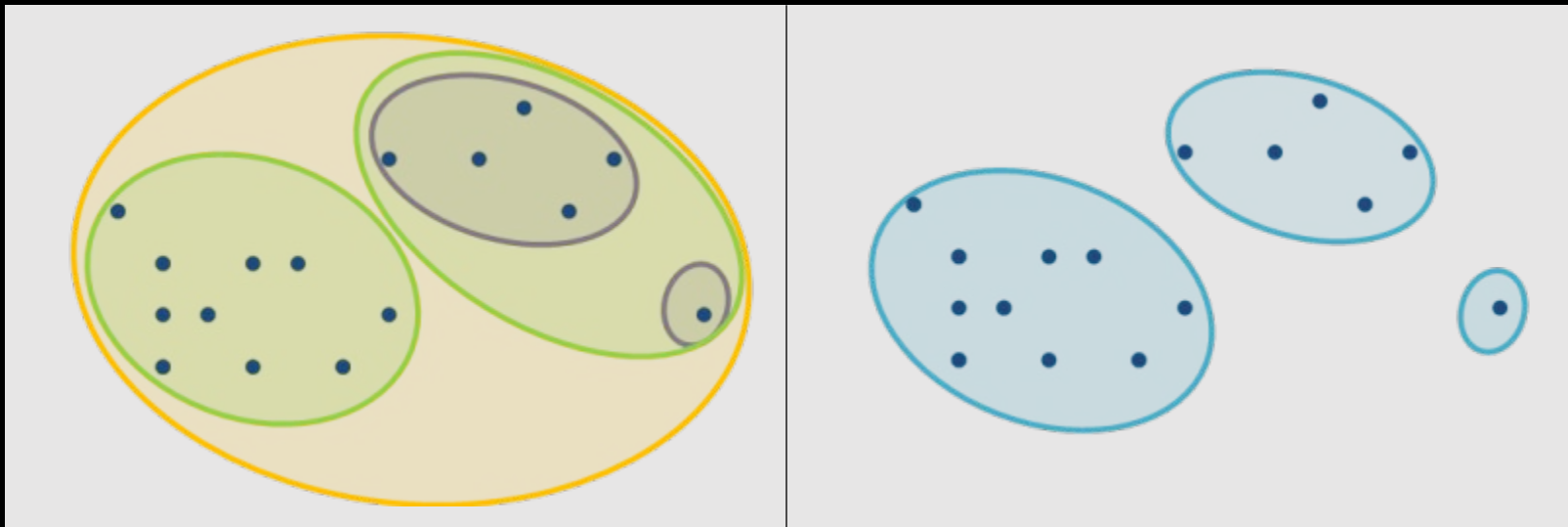
Clustering-based Anomaly Detection

- Cluster the data points
- Those in small clusters
→ candidate outliers
- Compute the distance between candidate points and non-candidate clusters
- Candidate points far from all other non-candidate points → outliers

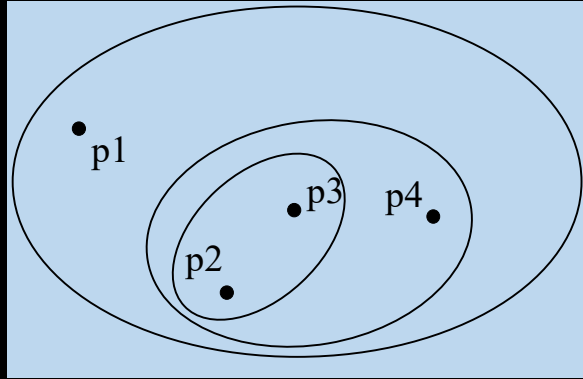


Hierarchical vs Partitional Clustering

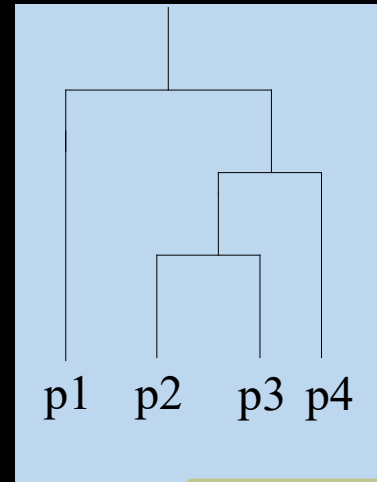
- Hierarchical: **nested** clusters as a hierarchical tree
 - Each node (cluster) in the tree (except for the leaf nodes) is the union of its children (subclusters)
 - The root of the tree → the cluster containing all data points
- Partitional: **non-overlapping** clusters
 - Each data point is in exactly one cluster



