Scalable Distributed Approximation of Internal Measures for Clustering Evaluation

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Abstract

An important step in cluster analysis is the evaluation of the quality of a given clustering through structural measures of goodness. Measures that do not require additional information for their evaluation (but the clustering itself), called internal measures, are commonly used because of their generality. The most widely used internal measure is the silhouette coefficient, whose naïve computation requires a quadratic number of distance calculations, which is clearly unfeasible for massive datasets. Surprisingly, there are no known general methods to efficiently approximate the silhouette coefficient of a clustering with rigorously provable high accuracy. In this paper, we present the first scalable algorithm to compute such a rigorous approximation for the evaluation of clusterings based on any metric distances. Our algorithm hinges on a Probability Proportional to Size (PPS) sampling scheme, and, for any fixed $\varepsilon, \delta \in (0, 1)$, it approximates the silhouette coefficient within a mere additive error $O(\varepsilon)$ with probability $1 - \delta$, using a very small number of distance calculations. We also prove that the algorithm can be adapted to obtain rigorous approximations of other internal measures of clustering quality, such as cohesion and separation. Importantly, we provide a distributed implementation of the algorithm using the MapReduce model, which runs in constant rounds and requires only sublinear local space at each worker, which makes our estimation approach applicable to big data scenarios. We perform an extensive experimental evaluation of our silhouette approximation algorithm, comparing its performance to a number of baseline heuristics on real and synthetic datasets. The experiments provide evidence that, unlike other heuristics, our estimation strategy not only provides tight theoretical guarantees but is also able to return highly accurate estimations while running in a fraction of the time required by the exact computation, and that its distributed implementation is highly scalable, thus enabling the computation of internal measures for very large datasets for which the exact computation is prohibitive.

1 Introduction

Clustering is a fundamental primitive for the unsupervised analysis of datasets, and finds applications in a number of areas including pattern recognition, bioinformatics and biomedicine, data management [2]. In its more general definition, clustering requires to identify groups of elements where each group exhibits high similarity among its members while elements in different groups are dissimilar. Starting from this common definition, several algorithms have been proposed to identify clusters in a dataset [11], often formalizing clustering as an optimization problem (based on a cost function). The resulting optimization problems are usually computationally hard to solve, and algorithms providing rigorous approximations are often sought in such cases. More recently the focus has been on developing efficient methods that scale to the massive size of modern datasets [3,4,7,17,18], while still providing rigorous guarantees on the quality of the solution.

A common step after clustering has been performed is clustering evaluation (sometimes called cluster validation). Cluster validation usually employs an evaluation measure capturing the goodness of a clustering structure. Evaluation measures are classified into unsupervised or internal measures, which do not rely on external information, and supervised or external measures, which assess how well a cluster structure matches the structure defined by external
information [21]. While external measures are useful only when additional external knowledge regarding the cluster structure of the data is available, internal measures find application in every scenario.

The most commonly used internal measure for clustering evaluation is the silhouette coefficient [22] (for brevity, called silhouette in this paper). The silhouette of a clustering is the average silhouette of all elements in the clusters, and, in turn, the silhouette \( s(e) \) of an element \( e \) in some cluster \( C \) is defined as the ratio \( (b(e) - a(e))/\max\{a(e), b(e)\} \), where \( a(e) \) is the average distance of \( e \) from the other elements of \( C \), and \( b(e) \) is the minimum average distance of \( e \) from the elements of another cluster \( C' \). In other words, \( s(e) \) provides and indication to what extent \( e \) is closer (on average) to elements in its cluster \( C \) than to elements in the “closest” cluster \( C' \neq C \). The naïve computation of the silhouette for a clustering of \( n \) elements requires \( \Theta(n^2) \) distance calculations, which is unfeasible for massive datasets. Surprisingly, while several methods have been proposed to efficiently cluster large datasets with rigorous guarantees on the quality of the solution, there are no methods to efficiently approximate the silhouette featuring provably high accuracy.

1.1 Related Work

While the silhouette is one of the most popular internal measures for clustering evaluation [19, 23, 25], the quadratic complexity of the naïve exact calculation makes its use impractical for clusterings of very large datasets. For this reason, some attempts have been made to propose variants that are faster to compute, or to simplify its calculation in some special cases.

Hruschka et al. [12] present the simplified silhouette for the evaluation of clusterings obtained on the basis of objective functions involving squared Euclidean distances (e.g., \( k \)-means clusterings [2]). The simplified silhouette is a variant of the silhouette, where for each element \( e \) in a cluster, the quantity \( a(e) \) (resp., \( b(e) \)) in the original definition is redefined as the (squared) distance between \( e \) and the centroid of its cluster (resp., the closest centroid of another cluster). In this fashion, the complexity of the whole computation reduces to \( O(nk) \), improving substantially over the naïve calculation of the exact silhouette for reasonable values of \( k \). While the case studies considered by Hruschka et al. [12] and Wang et al. [24] provide empirical evidence that the simplified silhouette can be an effective evaluation measure for clusterings returned by Lloyd’s algorithm [16], there is no evidence of its effectiveness for other types of clusterings (e.g., clusterings based on other distance functions). In fact, even for clusterings based on the \( k \)-means function, the analysis of Wang et al. [24] shows that the discrepancy between the original silhouette and the simplified silhouette can grow very large.

A heuristic trick for speeding-up the computation of the silhouette for clusterings based on Euclidean distances was proposed by Frahling and Sohler [10]. For each element \( e \) of a cluster \( C \), while the term \( a(e) \) is computed according to its definition, in an attempt to reduce the operations needed to compute the term \( b(e) \), the heuristic first determines the average distance \( d(e, C') \) between \( e \) and the elements of the cluster \( C' \neq C \), whose centroid is closest to \( e \), and then sets \( b(e) = d(e, C') \) in case the distance between \( e \) and the centroid of any other cluster \( C'' \not\in \{C, C'\} \) is larger than or equal to \( d(e, C') \), since in this case there is no need to compute any other average distance \( d(e, C'') \). However, when this is not the case, \( b(e) \) must be computed according to its definition. Despite the practicality of the heuristic, its worst case complexity remains clearly quadratic.

In Apache Spark\(^1\) one of the most popular programming frameworks for large-scale data processing, optimized methods are provided for computing the silhouette of clusterings under \( d \)-dimensional squared Euclidean and one formulation of cosine distance. Indeed, in these specific cases, simple algebra suffices to show that precomputing, for each of the \( k \) clusters, a limited number of values dependent on the coordinates of the cluster’s points, is sufficient to yield a fully parallelizable algorithm featuring \( O(nkd) \) work. We wish to observe that computing the silhouette by making use of squared distance measures tends to amplify distances and, consequently, differences between distances. The result is that the module of the silhouette is pushed closer to 1 than what would be obtained with linear distances, thus amplifying positive and negative scores.

1.2 Our Contributions

In this work, we target the problem of the efficient computation of an accurate estimate of the silhouette of a given clustering under general metric distances. In this regard, our contribution is fourfold:

- We develop the first efficient, sampling-based algorithm for estimating the silhouette with provable approximation guarantees. In our algorithm, we employ a Probability Proportional to Size (PPS) sampling scheme, pioneered in the context of distance query processing [8]. For any fixed \( \varepsilon, \delta \in (0, 1) \), our algorithm approximates the silhouette of a \( k \)-clustering of \( n \) elements within an additive error \( 4\varepsilon/(1-\varepsilon) \) with probability at least

\(^1\)https://spark.apache.org/
1 − δ, using only \( O(nk\varepsilon^{-2}\log(nk/\delta)) \) distance computations, which constitutes a dramatic improvement over the \( \Theta(n^2) \) distance computations required by the naive exact algorithm.

- We generalize our algorithm to compute rigorous approximations of other internal measures, such as cohesion and separation.
- We provide a distributed implementation of our algorithm using the Map-Reduce framework \([9][20]\), which runs in constant rounds, and requires only sublinear space at each worker.
- We perform an extensive suite of experiments on real and synthetic datasets to assess the effectiveness and efficiency of our algorithm, and to compare it with known approaches for fast silhouette computation/approximation. The experiments show that, in practice, our algorithm provides silhouette estimates featuring very low absolute error (less than 0.01 in most cases) with small variance \(< 10^{-3}\) using a very small fraction of the distance computations required by the exact calculation. Moreover, we demonstrate that the returned estimates are far superior in quality to those returned by a naive yet natural heuristics based on uniform sampling, or by a generalization of the method in \([12]\) to general distances, which are both affected by errors that can be so large to render the returned estimates of little use in the most typical scenario of application of the silhouette coefficient, that is, the choice of the correct cluster granularity. We also provide evidence that the MapReduce implementation of our algorithm enables the estimation of the silhouette for clusterings of massive datasets (e.g., 1 billion elements) for which the exact computation is out of reach, and show that our general (unoptimized) distributed implementation is also competitive with the specialized (optimized) Spark routine returning the exact silhouette value only in the case of squared Euclidean distances.

