COMP6237 Data Mining
Lecture 2: Discovering Groups

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Lecture slides available here:

http://comp6237.ecs.soton.ac.uk/jon.html

(Thanks to Prof. Jonathon Hare and Dr. Jo Grundy for providing the lecture materials used to develop the slides.)

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Recap – Recommendation System

Content-based

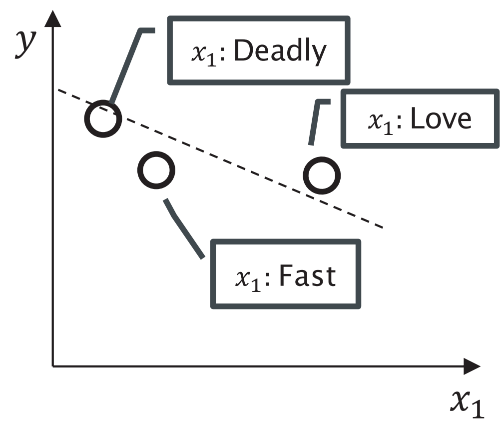
$$\min_{\theta} \frac{1}{m} \sum_{i=1}^{m} (\theta^T X_i - y)^2$$

$x(\text{Love}) = (x_1, x_2) = (1, 0.1)$

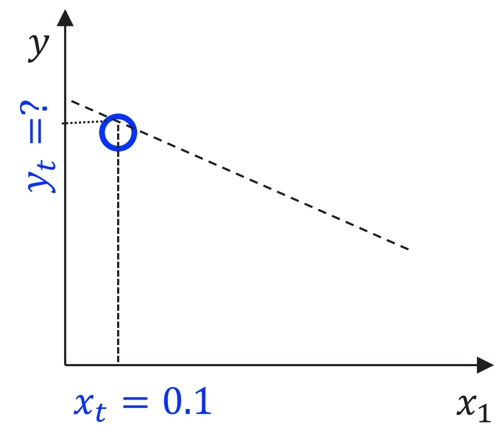
Film	Dave (y)	x_1 romance	x_2 action
Love Really	4	1	0.1
Deadly Weapon	5	0.1	1
Fast and Cross	4	0.2	0.9
Star Battles	?	0.1	1

$y_t = ?$

1. Fitting User Behavior



2. Prediction



User-based Collaborative

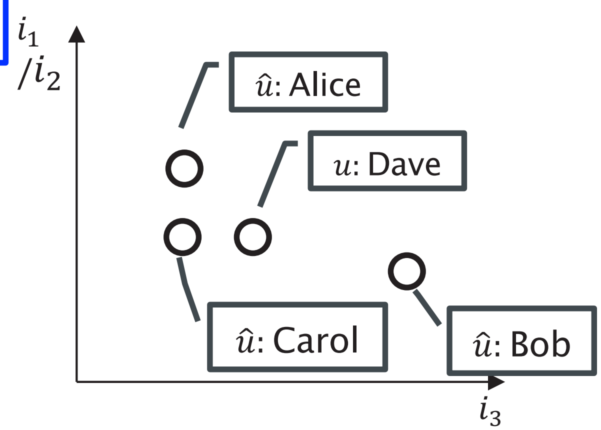
$$r_{u,i} = \frac{\sum_{\hat{u} \in U} sim(u, \hat{u}) r_{\hat{u},i}}{\sum_{\hat{u} \in U} |sim(u, \hat{u})|}$$

$\hat{u}(\text{Alice}) = (i_1, i_3) = (4, 5)$

	Film	Alice	Bob	Carol	Dave
i_1	Love Really	4	1		4
i_2	Deadly Weapon		1	4	5
i_3	Fast and Cross	5		5	4
	Star Battles	1	5	2	?

$r_{u,t} = ?$

1. Finding Similar Users



2. Prediction

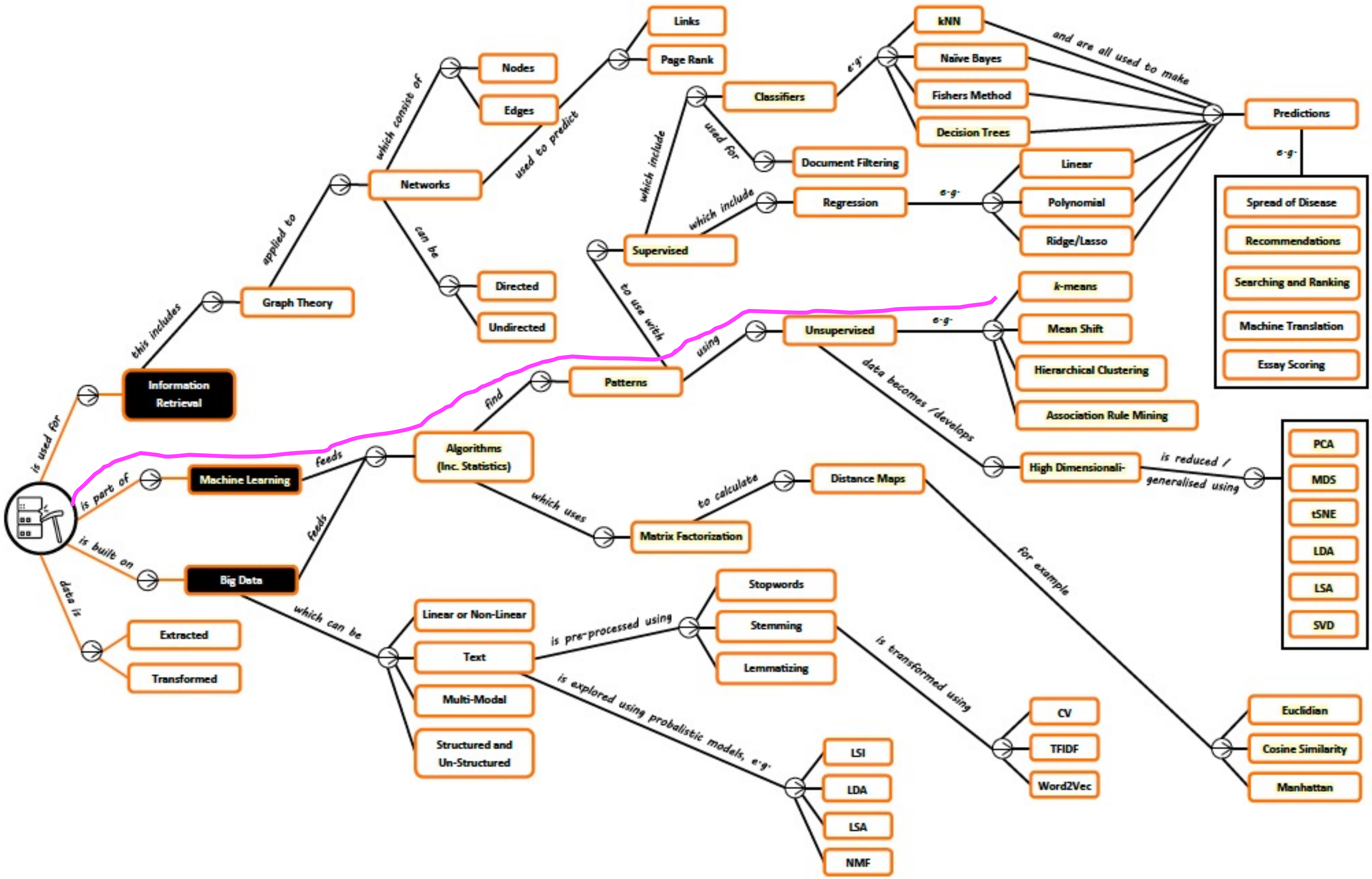
Sim(Dave, Alice) = 0.8
Sim(Dave, Carol) = 0.6

$$r_{u,t} = \frac{0.8 \times 1 + 0.6 \times 2}{0.8 + 0.6}$$

Cosine Similarity:

$$cos(\theta) = \frac{\boldsymbol{p}.\boldsymbol{q}}{|\boldsymbol{p}||\boldsymbol{q}|} = \frac{\sum_{i=1}^{N} p_i q_i}{\sqrt{\sum_{i=1}^{N} p_i^2}\sqrt{\sum_{i=1}^{N} q_i^2}}$$

Discovering Groups – **Roadmap**



Discovering Groups – **Textbook**

CHAPTER 3

Discovering Groups

- Programming Collective Intelligence: Building Smart Web 2.0 Applications *T. Segaran*.

Chapter 7

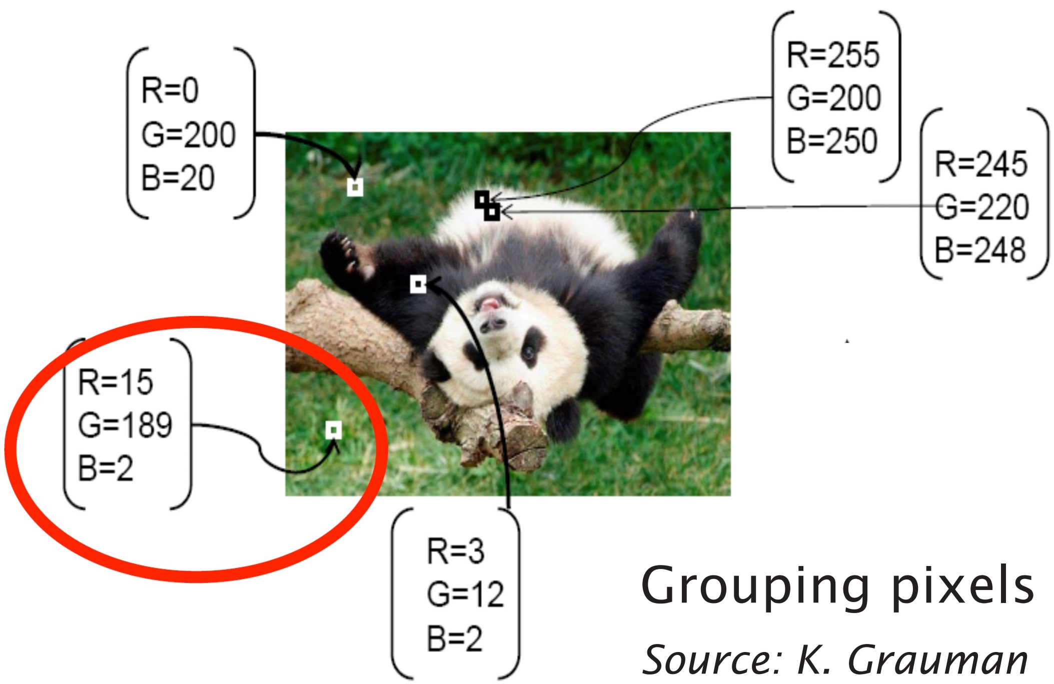
Clustering

Clustering is the process of examining a collection of "points," and grouping the points into "clusters" according to some distance measure. The goal is that points in the same cluster have a small distance from one another, while points in different clusters are at a large distance from one another. A suggestion of

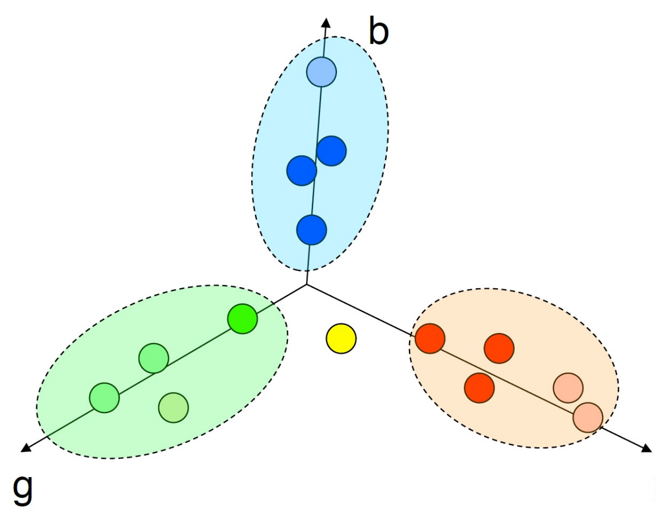
- Mining of Massive Datasets J. Leskovec *et al*

Discovering Groups – **Overview (1/5)**

- Grouping data, just using the feature vectors
  - Unsupervised: no group labels for training
  - Key idea: data with similar features grouped together
  - Can be
    - Soft (allow overlapping groups)
    - Hard (each item assigned to one group)



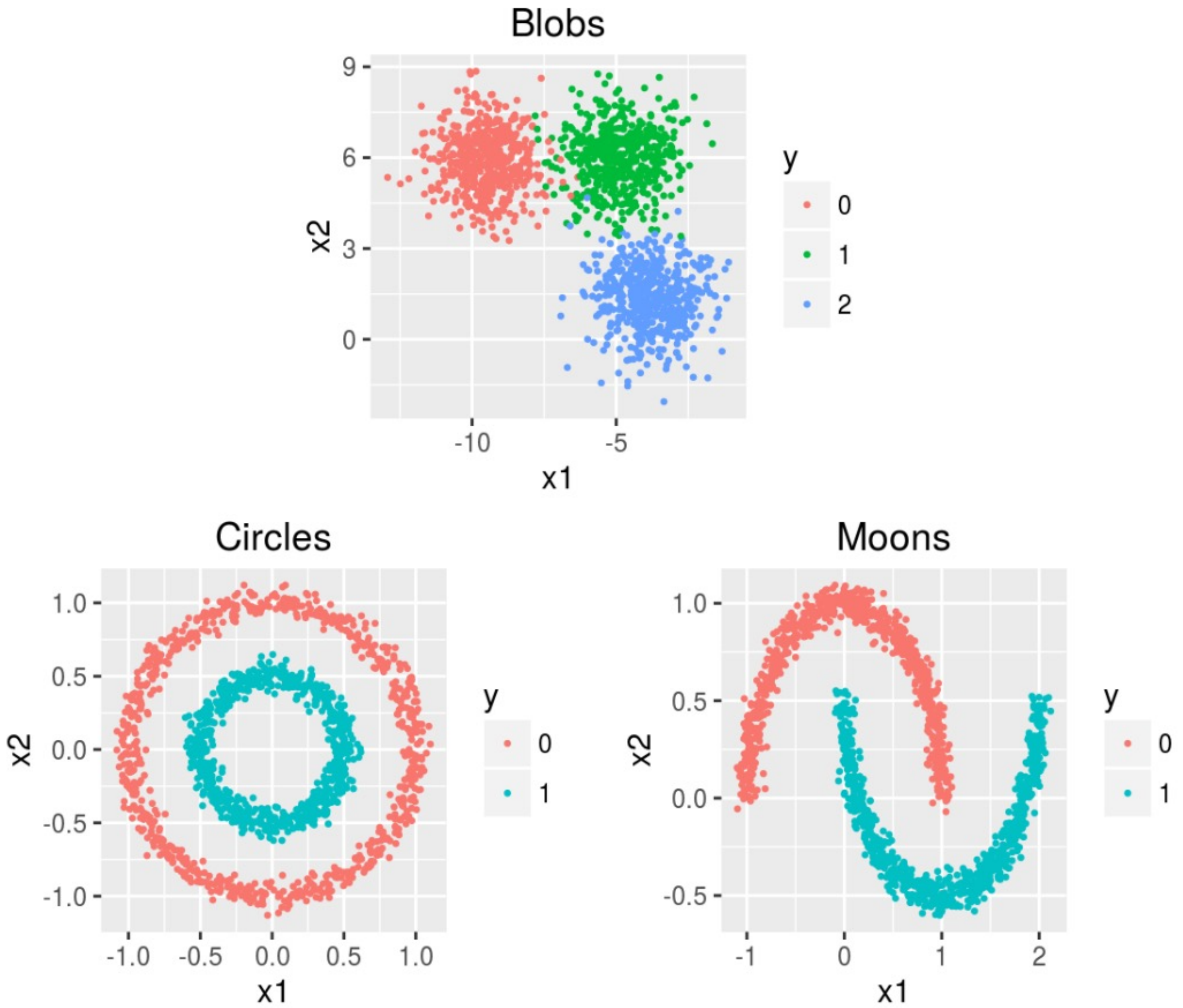
Feature space:
color value (3D)



