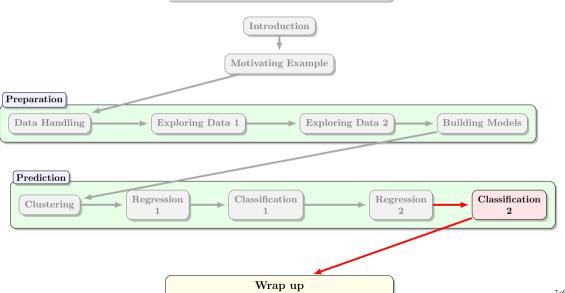
dm24s1 Topic 11: Clustering Part 01: Overview Dr Bernard Butler Data 2 Department of Computing and Mathematics, WIT. (bernard.butler@setu.ie) Autumn Semester, 2024 Outline How to compute distances between instances Algorithms that partition the data Wrap up

Data Mining (Week 11)



Overview — Summary

1. Introduction	4
2. Distance Measures	9
3. Hierarchical Clustering	14
4. Partioning Algorithms 4.1. K-means	25 28
4.2. Soft clustering	34
4.3. Expectation Maximisation (EM) iterations	37
4.4. Density-based clustering	39
4.5. Choosing <i>k</i> for centre-based clusters	44

Outline

1. Introduction	4
2. Distance Measures	9
3. Hierarchical Clustering	14
4. Partioning Algorithms	25
4.1. K-means	28
4.2. Soft clustering	34
4.3. Expectation Maximisation (EM) iterations	37
4.4. Density-based clustering	39
4.5 Choosing k for centre-based clusters	44

This week's aim is to introduce the main concepts and representative algorithms used in cluster analysis.

• Introduction to unsupervised learning

- Introduction to unsupervised learning
- Clustering as a means of understanding data

- Introduction to unsupervised learning
- Clustering as a means of understanding data
- Choice of distance function and metaparameters

- Introduction to unsupervised learning
- Clustering as a means of understanding data
- Choice of distance function and metaparameters
- Clusters that partition the data

- Introduction to unsupervised learning
- Clustering as a means of understanding data
- Choice of distance function and metaparameters
- Clusters that partition the data
 - Iris data: predicting which of three species

This week's aim is to introduce the main concepts and representative algorithms used in cluster analysis.

- Introduction to unsupervised learning
- Clustering as a means of understanding data
- Choice of distance function and metaparameters
- Clusters that partition the data
 - Iris data: predicting which of three species

Clustering is a long-established form of analysis, having much in common with exploratory data analysis. We look at the main concepts and algorithms today.

Background: Unsupervised Learning

Definition 1 (Unsupervised Learnng)

With unsupervised learning, the system receives input instances x_1, x_2, \ldots but obtains neither target outputs, nor rewards from its environment. Its goal is to build representations of the input that can be used for decision making, predicting future inputs, efficiently communicating the inputs to another machine, etc. It does this by finding patterns in the data beyond what would be considered pure unstructured noise (**Ghahramani2004**).

Regression and classification are examples of supervised learning because they require labeled *training* data.

We saw *dimensionality reduction* in Topic 8 (Regression 2). Other unsupervised learning techniques include *anomaly detection* and the very "hot" *Generative Adversarial Networks* of deep learning. We look at *clustering* today.

Introduction to Clustering

Definition 2 (Clustering)

Clustering is the operation of grouping objects into a smaller number of clusters (or segments), which have two properties. Firstly, they are not defined in advance by an analyst, but are discovered during the operation, unlike the classes used in classification. Secondly, the clusters combine objects having similar characteristics, which are separated from objects having different characteristics (resulting in *internal homogeneity* and *external heterogeneity* (**Tuffery2011**).

Clustering is usually called *segmentation* in marketing studies.

Usually clustering is not an end in itself: it generates insights that are used to motivate and inform other analyses.

The "quality" of a cluster analysis is difficult to determine objectively - there is no equivalent of recall, say.

Hierarchical

• Intermediate steps are interpretable

Partitional

Interpret the final clustering only

Hierarchical

- Intermediate steps are interpretable
- More than one clustering generated see *dendrogram*

- Interpret the final clustering only
- Single clustering returned; repeat with different conditions to improve it

Hierarchical

- Intermediate steps are interpretable
- More than one clustering generated see *dendrogram*
- Given choice of linkage, algorithm proceeds deterministically

- Interpret the final clustering only
- Single clustering returned; repeat with different conditions to improve it
- Optimisation by gradient descent, so

Hierarchical

- Intermediate steps are interpretable
- More than one clustering generated see *dendrogram*
- Given choice of linkage, algorithm proceeds deterministically
 - no concept of starting values

- Interpret the final clustering only
- Single clustering returned; repeat with different conditions to improve it
- Optimisation by gradient descent, so
 - result depends on starting values

Hierarchical

- Intermediate steps are interpretable
- More than one clustering generated see *dendrogram*
- Given choice of linkage, algorithm proceeds deterministically
 - no concept of starting values
 - no concept of local versus global optimum

- Interpret the final clustering only
- Single clustering returned; repeat with different conditions to improve it
- Optimisation by gradient descent, so
 - result depends on starting values
 - might find local rather than global optimum

Hierarchical

- Intermediate steps are interpretable
- More than one clustering generated see *dendrogram*
- Given choice of linkage, algorithm proceeds deterministically
 - no concept of starting values
 - no concept of local versus global optimum
- relatively few parameters to specify

- Interpret the final clustering only
- Single clustering returned; repeat with different conditions to improve it
- Optimisation by gradient descent, so
 - result depends on starting values
 - might find local rather than global optimum
- more parameters to specify

Hierarchical

- Intermediate steps are interpretable
- More than one clustering generated see *dendrogram*
- Given choice of linkage, algorithm proceeds deterministically
 - no concept of starting values
 - no concept of local versus global optimum
- relatively few parameters to specify
- more complex interpretation

- Interpret the final clustering only
- Single clustering returned; repeat with different conditions to improve it
- Optimisation by gradient descent, so
 - result depends on starting values
 - might find local rather than global optimum
- more parameters to specify
- interpretation is relatively easy

Outline

1. Introduction	4	
2. Distance Measures	9	
3. Hierarchical Clustering	14	
 4. Partioning Algorithms 4.1. K-means 4.2. Soft clustering 4.3. Expectation Maximisation (EM) iterations 4.4. Density-based clustering 4.5. Choosing k for centre-based clusters 	25 28 34 37 39 44	

Distance Measures and their role in clustering

Definition 3 (Distance Measure)

A distance measure (c.f., its complement, a similarity measure) is a scalar number $d(x_1, x_2)$ that quantifies the degree of agreement between two (usually vector-valued) observations x_1 and x_2 . When $x_1 = x_2$, $d(x_1, x_2) = 0$ and $d(x_1, x_2) > 0$ otherwise. It increases as the difference in the observations increases.

By definition, clustering is based on within-cluster homogeneity (measured by small d) versus large d between clusters. Thus choice of distance measure plays a critical part in generating useful clusters.

Distance Measures for numeric data

Definition 4 (Minkowski – norm)

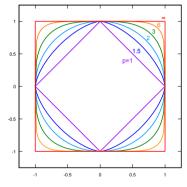
For a real number $1 \le p < \infty$, the *p*-norm of *x* is defined by

$$\|\mathbf{x}\|_p \equiv (|x_1|^p + |x_2|^p + \ldots + |x_n|^p)^{\frac{1}{p}}.$$

The limiting case of $p = \infty$ is defined as

$$||\mathbf{x}||_{\infty} \equiv \max\{|x_1|,|x_2|,\ldots,|x_n|\}.$$

See the visualisation of the "unit balls" alongside, for $p = 1, 1.5, 2, 3, 6, \infty$.



