Accelerating Spherical *k*-Means*

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Abstract. Spherical k-means is a widely used clustering algorithm for sparse and high-dimensional data such as document vectors. While several improvements and accelerations have been introduced for the original k-means algorithm, not all easily translate to the spherical variant: Many acceleration techniques, such as the algorithms of Elkan and Hamerly, rely on the triangle inequality of Euclidean distances. However, spherical k-means uses cosine similarities instead of distances for computational efficiency. In this paper, we incorporate the Elkan and Hamerly accelerations to the spherical k-means algorithm working directly with the cosines instead of Euclidean distances to obtain a substantial speedup and evaluate these spherical accelerations on real data.

1 Introduction

Clustering textual data is an important task in data science with applications in areas like information retrieval, topic modeling, and knowledge organization. Spherical k-means [8] is a widely used adaptation of the k-means clustering algorithm to high-dimensional sparse data, such as document vectors where cosine similarity is a popular choice. While it is generally used for clustering documents, it has also been applied to medical images [2,20], multivariate species occurrence data [14], and plant leaf images [1]. Because of its importance, several improvements and extensions have been suggested. Many optimizations improve the initialization of k-means cluster centers, such as k-means++ [3] and k-means|| [5,6], some of which have also been adapted to spherical k-means [11,22,19].

A key area of optimizations is focussed on the iterative optimization phase of k-means. The standard algorithm computes the distance of every point to every cluster in each iteration. Many of these computations are not necessary if cluster centers have not moved much, and hence a lot of research has been on how to avoid computing distances. The central work in this domain is the algorithm of Elkan [10], which is the base for many other variants such as Hamerly's algorithm [12], but also recently the Exponion algorithm [21], the Shallot algorithm [7], and the variants of Yu et al. [26], all of which rely on the Euclidean triangle inequality to avoid distance computations.

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This paper studies how to adapt such acceleration techniques to spherical k-means, thus providing a more efficient approach for clustering text documents.

2 Foundations

Cosine similarity (which we will simply denote using sim in the following) is commonly defined as the cosine of the angle θ between two vectors $\mathbf{x}$ and $\mathbf{y}$:

$$\operatorname{sim}(\mathbf{x},\mathbf{y}) := \operatorname{sim}_{\text{cosine}}(\mathbf{x},\mathbf{y}) := \frac{\langle \mathbf{x},\mathbf{y}\rangle}{\|\mathbf{x}\|_2 \cdot \|\mathbf{y}\|_2} = \frac{\sum_i x_i y_i}{\sqrt{\sum_i x_i^2}\cdot\sqrt{\sum_i y_i^2}} = \cos\theta$$

In the following, we will only consider vectors normalized to unit length, i.e., with Euclidean norm $\|\mathbf{x}\|_2 = 1$. It is trivial to see that on such vectors, the cosine similarity is simply the dot product. Consider the Euclidean distance of two *normalized* vectors $\mathbf{x}$ and $\mathbf{y}$, and expand using the binomial equations, we obtain:

$$d_{\text{Euclidean}}(\mathbf{x},\mathbf{y}) := \sqrt{\sum\nolimits_i (x_i - y_i)^2} = \sqrt{\sum\nolimits_i (x_i^2 + y_i^2 - 2x_i y_i)} \tag{1}$$

$$= \sqrt{\|\mathbf{x}\|^2 + \|\mathbf{y}\|^2 - 2\langle \mathbf{x},\mathbf{y}\rangle} = \sqrt{2 - 2\cdot\operatorname{sim}(\mathbf{x},\mathbf{y})} \tag{2}$$

where the last step relies on the vectors being normalized. Hence we have an extremely close relationship between cosine similarity and squared Euclidean distance on normalized vectors: $\operatorname{sim}(\mathbf{x},\mathbf{y}) = 1 - \frac{1}{2} d^2_{\text{Euclidean}}(\mathbf{x},\mathbf{y})$.

k-means minimizes the *squared* Euclidean distances of points to their cluster centers and hence can be used to maximize cosine similarities. Because the total variance of a data set is constant, by minimizing the within-cluster squared deviations, k-means also maximizes the between-cluster squared deviations. By adapting this to cosine, we obtain clusters where objects in the same cluster have to be more similar, while objects in different clusters are less similar.

Dhillon and Modha [8] popularized this idea as "spherical k-means" for clustering text documents and exploited exactly the above relationship between the squared Euclidean distance and cosine similarity. Only a tiny modification of the standard k-means algorithm is necessary to obtain the desired results: the arithmetic mean of a cluster usually does not have unit Euclidean length. Hence, after recomputing the cluster mean, we normalize it accordingly. This constrains the clustering to split the data at great circles (i.e., hyperplanes through the origin), rather than arbitrary Voronoi cells as with regular k-means.