Grouping pixels based on color similarity

Source: K. Grauman

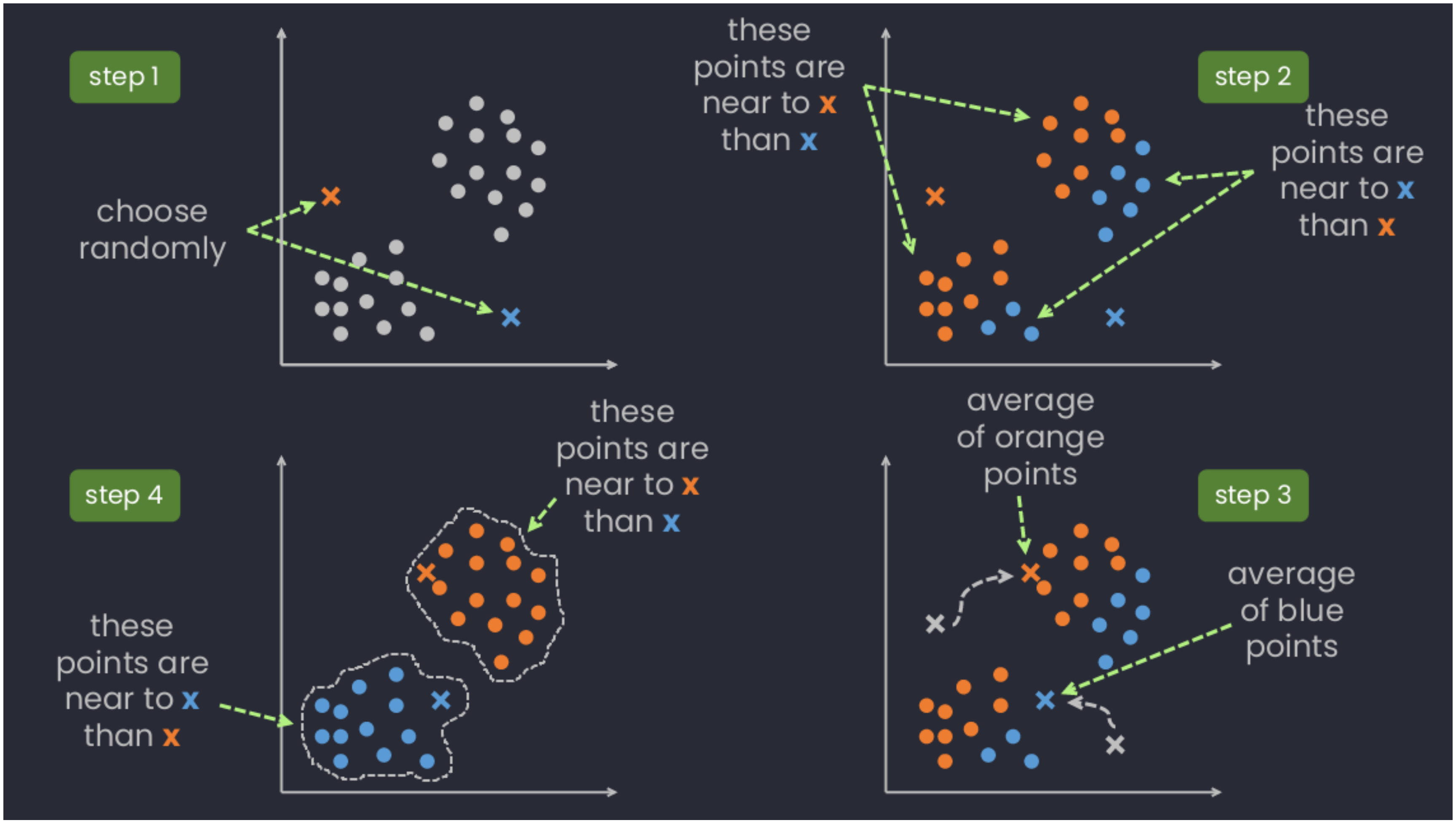
Discovering Groups – **Overview (2/5)**



https://marlabskochi.github.io

Discovering Groups – **Overview (3/5)**

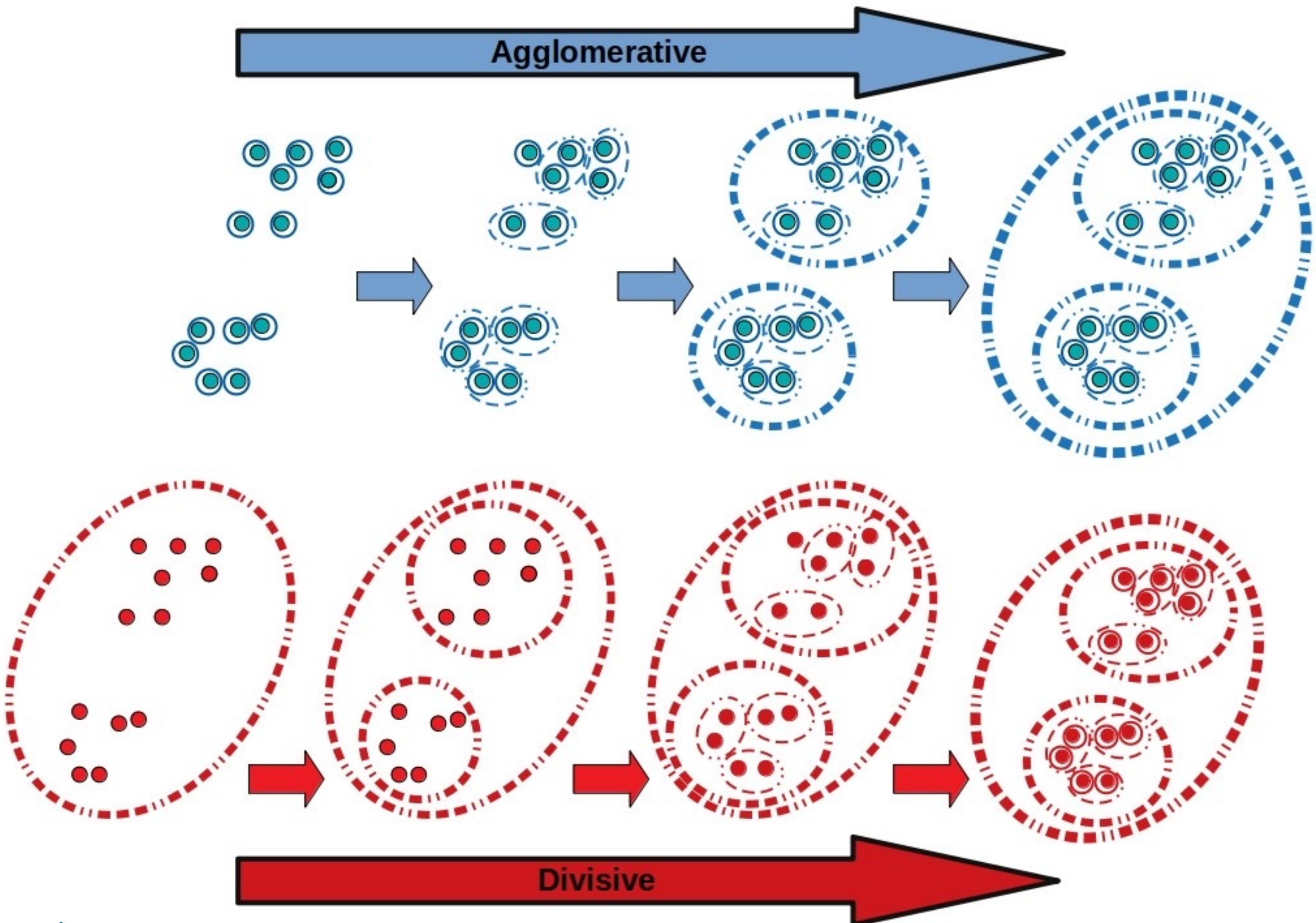
Clustering Algorithm (1/3) – K-means



Credict: Pratik Thorat

Discovering Groups – **Overview (4/5)**

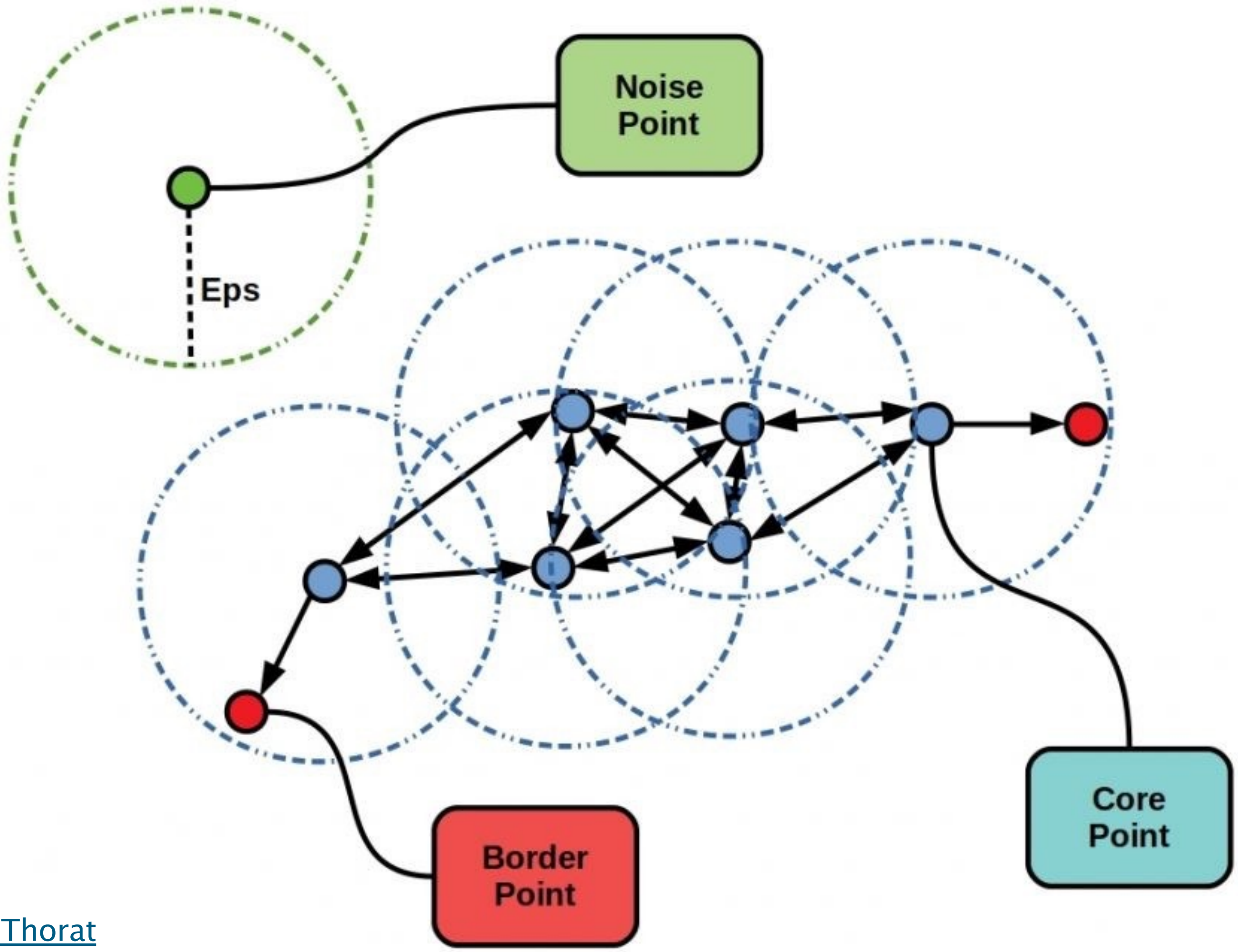
Clustering Algorithm (2/3) – Agglomerative (Divisive not learned in this lecture)



Credit: Pratik Thorat

Discovering Groups – **Overview (5/5)**

Clustering Algorithm (2/3) – DBSCAN



[Credit: Pratik Thorat]

Discovering Groups – **Learning Outcomes**

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- **LO1**: Comprehend the key ideas and the essential mathematical formulations employed in clustering methods (exam).
  - E.g., how is sum of squared error (SSE) defined?
  - E.g., understand the pros and cons of the learned algorithms
- **LO2**: Compute the fundamental stages of learned clustering approaches (exam).
  - E.g., given a dataset and a distance metric, be prepared to follow the selected clustering algorithm to cluster the instances in the dataset
- **LO3**: Implement and evaluate the learned clustering algorithms using Python (course work)

Assessment hints: Multi-choice Questions (single answer: concepts, calculation etc)

- *Textbook Exercises: textbooks (Programming + Mining)*
- *Other Exercises: https://www-users.cse.umn.edu/~kumar001/dmbook/sol.pdf*
- *ChatGPT or other AI-based techs*

Discovering Groups – K-means

- Given: data set $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, number of clusters K
- Goal: find cluster centers $\{\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K\}$ so that

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$

  is minimal, where $r_{nk} = 1$ if $\mathbf{x}_n$ is assigned to $\boldsymbol{\mu}_k$
- Idea: compute r_{nk} and $\boldsymbol{\mu}_k$ iteratively

Otherwise, $r_{n,k} = 0$

The used objective function is **Sum of Squared Error (SSE)**

Source: D. Cremers

Discovering Groups – K-means

Algorithm 1: K Means clustering

```
Data: X, K
initialise K centroids;
while positions of centroids change do
    for each data point do
        assign to nearest centroid
    end
    for each centroid do
        move to average of assigned data points
    end
end
return centroids, assignments;
```

A special case of Expectation Maximisation - why?