Source: wikipedia

Distance Measures for numeric data

Definition 4 (Minkowski – norm)

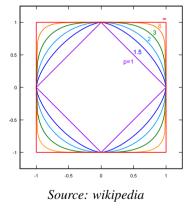
For a real number $1 \le p < \infty$, the *p*-norm of *x* is defined by

$$\|\mathbf{x}\|_p \equiv (|x_1|^p + |x_2|^p + \ldots + |x_n|^p)^{\frac{1}{p}}.$$

The limiting case of $p = \infty$ is defined as

$$||x||_{\infty} \equiv \max\{|x_1|, |x_2|, \dots, |x_n|\}.$$

See the visualisation of the "unit balls" alongside, for $p = 1, 1.5, 2, 3, 6, \infty$.



The most common norms are when $p = 1, 2, \text{ or}, \infty$. Choice of p depends on the application scenario. Can you think of when you would use each?

(Selected) Distance Measures for categorical data

Let $x_1 = [e_{1,1}, e_{1,2}, \dots e_{1,k}]^T$ and $x_2 = [e_{2,1}, e_{2,2}, \dots e_{2,k}]^T$. Furthermore let $e_{1,j}e_{2,j} = 1$ if $e_{1,j} = e_{2,j}$ and $e_{1,j}e_{2,j} = 0$ otherwise. To compute s, the number of matching attributes between x_1 and x_2 , we can just compute the dot product:

$$s = \boldsymbol{x}_1^T \boldsymbol{x}_2$$

and the number of mismatches is d = k - s, where k is the number of attributes in x.

(Selected) Distance Measures for categorical data

Let $x_1 = [e_{1,1}, e_{1,2}, \dots e_{1,k}]^T$ and $x_2 = [e_{2,1}, e_{2,2}, \dots e_{2,k}]^T$. Furthermore let $e_{1,j}e_{2,j} = 1$ if $e_{1,j} = e_{2,j}$ and $e_{1,j}e_{2,j} = 0$ otherwise. To compute s, the number of matching attributes between x_1 and x_2 , we can just compute the dot product:

$$s = \boldsymbol{x}_1^T \boldsymbol{x}_2$$

and the number of mismatches is d = k - s, where k is the number of attributes in x.

Definition 5 (Euclidean distance for categorical observations)

 $||x_1 - x_2|| = \sqrt{x_1^T x_1 - 2x_1^T x_2 + x_2^T x_2} = \sqrt{2(k-s)}$. So the maximum distance occurs when s = 0 (x_1 and x_2 share no attribute values in common, as expected).

(Selected) Distance Measures for categorical data

Let $x_1 = [e_{1,1}, e_{1,2}, \dots e_{1,k}]^T$ and $x_2 = [e_{2,1}, e_{2,2}, \dots e_{2,k}]^T$. Furthermore let $e_{1,j}e_{2,j} = 1$ if $e_{1,j} = e_{2,j}$ and $e_{1,j}e_{2,j} = 0$ otherwise. To compute s, the number of matching attributes between x_1 and x_2 , we can just compute the dot product:

$$s = \boldsymbol{x}_1^T \boldsymbol{x}_2$$

and the number of mismatches is d = k - s, where k is the number of attributes in x.

Definition 5 (Euclidean distance for categorical observations)

 $\|x_1 - x_2\| = \sqrt{x_1^T x_1 - 2x_1^T x_2 + x_2^T x_2} = \sqrt{2(k-s)}$. So the maximum distance occurs when s = 0 (x_1 and x_2 share no attribute values in common, as expected).

Definition 6 (Hamming Distance)

This is the number of mismatched values k - s.

(Selected) Distance Measures for categorical data - ratios

Definition 7 (Cosine similarity)

$$\cos \theta_{1,2} = \frac{x_1^T x_2}{\|x_1\| \|x_2\|} = \frac{s}{\sqrt{k}\sqrt{k}} = \frac{s}{k}.$$

because
$$||x|| \equiv \sqrt{x^T x} = \sqrt{k}$$
.

(Selected) Distance Measures for categorical data - ratios

Definition 7 (Cosine similarity)

$$\cos \theta_{1,2} = \frac{x_1^T x_2}{\|x_1\| \|x_2\|} = \frac{s}{\sqrt{k}\sqrt{k}} = \frac{s}{k}.$$

because $||x|| \equiv \sqrt{x^T x} = \sqrt{k}$.

Definition 8 (Jaccard Coefficient)

This is the ratio of the number of matching values s to the number of distinct values that appear in x_1 and x_2 , across the d distinct attributes of both. It is $J(x_1, x_2) = \frac{s}{2(k-s)+s} = \frac{s}{2k-s}$.

(Selected) Distance Measures for categorical data - ratios

Definition 7 (Cosine similarity)

$$\cos \theta_{1,2} = \frac{x_1^T x_2}{\|x_1\| \|x_2\|} = \frac{s}{\sqrt{k}\sqrt{k}} = \frac{s}{k}.$$

because $||x|| \equiv \sqrt{x^T x} = \sqrt{k}$.

Definition 8 (Jaccard Coefficient)

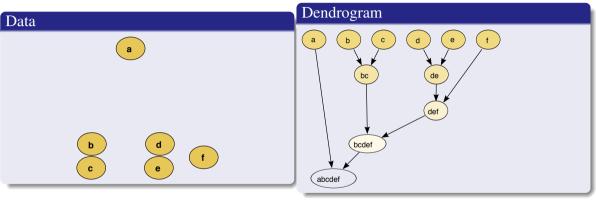
This is the ratio of the number of matching values s to the number of distinct values that appear in x_1 and x_2 , across the d distinct attributes of both. It is $J(x_1, x_2) = \frac{s}{2(k-s)+s} = \frac{s}{2k-s}$.

Note that all these distance measures are functions of s and k, where k is a constant and s is a count of the number of matching attribute values across the two observations in question.

Outline

1. Introduction	4
2. Distance Measures	9
3. Hierarchical Clustering	14
 4. Partioning Algorithms 4.1. K-means 4.2. Soft clustering 4.3. Expectation Maximisation (EM) iterations 4.4. Density-based clustering 4.5. Choosing k for centre-based clusters 	25 28 34 37 39 44

Simple example of data and its dendrogram



This illustrates how *agglomerative* clustering works. *Divisive* clustering works in the opposite direction, but the (flipped) dendrogram is the same in this case.

Sometimes, the vertical separation between Level i and i+1 of the tree indicates the distance between clusters that are merged at Level i+1.

Diagram Source: wikipedia

Definition 9 (dendrogram)

The dendrogram shows clusters and their subclusters, in the form of a tree. The root cluster contains all elements; each leaf contains a single element. Clusters are merged in order of their similarity.

Definition 9 (dendrogram)

The dendrogram shows clusters and their subclusters, in the form of a tree. The root cluster contains all elements; each leaf contains a single element. Clusters are merged in order of their similarity.

The dendrogram makes the internal similarity structure of the data more visible.

Definition 9 (dendrogram)

The dendrogram shows clusters and their subclusters, in the form of a tree. The root cluster contains all elements; each leaf contains a single element. Clusters are merged in order of their similarity.

The dendrogram makes the internal similarity structure of the data more visible.

