Home Installation
Documentation
Examples
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Searc
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«

Selecting the number of clusters with silhouette analysis on KMeans clustering

Silhouette analysis can be used to study the separation distance between the resulting clusters. The silhouette plot displays a measure of how close each point in one cluster is to points in the neighboring clusters and thus provides a way to assess parameters like number of clusters visually. This measure has a range of [-1, 1].

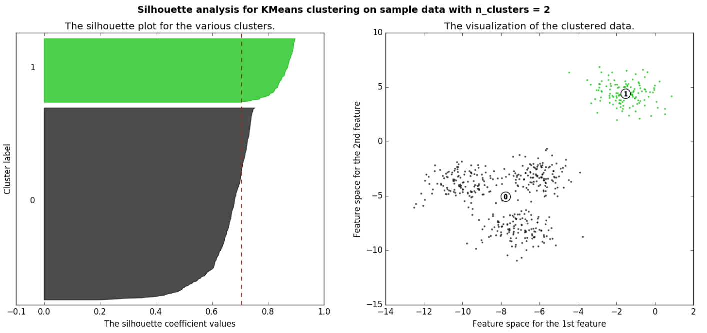
Silhouette coefficients (as these values are referred to as) near +1 indicate that the sample is far away from the neighboring clusters. A value of 0 indicates that the sample is on or very close to the decision boundary between two neighboring clusters and negative values indicate that those samples might have been assigned to the wrong cluster.

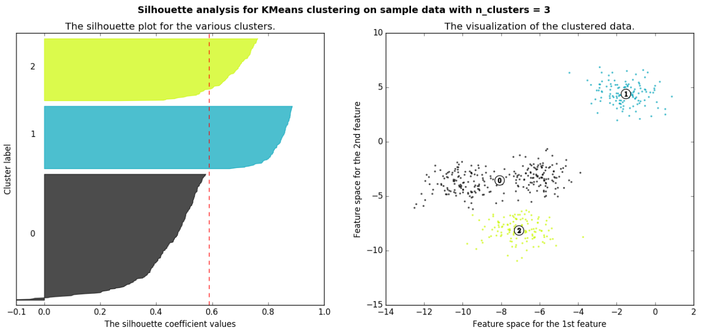
In this example the silhouette analysis is used to choose an optimal value for `n_clusters`. The silhouette plot shows that the `n_clusters` value of 3, 5 and 6 are a bad pick for the given data due to the presence of clusters with below average silhouette scores and also due to wide fluctuations in the size of the silhouette plots. Silhouette analysis is more ambivalent in deciding between 2 and 4.

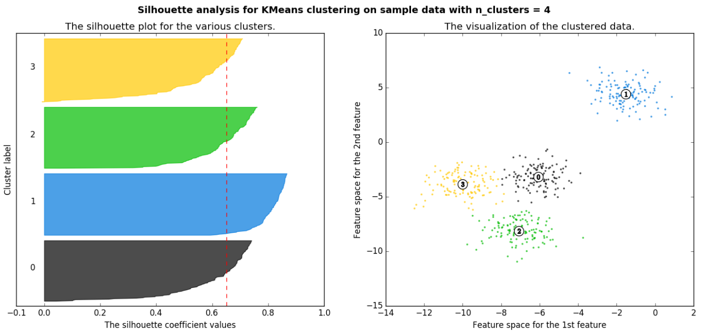
Also from the thickness of the silhouette plot the cluster size can be visualized. The silhouette plot for cluster 0 when `n_clusters` is equal to 2, is bigger in size owing to the grouping of the 3 sub clusters into one big cluster. However when the `n_clusters` is equal to 4, all the plots are more or less of similar thickness and hence are of similar sizes as can be also verified from the labelled scatter plot on the right.

