MADS-MMS – Mathematics and Multivariate Statistics

k Clustering

Prof. Dr. Stephan Doerfel

FACHHOCHSCHULE KIEL
University of Applied Sciences

SCAN ME

Moodle (SoSe 2025)

Agenda

Outline

Why k-Clustering?

- We have a fix number of groups that we want to split our data into.

Why k-Clustering?

- We have a fix number of groups that we want to split our data into.
- We have an intuition about the number of groups we want to split our data into.

Why k-Clustering?

- We have a fix number of groups that we want to split our data into.
- We have an intuition about the number of groups we want to split our data into.
- There are ways to determine "good" k, if we have none of the above.

Why k-Clustering?

- We have a fix number of groups that we want to split our data into.
- We have an intuition about the number of groups we want to split our data into.
- There are ways to determine "good" k, if we have none of the above.
- k clustering has simple algorithms, easy to implement and understand.

Chapter Goals

- understand the basic mechanics of well-known partitioning clustering algorithms (k-means and k-medoid)

Chapter Goals

- understand the basic mechanics of well-known partitioning clustering algorithms (k-means and k-medoid)
- understand the influence of the parameter k and methods for choosing it

Chapter Goals

- understand the basic mechanics of well-known partitioning clustering algorithms (k-means and k-medoid)
- understand the influence of the parameter k and methods for choosing it
- understand the influence of the initial clustering and approaches for mitigating it

Outline

Basics

Task: Partition a dataset into k disjoint subsets.

Basics

Task: Partition a dataset into k disjoint subsets.

Definition 1 (Partition)

For a set D, $\mathcal{C} \subseteq 2^D$ is a partition (a clustering) if the following holds:

Basics

Task: Partition a dataset into k disjoint subsets.

Definition 1 (Partition)

For a set D, $\mathcal{C} \subseteq 2^D$ is a partition (a clustering) if the following holds:

- $\emptyset \notin \mathcal{C}$ (no cluster is empty)

Basics

Task: Partition a dataset into k disjoint subsets.

Definition 1 (Partition)

For a set D, $\mathcal{C} \subseteq 2^D$ is a partition (a clustering) if the following holds:

- $\emptyset \notin \mathcal{C}$ (no cluster is empty)
- $\bigcup_{A \in \mathcal{C}} A = D$ (each instance belongs to one cluster)

Basics

Task: Partition a dataset into k disjoint subsets.

Definition 1 (Partition)

For a set D, $\mathcal{C} \subseteq 2^D$ is a partition (a clustering) if the following holds:

- $\emptyset \notin \mathcal{C}$ (no cluster is empty)
- $\bigcup_{A \in \mathcal{C}} A = D$ (each instance belongs to one cluster)
- $\forall A, B \in \mathcal{C} : A \neq B \Rightarrow A \cap B = \emptyset$ (no overlap)

Basics

Task: Partition a dataset into k disjoint subsets.

Definition 1 (Partition)

For a set D, $\mathcal{C} \subseteq 2^D$ is a partition (a clustering) if the following holds:

- $\emptyset \notin \mathcal{C}$ (no cluster is empty)
- $\bigcup_{A \in \mathcal{C}} A = D$ (each instance belongs to one cluster)
- $\forall A, B \in \mathcal{C} : A \neq B \Rightarrow A \cap B = \emptyset$ (no overlap)

Definition 2

The set of all partitions of D is denoted by $\mathfrak{C}(D)$.
The set of all partitions of D of size k is denoted by $\mathfrak{C}_k(D)$.

Formal Definition

Definition 3 (Partitioning Clustering)

Let D be a set of data instances, $k \in \mathbb{N}$ and a cost function

$$\mathrm{cost}\colon \mathfrak{C}_k(D) \to \mathbb{R}_{\geq 0},\, \mathcal{C} \mapsto \mathrm{cost}(\mathcal{C}).$$

Find a clustering $\mathcal{C}^{\mathrm{opt}} \in \mathfrak{C}_k(D)$ that minimizes $\mathrm{cost}(\mathcal{C}^{\mathrm{opt}})$, i.e.

$$\mathcal{C}^{\mathrm{opt}} = \arg\min_{\mathcal{C} \in \mathfrak{C}_k(D)} \mathrm{cost}(\mathcal{C})$$

Formal Definition

Definition 3 (Partitioning Clustering)

Let D be a set of data instances, $k \in \mathbb{N}$ and a cost function

$$\text{cost}\colon \mathfrak{C}_k(D) \to \mathbb{R}_{\geq 0}, \mathcal{C} \mapsto \text{cost}(\mathcal{C}).$$

Find a clustering $\mathcal{C}^{\text{opt}} \in \mathfrak{C}_k(D)$ that minimizes $\text{cost}(\mathcal{C}^{\text{opt}})$, i.e.

$$\mathcal{C}^{\text{opt}} = \arg\min_{\mathcal{C} \in \mathfrak{C}_k(D)} \text{cost}(\mathcal{C})$$

Finding the optimal clustering $\mathcal{C}^{\text{opt}}$ for given D,k, and cost is NP-complete. Hence: Find good approximations.

Solution: Local Optimization

Goal:

Solution: Local Optimization

Goal:

- partitioning into k clusters with approximately minimal costs

Solution: Local Optimization

Goal:

- partitioning into k clusters with approximately minimal costs

Locally Optimizing Method:

Solution: Local Optimization

Goal:

- partitioning into k clusters with approximately minimal costs

Locally Optimizing Method:

- choose k initial cluster representations

Solution: Local Optimization

Goal:

- partitioning into k clusters with approximately minimal costs

Locally Optimizing Method:

- choose k initial cluster representations
- optimize these representatives iteratively (lowering the costs)

Solution: Local Optimization

Goal:

- partitioning into k clusters with approximately minimal costs

Locally Optimizing Method:

- choose k initial cluster representations
- optimize these representatives iteratively (lowering the costs)
- stop when some given criterion is reached

Solution: Local Optimization

Goal:

- partitioning into k clusters with approximately minimal costs

Locally Optimizing Method:

- choose k initial cluster representations
- optimize these representatives iteratively (lowering the costs)
- stop when some given criterion is reached

Types of Cluster Representatives:

Solution: Local Optimization

Goal:

- partitioning into k clusters with approximately minimal costs

Locally Optimizing Method:

- choose k initial cluster representations
- optimize these representatives iteratively (lowering the costs)
- stop when some given criterion is reached

Types of Cluster Representatives:

- mean of a cluster's instances (construction of central points)

Solution: Local Optimization

Goal:

- partitioning into k clusters with approximately minimal costs

Locally Optimizing Method:

- choose k initial cluster representations
- optimize these representatives iteratively (lowering the costs)
- stop when some given criterion is reached

Types of Cluster Representatives:

- mean of a cluster's instances (construction of central points)
- element of cluster (selection of representative data instances)

Solution: Local Optimization

Goal:

- partitioning into k clusters with approximately minimal costs

Locally Optimizing Method:

- choose k initial cluster representations
- optimize these representatives iteratively (lowering the costs)
- stop when some given criterion is reached

Types of Cluster Representatives:

- mean of a cluster's instances (construction of central points)
- element of cluster (selection of representative data instances)
- (cluster probability distribution (maximizing expectation) ⧗)

Outline

Agenda

Idea

Assumption

data is grouped around a fix number (k) of central points in the data space (not data set!) – each such point represents one cluster

