Similarity search based on a distance function in metric spaces is a fundamental problem for many applications. Queries for similar objects lead to the well-known machine learning task of nearest-neighbours identification. Many data indexing strategies, collectively known as Metric Access Methods (MAM), have been proposed to speed up queries for similar elements in this context. Moreover, since exact approaches to solve similarity queries can be complex and time-consuming, alternative options have appeared to reduce query execution time, such as returning approximate results or resorting to distributed computing platforms. In this paper, we introduce MASK (Multilevel Approximate Similarity search with $k$-means), an unconventional application of the $k$-means algorithm as the foundation of a multilevel index structure for approximate similarity search, suitable for metric spaces. We show that inherent properties of $k$-means, like representing high-density data areas with fewer prototypes, can be leveraged for this purpose. An implementation of this new indexing method is evaluated, using a synthetic dataset and a real-world dataset in a high-dimensional and high-sparsity space. Results are promising and underpin the applicability of this novel indexing method in multiple domains.

**Keywords** Data indexing · Approximate similarity search · Metric distance · Unsupervised learning · Distributed computing · $k$-means
1 Introduction

Similarity search, also known as proximity search, [1, 2, 3] is a cornerstone for applications in many different fields such as databases [4], information retrieval [5], distributed data processing [6], computer vision [7] and bioinformatics [8, 9], among others. Elements from a dataset are represented by feature vectors in a multidimensional space, and the goal is to find which elements are similar (close) to a given query object, subject to a certain measure of similarity or, conversely, dissimilarity.

More formally, let $\mathcal{X}$ be the domain of elements represented by their descriptive features and $s : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ a similarity function that, for each pair of elements $a, b \in \mathcal{X}$, returns a real number $s(a, b)$ representing a similitude score between these two elements. In some cases, it is more convenient to define an equivalent dissimilarity function $\delta : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$, so that for $a, b, c \in \mathcal{X}$ it holds that $s(a, b) > s(a, c) \iff \delta(a, b) < \delta(a, c)$.

The pair $(\mathcal{X}, \delta)$ is known as a dissimilarity space, a kind of topological space [10]. In addition, if $\delta$ satisfies the properties $\delta(a, b) \geq 0$ (non-negativity), $\delta(a, a) = 0$ (reflexivity), $\delta(a, b) = \delta(b, a)$ (symmetry) and $\delta(a, b) + \delta(b, c) \geq \delta(a, c)$ (triangle inequality), then the dissimilarity function is a metric and it is usually termed as a distance [11, 12].

Given a query object $q \in \mathcal{X}$, the goal of similarity search is to resolve some of the following queries [2]:

- **Point query**: Finding elements in $\mathcal{X}$ with exactly the same feature values as $q$.
- **Range query**: Retrieving a subset of elements $\{o_i\} \in \mathcal{X}$ whose feature values lie within the scope of a given similarity threshold $r$ around $q$, so that $\forall o_i, \delta(o_i, q) \leq r$.
- **Nearest-neighbour query**: Recovering elements in $\mathcal{X}$ whose features are the most similar to the feature vector representing $q$. In this case, we may be interested in finding the single most similar element to $q$ (nearest neighbour), denoted by $NN_q$, or the k closest elements to $q$ ($k$-nearest neighbours), denoted by $k\cdot NN_q$.

Numerous data indexing methods, collectively known as access methods, have been proposed to speed up similarity queries. These methods create an index structure to partition the whole domain $\mathcal{X}$ in different regions, according to a distance function. After this, users employ different search algorithms to solve similarity queries using this index. There is a wide range of access methods, including exact approaches, approximate solutions and variants tailored to distributed computing systems.

Exact similarity search methods identify the completely accurate result set for a query. In vector spaces, multi-attribute access methods use the absolute position of objects to group elements and search for similar instances. In a $d$-dimensional Euclidean space, these indexing structures are jointly known as multidimensional access methods. These can be classified as Point Access Methods (PAM), for elements without a spatial extension, and Spatial Access Methods (SAM), to search extended elements such as lines, polygons or higher-dimensional polyhedra. In research literature, the general acronym SAM commonly designates both classes of indexing strategies in vector spaces [5].

However, SAM present several limitations. First, in applications like textual and multimedia databases, bioinformatics or pattern recognition, elements in $\mathcal{X}$ cannot always be described in a vector space. Second, to compare the similarity between any two elements we must use a distance function that avoids introducing any correlation between feature values [13]. A general distance function that meets this requirement is the Minkowski distance [14]. The Manhattan or city block distance ($L_1$ norm), the Euclidean distance ($L_2$ norm) and the Chebyshev distance ($L_\infty$ norm) are typical instances of this family. Third, SAM are prepared for data with spatial components or represented in a vector space with a relatively low number of dimensions. In high-dimensional spaces their data partition algorithms become unusable [15], due to the curse of dimensionality [16]. Hence, all elements tend to be very far from each other, disregarding the distance function chosen for the index. Feature selection [17] or dimensionality reduction techniques like multidimensional scaling [18] can mitigate this problem. However, these approaches will only be useful if the effective number of dimensions
in which the elements are actually represented is low. The so-called intrinsic dimensionality of a dataset $X$, accounts for this notion of “effective dimensions”, and is given by $\rho = \frac{\mu^2}{2\sigma^2}$, where $\mu$ and $\sigma^2$ are the mean and variance of the distribution of distance values between any pair of elements in $X$, respectively.

Metric Access Methods (MAM) provide a more general framework for similarity search problems set out in metric spaces [1, 3]. If $d : X \times X \rightarrow \mathbb{R}$ is a distance function (hence, a metric), then the pair $(X, d)$ defines a metric space. In this setting, MAM exploit the triangle inequality to partition the metric space into subspaces, so that they can filter out portions of the dataset that cannot contain valid results. This is a more general framework that subsumes SAM, since every normed vector space induces a metric. Additionally, alternative frameworks can leverage different properties, like Ptolemaic Access Methods (PtoAM) [19], that substitute the triangle inequality for Ptolemy’s inequality and use distances where it is applicable or Supermetric Search [20], which involves semimetric spaces where the so-called four-point property holds.

Nevertheless, MAM also present limitations. In certain complex problems there is no topological information about the application domain, so that only non-metric similarity or dissimilarity functions are available [21]. Examples include cosine similarity in information retrieval, dynamic time warping in time series and several edit distances in computational biology. This lack of information about the problem context impedes the development of MAM for those cases. In addition, exact search provided by MAM can be expensive, regarding computation time spent in the search process and updating the index structure in presence of dynamic data. Moreover, in high-dimensional problems MAM indexes have serious issues to narrow down the search of candidate elements for a query. As a result, these methods usually default to a sequential scan. In this situation users will accept a trade-off solution, sacrificing accuracy for a significant reduction in search time.

Approximate indexing methods implement compromise solutions for similarity search that may introduce some error in results, although not necessarily. In exchange, they provide faster response time by computing fewer distance values or decreasing usage of computing resources to complete the search. These methods are aimed at either vector spaces or metric spaces [2, 3, 22]. In this paper, we introduce MASK (Multilevel Approximate Similarity search with k-means), a novel indexing method based on a multilevel design for approximate similarity search. This method involves an unconventional application of the $k$-means partitioning algorithm [23, 24], that quickly reduces the number of regions to be checked when searching for results. For each level in the index structure, instead of fixing a low value for $k$ (number of centroids), as it would be customary in clustering problems, we force $k$-means to generate a high number of centroids that represent underlying data points with finer detail. Using a very large number of centroids, our indexing method can be applied to any metric space, including the particular case of vector spaces. We show that this unusual application of $k$-means has attractive properties and renders good performance, even with high-dimensional datasets, represented in a feature space that is usually sparse.

Scalability is another important limitation for many indexing methods, that struggle to work with large datasets [25]. Indexes whose design follows a top-down data partition strategy are not prepared for big data problems in distributed systems, where it is unfeasible to centralize metadata in a single node. Instead, successful indexing methods for large datasets usually follow a bottom-up partitioning strategy. We propose the same approach in MASK, which makes it suitable for distributed computing applications. In this case, an independent, multilevel index structure can be created for each data partition without the need of any information exchange between computing nodes, either to build the indexes or to solve queries. At search time, the top level index at each node can discard partitions that cannot contain a valid answer, to speed up the retrieval of candidate elements.

The rest of the paper is organized as follows. Section 2 reviews previous research related to multidimensional data indexing, in particular MAM and, within them, those based on clustering algorithms. Section 3 describes MASK, the new indexing method based on an unconventional application of $k$-means. Section 4 presents the results of two empirical experiments to gain intuition about the properties exploited by this new indexing method, as well as to evaluate its performance in high-dimensional, high-sparsity problems. In Section 5
we discuss further design considerations and possible applications of this indexing method, including its application for similarity search in distributed computing platforms. Finally, in Section 6 we recap the main conclusions for this work and lay out promising lines for future work.