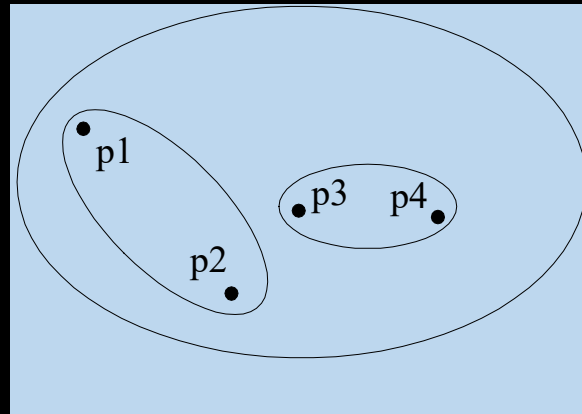
Hierarchical Clustering



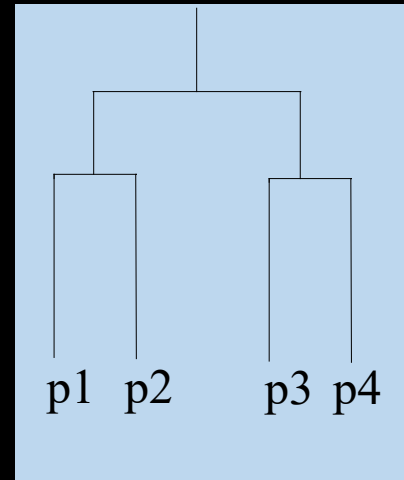
Traditional Hierarchical Clustering



Traditional Dendrogram



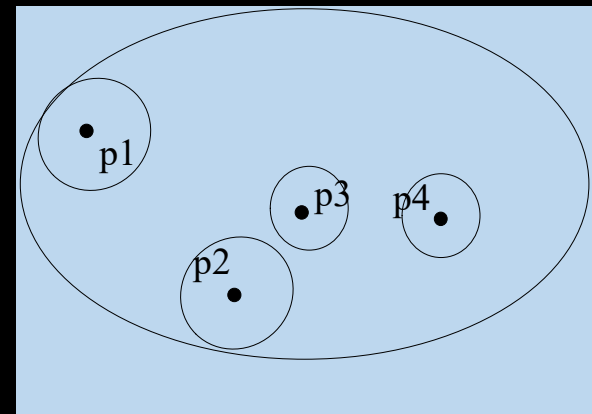
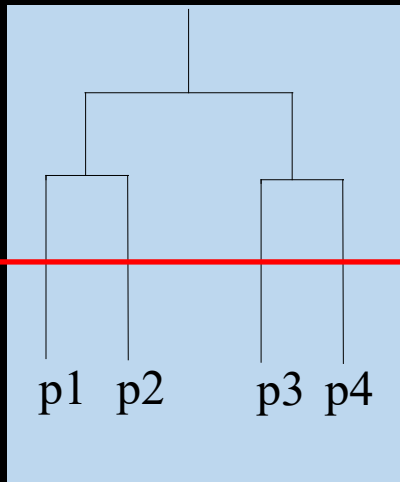
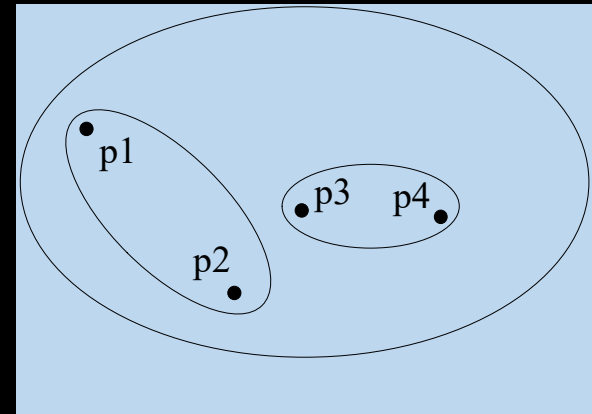
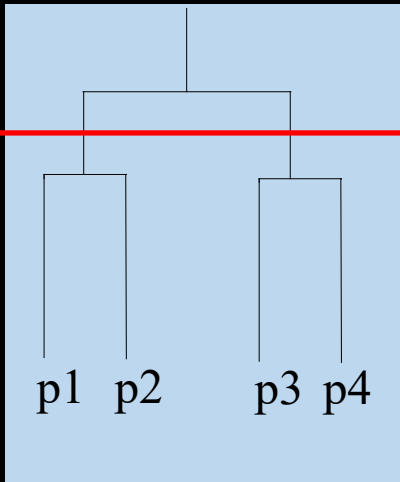
Non-traditional Hierarchical Clustering



Non-traditional Dendrogram

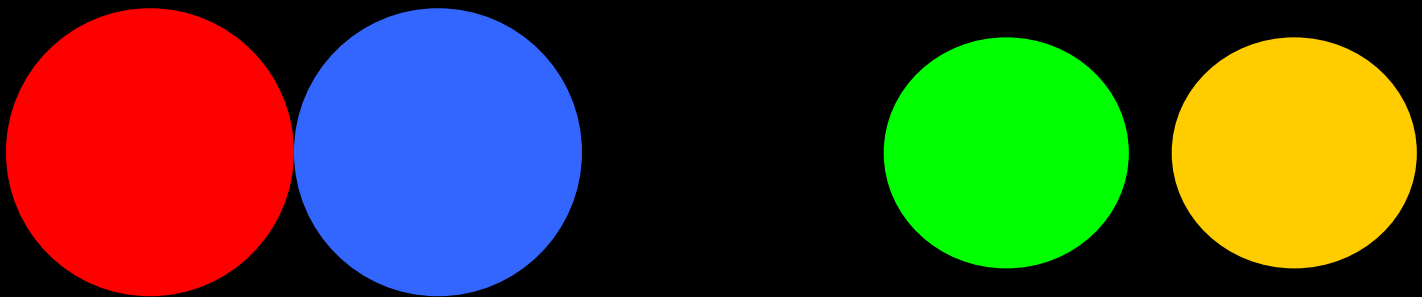
Hierarchical → Partitional

- **Hierarchical** = a sequence of partitional clustering cutting the hierarchical tree at a particular level



