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# Learning Cluster Representatives for Approximate Nearest Neighbor Search

*by*

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*Sometimes it is the people no one*
*imagines anything of who do the*
*things that no one can imagine.*

*— Alan Turing —*

# Abstract

Developing increasingly efficient and accurate algorithms for *approximate nearest neighbor search* is a paramount goal in modern information retrieval. A primary approach to addressing this question is *clustering*, which involves partitioning the dataset into distinct groups, with each group characterized by a representative data point. By this method, retrieving the top-$k$ data points for a query requires identifying the most relevant clusters based on their representatives—a *routing* step—and then conducting a nearest neighbor search within these clusters only, drastically reducing the search space.

The objective of this thesis is not only to provide a comprehensive explanation of *clustering-based approximate nearest neighbor search* but also to introduce and delve into every aspect of our novel state-of-the-art method, which originated from a natural observation: The routing function solves a ranking problem, making the function amenable to *learning-to-rank*. The development of this intuition and applying it to *maximum inner product search* has led us to demonstrate that learning cluster representatives using a simple linear function significantly boosts the accuracy of clustering-based approximate nearest neighbor search.

**Keywords**

Information Retrieval; Clustering; Approximate Nearest Neighbor Search; Learning to Rank.

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# Notation

This section offers a concise reference detailing the notation and special symbols used throughout this thesis.

| | |
|---|---|
| $a, b, c, \ldots$ | Vector |
| $q$ | Query point |
| $u^*$ | Resulting element of a problem |
| $A, B, C, \ldots$ | Matrix |
| $\mathcal{U}$ | Dataset |
| $\mathcal{X}$ | Collection of vectors |
| $\mathcal{D}$ | Collection of documents |
| $\mathcal{I}$ | Collection of items |
| $\mathcal{Q}$ | Collection of queries |
| $\mathcal{S}$ | Exact set of the $k$ most similar vectors to the query |
| $\tilde{\mathcal{S}}$ | Set of the top-$k$ most similar vectors to the query, returned by an ANN algorithm |
| $\{x_i\}_{i=1}^N$ | Set of $N$ elements |
| $\{\mu_i\}_{i=1}^L$ | Set of $L$ standard representative points |
| $\{\nu_i\}_{i=1}^L$ | Set of $L$ learnt representative points |
| $\boldsymbol{x}$, $(x_i)_{i=1}^N$ | Tuple of $N$ elements |
| $\mathbb{Z}^+$ | Set of positive integers |
| $\mathbb{R}^n$ | Euclidean $n$-dimensional vector space |
| $\mathcal{C}(\cdot)$ | Clustering function |
| $L$ | Number of clusters |
| $\{c_i\}_{i=1}^L$ | Set of L non-overlapping clusters |

| | |
|---|---|
| $\delta(\cdot, \cdot)$ | Distance function |
| $\langle \cdot, \cdot \rangle$ | Inner product of two vectors |
| $\|\cdot\|_i$ | L$i$ norm of a vector |
| $\|\cdot\|$ | Absolute value |
| $\|\cdot\|$ | Cardinality of a finite set |
| $[0, 1]$ | Unit interval |
| $f(\cdot, \cdot)$ | Ranking function |
| $\tau(\cdot)$ | Routing function |
| $\acute{\tau}(\cdot)$ | Learnt linear routing function |
| $\tilde{\tau}(\cdot)$ | Learnt nonlinear routing function |
| $\ell$ | Number of top clusters retrieved by a routing function |
| $\varphi(\cdot)$ | Encoder (embedding model) |
| $\eta(\cdot)$ | Numerical representation function |
| $l(\cdot, \cdot)$, $\mathcal{L}(\cdot, \cdot)$ | Loss function |
| $m(\cdot)$ | Evaluation metric |

# Code Implementation

To ensure transparency and reproducibility, the code underlying this thesis is publicly available at `https://github.com/tomvek/mips-learnt-ivf`.

This repository contains the official code implementation at the base of our paper "A Learning-to-Rank Formulation of Clustering-Based Approximate Nearest Neighbor Search" [95], thereby providing the specific implementation of our new proposed method. By utilizing this code, readers can replicate the experiments presented in this work, employ the code for future research, or integrate it into other systems or projects.

Specifically, the code implementation was exclusively carried out in Python[1]. The Python version and all required libraries are documented in the 'README.md' of the aforementioned repository. The experiments were conducted on a server running Ubuntu[2] 18.04.6 LTS equipped with an Intel[3] Xeon Platinum 8276L CPU, 503GiB of RAM, and an NVIDIA[4] Tesla T4 16GiB GPU.

[1] `https://www.python.org`
[2] `https://ubuntu.com`
[3] `https://www.intel.com`
[4] `https://www.nvidia.com`

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# Chapter 1

# Introduction

It may be opportune to begin with the definition of Information Retrieval:

> Information Retrieval (IR) is the scientific discipline concerned with the efficient and effective retrieval of relevant material from large collections to satisfy the information needs.

IR is having a profound and far-reaching impact, shaping the way we live, work, and learn. This is evident in every facet of contemporary society, as demonstrated by our use of search engines, recommendation systems, digital libraries, social media, and dialogue or question-answering systems among others. Extending its influence to significant fields such as education, research, healthcare, and business.

Taking an abstract standpoint, we can view IR as a gateway to knowledge. And, as the English philosopher Francis Bacon famously stated in 1597, *'knowledge is power'*.

This "game of knowledge" in IR is fundamentally defined by two major players: a collection of documents, representing the entirely of information available within a system; and the user's query, which describes the specific information the user seeks. The final objective is to return the best documents that most effectively address the query. In the IR community this "game" is called *top-k retrieval*.

One of the most prevalent and widely used methods for the top-$k$ retrieval problem is to map both documents and queries into a vector space. A well-defined distance function is then applied to calculate the similarity between the corresponding vector representations, enabling the system to determine how well a document matches the user's query. A visual representation is shown in Figure 1.1.

However, despite its simplicity and elegance, this methodology presents a significant challenge: how can we optimally represent our documents and queries as vectors, ensuring that the actual similarity between these entities is accurately reflected in the vector space?

The literature abounds with numerous works on the presented technique and to provide increasingly accurate answers to the aforementioned question. Among the earliest achievements, we find the vector space model based on the bag-of-words assumption [82, 84]. Subsequently, other noteworthy methods emerged, such as TF-IDF [83] and BM25 [80]. However, a significant advancement was achieved only when Machine Learning (ML) [12] and Deep Learning (DL) [39] techniques were used to obtain the vector representation [44, 88, 105, 57]. In particular, the turning point came with the Pre-trained Language

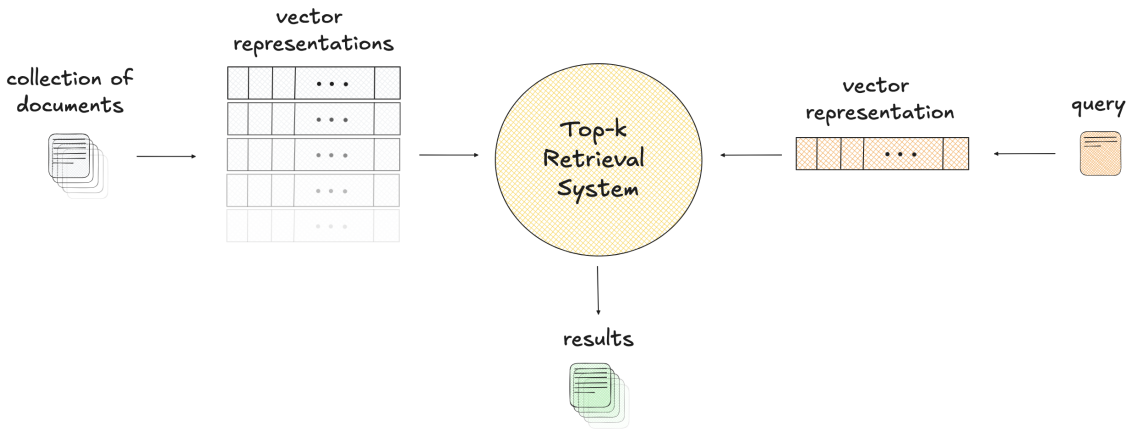



Figure 1.1: Top-$k$ retrieval problem based on the representation of documents and queries through vectors.

Models (PLMs), which, based on Transformer architectures [94], have a deep understanding of the language and consequently representing documents and queries in an optimal manner: the resulting vectors are referred to as *dense vectors* or *embeddings*. The remarkable success of PLMs, thanks especially to the *pre-training followed by fine-tuning* paradigm, has led to the creation of many retrieval models based on them, opening the door to *(PLM-based) dense retrieval models*, a new generation of effective retrieval methods [106].

With the dense vector representation in hand, the subsequent step involves retrieving the top-$k$ most relevant documents. To accomplish this, *Nearest Neighbor (NN) search algorithms* are applied. NN algorithms perform an exhaustive search, computing the distance function between the query vector and each individual document vector within our collection.

But NN search algorithms suffer from a significant computational cost issue. In fact, for extensive document collections, applying these algorithms during online search becomes infeasible. This poses another fundamental challenge given the ever-increasing volume of information and dataset sizes. *Approximate Nearest Neighbor (ANN) search* [16] has emerged as one of the most prevalent approach to tackle this problem and is currently a hot research topic in modern IR.

ANN search algorithms are a form of approximate retrieval and are designed to trade off accuracy for speed. This implies that the output of the algorithm is often an approximation of the exact solution, but results are achieved significantly faster. In order to accomplish this goal, ANN search algorithms rely on data structures known as *indexes*, which are constructed in an offline phase by processing the collection of vectors. Indexes are essential for space partitioning, enabling efficient navigation to locate the closest vectors to the query point, according to a distance function. Conceptually, indexes act as guides that direct the search to specific regions of the data space, without examining the entire dataset. Analogously, if one were searching for the Eiffel Tower, an index would guide the search directly to Paris, bypassing the need to search of all of France.

A prominent ANN search method is clustering-based approximation, where data points are grouped into $L$ geometric partitions using a clustering algorithm, and each partition is characterized by a representative vector. Partitions and their corresponding representative vectors constitute the index. At search time, in the online phase, a distance function is computed between the input query point and the representative vectors of the clusters to determine the $\ell$ closest partitions, a process referred to as *routing*. Once these partitions are identified, multiple strategies can be adopted to extract the top-$k$ documents, such as employing an another ANN algorithm or performing an exhaustive search with these partitions.

In the standard clustering-based ANN search, the design choice include: employing Standard KMeans [61] as the clustering algorithm to partition the data points into $L$ clusters; utilizing the mean of the cluster data points as the representative point; selecting the inner product (used in this work), $L1$ norm, $L2$ norm, or cosine similarity as the distance function; and setting $\ell$ significantly smaller than $L$ to substantially reduce the search space. At query time, to retrieve the top-$\ell$ partitions, the routing process is performed. Using the inner product as distance function, this process can be described by the function $\tau(q) = \arg\max^{\ell} Mq$, where $q \in \mathbb{R}^n$ is the query and $M \in \mathbb{R}^{L \times n}$ is a matrix whose rows correspond to the cluster centroids.