On text data, computing the cosine similarity is more efficient than computing Euclidean distance because of sparsity: rather than storing the vectors as a long array of values, most of which are zeros, only the non-zero values can be encoded as pairs (i, v) of an index i and a value v, and stored and kept in sorted order. The dot product of two such vectors can then be efficiently computed by a *merge* operation, where only those indexes i need to be considered that are contained in both vectors, because in $\langle \mathbf{x},\mathbf{y}\rangle = \sum_i x_i y_i$ only those terms matter where both x_i and y_i are not zero. A merge is most efficient if both vectors are sparse, but even the dot product of a sparse and a dense vector is often much

faster than that of two dense vectors. While we can also compute Euclidean distance this way (using Eq. 2), this computation is prone to the numerical problem called "catastrophic cancellation" for small distances that can be problematic in clustering (see, e.g., [24,16]). Hence, working with cosines directly is preferable.

Instead of recomputing the distances to all cluster centers, the idea of algorithms such as Elkan's is to keep an upper bound on the distance to the nearest cluster, and one or more lower bounds on the distances to the other centers. Let d_n be the distance to the nearest center, $d_n \leq u$ an upper bound, d_s the distance to the second nearest, and $l \leq d_s$ a lower bound. If we have $u \leq l$, then the nearest cluster must still be the same since $d_n \leq u \leq l \leq d_s$. Updating the distance bounds uses the triangle inequality: if the nearest center μ_n has moved to μ'_n, then $d(x, \mu'_n) \leq d(x, \mu_n) + d(\mu_n, \mu'_n)$; and we hence can obtain an upper bound u by adding every movement of a cluster center to the previous distance. Lower bounds are obtained similarly: starting with the initial distance as the lower bound, we subtract the distance the other center has moved to obtain a provable new lower bound. While Elkan stored a lower bound for each cluster (which needs $O(N \cdot k)$ memory), Hamerly [12] reduced the memory usage by using just one lower bound to the second nearest cluster, updated by the largest distance moved. Additional pruning rules involve the pairwise distances of centers [10], annuli around centers [21], and the relative movement of centers [26].

In the following, we describe how such accelerations can be applied to spherical k-means, i.e., for cosine similarity and high-dimensional data.

3 Pruning with Cosine Similarity

Many acceleration techniques rely on the triangle inequality of the (non-squared) Euclidean distance. Hence, we can adapt these methods by computing Euclidean distances from our cosine similarities using $d_{\text{Euclidean}}(\mathbf{x}, \mathbf{y}) = \sqrt{2 - 2 \cdot \text{sim}(\mathbf{x}, \mathbf{y})}$, but we wanted to avoid this because of (i) the square root takes 10–50 CPU cycles (depending on the exact CPU, precision, and input value) and (ii) the risk of numerical instability because of catastrophic cancellation. Hence we develop techniques that directly use similarities instead of distances, yet allow a similar pruning to these (very successful) acceleration techniques of regular k-means.

The arc length (i.e., the angle θ itself, rather than the cosine of the angle) satisfies the triangle inequality and hence we could use

$$\text{sim}(\mathbf{x}, \mathbf{y}) \geq \cos(\arccos(\text{sim}(\mathbf{x}, \mathbf{z})) + \arccos(\text{sim}(\mathbf{z}, \mathbf{y}))) \ , \tag{3}$$

but unforunately the trigonometric functions in here are even more expensive (60–100 CPU cycles each). Schubert [23] recently proposed reformulations avoiding the expensive trigonometric functions (but still using the square root):

$$\text{sim}(\mathbf{x}, \mathbf{y}) \geq \text{sim}(\mathbf{x}, \mathbf{z}) \cdot \text{sim}(\mathbf{z}, \mathbf{y}) - \sqrt{(1 - \text{sim}(\mathbf{x}, \mathbf{z})^2) \cdot (1 - \text{sim}(\mathbf{z}, \mathbf{y})^2)} \tag{4}$$

$$\text{sim}(\mathbf{x}, \mathbf{y}) \leq \text{sim}(\mathbf{x}, \mathbf{z}) \cdot \text{sim}(\mathbf{z}, \mathbf{y}) + \sqrt{(1 - \text{sim}(\mathbf{x}, \mathbf{z})^2) \cdot (1 - \text{sim}(\mathbf{z}, \mathbf{y})^2)} \tag{5}$$

In this paper, we explain how to integrate these triangle inequalities into spherical k-means, and discuss an easily overlooked pitfall therein.

4 Upper and Lower Bounds

In the following, we orient ourselves on the very concise presentation and notation of Hamerly [12] as well as Newling and Fleuret [21], except that we swap the names of u and l, because switching from distance to similarity requires us to swap the roles of upper and lower bounds. We will assume that all points are normalized to unit length, and hence $\text{sim}(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^T \cdot \mathbf{y}$.