Centre/Prototype-based Clusters

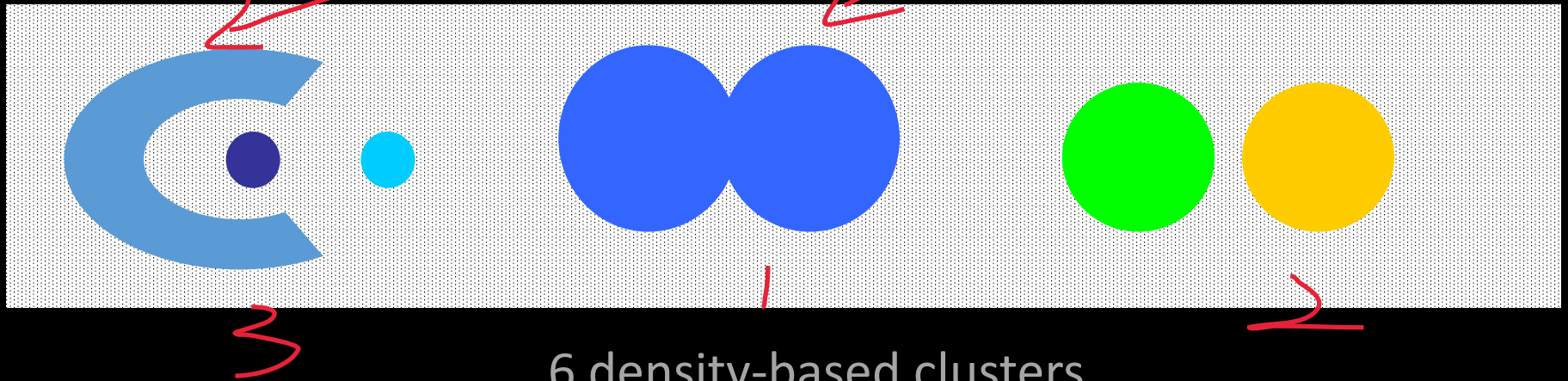
- Data points in a cluster are closer (more similar) to the centre of that cluster than to the centre of any others
- Centre
 - **Centroid**: the **average** of all the points in a cluster
 - **Medoid**: the most **representative** point of a cluster (e.g., categorical)



4 centre-based clusters

Density-based Clusters

- **Cluster**: a dense region of points separated by low-density regions from other regions of high density
- Used when the clusters are irregular/intertwined, and when noise and outliers are present



6 density-based clusters

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k -means Clustering

- A **centre-based, partitional** clustering approach
- Input: a set of n data points $X = \{x_1, x_2, \dots, x_n\}$ and the number of clusters k
- For a set $C = \{c_1, c_2, \dots, c_k\}$ of cluster centres, define the **Sum of Squared Error (SSE)** as:

$$SSE_X(C) = \sum_{x \in X} d(x, C)^2$$

$d(x, C)$: distance from x to the closest centre in C

- Goal: find C centres minimising $SSE_X(C)$

Lloyd Algorithm for k -means

- Start with k centres $\{c_1, c_2, \dots, c_k\}$ chosen uniformly at random from data points
- Assign clusters and compute centroids till convergence
 - Alternating optimisation again, similar to ALS
- Limitations
 - Many iterations to converge
 - Sensitive to initialisation
 - Random initialisation can get two centres in the same cluster \rightarrow stuck in a local optimum (example on next slide)

Initialisation → Stuck

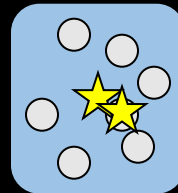
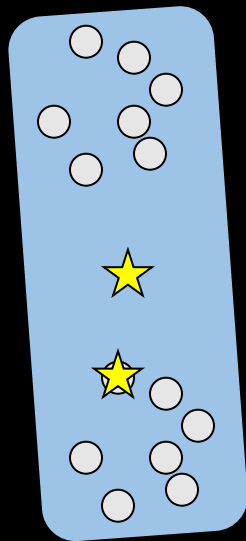