Credit: Jo Grundy

Discovering Groups – K-means

Algorithm 2: K Means clustering

```
Data: X, K
initialise K centroids;
while positions of centroids change do
    for each data point do
        assign to nearest centroid ;              // Expectation of
         associations
    end
    for each centroid do
        move to average of assigned data points ;
         // Maximisation of likelihood
    end
end
return centroids, assignments;
```

E-step: Estimate the posterior probabilities…

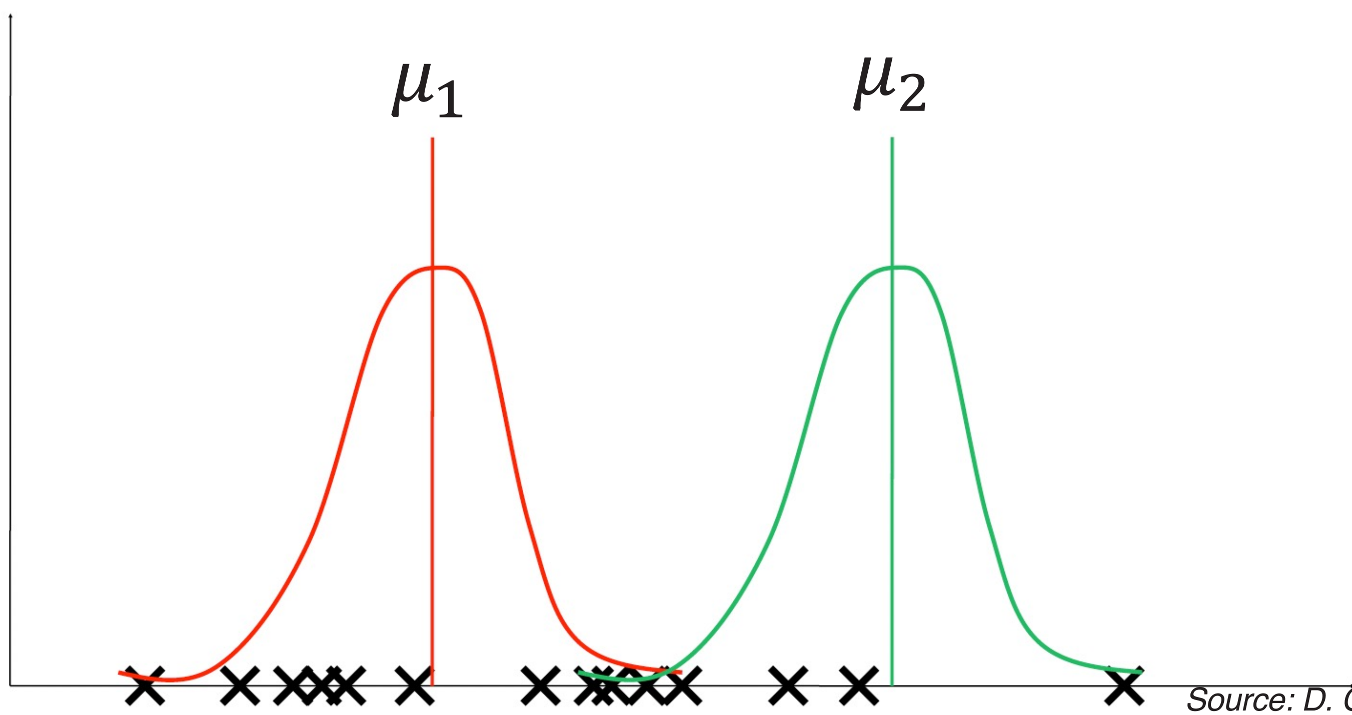
M-step: Estimate new parameters

Assumes spherical clusters

Credit: Jo Grundy

Discovering Groups – K-means
1D Example

Initialize cluster means: $\{\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K\}$

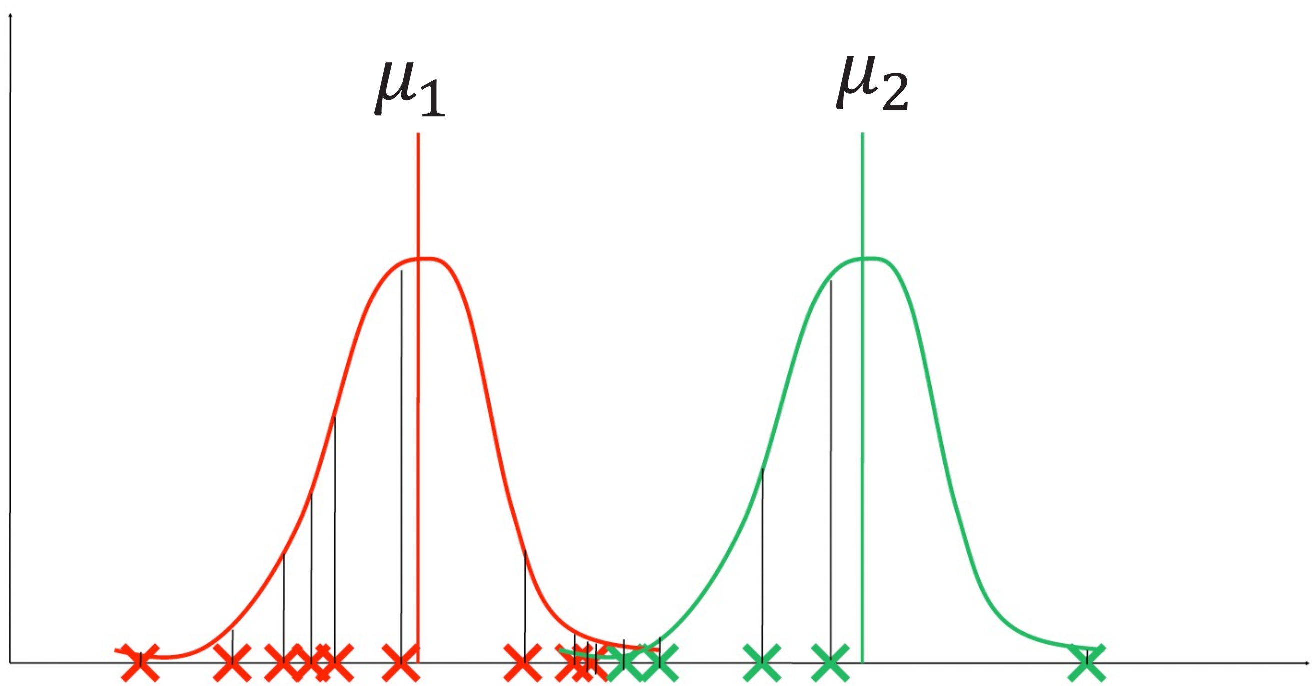


Source: D. Cremers

Discovering Groups – K-means
1D Example

Find optimal assignments:

$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\mathbf{x}_n - \boldsymbol{\mu}_j\| \\ 0 & \text{otherwise} \end{cases}$$



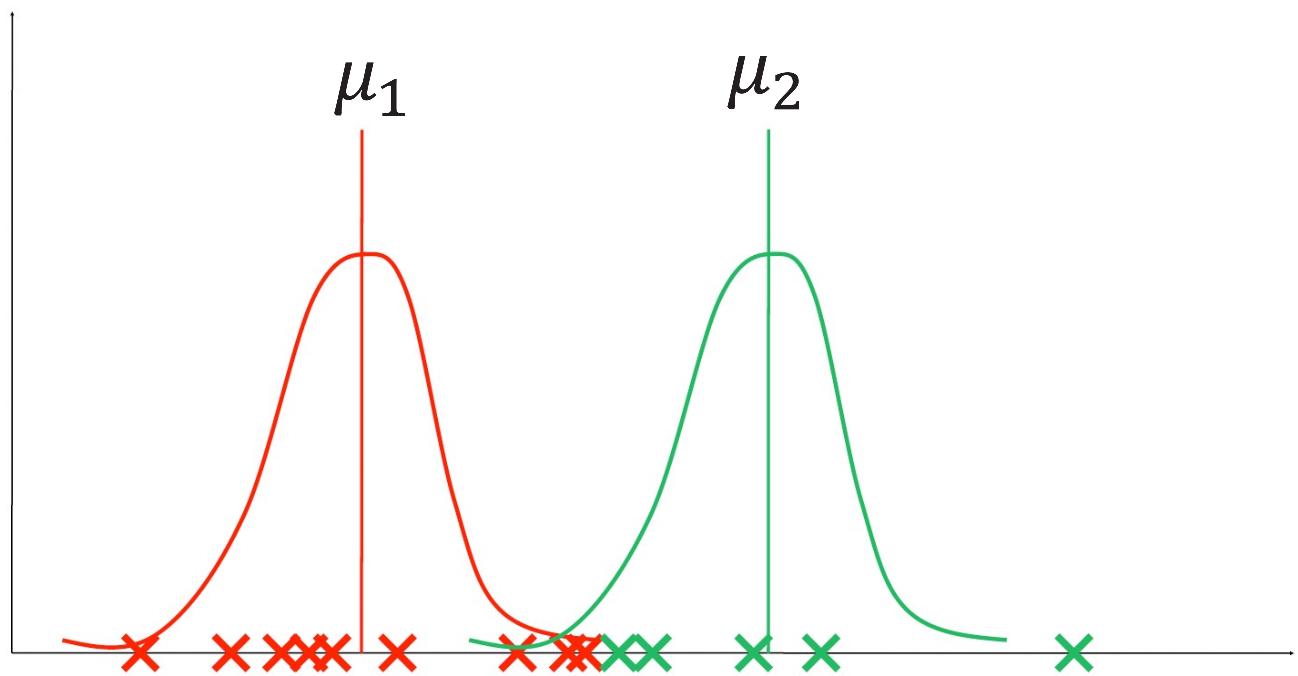
Source: D. Cremers

Discovering Groups – K-means
1D Example

Find new optimal means:

$$\frac{\partial J}{\partial \boldsymbol{\mu}_k} = 2\sum_{n=1}^{N} r_{nk}(\mathbf{x}_n - \boldsymbol{\mu}_k) \stackrel{!}{=} 0$$

$$\Rightarrow \boldsymbol{\mu}_k = \frac{\sum_{n=1}^{N} r_{nk}\mathbf{x}_n}{\sum_{n=1}^{N} r_{nk}}$$



Source: D. Cremers

Discovering Groups – K-means
1D Example

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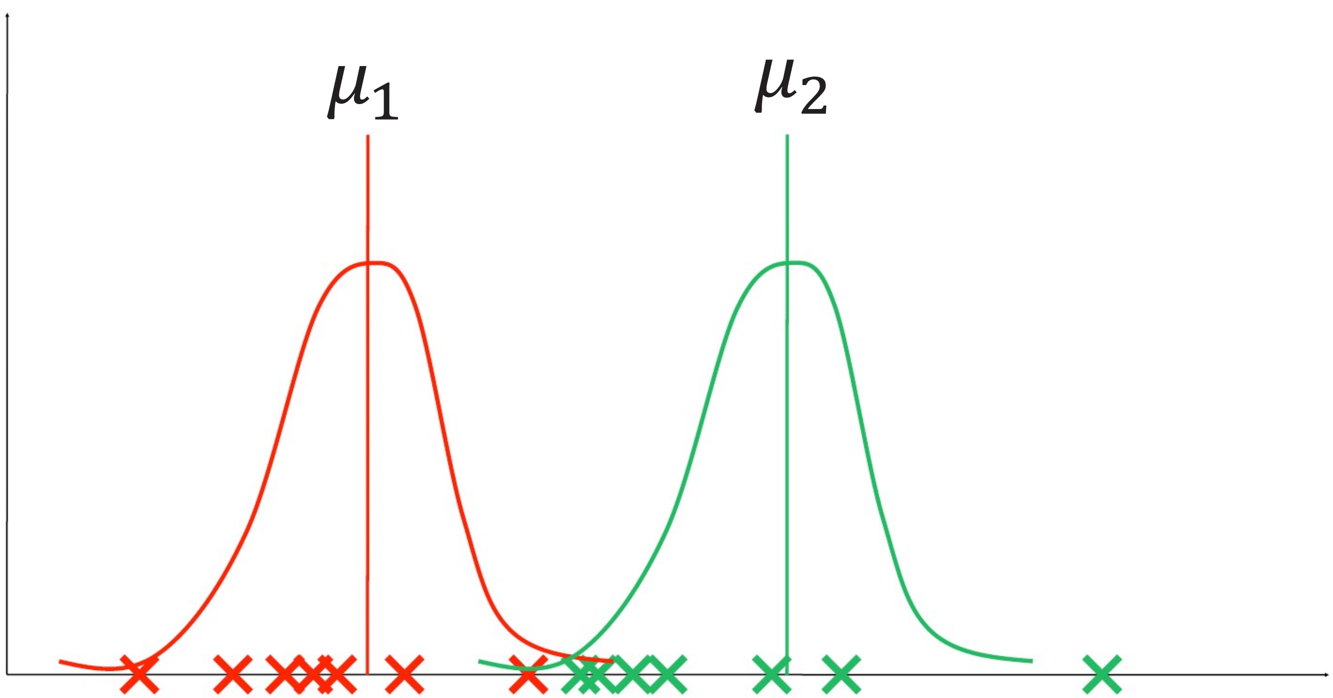
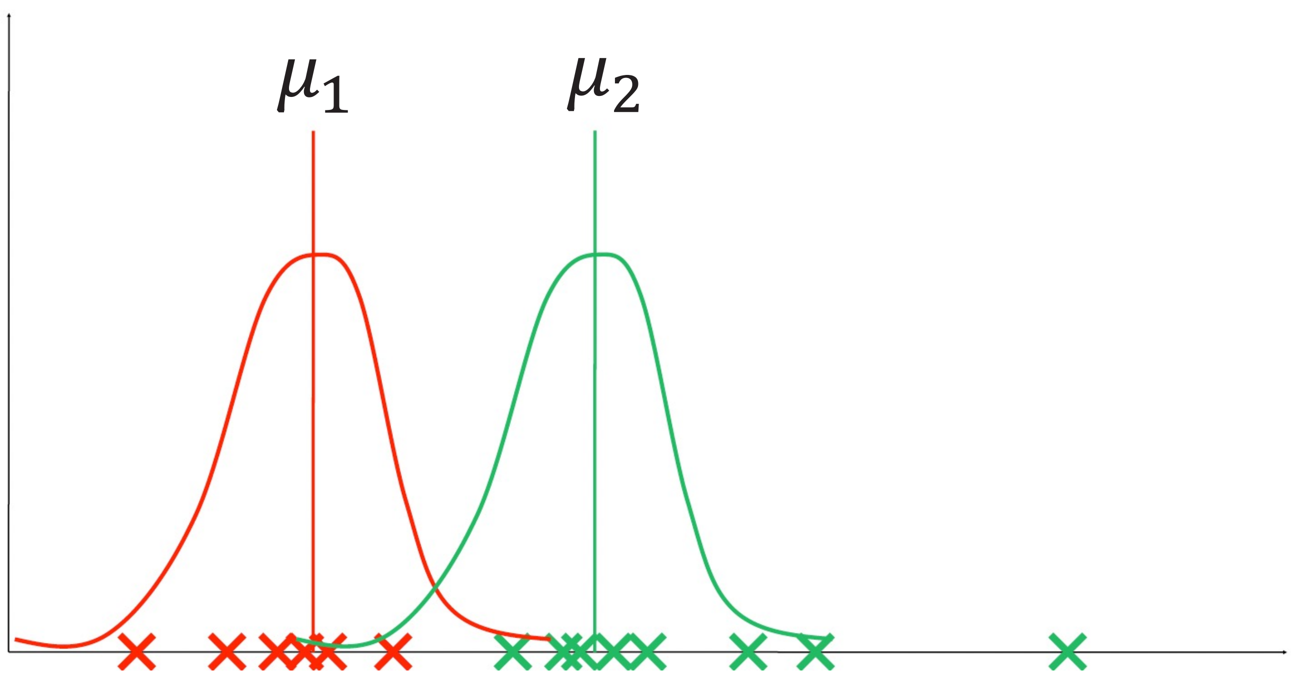