1.1 Contributions

MASK follows a multilevel, bottom-up design, similar to several methods found in previous research (see Section 2 for further details). However, unlike extant proposals for approximate indexing, it is based on an unconventional application of the \( k \)-means algorithm, that can take advantage of increasing resources in modern computing systems and distributed platforms. Following this strategy, data points can be assigned to closer \( k \)-means centroids, which are distributed in the feature space according to the density of data in different regions. Thanks to this, MASK can improve the performance of similarity search queries in high-dimensional problems which, oftentimes, also exhibit high sparsity. In consequence, it is characterized by two distinctive traits:

- The multilevel structure of clusters is built following a bottom-up approach. As a result, index construction can be distributed among several computing nodes, where each node can store one or several data partitions. Furthermore, we show that this strategy let the index recover underlying patterns in the dataset represented, in the general case, via pairwise dissimilarities between elements that define a dissimilarity space [10].

- Rather than determining a restrained number of prototype points (\( k \)-means centroids) to cluster elements at each level, our indexing method bombards each data partition with as many centroids as it can be afforded by available resources in each computing node. Once all centroids have been placed at their final location, they become the new set of elements to be clustered at the next layer above, using again as many \( k \)-means centroids as possible. This procedure is repeated at each additional level aggregated to the index structure, until the set of centroids at the final top level becomes of manageable size.

2 Background and related work

This section recaps the main concepts and strategies that constitute the basis for different similarity search methods. Featured access methods related to MASK are also described. Our main goal is to contextualize our work with previous research in this area and highlight the main novelties introduced by MASK, with respect to previous approaches.

2.1 Exact similarity search

As described above, access methods for exact similarity search include SAM (Spatial Access Methods) and MAM (Metric Access methods). Regarding SAM, surveys comparing dozens of indexing algorithms in this class can be found [26, 15]. Archetypal examples include the B-Tree [27, 28], Bloom filters [29, 30], the k-d tree [31, 32], linear quadtrees [33], as well as the R-tree [34] and its variants.

Except for few exceptions, these methods render very poor performance partitioning high-dimensional representation spaces. Experiments conducted by [35] suggest that they become unusable for a number of dimensions greater than 15. In the same way, according to [36] problems start at 10-15 dimensions in experiments with data following a uniform distribution. In that case, or when there is not even a clear representation of the elements in the set and only a distance function can be used to compare any pair of them, it is necessary to resort to MAM.

Different MAM have been proposed to implement indexing structures and query operations in metric spaces. Some of them use clustering algorithms, like \( k \)-means [37, 23, 24], to recursively partition the whole set of elements, leading to the creation of a hierarchical structure (tree) of nested clusters. This tree of clusters
is usually built following a top-down approach. Furthermore, in all cases the utilization of the $k$-means
algorithm in index creation follows the standard procedure of estimating a restricted number of centroids,
around which nested subgroups of elements can be grouped at each level.

As in the case of SAM, several surveys [1, 38, 39] and comprehensive monographs [2, 3] provide thorough
comparisons among alternative MAM and their properties. [40] introduces general properties of these
indexing structures, along with an initial taxonomy to classify MAM according to two possible data partition
strategies:

- **Ball partitioning**: In this type of indexing methods a subset of featured elements (sometimes referred
to as vantage points) \(\{v_i\} \in S, \ i = 1, \ldots, n\) are selected and a ball of radius \(r\) is defined around each
of them, with \(r = \text{median}(d(v_i, a)), \ \forall a \in S\). As a result, each ball defines a data partition separating
all points that lie within the scope of the ball from all other points outside the ball. For a dataset
distributed uniformly over the metric space this method is known to create many partitions that
will be intersected by the query region in many similarity search problems, thus providing poor
performance [40, 41].

- **Generalized hyperplane partitioning**: This class of MAM relies on a data partitioning scheme based
on defining a set of generalized hyperplanes (GH). Given two elements \(v_1, v_2 \in S | v_1 \neq v_2\) a GH
is defined as the subset of elements \(\{q_i\} \in S | d(q_i, v_1) = d(q_i, v_2), \ \forall i\). In consequence, each GH
partitions the space in two regions, one for all elements closer to \(v_1\) and the rest of elements closer to
\(v_2\). This strategy can produce more balanced partitioning schemes with GH defined using randomly
sampled elements.

The Vornoi-Tree [42] is a well-known example of a ball partitioning indexing algorithm. In the same way, one
of the most popular algorithms for indexing in metric spaces, the M-Tree [43], is also a prominent example
of a ball partitioning algorithm (although it partially incorporates some aspects of GH methods). In contrast,
the generalized hyperplane tree (GHT) [40] and its extension into an \(m\)-ary tree, the GNAT [41] are two
featured examples of GH-based indexing methods.

Complementing the previous taxonomy, [1] present a coherent framework to analyze data indexing methods
in metric spaces, mainly from the point of view of multimedia databases and information retrieval systems,
and introduce an alternative classification of MAM in two groups:

- **Pivoting algorithms**: A subset of reference elements \(\{v_i\} \in S, \ i = 1, \ldots, n\) (known as pivots) is
identified. Then, all remaining objects are classified according to their distances to the pivot objects.
Clearly, ball partitioning methods fall in this category, which also includes other MAM that make
use of precomputed distance matrices between pairs of elements in the dataset, such as AESA [44]
and LAESA [45]. AESA is very fast but it consumes a lot of resources (requires \(O(n^2)\) space and
construction time). LAESA uses \(k\) fixed pivots so that required space and construction time is
reduced to \(O(kn)\).

- **Compact partitioning algorithms**: In this case, the metric space is partitioned into clusters, according
to the proximity of elements to the centroids of each cluster. In this case, it is guaranteed that each
element is associated to its closest cluster center, whereas in pivoting algorithms that may not be the
case for elements associated to certain pivots. Methods based on the GH pertain to this category, as
well as algorithms defining a tree of nested clusters.

The Burkhard-Keller Tree [46] is probably one of the first examples of pivot-based indexing algorithm,
although it is conceived only for discrete distances. [40] introduces the metric tree, whose design is further
expanded in the VP-Tree [47] and introduces the alternative term vantage point to name the pivots. In contrast,
the hierarchical \(k\)-means tree [48] is one of the first examples of compact partitioning algorithm. Besides
GHT and GNAT, another example of compact partitioning algorithm is the list of clusters (LC) [49]. This
algorithm exhibits very good performance for indexing high-dimensional spaces, but at the cost of a quadratic
complexity in construction time, which invalidates it for distributed computing and big data settings.
Most of these indexing methods are designed for static datasets, and they are not well prepared for frequent insertions and deletions. Recent variants of MAM are specifically conceived for dynamic data, such as the DBM-Tree [50]. Its index structure is adapted to the density of local data regions, so that the height of the tree is higher in denser areas to attain a trade-off solution. Moreover, other recent proposals for MAM also include: probabilistic approximate indexing [51], which sacrifices accuracy for query resolution speed (see Section 2.2 below); redesigns of classic indexes such as the M-Tree, using cut-regions instead of ball regions [52]; specific methods to improve in-memory data indexing [53, 54]; a disk-based method to be integrated in commercial database management systems (SPB-Tree [55]) and new approaches to increase efficiency in dynamic data indexing [56].

2.2 Approximate similarity search

The approach proposed in this paper to resolve similarity queries pertains to the class of approximate search methods. Many examples of this kind of algorithms can be found in previous research. They usually aim at situations in which exact methods cannot provide a fast answer, such as in high-dimensional problems or using big data, where exact techniques default to a full scan of the entire dataset.

It is possible to find approximate similarity search methods designed for either vector spaces or metric spaces. [57] introduces a unified framework to study fast similarity search methods that can be either exact or approximate. Besides, [22] present a comparative summary of relevant approximate methods, introducing a taxonomy to classify them according to relevant traits, such as target space (vector, metric), strategy to obtain approximate results (changing the representation space, reducing the number of comparisons), guarantees provided on the quality of results (no guarantees, deterministic, probabilistic) and degree of interaction with users (static, interactive).

One of the first algorithms for approximate similarity search in metric spaces found in literature is FastMap [58]. It is based on a method to obtain a fast projection of elements in the original dataset into a $k$-dimensional space, where $k$ is a user-defined parameter and the projection preserves the distance between pairs of elements. Thus, it can reach an approximate answer via dimensionality reduction. Other popular exact algorithms also have their approximate versions, including three variants for the R-Tree [59] in vector spaces and three more based on the M-Tree [60] in metric spaces.

Certain approximate algorithms combine different strategies. An interesting example is the Integrated Progressive Search [61], which aims at vector spaces. This method first applies dimensionality reduction methods and, later on, applies conventional $k$-means clustering [62] on the resulting data points in a lower dimension space. This approach reduces the number of distance comparisons that must be performed. However, in general it is not straightforward to find a dimensionality reduction technique that works well for any problem. As we will see later, MASK takes a different approach, leveraging some interesting properties of the core $k$-means algorithm [63] to reach an approximate result without the need to reduce the number of dimensions of the original feature space.