Figure credited to David Arthur

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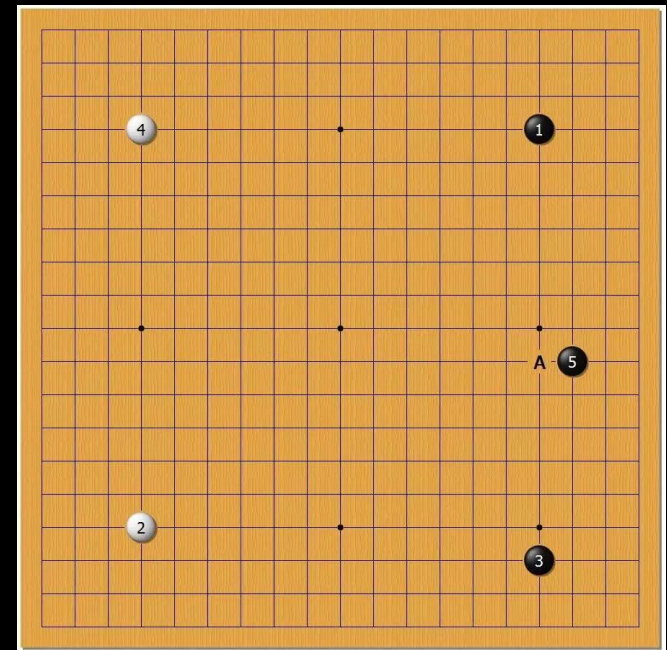
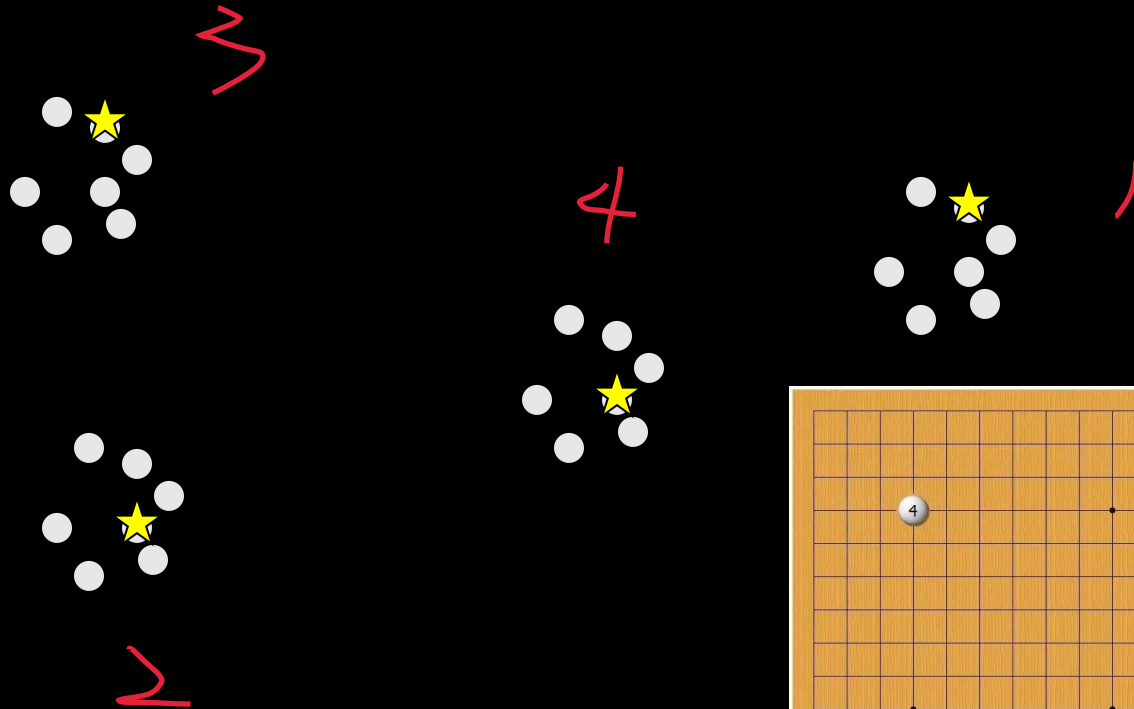
k -means++ [Arthur et al. '07]

- Key idea: **spread out the centres**
- Choose the first centre c_1 uniformly at random
- Repeat for $2 \leq i \leq k$:
 - Choose c_i to be equal to a data point x_0 **sampled** from the distribution:

$$\frac{d(x_0, C)^2}{SSE_X(C)} \propto d(x_0, C)^2$$

- Reminder: $d(x, C)$ = distance from x to the closest centre in C
- Theorem: $O(\log k)$ -approximation to the optimum