It is important to remark that while previously known approaches to efficiently compute or approximate the silhouette have been developed for specific distance functions, namely squared Euclidean and cosine distances, our algorithm provides provably accurate silhouette estimations for clusterings based on any metric distance.

1.3 Organization of the paper

The rest of the paper is structured as follows. Section 2 contains the description of our proposed strategy for silhouette estimation (Subsection 2.1), its accuracy and performance analysis (Subsection 2.2), the generalization of the approach to other internal evaluation measures (Subsection 2.3), and the MapReduce implementation (Subsection 2.4). Section 3 reports the results of an extensive suite of experiments performed to evaluate the effectiveness and scalability of our silhouette estimation algorithm on synthetic and real datasets. Section 4 concludes the paper with some final remarks.

2 Methods

Consider a metric space \( U \) with distance function \( d(\cdot, \cdot) \), and let \( V = \{e_1, \ldots, e_n\} \subseteq U \) be a dataset of \( n \) elements. Let also \( C = \{C_1, \ldots, C_k\} \) be a \( k \)-clustering of \( V \), that is, a partition of \( V \) into \( k \) disjoint non-empty subsets called clusters. A popular measure to assess clustering quality was introduced by Rousseeuw in 1987 \([22]\). Specifically, the silhouette of an element \( e \in V \) belonging to some cluster \( C_i \), is defined as

\[
s(e) = \frac{b(e) - a(e)}{\max\{a(e), b(e)\}},
\]

where

\[
a(e) = \frac{\sum_{e' \in C_i} d(e, e')}{|C_i| - 1},
\]

\[
b(e) = \min_{C_j \neq C_i} \frac{\sum_{e' \in C_j} d(e, e')}{|C_j|}
\]

denote, respectively, the average distance of \( e \) from the other elements in its cluster, and the minimum average distance of \( e \) from the elements in some other cluster. The silhouette of the clustering \( C \) is the average silhouette of all the elements of \( V \), namely:

\[
s(C) = \frac{\sum_{i=1}^{n} s(e_i)}{n}.
\]

From the above definitions it immediately follows that the values \( s(e) \), with \( e \in V \), and \( s(C) \) range in \([-1, 1]\). A positive value for \( s(e) \) implies that \( e \) has been assigned to an appropriate cluster, while a negative value implies that there might be a better cluster where \( e \) could have been placed. Therefore, \( s(e) \) can be interpreted as a measure of the
quality of the clustering from the perspective of element \( e \). In turn, \( s(C) \) provides a global measure of the quality of the whole clustering, where a value closer to 1 indicates higher quality. The exact computation of \( s(C) \) requires \( O(n^2) \) distance calculations, which is prohibitive when dealing with large datasets. In the following subsection, we present a randomized strategy to yield an estimate of \( s(C) \), which is accurate within a provable error bound, with sufficiently high probability, and amenable to an efficient distributed computation.

### 2.1 A Fast Algorithm for Silhouette Estimation

Consider the estimation of the silhouette \( s(C) \) for a \( k \)-clustering \( C = \{C_1, \ldots, C_k\} \) of a set \( V \) of \( n \) elements from a metric space \( U \). For each \( e \in V \) and \( C_j \in C \), define

\[
W_{C_j}(e) = \sum_{e' \in C_j} d(e, e').
\]

Let \( e \) belong to a cluster \( C \). It is easy to see that the quantities \( a(e) \) and \( b(e) \) in the definition of the silhouette \( s(e) \) can be rewritten as

\[
a(e) = W_{C}(e)/(|C| - 1) \quad \text{and} \quad b(e) = \min_{C_j \neq C} \{W_{C_j}(e)/|C_j|\}.
\]

Building on this observation, our approach to approximating \( s(C) \) is based on estimating the \( W_{C_j}(e) \)'s by exploiting the **Probability Proportional to Size** (PPS) sampling strategy inspired by the work of Chechik et al. \cite{chechik2012}. In particular, we determine a collection of \( k \) small samples, one for each cluster \( C_j \) of \( C \), which guarantees that \( W_{C_j}(e) \) can be estimated within a user-bounded error, with high probability. The details are given in what follows.

Consider a fixed error tolerance threshold \( 0 < \varepsilon < 1 \) and a probability \( 0 < \delta < 1 \). Our algorithm, dubbed PPS-SILHOUETTE (see Algorithm 1 for the pseudocode), consists of two steps. In Step 1, for each cluster \( C_j \in C \), the algorithm computes a sample \( S_{C_j} \) of expected size \( t = \left\lceil \frac{c}{\varepsilon^2 \ln (4nk/\delta)} \right\rceil \) for a suitably chosen constant \( c \), while in Step 2 the \( S_{C_j} \)'s are used to approximate the \( W_{C_j}(e) \)'s. In Step 1, each cluster \( C_j \) is processed independently. If \( |C_j| \leq t \), then \( S_{C_j} \) is set to \( C_j \), otherwise, the following actions are performed.

1. An initial sample \( S_{C_j}^{(0)} \) is obtained by performing Poisson sampling over \( C_j \) where each \( e \in C_j \) is included in \( S_{C_j} \) independently with probability \( (2/|C_j|) \ln(2k/\delta) \). (This initial sample will contain an element relatively close to a majority of the elements of \( C_j \), with sufficiently high probability, a property which is necessary to enforce the quality of the final sampling.)

2. For each \( e' \in S_{C_j}^{(0)} \) the value \( W_{C_j}(e') \) is computed. Then, for each \( e \in C_j \), a PPS coefficient \( \gamma_{e} \) is computed as the maximum between \( 1/|C_j| \) (which corresponds to uniform sampling) and the maximum of the values \( d(e, e')/W_{C_j}(e') \), with \( e' \in S_{C_j}^{(0)} \), which represent the relative contributions of \( e \) to the \( W_{C_j}(e') \)'s of the sample points.

3. Poisson sampling is performed over \( C_j \), where each element \( e \in C_j \) is included in the sample \( S_{C_j} \) independently with probability \( p_e = \min\{1, t\gamma_{e}\} \).

In Step 2, for each \( e \in V \) and each cluster \( C_j \), the sample \( S_{C_j} \) is used to compute the value

\[
\hat{W}_{C_j}(e) = \sum_{e' \in S_{C_j}} \frac{d(e, e')}{p_{e'}},
\]

which is an accurate estimator of \( W_{C_j}(e) \), as will be shown by the analysis. Once all these values have been computed, then, for each \( e \in V \) belonging to a cluster \( C \) we compute the estimates

\[
\hat{a}(e) = \frac{\hat{W}_{C_j}(e)}{|C| - 1},
\]

\[
\hat{b}(e) = \min_{C_j \neq C} \frac{\hat{W}_{C_j}(e)}{|C_j|},
\]

which are in turn used to estimate the silhouette as

\[
\hat{s}(e) = \frac{\hat{b}(e) - \hat{a}(e)}{\max\{\hat{a}(e), \hat{b}(e)\}}.
\]

Finally, we estimate the silhouette of the whole clustering as

\[
\hat{s}(C) = \frac{\sum_{e \in V} \hat{s}(e)}{n}. \quad (2)
\]
In this section we show that, with probability 1, Algorithm 1:

**PPS-S**

for each \( C \) in the following theorem, is a probabilistic upper bound on the relative error of the estimate \( \hat{s}(C) \) of \( s(C) \).