Idea

Assumption

data is grouped around a fix number (k) of central points in the data space (not data set!) – each such point represents one cluster

Approach

Idea

Assumption

data is grouped around a fix number (k) of central points in the data space (not data set!) – each such point represents one cluster

Approach

- try to determine those k central points, called **centroids**

Idea

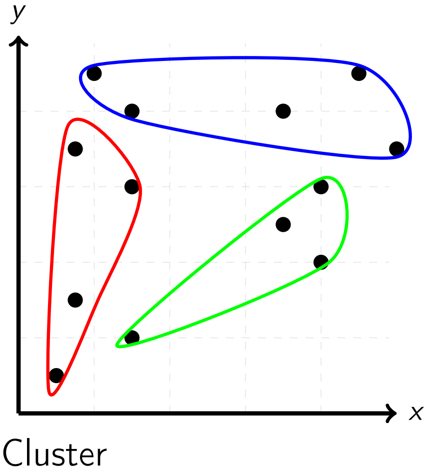
Assumption

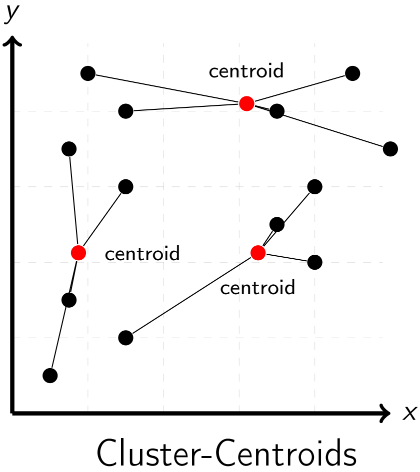
data is grouped around a fix number (k) of central points in the data space (not data set!) – each such point represents one cluster

Approach

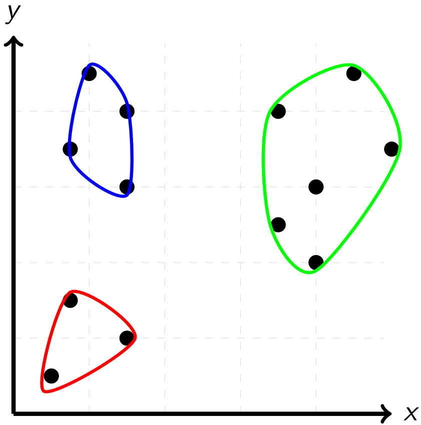
- try to determine those k central points, called **centroids**
- each data instance is assigned the closests of the central points

Examples, Bad/Good Clusterings, $k = 3$

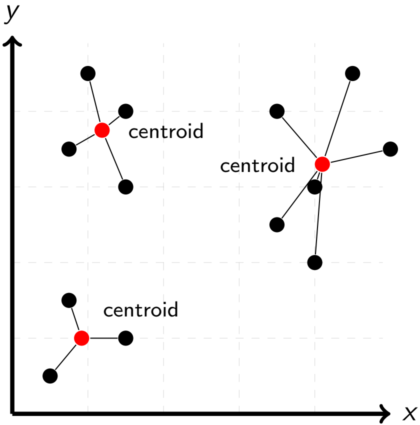




Examples, Bad/Good Clusterings, $k = 3$



Cluster



Cluster-Centroids

Construction of Central Points

Instances: vectors $p = (x_{p_1}, \ldots, x_{p_d})$ in a Euclidean vector space

Construction of Central Points

Instances: vectors $p = (x_{p_1}, \ldots, x_{p_d})$ in a Euclidean vector space

Distance: Euclidean distance

Construction of Central Points

Instances: vectors $p = (x_{p_1}, \ldots, x_{p_d})$ in a Euclidean vector space

Distance: Euclidean distance

Central Point: **Centroid** $\mu_C :=$ mean of the vectors in Cluster C

Construction of Central Points

Instances: vectors $p = (x_{p_1}, \ldots, x_{p_d})$ in a Euclidean vector space

Distance: Euclidean distance

Central Point: **Centroid** $\mu_C :=$ mean of the vectors in Cluster C

Cluster-Cost: measure for the (non-)compactness of a cluster C – **inertia**:

$$\text{cost}(C) = TD^2(C) := \sum_{p \in C} \text{dist}(p, \mu_C)^2$$

Construction of Central Points

Instances: vectors $p = (x_{p_1}, \ldots, x_{p_d})$ in a Euclidean vector space

Distance: Euclidean distance

Central Point: **Centroid** μ_C:= mean of the vectors in Cluster C

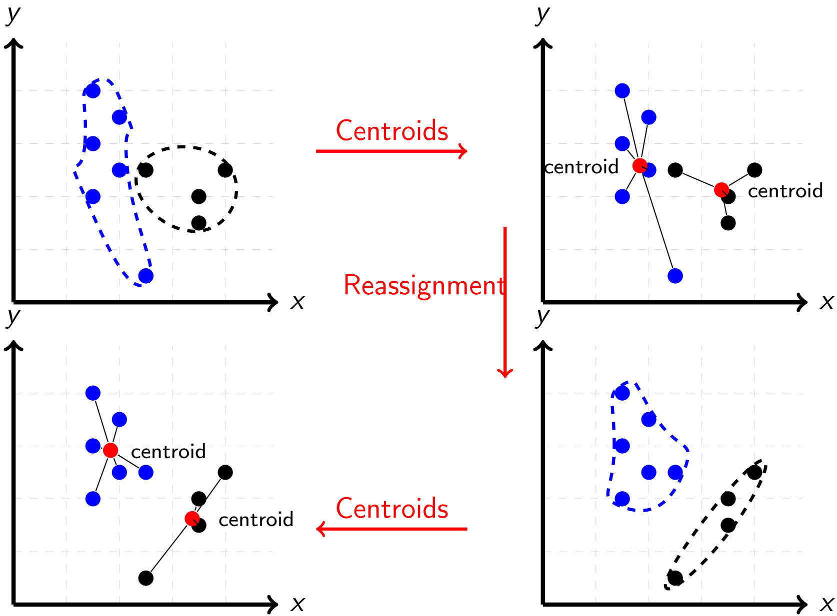
Cluster-Cost: measure for the (non-)compactness of a cluster C – **inertia**:

$$\mathrm{cost}(C) = TD^2(C) := \sum_{p \in C} \mathrm{dist}(p, \mu_C)^2$$

Clustering-Cost: measure for the (non-)compactness of a clustering $\mathcal{C}$:

$$\mathrm{cost}(\mathcal{C}) = TD^2(\mathcal{C}) := \sum_{C \in \mathcal{C}} TD^2(C)$$

Base-Algorithm



Base Algorithm – Variation Minimization

Initialization

Base Algorithm – Variation Minimization

Initialization

1. choose k data instances from the dataset as centroids

Base Algorithm – Variation Minimization

Initialization

1. choose k data instances from the dataset as centroids
2. assign each data instance to the closest centroid, thus create intial clustering $\mathcal{C}$

Base Algorithm – Variation Minimization

Initialization

1. choose k data instances from the dataset as centroids
2. assign each data instance to the closest centroid, thus create intial clustering $\mathcal{C}$
3. compute clustering inertia cost($\mathcal{C}$)

Base Algorithm – Variation Minimization

Initialization

1. choose k data instances from the dataset as centroids
2. assign each data instance to the closest centroid, thus create intial clustering $\mathcal{C}$
3. compute clustering inertia cost($\mathcal{C}$)