Approximate similarity search methods have become a frequent approach applied in previous research works, since they provide a convenient trade-off between speed and accuracy of results. Featured methods include Locality Sensitive Hashing (LSH) [64], which has interesting applications for similarity search under edit distance [65], and the DAHC-Tree [66], aimed at high-dimensional problems in metric spaces. The indexing method proposed in this paper takes advantage of certain properties of the $k$-means algorithm, along with available computational resources, to provide an approximate indexing method that is easy to construct, valid for the general case of metric spaces and can be used with both static and dynamic datasets. Therefore, it offers a versatile compromise solution for similarity search.
2.3 Scalable similarity search

Several indexing methods for similarity search have been designed to work with distributed systems [39], addressing large and complex datasets. Some initial examples of this kind are GHT* [67], MCAN [68], Metric Chord (M-Chord) [69] and an extension of GNAT (EGNAT) for parallel systems [70].

Later on, implementations in real systems started to appear, such as MD-HBase [71]. This method integrates multidimensional indexing in the open source key-value store HBase, focusing on location based services. Nevertheless, this application only implements two examples of SAM (K-d Tree and the Quad Tree) in the distributed data store, without considering metric spaces. Likewise, the A-Tree [72] implements a combination of R-trees and Bloom filters (both part of the SAM family) for multidimensional data indexing in cloud computing platforms. M-Grid [73] is a more recent example of a distributed multidimensional indexing structure for location based data, that claims to substantially improve the performance of MD-HBase.

Another innovative example in the MAM family is D-Cache [74]. This method is based on caching distance information that can be leveraged in distributed systems to speed up similarity queries.

Nowadays, distributed systems involving big data and high-dimensional, high-sparsity problems have proliferated. Technological frameworks like Apache Spark have been determinant for the widespread adoption of cluster-based systems in many areas, including machine learning. Recent advances show promising implementations of SAM on Apache Spark, specifically for similarity search with spatial data and IoT applications [75, 76]. However, to date there is no clear implementation of more general MAM in modern distributed data processing frameworks. As we describe in Section 3, the approximate similarity search method proposed in this paper can be naturally implemented on distributed computing platforms. The multilevel, bottom-up approach to build the index can be independently executed in each data partition, located in different nodes. Furthermore, the index construction does not imply any exchange of information or metadata between nodes storing different data partitions. The only coordination requirement would be to maintain the top level layer of representative points, to help in deciding which nodes should be involved in resolving a particular query.

2.4 Machine learning and similarity search

As we have seen, there is a close connection between machine learning and similarity search indexing. The foundations for designing data access methods repose on familiar concepts in machine learning classification, such as dissimilarity spaces and distance functions. They are also affected by the same limitations, namely the curse of dimensionality and the challenge of identifying the actual intrinsic dimension governing some problems.

Clustering algorithms play a central role in many indexing methods for similarity search. The \( k \)-means algorithm \([37, 23]\) stands out as a recurrent solution to build indexing structures, starting with hierarchical \( k \)-means \([48]\). In fact, according to \([2]\), the GHT and GNAT indexing methods can be regarded as special cases of a broader class of hierarchical clustering methods described by \([46]\) and \([48]\). However, the pivots selected by GNAT are not necessarily \( k \)-means centroids, which are \( k \) points that may not belong to \( S \) and that minimize the sum of squared distances of individual objects to their closest centroid.

Interestingly, the applicability of \( k \)-means for the construction of hierarchical indexing structures is already described, albeit without implementation details, by \([23]\). This application entails building tree clusters in a top-down fashion, so that the within cluster variance does not exceed an upper threshold \( R \). The set of centroids at each level act as a fair representation of data objects, effectively summarizing the clusters of all lower levels. Likewise, MacQueen also demonstrates that \( k \)-means can be readily extended beyond vector spaces to the general case of metric spaces. For example, \( k \)-means has been successfully applied in image indexing \([77]\). A recent application of \( k \)-means and Voronoi diagrams for multidimensional data indexing and spatial data query processing in sensor networks \([78]\) confirms the validity of multilevel \( k \)-means indexing for contemporary distributed data problems.
Nevertheless, this approach for building hierarchical indexes with $k$-means clusters is based on establishing an upper limit $R$ for within-cluster variance. In fact, this is just an alternative formulation of the typical problem in partitioning clustering, namely selecting the appropriate number of clusters that must be identified in the dataset [79, 80]. Many different methods have been proposed to solve this problem (see, for instance, [81, 82] for a detailed discussion), some of which rely on fixing a within-cluster variability threshold [83, 82].

To avoid these practical issues, it would be desirable to just let the multilevel clustering algorithm to adapt itself to the density of objects in different regions of the metric space to be indexed. In a certain way, this resembles the idea behind the DBM-Tree discussed in Section 2.1, but considering in this case a tree of clusters. Our indexing algorithm introduces an unconventional application of $k$-means because it completely eliminates the restriction of determining the optimal number of clusters in advance. Instead, we propose to create as many centroids at each level as it can be afforded by our computational resources.

As we show in Section 3, we can take advantage of the minimization of the sum of square distances from each object to the closest centroid to adjust the position of prototypes for each cluster, according to the density of elements in each region of the metric space. In a certain way, this approach also follows the recent strategy of learned indexes in databases [84], which states that traditional indexing structures can be substituted by multiple levels of machine learning algorithms that can help to approximate the underlying distribution of data. The Z-order Model (ZM) index is an example application of the learned index strategy to spatial index structures (for instance, the R-tree). In our method, we let the $k$-means algorithm to learn good locations to place the centroids representing each cluster, assuming that a sufficiently large number of centroids is used to map the set $S$.

3 Multilevel k-means structure for data indexing

This section describes the MASK method for approximate similarity search in metric spaces, using a multilevel index structure. The rationale behind the unconventional application of the $k$-means clustering algorithm is also explained. This method can be implemented in distributed systems, as different sections of the multilevel index can be independently created on data partitions stored in different nodes.

3.1 Multilevel index design

Figure 1 represents the design principles of MASK. At the lowest level, we have the data points in $X$ to be indexed. Blue boxes in the diagram represent different data partitions or groups. These groups could be stored in different nodes of a cluster although, for simplicity, in this case data partitions are considered to reside in the same node.

As described in Section 2 above, several MAM rely on building a hierarchy of clusters, using unsupervised machine learning algorithms like $k$-means. In the case of MASK, the multilevel structure of $k$-means centroids is created following a bottom-up approach. The first level of centroids (identified as $n_1$ in Figure 1) summarize the actual data points at the lowest level, so that the points assigned to each cluster are represented by its $k$-means prototype (centroid). The second level (identified as $n_2$), corresponds to centroids representing the prototypes calculated at the first level, $n_1$. The same procedure is recurrently applied, creating additional layers of prototypes summarizing the immediately lower group of centroids. The method stops when the number of centroids at the top layer of this multilevel index structure becomes manageable. Algorithm 1 details the construction of this multilevel index structure, using $k$-means.

The assembly process requires two initial parameters: the group length ($\text{lengthGroup}$) and the number of centroids calculated for each group ($n\text{Centroids}$). Group length refers to the number of elements in each data partition at the lowest level. In general, we assume that all partitions will have the same size, although this condition is not strictly necessary. The size of partitions should be configured according to available computing power (and the total number of nodes in distributed computing systems).
Algorithm 1: Multilevel index construction

**Input:** data, lengthGroup, nCentroids  
**Output:** layerPoints, layerLabels, layers

\[ \text{ngroups} \leftarrow \text{lengthData} / \text{lengthGroup}; \]
\[ \text{vector} \leftarrow \text{split}(\text{data, ngroups}); \]

Initialize lists \text{layerPoints} and \text{layerLabels}, and variable \text{idLayer};

\[ \text{while} \ \text{ngroups} \geq 1 \text{ do} \]
  \[ \text{// Initialize groupsPoints, groupsLabels and points} \]
  \[ \text{for} \ \text{idGroup} = 1 \text{ to } \text{ngroups} \text{ do} \]
    \[ \text{points} \leftarrow \text{vector[idGroup]}; \]
    \[ \text{groupsPoints.add(kmeans(nCentroids, points));} \]
    \[ \text{groupsLabels.add(kmeans.labels);} \]
    \[ \text{layerPoints.add(groupsPoints);} \]
    \[ \text{layerLabels.add(groupsLabels);} \]
    \[ \text{ngroups} \leftarrow \text{length(groupsPoints)} / \text{lengthGroup}; \]
    \[ \text{if} \ \text{ngroups} \geq 1 \text{ then} \]
      \[ \text{vector} \leftarrow \text{split(layerPoints, ngroups);} \]
      \[ \text{idLayer} += 1; \]
  \[ \text{layers} \leftarrow \text{idLayer} - 1 \]

Figure 1 shows a simple case example: 80 points in the dataset at the lowest level, with \text{lengthGroup} = 10 and \text{nCentroids} = 5. Thus, at the first level the algorithm assumes 8 groups of 10 points. In each group, the algorithm builds 5 clusters using \text{k-means}. Depending on the distance between points and their corresponding centroid, a different number of points can be assigned to each cluster. For this reason, regions with higher data density will also tend to receive a higher number of centroids. This clustering at the first level reduces the initial number of data points by a certain proportion, the \text{data summarization ratio}, determined by the relationship between the values of \text{lengthGroup} and \text{nCentroids}. In this example, this ratio is 2:1 and, hence, the size of each group of data is shrunk by a half, from 80 to 40.
At the second level, the algorithm takes 4 groups of 10 points (since $\text{lengthGroup} = 10$) and $k$-means is applied in each group to obtain 5 new clusters, each one represented by a centroid. This process is repeated recursively, until the number of points at the top level is small enough. The stop condition implemented in this case is that the total number of centroids at the top level must be less than or equal to $\text{lengthGroup}$. Therefore, the computational complexity of the problem gets lower as the total number of points is reduced after each iteration.