Sometimes, the vertical separation between Level i and i + 1 of the tree is proportional to the distance between clusters that are merged at Level i + 1.

Definition 9 (dendrogram)

The dendrogram shows clusters and their subclusters, in the form of a tree. The root cluster contains all elements; each leaf contains a single element. Clusters are merged in order of their similarity.

The dendrogram makes the internal similarity structure of the data more visible.

Sometimes, the vertical separation between Level i and i + 1 of the tree is proportional to the distance between clusters that are merged at Level i + 1.

An alternative representation is to display the data as a point cloud and to overlay nested clusters over the data.

Overview of Hierarchical Clustering Algorithm

Method (Agglomerative hierarchical clustering (AGNES))

```
Initialise the Cluster set C = \{x_i\}, i = 1, ..., n;
q \leftarrow |\{c_i\}| = n;
Compute the n \times n proximity matrix D where D_{ii} = d(c_i, c_i);
repeat
    Find i, j associated with \min_{i,j} D, where i, j are indices of clusters that are nearest each other;
    Create the merged cluster c'_i containing the elements of cluster c_i and c_i;
    Record the merge operation so the dendrogram data structure can be built;
    Drop the old c_i cluster since it is not needed any more;
    Delete row D(j,:) and column D(:,j) from D
    q \leftarrow q - 1;
    Update row D(i,:) and column D(:,i) to compute distance between new cluster c'_i and remaining
q-2 clusters;
until q = 1 and hence only one cluster remains;
```

Overview of Hierarchical Clustering Algorithm

Method (Agglomerative hierarchical clustering (AGNES))

```
Initialise the Cluster set C = \{x_i\}, i = 1, ..., n; q \leftarrow |\{c_i\}| = n; Compute the n \times n proximity matrix D where D_{ij} = d(c_i, c_j);
```

repeat

Find i, j associated with $\min_{i,j} D$, where i, j are indices of clusters that are nearest each other;

Create the merged cluster c'_i containing the elements of cluster c_i and c_i ;

Record the merge operation so the dendrogram data structure can be built;

Drop the old c_i cluster since it is not needed any more;

Delete row D(j,:) and column D(:,j) from D

$$q \leftarrow q - 1$$
;

Update row D(i,:) and column D(:,i) to compute distance between new cluster c'_i and remaining

q-2 clusters;

until q = 1 and hence only one cluster remains;

As can be seen, this is a deterministic search algorithm.

However, there is scope for different definitions of the distance function $d(c_i, c_j)$ between clusters c_i and c_j .

Distance between clusters: linkage

Earlier, we looked at different ways of computing the *distance between two points*. For hierarchical clustering, we need to compute the *distance between two clusters*.

Definition 10 (Linkage function)

For Complete Linkage: $D(X, Y) = \max_{x \in X, y \in Y} d(x, y)$.

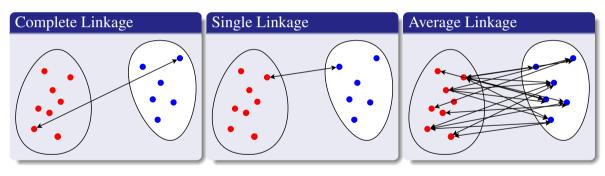
For Single Linkage: $D(X, Y) = \min_{x \in X, y \in Y} d(x, y)$.

For Average Linkage: $D(X,Y) = \frac{1}{|X||Y|} \sum_{x \in X, y \in Y} d(x,y)$. This is also known as Unweighted Pair Group Method with Arithmetic Mean (UPGMA) linkage.

For Ward linkage: the initial (single-point) cluster distances are simply the Euclidean distances between the points. The clusters are merged based on a minimum variance criterion. The distance between any point and a merged cluster is calculated using a recursive formula of Lance-Williams type (MurtaghLegendre2014).

Generally, Complete Linkage and Ward's minimum variance linkage give the most balanced and useful clusters.

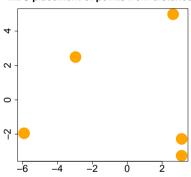
Distance between clusters: linkage visualisation



AGNES worked example: setting the scene

Distance	Mat	rix, S	Step	0			
		A	В	С	D	Е	
	A	0					
	В	9	0				
	C	3	7	0			
	D	6	5	9	0		
	Е	11	10	2	8	0	
							_

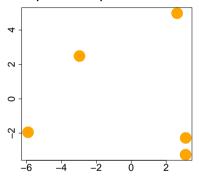
MDS placement of points from distances



AGNES worked example: setting the scene

Distance Matrix, Step 0 | A B C D E | | A | 0 | | B | 9 | 0 | | C | 3 | 7 | 0 | | D | 6 | 5 | 9 | 0 | | E | 11 | 10 | 2 | 8 | 0 |

MDS placement of points from distances



Use of distance matrices

Many algorithms in data mining either start from a distance matrix representation, or need to create it themselves. Reversing the process(from distances to locations) is not unique, but MultiDimensional Scaling often gives an attractive placement (as above, centred on origin).

AGNES worked example: Initial iterations

First clustering: CE, A, B, D

The smallest distance is 2 between C-E. We cluster these points and compute the distance of the remaining points from the CE cluster. Because of single linkage, we store the minimum such distance in the revised table beside.

Distance Matrix, Step 1

	CE	A	В	D
CE	0			
A B	3	0		
В	7	9	0	
D	8	6	5	0

AGNES worked example: Initial iterations

First clustering: CE, A, B, D

The smallest distance is 2 between C-E. We cluster these points and compute the distance of the remaining points from the CE cluster. Because of single linkage, we store the minimum such distance in the revised table beside.

Distance Matrix, Step 1

	CE	A	В	D
CE	0			
A B	3	0		
В	7	9	0	
D	8	6	5	0

Second clustering: ACE, B, D

The smallest distance is 3 between A and CE. We cluster these points and compute the distance of the remaining points from the ACE cluster. For example d(B,A) = 9, d(B,C) = 7, d(B,E) = 10, so by single linkage d(B,ACE) = 7 as in the revised table beside.

Distance Matrix, Step 2

		ACE	В	D
	ACE	0		
	В	7	0	
	D	6	5	0
Mi	nimum	distances	so	far: 2,3

AGNES worked example: Final iterations

Third clustering: CE, A, B, D

The smallest distance is 5, between B and D, so we create a BD cluster. The new distance matrix is shown alongside. The next step after this would be to merge ACE with BD, creating a single ABCDE cluster. The algorithm ends...

Distance Matrix, Step 3

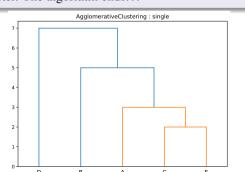
	ACE	BD
ACE	0	
BD	6	0

Minimum distances so far: 2,3,5,(6)

AGNES worked example: Final iterations

Third clustering: CE, A, B, D

The smallest distance is 5, between B and D, so we create a BD cluster. The new distance matrix is shown alongside. The next step after this would be to merge ACE with BD, creating a single ABCDE cluster. The algorithm ends...



Distance Matrix, Step 3

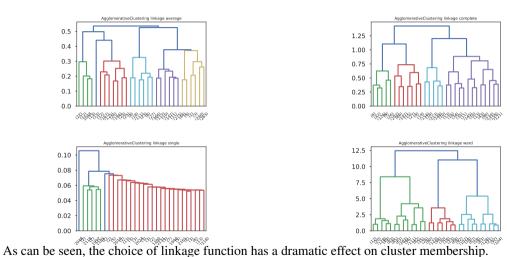
	ACE	BD
ACE	0	
BD	6	0

Minimum distances so far: 2,3,5,(6)

Resulting Dendrogram

The resulting dendrogram summarises the hierarchical clustering. Note that the joins/splits occur at distances 2, 3, 5 and 6, as noted above.