k -means++ Initialisation



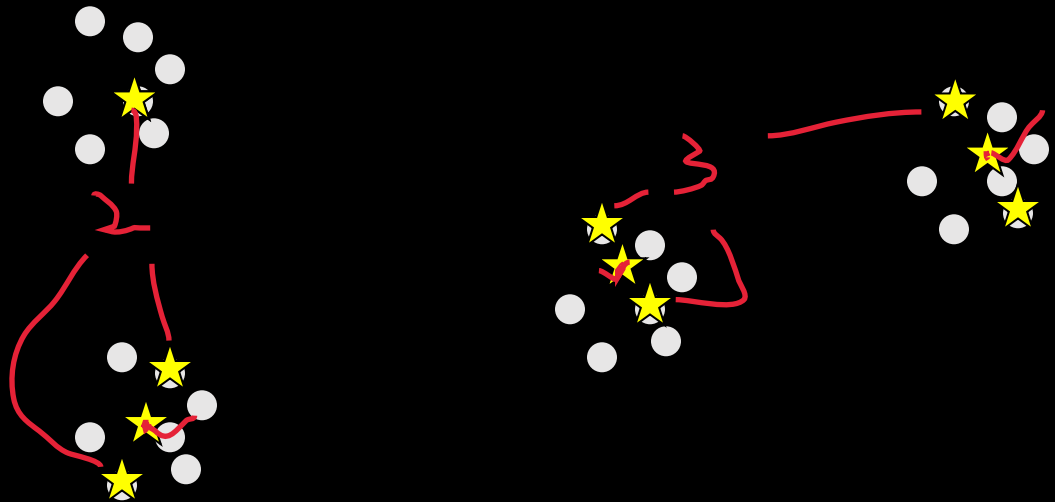
k -means++ \rightarrow k -means ||

- k -means++ limitations
 - Needs k passes over the data for initialisation
 - In big data applications, k is typically large (e.g., 1000) \rightarrow not scalable!
- A promising solution
 - k -means++ samples **just** one point per iteration
 - What if we **oversample** by sampling each point independently with a larger probability?
 - Equivalent to updating the distribution less frequently
 - **Coarser** sampling \rightarrow k -means || [Bahmani et al. '12]

k -means || Initialisation

$k=4$, oversampling factor $L=3$

Cluster the intermediate centres

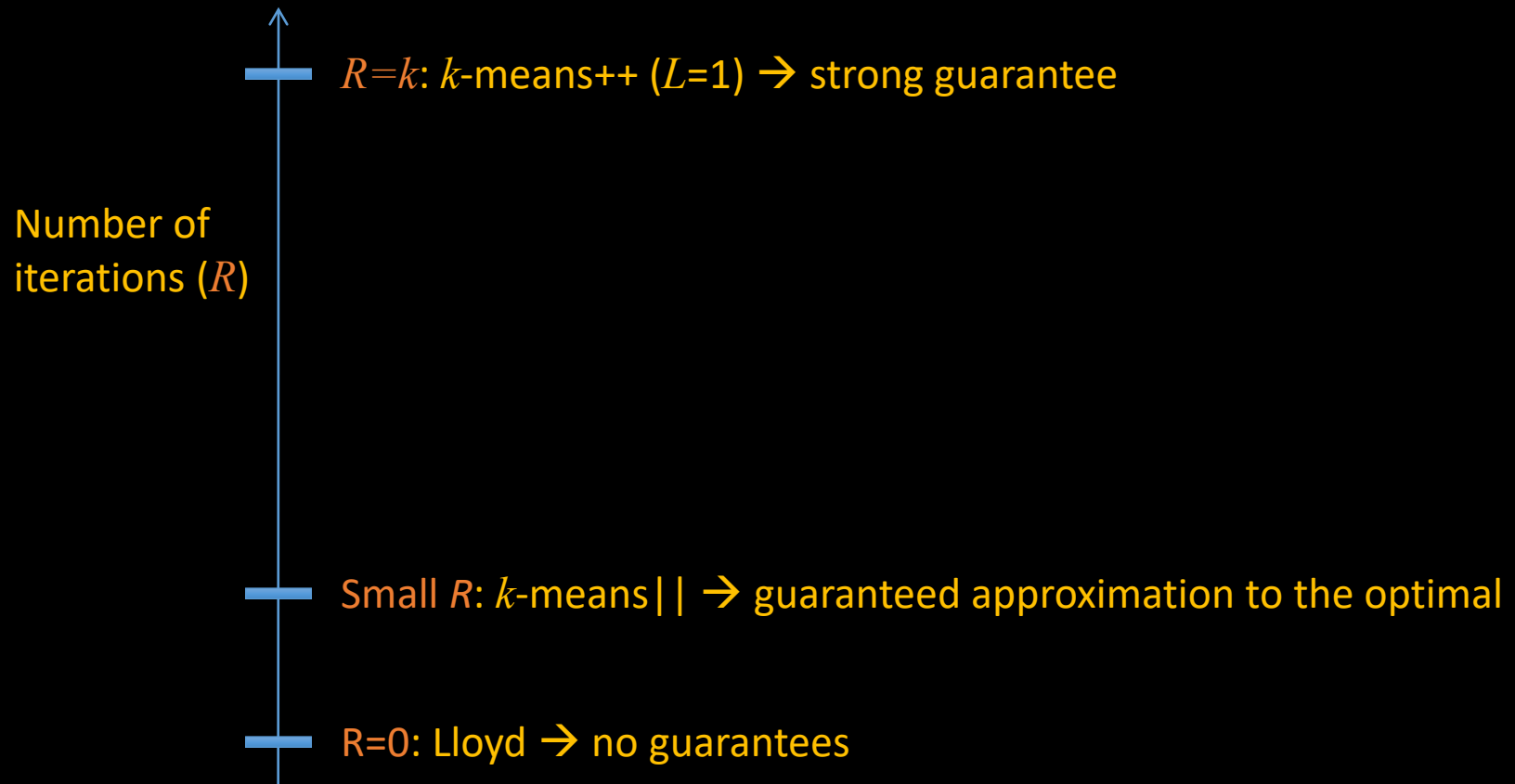


k -means | [Bahmani et al. '12]