**Proof.** Recall that \( \gamma : \) clustering

**Theorem 1.** There is a suitable choice of the constant \( c \) in the definition of the expected sample size \( t \) used by PPS-SILHOUETTE, which ensures that, with probability at least \( 1 - \delta \), for every element \( e \) and every cluster \( C_j \), the estimate \( \hat{W}_{C_j}(e) \) is such that

\[
\left| \frac{W_{C_j}(e) - \hat{W}_{C_j}(e)}{W_{C_j}(e)} \right| \leq \varepsilon.
\]

**Proof.** The proof mimics the argument devised in [8]. Recall that \( t = \left\lceil \frac{c}{2\pi} \ln \left( 4nk/\delta \right) \right\rceil \). Consider an arbitrary cluster \( C_j \) with more than \( t \) elements (in the case \( |C_j| \leq t \) the theorem follows trivially). For an element \( e \in C_j \), let \( m(e) \) denote the median of the distances from \( e \) to all other elements of \( C_j \). Element \( e \) is called well positioned if \( m(e) \leq 2 \min_{e' \in C_j} m(e') \). It is easy to see that at least half of the elements of \( C_j \) are well positioned. Hence, the initial random sample \( S^{(0)}_{C_j} \) will contain a well positioned element with probability at least \( \left( 1 - (2/|C_j|) \ln(2k/\delta) \right)^{|C_j|/2} \geq 1 - \delta/(2k) \). An easy adaptation of the proof of [8, Lemma 12], shows that if \( S^{(0)}_{C_j} \) contains a well positioned element and \( c \) is a
suitable constant, then the Poisson sample $S_{C_j}$ computed with the probabilities derived from $S_{C_j}^{(0)}$ is such that

$$\left| \frac{\hat{W}_{C_j}(e) - W_{C_j}(e)}{W_{C_j}(e)} \right| \leq \varepsilon,$$

with probability at least $1 - \delta/(2nk)$. By the union bound, it follows that the probability that there exists a cluster $C_j$ such that the initial sample $S_{C_j}^{(0)}$ does not contain a well positioned element is at most $k\delta/(2k) = \delta/2$. Also, by conditioning on the fact that for all clusters $C_j$ the initial sample $S_{C_j}^{(0)}$ contains a well positioned node, by using again the union bound we obtain that the probability that there exists an element $e$ and a cluster $C_j$ for which $|(|\hat{W}_{C_j}(e) - W_{C_j}(e)|)/W_{C_j}(e)| > \varepsilon$ is at most $nk\delta/(2nk) = \delta/2$, which concludes the proof. 

From now on, we assume that the relative error bound stated in Theorem holds for every element $e$ and every cluster $C_j$, an event which we will refer to as event $E$. Consider an arbitrary element $e \in V$ belonging to some cluster $C$ and let $\hat{a}(e), \hat{b}(e)$, and $\hat{s}(e)$ be the values computed by PPS-SILHOUETTE.

**Lemma 1.** If event $E$ holds, then

$$\left| \frac{\hat{a}(e) - a(e)}{a(e)} \right| \leq \varepsilon$$

*Proof.* The proof follows immediately from the definition of $\hat{a}(e)$ and the relative error bound assumed for $\hat{W}_{C_j}(e)$. 

**Lemma 2.** If event $E$ holds, then

$$\left| \frac{\hat{b}(e) - b(e)}{b(e)} \right| \leq \varepsilon$$

*Proof.* Consider an arbitrary cluster $C_j$ and let $b_{C_j}(e) = W_{C_j}(e)/|C_j|$ and $\hat{b}_{C_j}(e) = \hat{W}_{C_j}(e)/|C_j|$. As in the previous lemma we can immediately see that

$$\left| \frac{\hat{b}_{C_j}(e) - b_{C_j}(e)}{b_{C_j}(e)} \right| \leq \varepsilon.$$ 

Recall that $b(e) = \min_{C_j \in C} b_{C_j}(e)$ and that $\hat{b}(e) = \min_{C_j \in C} \hat{b}_{C_j}(e)$. Suppose that $b(e) = b_{C''}(e)$ and $\hat{b}(e) = \hat{b}_{C''}(e)$, for some, possibly different, clusters $C'$ and $C''$. We have:

$$(1 - \varepsilon)b(e) = (1 - \varepsilon)b_{C''}(e) \leq (1 - \varepsilon)b_{C''}(e) \leq \hat{b}_{C''}(e) = \hat{b}(e)$$

and

$$\hat{b}(e) = \hat{b}_{C''}(e) \leq \hat{b}_{C''}(e) \leq (1 + \varepsilon)b_{C''}(e) = (1 + \varepsilon)b(e),$$

and the lemma follows. 

Now we establish a bound on the relative error for the term appearing in the denominator of the formula defining $\hat{s}(e)$. Define $m(e) = \max\{a(e), b(e)\}$ and $\hat{m}(e) = \max\{\hat{a}(e), \hat{b}(e)\}$. We have:

**Lemma 3.** If event $E$ holds, then

$$\left| \frac{\hat{m}(e) - m(e)}{m(e)} \right| \leq \varepsilon.$$ 

*Proof.* Suppose that $m(e) = a(e)$, hence $a(e) \geq b(e)$ (the case $m(e) = b(e)$ can be dealt with similarly). If $\hat{m}(e) = \hat{a}(e)$, the bound follows directly from Lemma. Instead, if $\hat{m}(e) = \hat{b}(e)$, hence $\hat{b}(e) \geq \hat{a}(e)$, the bound follows since

$$\hat{m}(e) = \hat{b}(e) \leq (1 + \varepsilon)b(e) \quad \text{(by Lemma)}$$

$$\leq (1 + \varepsilon)a(e) = (1 + \varepsilon)m(e),$$
and
\[
\hat{m}(e) = \hat{b}(e) \geq \hat{a}(e) \geq (1 - \varepsilon)a(e) \quad \text{(by Lemma 1)}
= (1 - \varepsilon)m(e).
\]

As a last technical step, the following lemma establishes an error bound on the estimation of the silhouette \(s(e)\).

**Lemma 4.** If event \(E\) holds, then
\[
|\hat{s}(e) - s(e)| \leq \frac{4\varepsilon}{1 - \varepsilon}.
\]

**Proof.** By virtue of the relative error bounds established by Lemmas 1, 2 and 3, we have that
\[
\hat{s}(e) = \frac{\hat{b}(e) - \hat{a}(e)}{\hat{m}(e)} \leq \frac{(1 + \varepsilon)b(e) - (1 - \varepsilon)a(e)}{(1 - \varepsilon)m(e)}.
\]

Straightforward transformations show that
\[
(1 + \varepsilon)b(e) - (1 - \varepsilon)a(e)
= s(e) + \frac{2\varepsilon}{1 - \varepsilon} \left( s(e) + \frac{a(e)}{m(e)} \right).
\]

Since \(s(e) \leq 1\) and \(a(e) \leq m(e)\), we get
\[
\hat{s}(e) \leq s(e) + \frac{4\varepsilon}{1 - \varepsilon}.
\]

In a similar fashion, it follows that
\[
\hat{s}(e) = \frac{\hat{b}(e) - \hat{a}(e)}{\hat{m}(e)}
\geq \frac{(1 - \varepsilon)b(e) - (1 + \varepsilon)a(e)}{(1 + \varepsilon)m(e)}
= s(e) - \frac{2\varepsilon}{1 + \varepsilon} \left( s(e) + \frac{a(e)}{m(e)} \right)
\geq s(e) - \frac{4\varepsilon}{1 + \varepsilon} \geq s(e) - \frac{4\varepsilon}{1 - \varepsilon}.
\]

An upper bound to the absolute error incurred when estimating \(s(C)\) through the value \(\hat{s}(C)\) computed by PPS-SILHOUETTE, is established in the following theorem, whose proof is an immediate consequence of the definition of the two quantities (Equations 1 and 2) and of Theorem 1 and Lemma 4.

**Theorem 2.** Let \(V\) be a dataset of \(n\) elements, and let \(C\) be a \(k\)-clustering of \(V\). Let \(\hat{s}(C)\) be the estimate of the silhouette of the clustering \(s(C)\) computed by PPS-SILHOUETTE for given parameters \(\varepsilon\) and \(\delta\), with \(0 < \varepsilon, \delta < 1\), and for a suitable choice of constant \(c > 0\) in the definition of the sample size. Then,
\[
|\hat{s}(C) - s(C)| \leq \frac{4\varepsilon}{1 - \varepsilon}
\]

with probability at least \(1 - \delta\).