Comparison of Dendrograms



The underlying data in this instance appeared to have 6 clusters. Can you see this in these dendrograms?

• Hierarchical clustering can be very helpful for looking at data at a variety of scales, and hence for seeing hierarchical structure in a data set. This can lead to insights that other techniques, which focus on finding a single cluster mapping, cannot offer.

- Hierarchical clustering can be very helpful for looking at data at a variety of scales, and hence for seeing hierarchical structure in a data set. This can lead to insights that other techniques, which focus on finding a single cluster mapping, cannot offer.
- Hierarchical clustering offers a rich variety of objective functions (primarily relating to linkage), some of which might suit a specific scenario.

- Hierarchical clustering can be very helpful for looking at data at a variety of scales, and hence for seeing hierarchical structure in a data set. This can lead to insights that other techniques, which focus on finding a single cluster mapping, cannot offer.
- Hierarchical clustering offers a rich variety of objective functions (primarily relating to linkage), some of which might suit a specific scenario.
- It can be used as a means of estimating parameters for other, perhaps more focused techniques, e.g., to estimate the number of clusters/components in the data.

- Hierarchical clustering can be very helpful for looking at data at a variety of scales, and hence for seeing hierarchical structure in a data set. This can lead to insights that other techniques, which focus on finding a single cluster mapping, cannot offer.
- Hierarchical clustering offers a rich variety of objective functions (primarily relating to linkage), some of which might suit a specific scenario.
- It can be used as a means of estimating parameters for other, perhaps more focused techniques, e.g., to estimate the number of clusters/components in the data.
- Since hierarchical clustering provides more than one candidate clustering, it can be require more system resources (computation and memory) than other techniques. Thus it might not scale very well.

- Hierarchical clustering can be very helpful for looking at data at a variety of scales, and hence for seeing hierarchical structure in a data set. This can lead to insights that other techniques, which focus on finding a single cluster mapping, cannot offer.
- Hierarchical clustering offers a rich variety of objective functions (primarily relating to linkage), some of which might suit a specific scenario.
- It can be used as a means of estimating parameters for other, perhaps more focused techniques, e.g., to estimate the number of clusters/components in the data.
- Since hierarchical clustering provides more than one candidate clustering, it can be require more system resources (computation and memory) than other techniques. Thus it might not scale very well.
- We have seen agglomerative (bottom-up) clustering. Divisive (top-down) clustering (DIANA) is also available, but has worse scalability.

Outline

1. Introduction	4
2. Distance Measures	9
3. Hierarchical Clustering	14
4. Partioning Algorithms 4.1. K-means	25 28
4.2. Soft clustering	34
4.3. Expectation Maximisation (EM) iterations	37
4.4. Density-based clustering	39
4.5. Choosing <i>k</i> for centre-based clusters	44

• Often the purpose of clustering is to assign one or more labels to each observation, so that "similar" observations are given the same cluster membership label.

- Often the purpose of clustering is to assign one or more labels to each observation, so that "similar" observations are given the same cluster membership label.
- In the standard case, each observation is assigned a single label, and clustering defines a (hard) *partitioning* of the data. Lloyd's *k-means* algorithm does this.

- Often the purpose of clustering is to assign one or more labels to each observation, so that "similar" observations are given the same cluster membership label.
- In the standard case, each observation is assigned a single label, and clustering defines a (hard) *partitioning* of the data. Lloyd's *k-means* algorithm does this.
- If each observation is assigned a membership probability for each cluster, this is a *soft partitioning* of the data. A hard partition can be derived by choosing, for each observation, the cluster for which it has the highest probability of membership. *Gaussian Mixture* models can be used for this purpose.

- Often the purpose of clustering is to assign one or more labels to each observation, so that "similar" observations are given the same cluster membership label.
- In the standard case, each observation is assigned a single label, and clustering defines a (hard) *partitioning* of the data. Lloyd's *k-means* algorithm does this.
- If each observation is assigned a membership probability for each cluster, this is a *soft partitioning* of the data. A hard partition can be derived by choosing, for each observation, the cluster for which it has the highest probability of membership. *Gaussian Mixture* models can be used for this purpose.
- Some clustering algorithms, notably *density-based clustering*, do not always assign a label to each observation. However, if an observation is assigned a label, it will be just one such label.

- Often the purpose of clustering is to assign one or more labels to each observation, so that "similar" observations are given the same cluster membership label.
- In the standard case, each observation is assigned a single label, and clustering defines a (hard) *partitioning* of the data. Lloyd's *k-means* algorithm does this.
- If each observation is assigned a membership probability for each cluster, this is a *soft partitioning* of the data. A hard partition can be derived by choosing, for each observation, the cluster for which it has the highest probability of membership. *Gaussian Mixture* models can be used for this purpose.
- Some clustering algorithms, notably *density-based clustering*, do not always assign a label to each observation. However, if an observation is assigned a label, it will be just one such label.

Definition 11 (Representation-based clustering)

... finds a region around a *cluster centre* so that observations can be assigned to the cluster if they are found in that region.

- Often the purpose of clustering is to assign one or more labels to each observation, so that "similar" observations are given the same cluster membership label.
- In the standard case, each observation is assigned a single label, and clustering defines a (hard) partitioning of the data. Lloyd's *k-means* algorithm does this.
- If each observation is assigned a membership probability for each cluster, this is a *soft partitioning* of the data. A hard partition can be derived by choosing, for each observation, the cluster for which it has the highest probability of membership. *Gaussian Mixture* models can be used for this purpose.
- Some clustering algorithms, notably *density-based clustering*, do not always assign a label to each observation. However, if an observation is assigned a label, it will be just one such label.

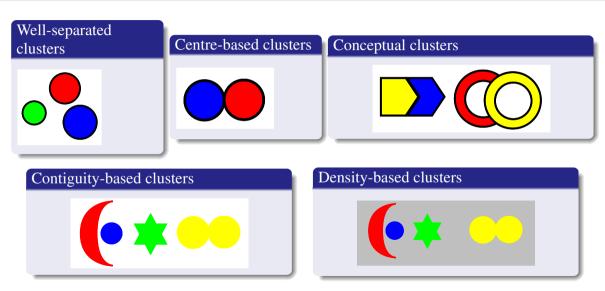
Definition 11 (Representation-based clustering)

... finds a region around a *cluster centre* so that observations can be assigned to the cluster if they are found in that region.

Definition 12 (Density-based clustering)

... looks for regions, possibly non-convex, where the data density is higher, and assigns observations in those regions to the relevant cluster. Any other observations are assumed to be either "noise" or "border" observations.

Types of partitional clustering



• The k-means algorithm assigns each observation to one of k clusters, by finding the nearest cluster centre for that observation (E-step).

- The k-means algorithm assigns each observation to one of k clusters, by finding the nearest cluster centre for that observation (E-step).
- Each cluster centre is calculated as the centroid of the observations assigned to that cluster (M-step).

- The k-means algorithm assigns each observation to one of k clusters, by finding the nearest cluster centre for that observation (E-step).
- Each cluster centre is calculated as the centroid of the observations assigned to that cluster (M-step).
- The algorithms proceeds in two steps (E-M). At each iteration, the algorithm finds the nearest centre for each observation, then assigns it to that centre and recomputes the centres.