It is evident that the representative point is crucial in the routing process, as it determines the selection of partitions. Thus, this point must effectively encapsulate its cluster to maximize the accuracy of retrieving top-$k$ documents relative to the query within the returned partitions. Consequently, the following inquiries present themselves: Is the use of the mean the optimal choice? How can we obtain the vector that best represents the partition?

In this work, we address these questions, developing a novel state-of-the-art clustering-based ANN search methodology and demonstrating that learning cluster representatives using a simple linear function significantly improves ANN search accuracy.

At the core of our research, we made a simple yet insightful observation:

> The *routing function* solves a ranking problem, making the function amenable to *Learning-to-Rank* (LTR) [17].

By developing this insight, we simply learn a linear function $\acute{\tau}(q;\ W) = Wq$, where given a query $q \in \mathbb{R}^n$ as input and the learnt matrix $W \in \mathbb{R}^{L \times n}$, it returns the ranking scores for each of the $L$ partitions. Each row of the matrix $W$ corresponds to the *learnt representative vector* for each cluster. Considering the top-1 scenario as an example, the function $\acute{\tau}$ ranks the partitions according to their likelihood of containing the nearest neighbor to the query.

Interestingly, all the required elements to learn this routing function are easily accessible: The training data consists of a set of queries; The ground-truth for each query comprises the partitions containing the exact top-$k$ documents; To determine the routing function's quality, we employ ranking metrics such as Mean Reciprocal Rank (MRR) [59], which is appropriate for our task; Cross-entropy as loss function to maximize MRR [19, 15] for the top-1 case, where each query has a single correct partition, and its generalization [15] for top-$k$ with $k > 1$.

Through experiments on diverse text datasets, embeddings and clustering algorithms,

we demonstrate empirically that learning a simple linear routing function leads to significant accuracy gains, establishing a new advancement in clustering-based ANN search.

## 1.1 Why This Thesis Matters

*Approximate Nearest Neighbor (ANN) search* is a hot topic today that implicitly influences our lives. Its pervasive use touches upon areas such as recommendation systems, image and video search, natural language processing, fraud detection, music streaming services, and many more. ANN search is a focal point of interest within the realm of vector databases. Numerous companies utilize ANN search algorithms and invest in them. Several prominent models, such as ColBERTv2 [87] and PLAID [86], incorporate this technique. Moreover, it is a widely studied research topic within the IR community due to its substantial impact.

*Clustering-based ANN search* is one of the primary methods for ANN search and is central to the aforementioned discussion. This thesis not only provides an in-depth explanation of this methodology, delving into its intricacies and foundational principles to ensure a comprehensive understanding, but also introduces a novel state-of-the-art for clustering-based ANN search through a method we have developed [95]. Additionally, our proposed method is distinguished by its ease of integration into existing production systems utilizing clustering-based ANN search. By merely replacing the old centroids with the newly learnt representatives, the overall implementation remains unchanged, while significant accuracy improvements are realized.

Our findings demonstrate the potential of merging two major IR fields: LTR and ANN. Motivating the community to explore this junction in future research.

In summary, we make the following contributions in this work:

- We provide an in-depth explanation of clustering-based ANN search and present a general overview of LTR, outlining its core concepts;
- We present our novel clustering-based ANN search algorithm that is based on learning cluster representatives;
- We show, by means of extensive experiments, significant gains in accuracy using our proposed method compared to the state-of-the-art baseline, for both top-1 and top-$k$ cases;
- We give a detailed analysis of our method, along with alternatives and variations.

## 1.2 Organization

The thesis is structured into six chapters.

Chapter 2, 3 and 4 respectively delve into Vector Search, Clustering-Based Approximate Nearest Neighbor Search and Learning-to-Rank. The following chapters are essential for a complete understanding of the research presented in the Chapter 5. In particular, Chapter 2 introduces Vector Search, starting from the concept of a vector and focusing on dense vectors. The chapter concludes by presenting the Maximum Inner Product Search problem. Chapter 3 discusses Clustering-Based Approximate Nearest Neighbor

Search, where the focus is on its two main components: clustering and approximate nearest neighbor search, which are explained. Regarding clustering, we concentrate on centroid-based clustering algorithms, specifically Standard Kmeans, Spherical Kmeans and Shallow Kmeans. Chapter 4 addresses Learning-to-Rank, providing an overview of the topic and explaining what it means to learn a ranking function and the necessary ingredients for doing so.

Chapter 5 provides our research project in detail. We start by offering a general overview and then delve into the technical methodology, ensuring a comprehensive understanding of learning cluster representatives for Approximate Nearest Neighbor search, building upon the concepts introduced in previous chapters. Subsequently, the experimental setup and results are presented, demonstrating empirically that our proposed approach outperforms the state-of-the-art baseline. The chapter concludes with further analysis of our method and by exploring variations of it.

The general strategy employed in Chapters 2, 3, 4 and 5 involves first presenting the intuition and the idea underlying the method under consideration, followed by a concrete explanation.

Finally, Chapter 6 conclude the thesis by recapitulating the main points and outlining potential avenues for future work.

The front and the end matter of the thesis contains: Abstract, Acknowledgements, Notation, Code Implementation, and Bibliography.

# Chapter 2

# Vector Search

*Vector search* is a retrieval technique based on finding similar items, represented as vectors, within large collections by considering their semantic and contextual meanings, all while maintaining efficiency. In essence, vector search transforms the vast and chaotic expanse of data into a navigable and manageable world through the utilization of vectors.

This technique leverages Machine Learning (ML) models, commonly referred to as encoders [97, 75], to transform data into high-dimensional vectors, also know as dense vectors or embeddings. As the term *embedding* implicitly suggests, these vectors encapsulate the semantic meaning behind the data they represent within their numerical representation. It is worth noting that the nature of the data we are discussing can be of various types, including text, images, audio, tabular data, and others. For the sake of simplicity, we will exclusively focus on textual data in the remainder of this document.

In this context, we can conceptualize an encoder model as a function $\varphi$ that maps a document $x \in \mathcal{D}$, where $\mathcal{D}$ is the collection of documents, to a vector $d$: $\varphi(x) \to d \in \mathbb{R}^n$.

A particularly effective strategy within this domain is to think of vectors as points in a multidimensional space, with each vector element defining a position along a particular dimension.

The fundamental property of the $\varphi$ function, which is exploited by this technique, is that the semantic and contextual similarity between items is reflected in their vector representation. Consequently, conceptually similar items will be located in close proximity within the high-dimensional space. This implies that we can employ a distance function $\delta$ between these vectors as a measure of similarity to determine which items are semantically related.

Given a query point $q \in \mathbb{R}^n$ and a collection of data points $\mathcal{X} \subset \mathbb{R}^n$ derived from $\mathcal{D}$ using $\varphi$, we can compute the distance function between $q$ and each individual data point $u \in \mathcal{X}$ and, based on the score of the distance metric, retrieve the top-$k$ most semantically similar documents, which will be in the nearest neighborhood of our query. Formally, we can write:

$$\underset{u \in \mathcal{X}}{\overset{(k)}{\arg\min}}\, \delta(q, u). \tag{2.1}$$

Since a lower distance value corresponds to a higher degree of similarity. Figure 2.1 provides a visual depiction of the concepts discussed thus far.

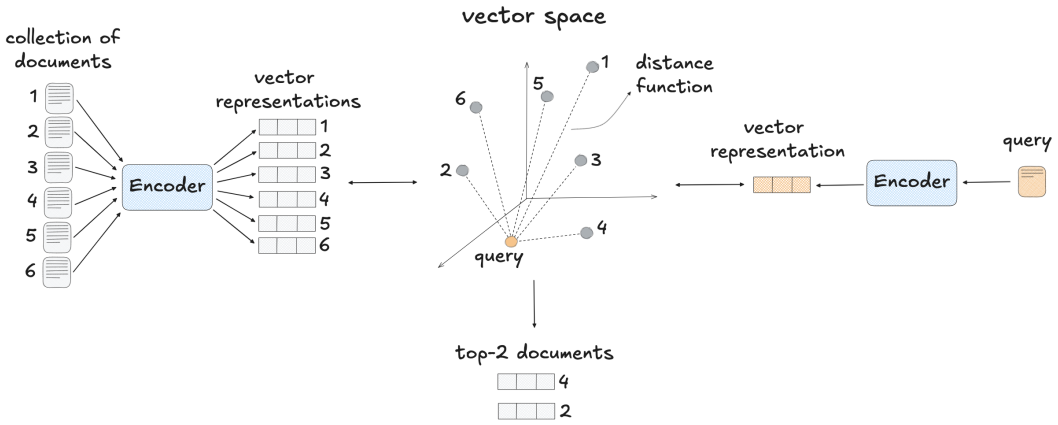



Figure 2.1: A visual representation of the vector search problem within the $\mathbb{R}^3$ space. Given a collection of documents, they are transformed into vector representations using an encoder. During online search, a query $q$ is vectorized using the same encoder, and a distance function is applied to retrieve the top-$k$ similar documents. In practical applications, not only are the number of documents extremely large, but the vectors themselves are often represented by hundreds or thousands of dimensions.

Having explored vector search and its three core components—dense vectors, encoders (embedding models), and distance functions—we will now delve deeper into each. Before proceeding, it's crucial to note that the relationship between items in the high-dimensional space vary based on the chosen encoder, which may focus on certain semantic aspects over others, and the distance function employed.

## 2.1 Dense Vector Retrieval

The concept of representing text as vectors is not new; early forms of such representations emerged between 1950 and 2000, with techniques like bag-of-words [82, 84], TF-IDF [83], PPMI [26, 28], LSI [30, 81], and BM25 [80]. Subsequent advancements were driven by Machine Learning (ML), initially leading to *static embedding* through models as Word2Vec [64, 65], GloVe [71], and FastText [13], and later with more sophisticated and expressive *dynamic (or contextual) embeddings*[1]. Among the first prominent models for obtaining dynamic embeddings was ELMo [72]. However, the real turning point came in 2018 with the introduction of Transformers [94], whose architecture radically changed the landscape of dynamic embedding representation. Since then, associated technologies like BERT [31], GPT [76], XLNet [101], and T5 [78] have consistently enhanced semantic vector representations, particularly after 2020 with the advent of *"Large" Transformers*. Large Transformers are Transformers with a larger architecture and trained on substantially larger datasets (e.g., GPT-3 [14] or GPT-4 [1]). These models have demonstrated an

[1]While static embeddings provide a single, global representation for a given word, subword o $n$-gram, contextual embeddings can assign also different representations based on the surrounding context, leading to a more accurate understanding of the word's, subword's or $n$-gram's meaning.

exceptional ability to understand the language and map text to high-dimensional vector spaces, capturing intricate semantic nuances.

While our focus lies on *dense vectors*, it is important to also acknowledge the existence of *sparse vectors* for text representation. Sparse vectors are extremely high-dimensional, containing many zero values, and the information is sparsely located. They are optimal for tasks that rely on syntax, lexicon, and exact or fuzzy text matching and are generated by algorithms such as BM25, TF-IDF, and SPLADE [35].

However, sparse vectors, due to their sparse nature, are generally less computationally efficient than dense vectors. Indeed, with the latter, we can operate on contiguous regions of memory, unlike the former. In addition, dense vectors, compared to sparse vectors, generally capture semantic meaning and underlying abstract concepts of a text more effectively. This makes them preferable for conducting efficient and high-performing semantic search.