- Choose the oversampling factor $L > 1$
- Initialise C to an arbitrary set of points
- For R iterations do:
 - Sample each point x in X independently with probability $p_x = Ld(x, C)^2 / SSE_X(C)$.
 - Add all the sampled points to C
- Cluster the intermediate centres in C using k -means++
- Benefits over k -means++
 - Less susceptible to noisy outliers
 - More reduction in the number of Lloyd iterations

k -means || : Relationships

- An interpolation between Lloyd and k -means++



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k -means in Spark

- Implemented in the RDD API Mllib - Kmeans
- Scala ml code: [org/apache/spark/ml/clustering/KMeans.scala](https://github.com/apache/spark/blob/master/mllib/src/main/scala/org/apache/spark/mllib/clustering/KMeans.scala)

```
29 import org.apache.spark.ml.util._
30 import org.apache.spark.ml.util.Instrumentation.instrumented
31 import org.apache.spark.mllib.clustering.{DistanceMeasure, KMeans => MllibKMeans, KMeansModel => MllibKMeansModel}
32 import org.apache.spark.mllib.linalg.{Vector => OldVector, Vectors => OldVectors}
33 import org.apache.spark.mllib.linalg.VectorImplicits._
34 ...
```

- Scala mllib: [org/apache/spark/mllib/clustering/KMeans.scala](https://github.com/apache/spark/blob/master/mllib/src/main/scala/org/apache/spark/mllib/clustering/KMeans.scala)

```
33 /**
34  * K-means clustering with a k-means++ like initialization mode
35  * (the k-means|| algorithm by Bahmani et al).
36  *
37  * This is an iterative algorithm that will make multiple passes over the data, so any RDDs given
38  * to it should be cached by the user.
39  */
40 @Since("0.8.0")
41 class KMeans private (
42   private var k: Int,
```

k -means API

- **k**: the number of desired clusters
- **maxIter**: the maximum number of iterations
- **initMode**: random or via k-means || (default) initialization
- **initSteps**: the number of steps in the k-means || algorithm (default=2, oversampling factor $L = \underline{2 \times k}$)
- **tol**: the distance threshold for checking convergence
- **seed**: the random seed
- **distanceMeasure**: Euclidean (default) or cosine dist measure
- **weightCol**: optional weighting of data points

```
375 // On each step, sample 2 * k points on average with probability proportional
376 // to their squared distance from the centers. Note that only distances between points
377 // and new centers are computed in each iteration.
378 var step = 0
379 val bcNewCentersList = ArrayBuffer[Broadcast[_]]()
380 while (step < initializationSteps) {
```