Source: D. Cremers

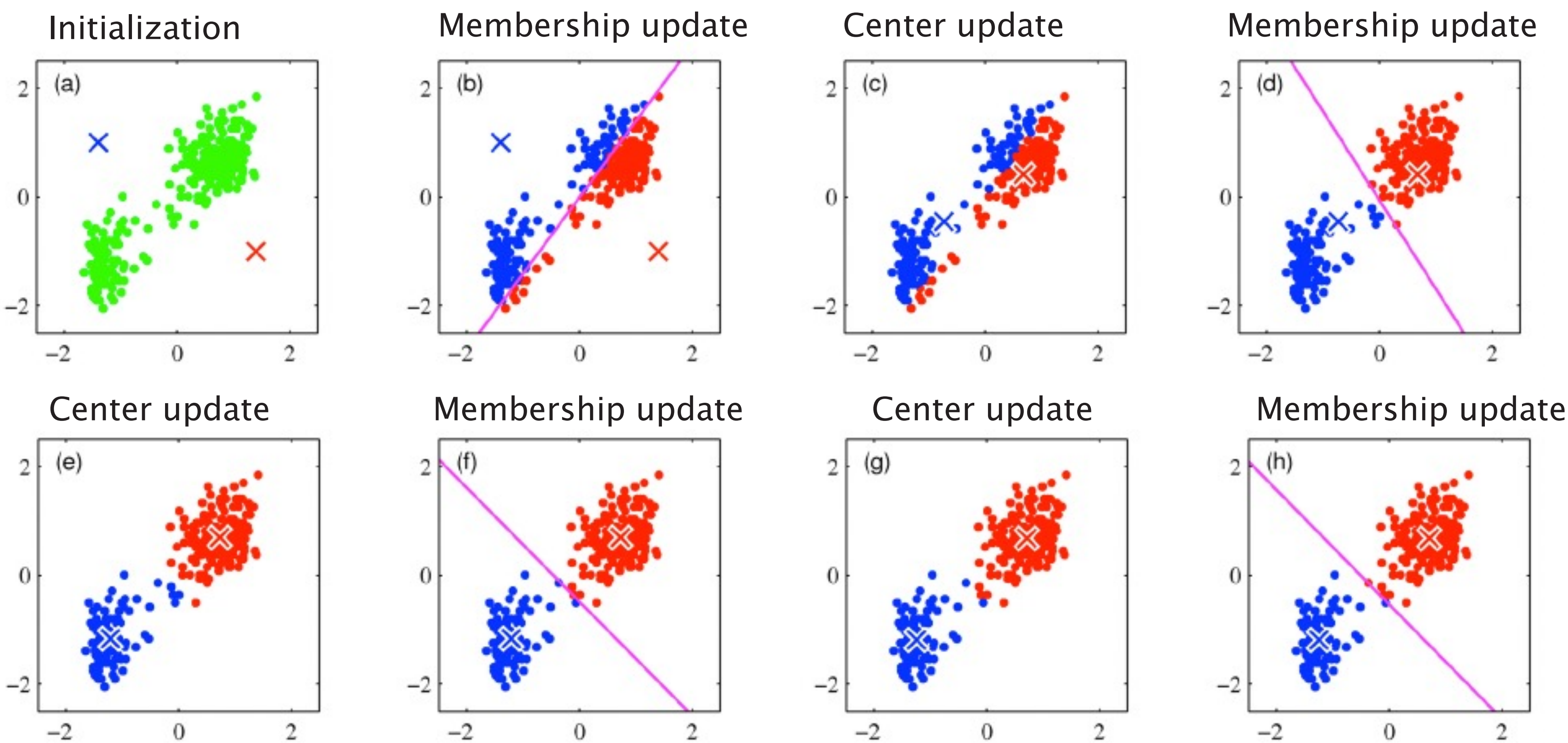
Discovering Groups – K-means
1D Example

Iterate these steps until means and assignments do not change any more



Source: D. Cremers

Discovering Groups – K-means
2D Example



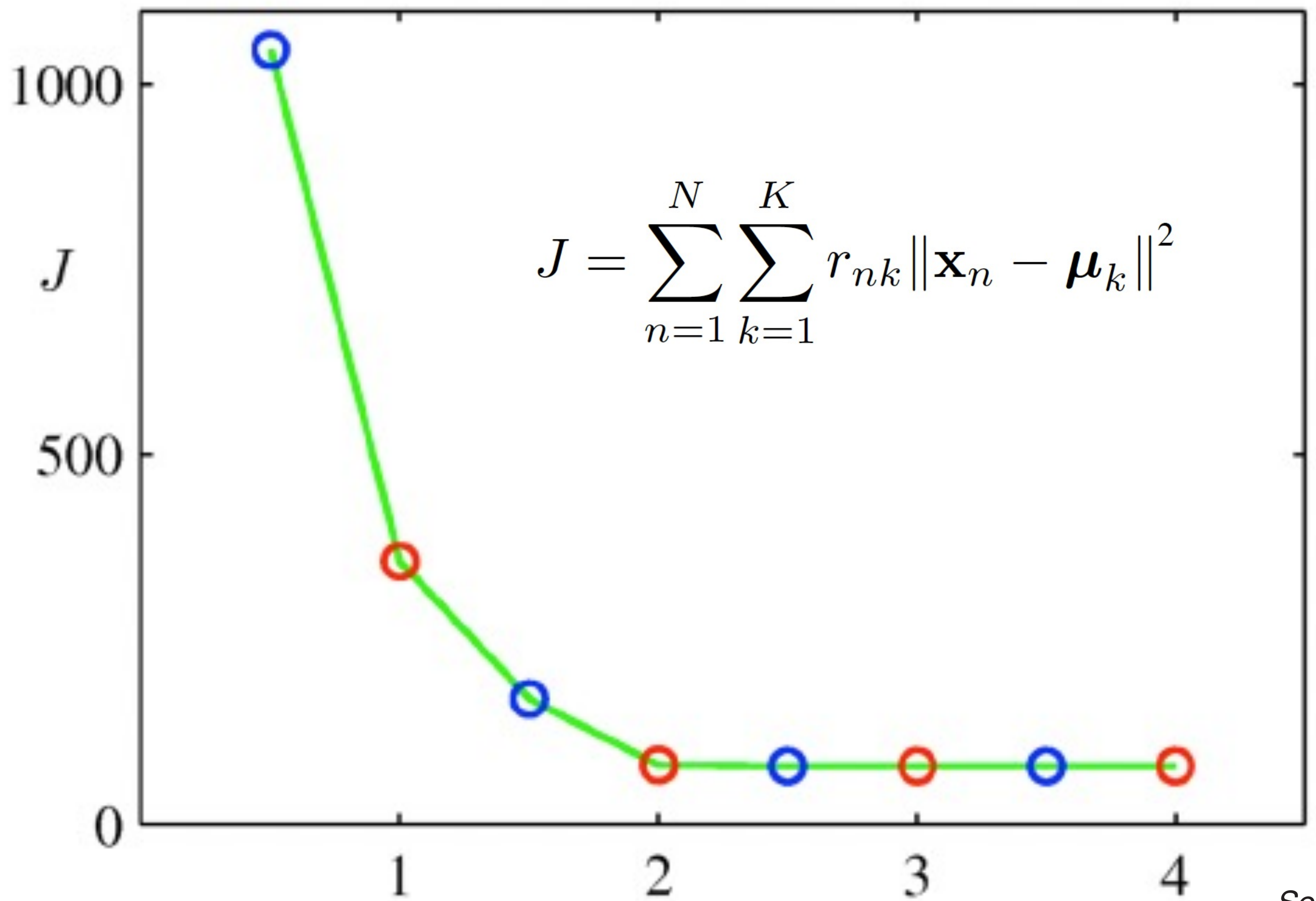
Source: D. Cremers

- Real data set
- Radom initialization

- Magenta line is ‘decision boundary’

Source: D. Cremers

Discovering Groups – K-means
Sum of Squared Error (SSE) Curve



Source: D. Cremers

- After every step the cost function J is minimized
- Blue steps: update assignments
- Red steps: update means
- Convergence after 4 rounds

Discovering Groups – K-means

K-means can quickly and cheaply cluster data.

Problems?

- need to specify the cluster number k
- depends on good initial centroid guesses
- may converge on local minimum
- assumes spherical data (or ellipsoid-shaped clusters, or at best convex clusters)

Gaussian Mixture models (GMM) can work better, using a generalization of K-means (assuming each cluster is Gaussian), not discussed in this lecture.

Discovering Groups – DBSCAN

- **Idea**: uses the **local density** of points to determine the clusters, rather than using only the distance between points

$$N_\epsilon(\mathbf{x}) = B_d(\mathbf{x}, \epsilon) = \{\mathbf{y} \mid \delta(\mathbf{x}, \mathbf{y}) \leq \epsilon\}$$

where $\delta(\mathbf{x}, \mathbf{y})$ represents the distance between **x** and **y,** ε indicates **Max radius,** and **x** is a **core point** if $|N_\epsilon(\mathbf{x})| \geq minpts$, where *minpts* is a **Min number** that is user-defined local density or frequency threshold

- **x** belongs to a density-based cluster when

$|N_\epsilon(\mathbf{x})| \geq minpts$ or $\mathbf{x} \in N_\epsilon(\mathbf{z})$

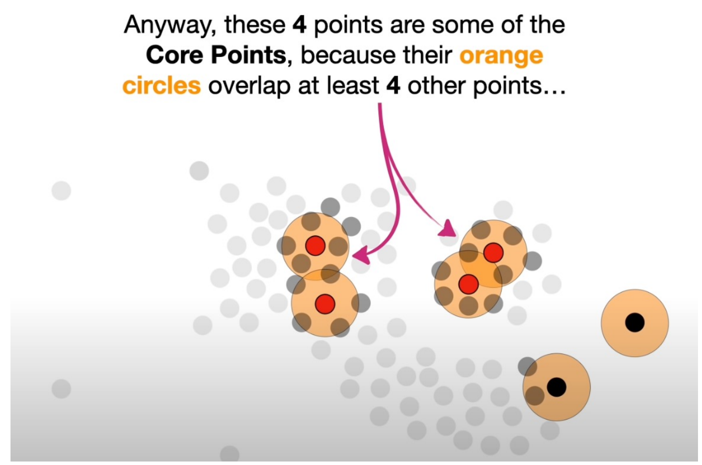
where **z** is another data point, *minpts* is a **Min number** that is user-defined local density or frequency threshold

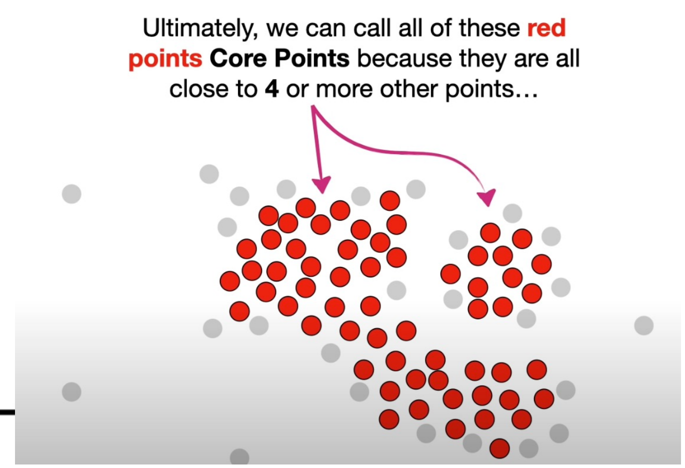
Max radius is the limit on which to look for neighbours
Min number is the lower limit on what can be in a cluster