- The k—means algorithm assigns each observation to one of k clusters, by finding the nearest cluster centre for that observation (E-step).
- Each cluster centre is calculated as the centroid of the observations assigned to that cluster (M-step).
- The algorithms proceeds in two steps (E-M). At each iteration, the algorithm finds the nearest centre for each observation, then assigns it to that centre and recomputes the centres.
- Lloyd's algorithm is an example EM-algorithm: Expectation-Maximisation (general algorithm, used in many scenarios, especially clustering).

- The *k*—means algorithm assigns each observation to one of *k* clusters, by finding the nearest cluster centre for that observation (E-step).
- Each cluster centre is calculated as the centroid of the observations assigned to that cluster (M-step).
- The algorithms proceeds in two steps (E-M). At each iteration, the algorithm finds the nearest centre for each observation, then assigns it to that centre and recomputes the centres.
- Lloyd's algorithm is an example EM-algorithm: Expectation-Maximisation (general algorithm, used in many scenarios, especially clustering).
- Variants include

- The *k*—means algorithm assigns each observation to one of *k* clusters, by finding the nearest cluster centre for that observation (E-step).
- Each cluster centre is calculated as the centroid of the observations assigned to that cluster (M-step).
- The algorithms proceeds in two steps (E-M). At each iteration, the algorithm finds the nearest centre for each observation, then assigns it to that centre and recomputes the centres.
- Lloyd's algorithm is an example EM-algorithm: Expectation-Maximisation (general algorithm, used in many scenarios, especially clustering).
- Variants include

Mini-batch k-means: work with a random sample of the data at each iteration: scales better, small loss of accuracy

- The k-means algorithm assigns each observation to one of k clusters, by finding the nearest cluster centre for that observation (E-step).
- Each cluster centre is calculated as the centroid of the observations assigned to that cluster (M-step).
- The algorithms proceeds in two steps (E-M). At each iteration, the algorithm finds the nearest centre for each observation, then assigns it to that centre and recomputes the centres.
- Lloyd's algorithm is an example EM-algorithm: Expectation-Maximisation (general algorithm, used in many scenarios, especially clustering).
- Variants include
 - Mini-batch k-means: work with a random sample of the data at each iteration: scales better, small loss of accuracy

kmeans++ : Choose initial centres that are well-separated from each other; "normal" k-means afterwards.

- The *k*—means algorithm assigns each observation to one of *k* clusters, by finding the nearest cluster centre for that observation (E-step).
- Each cluster centre is calculated as the centroid of the observations assigned to that cluster (M-step).
- The algorithms proceeds in two steps (E-M). At each iteration, the algorithm finds the nearest centre for each observation, then assigns it to that centre and recomputes the centres.
- Lloyd's algorithm is an example EM-algorithm: Expectation-Maximisation (general algorithm, used in many scenarios, especially clustering).
- Variants include
 - Mini-batch k-means: work with a random sample of the data at each iteration: scales better, small loss of accuracy
 - kmeans++ : Choose initial centres that are well-separated from each other; "normal" k-means afterwards.
 - k-medoids: Manhattan (ℓ_1) distance is used instead of Euclidean (ℓ_2), and centres are constrained to be data points); PAM and CLARA algorithms.

- The k-means algorithm assigns each observation to one of k clusters, by finding the nearest cluster centre for that observation (E-step).
- Each cluster centre is calculated as the centroid of the observations assigned to that cluster (M-step).
- The algorithms proceeds in two steps (E-M). At each iteration, the algorithm finds the nearest centre for each observation, then assigns it to that centre and recomputes the centres.
- Lloyd's algorithm is an example EM-algorithm: Expectation-Maximisation (general algorithm, used in many scenarios, especially clustering).
- Variants include
 - Mini-batch k-means: work with a random sample of the data at each iteration: scales better, small loss of accuracy
 - kmeans++ : Choose initial centres that are well-separated from each other; "normal" k-means afterwards.
 - k-medoids: Manhattan (ℓ_1) distance is used instead of Euclidean (ℓ_2) , and centres are constrained to be data points); PAM and CLARA algorithms.
- Generally Lloyd's algorithm is robust, although it is affected by the choice of initial centres, and care must be taken to avoid empty clusters

K-means algorithm: Detail

Method (k-means algorithm)

```
t \leftarrow 0;
Initialise centres \{\mu_j^t, j=1,\ldots,k\}: choose k points randomly, without replacement;
repeat
     t \leftarrow t + 1:
      C_i \leftarrow \emptyset, \forall j = 1, \ldots, k;
                                                                                                                           for all x do
                                                                      \triangleright Assign x_i to the nearest centroid from the previous iteration
           j^* \leftarrow \operatorname{arg\ min}_i \left\{ \| \boldsymbol{x}_j - \boldsymbol{\mu}_i^{t-1} \|^2 \right\};
            C_{i^*} \leftarrow C_{i^*} \cup \{\hat{\boldsymbol{x}}_i\};
      end for
                                                                                                                               ▷ Centroid Update Step M
      for all i = 1 to k do
           \mu_i^t \leftarrow \frac{1}{|C_i|} \sum_{x_i \in C_i} x_j;
      end for
end for until \sum_{i=1}^{k} \|\boldsymbol{\mu}_i^t - \boldsymbol{\mu}_i^{t-1}\|^2 \leq \epsilon
```

The termination condition is that the difference in centre positions should not exceed a small tolerance ϵ . This happens when points stay in their cluster from iteration p to p+1, so cluster centre stays same.

Clustering categorical data

• k-means uses centroids and Euclidean distance

Clustering categorical data

- k-means uses centroids and Euclidean distance
- So it cannot be applied directly to categorical data...

Clustering categorical data

- k-means uses centroids and Euclidean distance
- So it cannot be applied directly to categorical data...
- Options

- k-means uses centroids and Euclidean distance
- So it cannot be applied directly to categorical data...
- Options
 - Either encode categorical columns as integers can now compute distances

- k-means uses centroids and Euclidean distance
- So it cannot be applied directly to categorical data...
- Options
 - Either encode categorical columns as integers can now compute distances
 - Since this can dramatically increase the dimensionality, some dimensionality reduction might be needed

- k-means uses centroids and Euclidean distance
- So it cannot be applied directly to categorical data...
- Options
 - Either encode categorical columns as integers can now compute distances
 - Since this can dramatically increase the dimensionality, some dimensionality reduction might be needed
 - Or Use k-modes on the original data if *all* the data is categorical

- k-means uses centroids and Euclidean distance
- So it cannot be applied directly to categorical data...
- Options
 - Either encode categorical columns as integers can now compute distances
 - Since this can dramatically increase the dimensionality, some dimensionality reduction might be needed
 - Or Use k-modes on the original data if all the data is categorical
 - Or Use k-prototypes on the original data if some data is categorical and some is numerical

"K-means" for categorical data: k-modes

k-means uses centroids and Euclidean distance; k-modes uses modes and Hamming distance

Strengths and weaknesses: mostly similar to k-means

• Guaranteed to converge (eventually): helped by good choice of k and initial modes

"K-means" for categorical data: k-modes

k-means uses centroids and Euclidean distance; k-modes uses modes and Hamming distance

Strengths and weaknesses: mostly similar to k-means

- Guaranteed to converge (eventually): helped by good choice of k and initial modes
- Iterates to a local minimum: result quality depends on initial modes

"K-means" for categorical data: k-modes

k-means uses centroids and Euclidean distance; k-modes uses modes and Hamming distance

Strengths and weaknesses: mostly similar to k-means

- Guaranteed to converge (eventually): helped by good choice of k and initial modes
- Iterates to a local minimum: result quality depends on initial modes
- Distances are integers: need to choose between tied distances when assigning cases to clusters

k-means uses centroids and Euclidean distance; k-modes uses modes and Hamming distance

Strengths and weaknesses: mostly similar to k-means

- Guaranteed to converge (eventually): helped by good choice of k and initial modes
- Iterates to a local minimum: result quality depends on initial modes
- Distances are integers: need to choose between tied distances when assigning cases to clusters

Implementation

```
Installation: conda install -c conda-forge kmodes
 from kmodes.kmodes import KModes
 import pandas as pd
 import numpy as np
 model=KModes(n_clusters=3.random_state=42.n_init=4)
```

```
fittedModel=model.fit(df)
print("Cluster centroids - archetypal student grades")
print(fittedModel.cluster_centroids_)
```

clusters = fittedModel.predict(df) df["ClusterID"] = clusters print("Allocation of students to clu display(df)

Combine k-means (on numerical data) and k-modes (on categorical data) in one clustering algorithm.