We now analyze the running time of PPS-SILHOUETTE, assuming that the distance between two points can be computed in constant time. In Step 1, the running time is dominated by the computation of the distances between the points of each sufficiently large cluster \(C_j\) and the points that form the initial sample \(S_0^{\jmath}\). A simple application of the Chernoff bound shows that, with high probability, from each such cluster \(C_j\), \(O(\log(nk/\delta))\) points are included in \(S_0^{\jmath}\). Thus,
\[
O \left( \sum_{j=1}^{k} |C_j| \log(nk/\delta) \right) = O (n \log(nk/\delta)).
\]
distance computations are performed, altogether. For what concerns Step 2, its running time is dominated by the computation of the distances between all points of \( V \) and the points of the union of all samples extracted from the clusters. A simple adaptation of the proof of [8, Corollary 11] and a straightforward application of the Chernoff bound shows that there are \( O(kt) \) sample points overall, with high probability, where

\[
t = \left\lceil \frac{c}{2\varepsilon^2} \ln \left( 4nk/\delta \right) \right\rceil
\]

is the expected sample size for each cluster. Therefore, Step 2 performs

\[
O \left( \frac{nk}{\varepsilon^2} \log(nk/\delta) \right)
\]

distance computations overall. As a consequence, the running time of the algorithm is \( O \left( nk\varepsilon^{-2} \log(nk/\delta) \right) \) which, for reasonable values of \( k, \varepsilon \) and \( \delta \), is a substantial improvement compared to the quadratic complexity of the exact computation.

### 2.3 Generalization To Other Measures

The PPS-based sampling strategy adopted for approximating the silhouette of a clustering can be applied to other measures used for internal clustering evaluation, which are based on sums of distances between points of the dataset. This is the case, for instance, of measures that compare the cohesion (i.e., the average intracluster distance) and the separation (i.e., the average intercluster distance) of the clustering [21].

More precisely, consider a \( k \)-clustering \( C = \{C_1, \ldots, C_k\} \) and define the cohesion and separation of \( C \) as

\[
\text{Coh}(C) = \frac{1}{2} \sum_{j=1}^{k} \frac{\sum_{e',e'' \in C_j} d(e', e'')}{\binom{|C_j|}{2}}
\]

\[
\text{Sep}(C) = \frac{\sum_{1 \leq j_1 < j_2 \leq k} \sum_{e' \in C_{j_1}} \sum_{e'' \in C_{j_2}} d(e', e'')}{\sum_{1 \leq j_1 < j_2 \leq k} (|C_{j_1}| |C_{j_2}|)}
\]

respectively. (These measures have been also employed to assess the average cluster reliability for a clustering of a network where distances correspond to connection probabilities [6, 15].) We can rewrite the above measures in terms of the sums \( W_C(e) \) defined in the previous section, as follows

\[
\text{Coh}(C) = \frac{1}{2} \sum_{j=1}^{k} \frac{\sum_{e \in C_j} W_{C_j}(e)}{\binom{|C_j|}{2}}
\]

\[
\text{Sep}(C) = \frac{\sum_{1 \leq j_1 < j_2 \leq k} \sum_{e \in C_{j_1}} W_{C_{j_2}}(e)}{\sum_{1 \leq j_1 < j_2 \leq k} (|C_{j_1}| |C_{j_2}|)}
\]

Clearly, approximations of the \( W_C(e) \)'s with low relative errors immediately yield approximations with low relative error for \( \text{Coh}(C) \) and \( \text{Sep}(C) \). Specifically, define \( \hat{\text{Coh}}(C) \) and \( \hat{\text{Sep}}(C) \) as the respective approximations to \( \text{Coh}(C) \) and \( \text{Sep}(C) \) obtained by substituting each \( W_C(e) \) occurring in the above equations with the value \( \hat{W}_C(e) \) computed within PPS-SILHOUETTE. The following theorem is an immediate consequence of Theorem 1.

**Theorem 3.** Let \( V \) be a dataset of \( n \) elements, and let \( C \) be a \( k \)-clustering of \( V \). Let \( \hat{\text{Coh}}(C) \) and \( \hat{\text{Sep}}(C) \) be the respective approximations to \( \text{Coh}(C) \) and \( \text{Sep}(C) \) based on the values \( \hat{W}_C(e) \) computed within PPS-SILHOUETTE for given parameters \( \varepsilon \) and \( \delta \), with \( 0 < \varepsilon, \delta < 1 \), and for a suitable choice of constant \( c > 0 \) in the definition of the sample size. Then,

\[
\left| \frac{\hat{\text{Coh}}(C) - \text{Coh}(C)}{\text{Coh}(C)} \right| \leq \varepsilon
\]

\[
\left| \frac{\hat{\text{Sep}}(C) - \text{Sep}(C)}{\text{Sep}(C)} \right| \leq \varepsilon
\]

with probability at least \( 1 - \delta \).
2.4 Map-Reduce Implementation

A MapReduce algorithm\(^{[9][13][14][20]}\) executes in a sequence of parallel rounds. In a round, a multiset \(X\) of key-value pairs is first transformed into a new multiset \(X'\) of key-value pairs by applying a given map function independently to each pair, and then into a final multiset \(Y\) of pairs by applying a given reduce function independently to each subset of pairs of \(X'\) having the same key. The application of a reduce function to a set of pairs with same key is referred to as a reducer\(^{[14]}\). The model features two parameters, \(M_L\), the local memory available for each application of a map/reduce function, and \(M_A\), the aggregate memory ever required over the entire course of the algorithm. In what follows, we describe a 4-round MapReduce implementation of PPS-SILHOUETTE, analyzing the memory requirements of each round.

Throughout the algorithm, a key-value pair will be written as \((\text{key} | \text{value}_1, \ldots, \text{value}_r)\), where \(\{\text{value}_1, \ldots, \text{value}_r\}\) is an \(r\)-dimensional value. Consider a \(k\)-clustering \(C = \{C_1, \ldots, C_k\}\) of a dataset \(V = \{e_1, \ldots, e_n\}\) of \(n\) elements. We assume that, initially, the clustering is represented by the following set of key-value pairs:

\[
\{(i|e_i, j_i) : 1 \leq i \leq n \land e_i \in C_{j_i}\}.
\]

We also assume that the values \(n, k, t\) used in PPS-SILHOUETTE, as well as all \(|C_j|\)'s, are given to the program. In order to exploit parallelism, our implementation partitions the points of \(V\) into \(w\) subsets of size \(n/w\) each, to be processed in parallel, where \(w \in [0, n-1]\) is a design parameter which may be used to exercise suitable parallelism-memory tradeoffs. The four rounds are described in detail below.

Round 1:

- **Map**: Map each pair \((i|e_i, j_i)\) into the pair \((i \mod w | e_i, j_i, 0)\). Also, with probability \((2/(|C_{j_i}|))\ln(2k/\delta)\) select \(e_i\) to be part of the initial Poisson sample \(S_{C_{j_i}}^{(0)}\), and produce the \(w\) additional pairs \((\ell| e_i, j_i, 1)\), with \(0 \leq \ell < w\).

- **Reduce**: Let \(V_\ell\) be the set of elements \(e_i\) for which there is a pair \((\ell| e_i, j_i, 0)\). (Observe that the \(V_\ell\)'s form a balanced partition of \(V\) into \(w\) subsets.) For each pair \((\ell| e_i, j_i, 1)\) compute the sum \(W_{i,\ell}\) of the distances from \(e_i\) to all elements of \(V_\ell \cap C_{j_i}\), and produce the pair \((\ell| e_i, j_i, W_{i,\ell}, 1)\). Instead, for each pair \((\ell| e_i, j_i, 0)\) produce the pair \((\ell| e_i, j_i, 0, 0)\).

By the analysis of the previous subsection, we know that, with high probability, \(O(k \ln(nk/\delta))\) points have been selected to be part of the initial samples \(S_{C_{j_i}}^{(0)}\)'s (a copy of all these points, represented by pairs with 1 at the end, exists for each key \(\ell\)). Therefore, this round requires local memory \(M_L = O(n/w + k \ln(nk/\delta))\), with high probability, and aggregate memory \(M_A = O(wM_L)\).

Round 2:

- **Map**: Map each pair \((\ell| e_i, j_i, 0, 0)\) into itself, and each pair \((\ell| e_i, j_i, W_{i,\ell}, 1)\) into the \(w\) pairs \((\ell'| e_i, j_i, 0)\), with \(0 \leq \ell' < w\).

- **Reduce**: Each reducer, corresponding to some key \(\ell\), now contains all the information needed to compute the values \(W_C(e)\) for each cluster \(C\) and element \(e \in S_{C_{j_i}}^{(0)}\). This in turn implies that the reducer can also compute all sampling probabilities \(p(e_i)\) for \(e_i \in V_\ell\), by executing the operations specified in PPS-SILHOUETTE. The reducer computes these probabilities and produces the pairs \((\ell| e_i, j_i, p(e_i))\), one for each \(e_i \in V_\ell\).