Nevertheless, the important aspect of selecting the optimal number of centroids to calculate at each level remains open. In general, previous indexes based on trees of clusters generate a limited number of centroids at each level. In contrast, recent methods for metric spaces, such as DBM-Tree [50], adapt the height of the indexing tree to changes in data density of different regions in $\mathcal{X}$. However, the downside of the latter approach is that we may not attain uniform search performance, since the algorithm must traverse more or less levels depending on the density of the target region for each query. To solve this issue, the core novelty in MASK is an unconventional application of the $k$-means algorithm, tailored to the specific case of information indexing in modern computing platforms, that departs from the traditional strategy suggested in clustering problems.

### 3.2 Using $k$-means for information indexing

Typical usage of $k$-means in unsupervised machine learning dictates that the appropriate number of clusters for a given problem must be found beforehand, where each cluster is represented by a centroid. Therefore, the number of centroids should not be too large, since they would not summarize underlying data effectively, or too small, which would group unrelated data points together. In practice, the optimal number of centroids can be determined in different ways, such as using the elbow method [85], based on a plot of the total within-cluster sum of squares for different $k$, the Silhouette Coefficient Algorithm [86] or the Gap statistic [87]. Moreover, the final result can be quite sensible to the choice of initial locations for cluster centroids. To circumvent this limitation, algorithms such as $k$-means++ [63] propose spreading the initial random centroids more evenly which, generally, leads to better results.

However, the goal pursued by MASK is approximate data indexing, not clustering. As more powerful computational infrastructures become available, providing larger memory and storage capacity, prior restrictions about the number of clusters to maintain at each level become less relevant. In this new scenario, it is interesting to check what happens when the dataset is bombarded with a very high number of $k$-means centroids, as large as it can be afforded by the computing infrastructure capacity.

A conceptual experiment can be useful to illustrate this approach, on a dataset comprising 4 clouds generated from a t-distribution in $\mathbb{R}^2$, with 12 degrees of freedom and different means for each cloud, so that they are clearly separated from each other. The experiment consists of two tests:

- In the first test, an increasing number of $k$-means centroids (from 4 to 128) are generated on the complete dataset, following a top-down approach. That is, the complete set of points is provided to $k$-means to calculate the position of centroids in each case.
- In the second test, data points are first randomly assigned to 4 different data partitions (groups), simulating the situation that MASK would find in a distributed system. Then, each group is independently bombarded with a growing number of $k$-means centroids, so that, for each case, the aggregated number of centroids in all groups is the same as in the first test. This represents a bottom-up approach for data indexing.

The experiment aims to demonstrate that quite similar results can be attained disregarding the approach adopted for data indexing. Figure 2 shows the result of the first test. All panels depict the same 4 t-distribution clouds, which are bombarded with an increasing number of $k$-means centroids (in black). Interestingly, we observe that, as the number of centroids increases, more of them tend to concentrate in denser data regions. This behavior is in line with existing results on the consistency of the k-means method [88]. When using a
very large number of centroids, some of them even gravitate towards outliers, providing effective coverage also for extreme data points.

Figure 2: Results of bombarding 4 data clouds with an increasing number of $k$-means centroids, following a top-down approach. Labels on each pane indicate the total number of centroids generated for each case.

Figure 3 represents the bottom-up indexing procedure in the second test, and how partial outcomes from each group are combined to report the final result, so that each case can be compared with its counterpart in the first experiment.

Figure 4 presents the aggregated results for each case in the second test. As explained in Figure 3, each group can contain points that belong to any of the 4 initial clouds. Finally, the $k$-means algorithm is run independently on each group, using a growing value of $n$Centroids, from 1 to 32. Each pane in Figure 4 plots the aggregation of all partial results. Labels on top of each pane indicate the value of $n$Centroids calculated in each group, so that the total number of centroids for each case is the same as in the previous experiment. Results from this second test are comparable to those presented in Figure 2 above, provided that a high enough number of centroids is used for data indexing. This demonstrates that data partitions can be stored in separate nodes and, then, independent indexing structures can be created within each node. Hence, MASK can scale up to handle problems involving big data distributed in parallel computing clusters.

3.3 Searching and data insertion

When the index based on the multilevel structure with $k$-means centroids is ready, we can use it to accelerate similarity search queries. The hierarchy of centroids can help us discarding sections of the dataset where it is unlikely to find candidate results. However, the $k$-means algorithm usually provides a local optimum solution and cannot warrant to find the global optimum for the location of centroids. In consequence, we cannot assure that the search process using our multilevel index returns exact results.

For this reason, our algorithm pertains to the class of approximate similarity search methods. In spite of this apparent limitation, we will show that time and resources required to build the index are affordable and, depending on the characteristics of the dataset being indexed, the accuracy of results can be sufficiently high for many practical applications.
To solve any type of query using this multilevel index, we start at the top level of the hierarchy of centroids, steering the search according to the distance between the centroids at each level and the target query object $q \in \mathcal{X}$. Then, we can adapt this general approach to solve a specific type of query, as follows.

**Point query** At the top level, the distance from each centroid to $q$ is calculated, and the centroid with the minimum distance value is selected. Then, at the next level only the subset of centroids represented by the one previously selected at the top level is considered. Again, the distance from each centroid in this subset to $q$ is calculated and the centroid with the minimum distance is chosen. Subsequent iterations repeat the
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Figure 4: Results of bombarding the same dataset with an increasing number of k-means centroids, following a bottom-up approach with separate data partitions. Points are coloured according to the data partition (group) to which they have been assigned. Labels on each pane indicate the number of centroids generated within each group.

same procedure at each layer over the remaining levels, (focusing on children of the selected centroid at the previous level and taking the child with the minimum distance to \( q \)). Eventually, the algorithm reaches the subset of actual data points represented by the centroid selected at the lowest layer of the index. At this stage, it is easy to perform a full scan over this small subset of data points and return the one with the lowest distance to \( q \) as the result of the point query. Figure 5 illustrates this process, marking with arrows the centroid selected at each level of the index. This procedure is almost equivalent to the nearest-neighbour search described in Algorithm 2, below. The only difference is that, here, the algorithm seeks a perfect match within the data partition reached at the end of the search process.

Nearest neighbour and \( k \)-nearest neighbours queries The search for the nearest-neighbour can be performed in exactly the same way as to resolve the point query. However, instead of looking for an exact match, in this case the element with minimum distance to \( q \) found within the data partition is returned. If the query searches for the \( k \) closest elements to \( q \), the final subset of data points is ranked according to their distance to \( q \), and the query returns the \( k \) members with the lowest distance values from the rank. Algorithm 2 illustrates the case of the \( k \)-nearest-neighbour search.

Range query This type can be addressed considering, at each level, the subset of children centroids whose distance to \( q \) lies within a given ball \( r \) around \( q \). Then, the same search path is followed for every children selected in the lower layer. Finally, a set of candidate groups of points will be selected, and the query returns the aggregated collection of points that matches the query condition in each candidate set. Algorithm 3 details this approach.

Besides, the MASK method can also be applied to dynamic datasets, since new points can be stored using the index structure with a simple procedure:

- First, at the top level select the k-mean prototype with the minimum distance to the new point.
Algorithm 2: k-NN search algorithm.

Input: layerPoints, spoint, layers, nCentroids

for idLayer = layers to 1 do
  if idLayer ≠ layers then
    idGroup ← searchGroup(layerLabels, idLayer)
  else
    idGroup ← 0
  centroids ← layerPoints[idLayer][idGroup];
  matrixD ← euclideanDistance(spoint, centroids);
  posCentroid ← searchPosMin(matrixD);
  // Correction of the centroid identifier
  if idLayer ≠ layers then
    idGroup ← posCentroid/nCentroids;
    idCentroid ← posCentroid − (idGroup * nCentroids);
  else
    idGroup ← 0;
    idCentroid ← posCentroid;
  // Data layer
  selecPoints ← layerPoints[idGroup][idCentroid];
  matrixD ← euclideanDistance(spoint, selecPoints);
  idKPoints ← searchKNN(matrixD, k);

Algorithm 3: Range search algorithm.

