Dynamic User-Defined Similarity Searching in Semi-Structured Text Retrieval

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Abstract. Modern text retrieval systems often provide a similarity search utility, that allows the user to find efficiently a fixed number \( k \) of documents in the data set that are most similar to a given query (here a query is either a simple sequence of keywords or the identifier of a full document found in previous searches that is considered of interest). We consider the case of a textual database made of semi-structured documents. For example, in a corpus of bibliographic records any record may be structured into three fields: title, authors and abstract, where each field is an unstructured free text. Each field, in turns, is modelled with a specific vector space. The problem is more complex when we also allow each such vector space to have an associated user-defined dynamic weight that influences its contribution to the overall dynamic aggregated and weighted similarity. This dynamic problem has been tackled in a recent paper by Singitham et al. in [18] in VLDB 2004. Their proposed solution, which we take as baseline, is a variant of the cluster-pruning technique that has the potential for scaling to very large corpora of documents, and is far more efficient than the naive exhaustive search. We devise an alternative way of embedding weights in the data structure, coupled with a non-trivial application of a clustering algorithm based on the furthest point first heuristic for the metric k-center problem. The validity of our approach is demonstrated experimentally by showing significant performance improvements over the scheme proposed in [18]. We improve significantly tradeoffs between query time and output quality with respect to the baseline method in [18], and also with respect to a novel method by Chierichetti et al. to appear in ACM PODS 2007 [3]. We also speed up the pre-processing time by a factor at least thirty.

1 Introduction

Singitham et al. in [18] consider the following problem: given set \( S \) of \( s \) sources of evidence and a set \( E \) of \( n \) records, they define for each record \( e^j \in E \) and each source \( s_i \in S \) a source score \( \sigma_{s_i}(e^j) \), moreover for each source \( s_i \) we have a scalar positive weight \( w_i \) that is user-defined and changes dynamically for each query. The dynamic aggregated score of \( e^j \) is \( \sum_{i=1}^{s} w_i \sigma_{s_i}(e^j) \).

The Dynamic Vector Score Aggregation problem is to find the \( k \) elements in \( E \) with the highest dynamic aggregate score. The authors note that in absence of any further structure the only solution is an exhaustive computation of the aggregate score for all the elements in \( E \) and the determination of the \( k \) highest elements in the ranking induced by the aggregation score. Therefore they consider the special case when each feature of the records \( e^j \) is actually a vector, and the source score function \( \sigma_{s_i}(e^j) \) is a geometric distance function measuring the distance of \( e^j \) to a query point \( q \) (equivalently one can define a dual similarity function to the same purpose).

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They also observe that if \( s = 1 \) and the source score is a geometric proximity function (e.g. a metric) to a query point then this problem reduces to the classical \( k \)-nearest neighbor problem. The difficulty in handling the \( k \)-nearest-neighbor problem in the general case of a linear combination of \( s \geq 2 \) geometric proximity functions stems from the need of combining the scores form generally unrelated sources compounded with the presence of arbitrary positive weights. In [18] the Vector Score Aggregation problem is solved by extending the cluster pruning technique for the geometric \( k \)-nearest-neighbor.

1.1 Our contribution

In this paper we use the cluster pruning approach but we derive a new and much simpler way of (not) embedding dynamic weights in vector cluster pruning similarity searches. Moreover by using a different clustering strategies and techniques we obtain further benefits. In particular we will describe alternatives for the following key aspects:

(a) How weights are embedded in the scheme. In the general Vector Score Aggregation problem the user supplies a query (this can be either a document in the database or a collection of keywords that capture the concept being searched for) and a weight-vector that express the user’s perception of the relative importance of the document features in capturing the informal notion of "similarity". We show in Section 4 that, surprisingly, one need not be concerned with dynamic weights at all during pre-processing, the solution for the unweighted case is good also for the weighted one.

(b) Multiple clusterings. In cluster pruning search one decides beforehand to visit a certain number of clusters whose ”leaders” are closest to the query point. However, there is a hidden law of diminishing returns: clusters further away from the query are less likely to contain good \( k \)-neighbors. We use a different strategy: we form not one but several (three in our experiments) different independent clusterings and we search all three of them but looking into fewer clusters in each clustering.