Discovering Groups – DBSCAN

Algorithm 3: DBSCAN

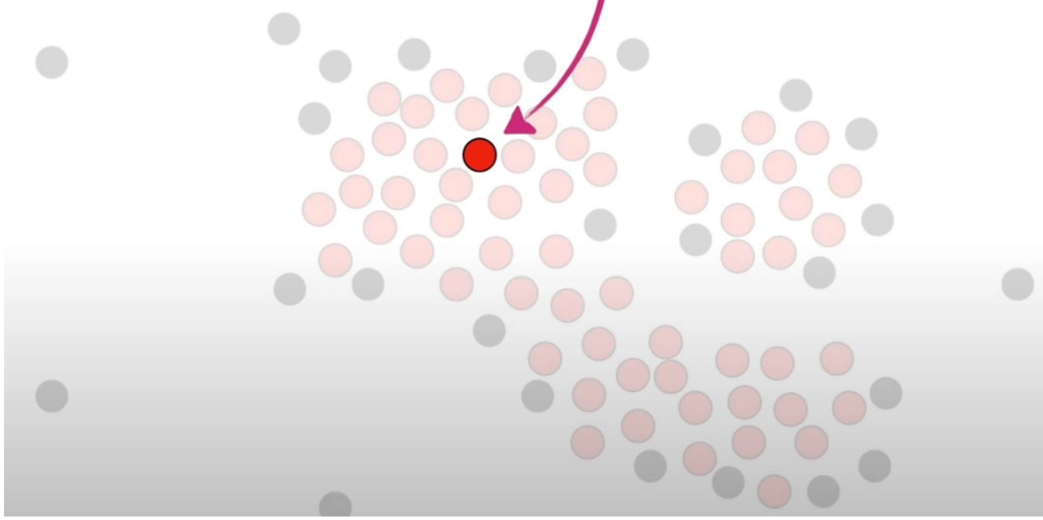
Data: X, *eps*, *min_pts*
initialse *labels* list as zeros, *count* list, *core* list;
Find neighbours for each point, Find core points; $|N_\epsilon(\mathbf{x})| \geq minpts$
class $= 1$;
for *each core point p* **do**
  add neighbours(p) to queue;
  while *queue not empty* **do**
    neighbours $=$ next(queue);
    for *q in neighbours* **do**
      set label($q =$ *class*;
      if *label(q) is 'core'* **then**
        add neighbours(q) to queue
      end
    end
  end
  class $=$ *class* $+ 1$
end
return labels;



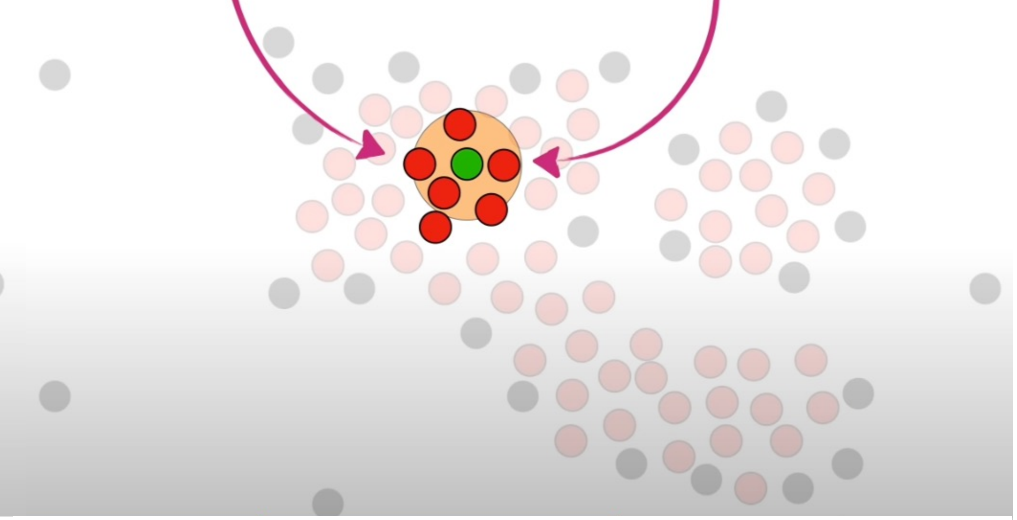


Credit: Jo Grundy

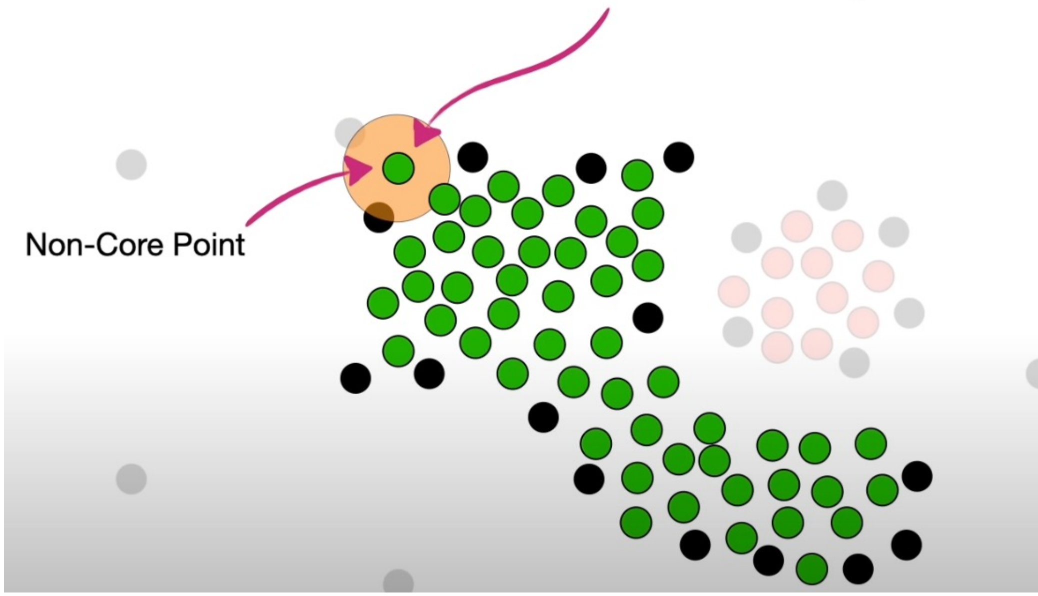
Now we randomly pick
a **Core Point**…



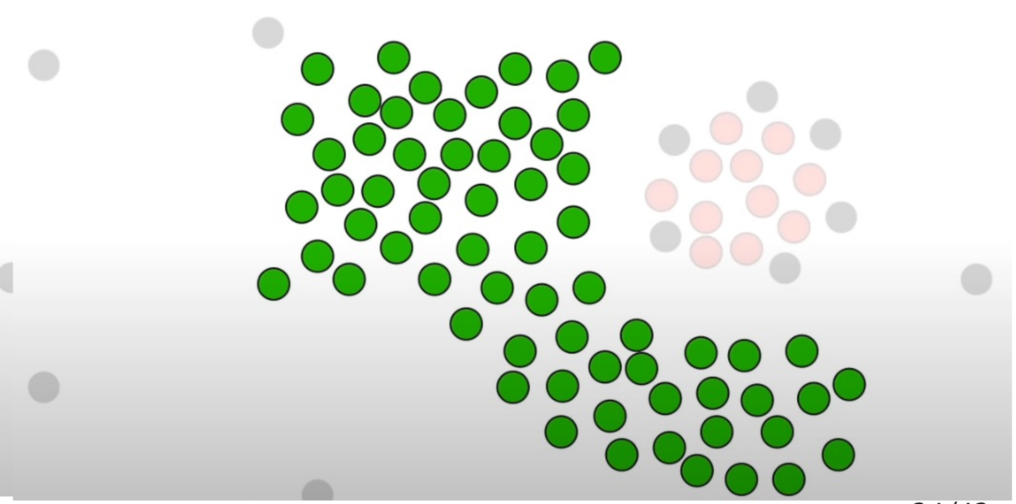
Next, the **Core Points** that are close
to the **first cluster**, meaning they
overlap the **orange circle**…



However, because this is not a **Core Point**, we do
not use it to extend the **first cluster** any further.



And now we are done
creating the **first cluster**.



https://www.youtube.com/watch?v=RDZUdRSDOok

Discovering Groups – DBSCAN

DBSCAN works well on any shape of data and is robust to outliers.

Problems?

- can struggle in high dimensions
- needs a distance parameter
- same parameter may not work for different cluster density
- need also minimum number specified

Credit: Jo Grundy

Discovering Groups – Hierarchical Clustering

Creates a **binary tree** that **recursively groups** pairs of similar items or clusters

Can be:

- Agglomerative (bottom up)
- Divisive (top down)

We will look at Agglomerative clustering. Needs a distance measure.

Credit: Jo Grundy

Discovering Groups – Hierarchical Clustering

Algorithm 4: Hierarchical Agglomerative Clustering

Data: N data points with feature vectors X_i $i = 1 \ldots N$

$numClusters = N$;

while $numClusters > 1$ **do**

    cluster1, cluster2 = FindClosestClusters();

    merge(cluster1, cluster2);

end

The distance between the clusters is evaluated using a linkage criterion.

If each merge is recorded, a binary tree structure linking the clusters can be formed.

This gives a **dendrogram**

Credit: Jo Grundy

Discovering Groups – Hierarchical Clustering

Linkage criterion: A measure of dissimilarity between clusters

Centroid Based:

- Dissimilarity is equal to distance between centroids
- Needs numeric feature vectors

Distance-Based:

- Dissimilarity is a function of distance between items in clusters
- Only needs precomputed measure of similarity between items

We could compute a distance matrix between points

Credit: Jo Grundy

Discovering Groups – Hierarchical Clustering

Centroid based linkage:

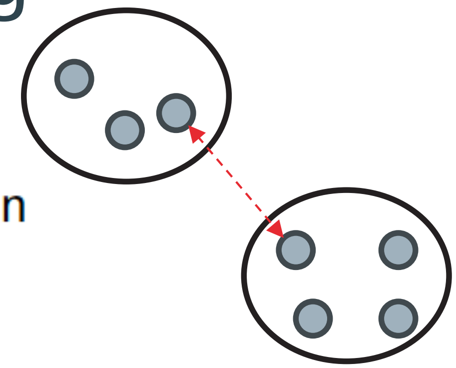
- WPGMC: Weighted Pair Group Method with Centroids. When two clusters are combined into a new cluster, the average of the two centroids is the new centroid

- UPGMC: Unweighted Pair Group Method with Centroids. When two clusters are combined into a new cluster, the new centroid is recalculated based on the positions of the items

Credit: Jo Grundy

Discovering Groups – Hierarchical Clustering

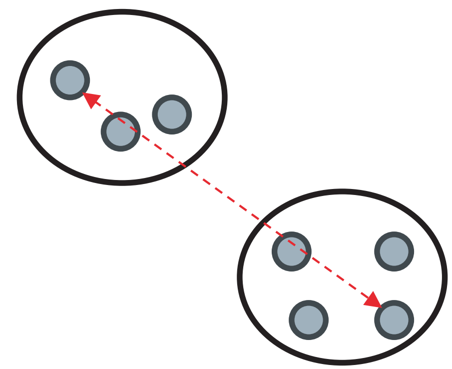
Distance based linkage:



- **Minimum**, or **single-linkage clustering** Distance between two closest members

  $$\min d(a, b) : a \in A, b \in B$$

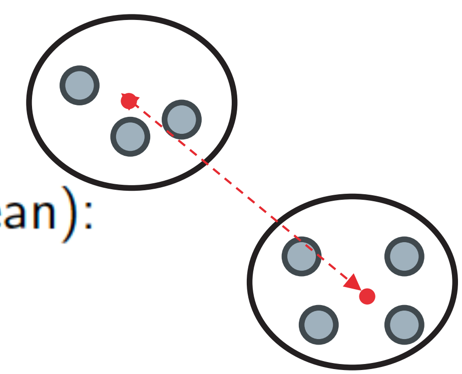
  Produces long, thin clusters



- **Maximum**, or **complete-linkage clustering** Distance between two most distant members

  $$\max d(a, b) : a \in A, b \in B$$

  Finds compact clusters, approximately equal diameter

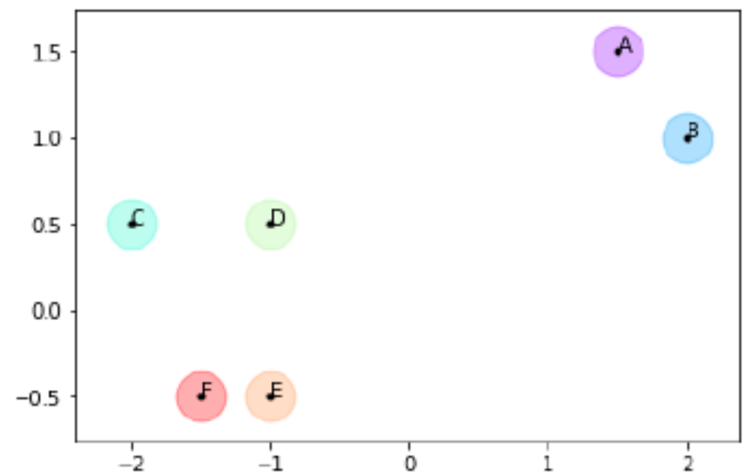


- **Mean** or **Average Linkage Clustering** (**UPGMA**: Unweighted Pairwise Group Method with Arithmetic Mean):

  $$\frac{1}{|A||B|} \sum_{a \in A} \sum_{b \in B} d(a, b)$$

Credit: Jo Grundy

Discovering Groups – Agglomerative Clustering



With sample data:

$$X = \begin{bmatrix} 1.5 & 1.5 \\ 2.0 & 1.0 \\ 2.0 & 0.5 \\ -1.0 & 0.5 \\ -1.5 & -0.5 \\ -1 & 0.5 \end{bmatrix}$$