Input: layerPoints, spoint, layers, nCentroids, radius

// Top layer
idGroup ← 0;
centroids ← layerPoints[layers][idGroup];
matrixD ← euclideanDistance(spoint, centroids);
sortVecCentroids ← sortDist(matrixD);
vecCandidates ← selectCandidates(sortVecCentroids, radius);
for idLayer = layers − 1 to 1 do
  // Initialize newCandidates, vecChildren
  for candidate ∈ vecCandidates do
    centroids ← layerPoints[idLayer][idGroup];
    matrixD ← euclideanDistance(spoint, centroids);
    sortVecCentroids ← sortDist(matrixD);
    vecChildren ← selectCandidates(sortVecCentroids, radius);
    // Correction of the centroid identifier
    for pos ∈ vecChildren do
      idGroup ← pos/nCentroids;
      newCandidates ← posCentroid − (idGroup * nCentroids);
    vecCandidates ← newCandidates;
  // Data layer
  matrixD ← euclideanDistance(spoint, centroids);
  sortVecCentroids ← sortDist(matrixD);
  idRangePoints ← selectCandidates(sortVecCentroids, radius);
• Then, from k-mean centroids at the second level that are children of the selected prototype at top level, choose again the one with the minimum distance to the data point.
• Repeat these steps, iterating over the layers of the multilevel index until we reach one of the group of data points with bounded within-group variance, and assign the new point to that group.

It is important to remark that, in case that many new elements are added to \( X \) following this procedure, the size of data partitions at the bottom of the hierarchy may become quite uneven. However, this is not a major problem, since new points are placed next to other similar elements, guided by the multilayer structure of centroids. As a result, if one partition grows beyond a certain threshold, it can be split in smaller data groups and reconstruct just the local part of the index covering that specific region, without affecting the rest of the structure.

### 3.4 Indexing distributed datasets

As noted above, MASK can be implemented in parallel and distributed computing systems, as shown in Figure 6. In this example, the dataset consists of four sets of elements, separated among each other in the feature space. Besides, let us assume that this dataset is split into several partitions, and each partition is stored in a different node. Hence, points from any of the four original sets can be found in any partition. Using MASK, each node can work with its own data partitions, in parallel with the rest of nodes. The algorithm is executed following a bottom-up approach, to obtaining a local multilevel index structure in each node. Then, at the management level of the distributed system, like the master node of the cluster, just the top level centroids from each node need to be recorded. Using these metadata, search queries can be launched and MASK can decide which nodes will be involved in their resolution.

In the example of Figure 6, MASK creates 4 centroids at the top level of each node and 2 groups with 4 centroids per group at the lower indexing level of each node. Using this distributed index structure, the algorithm can effectively summarize the original dataset, shrinking the size of hierarchical metadata that must be maintained by the centralized cluster management service to speed up the similarity search. Queries can be solved either searching in all nodes in parallel, or restricting the search only to nodes that have centroids whose distance to the target query object is lower than a given threshold \( \epsilon \).
Of course, several design parameters can be tuned in each particular application to adapt the multilevel index construction procedure to the peculiarities of any specific dataset:

- At the lowest level of the index structure, it is important to bombard data partitions with as many $k$-means centroids as it can be reasonably afforded by available computational resources. As we explained in Figure 4, the higher the number of centroids calculated on the data points, the better will be the accuracy of MASK to find the actual position of points, effectively mapping high-density regions, sparse regions or outliers.

- At higher layers of the multilevel index, a compromise can be attained between indexing accuracy and data summarization. This trade-off is determined by the data summarization ratio of centroids between one layer and its adjacent level, below it. For experiments described in Section 4, we have fixed a value of 2:1 for the ratio of centroids in adjacent layers, effectively halving the number of centroids to be calculated in each new iteration. However, further analysis must be conducted to evaluate the impact of this configuration parameter on the performance of MASK.

### 4 Experimental results

Several experiments have been conducted to evaluate the performance of MASK, using two different datasets:

- The first experiment is based on a synthetic dataset including 8 Gaussian clouds, generated using the standard procedure described in [89]. In this case, the main goal is to illustrate the behaviour of MASK against a dataset that exhibits well-known theoretical properties.

- For the second experiment, we use the Reuters-21578 dataset [90], a popular benchmark in high-dimensional and high-sparsity text classification, obtained from the UCI repository [91]. Here, we
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aim to evaluate the capacity of MASK to map and retrieve elements in an adverse scenario for many other alternative algorithms.

All experiments have been conducted using a server equipped with 2 AMD EPYC 7451 microprocessors (24 cores/48 threads, 2.30 GHz, 64 MB L3 caché), 128 GB of DDR4 RAM and an SSD Intel D3-S4510 (capacity 480 GB) for secondary storage. Next, the methodology developed to undertake these empirical tests is described, including the metrics to assess the performance of MASK. After this, experimental results are presented.

4.1 Performance evaluation

The main advantage of MASK is providing a rapid answer to queries, at the expense of returning approximate results. Thus, a straightforward strategy to assess the performance of this algorithm is to undertake an exhaustive search of all elements in a given dataset $\mathcal{X}$, so that the proportion of data points that were correctly retrieved can be determined. This is the common approach for all evaluation experiments developed in this study.

Besides, MASK performance could be improved even more by relocating points that were not correctly found after the first build of the multilevel structure of $k$-means centroids. Intuitively, when the point search reaches a partition at the bottom of the tree and the target element is not found in that group, if the target point is reassigned to that partition it will join other close elements, according to the distance function. Then, if the multilevel index is built again it can find similar points placed together, making it easier for the point search to retrieve more elements correctly. In our experiments, several iterations of data relocation and index rebuilding are performed, to check whether this strategy can help or not to decrease the error rate in some cases.

The main characteristics of the datasets used for performance evaluation experiments in this study are summarized in table 1.

| Dataset | Name Description |
|---------|------------------|
| $\mathcal{X}_{GNO}$ | Gaussian clouds (no overlap) |
| $\mathcal{X}_{GMO}$ | Gaussian clouds (moderate overlap) |
| $\mathcal{X}_{GRO}$ | Gaussian clouds (remarkable overlap) |
| $\mathcal{X}_{REUT}$ | Reuters-21578 (UCI repository) |

The first experiment evaluates the capacity of MASK to provide good approximations for similarity search, using a synthetic dataset with 8 Gaussian clouds in $\mathbb{R}^2$. This is a common benchmark in many previous studies on data indexing, since it is well characterized from a theoretical point of view [89, 11]. It is possible to adjust the mean and standard deviation of each Gaussian distribution to control the percentage of overlap between adjacent clouds. As a result, we create 3 different versions of this dataset:
• In the first version, the Gaussian clouds have clear separation between each other, as depicted in Figure 7a. This is a baseline test, where most data points should be correctly retrieved. This dataset is identified as $X_{GNO}$ in experiments.

• The second version represents a compromise benchmark, where there is a moderate overlap between contiguous Gaussian clouds, as shown in Figure 7b. This version will be used in experiments evaluating the effect of the problem size or configuration parameters on MASK performance. This dataset is identified as $X_{GMO}$ in our evaluation tests.

• The third version, depicted in Figure 7c, consists of Gaussian clouds with substantial overlap among each other. In this case, the error rate in point search should raise noticeably, since it is more difficult for MASK to retrieve data points inside overlapping regions accurately. In experiments, this dataset is referred to as $X_{GRO}$.

Figure 7: Synthetic datasets used in the first experiment, comprising 8 Gaussian clouds with 200 points each and different degrees of overlap between adjacent groups.

It is expected that MASK should retrieve without problems most data points in $X_{GNO}$, with clearly separated clouds. However, as the degree of overlap between contiguous clouds increases in datasets $X_{GMO}$ and $X_{GRO}$, the error rate is expected to grow, as well. In theory, for an exact indexing algorithm the error rate should tend to the Bayes (irreducible) error of the whole dataset \cite{11}. In this case, the classification error is determined by the 8 overlapping regions between contiguous clouds \cite{92}. However, in practice MASK will incur in certain additional error for exhaustive point search, on top of this threshold.
The performance of MASK in a real-world scenario is assessed in the second experiment, using a high-dimensional and high-sparsity problem. Many competing algorithms for similarity search in metric spaces struggle to deal with datasets of this kind. The Reuters-21578 dataset [90], from the UCI repository, represents a perfect case study. This is a widely used benchmark in supervised text classification, with a collection of more than 10,000 news documents, published in 1987 and categorized into 90 different topics. Some of these topics are very similar and present substantial overlap among them. Besides the results for topic categorization, this experiment measures the performance of MASK for indexing purposes. Henceforth, this dataset is identified as $X_{REUT}$.