(c) The ground clustering algorithm. When searching for nearest neighbors of a query point \( q \) it is natural to consider a cluster good for such a search when its diameter is small. This leads to considering the optimal K-center problem (i.e. finding a decomposition minimizing the maximum diameter of any cluster produced) as a better objective to attain with respect to other conceivable objectives. Thus we are led to consider the Furthest-Point-First heuristic, that is 2-competitive for this problem [15]. We attain two benefits: (1) quality of the output is increased, as demonstrated by the experiments in Section 7, (2) preprocessing time is reduced by orders of magnitude since we can use fast variants of this algorithm (see e.g. [12, 11]).

By introducing these three variations we significantly outperform state of the art algorithms for this problem.
1.2 Experimental results

We have run our algorithm against two baselines. The first baseline is the algorithm in [18] that uses k-means clustering. The second baseline is the algorithm in [18] modified so to use a simple cluster pruning randomized strategy proposed in a forthcoming paper by Chierichetti et al. [3]. We perform tests on data sets of 50K and 100K documents using a variety of weights and randomly chosen query documents. Figure 2 shows the query time/recall tradeoff of the three methods. Our method is clearly dominant giving consistently better quality results in less time. Quality data are also given in tabular form in Table 2.

The top portion of Table 2 corresponds to the case of equal weights, that is equivalent to the unweighted case, and already our method shows better time/quality tradeoffs than both the baselines. In the entries of Table 2 for unequal weights our scheme is vastly superior in recall, even doubling the number of true k-nearest neighbors found using less time over both baselines. The overall quality of the retrieved nearest neighbors, as measure via the normalized aggregated goodness, is also improved: this indicates that our method is robust and stable relative to the baselines.

The simpler clustering strategy in [3] has preprocessing time close to ours, but quality/cost performance inferior to our scheme and to that in [18]. Also the improvement in preprocessing time is noteworthy, we gain a factor 30 against [18] in a test with 100,000 documents. In practice we could complete the preprocessing in one day compared to one month required by [18].

1.3 Organization of the paper

This paper is organized as follows. In Section (2) we give a brief review of the state of the art methods more relevant to our setting, while a more extended survey is postponed in the full paper. In Section (3) we review known properties of the cosine similarity/distance metric. In Section (4) we show the main theoretical analysis underpinning our weight embedding technique. In Section (5) we describe and compare the algorithm that uses our new weight embedding scheme, and the scheme proposed in [18]. In Section (6) we describe how the output quality is measured. In Section (7) we give the experimental set up and the experimental results. Conclusions and future work are in Section (8).

2 Brief state of the Art

There is a vast literature on similarity searching and k-nearest neighbor problems (see extended surveys in [16, 2]). However, much less is known for the case when users are allowed to change the underlying metric dynamically at query time. Besides the work of [18] we mention work by P. Ciaccia and M. Patella [4] discussing which general relations should hold between two metrics A and B, that allow to build a data structure using the first metric (A), but perform searches according to the second one (B).

A series of papers by R. Fagin and co-authors [6, 8, 10, 9] deal with the problem of rank score aggregation in a general setting in which items are ranked independently according to several
sources (not necessarily due to geometric distance functions) and one seeks to find efficiently the best combined ranking. The same problem but in a distributed setting is discussed in [17]. In these papers the rankings are assumed to be statically available and the issue is only how to combine the rankings efficiently. Equivalently, in their model the cost for producing the independent rankings is not accounted for. Our setting is different since the total search cost is considered.

Many other schemes are known for the classical (unweighted, \( s = 1 \)) k-nearest neighbor computation that, however, are mostly useful in low dimensional spaces (or in high dimensional spaces with dense vectors). Applications in text retrieval are characterized by very high dimensionality of the corresponding vector space (in the region of tens of thousands) and sparse vector representations. In general, sophisticated tree-based schemes are ineffective on such data sets. For example the tree-based algorithm \( M^3 \)-tree proposed by Bustos and Skopal [1] has been tested on a data set in dimension 89. The rank-aggregation method of R. Fagin, R. Kumar and D. Sivakumar [7] has been tested on data sets in dimension 800, while the hashing based method of A. Gionis, P. Indyk and R. Motwani [13] has been tested data sets in on dimension 64. The p-sphere method [14] is used in [3] as base-line since it has been shown to be superior to a series of other data structures proposed in literature. Experiments in [3] found that their random clustering method performs better than the p-sphere method on textual data.

