Unsupervised Learning

Find groups in the data

- No labels nor response -> unsupervised
- Define groups based on similarity

Group customers, target ads

- A priori, you can’t really put labels on customers
- Group similar customers

You can then try to interpret the grouping, and send targeted ads to the groups

Note: you may want to assign labels to groups a posteriori

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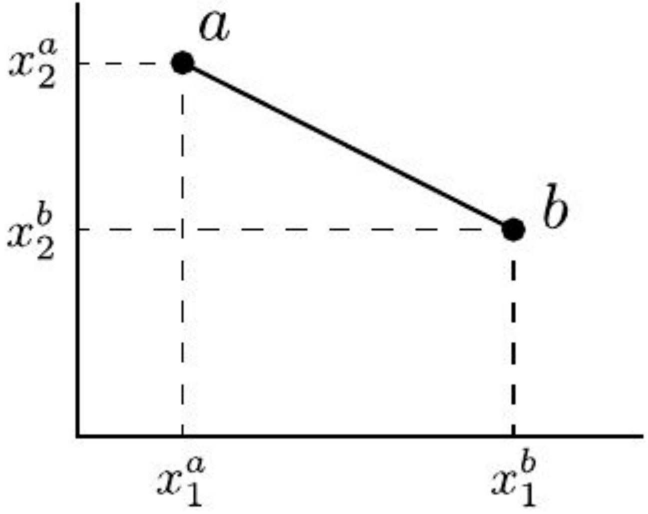
Defining similarity

After a pre-processing step, you have a data matrix with **n** rows (observations) and **p** columns (features). Each row is a “point”.

- How to define similarity between points?
- If the features are numerical, we can use the Euclidean distance
- What if some features are categorical?
    - Ignore
    - Embed into numerical

Euclidean distance



$$d(a, b)^2 = \sum_{i=1:2} (x_i^a - x_i^b)^2$$

Can be generalised from 2-D to n-D

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KMeans

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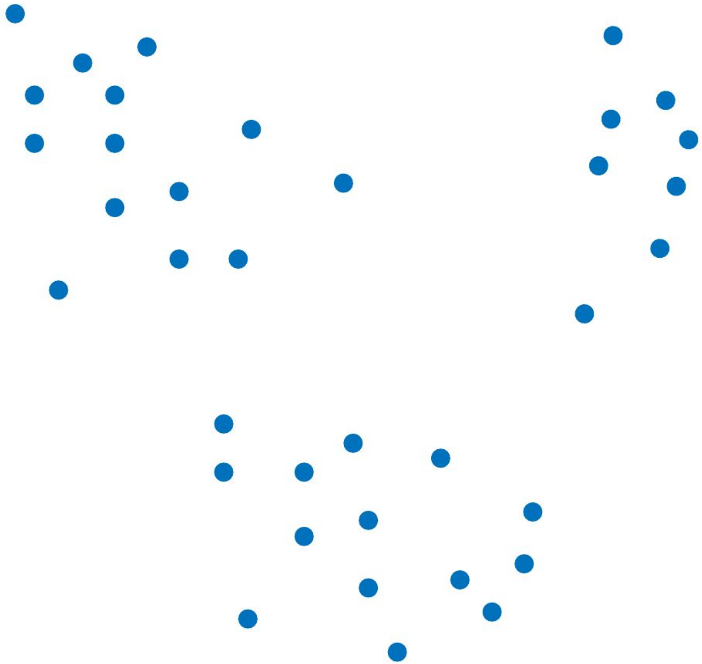
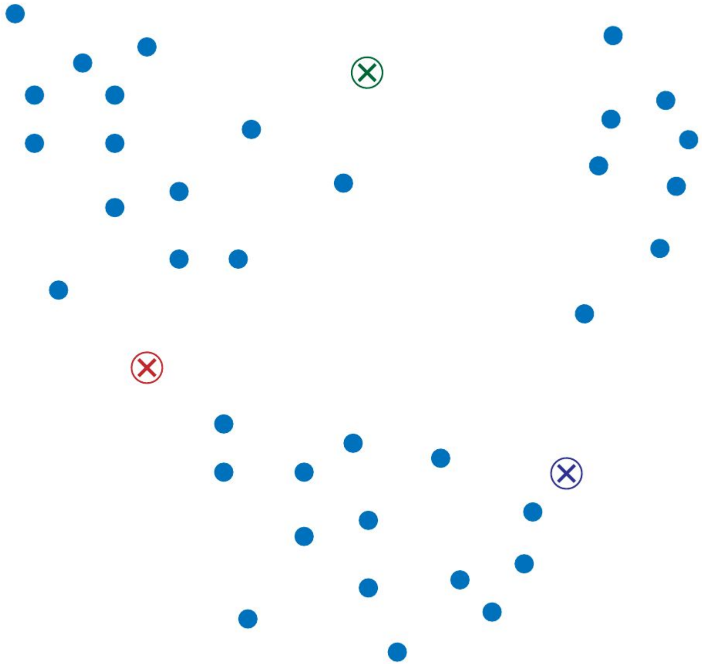
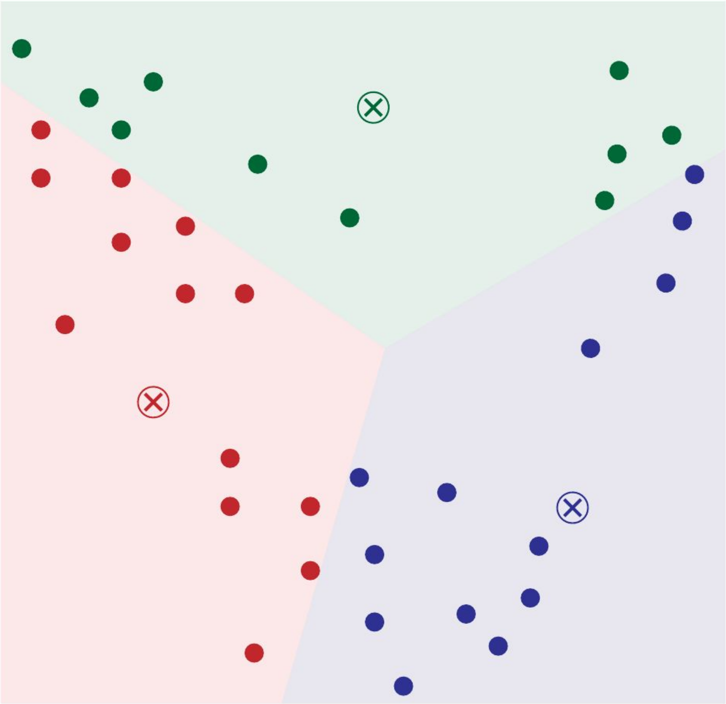
K-means