4.2 Synthetic dataset results

The first experiment starts comparing MASK performance against the two opposite versions of the synthetic dataset: $X_{GNO}$ (no overlap, see Figure 7a) and $X_{GRO}$ (remarkable overlap, see Figure 7c). In this execution, 8 Gaussian clouds in $\mathbb{R}^2$ are generated for each dataset, with 200 points per cloud. The distance function to measure dissimilarity between data elements is the Euclidean metric. The initial configuration parameters for MASK are $\text{lengthGroup} = 16$ and $\text{nCentroids} = 8$, which renders a data summarization ratio between adjacent index levels of 2:1. In both cases, MASK divides the initial dataset of 1,600 points into 100 groups, with 16 points per group. During this process, all data points are randomly assigned to one of these groups, so that each partition (group) may contain points from any of the 8 clouds. This simulates the situation in a distributed dataset, where data partitions are processed separately.

Once the data groups are created, we proceed to build the multilevel index. At the bottom level, the algorithm obtains 8 centroids per group, calculating a total of 800 centroids in this first layer. At the next level, the algorithm repeats this procedure, summarizing the 800 centroids obtained at the first level. Hence, in each iteration the centroids generated at the previous level are assigned to a new centroid at the next level above, according to the $k$-means algorithm and the Euclidean distance function.

Using this method, the algorithm eventually generates a multilevel index of $k$-means centroids, with a final depth of 8 layers, since the stop condition is that the number of centroids at the top layer must be lower than $\text{lengthGroup}$. Now, the index is ready to accept point queries that systematically search for all points in the original dataset, following Algorithm 2 to seek a perfect match. In the case of dataset $X_{GNO}$, the indexing method is able to correctly find all points without errors, as the original clouds are well-separated between each other. Due to this, there is no need to perform any iterations to relocate data points, since the error rate cannot be further reduced.

Nevertheless, working with dataset $X_{GRO}$ the error rate increases noticeably. In this case, the multilevel index cannot retrieve elements in the proximity or inside overlapping regions accurately, producing an error rate of 40.5% for a point search of all elements in $X_{GRO}$.

As mentioned above, an option to reduce this error rate is relocating data points not correctly found in the corresponding partition, reached at the end of the point search algorithm. After this relocation, the multilevel index is rebuilt and the exhaustive point search through all elements in the dataset is repeated to obtain the new error rate. Following this approach, the error rate decreases from the initial 40.5% at iteration 0 to 30.31% at iteration 3. Table 2 shows the error rates corresponding to each iteration. From these results, we can conclude that the algorithm converges to its best result very fast, even if it is still unable to determine the correct partition for some points pertaining to overlapping areas.

4.2.1 Influence of the dataset size

Since MASK is suitable for distributed computing platforms, it is crucial to evaluate how the problem size affects its performance. Nonetheless, dataset $X_{GRO}$ leads to a significant error rate, caused by the large overlap between Gaussian clouds. This large error may conceal the effects of other sources of variation on the index performance, such as the size of the dataset or changes in configuration parameters. For this reason, from this point we compare the performance between datasets $X_{GNO}$ (see Figure 7a) and $X_{GMO}$ (see Figure
Table 2: Change in error rate after each iteration of point relocation and index reconstruction for Gaussian clouds with remarkable overlap.

| Iteration | #0  | #1  | #2  | #3  | #4  | #5  | #6  | #7  | #8  |
|-----------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Error rate(%) | 40.5 | 39.06 | 32.56 | 30.31 | 32.56 | 30.62 | 34.19 | 36.25 | 36.56 |

7b). Different number of points per cloud are considered for both datasets (200, 1,000, 10,000 and 100,000), in order to analyze how this variation affects the error rate and computation time of MASK. All simulations have been performed with \( lengthGroup = 16 \) and \( nCentroids = 8 \).

In the case of dataset \( X_{GNO} \), Figure 8a displays the total time consumed during the index construction stage (tree time) and the time required to search the whole set of points (search time), for each problem size. Numerical results are presented in Table 3, along with the corresponding error rates. We can conclude that the error rate remains very low for any size of the dataset. However, as the problem size grows, the computation time for index construction and exhaustive point search also increases.

![Graph](image)

(a) Dataset \( X_{GNO} \) (no overlap).

(b) Dataset \( X_{GMO} \) (moderate overlap).

Figure 8: Comparison of tree time and search time (log scale) for different values of problem size.

Table 3: Index construction time (tree time), exhaustive point search duration (search time) for all elements in \( X_{GNO} \) (no overlap) and error rate, with different dataset sizes. The number of points per cloud in each problem \( (npc) \) is also indicated.

| Problem size | Tree time (sec.) | Search time (sec.) | Error rate(%) |
|--------------|------------------|--------------------|---------------|
| \( npc = 200 \) | 5.905             | 2.250              | 0.0           |
| \( npc = 1,000 \) | 28.601            | 13.892             | 0.11          |
| \( npc = 10,000 \) | 287.674           | 293.547            | 0.09          |
| \( npc = 100,000 \) | 2863.450          | 12415.074          | 0.05          |

The same analysis has been performed with dataset \( X_{GMO} \) (moderate overlap). It is clear, from computation times represented in Figure 8b and shown in Table 4, that when the problem size grows the time spent by MASK building the tree and searching for all points also increases. The error rate only experiments a small
variation, that can be mainly attributed to the overlap between clouds. As the number of points per cloud raises, the overlapping region is larger, incrementing the error rate.

Table 4: Index construction time (tree time), exhaustive point search duration (search time) for all elements in $\mathcal{X}_{GMO}$ (moderate overlap) and error rate, with different dataset sizes. The number of points per cloud in each problem (npc) is also indicated.

| Problem size | Tree time (sec.) | Search time (sec.) | Error rate(%) |
|-------------|-----------------|-------------------|--------------|
| npc = 200   | 5.842           | 2.284             | 11.937       |
| npc = 1,000 | 28.861          | 14.382            | 14.212       |
| npc = 10,000| 288.439         | 313.715           | 14.087       |
| npc = 100,000| 2874.815      | 13730.897         | 16.334       |

Figure 9 compares the error rate obtained with datasets $\mathcal{X}_{GNO}$ and $\mathcal{X}_{GMO}$. As expected, the error rate is higher for the moderate overlap case, but it does not raise significantly for larger problem sizes with any of these two datasets. Therefore, we can conclude that the degree of overlap between adjacent clouds has a greater impact on the error rate than the size of the problem.

Figure 9: Comparison of the error rate when there is no overlap between dataset clouds (bottom panel) and when there is some overlap between them (top panel).

4.2.2 Impact of configuration parameters

The evaluation continues analyzing the influence of configuration parameters, $lengthGroup$ and $nCentroids$, on MASK performance. Again, datasets $\mathcal{X}_{GNO}$ and $\mathcal{X}_{GMO}$ are used in these tests, fixing the number of points per cloud to 10,000 in both cases.

Figure 10 compares the computation time for the tree building phase and the exhaustive point search for dataset $\mathcal{X}_{GNO}$, using different values of $lengthGroup$ and $nCentroids$. In all cases, the data summarization ratio between these two configuration parameters is fixed at 2:1. As $lengthGroup$ and $nCentroids$ increase their values, the time to build the multilevel index decreases moderately, suggesting an inverse relationship
between these magnitudes. At the same time, since the number of indexing levels decreases when the group length and the number of centroids grows, a slight reduction in search time can be attained in some cases. Table 5 explores these differences in more detail.

Table 5: Computation time required for multilevel index construction (tree time) and exhaustive point query (search time), for different values of lengthGroup and nCentroids, with dataset $X_{GNO}$ (10,000 points per cloud). The number of levels created by the index structure in each case (tree depth) is also indicated.

| lengthGroup | nCentroids | Tree time (sec.) | Tree depth | Search time (sec.) | Error rate(%) |
|-------------|------------|------------------|------------|-------------------|---------------|
| 10          | 5          | 337.450          | 13         | 2653.897          | 0.158         |
| 30          | 15         | 321.383          | 12         | 2525.883          | 0.125         |
| 50          | 25         | 318.820          | 11         | 2550.783          | 0.06          |
| 70          | 35         | 312.977          | 11         | 2543.880          | 0.053         |
| 90          | 45         | 300.070          | 10         | 2491.706          | 0.061         |
| 110         | 55         | 301.053          | 10         | 2518.820          | 0.055         |

A similar situation occurs when MASK is applied to dataset $X_{GMO}$, using the same series of increasing values for lengthGroup and nCentroids and keeping the data summarization ratio between them at 2:1, for all cases. Results are presented in Figure 11 and Table 6. As lengthGroup and nCentroids are set to higher values, the computation time required by MASK for tree construction tends to decrease, as well as the time needed for exhaustive point search of the entire dataset. The values in column tree depth show that the number of layers in the multilevel index drops from 13 to 10 levels. This is the main cause behind time reduction in both tree
construction and point search. Since every individual point query must traverse less layers to return a result, the total time spent in exhaustive point search is reduced.