Iteration

Base Algorithm – Variation Minimization

Initialization

1. choose k data instances from the dataset as centroids
2. assign each data instance to the closest centroid, thus create intial clustering $\mathcal{C}$
3. compute clustering inertia cost($\mathcal{C}$)

Iteration

1. re-compute centroids for $\mathcal{C}$

Base Algorithm – Variation Minimization

Initialization

1. choose k data instances from the dataset as centroids
2. assign each data instance to the closest centroid, thus create intial clustering $\mathcal{C}$
3. compute clustering inertia cost($\mathcal{C}$)

Iteration

1. re-compute centroids for $\mathcal{C}$
2. assign each data instance to the closest centroid, thus create a new clustering $\mathcal{C}'$

Base Algorithm – Variation Minimization

Initialization

1. choose k data instances from the dataset as centroids
2. assign each data instance to the closest centroid, thus create intial clustering $\mathcal{C}$
3. compute clustering inertia $\text{cost}(\mathcal{C})$

Iteration

1. re-compute centroids for $\mathcal{C}$
2. assign each data instance to the closest centroid, thus create a new clustering $\mathcal{C}'$
3. compute clustering intertia $\text{cost}(\mathcal{C}')$

Base Algorithm – Variation Minimization

Initialization

1. choose k data instances from the dataset as centroids
2. assign each data instance to the closest centroid, thus create intial clustering $\mathcal{C}$
3. compute clustering inertia cost($\mathcal{C}$)

Iteration

1. re-compute centroids for $\mathcal{C}$
2. assign each data instance to the closest centroid, thus create a new clustering $\mathcal{C}'$
3. compute clustering intertia cost($\mathcal{C}'$)
4. repeat 1 through 3 with $\mathcal{C} := \mathcal{C}'$ until reaching some stop-criterion

Base Algorithm – Variation Minimization

Initialization

1. choose k data instances from the dataset as centroids
2. assign each data instance to the closest centroid, thus create intial clustering $\mathcal{C}$
3. compute clustering inertia cost($\mathcal{C}$)

Iteration

1. re-compute centroids for $\mathcal{C}$
2. assign each data instance to the closest centroid, thus create a new clustering $\mathcal{C}'$
3. compute clustering intertia cost($\mathcal{C}'$)
4. repeat 1 through 3 with $\mathcal{C} := \mathcal{C}'$ until reaching some stop-criterion

Stopping Criteria

Base Algorithm – Variation Minimization

Initialization

1. choose k data instances from the dataset as centroids
2. assign each data instance to the closest centroid, thus create intial clustering $\mathcal{C}$
3. compute clustering inertia $\text{cost}(\mathcal{C})$

Iteration

1. re-compute centroids for $\mathcal{C}$
2. assign each data instance to the closest centroid, thus create a new clustering $\mathcal{C}'$
3. compute clustering intertia $\text{cost}(\mathcal{C}')$
4. repeat 1 through 3 with $\mathcal{C} := \mathcal{C}'$ until reaching some stop-criterion

Stopping Criteria

- $\mathcal{C} = \mathcal{C}'$

Base Algorithm – Variation Minimization

Initialization

1. choose k data instances from the dataset as centroids
2. assign each data instance to the closest centroid, thus create intial clustering $\mathcal{C}$
3. compute clustering inertia $\text{cost}(\mathcal{C})$

Iteration

1. re-compute centroids for $\mathcal{C}$
2. assign each data instance to the closest centroid, thus create a new clustering $\mathcal{C}'$
3. compute clustering intertia $\text{cost}(\mathcal{C}')$
4. repeat 1 through 3 with $\mathcal{C} \coloneqq \mathcal{C}'$ until reaching some stop-criterion

Stopping Criteria

- $\mathcal{C} = \mathcal{C}'$
- $|\text{cost}(\mathcal{C}) - \text{cost}(\mathcal{C}')|$ below some threshold

Different Variations of the Base-Algorithm

k-means:

Different Variations of the Base-Algorithm

***k*-means:**

- similar, but instead of recomputing the full clustering, find one instance that should belong to a closer centroid and immediately recompute the centroids

Different Variations of the Base-Algorithm

***k*-means:**

- similar, but instead of recomputing the full clustering, find one instance that should belong to a closer centroid and immediately recompute the centroids
- k-means mainly has the properties of the base algorithm

Different Variations of the Base-Algorithm

***k*-means:**

- similar, but instead of recomputing the full clustering, find one instance that should belong to a closer centroid and immediately recompute the centroids
- *k*-means mainly has the properties of the base algorithm
- *k*-means depends on the order of the dataset

Different Variations of the Base-Algorithm

k-means:

- similar, but instead of recomputing the full clustering, find one instance that should belong to a closer centroid and immediately recompute the centroids
- k-means mainly has the properties of the base algorithm
- k-means depends on the order of the dataset
- computationally less expensive (easy centroid updates instead of full recomputation)

Different Variations of the Base-Algorithm

k-**means:**

- similar, but instead of recomputing the full clustering, find one instance that should belong to a closer centroid and immediately recompute the centroids
- k-means mainly has the properties of the base algorithm
- k-means depends on the order of the dataset
- computationally less expensive (easy centroid updates instead of full recomputation)
- faster convergence

Different Variations of the Base-Algorithm

***k*-means:**

- similar, but instead of recomputing the full clustering, find one instance that should belong to a closer centroid and immediately recompute the centroids
- k-means mainly has the properties of the base algorithm
- k-means depends on the order of the dataset
- computationally less expensive (easy centroid updates instead of full recomputation)
- faster convergence

***k*-means++:**

Different Variations of the Base-Algorithm

***k*-means:**

- similar, but instead of recomputing the full clustering, find one instance that should belong to a closer centroid and immediately recompute the centroids
- *k*-means mainly has the properties of the base algorithm
- *k*-means depends on the order of the dataset
- computationally less expensive (easy centroid updates instead of full recomputation)
- faster convergence

***k*-means++:**

- same as *k*-means but with sophisticated initialization

Different Variations of the Base-Algorithm

k-means:

- similar, but instead of recomputing the full clustering, find one instance that should belong to a closer centroid and immediately recompute the centroids
- k-means mainly has the properties of the base algorithm
- k-means depends on the order of the dataset
- computationally less expensive (easy centroid updates instead of full recomputation)
- faster convergence

k-means++:

- same as k-means but with sophisticated initialization
- initial centroids are chosen iteratively

Different Variations of the Base-Algorithm

***k*-means:**

- similar, but instead of recomputing the full clustering, find one instance that should belong to a closer centroid and immediately recompute the centroids
- k-means mainly has the properties of the base algorithm
- k-means depends on the order of the dataset
- computationally less expensive (easy centroid updates instead of full recomputation)
- faster convergence

***k*-means++:**

- same as k-means but with sophisticated initialization
- initial centroids are chosen iteratively
  - first centroid is chosen from the dataset at random

Different Variations of the Base-Algorithm

k-means:

- similar, but instead of recomputing the full clustering, find one instance that should belong to a closer centroid and immediately recompute the centroids
- k-means mainly has the properties of the base algorithm
- k-means depends on the order of the dataset
- computationally less expensive (easy centroid updates instead of full recomputation)
- faster convergence

k-means++:

- same as k-means but with sophisticated initialization
- initial centroids are chosen iteratively
  - first centroid is chosen from the dataset at random
  - each further centroid: chosen from dataset with probability proportional to the squared distance to its nearest centroid

Different Variations of the Base-Algorithm

k-means:

- similar, but instead of recomputing the full clustering, find one instance that should belong to a closer centroid and immediately recompute the centroids
- k-means mainly has the properties of the base algorithm
- k-means depends on the order of the dataset
- computationally less expensive (easy centroid updates instead of full recomputation)
- faster convergence

k-means++:

- same as k-means but with sophisticated initialization
- initial centroids are chosen iteratively
  - first centroid is chosen from the dataset at random
  - each further centroid: chosen from dataset with probability proportional to the squared distance to its nearest centroid
- longer initialization, speed-up of convergence, decrease of squared distance

k-means in Python

`sklearn.cluster.KMeans`

- default: k-means++

k-means in Python

`sklearn.cluster.KMeans`

- default: k-means++
- setup to run multiple times (`n_iter`) with different initialization, returns the best clustering

k-means in Python

`sklearn.cluster.KMeans`

- default: k-means++
- setup to run multiple times (`n_iter`) with different initialization, returns the best clustering
- abort criteria

k-means in Python

`sklearn.cluster.KMeans`

- default: k-means++
- setup to run multiple times (`n_iter`) with different initialization, returns the best clustering
- abort criteria
  - `max_iter`: maximum number of iterations

k-means in Python

`sklearn.cluster.KMeans`

- default: k-means++
- setup to run multiple times (`n_iter`) with different initialization, returns the best clustering
- abort criteria
  - `max_iter`: maximum number of iterations
  - `tol`: threshold on the change in the cluster centers between two iterations to assume convergence

k-means in Python

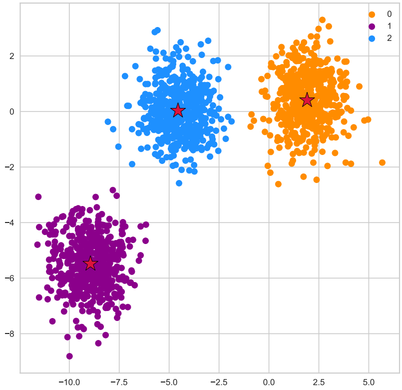
`sklearn.cluster.KMeans`

- default: *k*-means++
- setup to run multiple times (`n_iter`) with different initialization, returns the best clustering
- abort criteria
  - `max_iter`: maximum number of iterations
  - `tol`: threshold on the change in the cluster centers between two iterations to assume convergence

Notebook 06_1_k_means_synthetic

Agenda

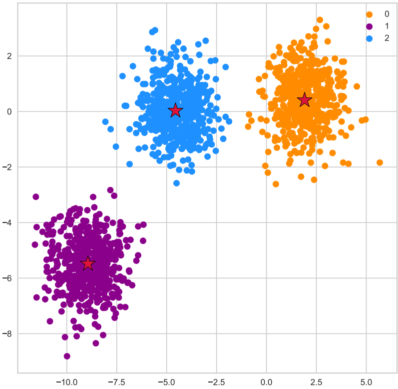
k-Means Example[1]



- $k = 3$

[1] adapted from an sklearn tutorial

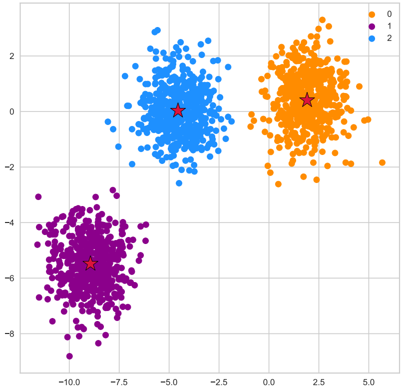
k-Means Example[1]



- $k = 3$
- stars mark the centroids

[1]adapted from an sklearn tutorial

k-Means Example[1]



- $k = 3$
- stars mark the centroids
- in 2D easy plausibility check

[1] adapted from an sklearn tutorial

Discussion of k-means

positive:

Discussion of k-means

positive:

- efficiency:

Discussion of k-means

positive:

- efficiency:
  - **Computational Effort**: $O(k \cdot n)$ per iteration,

Discussion of k-means

positive:

- efficiency:
  - **Computational Effort**: $O(k \cdot n)$ per iteration,
  - number of required iterations usually small (≈ 5 to 10).

Discussion of k-means

positive:

- efficiency:
  - **Computational Effort**: $O(k \cdot n)$ per iteration,
  - number of required iterations usually small (≈ 5 to 10).
- simple implementation

  → most popular partitioning clustering approach

Discussion of k-means

positive:

- efficiency:
  - **Computational Effort**: $O(k \cdot n)$ per iteration,
  - number of required iterations usually small (≈ 5 to 10).
- simple implementation
  → most popular partitioning clustering approach
- straightforward → easily applicable, easily explained

Discussion of k-means

positive:

- efficiency:
  - **Computational Effort**: $O(k \cdot n)$ per iteration,
  - number of required iterations usually small (≈ 5 to 10).
- simple implementation
  → most popular partitioning clustering approach
- straightforward → easily applicable, easily explained

negative:

Discussion of k-means

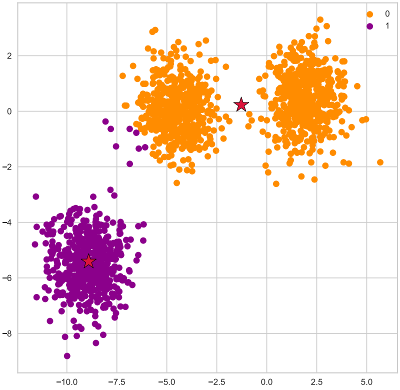
positive:

- efficiency:
  - **Computational Effort**: $O(k \cdot n)$ per iteration,
  - number of required iterations usually small (≈ 5 to 10).
- simple implementation
  ➔ most popular partitioning clustering approach
- straightforward ➔ easily applicable, easily explained

negative:

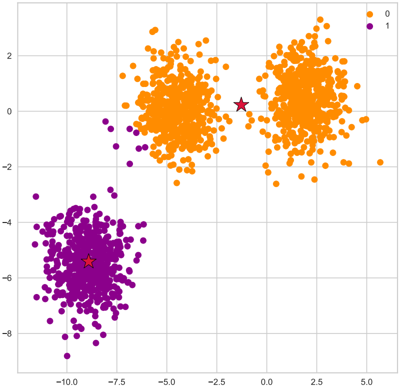
- let's look at a couple of examples

The k of k-Means [2]



[2] adapted from an sklearn tutorial

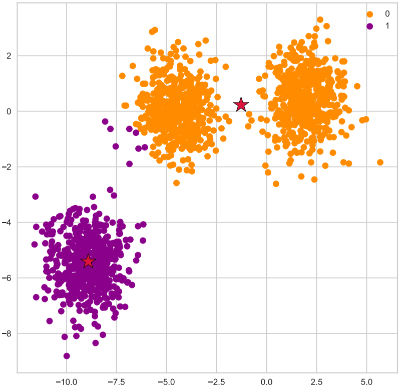
The k of k-Means [2]



- we need the "correct" k, upfront

[2] adapted from an sklearn tutorial

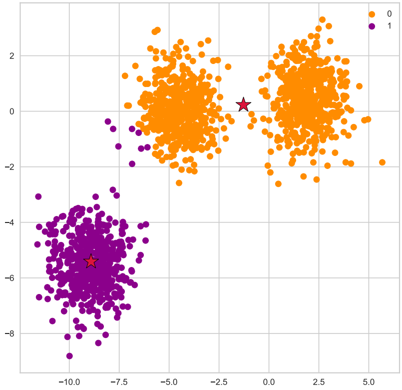
The k of k-Means [2]