By the observations made at the end of Round 1, this round requires local memory \(M_L = O(n/w + wk \log(nk/\delta))\), with high probability, and aggregate memory \(M_A = O(wM_L)\).

Round 3:

- **Map**: Map each pair \((\ell| e_i, j_i, p(e_i))\) into the pair \((\ell| e_i, j_i, 0)\). Also, with probability \(p(e_i)\) select \(e_i\) to be part of the Poisson sample \(S_{C_{j_i}}\), and produce the \(w\) additional pairs \((\ell'| e_i, j_i, 1)\), with \(0 \leq \ell' < w\).

- **Reduce Phase**: Each reducer, corresponding to some key \(\ell\), now contains all the information needed to compute the approximate silhouette values \(\hat{s}(e_i)\) for each element in \(e_i \in V_\ell\). The reducer computes the sum of these values, denoted by \(\hat{s}_\ell\), and produces the single pair \((0| \hat{s}_\ell)\).

\(^2\)We remark that the MapReduce algorithms presented in this paper also afford an immediate implementation and similar analysis in the Massively Parallel Computation (MPC) model\(^{[5]}\), which is popular in the database community.
By the analysis of the previous subsection, we know that, with high probability, the size of union of the Poisson samples $S_{C_j}$’s is $O(tk^2)$, with $t = \left\lceil c/(2\epsilon^2) \ln(4nk/\delta) \right\rceil$. Therefore, this round requires local memory $M_L = O(n/w + tk) = O(n/w + (k/\epsilon^2)(nk/\delta))$, with high probability, and aggregate memory $M_A = O(wM_L)$.

**Round 4:**

- **Map:** identity map.
- **Reduce:** The reducer corresponding to key 0 computes and returns $\hat{s}_e = (1/n) \sum_{t=1}^{w-1} \hat{s}_t$.

This round requires $M_L = M_A = O(w)$.

Overall, the above 4-round MapReduce algorithm requires local memory $M_L = O(n/w + (w + 1/\epsilon^2)k \log(nk/\delta))$, with high probability, and aggregate memory $M_A = O(wM_L)$. It is easy to see that for fixed values of $\epsilon$ and $\delta$, and for $k = O(n/\log n)$, by choosing $w = \Theta(\sqrt{n/(k \log n)})$, we obtain local memory $M_L = O(\sqrt{n}k \log n)$ and linear aggregate memory, with high probability. We remark, that for reasonable values of $k$, the required local memory is substantially sublinear, which is the “holy grail” of MapReduce algorithms [20].

### 3 Experimental Evaluation

We ran an extensive experimental evaluation of our PPS-SILHOUETTE algorithm. The goals of our experimental evaluation are threefold: first, to evaluate the accuracy of the approximation of the silhouette provided by our algorithm and to compare it against known heuristic baselines and exact (specialized) methods; second, to assess the impact of using the approximation provided by our algorithm in place of the exact value of the silhouette in a typical scenario (i.e., to identify the most suitable number of clusters); third, to evaluate experimentally the scalability of our MapReduce implementation on a distributed platform. The rest of this section is organized as follows: Subsection 3.1 describes the heuristic baselines considered in the evaluation of our algorithm; Subsection 3.2 provides details on the implementation and on the software/hardware environment used; Subsection 3.3 describes the datasets considered in our evaluation and the parameters used for their analysis; Subsection 3.4 discusses the results on the quality of the approximation provided by our algorithm; and, finally, Subsection 3.5 shows the scalability results.

#### 3.1 Baselines

We gauge the performance of our PPS-SILHOUETTE algorithm against two heuristics: one based on uniform sampling, and the other based on the simplified silhouette introduced in [24] for the evaluation of K-means clusterings, generalized to apply to arbitrary clusterings and metric spaces. More precisely, the first heuristic consists essentially in the execution of Step 2 of PPS-SILHOUETTE, where the samples $S_{C_j}$ are chosen via a uniform Poisson sampling, using the same probability $p(e) = t/|C_j|$ for each $e \in C_j$. The comparison with this heuristics aims at highlighting the added value of PPS vs straightforward uniform sampling. We refer to this heuristics as the uniform sampling algorithm.

The second heuristics adapts the simplified silhouette in [24] by substituting the use of the centroid of each cluster $C_j$ (which makes sense only when squared Euclidean distances are used) with that of the medoid $\text{med}(C_j)$, defined as

$$\text{med}(C_j) = \arg \min_{\{e \in C_j\}} \sum_{e' \in C_j} d(e,e').$$

The simplified silhouette of a point $e$ in cluster $C$ is then estimated as $\hat{s}(e) = (\hat{b}(e) - \hat{a}(e))/\max\{\hat{b}(e),\hat{a}(e)\}$, where $\hat{a}(e) = d(e,\text{med}(C))$ and $\hat{b}(e) = \min_{C_j \neq C} d(e,\text{med}(C_j))$. The simplified silhouette of the clustering is the arithmetic average of the simplified silhouette of its elements.

#### 3.2 Implementation and Environment

For the assessment of the accuracy of our approach, we devised Java-based sequential implementations of PPS-SILHOUETTE, the two heuristic baselines described in the previous subsection, and the exact computation of the silhouette (based on the definition). Also, for the assessment of scalability, we devised a MapReduce implementation of PPS-SILHOUETTE using the Apache Spark framework (with Java).

[3] All our implementations are available at [https://github.com/CalebTheGame/AppxSilhouette](https://github.com/CalebTheGame/AppxSilhouette) and [https://spark.apache.org](https://spark.apache.org)
the size of the initial samples \( S^{(0)}_{C_j} \) is obtained by fixing \( \delta = 0.1 \). Moreover, rather than fixing error tolerance thresholds \( \varepsilon \), we varied the accuracy by setting different values for the expected size \( t \) of samples \( S_{C_j} \).

The scalability experiments were run on CloudVeneto\(^4\), an institutional provider of cloud computing services, that granted us access to 9 PowerEdge M620 nodes, each with octa-core Intel Xeon E5-2670v2 2.50 GHz and 16 GB of RAM, running Ubuntu 16.04.3 LTS with Hadoop 2.7.4 and Apache Spark 2.4.4.

### 3.3 Datasets and Parameters

In our experimental evaluation we considered both synthetic datasets and real datasets. Synthetic datasets have been chosen so to contain a few outlier points, with the intent of making the accurate estimation of the silhouette more challenging. Specifically, for different values of \( n \) (ranging from tens of thousands to one billion), we generated \( n - 10 \) points uniformly at random within the sphere of unit radius, centered at the origin of the 3-dimensional Euclidean space, and 10 random points on the surface of the concentric sphere of radius \( 10^t \). For what concerns real datasets, we used reduced versions of “Covertype” and “HIGGS” datasets\(^5\). The former contains 100000 55-dimensional points, used to train learning algorithms for high-energy Physics experiments (as in previous works \(^7\,[17]\)), only the 7 summary attributes of the original 28 have been retained). For all datasets, the clusterings used to test the algorithms have been obtained by applying the \( k \)-medoids clustering algorithm implemented in the Java Machine Learning Library\(^6\,[1]\), using the Euclidean distance.

### 3.4 Quality of Approximation

In the first experiment, aimed at demonstrating the superiority of PPS over uniform sampling, we compared the accuracy of the silhouette estimations returned by our PPS-Silhouette algorithm and by the uniform sampling algorithm, using synthetic data. In order to make the computation of the exact value feasible, we considered instances of the synthetic dataset with a relatively small number of elements \( (n = 2 \times 10^4) \) and \( k \)-clusterings \( C \) with \( k \in \{2, \ldots, 10\} \). We ran both PPS-Silhouette and the uniform sampling algorithm with values of the (expected) sample size \( t \in \{64, 128, 256, 512, 1024\} \). We evaluated accuracy of an estimation \( \hat{s}(C) \) through the absolute error \( |\hat{s}(C) - s(C)| \). Table 1 reports maximum, average, and variance of the absolute error over 100 runs of the two algorithms, for each configuration of parameters \( k \) and \( t \). The results show that PPS-Silhouette provides a very accurate approximation to the silhouette already with \( t = 64 \), for which the average absolute error is at most 0.017 for all values of \( k \) and the maximum value is at most 0.084 for all cases but \( k = 6 \). The approximation quickly improves when larger values of \( t \) are considered, with an average error at most 0.01 and a maximum error of 0.064 when \( t = 128 \), and an average error at most 0.002 and a maximum error at most 0.01 when \( t = 1024 \). PPS-Silhouette also features a very low variance, which is \( < 10^{-5} \) in all cases. These results show that our PPS-Silhouette algorithm provides a very accurate approximation of the silhouette even with a limited number of samples.