3 Metric Spaces and Cosine Similarity

In this paper we will use mostly distance measures, therefore we will convert all results and algorithms for similarity measures into distances. As noted in [5] the inner product of two vectors \( x \) and \( y \) of length 1 (in norm 2) that is the standard cosine similarity of two normalized vector is turned into a distance \( d(x, y) = 1 - x \cdot y \). This distance function is not a metric in a strict sense since the triangular inequality is not satisfied, however the following derivation \( \|x-y\|^2_2 = x \cdot x + y \cdot y - 2x \cdot y = 2(1 - x \cdot y) = 2d(x, y) \) shows that the square root of the distance is indeed a metric. Equivalently one can say that it satisfies the extended triangular inequality \( (d(x, y))^\alpha + (d(y, z))^\alpha \geq d(x, z)^\alpha \) with parameter \( \alpha = 1/2 \). Moreover a linear combination of distance functions with positive weights defined on the same space is still a metric space \( D(x, y) = \sum w_i d_i(x, y) \) for \( w_i \geq 0 \). Thus the aggregate vector score function used in [18] although not giving rise to a metric in a strict sense is nonetheless closely related to a metric space.

4 Simplification of the vector score aggregation problem

In [18] the queries are of the form \( q = (q_1, \ldots, q_s) \) where each \( q_i \) is a vector of unit length, moreover the user supplies a weight vector \( w = (w_1, \ldots, w_s) \) where each \( w_i \) is a positive scalar weight, and the weights sum to 1. The element \( e^j \) in the input set \( E \) is of the form \( (e^1_j, \ldots, e^s_j) \) where each \( e^i_j \) is a vector of unit length. The aggregate distance function is \( d_{AD}(q, e^j) = 1 - \sum w_i(q_i \cdot e^i_j) \). While the aggregate similarity is: \( s_{AD}(q, e^j) = 1 - d_{AD}(q, e^j) = \sum w_i(q_i \cdot e^i_j) \).
**Linearity.** One should notice that because of the linearity of the summation and the inner product operators the weights can be associated to the vector space: \( \sum_i w_i (q_i \cdot e_j^i) = \sum_i q_i \cdot w_i e_j^i = q \cdot w e_j^i \). This association has been chosen in [18] thus the challenge arises from the fact that one has to do pre-processing without knowing the real weights that are supplied on-line at query time.

**A different aggregation.** Let \( q \) be a query point, \( c \) a center of cluster \( C(c) \), \( p \) a point in cluster \( C(c) \), and \( D \) a distance function that satisfies the extended triangular inequality with parameter \( \alpha \). The effectiveness of clustering search stems from the observation that the distance \( D(q, p) \) is bounded by an increasing function of \( D(q, c) \) and \( D(c, p) \). Moreover when \( p \in C(c) \), the distance \( D(c, p) \) has the smallest value over all centers in the clustering. Thus using the center \( c \) closest to \( q \) gives us the best possible upper estimate of the distance \( D(q, p) \). We have:

\[
D(q, p) \leq (D(q, c)^\alpha + D(c, p)^\alpha)^{1/\alpha}
\]

Consider now the weighted similarity \( WS \):

\[
WS(w, q, p) = \sum_i w_i (p_i \cdot q_i) = \sum_i (w_i q_i) \cdot p_i = Q_w \cdot p.
\]

where \( Q_w = [w_1 q_1, ..., w_s q_s] \) is the weighted query vector of vectors. Since the linear combination of weights and queries might not result in a unit length vector we perform a normalization (depending only in the weights and query point) and obtain a normalized weighted distance \( NWD \):

\[
NW D(w, q, p) = 1 - \frac{WS(w, q, p)}{|Q_w|} = 1 - Q_w / |Q_w| \cdot p = D(Q_w', p),
\]

where \( Q_w / |Q_w| = Q_w' \) is the normalized weighted query vector of vectors. Now we are in the condition of using the above generalized triangular inequality and establish that:

\[
NW D(w, q, p) = D(Q_w', p) \leq (D(Q_w', c)^\alpha + D(c, p)^\alpha)^{1/\alpha}.
\]