- we need the "correct" k, upfront
- sometimes easy to see in a plot

[2] adapted from an sklearn tutorial

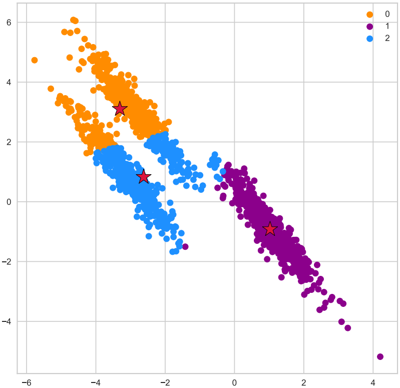
The k of k-Means [2]



- we need the "correct" k, upfront
- sometimes easy to see in a plot
- much more difficult for multidimensional data

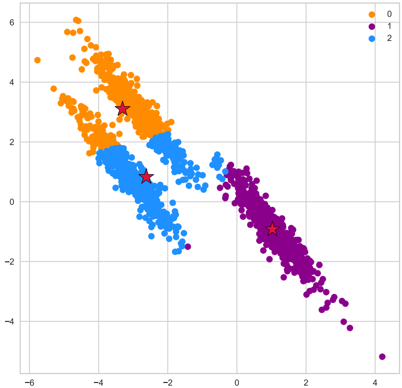
[2] adapted from an sklearn tutorial

The Form of k-Means Clusters [3]



[3] adapted from an sklearn tutorial

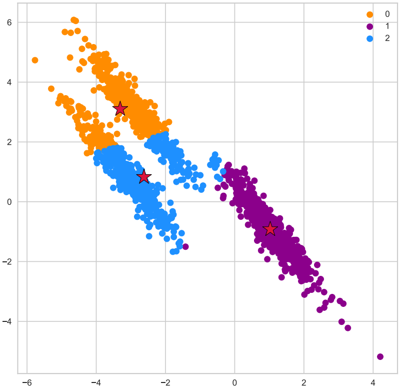
The Form of k-Means Clusters [3]



- k-means clusters are circular surroundings of the centroids

[3] adapted from an sklearn tutorial

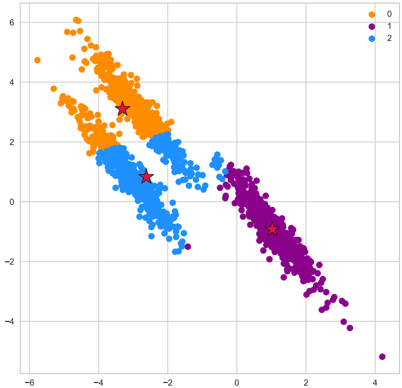
The Form of k-Means Clusters [3]



- k-means clusters are circular surroundings of the centroids
- the centroids induce a Voronoi diagram

[3] adapted from an sklearn tutorial

The Form of k-Means Clusters [3]



- k-means clusters are circular surroundings of the centroids
- the centroids induce a Voronoi diagram
- the form does not necessarily reflect the real data structure

[3] adapted from an sklearn tutorial

Discussion of k-means

negative:

Discussion of k-means

negative:

- choosing k properly is often difficult → ⌛ silhouette coefficient

Discussion of *k*-means

negative:

- choosing *k* properly is often difficult → ⌛ silhouette coefficient
- "real" clusters must have convex form for a good fit → ⌛ density-based clustering

Discussion of *k*-means

negative:

- choosing *k* properly is often difficult → ⌛ silhouette coefficient
- "real" clusters must have convex form for a good fit → ⌛ density-based clustering
- sensitive to noise and outliers (all instances enter the computation of centroids) →

Discussion of *k*-means

negative:

- choosing k properly is often difficult → ⌛ silhouette coefficient
- "real" clusters must have convex form for a good fit → ⌛ density-based clustering
- sensitive to noise and outliers (all instances enter the computation of centroids) →
  - drop outliers before running the algorithm

Discussion of k-means

negative:

- choosing k properly is often difficult → ⌛ silhouette coefficient
- "real" clusters must have convex form for a good fit → ⌛ density-based clustering
- sensitive to noise and outliers (all instances enter the computation of centroids) →
  - drop outliers before running the algorithm
  - ⌛ density-based clustering

Discussion of k-means

negative:

- choosing k properly is often difficult → ⌛ silhouette coefficient
- "real" clusters must have convex form for a good fit → ⌛ density-based clustering
- sensitive to noise and outliers (all instances enter the computation of centroids) →
  - drop outliers before running the algorithm
  - ⌛ density-based clustering
- result strongly depends on initial choice of centroids → run multiple times, use best result

Discussion of k-means

negative:

- choosing k properly is often difficult → ⧗ silhouette coefficient
- "real" clusters must have convex form for a good fit → ⧗ density-based clustering
- sensitive to noise and outliers (all instances enter the computation of centroids) →
  - drop outliers before running the algorithm
  - ⧗ density-based clustering
- result strongly depends on initial choice of centroids → run multiple times, use best result
- no confidence for cluster memberships → ⧗ probabilistic clustering

Agenda

Choosing k

method:

- create a clustering for each $k = 2, \ldots, n-1$
- choose k with the best clustering – according to a quality measure

measure for a clustering's quality:

- needs to be independent of k
- TD^2 decreases monotonously with increasing k
- TD^2 is thus unsuitable as quality measure
- similar effect for k-Medoid and EM ⌛

Choosing k – The Silhouette Coefficient

Definition 4 (Silhouette Coefficient)

For a given clustering $\mathcal{C}$ on a dataset D, the **silhouette** $s(o)$ of an instance $o \in D$ is given as $s(o) = 0$ if o's cluster has only the one element, and otherwise

$$s(o) = \frac{b(o) - a(o)}{\max\{a(o), b(o)\}}$$

where

- $a(o)$ is the mean distance to the other elements in o's cluster, and
- $b(o)$ the mean distance to the elements of the "nearest" cluster.

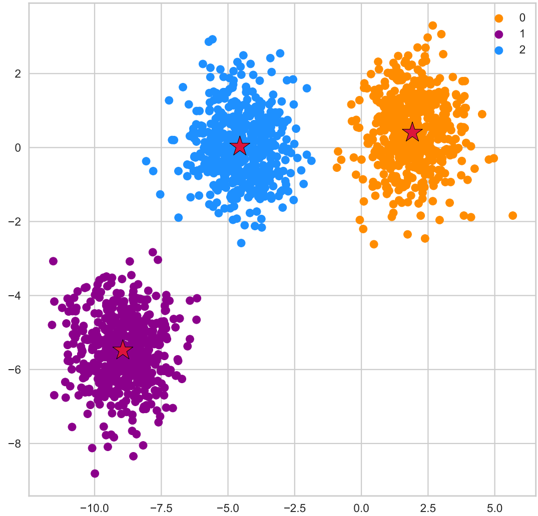
The nearest cluster is the one with the lowest mean distance to o. The silhouette coefficient of a clustering is the mean of the objects' silhouettes.

