Silhouette Score and Coefficient: Explanation, Math, and Example

The **Silhouette Score** is a metric used to evaluate the quality of a clustering. It measures how similar an object is to its own cluster compared to other clusters. The Silhouette Coefficient provides an indication of how well each data point has been clustered.

1. Explanation

- **Silhouette Score**: It is a measure of how close each sample in one cluster is to the samples in the neighboring clusters. A higher score indicates that the samples are well-clustered, while a lower score suggests that the clustering might be poor.
- The Silhouette Coefficient for a point can range from -1 to +1:
 - +1: indicates that the point is far away from the neighboring clusters, meaning it is well-clustered.
 - **0**: indicates that the point is on or very close to the decision boundary between two neighboring clusters.
 - -1: indicates that the point is incorrectly clustered and would be better off in another cluster.

2. Mathematics of Silhouette Score

The Silhouette Coefficient for a single sample i is defined as:

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

Where:

- a(i) = The average distance between the sample i and all other points in the same cluster (cohesion).
- b(i) = The average distance between the sample i and all points in the nearest cluster (separation).

The Silhouette Score for a clustering solution is the average silhouette score of all samples in the dataset:

$$S = \frac{1}{n} \sum_{i=1}^{n} s(i)$$

Where:

- n = total number of samples.
- s(i) = Silhouette Coefficient for sample i.

3. Example

Let's consider a simple example with a set of points belonging to two clusters:

- Cluster 1: Points A, B, and C
- Cluster 2: Points D, E, and F

Now, let's calculate the Silhouette Score for a point, say A, in Cluster 1.

1. **Cohesion**: Calculate the average distance from point A to other points in its own cluster (Cluster 1). Suppose the distances from A to B and A to C are 1.2 and 1.5, respectively.

$$a(A) = \frac{1.2 + 1.5}{2} = 1.35$$

2. **Separation**: Calculate the average distance from point A to points in the nearest cluster (Cluster 2). Suppose the distances from A to D, E, and F are 4.5, 4.0, and 4.3, respectively.

$$b(A) = \frac{4.5 + 4.0 + 4.3}{3} = 4.27$$

3. Silhouette Coefficient for A:

$$s(A) = \frac{b(A) - a(A)}{\max(a(A), b(A))} = \frac{4.27 - 1.35}{\max(1.35, 4.27)} = \frac{2.92}{4.27} \approx 0.68$$

This score (0.68) indicates that point A is fairly well-clustered with respect to the other points, but not perfectly.

4. **Silhouette Score for the Clustering**: To calculate the overall Silhouette Score for the clustering, we would repeat this process for each point and take the average of the individual scores.

4. Interpretation

- A higher Silhouette Score (close to +1) indicates that the clusters are well-separated and compact.
- A score close to 0 indicates that the clusters are overlapping, and the points are near the decision boundary.
- A negative score indicates that the points may be assigned to the wrong clusters.

In summary:

- Silhouette Score is a useful method for evaluating clustering performance.
- It provides insight into both **cohesion** (how close points within a cluster are) and **separation** (how distinct clusters are).