The algorithms we discuss will employ upper and lower bounds for the similarities of each sample $x(i)$ to the cluster centers $c(j)$. $l(i)$ is a lower bound for the similarity to the current cluster $a(i)$, $u(i,j)$ are upper bounds on the similarity of each point to each cluster center, respectively $u(i)$ is an upper bound on the similarity to all other cluster centers ($u(i,j)$ and $u(i)$ are used in different variants, not at the same time). These bounds are maintained to satisfy:

$$l(i) \leq \langle x(i), c(a(i)) \rangle \qquad u(i,j) \geq \langle x(i), c(j) \rangle \qquad u(i) \geq \max_{j \neq a(i)} \langle x(i), c(j) \rangle$$

The central idea of all the discussed variants is that if we have $l(i) \geq u(i,j)$, then $\langle x(i), c(a(i)) \rangle \geq l(i) \geq u(i,j) \geq \langle x(i), c(j) \rangle$ implies that the current cluster assignment of object $x(i)$ is optimal, and we do not need to recompute the similarities.

The bounds $l(i)$ and $u(i,j)$, can be maintained using above triangle inequality if we know how much the cluster centers $c(j)$ moved from their previous location $c'(j)$. Let $p(j) := \langle c(j), c'(j) \rangle$ denote this similarity. Based on the triangle inequalities Eq. 4 and Eq. 5, we obtain the following bound update equations:

$$l(i) \leftarrow l(i) \cdot p(a(i)) - \sqrt{(1 - l(i)^2) \cdot (1 - p(a(i))^2)} \tag{6}$$

$$u(i,j) \leftarrow u(i,j) \cdot p(j) + \sqrt{(1 - u(i,j)^2) \cdot (1 - p(j)^2)} \tag{7}$$

5 Accelerated Spherical *k*-Means

The algorithms discussed here all follow the outline of the standard k-means algorithm of alternating optimization. During initialization, all data samples $x(i)$ are normalized to have length $\|x(i)\| = 1$. In the first step, all objects are reassigned to the nearest cluster, in the second step, the cluster center is optimized. However, we switch the notation from distance to similarity. Let the variable $a(i)$ denote the current cluster assignment of sample $x(i)$, and denote the current cluster centers using $c(j)$, the two steps can be written as:

$$a(i) \leftarrow \arg\max_j \langle x(i), c(j) \rangle \qquad i \in 1..N$$

$$c(j) \leftarrow \frac{\sum_{i|a(i)=j} x(i)}{\left\| \sum_{i|a(i)=j} x(i) \right\|} \qquad j \in 1..k$$

When computing $a(i)$ we maximize the cosine similarity instead of the squared Euclidean distance in regular k-means. For $c(j)$, note that the denominator is different here, as we want to have $\|c(j)\| = 1$ for all j. We hence do not need to compute the arithmetic mean, but we can scale the sum directly to length 1.

There are several optimizations we can do for the baseline algorithm that make a difference: (i) By normalizing the vectors, we do not have to take the vector lengths of $x(i)$ into account when updating $c(j)$, and by also normalizing the $c(j)$ we can use the dot product when computing $a(i)$. (ii) Both the dot product as well as the sum operation when computing $c(j)$ can be optimized for sparse data. (iii) Instead of recomputing $c(j)$ each time, it is better to store the sums before normalization and update them when a cluster assignment changes.

5.1 Spherical Simplified Elkan's Algorithm

As the name suggests, this algorithm is a simplified version of Elkan's approach, introduced by Newling and Fleuret [21]. As it uses a subset of the pruning rules, we introduce it before Elkan's full algorithm. Both are presented directly in the adaptation for spherical k-means.

Simplified Elkan uses the test $u(i,j) \leq l(i)$ to skip computing the similarity between $x(i)$ and $c(j)$ when it is not necessary. If this test fails, $l(i) \leftarrow \langle x(i), c(a(i)) \rangle$ is updated first (as the current assignment is clearly the best guess), and only if the condition still is violated, $u(i,j) \leftarrow \langle x(i), c(j) \rangle$ is computed next, and the point is reassigned if necessary (updating $l(i)$ and $a(i)$ then).

5.2 Spherical Elkan's Algorithm

Elkan's algorithm [10] uses additional tests based on the pairwise distance of centers, respectively pairwise cluster similarities here. The idea is that cluster centers are supposedly well separated, whereas points are close to their nearest cluster, and we can use half the distance between two centers as a threshold. We simplify the computation of half of the angle per $\cos(\frac{1}{2}\arccos(x)) = \sqrt{(x+1)/2}$. Let $cc(i,j) := \sqrt{(\langle c(i), c(j) \rangle + 1)/2}$ be this lower bound (cc for center-center bounds, as in [21]). Let $s(i) := \max_{j \neq i} cc(i,j)$ denote the maximum such bound for each i.