Intuition

• A prototype instance has representative values of numerical and categorical features.

Combine k-means (on numerical data) and k-modes (on categorical data) in one clustering algorithm.

Intuition

- A prototype instance has representative values of numerical and categorical features.
- Distance is a linear combination of the Euclidean (numerical) and Hamming (categorical) distances

Combine k-means (on numerical data) and k-modes (on categorical data) in one clustering algorithm.

Intuition

- A prototype instance has representative values of numerical and categorical features.
- Distance is a linear combination of the Euclidean (numerical) and Hamming (categorical) distances
- With this interpretation, the algorithm is much the same as k-means or k-modes, with similar strengths and weaknesses

Combine k-means (on numerical data) and k-modes (on categorical data) in one clustering algorithm.

Intuition

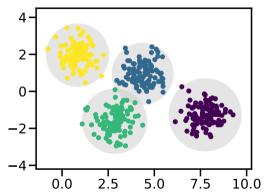
- A prototype instance has representative values of numerical and categorical features.
- Distance is a linear combination of the Euclidean (numerical) and Hamming (categorical) distances
- With this interpretation, the algorithm is much the same as k-means or k-modes, with similar strengths and weaknesses

Implementation

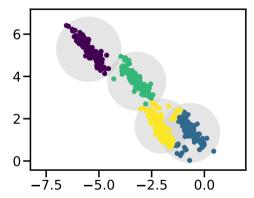
```
kRange = range(1.8)
allCols = numCols + allCatCols
catColIDs = list(range(len(numCols).len(numCols)+len(allCatCols)))
scores = dict()
for k in kRange:
  # Use Huang initialisation, use 5 random starting starting points, turn off logging
 model = KPrototypes(n_clusters=k, init='Huang', verbose=0, random_state=42, n_init=5)
  # Note that we need to tell the model which are the categorical columns
 fittedModel = model.fit(df[allCols], categorical=catColIDs)
  scores[k] = fittedModel.cost_
```

32 of 53

K-means algorithm: In practice



With the original globular clusters, *k*-means was able to find the centres and clusters easily.



With the stretched clusters, k-means had more difficulty, e.g., with the yellow and purple clusters.

k-means minimises the within-cluster sum of squared distances (also known as inertia) so the choice of distance function is critical.

• k-means is an example of hard clustering, where each data point is mapped to a single cluster

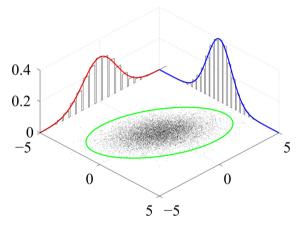
- k-means is an example of hard clustering, where each data point is mapped to a single cluster
- As such it is best suited to well-separated clusters but what if they are close or even overlap?

- k-means is an example of hard clustering, where each data point is mapped to a single cluster
- As such it is best suited to well-separated clusters but what if they are close or even overlap?
- fuzzy clustering: points are assigned to multiple clusters, and are given a membership score in [0,1] for each cluster

- k-means is an example of hard clustering, where each data point is mapped to a single cluster
- As such it is best suited to well-separated clusters but what if they are close or even overlap?
- fuzzy clustering: points are assigned to multiple clusters, and are given a membership score in [0,1] for each cluster
- fuzzy c-means algorithm is a straightforward extension of k-means, just using probability $P(x_i, \mu_i)$ to weight each point x_i when calculating the centroid of each cluster μ_i (M-step)

- k-means is an example of hard clustering, where each data point is mapped to a single cluster
- As such it is best suited to well-separated clusters but what if they are close or even overlap?
- fuzzy clustering: points are assigned to multiple clusters, and are given a membership score in [0,1] for each cluster
- fuzzy c-means algorithm is a straightforward extension of k-means, just using probability $P(x_i, \mu_j)$ to weight each point x_i when calculating the centroid of each cluster μ_i (M-step)
- P is a function of the relative Euclidean distances to the cluster centres $\{\mu_i\}$

- k-means is an example of hard clustering, where each data point is mapped to a single cluster
- As such it is best suited to well-separated clusters but what if they are close or even overlap?
- fuzzy clustering: points are assigned to multiple clusters, and are given a membership score in [0,1] for each cluster
- fuzzy c-means algorithm is a straightforward extension of k-means, just using probability $P(x_i, \mu_j)$ to weight each point x_i when calculating the centroid of each cluster μ_j (M-step)
- P is a function of the relative Euclidean distances to the cluster centres $\{\mu_i\}$
- This probability function can be generalised, notably to take account of the *shape* of the clusters and not just their centres, leading to *Gaussian Mixture Model* (GMM) probabilistic clustering



- The distribution can have different dimensions that do not need to align with the coordinate axes; captured as a 2x2 covariance matrix C
- The distribution stretches to infinity in the plane, but points far from the centre of the distribution have very low probability.
- A collection of clusters can be modelled by overlaying a *mixture* of such Gaussian distributions on the plane.

Review of Bayes Theorem

Use of Bayes Theorem in Classification

Likelihood is the probability of the data given the label. **Prior** measures our belief about how likely each label is *before* we have seen any data. The **Posterior** includes influences of both the Prior and the Likelihood.

$$P(y = c|x) = \frac{P(x|y = c)P(y = c)}{P(x)}$$

The Posterior here is P(y = c|x), the Likelihood is P(x|y = c) and the Prior is P(y = c). P(x) is a normalizing constant that measures how likely the observed data x is.

Use of Bayes Theorem in Classification

Likelihood is the probability of the data given the label. **Prior** measures our belief about how likely each label is *before* we have seen any data. The **Posterior** includes influences of both the Prior and the Likelihood.

$$P(y = c|x) = \frac{P(x|y = c)P(y = c)}{P(x)}$$

The Posterior here is P(y = c|x), the Likelihood is P(x|y = c) and the Prior is P(y = c). P(x) is a normalizing constant that measures how likely the observed data x is.

When used for Gaussian Mixture Models, there is not just a *single* cluster label c, but a linear combination of many.

Overview of EM algorithm for GMM clustering

E-step For each x_i , calculate the probability that x_i belongs to the j^{th} distribution

$$P(\Theta_j|x_i,\Theta) = \frac{P(x_i|\Theta_j)}{\sum_{l=1}^k P(x_i|\Theta_l)},$$

where Θ_j is the set of parameters defining Gaussian distribution j, namely its centre μ_j and covariance matrix C_j .