Since \( D(c, p) \) is independent of the pair \( q, w \) we can do at preprocessing time a clustering based on the input set \( E \) and the distance \( D(., .) \), regardless of weights and queries. At query time we can compute \( D(Q_w', c) \) and combine this value with \( D(c, p) \) to get the upper estimate of \( NW D(w, q, p) \) that guides the searching. The conclusion of this discussion is that using cosine similarity the multi-dimensional weighted case can be reduced to a mono-dimensional (i.e. not weighted case) for which we have good data structures.

5 Algorithms

5.1 Basic Cluster Pruning Searching

For \( s = 1 \) the cluster pruning technique works as follows. Let \( E \) be a set of points in \( d \)-dimensional space, and \( D(., .) \) the distance function among pairs of points. The set \( E \) is clustered
into $K$ groups so to minimize some functional depending on the distance. Then for each cluster a representative point is elected. When a query point $q$ is given, first one finds out a set of $k'$-nearest neighbors among the representative points, for example by exhaustive search. Afterwards only the clusters whose representative have been selected are searched exhaustively for the $k$-nearest neighbors. All other clusters are not examined, thus avoiding computing distances from $q$ and the majority of the points in $E$. This procedure is heuristic insofar as there is no guarantee that all true $k$-nearest neighbors are found, however in practice, by a careful choice of $k$, $k'$ and $K$ one can detect a large fraction of the true $k$-nearest neighbors, while accessing only a small portion of the input data set.

5.2 Our weight embedding scheme and algorithm

The discussion in Section (4) shows that the pre-processing can be done independently of the user provided weights and that any distance based clustering scheme can be used in principle. Weights are used to modify directly the input query point and are relevant only for the query procedure. The basic clustering algorithm we use is described in detail in [11]. It is an algorithm based on the further-point-first (FPF) heuristic for the k-center problem that was proposed by [15]. Summarizing, to produce $K$ clusters we start by taking a sample of $\sqrt{Kn}$ points out of $n$ points, and we apply the furthest-point-first method on the sample to produce $K$ centers. The remaining points are associated to the closest center iteratively, while adjusting the representative point (medoid) of the cluster at each addition of a point to that cluster.

The new twist is that we apply [11] three times on three different random samples and we collect all the (overlapping) clusters so produced. There is an extra overhead cost in terms of number of distance computations to be paid at query time when searching multiple clusterings. However, since each our distance computation involves only sparse vectors (i.e. we do not use dense centroids), each distance computation is less expensive. The balance of the two effects is still positive for us as demonstrated by the graphs in figure 1.

5.3 The weight embedding scheme of [18]

In [18] several schemes and variants are compared but experiments show that the best performance is consistently attained by Query Algorithm 3 (CellDec) described in [18, Section 5.4]. The preprocessing is as follows. For simplicity we consider the 3-dimensional case, that is a data set where each record has 3 distinct sources of evidence (e.g. in out tests, title, author and abstract of a paper). We consider the set $T$ of positive weight-vectors summing to one (this is the intersection of the hyperplane $w_1 + w_2 + w_3 = 1$ with the positive coordinate octant). We split $T$ into 4 regular triangles $T_1$, $T_2$ and $T_3$ each incident to a vertex of $T$ and the central region $T_4$. Let $V_i^j$ be the vector corresponding to record $j$ and source $i$. Region $T_4$ is the central one and weights in $T_4$ are not too different form each other, therefore we form a composite vector as follows $V(T_4)^j = V_1^j + V_2^j + V_3^j$. For the other four regions we apply a squeeze factor $\theta$ for the vector spaces corresponding to the lower weights. $V(T_i)^j = V_1^j + \theta V_2^j + \theta V_3^j$. We build
similarly $V(T_2)^j$ and $V(T_3)^j$. Experiments in [18] show that a value of $\theta = 0.5$ attains the best results. At query time, given the query $Q = (q, w)$ one first detects the region of $T$ containing $w$, then uses $q$ in the associated indexing data structure for cluster-pruning.