Properties of the Silhouette Coefficient

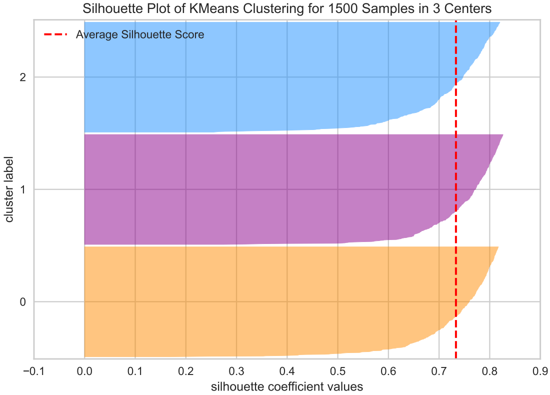
- higher means more structure
- $-1 \leq s(o) \leq 1$, where $s(o) = -1$ means a bad cluster assignment, 0 is indifferent and $+1$ a good assignment
- measure is independent of the number of clusters
- rule of thumb:
  - $s_{\mathcal{C}} > 0.7$: strong structure,
  - $0.7 \geq s_{\mathcal{C}} > 0.5$: usable structure,
  - $0.5 \geq s_{\mathcal{C}} > 0.25$: weak structure,
  - $0.25 \geq s_{\mathcal{C}}$: no structure.

Admit when the coefficient is low, that the algorithm found no real clustering.

Plotting the Silhouette

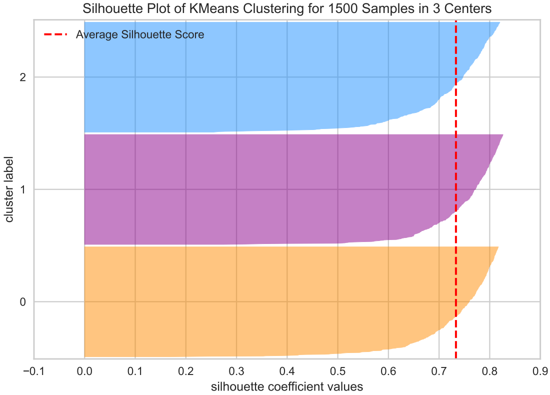


Plotting the Silhouette



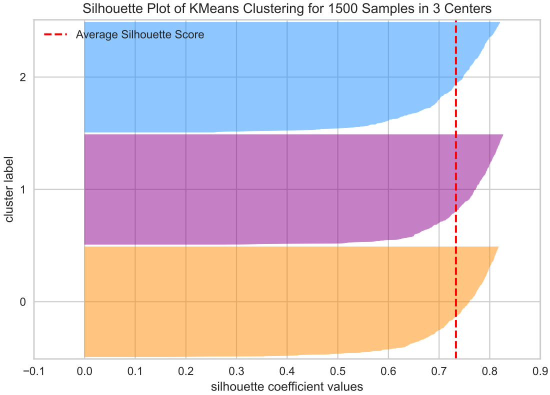
- silhouette score: $s = 0.73$

Plotting the Silhouette



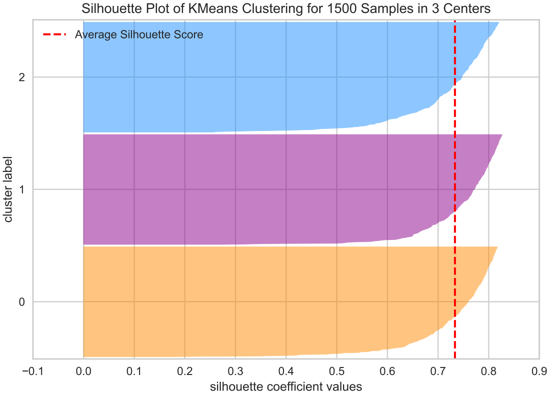
- silhouette score: $s = 0.73$
- one row for each data instance, orderd by cluster and silhouette

Plotting the Silhouette



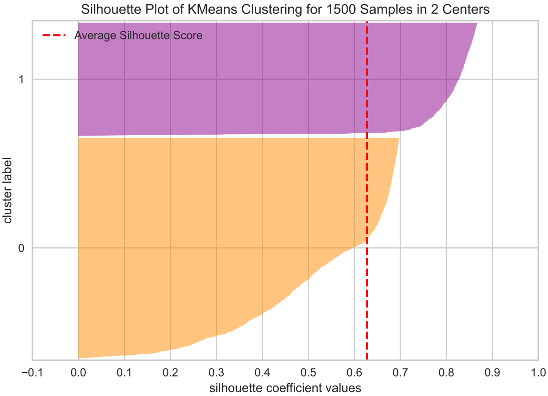
- silhouette score: $s = 0.73$
- one row for each data instance, orderd by cluster and silhouette
- we can assess quality per cluster

Plotting the Silhouette

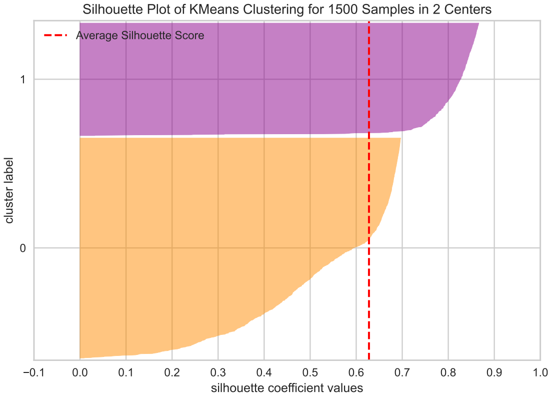


- silhouette score: $s = 0.73$
- one row for each data instance, orderd by cluster and silhouette
- we can assess quality per cluster
- visualization independent of dataset dimension!

Interpreting Silhouette Plots 1

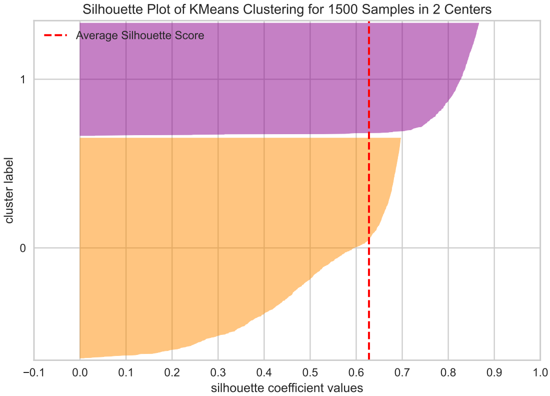


Interpreting Silhouette Plots 1



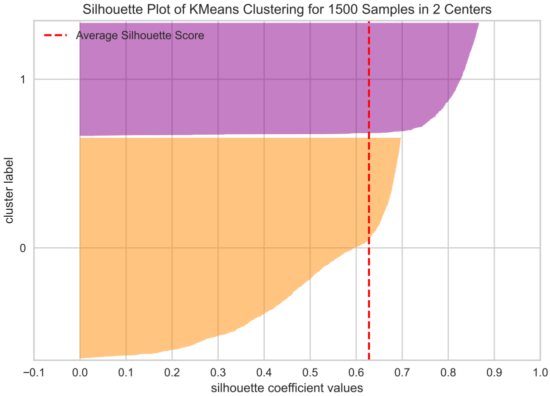
- overall structure not as strong as before ($s = 0.63$) (same dataset!)