K-means



K-means



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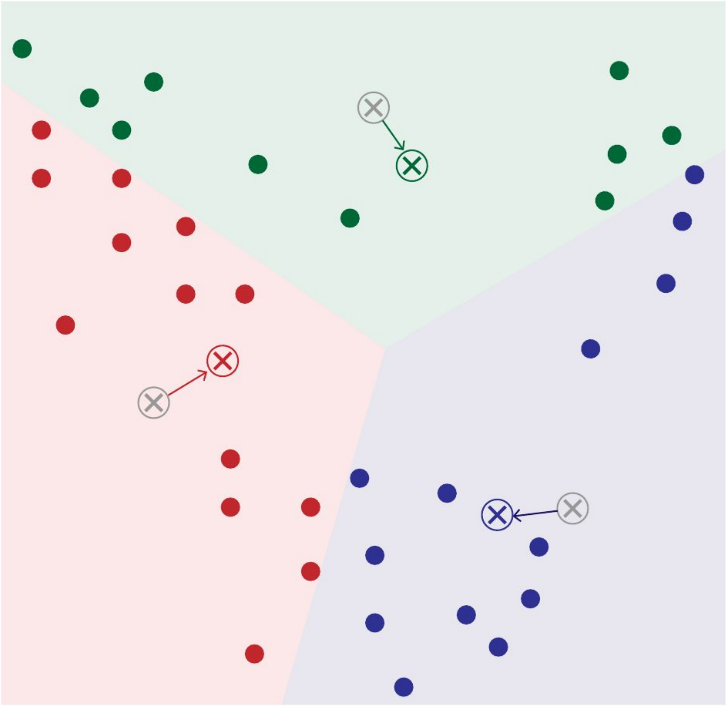
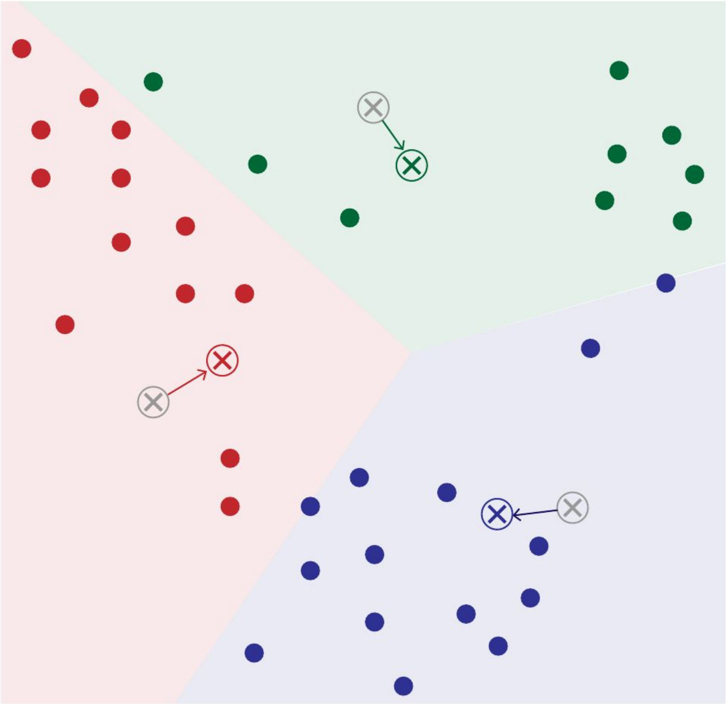
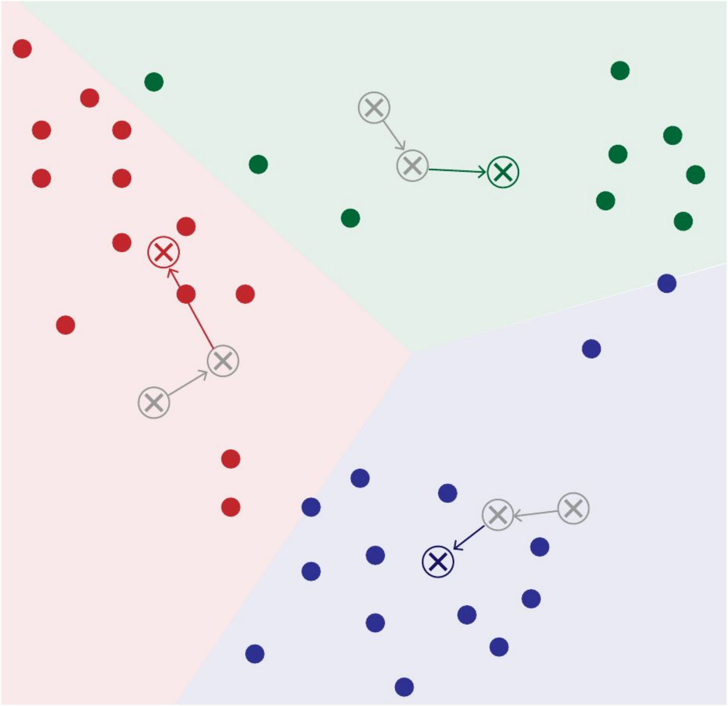
K-means