Note that the E-step computes a membership probability for each point based on all the Gaussian models and their parameters.

Overview of EM algorithm for GMM clustering

E-step For each x_i , calculate the probability that x_i belongs to the j^{th} distribution

$$P(\Theta_j|x_i,\Theta) = \frac{P(x_i|\Theta_j)}{\sum_{l=1}^k P(x_i|\Theta_l)},$$

where Θ_j is the set of parameters defining Gaussian distribution j, namely its centre μ_j and covariance matrix C_i .

M-step Maximise the expected likelihood $P(\{x_i\}|\Theta)$ by updating the Gaussian mixture. That is, for each μ_j and C_j , use all x_i and the $P(\Theta_j|x_i,\Theta)$ computed in the E-step) to derive the new Gaussian distribution parameters.

Note that the E-step computes a membership probability for each point based on all the Gaussian models and their parameters.

By contrast, the M-step computes the new Gaussian models based on all the points and their membership probabilities.

Overview of EM algorithm for GMM clustering

E-step For each x_i , calculate the probability that x_i belongs to the j^{th} distribution

$$P(\Theta_j|x_i,\Theta) = \frac{P(x_i|\Theta_j)}{\sum_{l=1}^k P(x_i|\Theta_l)},$$

where Θ_j is the set of parameters defining Gaussian distribution j, namely its centre μ_j and covariance matrix C_j .

M-step Maximise the expected likelihood $P(\{x_i\}|\Theta)$ by updating the Gaussian mixture. That is, for each μ_j and C_j , use all x_i and the $P(\Theta_j|x_i,\Theta)$ computed in the E-step) to derive the new Gaussian distribution parameters.

Note that the E-step computes a membership probability for each point based on all the Gaussian models and their parameters.

By contrast, the M-step computes the new Gaussian models based on all the points and their membership probabilities.

Lloyd's k-means algorithm is equivalent: the membership probability is either 1 (allocated to this cluster) or 0 (not allocated to this cluster) for each point. The M-step re-computes the cluster centres based on all the points and their cluster assignment.

GMM compared with k-means

	k-means	GMM
E-step	Compute membership probability which is either 1 (allocated to this cluster) or 0 (not allocated to this cluster) for each point	Compute membership probability for each point based on all the Gaussian models and their parameters.

GMM compared with k-means

	k-means	GMM
E-step	Compute membership probability which is either 1 (allocated to this cluster) or 0 (not allocated to this cluster) for each point	Compute membership probability for each point based on all the Gaussian models and their parameters.
M-step	Recompute the new cluster centres based on all the points and their cluster assignment	Recompute the new Gaussian models based on all the points and their membership probabilities

GMM compared with k-means

	k-means	GMM
E-step	Compute membership probability which is either 1 (allocated to this cluster) or 0 (not allocated to this cluster) for each point	Compute membership probability for each point based on all the Gaussian models and their parameters.
M-step	Recompute the new cluster centres based on all the points and their cluster assignment	Recompute the new Gaussian models based on all the points and their membership probabilities
Use for	Well-separated	Centre-based or well-separated

	k-means	GMM
E-step	Compute membership probability which is either 1 (allocated to this cluster) or 0 (not allocated to this cluster) for each point	Compute membership probability for each point based on all the Gaussian models and their parameters.
M-step	Recompute the new cluster centres based on all the points and their cluster assign- ment	Recompute the new Gaussian models based on all the points and their membership probabilities
Use for	Well-separated	Centre-based or well-separated
Shape	nondirectional ("spherical")	directional ("ellipsoidal") or nondirectional

k-means and GMM are both characterised by the following properties:

- the number of clusters k must be specified beforehand
- clusters have a convex shape
- they work best when the clusters are linearly separable
- all points are assigned to clusters, so can be sensitive to outliers

k-means and GMM are both characterised by the following properties:

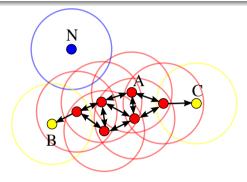
- the number of clusters k must be specified beforehand
- clusters have a convex shape
- they work best when the clusters are linearly separable
- all points are assigned to clusters, so can be sensitive to outliers

Density-based clustering relaxes these conditions

It uses the heuristic that clusters are (arbitrarily-shaped) contiguous regions with high datapoint density.

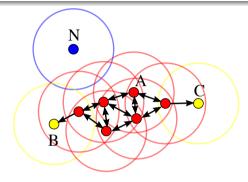
Datapoints outside these regions represent *noise* and are ignored.

Rather than specifying k, the user specifies density thresholds.

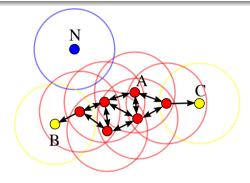


Source: wikipedia

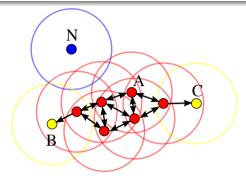
• A, B and C are directly connected points.



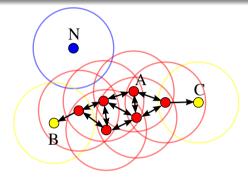
- A, B and C are directly connected points.
- A is a core point



- A, B and C are directly connected points.
- A is a core point
- B and C are border points.



- A, B and C are directly connected points.
- A is a core point
- B and C are border points.
- N is a noise point and so is not assigned to a cluster.



- A, B and C are directly connected points.
- A is a core point
- B and C are border points.
- N is a noise point and so is not assigned to a cluster.
- The connected component of the 8 points (6 red, 2 yellow; including A,B,C) forms a cluster.

DBSCAN algorithm and its concepts

Definition 13 (DBSCAN)

Density-Based Spatial Clustering of Applications with Noise (DBSCAN): an algorithm for deriving clusters in areas of high data density.

Definition 14 (eps-neighbourhood)

Epsilon ϵ parameter defines a region of points t around a point x where $||t-x|| < \epsilon$.

Definition 15 (core point)

Point with at least MinPts-1 other points in its eps-neighbourhood.

Definition 16 (border point)

Point with less than MinPts-1 other points in its eps-neighbourhood, but at least one is a core point.

Definition 17 (noise point)

Point with less than MinPts-1 other non-core points in its eps-neighbourhood.

Development of the algorithm

Definition 18 (Direct density reachable)

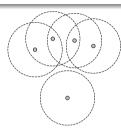
Point x_A is directly density reachable from x_B iff x_A is in the eps-neighborhood of x_B and x_B is a core point.

Definition 19 (Density reachable)

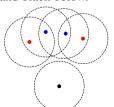
Point x_A is density reachable from x_B if there is a set of core points in each other's eps-neighbourhood between x_A and x_B .

Definition 20 (Density connected)

Points x_A and x_B are density connected if there exists a core point x_C so that both x_A and x_B are density reachable from x_C .



Core, border and noise points are coloured blue, red and black below.



Steps of the DBSCAN algorithm

Method (DBSCAN)

- Find the ϵ neighbors of every point.
- ② Identify the core points with more than minPts neighbors.
- **②** Derive the *connected component* graphs of core points, assigning edges between core points that are less than ϵ apart.
- Identify the border points and assign them to their nearest cluster.
- **1** Label any remaining points as *noise*.
- A variant (HDBCSAN) excludes border points from the cluster, treating them as noise points (can be more robust).
- Another vatiant (OPTICS) places the points in a priority queue, ordered by reachability distance (updating is slower, but handles varying density better).

How can we decide on k for k-means and GMM?