Figure 11: Computation time spent in multilevel index construction (tree) and exhaustive point query (search), for different values of lengthGroup and nCentroids, with dataset X_{GMO} (10,000 points per cloud).

Table 6: Numeric results for the computation time required for multilevel index construction (tree time) and exhaustive point query (search time), for different values of lengthGroup and nCentroids, with dataset X_{GMO} (10,000 points per cloud). The number of levels created by the index structure in each case (tree depth) is also indicated.

| lengthGroup = 10 | Tree time (sec.) | Tree depth | Search time (sec.) | Error rate(%) |
|------------------|------------------|------------|--------------------|---------------|
| nCentroids = 5   | 325.294          | 13         | 2891.359           | 13.791        |
| lengthGroup = 30 | 322.588          | 12         | 2762.296           | 13.631        |
| nCentroids = 15  | 318.593          | 11         | 2769.591           | 12.775        |
| lengthGroup = 50 | 317.898          | 11         | 2745.472           | 11.853        |
| nCentroids = 25  | 318.403          | 10         | 2618.803           | 11.712        |
| lengthGroup = 70 | 309.307          | 10         | 2676.827           | 11.448        |
| nCentroids = 35  |                  |            |                    |               |
| lengthGroup = 90 |                  |            |                    |               |
| nCentroids = 45  |                  |            |                    |               |
| lengthGroup = 110|                  |            |                    |               |
| nCentroids = 55  |                  |            |                    |               |

The main effect when the values of lengthGroup and nCentroids are increased is the progressive improvement of the error rate in exhaustive point search. Figure 12 compares the error rate variation for datasets X_{GNO} (no overlap) and X_{GMO} (moderate overlap), respectively. Even though the error rate values for dataset X_{GNO} are much lower than for X_{GMO}, we observe similar trends in both graphs, as lengthGroup and nCentroids values raise. From these results, it can be inferred that the influence of both lengthGroup and nCentroids on the performance of MASK is consistent, disregarding the degree of overlap between the Gaussian clouds.
Index structures with fewer layers need less time to be constructed and lead to a more precise point search, with lower error rate. Therefore, there is a performance advantage in MASK when larger size of data groups (partitions) are configured. In spite of this, after a certain point the error rate levels off, and no further improvement can be achieved.

![Figure 12](image.png)

Figure 12: Comparison of changes in the error rate values with dataset $\mathcal{X}_{GNO}$ (no overlap) and $\mathcal{X}_{GMO}$ (moderate overlap), as $\text{lengthGroup}$ and $n\text{Centroids}$ are increased.

### 4.2.3 Role of the data summarization ratio

So far, the data summarization ratio between $\text{lengthGroup}$ and $n\text{Centroids}$ has been kept at a fixed value of 2:1 in all experiments. Here, we explore how changes in this data summarization ratio affect MASK performance, using again the $\mathcal{X}_{GNO}$ and $\mathcal{X}_{GMO}$ synthetic datasets. In both cases, we generate 10,000 points per cloud.

Three situations are studied, corresponding to $\text{lengthGroup} = 10$, 50 and 90, respectively. Figure 13 presents the results for $\mathcal{X}_{GNO}$ (no overlap case). The left panel display changes in computation time for tree assembly (blue line) and during the search process (red line), for $\text{lengthGroup} = 10$. On the horizontal axis, $n\text{Centroids}$ gets values 2, 5 and 8, respectively. The graph shows that the computation time for both stages directly depends on the number of centroids per group, as expected. That is, if the number of centroids increases, computation time for both index construction and exhaustive point search also raises. The same effect is observed in the other two cases, for $\text{lengthGroup} = 50$ and 90. When $\text{lengthGroup} = 50$, $n\text{Centroids}$ is set to 10, 25 and 40, and when $\text{lengthGroup} = 90$ the number of centroids are 18, 45 and 72. In this way, the same sequence of data summarization ratios as for the case of $\text{lengthGroup} = 10$ is used. The difference between computation time during the index construction stage and for the search process remains approximately constant over the three cases of $\text{lengthGroup}$.

Figure 14 displays the computation time for the moderate overlap case (dataset $\mathcal{X}_{GMO}$). The same three scenarios with $\text{lengthGroup} = 10$, 50 and 90 are considered, with identical variation in the number of centroids for each case. Results are very similar to the previous ones in Figure 13. Therefore, it can be concluded that the overlap between adjacent clouds does not increase computation time for tree building or search queries, when different data summarization ratios are configured.

Figure 15 displays changes in the error rate for datasets $\mathcal{X}_{GNO}$ (no overlap) and $\mathcal{X}_{GMO}$ (moderate overlap), in the three previous situations (with $\text{lengthGroup} = 10$, 50 and 90), respectively. As seen above, the
error rate decreases when lengthGroup and nCentroids increase their values. This difference becomes more remarkable in the moderate overlap case. In spite of this, if we keep the value of lengthGroup constant, the error rate drops or remains stable when the number or centroids per group is increased. A satisfactory compromise solution between computation time (for index construction and search) and error rate is found for a data summarization ratio of 2:1.
4.3 High-dimensional and sparse dataset results

One of the most problematic aspects of MAM is that, in many cases, they render very poor performance in high-dimensional and sparse dissimilarity spaces. As we explained in Section 1, this issue is linked to the intrinsic dimensionality of our dataset, \( \delta \), which determines the number of effective dimensions that represent all elements. The higher the number of dimensions and the sparsity of our dataset, the more difficult it will be for our indexing method to effectively locate query objects.

However, a key advantage of MASK is that, if we bombard data partitions with enough \( k \)-means centroids, the indexing structure can still retrieve data elements with good accuracy, at the expense of returning approximate results. As shown in Section 3.2, when a high number of \( k \)-means centroids are used for the first layer, MASK place them according to the density of the underlying data elements. In this way, we are able to index not only high density data regions, but also outliers and clusters of elements separated from the main concentrations of points.

Several experiments were conducted to evaluate the performance of MASK in this kind of problems, using dataset \( X_{\text{REUT}} \). Individual documents are tagged according to their topic, and there exists substantial overlap between different categories. The goal in this evaluation tests is to classify documents as belonging to a particular category.

Following conventional text mining procedures [93], stop words (common words that usually do not add useful information for the analysis), numbers, punctuation marks and white spaces were removed from documents. After this, the text in each document is converted to lower-case and the corresponding term-document matrix is created. Thus, each set of documents is represented as an \( m \times n \) matrix, where \( m \) is the number of unique terms in the dictionary and \( n \) is the number of documents in the data set. Each element \( w_{ij} \) of the term-document matrix represents the importance or weight of the term \( i \) in document \( j \). To obtain the value of \( w_{ij} \), we use the TF-IDF measure [94], calculated through equation (1)

\[
w_{ij} = tf_{ij} \times \log \left( \frac{n}{df_i} \right),
\]

where \( tf_{ij} \) is the term frequency of term \( i \) in document \( j \), \( df_i \) is the document frequency of term \( i \), and \( n \) is the number of documents in the data set.
where $t_{f_{ij}}$ denotes the number of occurrences of the term $i$ in document $j$; $n$ is the total number of documents in the dataset and $df_i$ represents the number of documents in which term $i$ appears. Given these initial conditions, data elements are represented in a dissimilarity space with many dimensions, where components are the TF-IDF measures for each document, and high sparsity, since many terms will be absent from numerous documents.

In a first round of experiments, documents are encoded applying TF-IDF with stemming [93]. Results are compared with a second round of experiments, in which the document encoding does not include stemming, to assess the impact of this step on MASK search accuracy. Several pairs of document categories have been considered for the sake of clarity to illustrate the results: ‘alum’ vs. ‘barley’; ‘ipi’ vs. ‘iron-steel’; ‘carcass’ vs. ‘cocoa’; ‘palm-oil’ vs. ‘pet-chem’ and ‘palm-oil’ vs. ‘barley’. In all cases, the input parameters for our algorithm will be $\text{lengthGroup} = 16$ and $\text{nCentroids} = 8$ (thus, the data summarization ratio is 2:1). The algorithm builds the search tree with a maximum depth of 3 levels.

Figure 16 presents the comparison of the classification error rate with and without stemming, for 10 iterations of the algorithm (relocating data elements in each iteration, to try to improve the performance of MASK).

![Figure 16: Boxplots comparing the classification error of documents in each pair of categories, obtained with and without stemming.](image)

Since the maximum classification error rate is less than 25%, this confirms that results obtained for both cases are very accurate. However, there is a slight improvement in several tests, when no stemming is applied. Tables 7 and 8 present the classification and indexing error for each pair of categories when stemming is applied and without this step, respectively. Results indicate that, in many cases, the best iteration is either the first or the second attempt to relocate data points, according to the previous position of centroids in the multilevel index. Hence, in many practical situations, the actual performance gain attained with this iterative process is low. Due to this, it can be assumed that the approximation provided by the initial construction of the multilevel indexing structure is quite acceptable for high-dimensional problems.