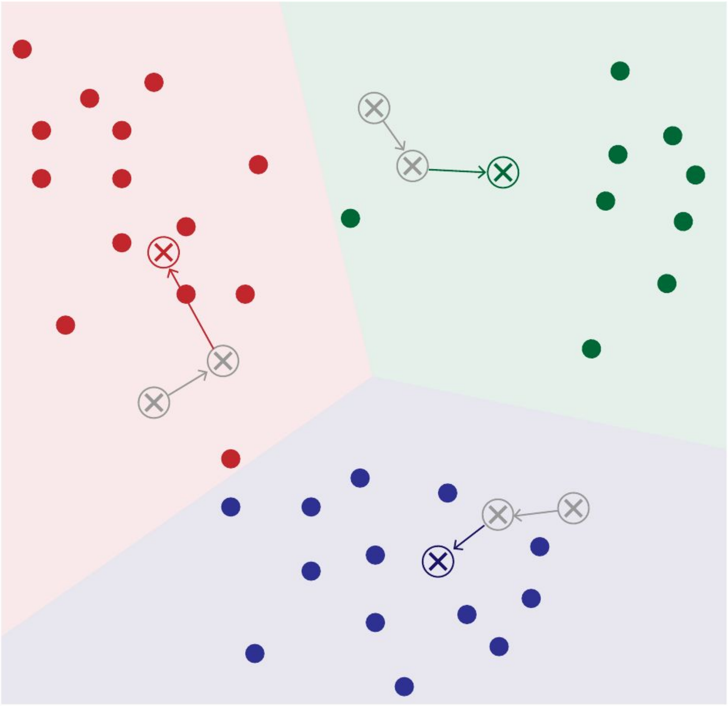
K-means



K-means



K-means



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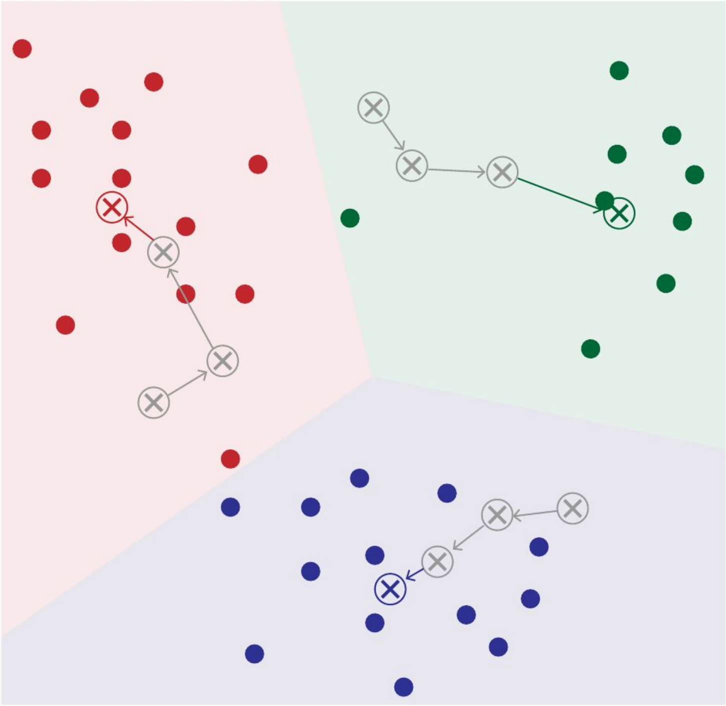
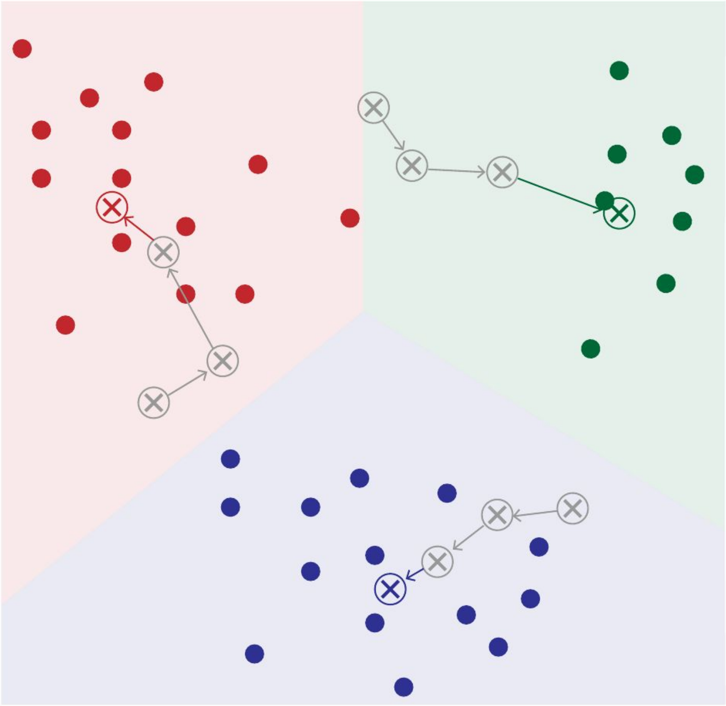
K-means



K-means



K-means - Summary

- Start with K “means” drawn at random
- Assign data points to the nearest one
- Update the position of the means to correspond to the mean of those points
- Repeat...

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K-means - Pros and cons

Pros

- Cheap to compute
- Easy to interpret
- Efficient implementations available
- Assigning a new point is straightforward

Cons

- Need to guess K
- Clusters are globular
- Sensitive to initialisation
- Sensitive to noise

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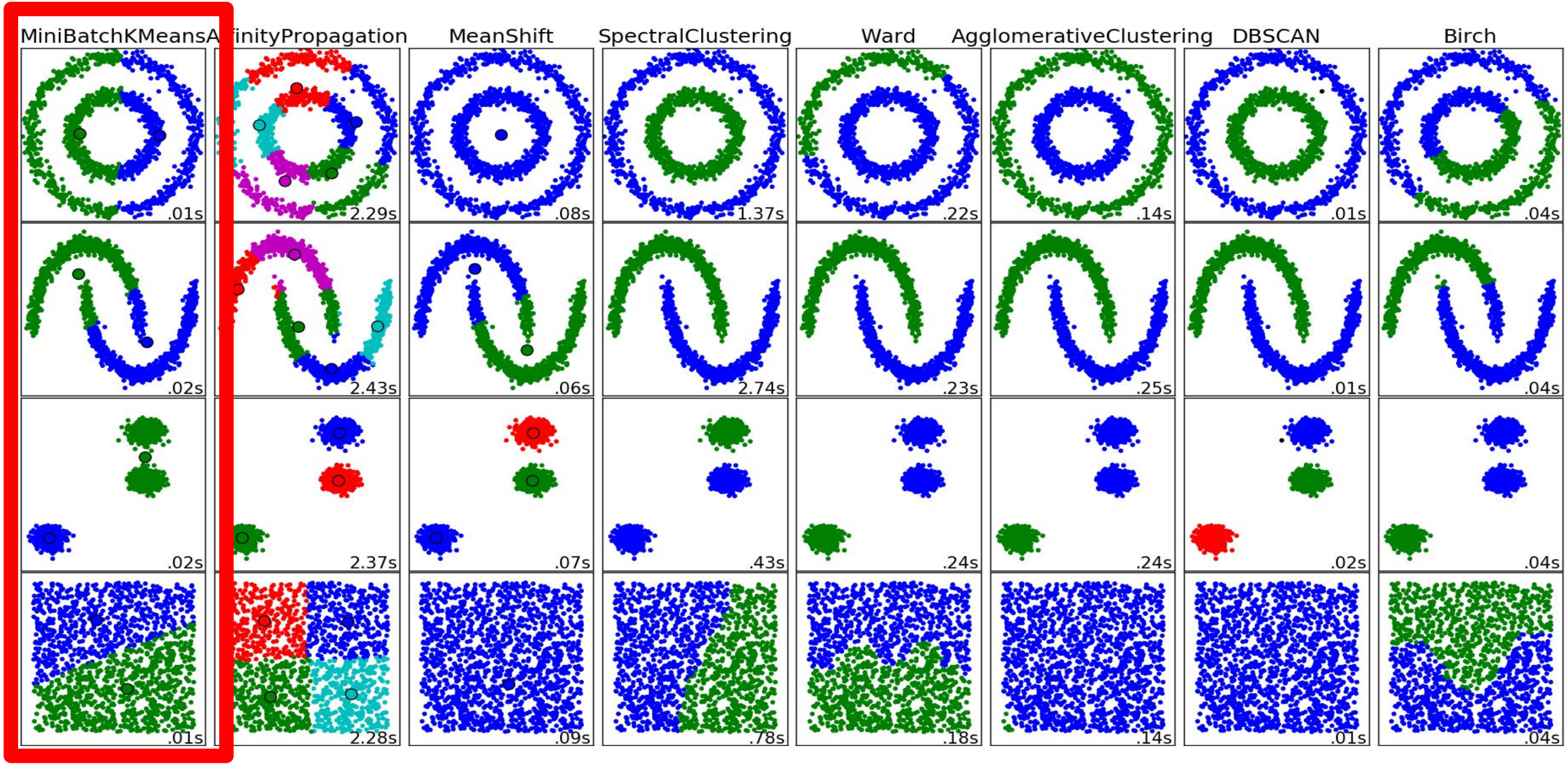
Comparisons of clustering algorithms