Distance matrix: *demo distances, not ground truth*

	A	B	C	D	E	F
A	0	0.7	2.7	1.8	...	
B	0.7	0	...			
C	2.7		0	...		
D	1.8			0	...	
E	⋮				0	

Credit: Jo Grundy

Discovering Groups – Agglomerative Clustering

Algorithm 4: Hierarchical Agglomerative Clustering

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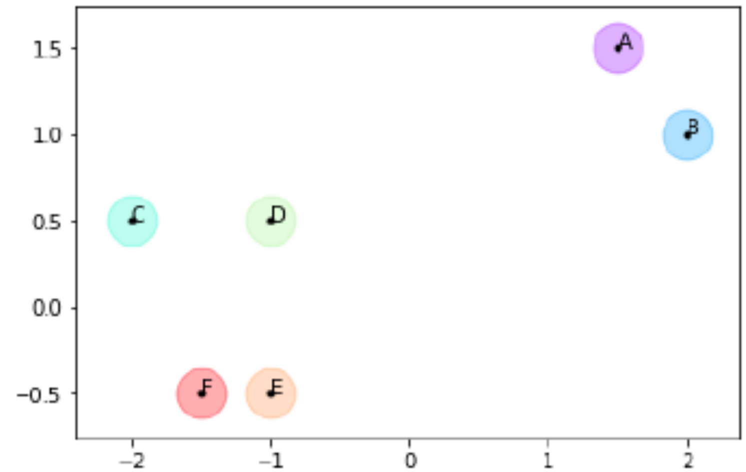
$numClusters = N$;

while $numClusters > 1$ **do**

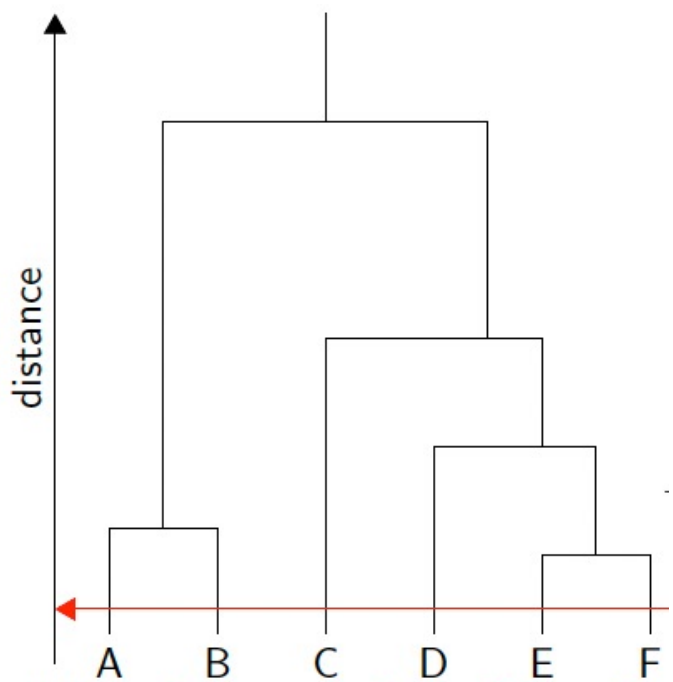
  cluster1, cluster2 = FindClosestClusters();

  merge(cluster1, cluster2);

end

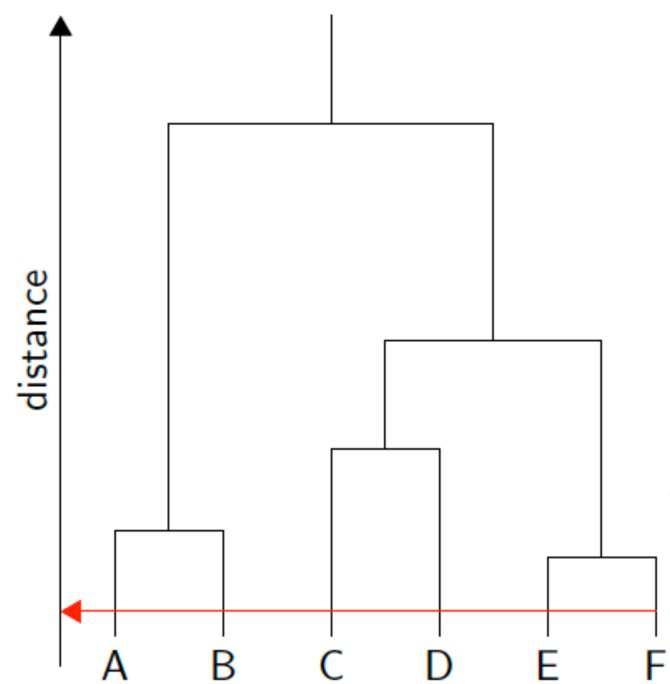


Dendrograms



Using minimum or single-linkage clus

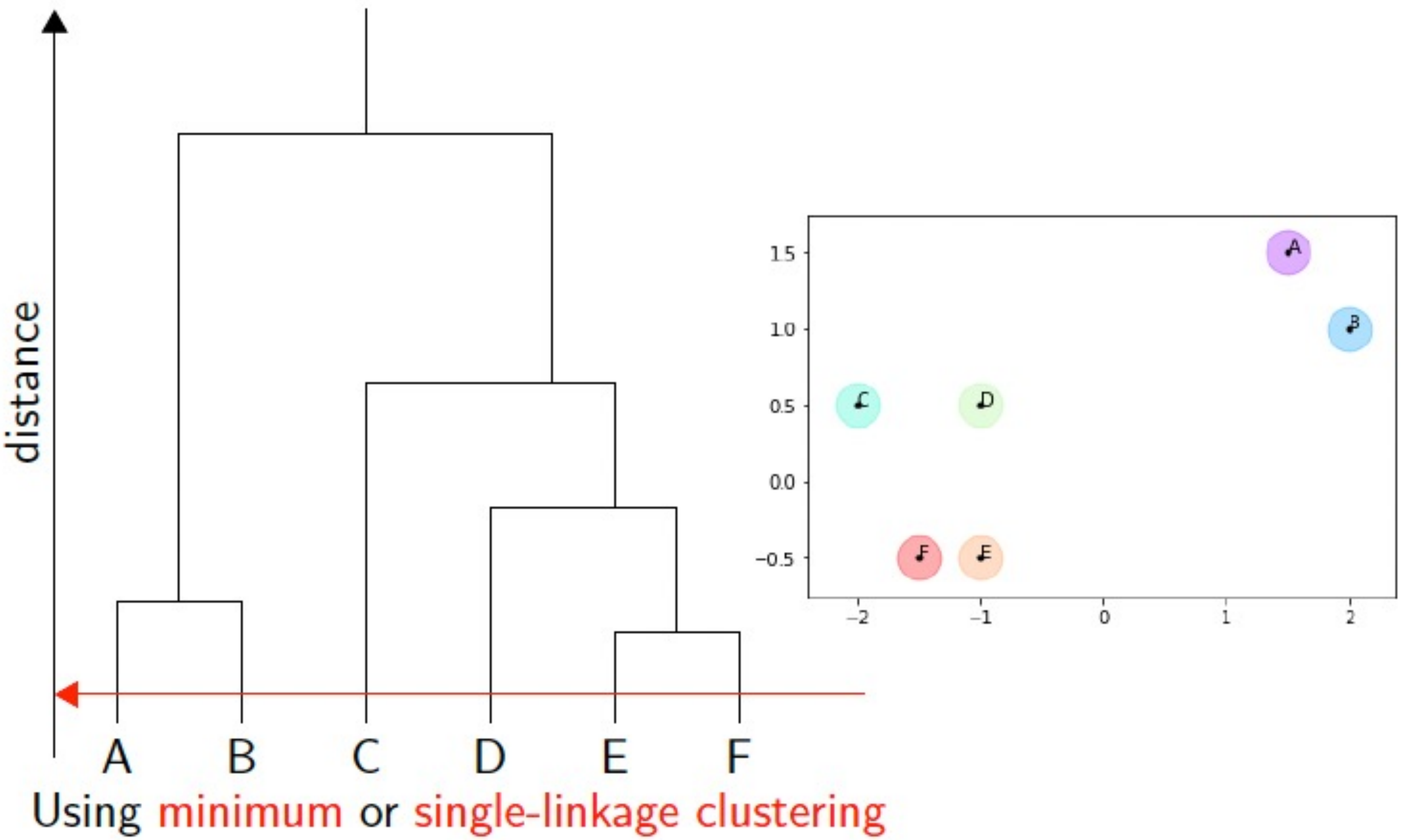
d_{min}



Using maximum or complete-linkage

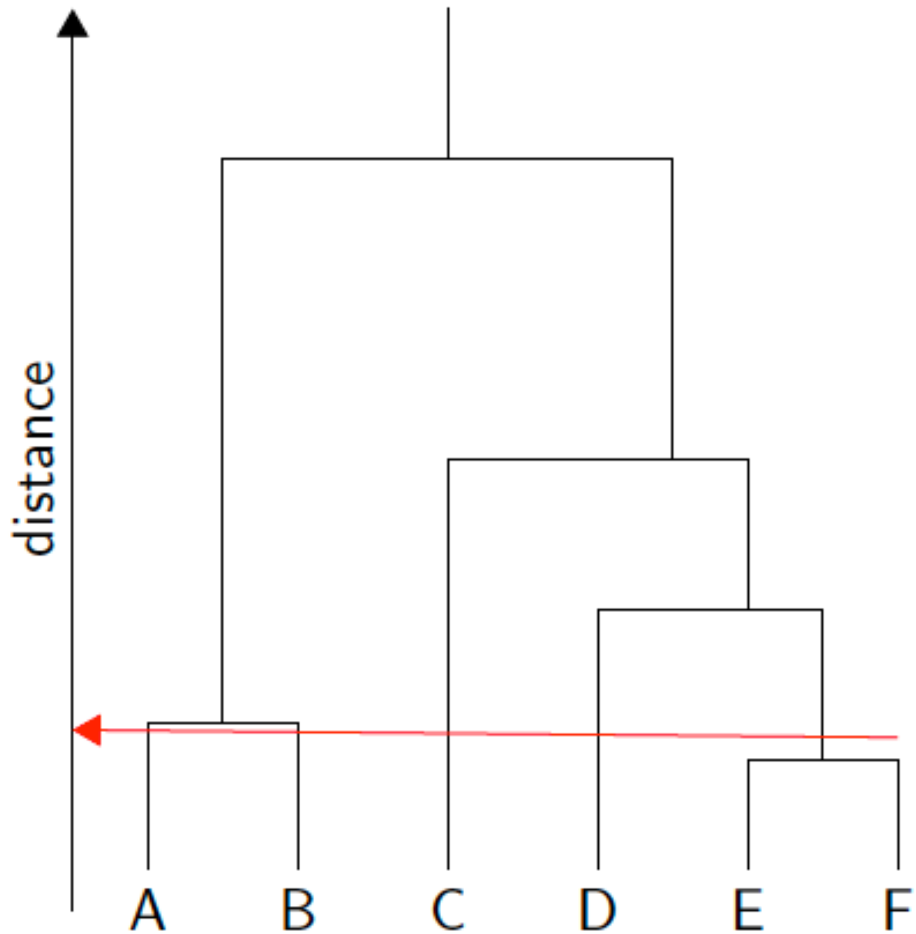
d_{max}

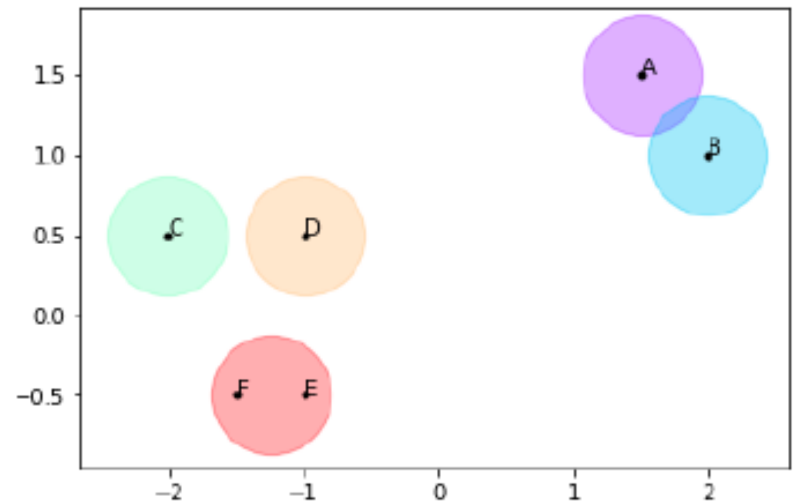
Discovering Groups – Agglomerative Clustering