While still high-dimensional, dense vectors have a significantly lower dimensionality than sparse vectors, containing mostly non-zero values, and effectively utilize the entire space to represent the text. Vector search models are based on dense vectors. Dense vectors are typically generated by machine learning models such as Transformers.

The vector space where dense vectors, generated by a given model, reside has a well-defined structure: semantically and contextually similar objects are mapped close together, while dissimilar objects are mapped far apart. The concept of distance and proximity within this space, and thus the similarity or dissimilarity between elements, is precisely defined by a distance function $\delta$. This structure is particularly well-suited for the fundamental problem of top-$k$ retrieval, where vectors serve as retrieval units and the relevance between a query and a document is determined by measuring their similarity.

At the heart of numerous applications, including web search, recommendation systems, question answering systems, legal search, chatbots, and more, lies the fundamental problem of top-$k$ retrieval [16]. This problem is central to vector search and involves finding and retrieving the $k$ most similar objects within a collection given a query $q$. By representing objects as vectors and defining similarity using a distance function $\delta$, the top-$k$ retrieval problem reduces to finding the $k$ points that minimize $\delta$ with respect to the query.

Let us now formalize the aforementioned intuition in Definition 2.1.1.

**Definition 2.1.1** (Top-$k$ Retrieval)**.** Let be given a query point $q \in \mathbb{R}^n$, a collection of data points $\mathcal{X} \subset \mathbb{R}^n$ and a distance function $\delta(\cdot, \cdot)$, the data point $u^* \in \mathcal{X}$ is one of the top-$k$ data points, if

$$u^* \in \underset{u \in \mathcal{X}}{\overset{(k)}{\arg\min}}\, \delta(q, u). \tag{2.2}$$

Thus far, we have considered the embedding function (encoder) $\varphi$ and the distance function $\delta$ as given. In Section 2.2 and 2.3, we will explore their internal mechanisms.

## 2.2 Embedding Models

There exist various embedding models for creating dense vector representations, some of which were mentioned in the previous section. However, the predominant approach

involves the use of Transformer-based Pre-trained Language Models (PLMs), due to their superior performance [27].

PLMs are (Large) Language Models (LLMs) [67] pre-trained on massive datasets in a self-supervised [8] manner, enabling them to understand language and capture a wide range of syntactic and semantic properties across diverse linguistic contexts. Moreover, these models can be fine-tuned for specific downstream tasks. Fine-tuning involves further training the PLM on specific task-oriented datasets, leveraging the pre-acquired knowledge to specialize it for a particular domain. This paradigm of *"pre-training followed by fine-tuning"* has enable state-of-the-art performance across a broad spectrum of tasks [72, 43, 31, 78].

Transformer-based PLMs are built upon the Transformer architecture, an encoder-decoder neural network model, based on the *self-attention* mechanism [94]. Self-attention is the cornerstone for enabling the model to understand the underlying meaning of language and construct an internal mathematical representation of it. Specifically, self-attention effectively captures the relationships and dependencies inherent in data by attending to how the different components of the text influence each other. Transformers are inherently highly parallelizable, enabling them to process large amounts of data simultaneously. This characteristic allows for efficient pre-training of large language models. Additional characteristics include the ability to effectively handle long text sequences and scale very well with massive datasets.

Based on variations in the original Transformer architecture, training methods, model dimensionality in terms of parameters, dataset type and size, number of encoder and/or decoder layers, and other differences, a multitude of Transformer-based Pre-trained Language Models (PLMs) have emerged, including BERT [31], DistilBERT [85] RoBERTa [60], ALBERT [55], XLNet [101], LLaMA [93], GPT-1 [76], GPT-2 [77], GPT-3 [14], GPT-4 [1], T5 [78], mT5 [100], BART [56], and many others.

The key point of interest is that all Transformer-based Pre-trained Language Models, whether fine-tuned or not, and regardless of their specific characteristics, can generate dense vector representations of input texts that encapsulate their semantic meaning.

This section has introduced modern embedding models and provided a basic understanding of the $\varphi$ function. A more in-depth discussion of the presented models and their specific operations is beyond the scope of this work. Readers interested in a deeper dive into this topic may consult [67, 34, 107, 40, 66, 74, 58, 106, 57, 97].

## 2.3 Distance Functions

Once vector representations of both the corpus documents and the input query are obtained, the subsequent and necessary step to retrieve the top-$k$ documents is to compute the distance function between the query point and each document point in the collection (Definition 2.1.1). We will now define the distance function, reformulating the top-$k$ retrieval problem according to the specific metric used.

*Manhattan distance*, *Euclidean distance*, *Cosine distance*, and *Inner Product distance* are the most frequently employed metrics for vector distance calculation.

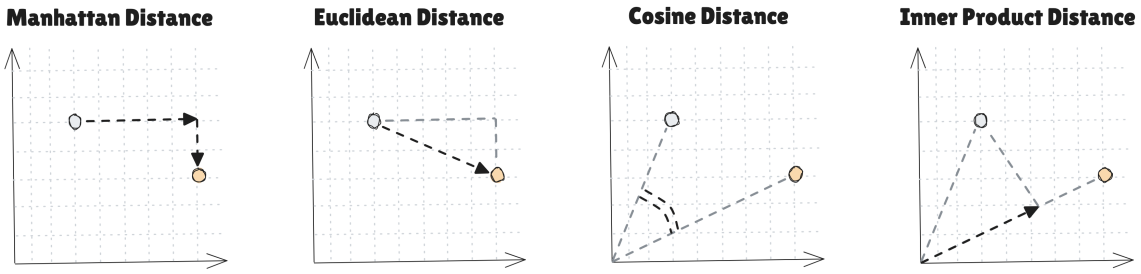



Figure 2.2: Distance metrics applied to two vectors, represented by the gray and orange dots, in a two-dimensional space $\mathbb{R}^2$. (a) Manhattan distance, L1 norm; (b) Euclidean distance, L2 norm; (c) Cosine distance; (d) Inner Product distance.

### 2.3.1 Manhattan Distance

The Manhattan distance, or L1 norm, (Figure 2.2a) measures the distance between two points in a grid-like pattern, analogous to the distance traveled by a taxicab along city blocks in $\mathbb{R}^2$. It is computed by summing the absolute differences of the corresponding coordinates of the two points. In other words, imagine two points in an n-dimensional space $\mathbb{R}^n$; the Manhattan distance from one point to the other is the sum of the distances traveled along each coordinate axis to reach the destination.

Formally, L1 norm between two points $q, u \in \mathbb{R}^n$ is defined as:

$$\delta(q, u) = \|q - u\|_1 = \sum_{i=1}^{n} |q_i - u_i| \tag{2.3}$$

The top-$k$ retrieval problem using the L1 norm as a distance function to compute similarity between the query and documents is referred to as $k$-Nearest Neighbors search with L1 norm ($k$-NN$_1$).

**Definition 2.3.1** ($k$-Nearest Neighbors search with L1 norm)**.** Let be given a query point $q \in \mathbb{R}^n$ and a collection of data points $\mathcal{X} \subset \mathbb{R}^n$, the $k$-Nearest Neighbors search with L1 norm ($k$-NN$_1$) consists in finding:

$$\{u_1^*, u_2^*, \cdots, u_k^*\} \subseteq \underset{u \in \mathcal{X}}{\overset{(k)}{\arg\min}} \|q - u\|_1. \tag{2.4}$$

### 2.3.2 Euclidean Distance

The Euclidean distance, also known as the L2 norm, (Figure 2.2b) measures the distance between two points in straight-line. It is computed by taking the square root of the sum of the squared differences of the corresponding coordinates of the two points under consideration. In simple terms, the Euclidean distance is the length of the line segment connecting the two points.

Formally, L2 norm between two vectors $q, u \in \mathbb{R}^n$ is defined as:

$$\delta(q, u) = \|q - u\|_2 = \sqrt{\sum_{i=1}^{n} (q_i - u_i)^2} \tag{2.5}$$

The top-$k$ retrieval problem using the L2 norm as a distance function is known as $k$-Nearest Neighbors search with L2 norm ($k$-NN$_2$).

**Definition 2.3.2** ($k$-Nearest Neighbors search with L2 norm)**.** Let be given a query point $q \in \mathbb{R}^n$ and a collection of data points $\mathcal{X} \subset \mathbb{R}^n$, the $k$-Nearest Neighbors search with L2 norm ($k$-NN$_2$) consists in finding:

$$\{u_1^*, u_2^*, \cdots, u_k^*\} \subseteq \underset{u \in \mathcal{X}}{\overset{(k)}{\arg\min}} \|q - u\|_2 = \underset{u \in \mathcal{X}}{\overset{(k)}{\arg\min}} \|q - u\|_2^2. \tag{2.6}$$

### 2.3.3 Cosine Distance

The cosine distance (Figure 2.2c) is defined as one minus the cosine similarity. The cosine similarity measures the similarity between two vectors in $\mathbb{R}^n$ based on the cosine of the angle between them, irrespective of their magnitude. It is calculated by computing the dot product of the two vectors and dividing it by the product of their Euclidean norms. Intuitively, the smaller the angular distance between vectors, the greater their similarity.

Formally, the cosine distance between two vectors $q, u \in \mathbb{R}^n$, with an angle $\theta$ between them, is defined as:

$$\delta(q, u) = 1 - cos(\theta) = 1 - \frac{\langle q, u \rangle}{\|q\|_2 \|u\|_2} = 1 - \frac{\sum_{i=1}^n q_i u_i}{\sqrt{\sum_{i=1}^n q_i^2} \sqrt{\sum_{i=1}^n u_i^2}} \tag{2.7}$$

The top-$k$ retrieval problem using the cosine distance as a distance function is referred to as $k$-Maximum Cosine Similarity Search ($k$-MCS).

**Definition 2.3.3** ($k$-Maximum Cosine Similarity Search)**.** Let be given a query point $q \in \mathbb{R}^n$ and a collection of data points $\mathcal{X} \subset \mathbb{R}^n$, the $k$-Maximum Cosine Similarity Search ($k$-MCS) consists in finding:

$$\{u_1^*, u_2^*, \cdots, u_k^*\} \subseteq \underset{u \in \mathcal{X}}{\overset{(k)}{\arg\min}}\, 1 - \frac{\langle q, u \rangle}{\|q\|_2 \|u\|_2} = \underset{u \in \mathcal{X}}{\overset{(k)}{\arg\max}} \frac{\langle q, u \rangle}{\|q\|_2 \|u\|_2}. \tag{2.8}$$

### 2.3.4 Inner Product Distance

The inner product distance, also known as the dot product distance, (Figure 2.2d) between two vectors is defined as the negative of their inner product. The inner product measures the similarity between two vectors in $\mathbb{R}^n$, considering both their magnitude and direction. In simple terms, the longer two vectors are, i.e., the greater their magnitude, and the more closely aligned they are, i.e., the smaller the angle between them, the higher their similarity.

Geometrically, the inner product can be interpreted as the projection of one vector onto the line defined by the other. The similarity between the two vectors is then computed by multiplying the length of this projection by the length of the vector that defines the line. The result is positive if the vectors point in the same direction and negative otherwise.