RK

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Hierarchical Clustering

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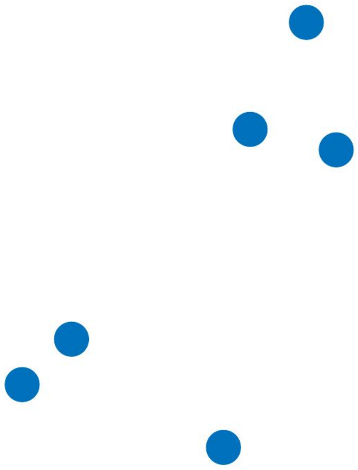
Hierarchical clustering

Building a hierarchy of clusters sequentially.

- **Agglomerative** (bottom-up): Start considering each point as a cluster then merge the closest ones and repeat
- **Divisive** (top-down): Start with one single cluster and divide to have groups with reduced variance

Let’s take a look at agglomerative hierarchical clustering (a.k.a. linkage)

Linkage algorithm



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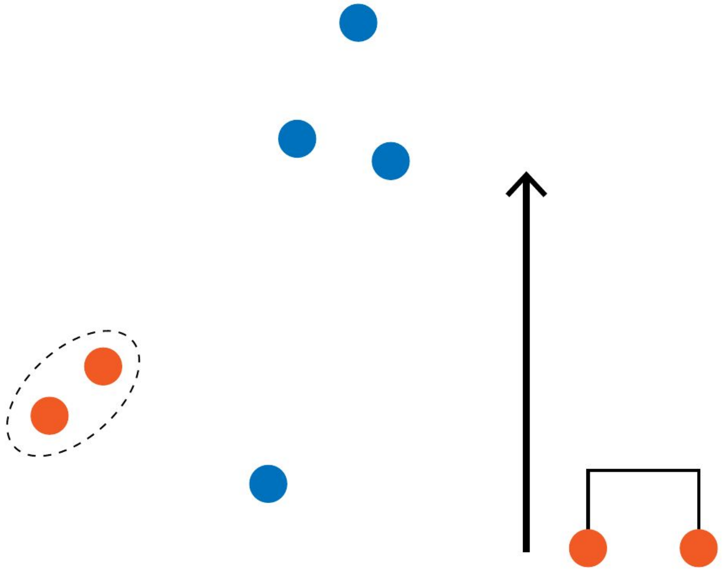
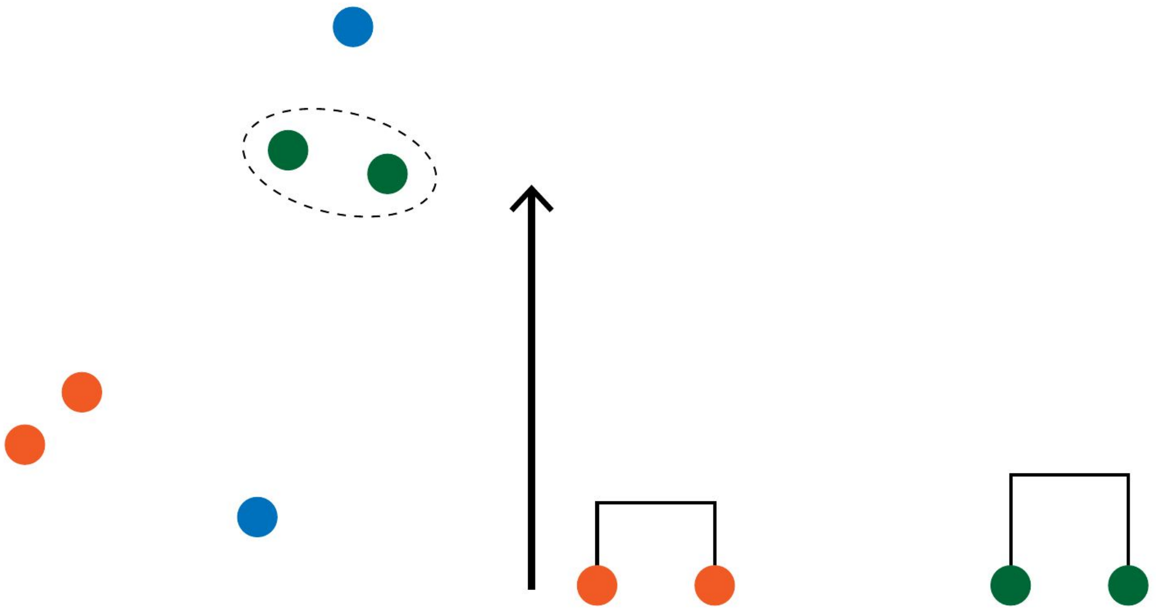
Linkage algorithm