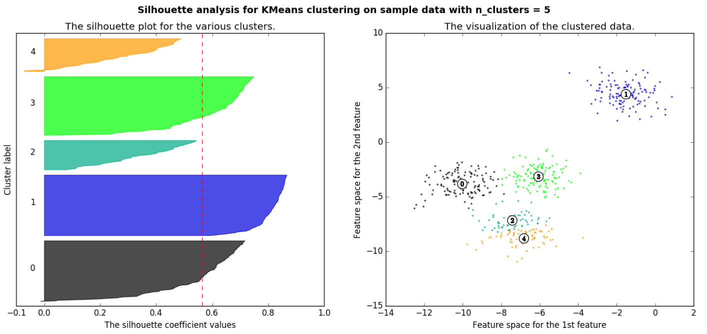
Previous **Next**

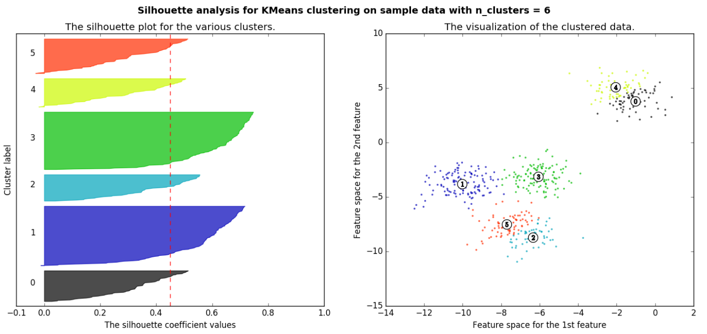
«


Silhouette analysis for KMeans clustering on sample data with n_clusters = 2
The silhouette plot for the various clusters.
Cluster label
1
0
−0.1
0.0
0.2
0.4
0.6
0.8
1.0
The silhouette coefficient values
The visualization of the clustered data.
Feature space for the 2nd feature
10
5
0
−5
−10
−15
−14
−12
−10
−8
−6
−4
−2
0
2
Feature space for the 1st feature
0
1


Silhouette analysis for KMeans clustering on sample data with n_clusters = 3
The silhouette plot for the various clusters.
Cluster label
2
1
0
−0.1
0.0
0.2
0.4
0.6
0.8
1.0
The silhouette coefficient values
The visualization of the clustered data.
Feature space for the 2nd feature
10
5
0
−5
−10
−15
−14
−12
−10
−8
−6
−4
−2
0
2
Feature space for the 1st feature
1
0
2


Silhouette analysis for KMeans clustering on sample data with n_clusters = 4
The silhouette plot for the various clusters.
Cluster label
3
2
1
0
−0.1
0.0
0.2
0.4
0.6
0.8
1.0
The silhouette coefficient values
The visualization of the clustered data.
Feature space for the 2nd feature
10
5
0
−5
−10
−15
−14
−12
−10
−8
−6
−4
−2
0
2
Feature space for the 1st feature
1
3
0
2


Silhouette analysis for KMeans clustering on sample data with n_clusters = 5
The silhouette plot for the various clusters.
Cluster label
4
3
2
1
0
−0.1
0.0
0.2
0.4
0.6
0.8
1.0
The silhouette coefficient values
The visualization of the clustered data.
Feature space for the 2nd feature
10
5
0
−5
−10
−15
−14
−12
−10
−8
−6
−4
−2
0
2
Feature space for the 1st feature
1
0
3
2
4


Silhouette analysis for KMeans clustering on sample data with n_clusters = 6
The silhouette plot for the various clusters.
Cluster label
5
4
3
2
1
0
−0.1
0.0
0.2
0.4
0.6
0.8
1.0
The silhouette coefficient values
The visualization of the clustered data.
Feature space for the 2nd feature
10
5
0
−5
−10
−15
−14
−12
−10
−8
−6
−4
−2
0
2
Feature space for the 1st feature
4
0
1
3
5
2

Previous

Out:

```
  For n_clusters = 2 The average silhouette_score is : 0.70497
For n_clusters = 3 The average silhouette_score is : 0.5882004
For n_clusters = 4 The average silhouette_score is : 0.6505186
For n_clusters = 5 The average silhouette_score is : 0.5637646
For n_clusters = 6 The average silhouette_score is : 0.4504666
```

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```
from __future__ import print_function

from sklearn.datasets import make_blobs
from sklearn.cluster import KMeans
from sklearn.metrics import silhouette_samples, silhouette_score

import matplotlib.pyplot as plt
import matplotlib.cm as cm
import numpy as np

print(__doc__)