Formally, the inner product distance between two vectors $q, u \in \mathbb{R}^n$ is defined as:

$$\delta(q, u) = -\langle q, u \rangle = -\sum_{i=1}^n q_i u_i \tag{2.9}$$

$k$-Maximum Inner Product Search ($k$-MIPS) is a variant of the top-$k$ retrieval problem where similarity between the query point and a data point is measured using the inner product.

The $k$-$\text{NN}_2$ and $k$-MCS problems are both particular cases of the broader $k$-MIPS problem [16].

**Definition 2.3.4** ($k$-Maximum Inner Product Search)**.** Let be given a query point $q \in \mathbb{R}^n$ and a collection of data points $\mathcal{X} \subset \mathbb{R}^n$, the $k$-Maximum Inner Product Search ($k$-MIPS) consists in finding:

$$\{u_1^*, u_2^*, \cdots, u_k^*\} \subseteq \underset{u \in \mathcal{X}}{\overset{(k)}{\arg\min}} -\langle q, u \rangle = \underset{u \in \mathcal{X}}{\overset{(k)}{\arg\max}} \langle q, u \rangle. \tag{2.10}$$

This work focuses on the $k$-MIPS problem.

# Chapter 3

# Approximate Nearest Neighbor Search

Having explored the most widely used vector similarity metrics and defined the variants of the top-$k$ retrieval problem ($k$-NN$_1$, $k$-NN$_2$, $k$-MCS, and $k$-MIPS) in relation to them, we now turn our attention to applying an algorithm to retrieve the top-$k$ data points given a query point. For simplicity and given that the distance function used in this work is the inner product distance, we focus our discussion on the $k$-MIPS problem.

In order to accurately retrieve the top-$k$ most relevant documents for a given query, thus providing an exact solution to the $k$-MIPS problem, an *exhaustive search algorithm*, also known as a brute-force algorithm, is required. This algorithm first computes the inner product between the query point and every data point within the collection, and then retrieves the $k$ data points with the highest similarity scores.

Although this approach is conceptually straightforward, the associated computational cost is substantial, rendering it impractical and highly inefficient at query time, especially in modern systems that handle extremely large numbers of high-dimensional vectors. As evidence, we can consider the time complexity of computing the dot product between a query point and every data point in the collection, which is $\mathcal{O}(|\mathcal{X}|n)$, where $|\mathcal{X}|$ represents the number of data points and $n$ represents the dimensionality of the vector space. This makes it evident that exhaustive search algorithm is prohibitive for billions of vectors with thousands of dimensions.

*Approximate Nearest Neighbor (ANN) search* emerges as the technique to address this challenge, providing an efficient and scalable solution. The efficiency and scalability of an ANN search method are achieved by sacrificing perfect accuracy and introducing a degree of approximation in the search results. Indeed, ANN is an approximate retrieval technique that returns an approximate top-$k$ set as output, rather than an exact one.

In order to assess the effectiveness of an approximate top-$k$ solution provided by an ANN search algorithm, and quantify the accuracy of the search, we calculate the proportion of data points in the returned solution that are also present in the exact top-$k$ set. Formally, this can be expressed as: $|\mathcal{S} \cap \tilde{\mathcal{S}}|/k$, where $\mathcal{S}$ represents the set of relevant items (exact top-$k$) and $\tilde{\mathcal{S}}$ represents the set of retrieved items returned by the ANN algorithm.

ANN search algorithms are instrumental in modern vector search systems, offering an optimal trade-off between accuracy and efficiency. By sacrificing a small degree of

precision, ANN can rapidly identify a promising subset of vectors from the vector collection that is likely to contain the desired results. This subset is then subjected to more rigorous search methods, such as a secondary ANN algorithm with a stronger emphasis on accuracy or, for sufficiently small subsets, an exhaustive search.

In essence, vector search systems operate as pipelines, beginning with the entire corpus and primarily leveraging ANN algorithms to iteratively reduce the search space, where at each stage, the algorithm selects a smaller subset of vectors, ultimately returning the top-$k$ most relevant results. These results can subsequently be fed into more sophisticated ranking algorithms for further refinement.

This approach enables the development of extremely fast search systems capable of achieving nearly flawless accuracy.

Technically, an ANN setup first builds a data structure—the index—from the given collection of vectors, in an offline phase. This index is then used to rapidly identify the most similar vectors to a new query point.

The landscape of ANN algorithms is vast, encompassing a wide array of approaches, including tree-based [16, 9, 37, 29, 11, 5], hashing-based [16, 47, 45, 38, 96], graph-based [16, 62, 36, 69, 51], and clustering-based [16, 52, 18, 25, 7] methods. This work concentrates on the clustering-based approach, also known as the Inverted File (IVF) method.

## 3.1 Clustering-Based ANN Search

Clustering-based ANN search is a prominent ANN search method, demonstrating strong empirical performance [7] and widespread adoption in production systems[1]. This methodology is grounded in a simple yet acute intuition: Leveraging the intrinsic clustering behavior of data points within the search space. By exploiting these natural partitions, top-$k$ data points for a query can be retrieved by examining solely the most similar clusters, thus significantly reducing the search space while maintaining a high level of retrieval accuracy.

More specifically, the clustering-based ANN methodology first takes the given collection of $P$ data points $\mathcal{X} \subset \mathbb{R}^n$ and applies a *clustering* function to them, mapping each point to a specific cluster, $\mathcal{C} : \mathbb{R}^n \to \{1, 2, \ldots, L\}$, thereby partitioning the vectors under consideration. Subsequently, each partition is represented by a vector. The resulting partitions and their respective representative vectors constitute the *index*.

At query time, when a query point $q$ is provided as input, a *routing* function $\tau : \mathbb{R}^n \to \arg\max^{\ell} \mathbb{R}^L$ is invoked to calculate the similarity between the representative vectors and $q$. The function then returns the clusters associated with the top-$\ell$ most similar representative points to the query $q$. Put differently, the routing function $\tau$ maps a query vector $q$ to the $\ell$ most similar partitions to it, within which the top-$k$ data points are most likely to be found. In order to retrieve the $\ell$ most similar partitions, $\tau$ essentially solves a top-$\ell$ retrieval problem where the collection of points is represented by the representatives points of clusters. Figure 3.1 offers a visual depiction of the core ideas underlying the clustering-based ANN method discussed so far.

[1] `https://turbopuffer.com/blog/turbopuffer`, `https://www.pinecone.io/blog/serverless-architecture`

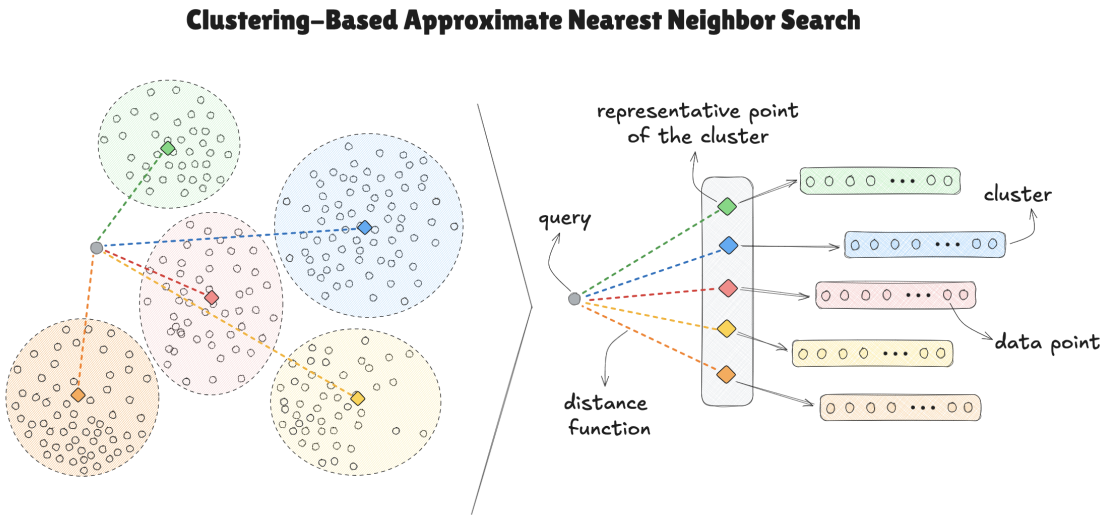



Figure 3.1: Clustering-Based Approximate Nearest Neighbor (ANN) Search. The left-hand side presents a visual representation of the space partitioned into clusters, while the right-hand side illustrates the corresponding index structure. Both figures depict the process of computing the similarity between a query point and the cluster representative points.

Once the $\ell$ partitions have been obtained, to retrieve the top-$k$ data points relative to the query $q$, a second search phase is conducted considering only the data points within those partitions. The search within these clusters can be exhaustive—as performed in this work—using a brute-force algorithm, or by employing another ANN algorithm. It is trivial to observe that by using $\ell \ll L$, the search space for the second phase is significantly reduced, leading to more efficient search at the cost of potential accuracy loss.

A standard choice [7, 16, 52] for clustering-based ANN is to use the Standard KMeans [61] as the clustering algorithm $\mathcal{C}$, setting the number of clusters to $L = \mathcal{O}(\sqrt{P})$, and defining the routing function $\tau$ as:

$$\tau(q) = \underset{i=1,\dots,L}{\arg\min^{(\ell)}} \delta(q, \mu_i), \tag{3.1}$$

where $\mu_i$, the representative of the $i$-th cluster, is the cluster centroid defined as the mean of the data points within it: $\mu_i = \frac{1}{|\mathcal{C}^{-1}(i)|} \sum_{u \in \mathcal{C}^{-1}(i)} u$, with $\mathcal{C}^{-1}(i) \coloneqq \{u \,|\, u \in \mathcal{X}, \mathcal{C}(u) = i\}$.

As we have observed, clustering plays a pivotal role in this approach, with the Standard KMeans algorithm serving as the default choice. Consequently, in the subsequent section, we delve deeper into these concepts. Firstly, we provide an overview of clustering, followed by a detailed explanation of the Standard KMeans and two other interesting variants employed in this work: Spherical KMeans [32] and Shallow KMeans [25].

### 3.1.1 Clustering

The initial question that must be addressed is: what is clustering?

> Given a collection of objects, *clustering* is a technique designed to group similar objects into the same cluster and dissimilar objects into different clusters.

The application of clustering is ubiquitous, finding utility in fields such as machine learning, bioinformatics, pattern recognition, social network analysis, information retrieval, computer vision, climatology, healthcare, economics, and many more. Its application across such diverse fields is not surprising, given the inherent tendency of objects or data points to form natural clusters. This makes clustering an optimal approach for many applications.

It is crucial to emphasize that a clustering function, designed to uncover structures and patterns within a given collection of objects to create groups or partitions, necessitates a key element: a metric for comparing these objects. This metric is the core of the objective function. Indeed, clustering is an optimization problem where the goal is to achieve groups with the highest intra-cluster similarity and the lowest inter-cluster similarity.

In relation to the problem described in the preceding chapters of retrieving the top-$k$ documents with the highest accuracy and efficiency from a large collection of data points, it is intuitive that clustering aligns well with this task. As discussed in Section 2.1, the vector representation has the property that semantically similar objects are mapped close together in the space, while dissimilar objects are mapped far apart. Hence, by clustering semantically similar objects, we can accelerate the search for the top-$k$ documents, because we can focus our attention solely on the vectors within the clusters most similar to a given query $q$. Resulting in an effective ANN algorithm.