Suppose that $cc(a(i), j) \leq l(i)$ and $l(i) \geq 0$, then $\langle c(i), c(j) \rangle \leq 2l(i)^2 - 1$. We can then use Eq. 5 to bound the distance to another cluster $c(j) \neq c(a(i))$ per

$$\begin{aligned}
\langle x(i), c(j) \rangle &\leq \langle x(i), c(a(i)) \rangle \cdot \langle c(a(i)), c(j) \rangle \\
&\quad + \sqrt{(1 - \langle x(i), c(a(i)) \rangle^2) \cdot (1 - \langle c(a(i)), c(j) \rangle^2)} \\
&\leq l(i)(2l(i)^2 - 1) + \sqrt{(1 - l(i)^2) \cdot (1 - (2l(i)^2 - 1)^2)} \\
&= 2l(i)^3 - l(i) + \sqrt{(1 - l(i)^2) \cdot 4l(i)^2(1 - l(i)^2)} \\
&= 2l(i)^3 - l(i) + 2l(i)(1 - l(i)^2) = l(i) \quad ,
\end{aligned}$$

and hence do not have to consider other cluster centers $c(j)$ *if* $cc(a(i), j) \leq l(i)$. Because $s(i)$ is the maximum of these values, we can skip iterating over the means if $s(i) \leq l(i)$ altogether. While these additional tests are fairly cheap to compute, they were found to not always be effective by Newling and Fleuret [21] (who, hence, suggested the simplified variant discussed in the previous section).

For spherical k-means clustering, these bounds may not be very effective because of the high dimensionality. Using these bounds adds $k \cdot (k-1)/2 = O(k^2)$

similarity computations to each iteration. Furthermore, the necessary computations can become more expensive because the centers are best stored using dense vectors because (i) we aggregate many vectors into each center, and only attributes zero in all of the assigned vectors will be zero in the resulting center, i.e., the sparsity decreases often to the point where a dense representation is more compact, and (ii) the efficient sparse data structures we use for the $x(i)$ are not well suited for adding and removing attributes. We could aggregate into a dense vector and convert it to a sparse representation when normalizing the center, but the resulting vectors will still often be too dense to be efficient.

5.3 Spherical Hamerly's Algorithm

Where Elkan's algorithm used one upper bound for each cluster, Hamerly [12] only uses a single bound for all clusters. This does not only saves memory (for large k, memory consumption of Elkan's algorithm can be an issue) but updating the $N{\cdot}k$ bounds each iteration even if the clusters change only very little takes a considerable amount of time. Hamerly's idea is to make a worst-case assumption, where we use the distance to the second nearest center as the initial bound, and update it based on the largest cluster movement (of all clusters, except the one currently assigned to). Because of this, the bound will become loose much faster, and hence we need to recompute more often (and then we need to recompute the distances to all clusters). Because of this, it is hard to predict which algorithm works better, we are trading reduced memory and fewer bound updates against additional distance computations. Nevertheless, many later works have confirmed that it is often favorable to only keep one bound.

At first, adapting Hamerly to cosine similarity appears to be straightforward. To obtain the lowest upper bound per object $u(i) \leq \min_{j \neq a(i)} u(i,j)$, we would compute the smallest similarity of a cluster center to its previous location (as well as the second smallest, in case the point is currently assigned to that center), then use Eq. 7 with $p'(i) := \min_{j \neq i} p(j)$ (which is either the smallest or the second smallest $p(j)$). Most of the time this is fine, but there is a subtly hidden catch here because of the underlying non-monotone trigonometric functions.

Recall the update equation (7), rewritten to $u(i)$ instead of $u(i,j)$ already:

$$u(i) \leftarrow u(i) \cdot p(j) + \sqrt{(1 - u(i)^2) \cdot (1 - p(j)^2)}$$

This equation is not necessarily minimized by the smallest $p(j)$, because of the square root term. For large $u(i)$ (e.g., 1), the result will be determined by the first term, and a smaller $p(j)$ is what is needed. But for small $u(i)$ (e.g., 0), the second term becomes influential, and a larger $p(j)$ causes a smaller bound. This is because we are working with the cosines $\cos\theta$, not the angles θ themselves. Unfortunately, this depends on the previous value of $u(i)$, and we probably cannot use just one $p(j)$ for all points.

One option would be to use both the minimum $p'(i) := \min_{j \neq i} p(j)$ and the maximum $p''(i) := \max_{j \neq i} p(j)$ to update the bound with:

$$(7) \leq u(i) \cdot p''(a(i)) + \sqrt{(1 - u(i)^2) \cdot (1 - p'(a(i))^2)} \ . \tag{8}$$

Because $p''(j) \to 1$ as the algorithm converges, we may omit this term entirely:

$$(8) \leq u(i) + \sqrt{(1 - u(i)^2) \cdot (1 - p'(a(i))^2)} \tag{9}$$

This has almost identical pruning power once $p''(j)$ becomes large enough in later iterations. As we can precompute $(1 - p'(j))$ for all j, this is quite efficient. We cannot rule out that a tighter and computationally efficient bound exists.

If the condition $l(i) \geq u(i)$ is violated, first $l(i)$ is made tight again, and if it still is violated, all remaining similarities are computed to update $u(i)$, or to potentially obtain a new cluster assignment (updating $a(i)$, $l(i)$, and $u(i)$).