Interpreting Silhouette Plots 1



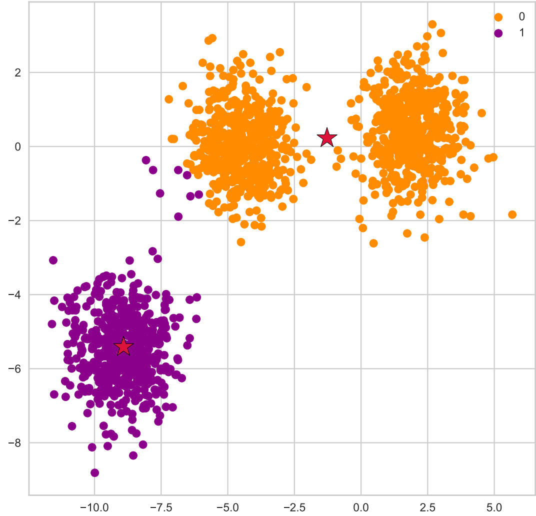
- overall structure not as strong as before ($s = 0.63$) (same dataset!)
- only two clusters

Interpreting Silhouette Plots 1

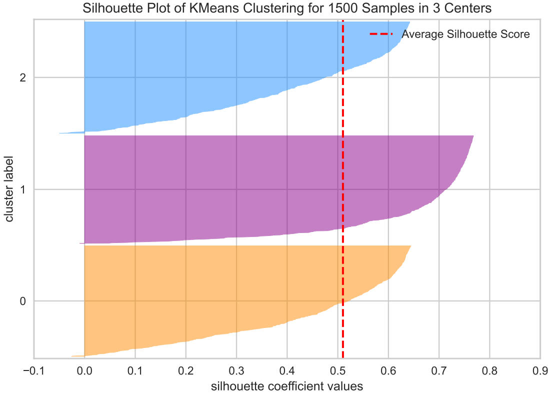


- overall structure not as strong as before ($s = 0.63$) (same dataset!)
- only two clusters
- cluster 0 seriously lacks structure (many instances with small silhouettes)

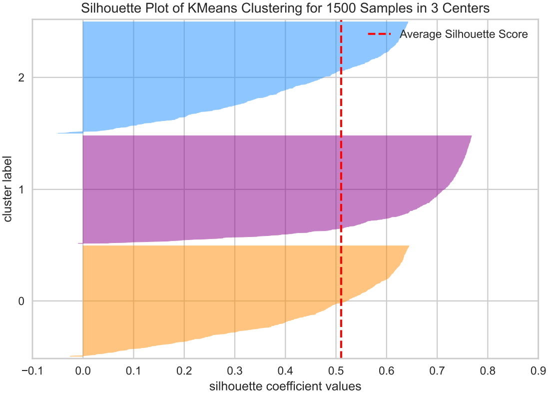
Interpreting Silhouette Plots 1



Interpreting Silhouette Plots 2

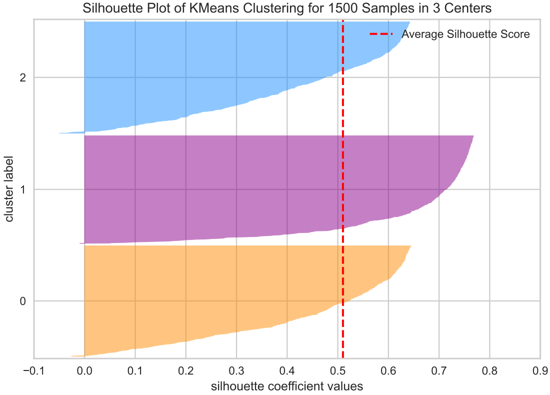


Interpreting Silhouette Plots 2



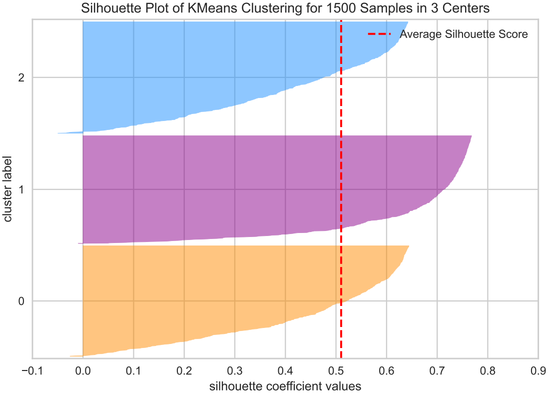
- overall structure close to unusable ($s = 0.51$)

Interpreting Silhouette Plots 2



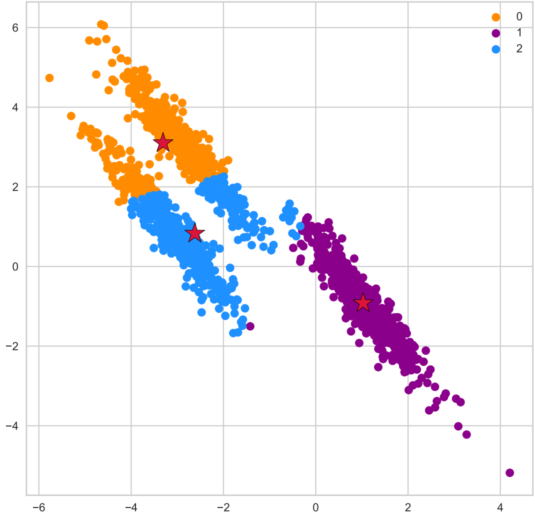
- overall structure close to unusable ($s = 0.51$)
- three cluster, one with good structure, two without

Interpreting Silhouette Plots 2

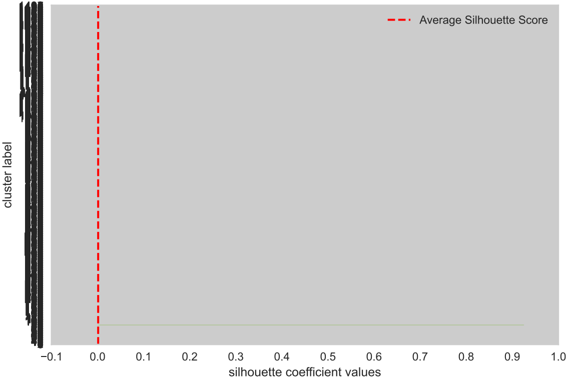


- overall structure close to unusable ($s = 0.51$)
- three cluster, one with good structure, two without
- some instances even have negative silhoutte

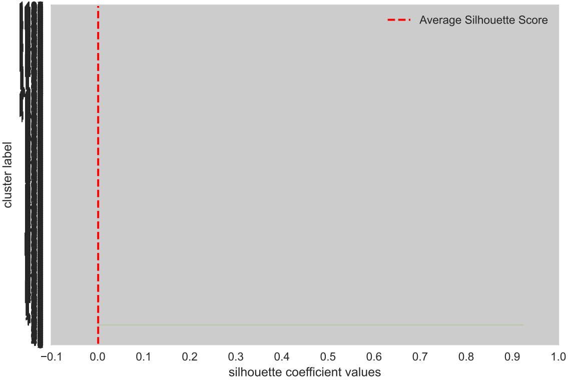
Interpreting Silhouette Plots 2



Interpreting Silhouette Plots 3

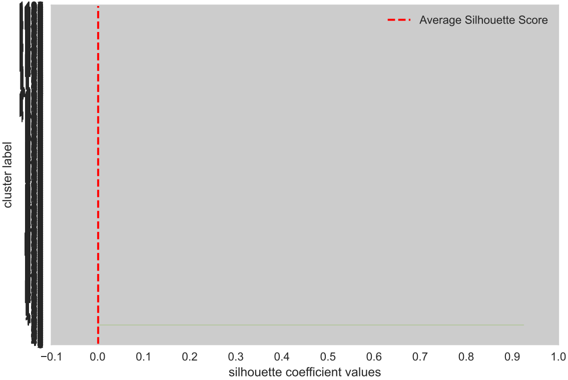


Interpreting Silhouette Plots 3



- silhouette coefficient is close to 0: $s = 0.0012$

Interpreting Silhouette Plots 3



- silhouette coefficient is close to 0: $s = 0.0012$
- 1500 instances and 1499 clusters

Interpreting Silhouette Plots 4

The silhouette plot:

- visualizes the data in 2D for arbitrary dimensional data!