The literature presents a variety of types of clustering [98], including partition-based, density-based, distribution-based, hierarchical, and graph-based, each optimal in specific scenarios. However, in this context, we will focus on the partitioning approach and examine the default algorithm employed for clustering-based ANN, namely the KMeans algorithm.

### 3.1.2 Standard KMeans

Partition-based clustering is a type of clustering that groups data points into non-overlapping partitions. The KMeans algorithm is a prominent example of this type of clustering.

The KMeans algorithm is an iterative clustering algorithm that returns a local optimum for the KMeans optimization problem, which is defined in 3.1.1.

**Definition 3.1.1** (KMeans problem)**.** The KMeans problem, given $L \in \mathbb{Z}^+$ and a collection of data points $\mathcal{X} \subset \mathbb{R}^n$, consists of identifying $L$ centroids $\{\mu_i\}_{i=1}^L$ that minimize the objective function $\mathcal{E}$, defined as:

$$\mathcal{E}(\{\mu_i\}_{i=1}^L) = \sum_{x \in \mathcal{X}} \|x - \underset{\mu_i \in \{\mu_i\}_{i=1}^L}{\arg\min} \|x - \mu_i\|_2^2\|_2^2. \tag{3.2}$$

Considering the definition 3.1.1, it is clear that problem is intrinsically linked to the concept of clustering. Specifically, the KMeans problem can be reformulated as finding the $L$ partitions of a collection of data points $\mathcal{X}$ such that the centroids of these partitions minimize the Equation 3.2.

The KMeans clustering algorithm aims to create $L$ partitions that minimize the objective function $\mathcal{E}$ (Equation 3.2), also known as inertia. To achieve this, after an initial

centroids initialization phase, the algorithm iteratively performs two steps: first, each data point is assigned to the nearest centroid; then, the centroids are recalculated based on the new cluster memberships. This iterative process ensures a decrease in inertia until a local optimum is reached [6]. The algorithm terminates when a stopping criterion is satisfied, such as after $t$ iterations or when the change in $\mathcal{E}$ is less than a specified threshold, $|\mathcal{E}(\{\mu_i\}_{i=1}^{L})^{(i)} - \mathcal{E}(\{\mu_i\}_{i=1}^{L})^{(i+1)}| < \epsilon$.

The pseudocode for the Standard KMeans clustering algorithm is presented in Algorithm 1.

**Algorithm 1** Standard KMeans Algorithm

**Input:** number of clusters $L$, collection of data points $\mathcal{X} \subset \mathbb{R}^n$
**Output:** cluster centroids $[\mu_1, \ldots, \mu_L] \in \mathbb{R}^{n \times L}$, non-overlapping partitions $\{c_i\}_{i=1}^{L}$
Randomly select $L$ cluster centroids $\mu_1, \ldots, \mu_L$
**repeat**
    $\{c_i\}_{i=1}^{L} = \{\}$
    **for each** $x \in \mathcal{X}$ **do**
        $c_i = c_i \cup \{x\}$, where $i \coloneqq \arg\min_{i=1,\ldots,L} \|x - \mu_i\|_2^2$
    **for** $i \in \{1, \ldots, L\}$ **do**
        $\mu_i = \frac{1}{|c_i|} \sum_{x \in c_i} x$
**until** $\mu_1, \ldots, \mu_L$ converge

The KMeans algorithm is one of the most widely used, recognized, and popular clustering algorithms [49, 103, 98, 46, 3, 10]. In general, the Standard KMeans algorithm and its variants, in addition to being intrinsically simple to understand and implement, are also efficient algorithms with low time complexity and high computational efficiency, making them well-suited to use on massive datasets [98, 103, 46, 23, 89, 99].

However, the KMeans algorithm is not without its drawbacks, such as sensitivity to the initial choice of centroids, the requirement of specifying the number of clusters a priori, difficulties in achieving a global minimum for complex datasets, sensitivity to noise data and outliers, and suboptimal performance on non-convex data; although numerous studies and variants have been proposed to address these issues [98, 46, 3, 10, 6].

Let us now turn our attention to two variants of the Standard KMeans algorithm: Spherical KMeans and Shallow KMeans.

### 3.1.3 Spherical KMeans

Both Spherical KMeans [32] and Standard KMeans are commonly employed in clustering-based ANN [18].

The fundamental distinction between the two aforementioned algorithms lies in their respective focus on similarity measures and the consequent objective functions. While Standard KMeans algorithm minimizes an objective function based on Euclidean distance (Definition 3.1.1), Spherical KMeans minimizes an objective function that employs cosine distance (Equation 2.7) to form L partitions. By L2-normalizing all $x \in \mathcal{X}$ to unit length, Spherical KMeans is an iterative algorithm that aims to find $L$ partitions maximizing the

following objective function:

$$\mathcal{P}(\{\mu_i\}_{i=1}^{L}) = \sum_{x \in \mathcal{X}} \langle x, \underset{\mu_i \in \{\frac{\mu_i}{\|\mu_i\|_2}\}_{i=1}^{L}}{\arg\max} \langle x, \mu_i \rangle \rangle. \tag{3.3}$$

As with the KMeans problem [4], determining the globally optimal partitions in this case is also NP-hard [54]. Thus, Spherical KMeans, like Standard Kmeans, is an approximation algorithm for the optimal solution. Nonetheless, it is an efficient and effective iterative heuristic, prone to local optima, and capable of yielding reasonable results [32].

Algorithm 2 provides the pseudocode for the Spherical KMeans clustering algorithm.

**Algorithm 2** Spherical KMeans Algorithm

**Input:** number of clusters $L$, collection of data points $\mathcal{X} \subset \mathbb{R}^n$
**Output:** cluster centroids $[\mu_1, \ldots, \mu_L] \in \mathbb{R}^{n \times L}$, non-overlapping partitions $\{c_i\}_{i=1}^{L}$
Randomly select $L$ cluster centroids $\mu_1, \ldots, \mu_L$ on the unit sphere
$x = \frac{x}{\|x\|_2} \; \forall x \in \mathcal{X}$
**repeat**
    $\{c_i\}_{i=1}^{L} = \{\}$
    **for each** $x \in \mathcal{X}$ **do**
        $c_i = c_i \cup \{x\}$, where $i := \arg\max_{i=1,\ldots,L} \langle x, \mu_i \rangle$
    **for** $i \in \{1, \ldots, L\}$ **do**
        $\mu_i = \frac{1}{|c_i|} \sum_{x \in c_i} x$
        $\mu_i = \frac{\mu_i}{\|\mu_i\|_2}$ ▷ $\mu_i$ is projected on the unit sphere
**until** $\mu_1, \ldots, \mu_L$ converge

Comparing Algorithm 1 with Algorithm 2, the Spherical KMeans algorithm introduces the following modifications: initial L2-normalization of all vectors $x \in \mathcal{X}$; cluster assignment based on inner products between data points and centroids during iterations; and, the projection of centroids onto the unit sphere at the end of each iteration.

The Spherical KMeans clustering algorithm, as defined, is a suitable choice for clustering-based ANN with cosine distance (Equation 2.7) or inner product distance (Equation 2.9) as the distance metric of interest.

### 3.1.4 Shallow KMeans

We now turn our attention to a particularly simple, computationally efficient, and interesting clustering algorithm, which we refer to as Shallow KMeans. The corresponding pseudocode is presented in Algorithm 3.

Shallow KMeans can be viewed as a single iteration of the KMeans algorithm. It involves randomly selecting $L$ data points from $\mathcal{X}$ as initial cluster representatives, followed by assigning each data point to the nearest representative. The cluster representatives can then be updated, for example, by computing the mean of the points in each cluster or employing other strategies. However, this update step is not mandatory, and the initial $L$ points can be used as final representatives. In our implementation, the distance function employed is the inner product distance (Equation 2.9), and the final cluster representatives coincide with the initial ones.

**Algorithm 3** Shallow KMeans Algorithm

**Input:** number of clusters $L$, collection of data points $\mathcal{X} \subset \mathbb{R}^n$
**Output:** cluster representatives $[r_1, \ldots, r_L] \in \mathbb{R}^{n \times L}$, non-overlapping partitions $\{c_i\}_{i=1}^{L}$
Randomly select $L$ data points $s_1, \ldots, s_L$ from $\mathcal{X}$
$\{c_i\}_{i=1}^{L} = \{\}$
**for each** $x \in \mathcal{X}$ **do**
    $c_i = c_i \cup \{x\}$, where $i \coloneqq \arg\min_{i=1,\ldots,L} \delta(x, s_i)$
Select a representative point for each cluster $r_1, \ldots, r_L$

The Shallow KMeans clustering algorithm was originally introduced in [25], where the authors proposed an extremely simple pruning scheme, termed *cluster pruning*, to efficiently address the top-$k$ retrieval problem (Definition 3.1.1) while maintaining good retrieval quality. The clustering algorithm, in particular, is used in the preprocessing phase of cluster pruning scheme with some variations. Furthermore, [25] demonstrated that the proposed approach, and consequently the underlying clustering algorithm, is both efficient and accurate in retrieving the top-$k$ documents for a given query, achieving remarkable performance. As we will also see in this work.

# Chapter 4

# Learning-to-Rank

To realize the proposed method, which will be detailed in the subsequent chapter, we have employed a widely studied and researched technique within the scientific community: *Learning-to-Rank (LTR)*. By developing a model that harnesses the power of LTR to enhance ANN search. The results obtained highlight the potential of combining these two fields, thus motivating the community to further investigate into this intersection.

The objective of this chapter is to provide an overview of LTR and equip readers with the necessary knowledge to fully understand the ranking model employed in our work. For a deeper dive into LTR, we suggest referring to [59, 17].

We will now introduce Learning-to-Rank through the following fundamental question: what is LTR?

> *Learning-to-Rank (LTR)* is a supervised Machine Learning (ML) technique aimed at *learning* a function to solve a *ranking* problem.

More specifically, the learnt function is a ranking model or ranking function $f : \mathcal{Q} \times \mathcal{I}^U \rightarrow \mathbb{R}^U$, which, given a query $q \in \mathcal{Q}$ and a set of $U$ items $\boldsymbol{d} = (d_i)_{i=1}^U \in \mathcal{I}^U$ as input, computes a score $s_i \in \mathbb{R}$ for each query-item pair: $f(q, (d_i)_{i=1}^U) = (s_i)_{i=1}^U = \boldsymbol{s} \in \mathbb{R}^U$. These scores are then used to order the items by relevance. A visual depiction is provided in Figure 4.1.

To illustrate LTR more clearly, image our ranking function $f$ as a pastry chef. The chef's task is to arrange a set of pastries according to a customer's preferences. By assigning a relevance score to each pastry based on the customer's order, the chef create a ranked list. Through training and learning from mistakes, the chef can improve their ability and generate more accurate rankings.

Staying within the analogy, in the next section we will delve deeper into the pastry chef and explore how they actually learn.

## 4.1 Learnt Ranking Function

The learnt ranking function is the mathematical function learnt through supervised learning techniques by LTR models. To learn this function, we need the following key ingredients.