On the other hand, the table shows that for \( t = 64 \) the estimate provided by the uniform sampling algorithm incurs considerably larger average and maximum absolute errors for most values of \( k \). In fact, for seven out of nine values of \( k \) the average error of the uniform sampling algorithm is one order of magnitude larger than the average error of PPS-Silhouette, and, in the remaining two cases, two orders of magnitude larger. Interestingly, the accuracy of the uniform sampling algorithm does not significantly improve even for \( t = 1024 \) since for four out of nine values of \( k \) the average error is greater than 0.11, and maximum error greater than 0.19, and in four cases the error is two orders of magnitude larger than the one of PPS-Silhouette. These results show that the use of PPS sampling is crucial to obtain good approximations of the silhouette while keeping the sample size small.

In the second experiment, we assessed the impact of relying on estimated rather than exact values in the most typical scenario of use of the silhouette, suggested in the original paper \(^{22}\), that is, identifying the best granularity \( k \) when the same clustering algorithm is applied to a dataset with different values \( k \). To this end, we performed the following experiment. Given the synthetic dataset described above, we ran \( k \)-medoids clustering for all values of \( k \) in an interval \( [2, \ell] \) and we checked whether the best clustering (according to the exact silhouette) was identified using the silhouette estimations returned by PPS-Silhouette and by the uniform sampling algorithm. We ran the experiment for \( \ell = 3, \ldots, 10 \), and expected sample sizes \( t \in \{64, 128, 256, 512, 1024\} \). For each combination of \( \ell \) and \( t \), we considered 100 trials (corresponding to 100 estimates of the silhouette by the two algorithms). Table 2 displays the fraction of times the correct value of \( k \) was identified by the two algorithms. Strikingly, PPS-Silhouette identified the correct

\(\text{http://cloudevneto.it}\)

\(\text{https://archive.ics.uci.edu/ml/datasets/}\)

\(\text{https://github.com/AbeelLab/javaml}\)
Table 1: Maximum, average, and variance of the absolute error of the silhouette estimates returned by PPS-SILHOUETTE (label “PPS”) and the uniform sampling algorithm, (label “uniform”) relative to the $k$-medoid clustering of the synthetic dataset with $n = 2 \cdot 10^4$ points, with $k = 2, 3, \ldots, 10$ and $t = 64, 128, \ldots, 1024$. Values $< 10^{-3}$ are denoted by 0*.

| $k$ | Algorithm | $t=64$ | | | $t=128$ | | | $t=256$ | | | $t=512$ | | | $t=1024$ |
|-----|-----------|-------|-----|-----|-------|-----|-----|-------|-----|-----|-------|-----|-----|-------|
|     |           | max   | avg | var | max   | avg | var | max   | avg | var | max   | avg | var | max   |
| 2   | PPS       | .005  | .001 | 0*  | .004  | .001 | 0*  | .002  | .0*  | 0*  | .001  | .0*  | 0*  | .001  |
|     | uniform   | .207  | .145 | 0*  | .207  | .150 | 0*  | .206  | .143 | 0*  | .204  | .153 | .001 | .199  |
| 3   | PPS       | .018  | .005 | 0*  | .014  | .003 | 0*  | .008  | .002 | 0*  | .009  | .002 | 0*  | .004  |
|     | uniform   | .369  | .235 | .008 | .407  | .247 | .008 | .403  | .217 | .013 | .400  | .177 | .017 | .392  |
| 4   | PPS       | .012  | .003 | 0*  | .007  | .002 | 0*  | .005  | .001 | 0*  | .003  | .001 | 0*  | .002  |
|     | uniform   | .482  | .284 | .007 | .509  | .297 | .006 | .473  | .301 | .005 | .539  | .267 | .015 | .392  |
| 5   | PPS       | .015  | .005 | 0*  | .014  | .003 | 0*  | .008  | .002 | 0*  | .006  | .001 | 0*  | .004  |
|     | uniform   | .174  | .101 | .005 | .498  | .380 | .011 | .478  | .322 | .022 | .482  | .220 | .019 | .438  |
| 6   | PPS       | .047  | .010 | 0*  | .064  | .008 | 0*  | .016  | .004 | 0*  | .011  | .003 | 0*  | .010  |
|     | uniform   | .280  | .174 | .003 | .263  | .147 | .003 | .273  | .121 | .003 | .119  | .002 | .001 | .097  |
| 7   | PPS       | .084  | .017 | 0*  | .043  | .010 | 0*  | .028  | .006 | 0*  | .017  | .003 | 0*  | .008  |
|     | uniform   | .168  | .075 | .001 | .140  | .056 | .001 | .149  | .049 | 0*  | .063  | .012 | 0*  | .013  |
| 8   | PPS       | .078  | .013 | 0*  | .056  | .008 | 0*  | .015  | .003 | 0*  | .009  | .001 | 0*  | .003  |
|     | uniform   | .295  | .187 | .002 | .294  | .159 | .002 | .254  | .188 | .003 | .174  | .050 | .001 | .068  |
| 9   | PPS       | .050  | .013 | 0*  | .057  | .007 | 0*  | .013  | .003 | 0*  | .007  | .001 | 0*  | .003  |
|     | uniform   | .284  | .180 | .003 | .269  | .156 | .003 | .246  | .108 | .003 | .160  | .049 | .002 | .071  |

Table 2: Identification of the value of $k$ yielding the highest silhouette using PPS-SILHOUETTE (label “PPS”) and the uniform sampling algorithm (label “uniform”). For each range of $k \in [2, \ell]$, with $\ell = 3, \ldots, 10$ and $t = 64, 128, \ldots, 1024$, the table shows the percentage of the runs (over 100) where the correct value was identified.

| Range of $k$ | $t=64$ | | | $t=128$ | | | $t=256$ | | | $t=512$ | | | $t=1024$ |
|--------------|--------|-----|-----|--------|-----|-----|--------|-----|-----|--------|-----|-----|--------|
|              | PPS    | uniform | PPS    | uniform | PPS    | uniform | PPS    | uniform | PPS    | uniform | PPS    | uniform |
| 2-3          | 100%   | 66%   | 100%   | 56%   | 100%   | 57%   | 100%   | 71%   | 100%   | 85%   |       |       |
| 2-4          | 100%   | 1%    | 100%   | 2%    | 100%   | 3%    | 100%   | 31%   | 100%   | 72%   |       |       |
| 2-5          | 100%   | 0%    | 100%   | 0%    | 100%   | 6%    | 100%   | 25%   | 100%   | 64%   |       |       |
| 2-6          | 100%   | 0%    | 100%   | 2%    | 100%   | 4%    | 100%   | 28%   | 100%   | 50%   |       |       |
| 2-7          | 100%   | 2%    | 100%   | 1%    | 100%   | 5%    | 100%   | 20%   | 100%   | 53%   |       |       |
| 2-8          | 100%   | 3%    | 100%   | 2%    | 100%   | 5%    | 100%   | 13%   | 100%   | 53%   |       |       |
| 2-9          | 100%   | 2%    | 100%   | 1%    | 100%   | 7%    | 100%   | 25%   | 100%   | 53%   |       |       |
| 2-10         | 100%   | 1%    | 100%   | 3%    | 100%   | 5%    | 100%   | 19%   | 100%   | 57%   |       |       |

For what concerns the uniform sampling algorithm, Table 2 shows that, except for the range $k \in \{2, 3\}$ or $t = 1024$, the algorithm leads to the wrong choice of $k$ more than half of the times. In fact, when $t \leq 256$, the correct value of $k$ is identified no more than 7% of the times, which is less than expected if a random choice among the considered values of $k$ was made. The results clearly improve with $t = 1024$, but still the wrong value of $k$ is identified at least 15% of the times, and close to 50% of the times in most cases. These results provide further evidence of the superiority of PPS sampling.