5.4 Spherical Simplified Hamerly's Algorithm

Hamerly's algorithm contains a bounds test similar to Elkan's algorithm, but using only the distance of each center to its nearest neighbor center instead of keeping all pairwise center distances, i.e., only the threshold $s(i) := \max_{j \neq i} cc(i, j)$ to prune objects with $l(i) \geq s(a(i))$. We also consider a "simplified" variant of Hamerly's algorithm in our experiments with this bound check removed for the same reasons as discussed with Elkan's algorithm.

5.5 Further *k*-Means Variants

An obvious candidate to extend this work is Yin-Yang k-means [9], which groups the cluster centers and uses one bound for each group. This is a compromise between Elkan's and Hamerly's approaches, encompassing both as extreme cases (k groups respectively one group). The results of this paper will trivially transfer to this method. The Annulus algorithm [13] additionally uses the distance from the origin for pruning. As all our data is normalized to unit length, this approach clearly will not help for spherical k-means. The Exponion [21] and Shallot [7] algorithms transfer this idea to using pairwise distances of cluster centers, where our considerations may be applicable again.

5.6 Spherical *k*-means++

We experiment with the canonical adaptation of k-means++, using the analogy with squared Euclidean distance. The first sample is chosen uniformly at random, the remaining instances are sampled proportional to $1 - \max_c \langle x(i), c \rangle$ which is proportional to the squared Euclidean distance used by k-means++. This can be done in $O(nk)$ by caching the previous maximum, and the scalar product is efficient for two sparse vectors. Endo and Miyamoto [11] prove theoretical guarantees for a slight modification of spherical k-means using the dissimilarity of $\alpha - \langle \mathbf{x}, \mathbf{y} \rangle$ with $\alpha \geq \frac{3}{2}$ to make it metric, and hence sample proportionally to $1 - \max_c \langle x(i), c \rangle$. Pratap et al. [22] use the same trick to apply the AFK-MC^2 algorithm [4] to spherical k-means-clustering.

Table 1: Data sets used in the experiments.

Data set	Rows	Columns	Non-zero
DBLP Author-Conference	1842986	5236	0.056%
DBLP Conference-Author	5236	1842986	0.056%
DBLP Author-Venue	2722762	7192	0.099%
Simpsons Wiki	10126	12941	0.463%
20 Newsgroups	11314	101631	0.096%
Reuters RCV-1	804414	47236	0.160%

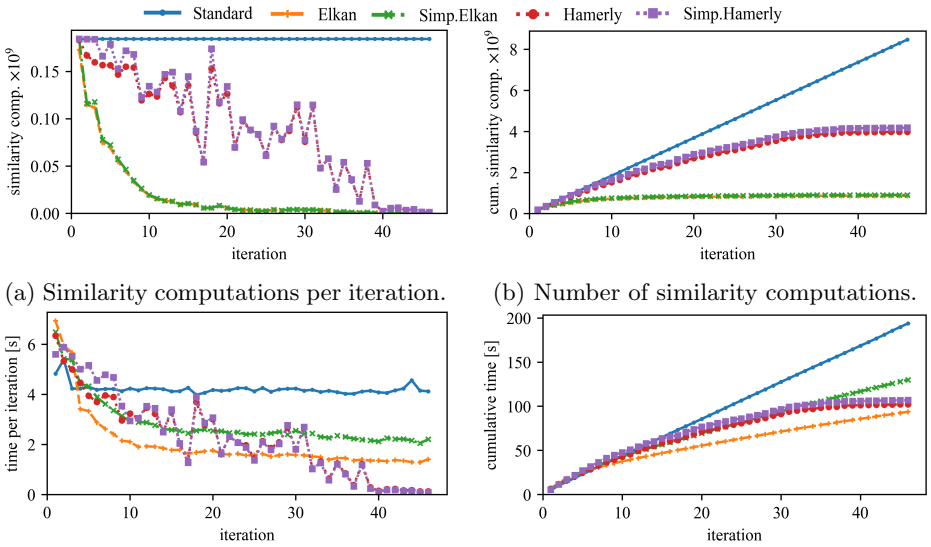
6 Experiments

We implemented our algorithms in the Java framework ELKI [25], which already contained a large collection of k-means variants. By keeping the implementation differences to a minimum, we try to make the benchmark experiments more reliable (c.f., [15]), but the caveats of Java just-in-time compilation remain.