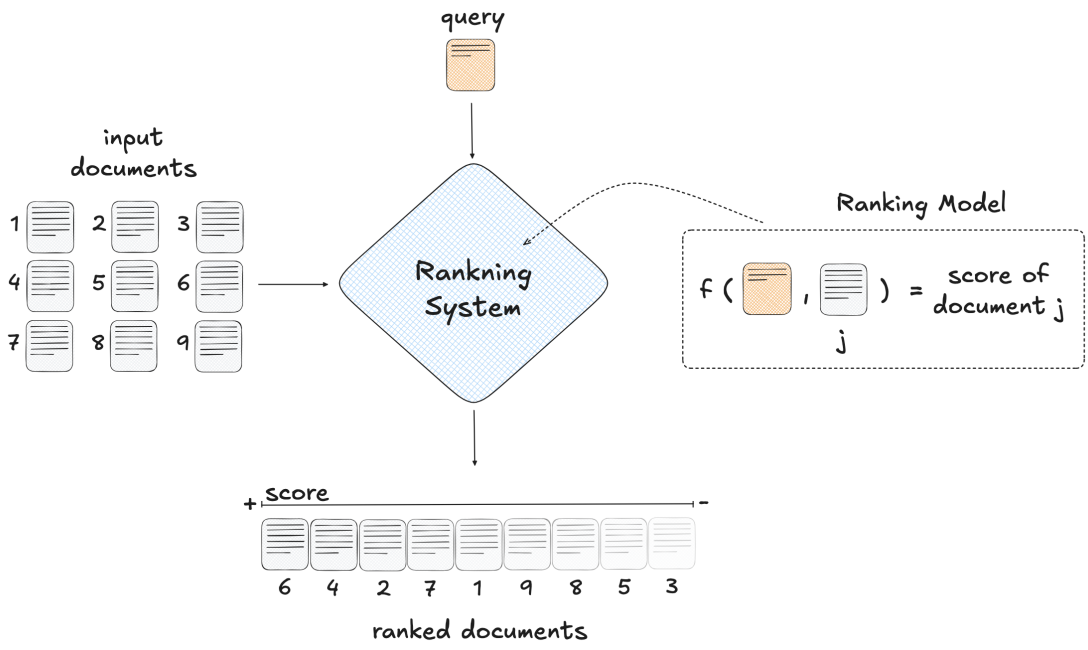



Figure 4.1: A ranking system is proposed that, given a set of documents and a query as input, outputs the documents ordered by their relevance to the query. This relevance is obtained through a ranking model, which assigns a score to each document-query pair, reflecting the document's pertinence to the query.

- **Dataset $\mathcal{U}$**

  The dataset $\mathcal{U}$ serves as the raw material for learning the function $f$, providing the data required to train, validate, and test it. Typically, an LTR dataset consists of a set of triplets $(q, \boldsymbol{d}, \boldsymbol{y}) \in \mathcal{Q} \times \mathcal{I}^U \times \mathcal{Y}^U$, where $q$ symbolizes the query, $\boldsymbol{d} = (d_i)_{i=1}^U$ is the collection of items to be ranked in relation to $q$, and $\boldsymbol{y} = (y_i)_{i=1}^U$ represents the ground-truth relevance judgment for each query-item pair.

  Formally, $\mathcal{U} \coloneqq \{(q_j, \boldsymbol{d}_j, \boldsymbol{y}_j)\}_{j=1}^N$.

- **Numerical Representation Function $\eta$**

  The function $\eta$ takes as input a triplet from the dataset $\mathcal{U}$ and outputs the corresponding numerical representation that will be used to train, validate, or test $f$ in practice. The nature of the $\eta$'s output is determined by the strategy employed to solve the ranking problem, and consequently on the learning algorithm, the input and output spaces, and additional relevant factors.

  To illustrate the function more clearly, let us consider some examples. $\eta$ might take as input an image query, a collection of text documents, and a binary ground-truth with 'yes' and 'no' labels; it could then generate a vector representation of the image using ResNet [41], a vector representation of the documents using BERT [31], and a binary vector representing relevance. Alternatively, $\eta$ could receive a textual query, a collection of textual documents, and a relevance score for each query-document pair; producing a feature vector for each pair and a corresponding vector where the relevance score is normalized between 0 and 1.

- **Evaluation Metric** $m$

  The evaluation metric $m$ is indispensable for assessing the quality of rankings produced by the ranking function, providing an objective measure of the model's performance and effectiveness on the specific ranking task. In other words, it offers a quantitative evaluation that enables us to understand how well the model is performing.

  Various metrics exist, each measuring different aspects of the ranking. The choice of the most appropriate metric depends on the specific ranking problem. In the following, we provide a selection of ranking metrics: *Mean Reciprocal Rank* [104], *Mean Average Precision* [104], *Normalized Discounted Cumulative Gain* [50], *Rank-Biased Precision* [68], and *Expected Reciprocal Rank* [24].

- **Loss Function** $l$

  The loss function $l$, also known as the error function, cost function, or objective function, quantifies the error between the predicted value (output of $f$) and the true value (ground-truth). The loss function is instrumental in training the function $f$, serving as a guiding objective for optimization algorithms [90]. During training, optimization algorithms aim to minimize the loss function by updating the parameters of $f$, thereby improving the accuracy of the resulting rankings. The mathematical formalization of the loss function is as follows: $l(f(q, \boldsymbol{d}), \boldsymbol{y}) = l(\hat{\boldsymbol{y}}, \boldsymbol{y})$.

  In the context of ranking, minimizing a loss function is equivalent to maximizing a ranking metric. However, the non-continuous and non-differentiable nature of ranking metrics presents an obstacle for optimization algorithms. To circumvent this issue, *surrogate objective functions* [20, 21, 22, 15, 73, 91] are utilized. These are continuous and differentiable functions derived from ranking metrics. Their use allows optimization algorithms to run smoothly and optimize objective functions consistent with ranking metrics.

- **Hypothesis Class of** $f$

  The hypothesis class represents the family of functions to which $f$ belongs. Hypothesis classes can be linear functions, polynomial functions, and, among the most commonly used in LTR, decision forests and deep neural networks [17]. The goal is to identify the most suitable hypothesis class for a given problem, as using all the other aforementioned ingredients ($\mathcal{U}$, $\eta$, and $l$ with an optimization algorithm), we will obtain the optimal function within that class, which will be our learnt ranking function $f(\cdot, \cdot; \theta)$, where $\theta$ represents the learnt parameters that minimize the loss function.

  To make this more intuitive, consider the analogy of a nail in a wall. Our goal is to remove this nail using a specific tool ($f$). To achieve this, we can employ various tools (which represent the hypothesis classes), such as the 'class of pliers', the 'class of hammers', the 'class of screwdrivers', and many others. After careful analysis, we decide, based on our considerations, to select the 'class of pliers' (the chosen hypothesis class), which contains a variety of pliers (family of functions), including the particular pair of pliers ($f$) recommended by a domain expert who selected it according to specific analyses.

Through the careful selection and combination of these ingredients, it is possible to develop highly effective learnt ranking functions capable of solving ranking problems satisfactorily.

To gain a more comprehensive understanding of the learning process for the ranking function $f$, we revisit the necessary components and illustrate how these elements interact.

Central to our learning and evaluation process for function $f$ is the dataset $\mathcal{U} \coloneqq \{(q_j, \boldsymbol{d}_j, \boldsymbol{y}_j)\}_{j=1}^{N}$, which is typically partitioned into three subsets: training, validation, and test sets [12]. The training set comprises the triples used to train the ranking function, the validation set is used to evaluate the model's performance during training and to tune hyperparameters, and the test set is used to assess the performance of the final learnt ranking function $f$.

Once the dataset is acquired, the subsequent step involves applying a numerical representation function, $\eta$. This function transforms each dataset instance into a numerical representation tailored to the specific ranking problem and chosen solution strategy. The resulting representations are then employed to train and evaluate the ranking function $f$. The quality and characteristics of $f$ are heavily influenced by $\eta$.

While $\eta$ plays a vital role, the selection of a suitable ranking metric $m$ is equally important. A ranking metric is essential for objectively evaluating the performance of a ranking function. Our goal is to learn a function $f$ that maximizes the chosen ranking metric, which is achieved by minimizing a surrogate objective function $l$ that is correlated with the metric to be maximized. The function $l$ is then employed to train $f$.

The final step prior to training the ranking function $f$ involves selecting the hypothesis class. This choice defines the space of possible functions from which the learnt ranking function will be extracted. It is important to note that, similar to the selection of the numerical representation function $\eta$, the ranking metric $m$, and the loss function $l$, there is no universally optimal choice for the hypothesis class. Instead, this selection requires careful consideration of the specific ranking problem.

Having prepared all the necessary components, we can now proceed with the actual training of the ranking function $f$. Specifically, we utilize the training set and validation set, appropriately transformed by $\eta$, along with the loss function $l$ and an optimization algorithm [90]. The training process involves optimizing the parameters of $f(\cdot, \cdot; \theta)$ using an optimization algorithm to minimize the loss function on the training set. Beyond the training set, which is essential for parameter estimation, the validation set plays a pivotal role for hypothesis (function) selection. By assessing the predictive performance of different functions within the hypothesis class on the validation set, we can determine the function that is most likely to generalize well to new, unseen data, thereby enabling us to select the optimal learnt ranking function $f$.

Once the final learnt ranking function, $f$, has been obtained, it is evaluated on the test set using the selected metric, $m$, to determine its effectiveness in solving the given ranking task.

# Chapter 5

# Learning Cluster Representatives

In this chapter, we delve into the details of our novel methodology for MIPS-based clustering-based ANN search, which represents the state-of-the-art in the field. This methodology was presented at SIGIR 2024[1] in paper [95]. In this thesis, we expand upon [95] and provide a more in-depth analysis. We begin by exploring the intuition and motivations behind our research. Subsequently, we formalize the methodology rigorously, outlining its fundamental principles and components. We then present the experimental setup and discuss the obtained results, extending beyond those reported in the aforementioned paper. Finally, we dedicate a section to further analysis, where we explore a variation of the methodology and evaluate its corresponding results.

## 5.1 Intuition

In Section 3.1 on clustering-based ANN search, we saw that at query time, the fundamental element analyzed by the routing function $\tau$, to return the $\ell$ most similar partitions to a given query, is the representative element of each cluster. The standard approach consists of computing the mean of the points within the cluster as the representative point (Equation 3.1).

However, a natural question arises: Does there exist a representative point that better captures the semantics of the cluster and its internal elements, such that when a distance function $\delta$ is applied, the returned score more accurately reflects the true similarity between the query and the cluster? Our work provides an affirmative answer to this question by introducing *learnt representative points*.

Let us begin with a simple yet crucial observation to understand how the learnt representative points are obtained: The routing function $\tau$ is a ranking function that addresses the problem of ordering partitions from the most similar, which has the highest probability of containing the actual top-$k$ documents for a given query, to the least similar, where we have the lowest probability of finding the resulting top-$k$ documents.