# Generating the sample data from make_blobs
# This particular setting has one distinct cluster and 3 clusters
# together.
X, y = make_blobs(n_samples=500,
                  n_features=2,
                  centers=4,
                  cluster_std=1,
                  center_box=(-10.0, 10.0),
                  shuffle=True,
                  random_state=1)  # For reproducibility

range_n_clusters = [2, 3, 4, 5, 6]

for n_clusters in range_n_clusters:
    # Create a subplot with 1 row and 2 columns
    fig, (ax1, ax2) = plt.subplots(1, 2)
    fig.set_size_inches(18, 7)

    # The 1st subplot is the silhouette plot
    # The silhouette coefficient can range from -1, 1 but in this
    # lie within [-0.1, 1]
    ax1.set_xlim([-0.1, 1])
    # The (n_clusters+1)*10 is for inserting blank space between s
    # plots of individual clusters, to demarcate them clearly.
    ax1.set_ylim([0, len(X) + (n_clusters + 1) * 10])

    # Initialize the clusterer with n_clusters value and a random
    # seed of 10 for reproducibility.
    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 sam
    # This gives a perspective into the density and separation of
    # clusters
    silhouette_avg = silhouette_score(X, cluster_labels)
    print("For n_clusters =", n_clusters,
          "The average silhouette_score is :", silhouette_avg)

    # Compute the silhouette scores for each sample
    sample_silhouette_values = silhouette_samples(X, cluster_label

    y_lower = 10
    for i in range(n_clusters):
        # Aggregate the silhouette scores for samples belonging to
        # cluster i, and sort them
```

Previous

«

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        ith_cluster_silhouette_values = \
            sample_silhouette_values[cluster_labels == i]

        ith_cluster_silhouette_values.sort()

        size_cluster_i = ith_cluster_silhouette_values.shape[0]
        y_upper = y_lower + size_cluster_i

        color = cm.spectral(float(i) / n_clusters)
        ax1.fill_betweenx(np.arange(y_lower, y_upper),
                          0, ith_cluster_silhouette_values,
                          facecolor=color, edgecolor=color, alpha=

        # Label the silhouette plots with their cluster numbers at
        ax1.text(-0.05, y_lower + 0.5 * size_cluster_i, str(i))

        # Compute the new y_lower for next plot
        y_lower = y_upper + 10  # 10 for the 0 samples

    ax1.set_title("The silhouette plot for the various clusters.")
    ax1.set_xlabel("The silhouette coefficient values")
    ax1.set_ylabel("Cluster label")

    # The vertical line for average silhouette score of all the va
    ax1.axvline(x=silhouette_avg, color="red", linestyle="--")

    ax1.set_yticks([])  # Clear the yaxis labels / ticks
    ax1.set_xticks([-0.1, 0, 0.2, 0.4, 0.6, 0.8, 1])

    # 2nd Plot showing the actual clusters formed
    colors = cm.spectral(cluster_labels.astype(float) / n_clusters
    ax2.scatter(X[:, 0], X[:, 1], marker='.', s=30, lw=0, alpha=0.
                c=colors)

    # Labeling the clusters
    centers = clusterer.cluster_centers_
    # Draw white circles at cluster centers
    ax2.scatter(centers[:, 0], centers[:, 1],
                marker='o', c="white", alpha=1, s=200)

    for i, c in enumerate(centers):
        ax2.scatter(c[0], c[1], marker='$%d$' % i, alpha=1, s=50)

    ax2.set_title("The visualization of the clustered data.")
    ax2.set_xlabel("Feature space for the 1st feature")
    ax2.set_ylabel("Feature space for the 2nd feature")

    plt.suptitle(("Silhouette analysis for KMeans clustering on sa
                  "with n_clusters = %d" % n_clusters),
                 fontsize=14, fontweight='bold')

    plt.show()
```

Total running time of the script: (0 minutes 1.241 seconds)

Download Python source code: `plot_kmeans_silhouette_analysis.py`

Download IPython notebook: `plot_kmeans_silhouette_analysis.ipynb`

Previous **Next**