Linkage algorithm



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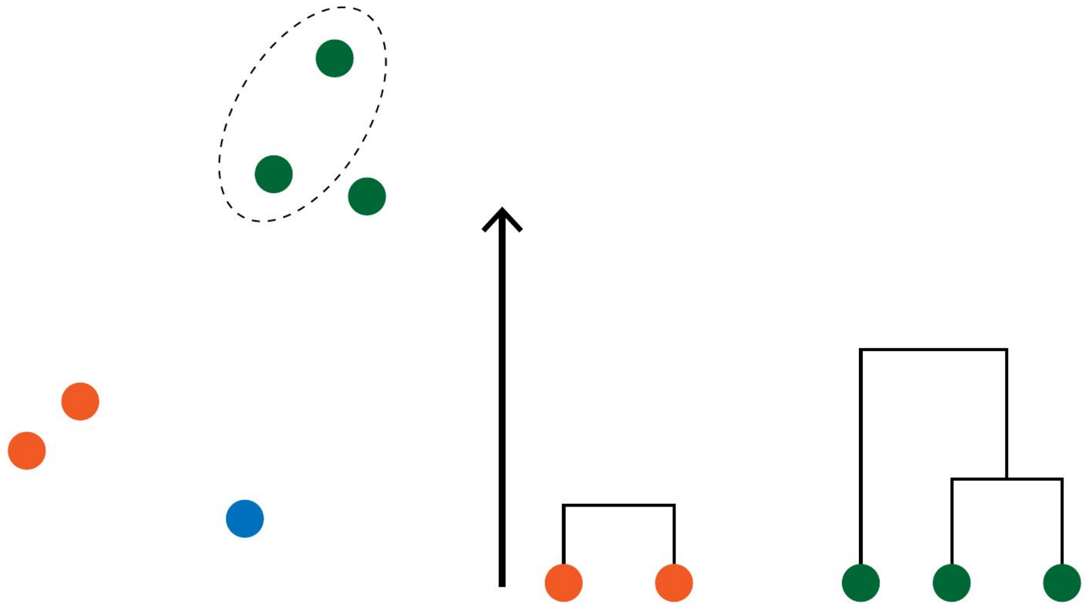
Linkage algorithm



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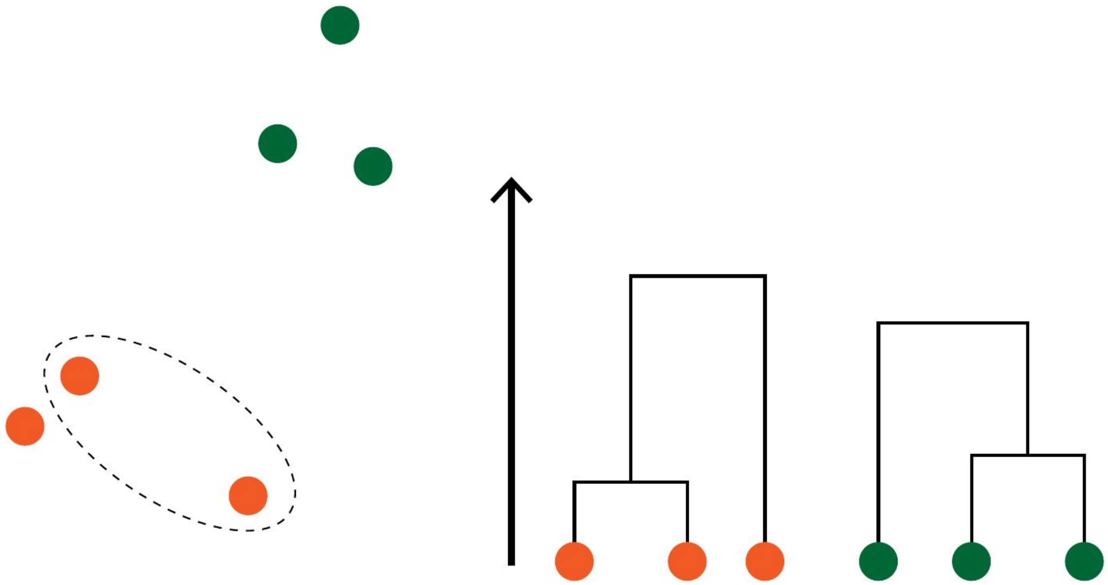
Linkage algorithm



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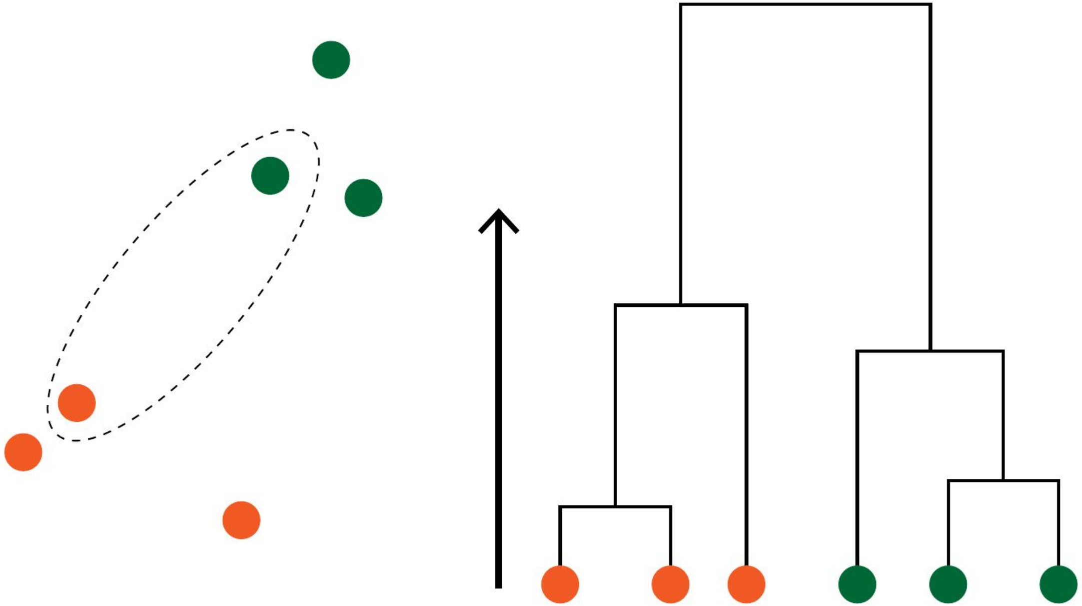
Linkage algorithm