One might argue that the poor performance of uniform sampling in the previous experiments could be due to the large variance affecting the silhouette estimates. A natural way to reduce variance is to adopt a Monte Carlo approach where the average of several independent estimates is used in lieu of a single estimate. To ascertain the effect of variance reduction, in the third experiment, we considered the largest range $k \in [2, 10]$ of the previous experiment and tested to what extent the two algorithms are able to spot the best granularity when using, for each value of $k$, the average of 100 silhouette estimates. In this experiment, for each $k$ we also computed the (unique) value of the generalized simplified
silhouette described in Subsection 3.1 to compare its effectiveness against the two sampling strategies. The results are shown in Table 3, where the exact value of the silhouette is also shown.

As expected, PPS-SILOUETTE always identifies the correct value already for \( t = 64 \), and, for all \( k \) and \( t \), it provides extremely accurate approximations. On the other hand, the uniform sampling algorithm identifies the correct value of \( k \) only for \( t = 1024 \), and, for smaller values of \( t \), it provides much weaker approximations (indeed, \( t = 512 \) is needed merely to hit the correct sign of the silhouette value). Also, the table shows that the generalized simplified silhouette is not able to identify the correct value of \( k \), which is not surprising considering the weak relation between simplified silhouette and silhouette quantified by \( ILHOUETTE \) for the case of squared Euclidian distances.

Table 3: Comparison between exact silhouette, generalized simplified silhouette, and Monte Carlo estimates obtained by averaging 100 estimates returned by PPS-SILOUETTE (label “PPS”) and the uniform sampling algorithm (label “uniform”), for \( k = 2, 3, \ldots, 10 \) and \( t = 64, 128, \ldots, 1024 \). The highest value identified by each algorithm (one for each \( t \) for PPS and uniform) is highlighted in boldface. Observe that the “correct” value of \( k \) corresponds to the value with highest exact silhouette.

| \( k \) | Exact | Simplified | \( k \) | PPS | Silhouette |
|---|---|---|---|---|---|
| \( t = 64 \) | \( t = 128 \) | \( t = 256 \) | \( t = 512 \) | \( t = 1024 \) | \( t = 64 \) | \( t = 128 \) | \( t = 256 \) | \( t = 512 \) | \( t = 1024 \) |
| 2 | 0.064 | 0.347 | 0.064 | 0.064 | 0.064 | 0.064 | 0.064 | 0.064 | 0.064 | 0.192 | 0.169 | 0.176 | 0.134 | 0.074 |
| 3 | -0.072 | 0.332 | -0.070 | -0.072 | -0.072 | -0.726 | -0.727 | -0.072 | -0.072 | 0.151 | 0.130 | 0.081 | -0.084 | -0.191 |
| 4 | 0.343 | 0.369 | 0.343 | 0.343 | 0.344 | 0.343 | 0.343 | 0.343 | 0.343 | 0.049 | 0.045 | 0.039 | 0.099 | 0.183 |
| 5 | -0.228 | 0.333 | -0.223 | -0.223 | -0.228 | -0.228 | -0.228 | -0.228 | -0.228 | 0.158 | 0.115 | 0.031 | -0.081 | -0.244 |
| 6 | 0.034 | 0.348 | 0.022 | 0.029 | 0.032 | 0.033 | 0.034 | 0.034 | 0.034 | 0.121 | 0.096 | 0.071 | 0.057 | 0.040 |
| 7 | -0.143 | 0.306 | -0.148 | -0.144 | -0.145 | -0.144 | -0.144 | -0.143 | -0.143 | 0.033 | 0.010 | -0.030 | -0.091 | -0.130 |
| 8 | 0.059 | 0.380 | 0.038 | 0.046 | 0.055 | 0.057 | 0.058 | 0.058 | 0.058 | 0.134 | 0.124 | 0.094 | 0.045 | 0.057 |
| 9 | -0.087 | 0.368 | -0.102 | -0.093 | -0.091 | -0.089 | -0.089 | -0.088 | -0.088 | 0.102 | 0.070 | 0.021 | -0.040 | -0.087 |
| 10 | -0.104 | 0.353 | -0.116 | -0.110 | -0.017 | -0.105 | -0.104 | -0.104 | -0.104 | 0.073 | 0.046 | 0.005 | -0.060 | -0.103 |

In the fourth experiment, we compared maximum and average absolute errors (over 100 runs) of the silhouette estimates computed by PPS-SILOUETTE and by the uniform sampling algorithm on the real datasets HIGGS and Covertype described in Subsection 3.3. For this comparison we used two clustering granularities (\( k = 5, 10 \)) and the same range of expected sample sizes as in the previous experiments (\( t = 64, 128, 256, 512, 1024 \)). Table 4 reports the results of the experiments, together with the values of the exact silhouette and of the generalized simplified silhouette, for each dataset and for each configuration of the parameters. Similarly to the case of the synthetic dataset, the table shows that PPS-SILOUETTE provides very accurate estimates already for \( t = 64 \), with an average error smaller than 0.03, and for \( t \geq 256 \) it features an average error below 0.01. The variance (not reported in the table) is below \( 10^{-3} \) in all cases. On these datasets, the uniform sampling algorithm also provides fairly accurate estimates (with variance \( < 10^{-3} \) in all cases). However, for no combination of \( k \) and \( t \) the average error of the uniform sampling algorithm is lower than the one of PPS-SILOUETTE, while its maximum error is slightly better only in four out of twenty configurations. Also, the table shows the poor accuracy of the generalized simplified silhouette, which is worse than the one of PPS-SILOUETTE already for \( t = 64 \). Once again, this experiment confirms the superiority of our PPS-SILOUETTE estimation algorithm with respect to the two competitors.

Finally, in a fifth experiment, we tested our general PPS-SILOUETTE algorithm using squared Euclidean distances (which do not satisfy the triangle inequality) against the routine available in Apache Spark to compute the exact value in this special case. For this experiment, we considered our synthetic dataset with \( n = 10^8 \) points, and two clustering granularities (\( k = 5, 10 \)). We ran PPS-SILOUETTE with expected sample size \( t = 64 \). For \( k = 5 \), PPS-SILOUETTE provides estimates with an average error smaller than 0.005 and a maximum error of 0.008, while for \( k = 10 \) the average error is smaller than 0.058 and the maximum error is 0.069. These results show that our PPS-SILOUETTE algorithm can be used to provide accurate estimates of the silhouette with a limited number of samples even for squared Euclidean distances.

### 3.5 Scalability Evaluation

We assessed the scalability of the MapReduce version of PPS-SILOUETTE. For this experiment, we used four instances of the synthetic dataset described in Subsection 3.3 with \( n = 10^6, 10^7, 10^8, 10^9 \) points. We clustered each dataset using \( k \)-medoids with \( k = 5 \). We then run the MapReduce implementation of PPS-SILOUETTE with \( t = 64 \) using \( w = 1, 2, 4, 8, 16 \) workers, each running on a single core. For the dataset with \( n = 10^9 \) points, we considered only \( w = 8, 16 \) since for lower levels of parallelism the local memory available to each core was not sufficient to process the \( n/w \) points assigned to each worker. The four graphs in Figure 4 report, on a logarithmic scale, the median...
Table 4: Comparison between exact silhouette, generalized simplified silhouette, and maximum and average absolute error of the silhouette estimates returned by PPS-SILHOUETTE (label “PPS”) and the uniform sampling algorithm, (label “uniform”), relative to the \( k \)-medoid clustering of the real datasets Covertype and HIGGS, with \( k = 5, 10 \) and \( t = 64, 128, \ldots, 1024 \).

| Dataset | \( k \) | Silhouette | Algorithm | \( t = 64 \) | \( t = 128 \) | \( t = 256 \) | \( t = 512 \) | \( t = 1024 \) |
|---------|-------|------------|-----------|-------------|-------------|-------------|-------------|---------------|
|         |       |            |           | max avg     | max avg     | max avg     | max avg     | max avg       |
|         |       |            |           | \( k \)     | \( n \)     | \( n \)     | \( n \)     | \( n \)        |
| Covertype | 5     | 0.344      | PPS       | .084 .016   | .058 .008   | .042 .006   | .014 .003   | .007 .002     |
|          |       | 0.474      | uniform   | .108 .019   | .044 .010   | .027 .007   | .017 .003   | .014 .003     |
|          | 10    | 0.266      | PPS       | .120 .023   | .046 .012   | .025 .006   | .015 .005   | .014 .002     |
|          |       | 0.394      | uniform   | .160 .031   | .070 .018   | .040 .009   | .023 .005   | .014 .002     |
| HIGGS   | 5     | 0.244      | PPS       | .114 .016   | .073 .010   | .024 .006   | .019 .004   | .008 .003     |
|          |       | 0.368      | uniform   | .110 .017   | .087 .011   | .045 .008   | .019 .005   | .019 .003     |
|          | 10    | 0.151      | PPS       | .107 .028   | .088 .018   | .047 .010   | .033 .007   | .020 .004     |
|          |       | 0.289      | uniform   | .155 .033   | .097 .020   | .081 .012   | .046 .009   | .019 .005     |

running times, over 5 runs, for the four datasets, as a function of the number of workers \( w \). We observe that for the two largest datasets PPS-SILHOUETTE exhibits linear scalability. For \( n = 10^7 \), the algorithm still exhibits linear scalability for up to 8 workers, while there is a limited gain in using 16 workers. For \( n = 10^8 \), scalability is linear from 2 workers onwards, however, due to the relatively small size of the dataset, the behavior is less regular due to the stronger incidence of communication overheads and caching effects. Also, for a fixed number of workers, we observe that the algorithm scales almost linearly with the number of points, in accordance with our theoretical analysis.