Finally, we study the convergence of the algorithm as the size groups and the number of centroids to map each group vary. In this experiment, categories ‘jobs’, ‘iron-steel’ and ‘cotton’ are considered, whereas
Table 7: Classification and indexing error in the best iteration of data relocation in MASK, for each pair of document categories, when stemming is applied. All simulations have been performed with $lengthGroup = 16$ and $nCentroids = 8$.

| Categories              | Classification Error |  | Indexing Error |
|-------------------------|----------------------|---|----------------|
| Best Iter. | Error | Best Iter. | Error |
| alum / barley | 2 | 5.55 | 1 | 8.33 |
| ipi / iron-steel | 4 | 3.7 | 0 | 12.34 |
| carcass / cocoa | 0 | 10.47 | 0 | 16.19 |
| palm-oil / pet-chem | 0 | 4.0 | 0 | 2.0 |
| palm-oil / barley | 0 | 2.98 | 1 | 17.91 |

Table 8: Classification and indexing error in the best iteration of data relocation in MASK, when stemming is not applied. All simulations have been performed with $lengthGroup = 16$ and $nCentroids = 8$.

| Categories              | Classification Error |  | Indexing Error |
|-------------------------|----------------------|---|----------------|
| Best Iter. | Error | Best Iter. | Error |
| alum / barley | 3 | 5.55 | 0 | 6.94 |
| ipi / iron-steel | 5 | 9.87 | 3 | 12.34 |
| carcass / cocoa | 0 | 19.04 | 0 | 15.23 |
| palm-oil / pet-chem | 0 | 2.0 | 4 | 0.0 |
| palm-oil / barley | 1 | 5.97 | 0 | 11.94 |

$lengthGroup$ and $nCentroids$ are set to values ranging from 8-4 to 60-30, so that the data summarization ratio in all cases is kept at 2:1. Figure 17 shows the classification error rate for each case. No stemming has been applied in these simulations. The classification error rate decreases when both input parameters increase their values. Results are quite similar when stemming is not applied, suggesting that this encoding step does not affect the accuracy of MASK, as size of data partitions and the number of centroids increase. Again, this is consistent with the effect of using a high number of centroids to map the underlying dataset, as explained in Section 3.2. As a higher number of centroids is used to map the dataset, their location will become more advantageous for indexing purposes.

5 Discussion

MASK is an approximate method for similarity search based on $k$-means, that builds multilevel index structures suitable for different scenarios, from low-dimensional problems to high-dimensional and high-sparcity datasets in metric spaces. Algorithms to solve the principal types of similarity search requests can be deployed using MASK. Likewise, this method offers a good performance without the need to relocate data points after the initial index construction. The multilevel structure created by MASK in the first iteration already provides a good approximation to solve similarity queries with reasonable efficiency.

One of the main contributions of MASK is an unconventional application of the $k$-means algorithm for information indexing, demonstrated in Section 3. The classical approach in clustering problems dictates that the number of centroids to group data points must be chosen beforehand. Unlike this common strategy,
our approach simply suggest that, for information indexing, one should use as many centroids as the infrastructure can afford. This is specially important in the lowest layer of the multilevel index, next to the actual data points. When the number of centroids per data partition is incremented, there is a rapid improvement in the capacity of $k$-means to distribute centroids in optimal locations, including denser data regions, scattered sections or even outliers. The theoretical approach of using $k$-means for information indexing was already considered since the inception of this method [23]. In addition, several algorithms for both exact and approximate similarity search use $k$-means to build their index [48, 61, 7]. However, to the best of our knowledge, none of them follow this unconventional application of $k$-means to map data in a flexible manner, according to available system resources.

On top of this, MASK is also adequate for distributed datasets with partitions stored in different nodes, thanks to its bottom-up design. As a result, a multilevel index can be created in parallel for data partitions in different nodes, in contrast with current approaches for similarity search in distributed systems [6, 95]. In general, other alternative methods involve substantial data interchange between nodes to build the index. In MASK, index metadata corresponding to the top level of all nodes can be aggregated in the management node to select the nodes that should be involved in resolving a query. Thanks to its multilayer design, MASK input configuration parameters can be tuned to achieve the desired reduction in the total number of centroids stored at higher levels. Indeed, as the number of layers increase, the set of calculated prototypes for each level is reduced by a factor equal to the data summarization ratio ($\text{groupLength}/n\text{Centroids}$) for that level.

Another advantage of MASK is that it can handle geographically distributed datasets. For instance, consider the case of a large organization with subsidiaries in different locations that are geographically scattered. Using other indexing algorithms, it would be very difficult to coalesce index metadata stored in each location in a centralized management system. However, MASK can also tackle this situation, aggregating the top-level centroids from each venue. Even more complex hierarchies of data centers, involving intermediate
headquarters, can also be supported. In this case, each intermediate center stores an aggregation of the centroids coming from all venues under its direct oversight, and it forward this aggregated set of centroids upstream as required.

One of the most important limitations of this new indexing method is that it can only provide approximate results. The only warranty that MASK can offer is that accuracy will be higher as the number of centroids in each layer increases. Again, the data summarization ratio steers this trade-off. The trivial scenario where one centroid is assigned each data point (1:1 ratio) does not provide any improvement in storage space for indexing purposes, although it renders perfect accuracy (exact search). Conversely, when the number of centroids per layer is gradually reduced, the storage gain improves, at the expense of greater loss in search accuracy. Specific applications should test different values for configuration parameters and the number of layers in the indexing structure, to find the best fit for particular problems.

Another limitation is the need to use a powerful computing infrastructure to store both the dataset and the index metadata described in this approach. Nevertheless, continuous features improvements in computing hardware and cloud architectures counteract this shortcoming to a certain extent. Nowadays, nodes shipping large RAM units, fast secondary storage and distributed file systems are becoming prevalent in many organizations. This paves the way for the design of new indexing algorithms that take advantage of extant improvements in computing infrastructure.

In spite of these shortcomings, results from experiments show that this new method achieves good accuracy, even in complex scenarios involving high-dimensional and high-sparsity datasets, provided that the problem is set in a metric space. The flexibility and simplicity of configuration parameters allows MASK to cover a wide spectrum of possible applications in many different domains.

6 Conclusion

In this paper we have presented MASK, a new method for approximate similarity search based on an unconventional application of the $k$-means algorithm, to create a multilevel index in metric spaces. Departing from the typical utilization of $k$-means in clustering problems, where the number of centroids must be specified in advance, we demonstrate that, for data indexing, one should use as many centroids as it can be afforded by the computing infrastructure, to effectively map the target dataset. Following this novel approach, the $k$-means algorithm will place the centroids at each level in convenient positions to map dense data regions, scattered subsets of elements or even outliers.

Moreover, the bottom-up design of this new method makes it suitable for distributed computing systems, since each node can create a local multilayered index in parallel, without the need of any data transfer between nodes. Even geographically scattered data centers that must be managed coordinately can also benefit from using this method. The index can be configured to meet different design goals, like storage capacity consumption, speed and accuracy of query resolution. This balance between computational requirements and search performance makes it a good candidate for a wide range of applications demanding approximate similarity search.

Regarding future research on this topic, applying MASK to solve distributed indexing problems in wireless sensor networks and other similar types of federated and ubiquitous computing systems is a line that deserves to be explored. Recent research in this regard [78] emphasize the relevance of effective indexing in this kind of technologies, that play an essential role in smart cities, Industry 4.0 and many other settings. MASK provide clear advantages, such as eliminating the need of data exchange among device clusters, which reduces energy consumption. Likewise, MASK enables independent construction of local indexes covering specific regions of the network, that can work either in isolation or cooperating with each other to broaden the total coverage of the multilevel index. This is another important asset, as the algorithm is flexible enough to prepare an index structure that could operate in any of these two different modes, seamlessly changing between them.
Further experiments evaluating the performance of MASK on different datasets must be conducted, as well. This includes assessing the performance of the new algorithm for specific applications such as multimedia and spatial datasets, and high-dimensional problems. In the last case, it will be critical to study the influence of the number of dimensions in the feature space over MASK indexing performance. In the same way, this study must be complemented with a detailed analysis of MASK behaviour and performance using alternatives to the Euclidean distance [96] in metric spaces. Although, in classical clustering applications \( k \)-means is widely known to be tightly connected with the Euclidean distance, in data indexing and using a large number of centroids it is possible to adopt alternative distance functions for categorical data, strings, etc. Once the distance function is calculated for the necessary cases, \( k \)-means can build the multilevel structure as described here, based on this information. Results from these experiments will lead to discern which combination of distance function and initial configuration parameters is more adequate to resolve a particular similarity search problem.

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