As our method is designed for sparse and high-dimensional data sets, we focus on textual and graph data as input. From the Digital Bibliography & Library Project (DBLP, [18]) we extracted graphs that connect authors and conferences. As this includes many authors with just a single paper, the data set is very sparse. We can either use the authors as samples and the conferences as columns or transposed. But because we use TF-IDF weighting afterward the semantics will be different. Spherical k-means clustering has been used successfully for community detection on such data sets (although we have to choose the number of communities as a parameter). If we also include journals, the data set becomes both larger and denser. A second data set was obtained from the Simpsons Fandom Wiki,[1] from which we extracted the text of around 10000 articles. The text was tokenized and lemmatized, stop words were removed as well as infrequent tokens (reducing the dimensionality from 42124 to 12941, and increasing the density of non-zero values from 0.153% to 0.463%). This data set is more typical of a smaller domain-specific text corpus. The 20 Newsgroups data set is a classic, popularized by the textbook of Tom Mitchell. We use a version available via scikit-learn, with headers, footers, and quotes removed and vectorized using the default settings (i.e., TF-IDF weighting). This is much more sparse than the Simpsons wiki because of the poor input data quality (including Base64-encoded attachments). After removing stop words and rare words as above, the density would have been 0.317%, but we opted for the default scikit-learn version instead. Reuters RCV-1 [17] is another classic text categorization benchmark, with a density between the Simpsons and the 20news data.

We first discuss the algorithms on a single data set, with a single random seed, averaged over 10 re-runs, to observe some characteristic behavior. The reason that we do not average over different random initializations is that we want to observe individual iterations of the algorithms, which depend on the initialization. Fig. 1 shows the results on the DBLP author-conference data set with

[1] `https://simpsons.fandom.com/wiki/Simpsons_Wiki`



(a) Similarity computations per iteration.

(b) Number of similarity computations.

(c) Run time per iteration.

(d) Cumulative run time.

Fig. 1: Distance computations and resulting run time for one initialization.

a large k=100. Considering only similarity computations (Fig. 1a and Fig. 1b), both Elkan and Simplified Elkan shine (as expected) and use the fewest computations as they have the tightest bounds. There is next to no difference among the two concerning the number of computations, but considering the run time (Fig. 1c and Fig. 1d) the simplified variant is much worse. Perhaps unexpectedly, this can be explained by the high k. The additional pruning rule of the full algorithm allows skipping the loop over all clusters k, which would otherwise each have to be checked against their bounds. The behavior of the Hamerly variants is much more chaotic because it only depends on the cluster center that changed most. Because of this, Hamerly computes many more similarities than Elkan until the last few iterations. Nevertheless, its total run time is initially similar to that of Simplified Elkan, and after around 30 iterations its run time per iteration (c.f., Fig. 1c) becomes even lower than the full Elkan algorithm's. These savings arise once clusters do not change much anymore because only 2 bounds need to be updated instead of k+1 bounds per iteration. For k=10 (not shown in the figures), both Hamerly variants outperform Elkan, while for k=1000 even Simplified Elkan clearly outperforms both Hamerly variants. Note that we used random sampling as initialization. If we had known the optimal initial cluster centers, all methods would have converged instantly.

Next, we compare the quality and run time of the initialization methods. Table 2 shows the difference in the sum of variances, averaged over 10 random seeds, compared to the uniform random initialization. It shows that the quality difference of the converged solutions between all initialization methods is small

Table 2: Relative change in the objective function compared to the random initialization (lower is better).