5.4 The clustering scheme of [3]

In a forthcoming paper [3] Chierichetti et al. propose a very simple but effective scheme for doing approximate k-nearest neighbor search for documents. In a nutshell, after mapping $n$ documents in a vector space they choose randomly $K = \sqrt{n}$ such documents as representatives, and associated each other document to its closest representative. Afterwards, for each group the centroid is computed as “leader” of the group to be used during the search. In [3] the authors are able to prove probabilistic bounds on the size of each group which is an important parameter that directly influences the time complexity of the cluster prune search. Dynamically weighted queries are not treated in [3], therefore we choose as a second base-line to employ [3], in place of K-means, within the weighting framework of [18].

6 Measuring Output Quality

We compare the results provided by the three algorithms using two quality indexes (employed also in [18] and [3]): the mean competitive recall and the mean normalized aggregate goodness.

Mean Competitive Recall. Let $k$ be the number of similar documents we want to find (in our experiments $k=10$) and $A(k, q, E)$ the set of the $k$ retrieved document by algorithm $A$ on data set $E$, and $GT(k, q, E)$ the ”Ground truth”, the set of the $k$ closest points in $E$ to the query $q$ which is found through an exhaustive search; the competitive recall is $CR(A, q, k) = |A(k, q, E) \cap GT(k, q, E)|$. Note that the Competitive recall is a real number in the range $[0, ..., k]$ and a higher value indicated higher quality. The Mean Competitive Recall $\overline{CR}$ is the average of the competitive recall over a set of queries $Q$:

$$\overline{CR}(A, Q, E) = \frac{1}{|Q|} \sum_{q \in Q} CR(A, q, k)$$

This measure tell us how many of the true $k$ nearest neighbors are our algorithm is able to find.

Mean Normalized Aggregate Goodness. We define as the Farthest Set $FT(k, q, E)$ the set of $k$ points in $E$ farthest from $q$. Let the sum of distances of the $k$ furthest points from $q$ be $W(k, q, E) = \sum_{p \in FS(k, q, E)} \mu(q, p)$. The normalized aggregate goodness:

$$NAG(k, q, A) = \frac{W(k, q, E) - \sum_{p \in A(k, q, E)} \mu(q, p)}{W(k, q, E) - \sum_{p \in GT(k, q, E)} \mu(q, p)}.$$
Note that the Normalized Aggregate goodness is a real number in the range $[0, \ldots, 1]$ and a higher value indicated higher quality. The Mean Normalized Aggregate Goodness $\overline{NAG}$ is the average of the normalized aggregate goodness over a set of queries $Q$:

$$\overline{NAG}(A, Q, E) = \frac{1}{|Q|} \sum_{q \in Q} NAG(A, q, k).$$

Among the possible distance functions there is a large variability in behavior (for example some distance functions are bounded, some are not). Moreover for a given $E$ and $q$ there could be very different range of possible distance values. To filter out all these distortion effects we normalize the outcome of the algorithm against the ground truth by considering the shift against the $k$ worst possible results. This normalization allows us a finer appreciation of the different algorithms by factoring out distance idiosyncratic or border effects.

### 7 Experiment

In our experiment we compared the following algorithms:

A) The CellDec algorithm described in [18] with k-means clustering and weighted cosine distance.

B) The algorithm proposed in [3] based on random cluster algorithm and weighted cosine distance, christened PODS07 for lack of a better name.

C) The algorithm proposed here based on the furthest point first algorithm and weighted cosine distance (referred to as Our).

We implemented all the algorithms in Python. Data were stored in textual bsd databases. Tests have been run on an Intel(R) Pentium(R) D CPU 3.20GHz with 4GB of RAM and with operating System Linux.

Following [18] we have downloaded the first one hundred thousands Citeseer bibliographic records\(^1\). Each record contains three fields: paper title, authors and abstract. We built two data sets: TS1 with the first 53722 documents and TS2 with all 100000 downloaded documents. After applying standard stemming and stop words removal, three vector spaces were created: one for each field of the documents. Terms in the vector are weighted according to the standard tf-idf schema. Details are in Table 1.