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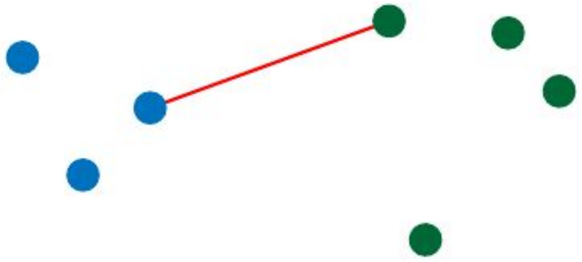
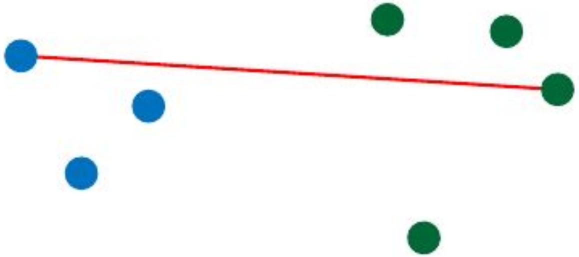
Linkage algorithm

Two strategies to merge clusters:

- **Single linkage**: closest point distance (build spanning trees)
- **Complete linkage**: furthest point distance (to avoid elongated clusters)





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Linkage: pros and cons

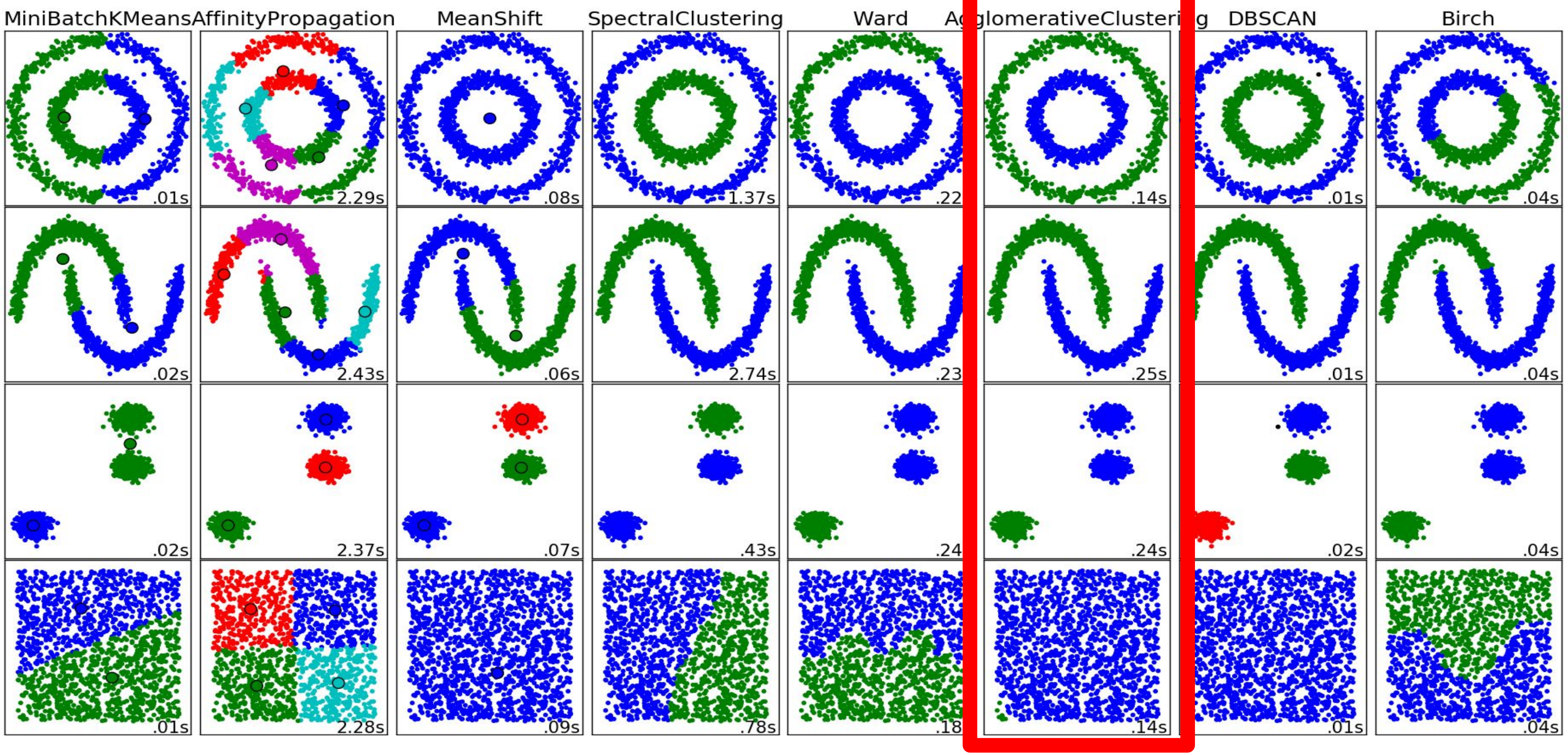
Pros

- Clusters are not necessarily globular
- No dependence upon initialisation
- Dendogram shows a good summary

Cons

- Slower than K-means
- Still need to pick a number of clusters
- Assigning a new point is not straightforward
- Sensitive to noise

Comparisons of clustering algorithms



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DBSCAN

DBSCAN

Clusters = Zones of **high-density**
Two parameters: **min_samples** and **eps**

Algorithm:

- Start at a random point, consider all points within radius **eps**
- If that covers **min_samples**, keep that ball
    - Expend by considering esp-balls around every point of the current ball and iterate
- Otherwise mark the point as **noise**

… let's see this in action

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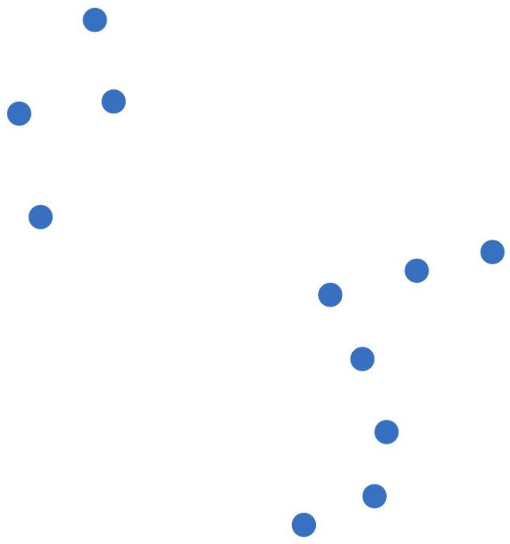
DBSCAN