Remember to Cache

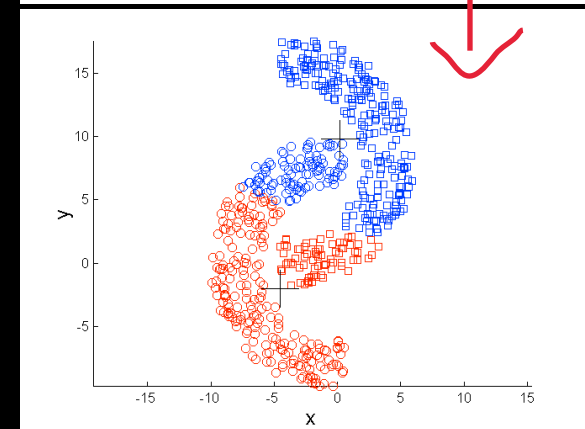
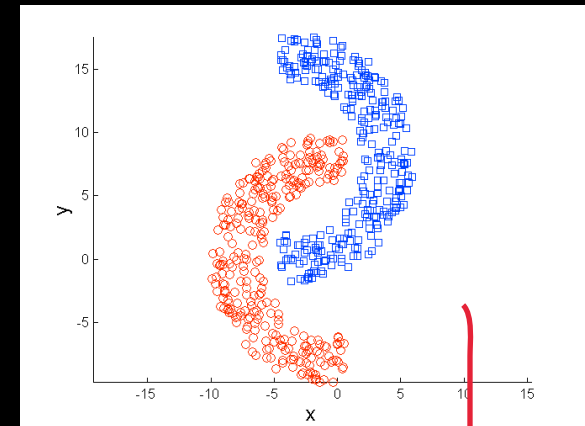
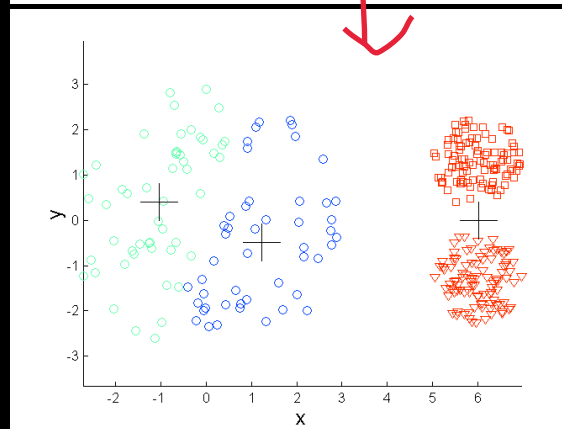
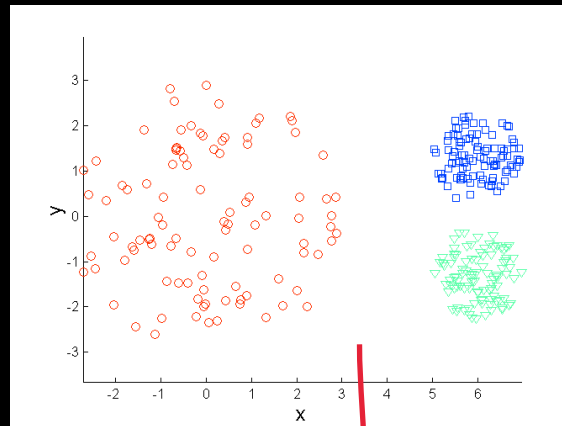
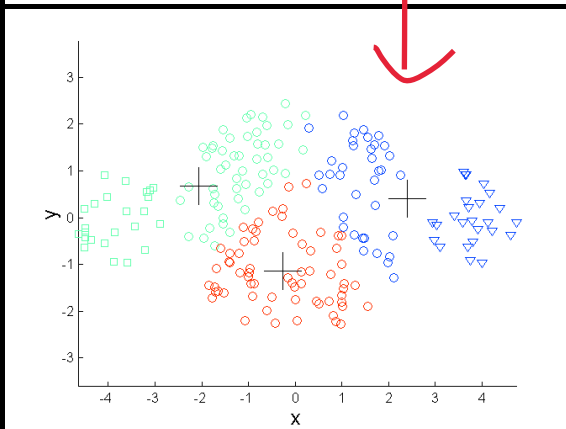
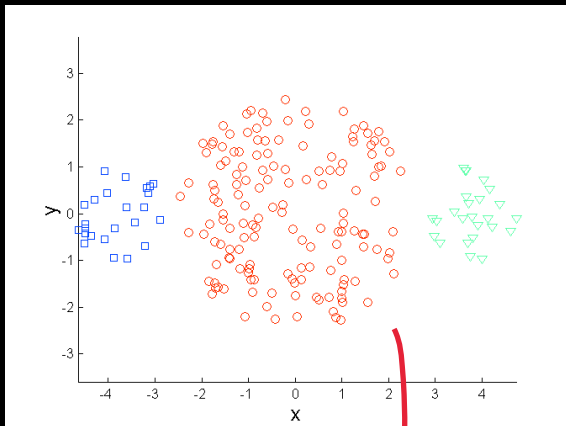
- Data need to be **cached** for high performance
- See from the source code

```
33  /**
34   * K-means clustering with a k-means++ like initialization mode
35   * (the k-means|| algorithm by Bahmani et al).
36   *
37   * This is an iterative algorithm that will make multiple passes over the data, so any RDDs given
38   * to it should be cached by the user.
39   */
40  @Since("0.8.0")
41  class KMeans private (

207   * Train a K-means model on the given set of points; `data` should be cached for high
208   * performance, because this is an iterative algorithm.
209   */
210  @Since("0.8.0")
211  def run(data: RDD[Vector]): KMeansModel = {
212    val instances = data.map(point => (point, 1.0))
213    val handlePersistence = data.getStorageLevel == StorageLevel.NONE
```