Interpreting Silhouette Plots 4

The silhouette plot:

- visualizes the data in 2D for arbitrary dimensional data!
- shows the distribution of instances over the clusters (larger and smaller clusters).

Interpreting Silhouette Plots 4

The silhouette plot:

- visualizes the data in 2D for arbitrary dimensional data!
- shows the distribution of instances over the clusters (larger and smaller clusters).
- shows the overall silhouette coefficients.

Interpreting Silhouette Plots 4

The silhouette plot:

- visualizes the data in 2D for arbitrary dimensional data!
- shows the distribution of instances over the clusters (larger and smaller clusters).
- shows the overall silhouette coefficients.
- shows the distribution per cluster.

Interpreting Silhouette Plots 4

The silhouette plot:

- visualizes the data in 2D for arbitrary dimensional data!
- shows the distribution of instances over the clusters (larger and smaller clusters).
- shows the overall silhouette coefficients.
- shows the distribution per cluster.
- shows negative silhouettes, meaning points have closer average distance to points in another cluster than to their own.

Interpreting Silhouette Plots 4

The silhouette plot:

- visualizes the data in 2D for arbitrary dimensional data!
- shows the distribution of instances over the clusters (larger and smaller clusters).
- shows the overall silhouette coefficients.
- shows the distribution per cluster.
- shows negative silhouettes, meaning points have closer average distance to points in another cluster than to their own.
- can be used to discuss clusterings for different k on the same data.

Interpreting Silhouette Plots 4

The silhouette plot:

- visualizes the data in 2D for arbitrary dimensional data!
- shows the distribution of instances over the clusters (larger and smaller clusters).
- shows the overall silhouette coefficients.
- shows the distribution per cluster.
- shows negative silhouettes, meaning points have closer average distance to points in another cluster than to their own.
- can be used to discuss clusterings for different k on the same data.
- must be used with care when interpreting individual clusters!

Interpreting Silhouette Plots 4

The silhouette plot:

- visualizes the data in 2D for arbitrary dimensional data!
- shows the distribution of instances over the clusters (larger and smaller clusters).
- shows the overall silhouette coefficients.
- shows the distribution per cluster.
- shows negative silhouettes, meaning points have closer average distance to points in another cluster than to their own.
- can be used to discuss clusterings for different k on the same data.
- must be used with care when interpreting individual clusters!

When using k-means, ALWAYS discuss silhouette plots.
For other clustering algorithms, silhouettes often are NOT meaningful.

Exercises

Exercises 1–2

Outline

Idea

Assumption

data is grouped around a fix number of central instances, called **medoids**

Idea

Assumption

data is grouped around a fix number of central instances, called **medoids**

Use Case

we want the center to be an actual representative (member) of the data, a prototypical element of the cluster

Idea

Assumption
data is grouped around a fix number of central instances, called **medoids**

Use Case
we want the center to be an actual representative (member) of the data, a prototypical element of the cluster

Approach

Idea

Assumption

data is grouped around a fix number of central instances, called **medoids**

Use Case

we want the center to be an actual representative (member) of the data, a prototypical element of the cluster

Approach

- try determine those representatives

Idea

Assumption

data is grouped around a fix number of central instances, called **medoids**

Use Case

we want the center to be an actual representative (member) of the data, a prototypical element of the cluster

Approach

- try determine those representatives
- each instance is assigned to the representative it is closest to

Selecting Representative Instances

Instances: vectors $p = (x_{p_1}, \ldots, x_{p_d})$ in a Euclidean vector space

Distance: Euclidean distance

Representative: **Medoid** $m_C \in D$ as central element of a cluster

Cluster-Cost: measure for the (non-)compactness of a Cluster C:

$$\text{cost}(C) = TD(C) := \sum_{p \in C} \text{dist}(p, m_C)$$

Clustering-Cost: measure for the (non-)compactness of a clustering:

$$\text{cost}(\mathcal{C}) = TD(\mathcal{C}) := \sum_{C \in \mathcal{C}} TD(C)$$

Search space of the clustering algorithm: all k-element partitions of D

➔ runtime of exhaustive search: $O(|D|^k)$

Algorithms PAM and CLARANS

PAM

Algorithms PAM and CLARANS

PAM

- greedy-Algorithm: in each step exchange a medoid with a non-medoid

Algorithms PAM and CLARANS

PAM

- greedy-Algorithm: in each step exchange a medoid with a non-medoid
- choose the pair that reduces the cost *TD* the most

Algorithms PAM and CLARANS

PAM

- greedy-Algorithm: in each step exchange a medoid with a non-medoid
- choose the pair that reduces the cost *TD* the most

CLARANS two additional parameters: `maxneighbor` und `numlocal`

Algorithms PAM and CLARANS

PAM

- greedy-Algorithm: in each step exchange a medoid with a non-medoid
- choose the pair that reduces the cost *TD* the most

CLARANS two additional parameters: `maxneighbor` und `numlocal`

- at most `maxneighbor` many randomly chosen pairs (medoid, non-medoid) are considered

Algorithms PAM and CLARANS

PAM

- greedy-Algorithm: in each step exchange a medoid with a non-medoid
- choose the pair that reduces the cost TD the most

CLARANS two additional parameters: `maxneighbor` und `numlocal`

- at most `maxneighbor` many randomly chosen pairs (medoid, non-medoid) are considered
- the first replacement reducing TD is applied

Algorithms PAM and CLARANS

PAM

- greedy-Algorithm: in each step exchange a medoid with a non-medoid
- choose the pair that reduces the cost TD the most

CLARANS two additional parameters: `maxneighbor` und `numlocal`

- at most `maxneighbor` many randomly chosen pairs (medoid, non-medoid) are considered
- the first replacement reducing TD is applied
- search for k optimal medoids is repeated `numlocal` times

Algorithms PAM and CLARANS

PAM

- greedy-Algorithm: in each step exchange a medoid with a non-medoid
- choose the pair that reduces the cost *TD* the most

CLARANS two additional parameters: `maxneighbor` und `numlocal`

- at most `maxneighbor` many randomly chosen pairs (medoid, non-medoid) are considered
- the first replacement reducing *TD* is applied
- search for k optimal medoids is repeated `numlocal` times
- sacrifice *TD* (non-optimal choices in every step) for runtime (significantly fewer candidates).

Algorithms PAM and CLARANS

PAM

- greedy-Algorithm: in each step exchange a medoid with a non-medoid
- choose the pair that reduces the cost *TD* the most

CLARANS two additional parameters: `maxneighbor` und `numlocal`

- at most `maxneighbor` many randomly chosen pairs (medoid, non-medoid) are considered
- the first replacement reducing *TD* is applied
- search for k optimal medoids is repeated `numlocal` times
- sacrifice *TD* (non-optimal choices in every step) for runtime (significantly fewer candidates).

Notebook 06_2_clarans_iris