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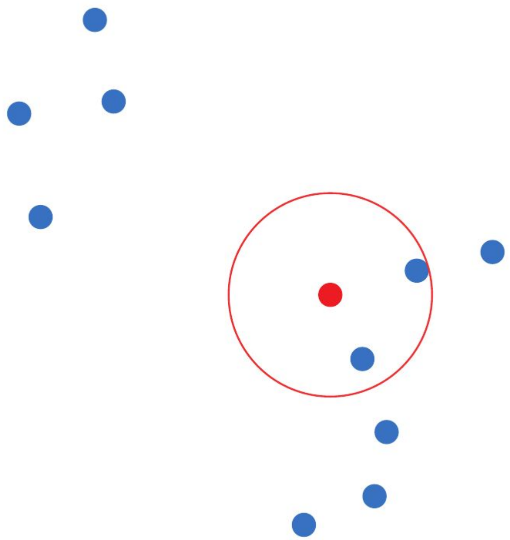

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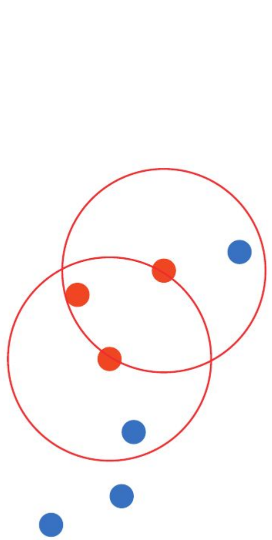

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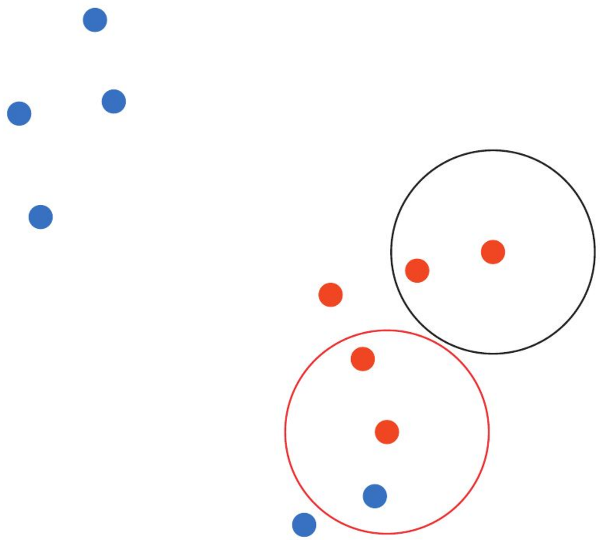
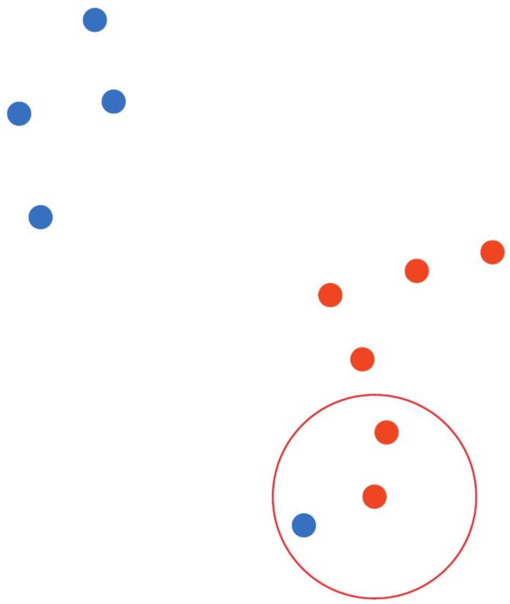
DBSCAN



DBSCAN



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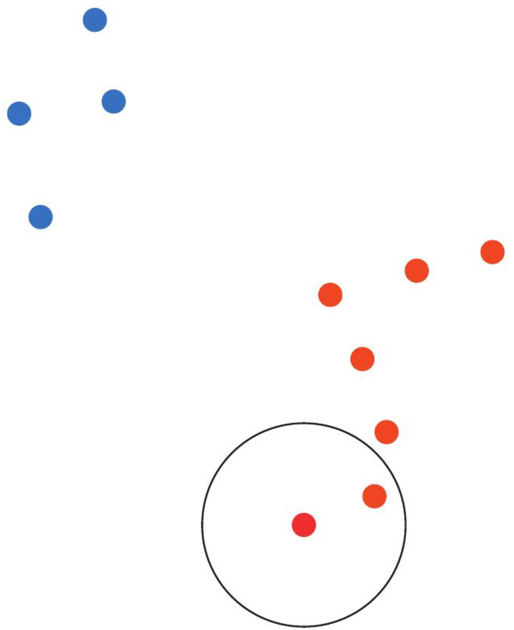

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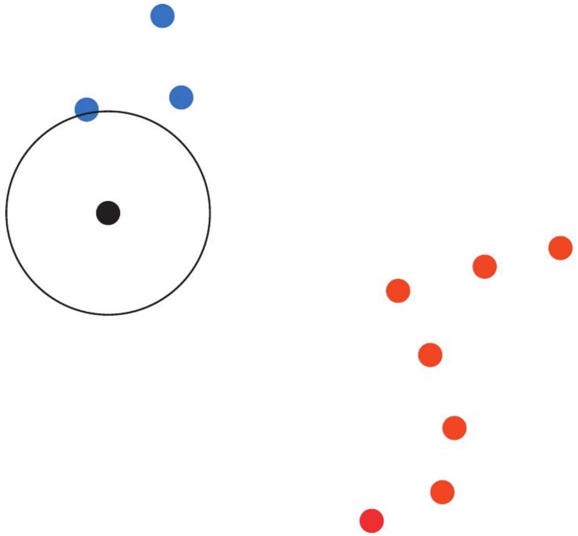

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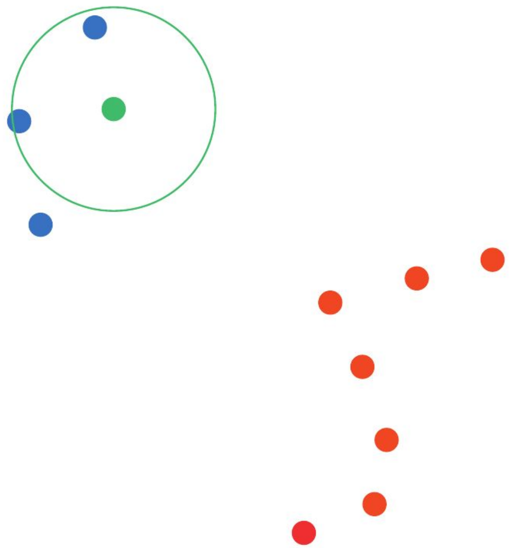