Credit: Jo Grundy

Discovering Groups – Agglomerative Clustering

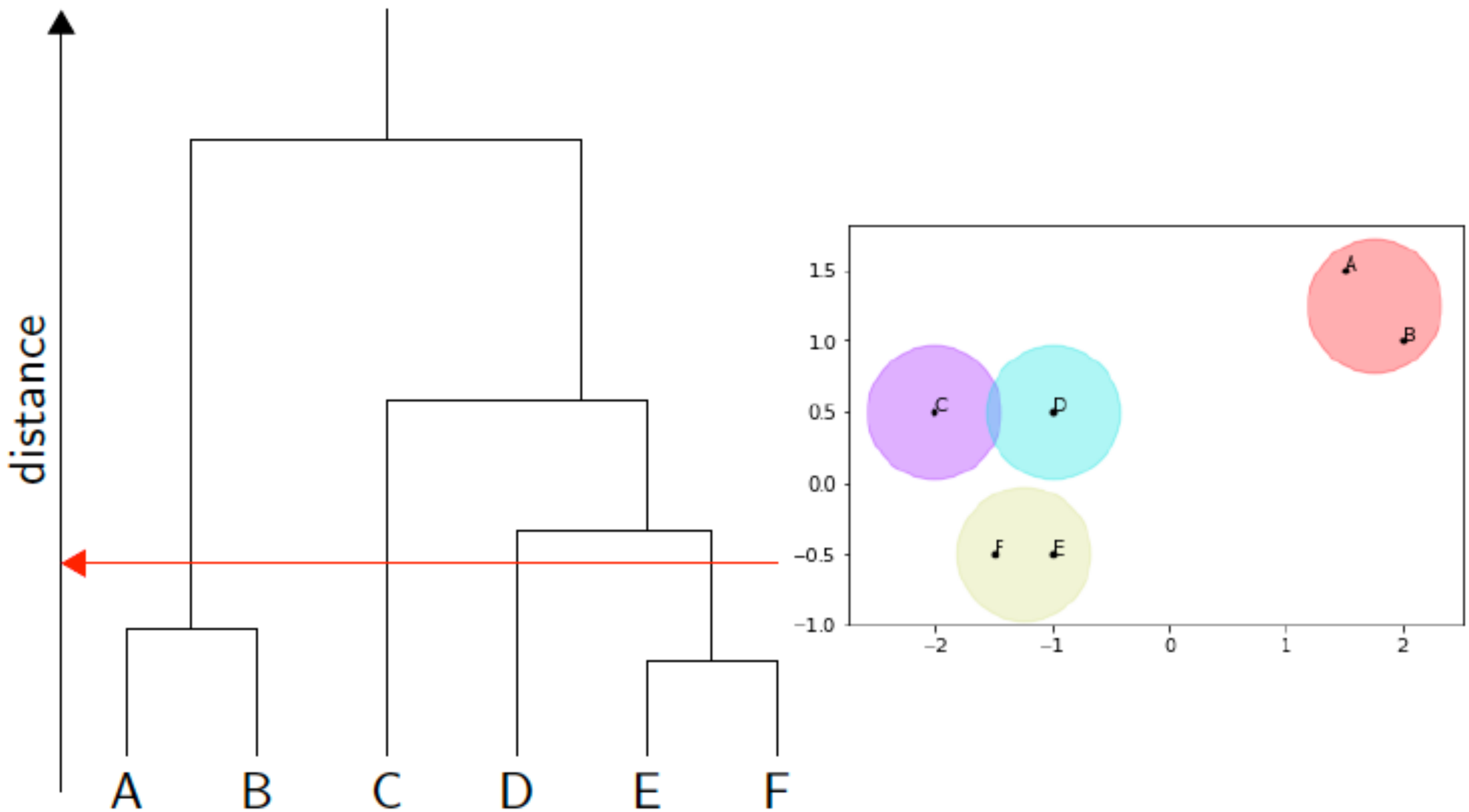




Using minimum or single-linkage clustering

Credit: Jo Grundy

Discovering Groups – Agglomerative Clustering



Using minimum or single-linkage clustering

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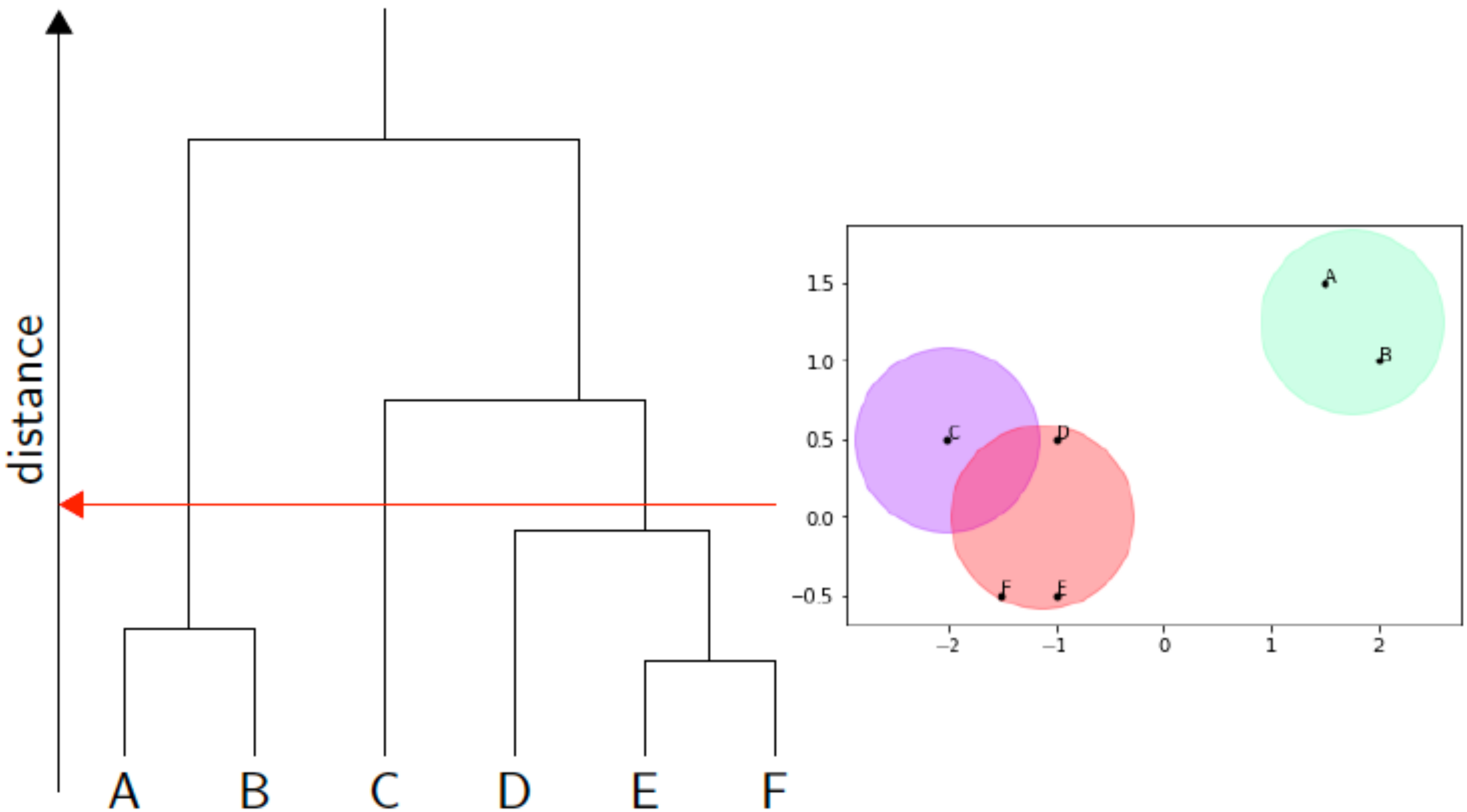
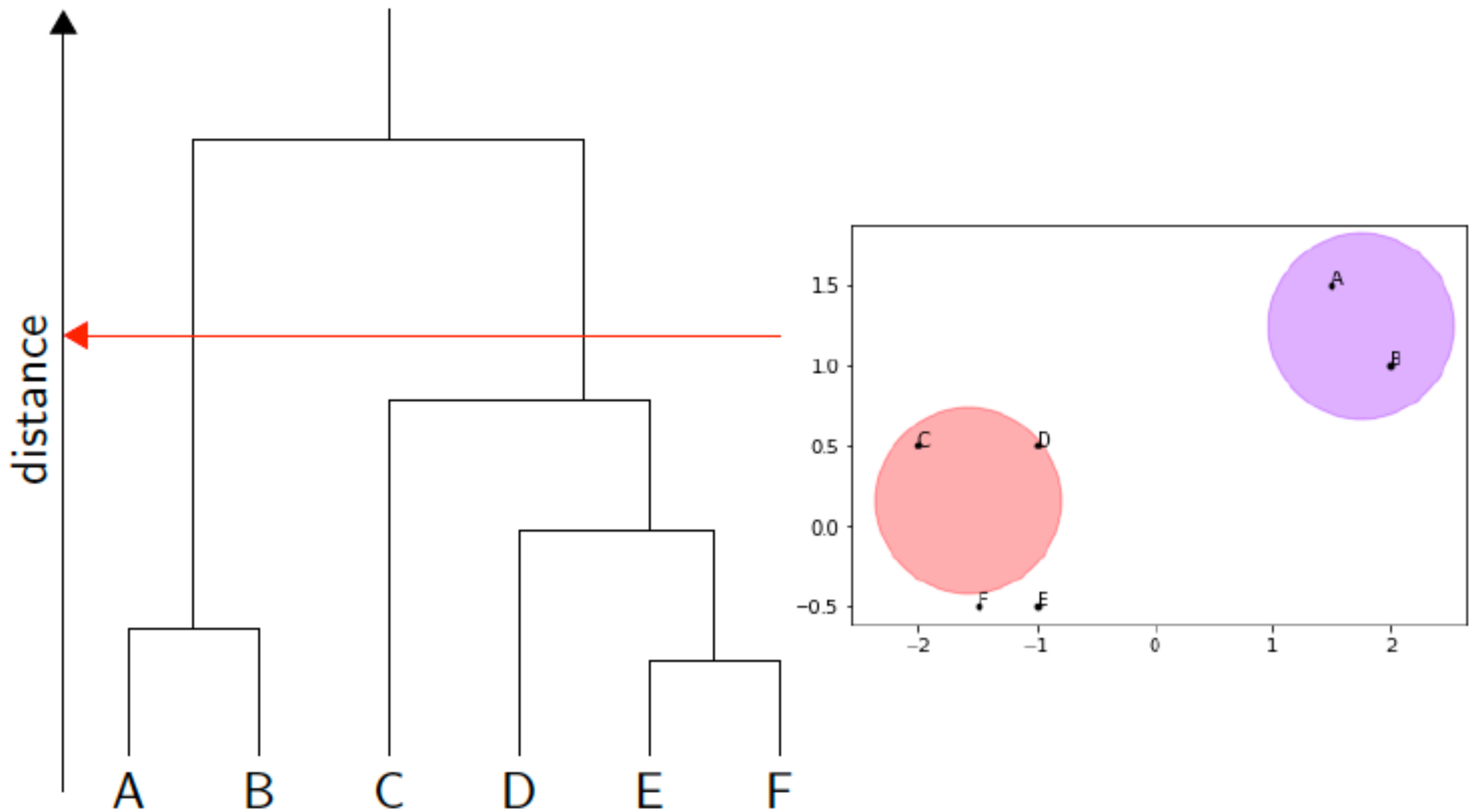
Discovering Groups – Agglomerative Clustering



Using minimum or single-linkage clustering

Credit: Jo Grundy

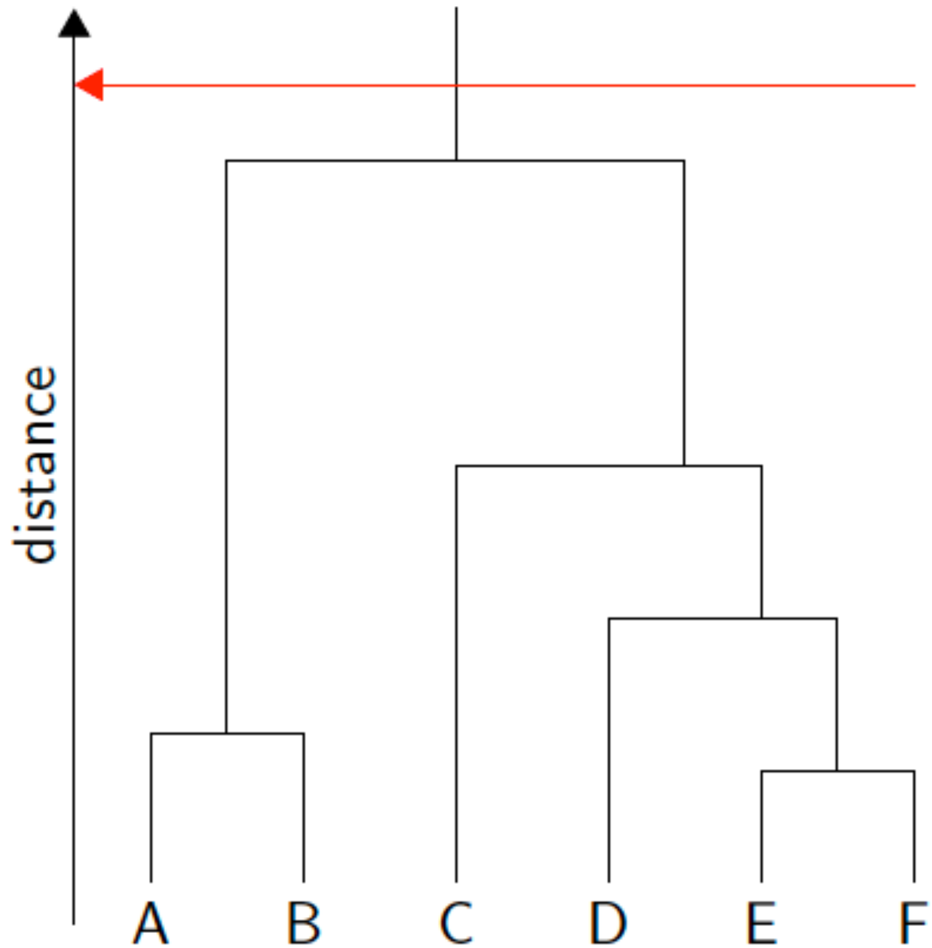
Discovering Groups – Agglomerative Clustering

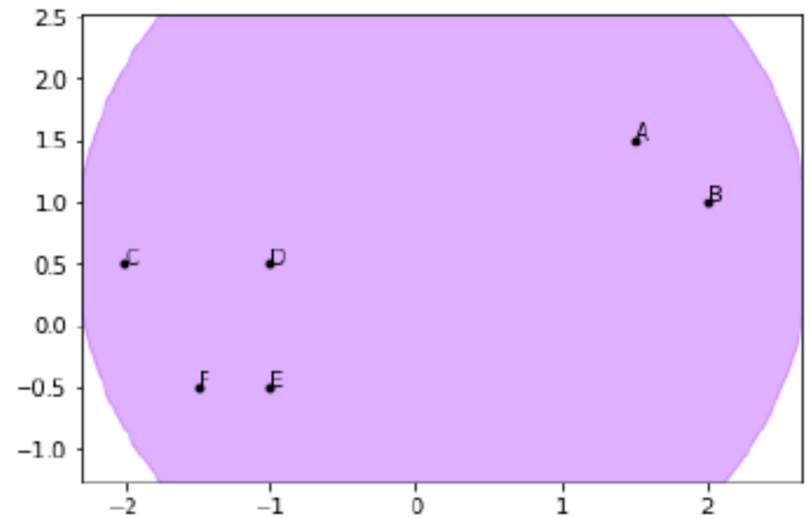


Using minimum or single-linkage clustering

Credit: Jo Grundy

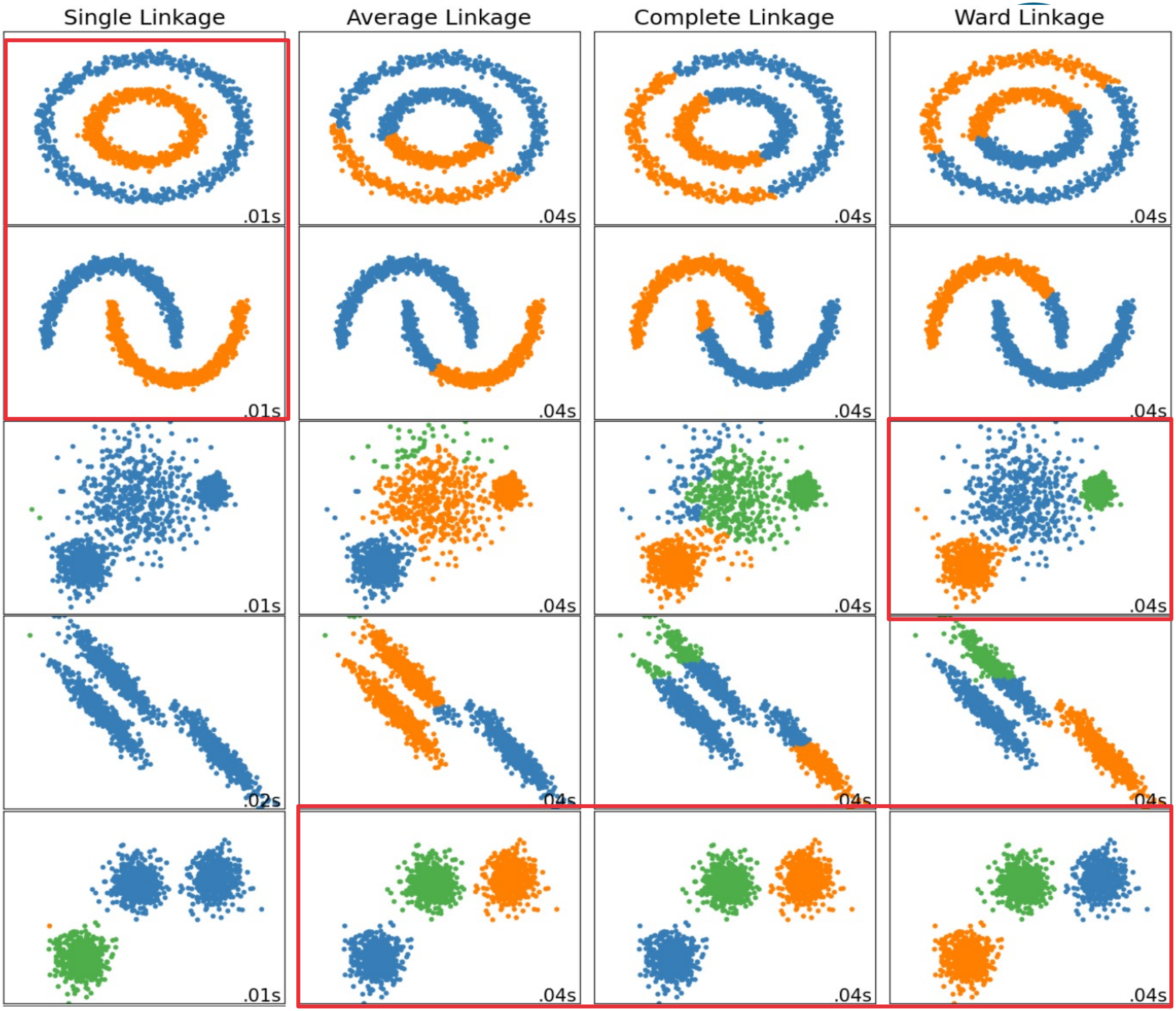
Discovering Groups – Agglomerative Clustering