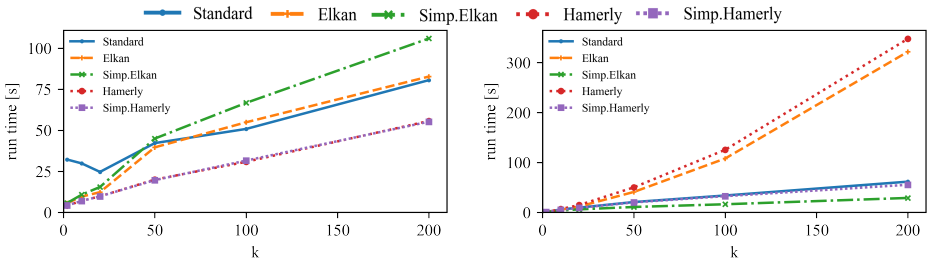
Data set	Initialization	k=2	k=10	k=20	k=50	k=100	k=200
Simpsons Wiki	Uniform	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
	k-means++ α=1	-0.27%	**-0.16%**	**-0.24%**	-0.07%	-0.18%	-0.07%
	k-means++ α=1.5	-0.16%	-0.13%	-0.17%	-0.01%	-0.18%	**-0.09%**
	AFK-MC^2 α=1	**-0.44%**	0.12%	-0.15%	**-0.15%**	**-0.24%**	-0.08%
	AFK-MC^2 α=1.5	-0.31%	0.21%	0.09%	0.09%	-0.05%	-0.02%
DBLP Author-Conf.	Uniform	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
	k-means++ α=1	**-0.11%**	0.12%	-0.07%	0.27%	0.14%	**-1.67%**
	k-means++ α=1.5	-0.03%	0.11%	0.33%	0.68%	0.53%	-0.74%
	AFK-MC^2 α=1	-0.01%	**-0.06%**	**-0.87%**	**-0.47%**	-0.48%	-1.03%
	AFK-MC^2 α=1.5	-0.03%	0.34%	-0.32%	0.09%	**-0.56%**	-1.10%
DBLP Author-Venue	Uniform	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
	k-means++ α=1	-0.13%	0.09%	-0.12%	0.13%	**-0.74%**	**-1.70%**
	k-means++ α=1.5	-0.01%	0.18%	0.00%	0.23%	0.39%	-0.17%
	AFK-MC^2 α=1	-0.17%	0.10%	-0.05%	0.47%	-0.20%	-0.68%
	AFK-MC^2 α=1.5	**-0.19%**	**-0.33%**	**-0.68%**	**-0.04%**	-0.50%	-1.41%
DBLP Conf.-Author	Uniform	**0.00%**	**0.00%**	**0.00%**	0.00%	0.00%	0.00%
	k-means++ α=1	0.01%	0.04%	0.05%	-0.02%	-0.13%	-0.09%
	k-means++ α=1.5	**0.00%**	0.11%	0.08%	**-0.15%**	-0.18%	**-0.13%**
	AFK-MC^2 α=1	0.04%	**0.00%**	0.05%	-0.10%	**-0.19%**	-0.02%
	AFK-MC^2 α=1.5	0.04%	**0.00%**	0.06%	-0.12%	-0.15%	-0.06%
20 Newsgroups	Uniform	**0.00%**	**0.00%**	**0.00%**	**0.00%**	**0.00%**	**0.00%**
	k-means++ α=1	0.38%	0.52%	0.78%	1.83%	4.09%	7.34%
	k-means++ α=1.5	0.72%	0.93%	0.89%	2.39%	4.65%	7.87%
	AFK-MC^2 α=1	0.24%	0.31%	0.31%	0.41%	0.11%	0.23%
	AFK-MC^2 α=1.5	0.37%	0.17%	0.26%	0.30%	0.08%	0.23%
RCV-1	Uniform	0.00%	0.00%	0.00%	0.00%	0.00%	**0.00%**
	k-means++ α=1	0.13%	**-0.11%**	0.08%	**-0.25%**	**-0.17%**	0.06%
	k-means++ α=1.5	-0.03%	0.21%	0.53%	0.44%	0.04%	0.16%
	AFK-MC^2 α=1	**-0.24%**	-0.01%	**-0.03%**	0.39%	0.05%	0.24%
	AFK-MC^2 α=1.5	0.13%	0.07%	**-0.03%**	0.22%	-0.09%	0.15%

except for the 20-news data set where k-means++ performs up to 8% worse. Supposedly, because this data set contains anomalies. AFK-MC^2 [4] with α=1 finds the best initialization most of the time. While k-means++ with α=1.5 does not quite reach same the quality, it performs generally better than uniform random. With α=1.5, both initialization methods are worse and more often than not are below the quality of the random uniform initialization. The run time behavior is similar on all data sets. The uniform initialization is nearly instantaneous, while the $k$means++ and AFK-MC^2 initialization generally stay below the time needed for one iteration. They only have a small impact on the overall run time. Usually, α=1 seems to work better than α=1.5, where the first is the standard cosine similarity, while the latter was used in the proofs to obtain a metric.

Table 3: Run times of all k-means variants in milliseconds.

Data set	Algorithm	k=2	k=10	k=20	k=50	k=100	k=200
Simpsons Wiki	Standard	166	457	845	1,646	3,015	10,047
	Elkan	161	352	532	1,198	2,657	8,247
	Simp.Elkan	**145**	**312**	**436**	**800**	**1,230**	**3,100**
	Hamerly	171	434	732	1,860	3,976	14,386
	Simp.Hamerly	166	421	657	1,450	2,471	9,858
DBLP Author-Conf.	Standard	32,228	29,865	24,687	42,229	50,851	80,553
	Elkan	5,675	9,650	12,366	39,652	54,901	82,732
	Simp.Elkan	5,732	10,841	15,514	44,991	66,731	105,905
	Hamerly	**4,220**	7,072	9,834	19,988	**30,846**	55,687
	Simp.Hamerly	4,285	**7,002**	**9,810**	**19,690**	31,589	**55,250**
DBLP Author-Venue	Standard	33,359	46,328	50,596	70,772	80,218	199,230
	Elkan	5,730	14,593	22,733	59,725	84,011	165,756
	Simp.Elkan	5,986	16,822	27,200	68,577	103,678	209,835
	Hamerly	4,321	11,410	18,056	33,881	**51,242**	125,066
	Simp.Hamerly	**4,188**	**11,096**	**17,799**	**33,017**	52,593	**123,931**
DBLP Conf.-Author	Standard	1,149	6,017	9,672	20,908	33,973	61,680
	Elkan	943	5,549	11,907	41,078	108,028	32,103
	Simp.Elkan	**894**	**4,018**	**6,184**	**10,998**	**16,435**	**29,093**
	Hamerly	944	6,840	14,760	50,282	125,513	347,668
	Simp.Hamerly	944	5,347	9,158	20,115	32,640	55,421
20 Newsgroups	Standard	**101**	**234**	1,223	6,755	16,394	38,131
	Elkan	118	269	498	6,683	19,917	83,407
	Simp.Elkan	118	251	**342**	**1,876**	**3,915**	**7,891**
	Hamerly	111	272	536	9,542	28,005	109,204
	Simp.Hamerly	121	266	443	5,298	12,653	29,915
RCV-1	Standard	24,569	153,170	224,939	917,894	2,669,733	6,064,203
	Elkan	7,639	38,199	47,963	**115,275**	**260,924**	547,110
	Simp.Elkan	8,825	**41,162**	**50,161**	123,428	263,728	**474,800**
	Hamerly	**5,424**	49,041	80,793	325,433	1,132,352	3,181,667
	Simp.Hamerly	5,498	47,977	81,593	320,677	1,144,947	3,266,234