• We can do this *graphically* (plot clusters for each *k*) or by using *scores*.

How can we decide on k for k-means and GMM?

- We can do this *graphically* (plot clusters for each *k*) or by using *scores*.
- Plot within-cluster sum of squared distances (inertia) against k and look for k at the "elbow".

How can we decide on k for k-means and GMM?

- We can do this *graphically* (plot clusters for each *k*) or by using *scores*.
- Plot within-cluster sum of squared distances (inertia) against k and look for k at the "elbow".
- Use kmeans.inertia_ as the score for a given instance of the kmeans classifier.

How can we decide on k for k-means and GMM?

- We can do this *graphically* (plot clusters for each *k*) or by using *scores*.
- Plot within-cluster sum of squared distances (inertia) against k and look for k at the "elbow".
- Use kmeans.inertia_ as the score for a given instance of the kmeans classifier.
- Can also compute inertia for other partitional clustering techniques, but this is more work and interpretation is more difficult.

Silhouette scores - derivation

How much is any point in a cluster nearer its peers than it is to points in the nearest of the other clusters?

Method (Silhouette score)

Require: Clustering where the *i* point is assigned to cluster C(i) and there are *k* such clusters **for all** point *i* in cluster C(i) **do**

Calculate a(i), the mean distance between i and all the other points in C(i). $\triangleright a(i) \equiv 0$ is there is no other point in C(i).

Calculate b(i), minimum of the mean distances between i and all the other points in each of C(j) where $j \neq i$.

Silhouette
$$s(i) = 1 - a(i)/b(i)$$
 if $a(i) < b(i)$, $s(i) = 0$ if $a(i) = b(i)$ and $s(i) = b(i)/s(i) - 1$ if $a(i) > b(i)$.

end for

The mean of s(i) over all points (\bar{s}_k) is a measure of the clustering efficiency for that value of k.

The k associated with the maximum of these \bar{s}_k silhouette scores is the best choice of k.

There are many other scores but they require more advanced mathematics and are out of scope for this module.

Code to compute the silhouette score

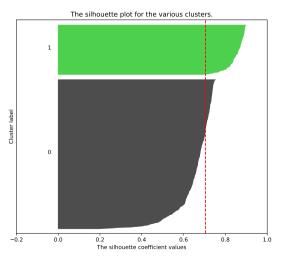
```
from sklearn.metrics import silhouette_samples, silhouette_score

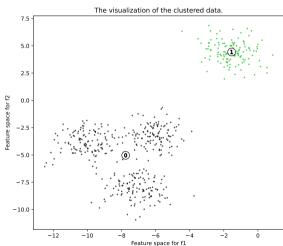
clusterer = KMeans(n_clusters=n_clusters, random_state=10)
cluster_labels = clusterer.fit_predict(X)

# The silhouette_score gives the average value for all the samples.
silhouette_avg = silhouette_score(X, cluster_labels)
```

Silhouette score with k = 2 - looking good

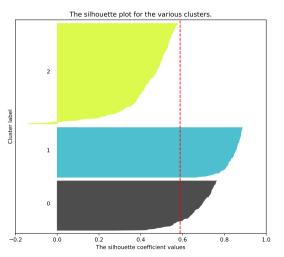
Silhouette analysis for KMeans clustering on sample data with n clusters = 2

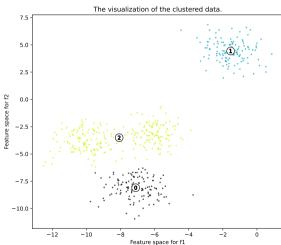




Silhouette score with k = 3 - not looking good

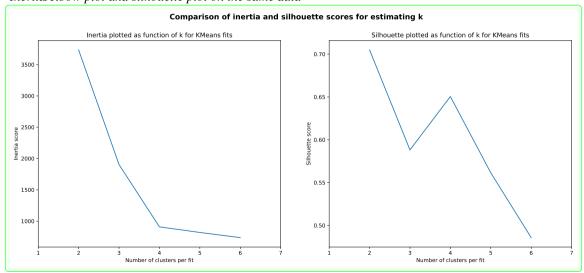
Silhouette analysis for KMeans clustering on sample data with n clusters = 3





Comparing both scoring systems

Inertia/elbow plot and silhouette plot on the same data



Outline

5. Review and resources

1. Introduction	4
2. Distance Measures	9
3. Hierarchical Clustering	14
4. Partioning Algorithms 4.1. K-means	25 28
4.2. Soft clustering	34
4.3. Expectation Maximisation (EM) iterations	37
4.4. Density-based clustering	39
4.5. Choosing <i>k</i> for centre-based clusters	44

50

AGNES: choose distance function and linkage. Usually Ward or single linkage work best.

AGNES: choose distance function and linkage. Usually Ward or single linkage work best.

k-means, etc. : choose distance function, starting condition (cf kmeans++), aggregation (cf k-medoids), k

AGNES: choose distance function and linkage. Usually Ward or single linkage work best.

k-means, etc. : choose distance function, starting condition (cf kmeans++), aggregation (cf k-medoids), k

GMM: choose distance function, k

AGNES: choose distance function and linkage. Usually Ward or single linkage work best.

k-means, etc. : choose distance function, starting condition (cf kmeans++), aggregation (cf k-medoids), k

GMM: choose distance function, k

DBSCAN: choose distance function, minpts, eps

AGNES: choose distance function and linkage. Usually Ward or single linkage work best.

k-means, etc. : choose distance function, starting condition (cf kmeans++), aggregation (cf k-medoids), k

GMM: choose distance function, k

DBSCAN: choose distance function, minpts, eps

Tips

• Good idea to scale so that clusters are approximately (hyper)spherical.

AGNES: choose distance function and linkage. Usually Ward or single linkage work best.

k-means, etc. : choose distance function, starting condition (cf kmeans++), aggregation (cf k-medoids), k

GMM: choose distance function, k

DBSCAN: choose distance function, minpts, eps

Tips

- Good idea to scale so that clusters are approximately (hyper)spherical.
- Can be good idea to transform data before clustering.

AGNES: choose distance function and linkage. Usually Ward or single linkage work best.

k-means, etc. : choose distance function, starting condition (cf kmeans++), aggregation (cf k-medoids), k

GMM: choose distance function, k

DBSCAN: choose distance function, minpts, eps

Tips

- Good idea to scale so that clusters are approximately (hyper)spherical.
- Can be good idea to transform data before clustering.
- Dendrogram is good for visualising structure when data is more than 3-D.

• Clustering is perhaps the best known form of unsupervised learning

- Clustering is perhaps the best known form of unsupervised learning
- Hierarchical clustering can provide insights into the structure of a data set very useful when exploring data for other techniques

- Clustering is perhaps the best known form of unsupervised learning
- Hierarchical clustering can provide insights into the structure of a data set very useful when exploring data for other techniques
- Partitional clustering can be used to label points according to which cluster they belong to

- Clustering is perhaps the best known form of unsupervised learning
- Hierarchical clustering can provide insights into the structure of a data set very useful when exploring data for other techniques
- Partitional clustering can be used to label points according to which cluster they belong to
- Partitional classification has many approaches: centre-based and density based are most common

- Clustering is perhaps the best known form of unsupervised learning
- Hierarchical clustering can provide insights into the structure of a data set very useful when exploring data for other techniques
- Partitional clustering can be used to label points according to which cluster they belong to
- Partitional classification has many approaches: centre-based and density based are most common
- Clustering can be used to help create training data for classification purposes (c.f., the digits notebook used in the practical)