Using minimum or single-linkage clustering

Credit: Jo Grundy



Source: https://scikit-learn.org/stable/auto_examples/cluster/plot_linkage_comparison.html#sphx-glr-auto-examples-cluster-plot-linkage-comparison-py

Discovering Groups – Hierarchical Clustering

Pros:

- No need to pre-specify cluster numbers; cut the dendrogram at the desired level for the clusters.
- Dendrograms easily summarize data into a hierarchy, facilitating cluster examination and interpretation.

Cons:

- Needs a threshold to determine the number of clusters
- Non-trivial to select the best linkage method

Discovering Groups – Summary

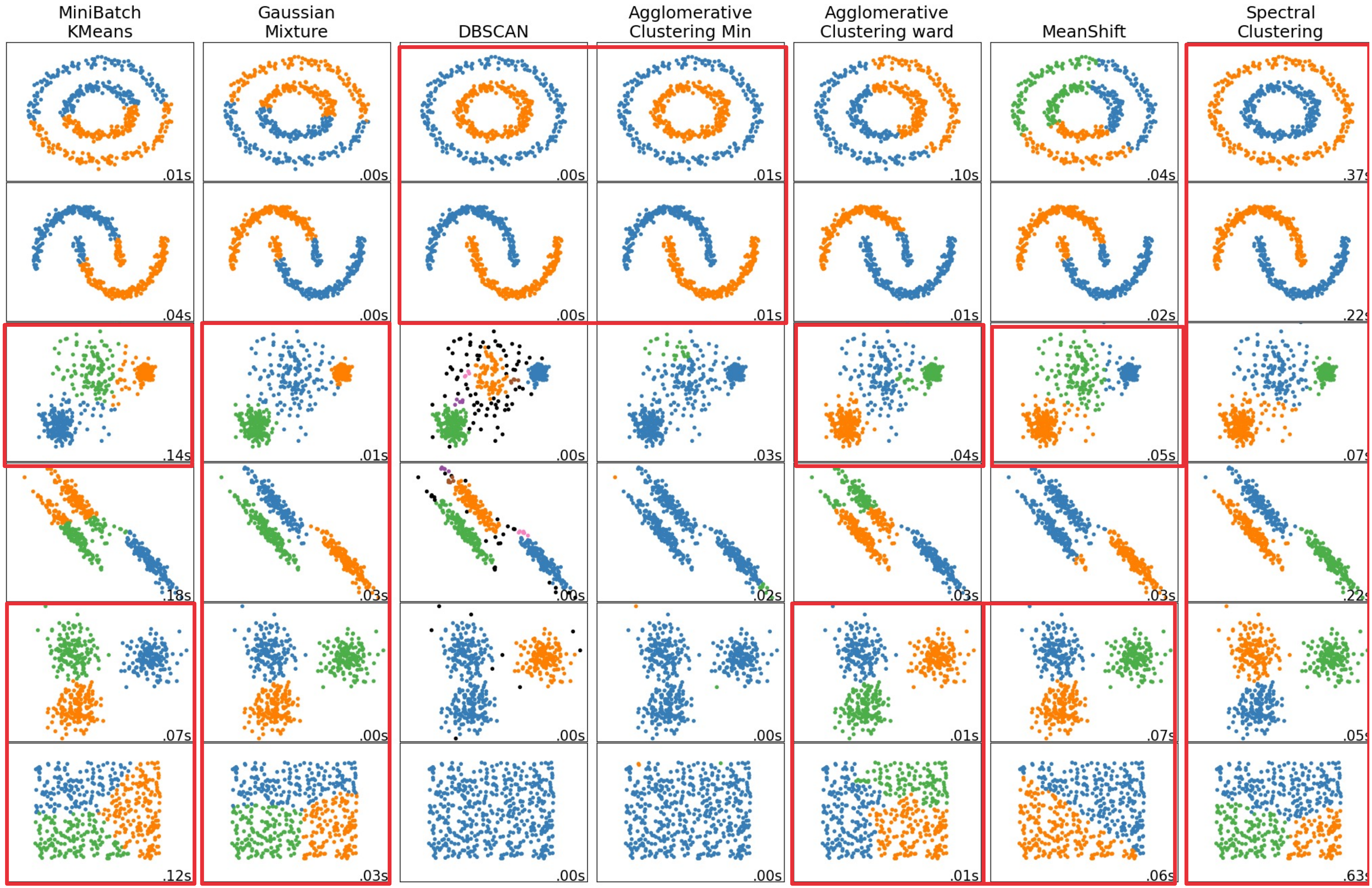
Clustering is a key way to understand your data.

There are many different approaches

- K Means - Need to chose K
- DBSCAN - need to choose min points and radius
- Hierarchical Agglomerative Clustering - needs a threshold or number of clusters

They are a very good way to start exploring a dataset

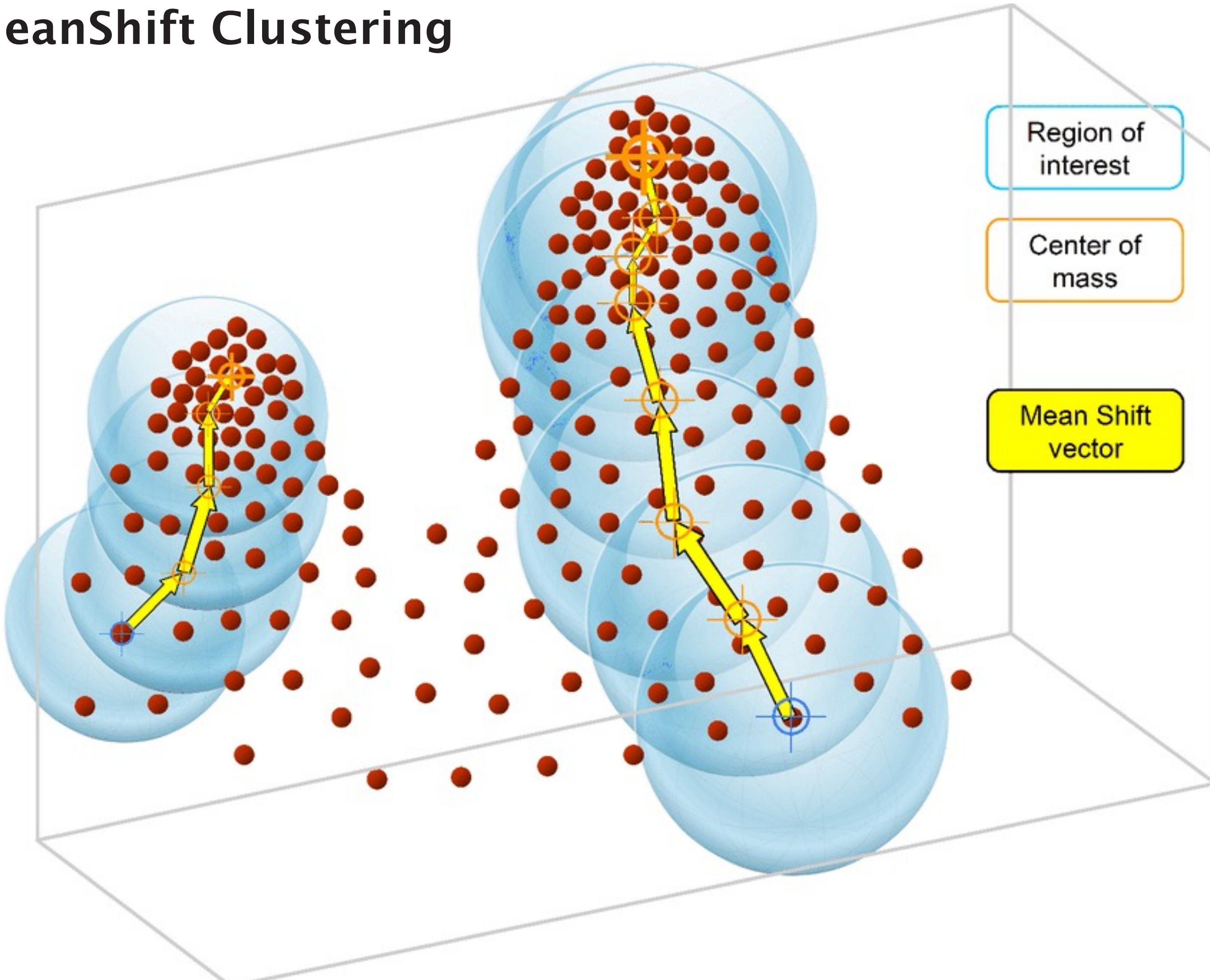
Credit: Jo Grundy



Source: https://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html#sphx-glr-auto-examples-cluster-plot-cluster-comparison-py

Discovering Groups – **Appendix (1/2)**

MeanShift Clustering



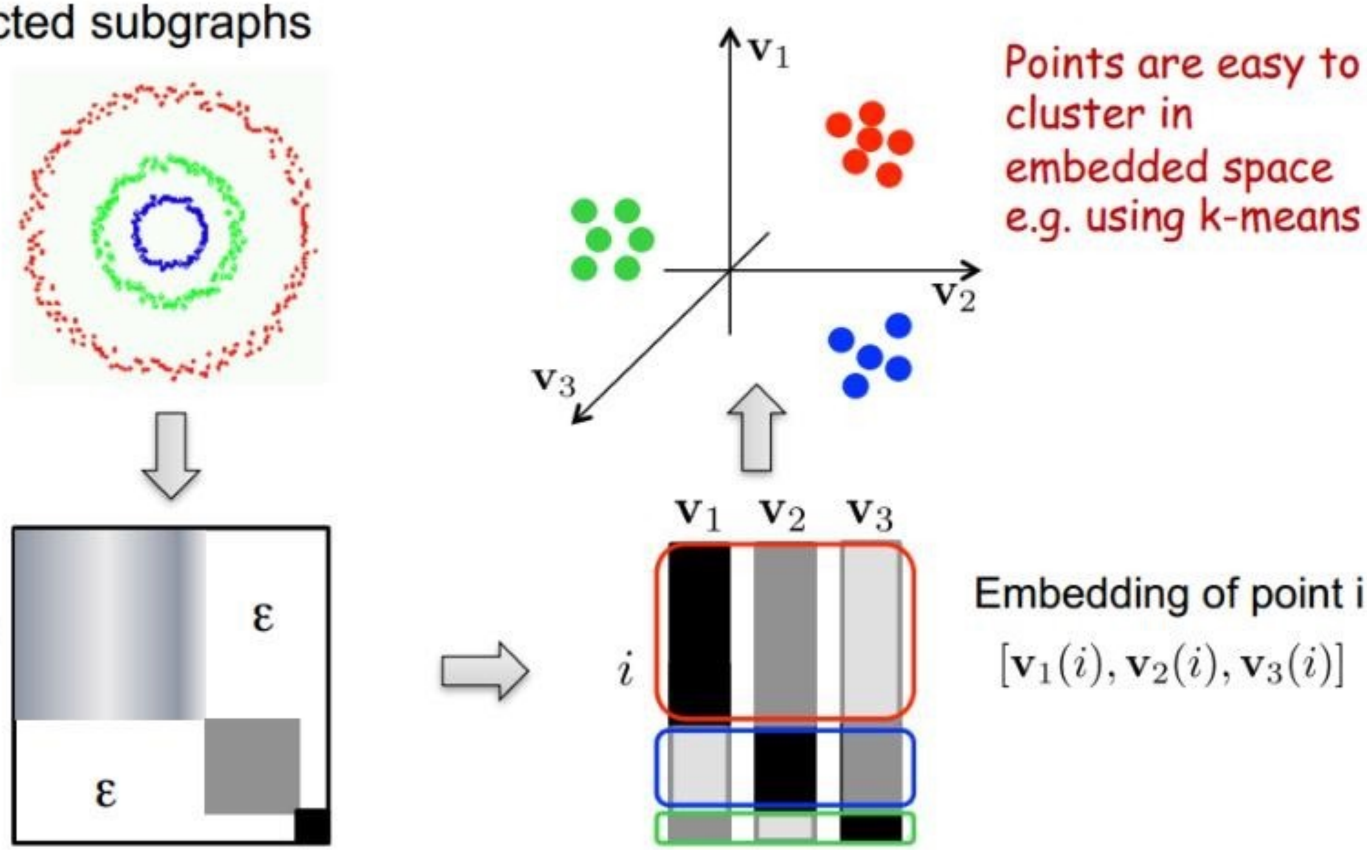
https://ailephant.com/how-to-program-mean-shift/

Discovering Groups – **Appendix (2/2)**

Spectral Clustering

Eigenvectors of the Laplacian matrix provide an embedding of the data based on similarity.

Disconnected subgraphs



Slides Courtesy: Eric Xing, M. Hein & U.V. Luxburg