We also compared (results not shown) the sequential running time of PPS-SILHOUETTE against the one of the exact silhouette computation and of the uniform sampling algorithm (with the same value of \( t \)). Even for the smallest dataset (\( n = 10^5 \)) the exact computation requires dozens of hours, while PPS-SILHOUETTE and the uniform sampling algorithm require less than one minute. Also, in general, the uniform sampling algorithm exhibits a running time which is comparable, although slightly lower (by \( 10 - 20\% \) in all experiments), than PPS-SILHOUETTE. In addition, we compared the running time of PPS-SILHOUETTE using squared Euclidean distances with the running time of the optimized routine available in Apache Spark for such distances, using our synthetic dataset with \( n = 10^8 \) points and for \( k = 5, 10 \). Since our goal in this experiment is to compare the best performance achievable by the two implementations, and since our PPS-SILHOUETTE algorithm provides very accurate estimates already with a limited number \( t \) of samples (see Section 3.4), we fixed \( t = 32 \) and \( w = 16 \) workers. For both values of \( k \) the estimates from PPS-SILHOUETTE are very precise (average error 0.007 for \( k = 5 \) and 0.087 for \( k = 10 \)), while the running time of PPS-SILHOUETTE is comparable to, even if higher than (up to approximately three times), the running time of the optimized Apache Spark routine.

Finally, we wish to remark that the MapReduce implementation of PPS-SILHOUETTE has not been optimized and must be regarded as a mere proof-of-concept needed to argue the scalability of our approach. In this respect, we believe that there is much room for improving the absolute times reported in Figure 1 through an optimized implementation.

4 Conclusions

In this work, we studied the problem of efficiently computing an accurate estimate of the silhouette coefficient for a given clustering. We developed the first efficient, sampling-based algorithm for estimating the silhouette coefficient with provable approximation guarantees. Our algorithm employs a PPS sampling scheme, and we show that, that for a \( k \)-clustering of \( n \) elements, our algorithm approximates the silhouette coefficient within an additive error \( \varepsilon \) with probability at least \( 1 - \delta \) using only \( O(\varepsilon^{-22} \log \frac{n}{\varepsilon^2}) \) distance computations, dramatically improving over the \( \Theta \left( n^2 \right) \) distance computations required by the naïve exact algorithm. We also generalize our algorithm to compute rigorous approximations of other internal measures. We provided a distributed implementation of our algorithm in Map-Reduce which runs in constant rounds, and requires only sublinear space at each worker. We performed an extensive experimental evaluation on real and synthetic datasets, showing that, in practice, our approach is superior to other known heuristics and yields highly accurate estimates in a tiny fraction of the time required by the exact computation. The experimental evaluation demonstrates that our algorithm enables the estimation of the silhouette coefficient for clusterings of massive datasets for which the exact computation is out of reach.
Figure 1: Running time of our PPS-SILHOUETTE algorithm as function of the number $w$ of workers, for datasets of different sizes.

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References

[1] T. Abeel, Y. V. d. Peer, and Y. Saeys. Java-ml: A machine learning library. Journal of Machine Learning Research, 10(Apr):931–934, 2009.
[2] C. C. Aggarwal and C. K. Reddy. Data Clustering: Algorithms and Applications. CRC Press, 2013.
[3] P. Awasthi and M. Balcan. Center based clustering: A foundational perspective. In Handbook of cluster analysis. CRC Press, 2015.
[4] A. Barger and D. Feldman. $k$-means for streaming and distributed big sparse data. In Proc. SDM, pages 342–350, 2016.
[5] P. Beame, P. Koutris, and D. Suciu. Communication Steps for Parallel Query Processing. In Proc. PODS, pages 273–284, 2013.
[6] M. Ceccarello, C. Fantozzi, A. Pietracaprina, G. Pucci, and F. Vandin. Clustering Uncertain Graphs. PVLDB, 11(4):472–484, 2017.
[7] M. Ceccarello, A. Pietracaprina, and G. Pucci. Solving $k$-center clustering (with outliers) in mapreduce and streaming, almost as accurately as sequentially. PVLDB, 12(7):766–778, 2019.
[8] S. Chechik, E. Cohen, and H. Kaplan. Average distance queries through weighted samples in graphs and metric spaces: high scalability with tight statistical guarantees. In Proc. APPROX/RANDOM, pages 659–679, 2015.
[9] J. Dean and S. Ghemawat. Mapreduce: simplified data processing on large clusters. Communications of the ACM, 51(1):107–113, 2008.
[10] G. Frahling and C. Sohler. A fast $k$-means implementation using coresets. Int. J. Comput. Geometry Appl., 18(6):605–625, 2008.
[11] C. Hennig, M. Meila, F. Murtagh, and R. Rocci. Handbook of cluster analysis. CRC Press, 2015.
[12] E. R. Hruschka, L. N. de Castro, and R. J. Campello. Evolutionary algorithms for clustering gene-expression data. In Proc. ICDM, pages 403–406, 2004.
[13] H. J. Karloff, S. Suri, and S. Vassilvitskii. A model of computation for mapreduce. In Proc. SODA, pages 938–948, 2010.
[14] J. Leskovec, A. Rajaraman, and J. D. Ullman. *Mining of Massive Datasets, 2nd Ed.* Cambridge University Press, 2014.

[15] L. Lin, J. Ruoming, C. Aggarwal, and S. Yelong. Reliable clustering on uncertain graphs. In *Proc. ICDM*, pages 459–468. IEEE, Dec 2012.

[16] S. P. Lloyd. Least squares quantization in PCM. *IEEE Trans. on Information Theory*, 28(2):129–137, 1982.

[17] G. Malkomes, M. Kusner, W. Chen, K. Weinberger, and B. Moseley. Fast Distributed k-Center Clustering with Outliers on Massive Data. In *Proc. NIPS*, pages 1063–1071, 2015.

[18] A. Mazzetto, A. Pietracaprina, and G. Pucci. Accurate mapreduce algorithms for k-median and k-means in general metric spaces. In *Proc. ISAAC*, pages 34:1–34:16, 2019.

[19] D. Moulavi, P. A. Jaskowiak, R. J. G. B. Campello, A. Zimek, and J. Sander. Density-based clustering validation. In *Proc. SDM*, pages 839–847, 2014.

[20] A. Pietracaprina, G. Pucci, M. Riondato, F. Silvestri, and E. Upfal. Space-round tradeoffs for mapreduce computations. In *Proc. ICS*, pages 235–244, 2012.

[21] P.N.Tan, M.Steinbach, and V.Kumar. *Introduction to Data Mining*. Addison Wesley, 2006.

[22] P. J. Rousseuw. Silhouettes: a graphical aid to the interpretation and validation of cluster analysis. *Journal of Computational and Applied Mathematics*, 20:53–65, 1987.

[23] C. Tomasini, L. R. Emmendorfer, E. N. Borges, and K. S. Machado. A methodology for selecting the most suitable cluster validation internal indices. In *Proc. SAC*, pages 901–903, 2016.

[24] F. Wang, H.-H. Franco-Penya, J. D. Kelleher, J. Pugh, and R. Ross. An analysis of the application of simplified silhouette to the evaluation of k-means clustering validity. In P. Perner, editor, *Machine Learning and Data Mining in Pattern Recognition*, pages 291–305, Cham, 2017. Springer International Publishing.

[25] H. Xiong and Z. Li. Clustering validation measures. In C. Aggarwal and C. Reddy, editors, *Data Clustering: Algorithms and Applications*, chapter 23. CRC Press, 2014.