This observation implies that the function $\tau$ can be learnt using Learning-to-Rank (Section 4), and in particular, we can learn it using a simple linear function $\hat{\tau}(q;\ W) = Wq$, with $q \in \mathbb{R}^n$ and $W \in \mathbb{R}^{L \times n}$, where the $i$-th row of $W$ is the learnt representative vector

[1] `https://sigir-2024.github.io/`

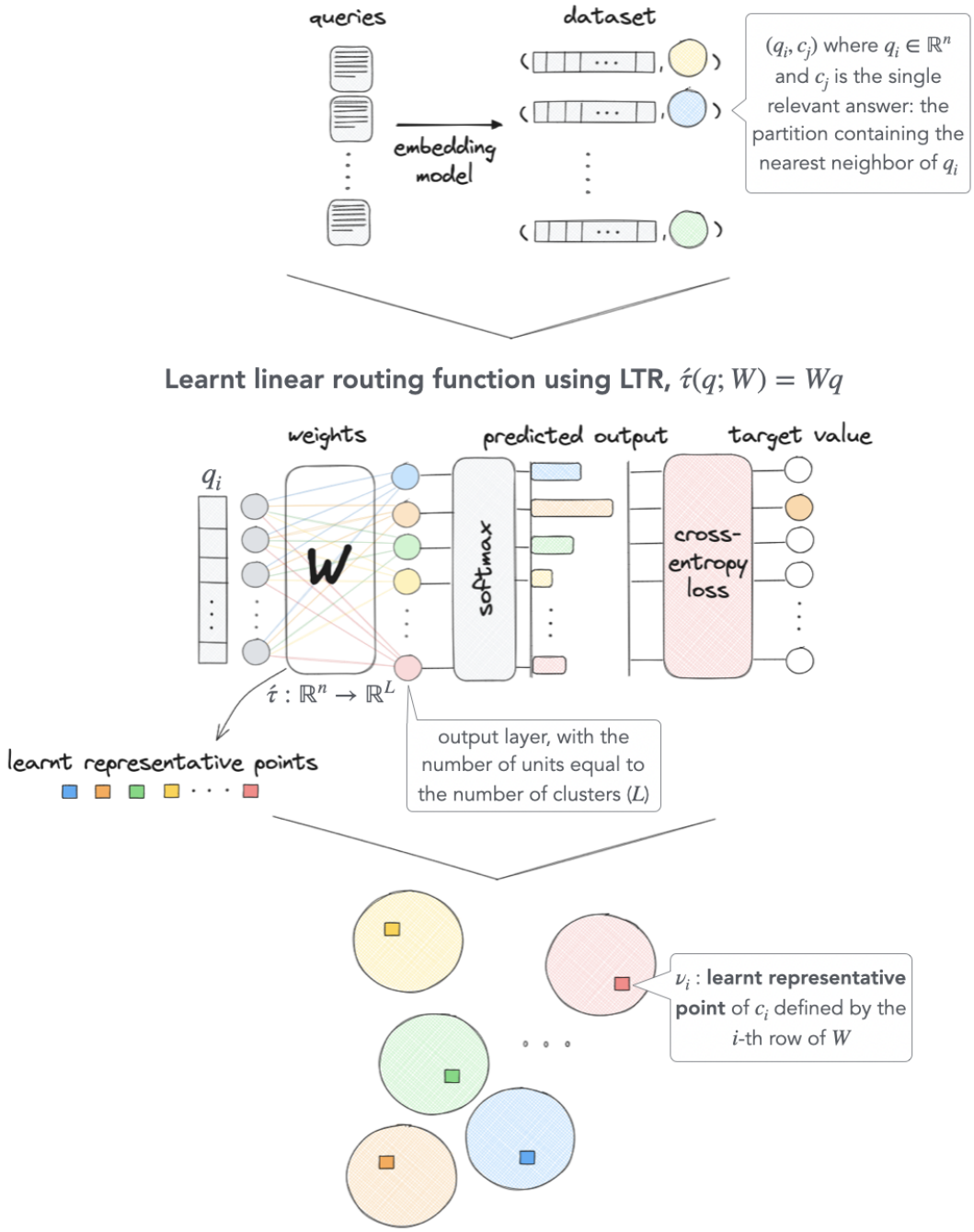



Figure 5.1: Visual representation of the learning process of the routing function $\acute{\tau}$ using LTR to obtain the learnt representative points. Specifically, three phases are depicted: dataset creation, learning the routing function, and visualization of clusters with the learnt points.

of the $i$-th partition. This yields a learnt ranking function $\acute{\tau}(q;\ W) = Wq$ that, given a query $q$, outputs a ranking score for each of the $L$ partitions under consideration, with $W$ containing the new representatives of the partitions.

Concretely, to learn the routing function $\acute{\tau}$, we consider the top-$k$ case with $k = 1$.

It is straightforward to observe that the quality of routing can be evaluated using a ranking metric: Given a query, the routing function assigns to each partition a likelihood of containing the nearest neighbor, while the single relevant response (ground-truth) is the partition that actually contains the nearest neighbor. An appropriate metric we can use is MRR [104]. Consequently, with MRR as the appropriate metric and since each query has a single relevant answer, the most suitable surrogate objective to optimize is cross-entropy loss [15, 19].

Regarding the dataset, it is also easily obtainable. All that is needed is a set of queries where, for each query, as ground-truth relevance label, we have the corresponding partition that contains its nearest neighbor. The corresponding partition can be found by simply retrieving the relevant top-1 document with an exhaustive search and subsequently identifying its cluster of belonging.

Finally, by representing the query as a vector in $\mathbb{R}^n$ and the ground-truth as a binary vector with a 1 set for the partition containing the top-1 document, and selecting a hypothesis class of linear neural networks [39] with only an input layer (with the number of units equal to the dimension of the query vector) and an output layer (with units equal to the number of clusters) followed by with a softmax function, we have all the necessary components to learn $\acute{\tau}$, where the learnt representative points in this case are the weights $W$ of the neural network. A graphical illustration of the aforementioned is presented in Figure 5.1.

Building upon this intuition, we have experimentally demonstrated that the learnt representative points significantly improve the accuracy of clustering-based ANN search. Moreover, an appealing aspect of this methodology lies in its easy integration into a production system that already implements a routing mechanism. By merely replacing the old representative points with the learnt points, without any additional modifications.

## 5.2 Methodology

In this section, we formally introduce the methodology employed to learn the $L$ representative points, where $L$ denotes the number of clusters. We provide a rigorous mathematical formulation, detailing the steps involved, starting from the problem to be solved.

Given a collection of data points $\mathcal{X} \subset \mathbb{R}^n$ and a query $q \in \mathbb{R}^n$, obtained from an embedding function $\varphi$, we aim to retrieve the top-$k$ most similar data points to $q$, as measured by the inner product, thereby solving the $k$-MIPS problem (Definition 2.3.4): $\{u_1^*, u_2^*, \cdots, u_k^*\} \subseteq \arg\max_{u \in \mathcal{X}}^{(k)} \langle q, u \rangle$ (Equation 2.10). As shown in Section 3.1, an efficient practical solution for this problem, though approximate, involves employing clustering-based ANN search approach.

Clustering-based ANN search applies a clustering algorithm $\mathcal{C} : \mathbb{R}^n \to \{1, 2, \ldots, L\}$ to partition the dataset $\mathcal{X}$ into a set of $L$ non-overlapping clusters $\{c_i\}_{i=1}^{L}$, where each cluster is represented by a representative point $\mu_i$. In the standard approach, $\mu_i$ is computed as the mean of the points in cluster $c_i$. Subsequently, given a query $q$, a routing function

$\tau : \mathbb{R}^n \to \arg\max^{\ell} \mathbb{R}^L$ retrieves the top-$\ell$ clusters. To retrieve the top-$\ell$ clusters, $\tau$ first assigns a similarity score to each cluster by computing the inner product between $q$ and each $\mu_i$, and then returns the $\ell$ clusters with the highest scores.

Mathematically, $\tau$ can be represented as $\tau(q;\ M) = \arg\max^{(\ell)}_{i=1,\dots,L}(Mq)$, where $q \in \mathbb{R}^n$ and $M \in \mathbb{R}^{L\times n}$ whose $i$-th row is $\mu_i$. The search space for the final top-$k$ documents will be restricted to points contained in the top-$\ell$ clusters.

In this work, we propose to replace $\{\mu_i\}_{i=1}^L$ with learnt representative points $\{\nu_i\}_{i=1}^L$. To this end, we learn a routing function $\acute{\tau}(q;\ W) = Wq$, where $W \in \mathbb{R}^{L\times n}$, using LTR. $W$ will substitute $M$ in the original formulation.

In order to learn the linear function $W$, the training dataset consists of a set of pairs: $(q, (b_i)_{i=1}^L)$. Here, $q$ is a query point $\in \mathbb{R}^n$, and $(b_i)_{i=1}^L$ is a binary vector of length equal to the number of clusters, with exactly one element set to 1. The 1 is located in the $i$-th position corresponding to the $i$-th cluster, $c_i$, that contains the top-1 document for query $q$. $(b_i)_{i=1}^L$ represents the ground-truth for $q$.

To train $\acute{\tau}$ another necessary ingredient is to define a loss function. Given that we aim to maximize the Mean Reciprocal Rank (MRR), a metric well-suited for this task, the cross-entropy loss emerges as an appropriate choice. Notably, prior research, as demonstrated in [15] and [19], has established cross-entropy loss as a consistent surrogate for MRR under the assumption that each query has at most one relevant item with probability 1, as is the case in our setting.

For completeness, we provide the mathematical definitions of MRR and cross-entropy loss for a single query $q$. MRR is given by:

$$\mathrm{MRR}(\boldsymbol{q}) = \frac{1}{|\boldsymbol{q}|}\sum_{i=1}^{|\boldsymbol{q}|}\frac{1}{r(\boldsymbol{q}_i)}, \tag{5.1}$$

in which $|\boldsymbol{q}|$ is the cardinality of the query set, and $r(\boldsymbol{q}_i)$ represents the rank position of the first relevant item for the query $\boldsymbol{q}_i$. The cross-entropy loss (CE) for a single query $q$ is computed as:

$$l_{\mathrm{CE}}(\boldsymbol{s},\boldsymbol{b}) = -\sum_{i=1}^{L}\boldsymbol{b}_i \log \mathrm{softmax}(\boldsymbol{s})_i = -\sum_{i=1}^{L}\boldsymbol{b}_i \log\frac{\exp(\boldsymbol{s}_i)}{\sum_{j=1}^{L}\exp(\boldsymbol{s}_j)}, \tag{5.2}$$

whereby $\boldsymbol{s} = Wq = \acute{\tau}(q;\ W)$ and $\boldsymbol{b} = (b_i)_{i=1}^L$.

Specifically, our final objective function, which we aim to minimize to learn the function $\acute{\tau}$, is the cross-entropy loss across the entire training query set, defined as:

$$\mathcal{L}_{\mathrm{CE}}(S,B) = \frac{1}{N}\sum_{i=1}^{N} l_{\mathrm{CE}}(S_i, B_i), \tag{5.3}$$

where $S = (\boldsymbol{s}_i)_{i=1}^N = (Wq_i)_{i=1}^N$ and $B = (\boldsymbol{b}_i)_{i=1}^N$. $N$ is the number of samples in the training query set.

With the training query set and cross-entropy loss in place, coupled with the selection of an optimizer, we are now equipped to learn $\acute{\tau}$ and obtain the learnt representative points $\{\nu_i\}_{i=1}^L$.

### 5.2.1 Generalizing to Top-$k$

The foregoing provides a formal description of how to learn a function that, given a query, accurately identifies the cluster containing the top-1 document. This approach will be used throughout our experiments, demonstrating satisfactory performance not only in the 1-MIPS case but also in the 10-MIPS and 100-MIPS scenarios.