At last, we discuss the achieved improvements in run time for the accelerated spherical k-means algorithms. As with the other experiments, each one was repeated 10 times with various random seeds. Table 3 shows that for most data sets the simplified Elkan algorithm is the fastest, but there are several interesting observations to be made. On the Author-Conference data set, which has the most rows of all data sets but also the lowest number of columns, the normal Elkan and both Hamerly variants are faster. Interestingly, this changes when we increase the number of columns in relation to the number of rows by transposing the data (before applying TF-IDF), shown in Fig. 2. Here, the normal Elkan and Hamerly variants increase drastically in their run time when k increases. This effect originates in the increasing cost of calculating the distances between cluster centers for the additional pruning step. By transposing the data (to cluster conferences, not authors), we increased the dimensionality by 350×,



(a) Run time of the different algorithms on Authors-Conf. (higher N, lower d).

(b) Run time of the different algorithms on Conf.-Authors (lower N, higher d).

Fig. 2: Run times of the different algorithms on the DBLP author-conference data set, and its transpose, with very different characteristics.

while at the same time reducing the number of instances by the same factor. Computing the pairwise cluster distances now became a substantial effort. This shows that there is no "one size fits all", but the best k-means variant needs to be chosen depending on data characteristics such as dimensionality and the number of instances. While Simplified Hamerly is among the best methods in both situations, it barely outperforms the standard algorithm on the latter data set. Supposedly because of the very high dimensionality, its pruning power is rather limited. While the spherical Hamerly and Elkan implementations can be faster than the standard spherical k-means algorithms, this depends on the data, and with an unfavorable data set they can be much worse. The simplified version of spherical Hamerly seems to be a reasonable default choice, but for small k, it may often be outperformed by the Elkan variants. On the well-known RCV-1 data set, speedups of over 10× are achievable for $k \geq 100$. It may be a bit disappointing that there is no "winner" solution, but data sets simply may have very different characteristics. Possibly some simple heuristics can be identified to automatically choose an appropriate alternative based on empirical thresholds (which need to be determined for a particular implementation and hence are outside the scope of a scientific paper) on the data dimensionality and data set size. In many cases, the limiting factor may be the memory usage and bandwidth for the Elkan variants. Consider the DBLP authors-conference data set with $k = 100$, the bounds used by Elkan with double precision require 2 GB of RAM for the bounds alone, and have to be read and written each iteration. The Hamerly variants only add an overhead of 44 MB. The Yin-Yang variant which we did not yet implement allows choosing the number of bounds to use, and hence make better use of the available RAM.

7 Conclusions

In this article, we use the triangle inequality for cosine similarity of Schubert [23], to accelerate spherical k-means clustering by avoiding unnecessary similarity computations. We were able to adapt the well-known algorithms of Elkan and Hamerly (along with some simplified variants) to work with similarities rather than distances throughout the algorithm. This is desirable because the similarities are more efficient to compute, and the trigonometric bounds are tighter than the Euclidean bounds [23] (with the first corresponding to the arc length, the latter to the chord length). Both require the computation of a square root and hence require similar effort.

We integrated the new triangle inequality into Elkan's and Hamerly's algorithm as two prominent and popular choices, but acknowledge there exist further improved algorithms such as the Yin-Yang, Exponion, and Shallot algorithms that deserve attention in future work. The purpose of this paper is to demonstrate that we can perform pruning directly on the cosine similarities now and that it can speed up the algorithm run times considerably (we observed speedups of over 10× for the well-known RCV-1 data set).

For further speedups, the new technique can also be combined with improved initialization methods from literature. There exists a synergy between some initialization methods that we are not yet exploiting in our implementation, where, e.g., the k-means++ initialization can pre-initialize the bounds used here, and will then allow pruning computations already in the first iteration of the main algorithm.

We hope that this article spurs new research on further accelerating spherical k-means clustering using the triangle inequality, similar to Euclidean k-means.

Acknowledgments A simpler approach of adapting Hamerly's and Elkan's algorithms for spherical k-means clustering still using Euclidean distances and not the cosine triangle inequalities was explored by our student, Alexander Voß, in his bachelor thesis.

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