Without loss of generality, as queries we used documents extracted from the data set. Test queries have been selected by picking a random set of 250 documents. During searches the exact match of the query document is not counted. In our experiments we adopted the 7 sets of weights used in [18]. For each set of weights, we always used the same query set. This gave us the opportunity of comparing results for different choices of the weights vector. The query time as a function of the number of clusters visited is in Figure 1 and shows clearly the speed up factor of two.

\(^1\) [http://citeseer.ist.psu.edu/](http://citeseer.ist.psu.edu/)
| Dataset | TS1     | TS2    |
|---------|---------|--------|
| Input size (MB) | 41.80   | 76.13  |
| # Records    | 53722   | 100000 |
| # Clusters   | 500     | 1000   |
| Algorithm    | Our     | CellDec | PODS07 | Our | CellDec | PODS07 |
| Preprocessing time | 5:28    | 215:48 | 7:18   | 20:13 | 636.80 | 22:56 |
| Space (MB)   | 332.078 | 1407.656 | 1402.140 | 645.765 | 2738.671 | 2725.078 |

Table 1. Measure of input complexity. Preprocessing time (in hours and minutes) and storage (in Megabytes) of the two data structures generated by CellDec, PODS07 and our algorithm.

![Graph](image1.png)

(a) Data Set TS1

![Graph](image2.png)

(b) Data Set TS2

Fig. 1. Average query time (in seconds) over all queries in function of the number of visited clusters.

8 Conclusions and future work

We have shown that a difficult searching problem with dynamically chosen weights can be reduced, thanks to the linearity properties of the cosine similarity metric, to a simpler static search problem. For this problem we provide efficient and effective method that are competitive with state of the art techniques for large semi-structured textual databases. We plan in future work to extend and test our techniques to handling other types of data (e.g. images, and sound). We wish to thank P. Raghavan for introducing us to cluster pruning techniques and A. Panconesi for many useful discussions and for providing a preprint of [3].

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Fig. 2. Recall of 10 nearest neighbors as a function of query time. Each point in the graph is the average of measurements of all queries for a class of weights and a number of visited clusters. The points in the upper left corner of the graphs corresponding to our algorithm show clear dominance.

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| Visited clusters | Data Set TS1 = 50K docs. | Data Set TS2 = 100K docs. |
|-----------------|-----------------|-----------------|
|                 | Recall           | NAG             | Recall           | NAG             | Recall           | NAG             | Recall           | NAG             |
| CellDec         | 4.812 5.184 5.336 | 5.472 5.544 5.644 | 4.592 5.536 5.704 | 5.776 5.86 5.904 | 5.972 5.972 5.972 |
| PODS07          | 4.512 5.032 5.196 | 5.284 5.372 5.444 | 4.852 5.18 5.308 | 5.444 5.528 5.6  | 5.652 5.652 5.652 |
| Our             | 6.128 7.168 7.64  | 7.832 7.916 7.984 | 6.848 7.708 8.08 | 8.268 8.392 8.448 | 8.48 8.48 8.48  |
| NAG             | 0.769 0.811 0.830 | 0.844 0.855 0.866 | 0.852 0.869 0.889 | 0.908 0.914 0.918 | 0.918 0.918 0.918 |
| PODS07          | 0.743 0.807 0.821 | 0.832 0.842 0.853 | 0.771 0.819 0.843 | 0.860 0.875 0.881 | 0.881 0.881 0.881 |
| Our             | 0.778 0.833 0.856 | 0.869 0.872 0.875 | 0.836 0.883 0.903 | 0.909 0.916 0.921 | 0.921 0.921 0.921 |
| Query weights   | 0.2-0.4-0.2      | 0.2-0.4-0.4     | 0.2-0.4-0.4     | 0.2-0.4-0.4     | 0.2-0.4-0.4     | 0.2-0.4-0.4     | 0.2-0.4-0.4     | 0.2-0.4-0.4     |

Table 2. Quality results of the compared algorithms. Recall is a number in [0,10]. Normalized Aggregated Goodness is a number in [0,1]. Data as a function of the number of visited clusters.