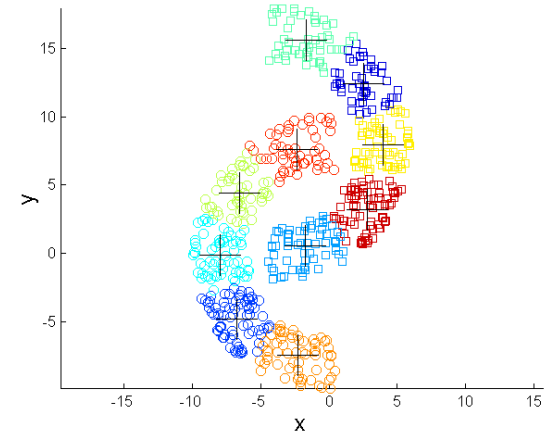
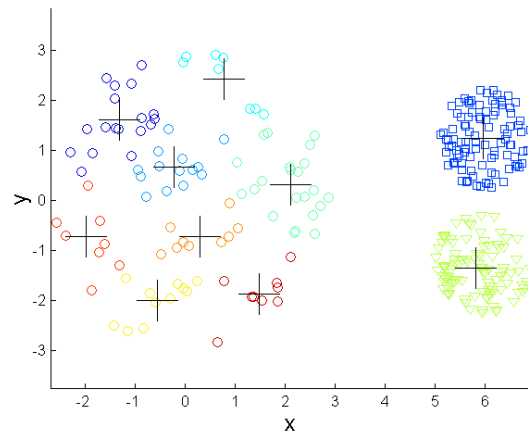
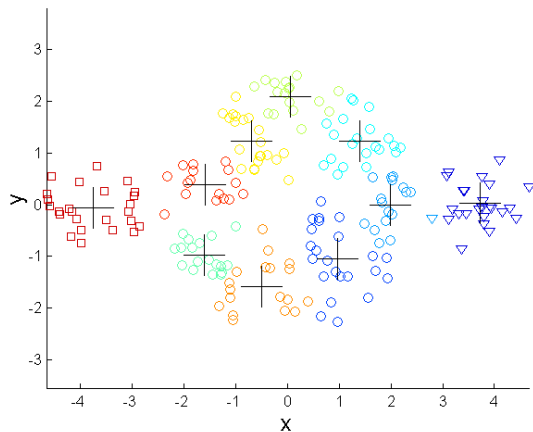
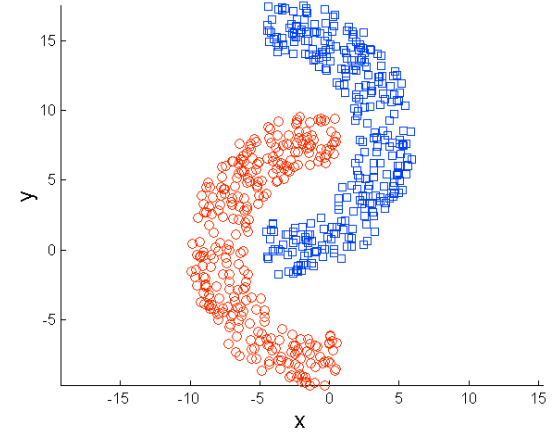
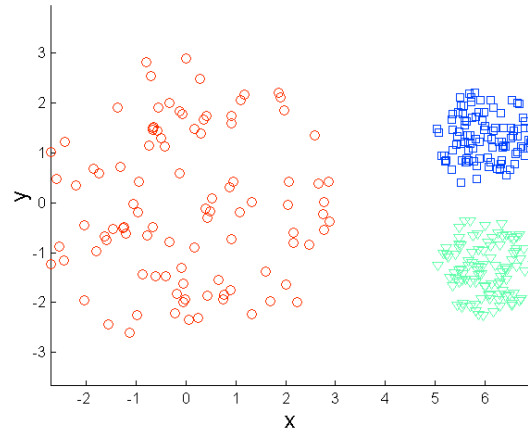
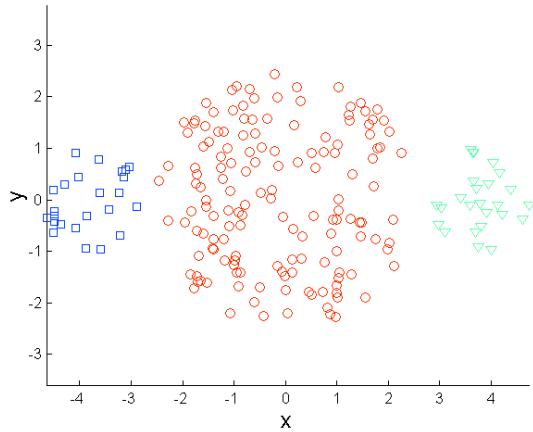
Limitations of k -means

- Problems when clusters are of differing sizes, densities, or non-globular shapes



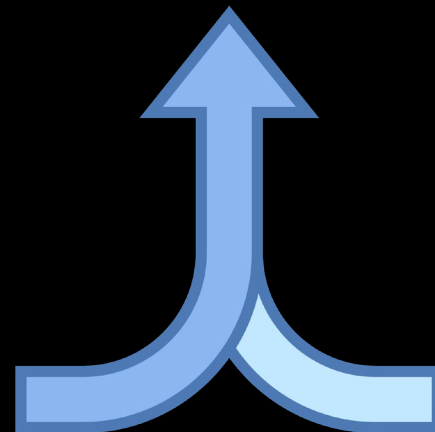
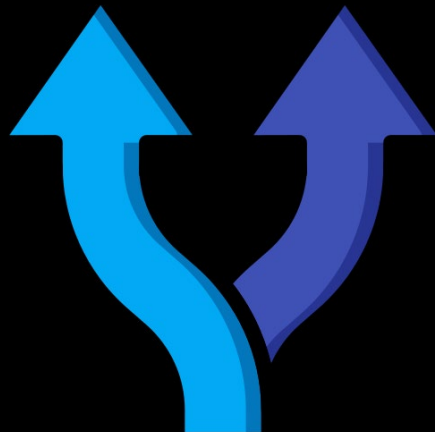
Overcoming k -means Limitations

- Use many clusters to find parts of clusters → put together



Pre-processing & Post-processing

- Pre-processing
 - Normalise the data (distance measure)
 - Eliminate outliers
- Post-processing
 - Eliminate small clusters that may represent outliers
 - Split **loose** clusters (with relatively high SSE)
 - Merge clusters that are **close** (with relatively low SSE)



Acknowledgement & References

- Acknowledgement

- Some slides are adapted from 1) the [k-means || slides](#) by Bahman Bahmani, Stanford University, 2012, and 2) Tan, Steinbach, Kumar's slides for the book [Introduction to Data Mining](#)

- References

- [Chapter on clustering from the book above](#) (88 pages)
- [k-means overview](#)
- [k-means ++ paper](#)
- [k-means || paper](#) and [video](#)