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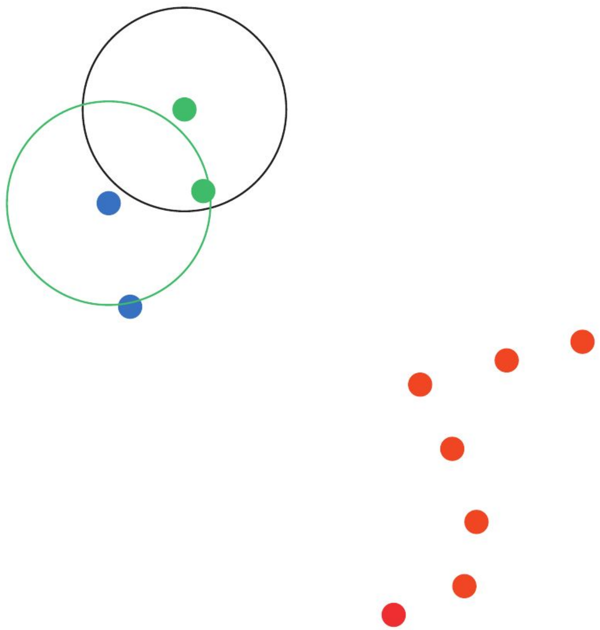
DBSCAN



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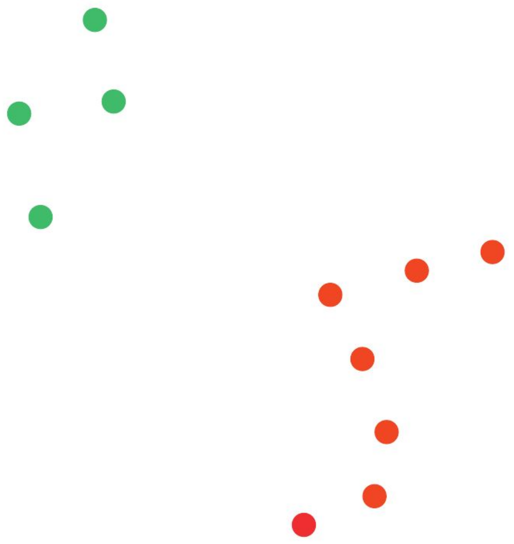

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DBSCAN: pros and cons

Pros

- Clusters are not necessarily globular
- No choice of number of clusters
- Very efficient implementations exist
- Robust to noise

Cons

- The **eps** and **min_samples** can be hard to tune
- If clusters have significantly different densities it is hard to find a meaningful **eps**, **min_samples**

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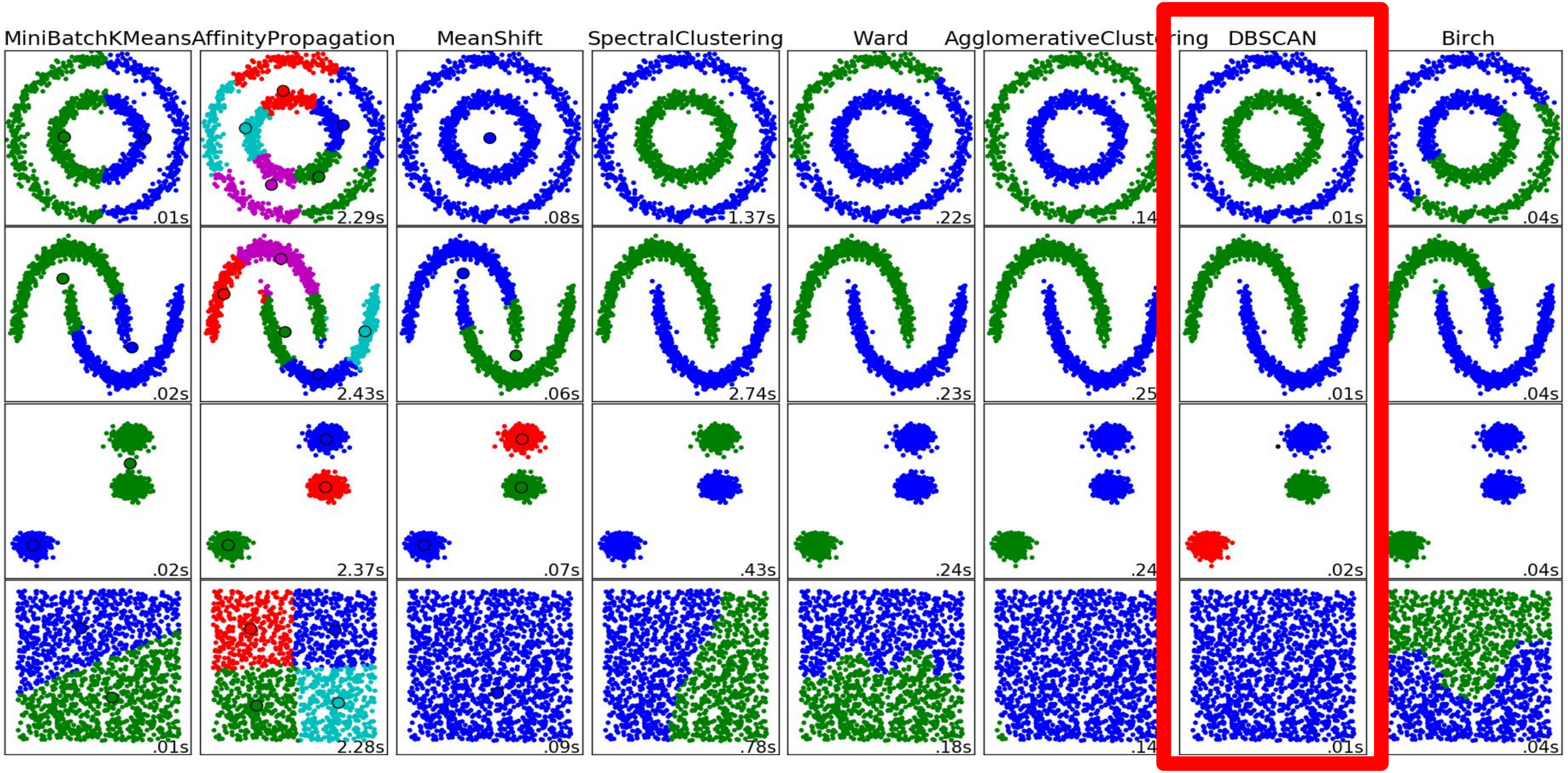
Comparisons of clustering algorithms



Hands-on session

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