However, generalizing the learning approach for the routing function $\acute{\tau}$ to the top-$k$ problem with $k > 1$ is straightforward. We will now demonstrate why, by defining the training query set and loss function for this context.

The training query set consists of a collection of pairs: $(q, (b_i)_{i=1}^L)$, where $q$ represents a query, and $(b_i)_{i=1}^L$ is a binary vector. The $i$-th position of $(b_i)_{i=1}^L$ is set to 1 if and only if the $i$-th cluster contains at least one of the top-$k$ documents relevant to $q$. Formally, given a set $\mathcal{S}$ containing the top-$k$ data points for query $q$, the set of clusters that contain at least one element of $\mathcal{S}$ is defined as: $\{c_i \,|\, c_i \in \{c_i\}_{i=1}^L,\, c_i \cap \mathcal{S} \neq \emptyset\}$.

Regarding the cross-entropy loss function over the entire training query set, it can be updated following the formulation outlined in [15] as follows:

$$\mathcal{L}_{\text{CE}}^{\text{top}-k}(S, B) = -\frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{L}\frac{2^{B_{ij}} - \gamma_{ij}}{\sum_{z=1}^{L} 2^{B_{iz}} - \gamma_{iz}} \log \frac{\exp(S_{ij})}{\sum_{z=1}^{L}\exp(S_{iz})} \tag{5.4}$$

with $S$, $B$ and $N$ as defined in $\mathcal{L}_{\text{CE}}(S, B)$, and $\gamma$'s sampled uniformly from $[0, 1]$.

With this formulation, it is possible to learn a function $\acute{\tau}$ that, given a query, is trained to identify the partitions containing the top-$k$ documents, thus generalizing from the top-1 training case.

## 5.3 Experimental Setup

The following section presents the experimental setup used in this work.

#### Datasets

Three publicly available datasets were utilized for this research[2].

- MS MARCO [70]: Large scale MAchine Reading COmprehensive dataset focused on deep learning in search. It comprises of 8,841,823 short passages and 909,824 train queries.

- HotpotQA [102]: Large scale Wikipedia-based question answering dataset, comprising of 5,233,235 documents and 97,852 queries.

- FEVER [92]: Fact Extraction and VERification dataset consists of 5,396,138 documents and 13,332 queries.

[2] `https://ir-datasets.com`

### Embedding Models

To transform queries and documents into $n$-dimensional dense vectors, we employed embedding models. Specifically, we utilized the following Transformer-based Pre-trained Language Models (PLMs).

- `TAS-B`[3] [42]: The model projects text inputs into 768-dimensional dense vectors. A distinguishing feature of this model is the employment of balanced topic aware sampling.
- `Contriever`[4] [48]: The model outputs 768-dimensional dense vector representations of the input texts. Contrastive learning is the principal distinguishing technique in the model.
- `all-MiniLM-L6-v2`[5], `all-mpnet-base-v2`[6] and `all-distilroberta-v1`[7] [79]: Sentence transformer models that map text into dense vector spaces of dimensionality 384, 768, and 768, respectively. These models were obtained by fine-tuning a pre-trained base model[8] on a massive and diverse dataset comprising over 1 billion text pairs.

### Baseline

The baseline used for comparison with our learnt routing function is defined as follows: $\tau(q) = Mq$, where the rows of $M$ represent the centroids of the clusters returned by the clustering algorithm. In other words, to assess the effectiveness of our strategy, we compare the learnt representative points $\{\nu_i\}_{i=1}^{L}$ with the standard representative points $\{\mu_i\}_{i=1}^{L}$.

### Implementation Details

The routing function $\acute{\tau}$ is learnt via a linear neural network with a single input and output layer, no biases, and a final softmax activation function. The input layer has a dimensionality equal to that of the vector space in which the query and document points reside, while the output layer has a dimensionality equal to the number of clusters. The softmax activation function transforms the network's output into probability scores, allowing for the computation of the cross-entropy loss $l_{\text{CE}}$, Equation 5.2. To minimize the loss function, the Adam [53] optimizer is employed with a learning rate of $10^{-4}$. A batch size of 512 is used, and training is conducted for a maximum of 100 epochs. Upon training completion, the network weights $W$ correspond to the learnt representative points, resulting in the learnt routing function $\acute{\tau}(q; W) = Wq$, with $W \in \mathbb{R}^{L \times n}$.

The pipeline for obtaining learnt representative points and evaluating their effectiveness is as follows. First, a dataset and an embedding model are employed to transform

[3] `https://huggingface.co/sentence-transformers/msmarco-distilbert-base-tas-b`
[4] `https://huggingface.co/facebook/contriever`
[5] `https://huggingface.co/sentence-transformers/all-MiniLM-L6-v2`
[6] `https://huggingface.co/sentence-transformers/all-mpnet-base-v2`
[7] `https://huggingface.co/sentence-transformers/all-distilroberta-v1`
[8] `https://www.sbert.net/docs/sentence_transformer/pretrained_models.html`

queries and documents within the dataset into vector representations using the given embedding. Subsequently, a clustering algorithm is applied to partition the set of document vector points $\{d_i\}_{i=1}^{P} \subset \mathbb{R}^n$ into $L = \sqrt{P}$ clusters. In this study, we consider Standard KMeans, Spherical KMeans (implemented using the FAISS library [33]), and Shallow KMeans. Following clustering, for each query $q_i \in \mathbb{R}^n$ in the query set $\{q_i\}_{i=1}^{N} \subset \mathbb{R}^n$, we obtain the pair $(q_i, \boldsymbol{b}_i)$ as described in Section 5.2. The resulting set of pairs is divided into training (60%), validation (20%), and test (20%) sets. Finally, our neural network is trained on the training set, with the best model selected based on the loss function on the validation set. The learnt representative vectors $\{\nu_i\}_{i=1}^{L}$ and the standard representative points $\{\mu_i\}_{i=1}^{L}$ are evaluated on the test set.

### 5.3.1 Evaluation Metric

The learnt representative points $\{\nu_i\}_{i=1}^{L}$ and standard representative points $\{\mu_i\}_{i=1}^{L}$ are evaluated in terms of *top-k accuracy*. Top-$k$ accuracy is obtained by retrieving the top-$\ell$ partitions for each query $q$ based on the routing function, i.e., $\tau(q) = Mq$ for the baseline and $\acute{\tau}(q) = Wq$ for our method, and then computing the percentage of the top-$k$ documents contained within these top-$\ell$ partitions.

## 5.4 Experimental Results

In this section, we present the experimental results obtained by evaluating the performance of our proposed method, *Learnt*, against the standard clustering-based ANN search, *Baseline*. The evaluation is conducted on the datasets, embedding models, and clustering algorithms discussed in the previous section using the top-$k$ accuracy metric.

### 5.4.1 Top-1 Retrieval

Tables 5.1 and 5.2 represent the top-1 accuracy of the Baseline method, with standard representative points $\{\mu_i\}_{i=1}^{L}$, and the Learnt method, with learnt representative points $\{\nu_i\}_{i=1}^{L}$, on the MS MARCO, HotpotQA, and FEVER text datasets. Table 5.1 employs

Table 5.1: Top-1 accuracy of Baseline and Learnt methods using `all-MiniLM-L6-v2` on MS MARCO, HotpotQA, and FEVER datasets. Results are reported for Standard, Spherical, and Shallow KMeans clustering algorithms, considering top-$\ell$ partitions with $\ell$ equal to 0.1% and 1% of $L$.

| Dataset | Method | Standard | | Spherical | | Shallow | |
|---|---|---|---|---|---|---|---|
| | | 0.1% | 1% | 0.1% | 1% | 0.1% | 1% |
| MS MARCO | Baseline | 0.392 | 0.779 | 0.627 | 0.869 | 0.517 | 0.815 |
| | Learnt | 0.746 | 0.940 | 0.751 | 0.938 | 0.670 | 0.923 |
| HotpotQA | Baseline | 0.089 | 0.481 | 0.328 | 0.684 | 0.258 | 0.724 |
| | Learnt | 0.488 | 0.844 | 0.493 | 0.833 | 0.412 | 0.827 |
| FEVER | Baseline | 0.102 | 0.443 | 0.249 | 0.562 | 0.279 | 0.621 |
| | Learnt | 0.663 | 0.865 | 0.662 | 0.872 | 0.633 | 0.912 |

Table 5.2: Top-1 accuracy of Baseline and Learnt methods using `TAS-B` on MS MARCO, HotpotQA, and FEVER datasets. Results are reported for Standard, Spherical, and Shallow KMeans clustering algorithms, considering top-$\ell$ partitions with $\ell$ equal to 0.1% and 1% of $L$.

| Dataset | Method | Standard | | Spherical | | Shallow | |
|---|---|---|---|---|---|---|---|
| | | 0.1% | 1% | 0.1% | 1% | 0.1% | 1% |
| MS MARCO | Baseline | 0.480 | 0.835 | 0.680 | 0.915 | 0.553 | 0.869 |
| | Learnt | 0.727 | 0.936 | 0.724 | 0.933 | 0.612 | 0.896 |
| HotpotQA | Baseline | 0.258 | 0.724 | 0.372 | 0.783 | 0.345 | 0.756 |
| | Learnt | 0.525 | 0.882 | 0.507 | 0.867 | 0.405 | 0.797 |
| FEVER | Baseline | 0.235 | 0.675 | 0.314 | 0.690 | 0.303 | 0.704 |
| | Learnt | 0.836 | 0.930 | 0.834 | 0.925 | 0.819 | 0.917 |

the `all-MiniLM-L6-v2`, while Table 5.2 uses the `TAS-B` embedding. Standard, Spherical, and Shallow KMeans clustering algorithms are employed to generate partitions. For each algorithm, top-1 accuracy is measured considering the top 0.1% and 1% of clusters relative to the total number, i.e., $\ell = 0.1\% \times L$ and $\ell = 1\% \times L$.

Tables 5.1 and 5.2 clearly demonstrate that our proposed Learnt method consistently outperforms the Baseline. For instance, considering Standard KMeans with $\ell = 0.1\% \times L$, $\{\nu_i\}_{i=1}^{L}$ exhibit a significant accuracy improvement compared to $\{\mu_i\}_{i=1}^{L}$, achieving +90.3% on MS MARCO, +448.3% on HotpotQA, and +550.0% on FEVER when using `all-MiniLM-L6-v2`, and +51.5% on MS MARCO, +103.5% on HotpotQA, and +255.7% on FEVER when using `TAS-B`.

Additionally, analysis of the tables reveals a more pronounced difference in accuracy for $\ell = 0.1\% \times L$ compared to $\ell = 1\% \times L$. Generally, our results indicate that a smaller value of $\ell$ correlates with a larger gap in accuracy between the two methods, indicating that partitions closer to query points are of much higher quality. This is intuitively expected, as our learning objective is specifically tailored to identify and retrieve the top-1 cluster.

Another notable observation from the results is that, across clustering algorithms, the accuracy difference between the Learnt and Baseline methods is most marked for Standard KMeans, followed by Shallow KMeans, and is least marked for Spherical KMeans. These findings are not unexpected for Standard and Spherical KMeans, considering their distance metric used in the objective function. Standard KMeans utilizes the Euclidean distance (Equation 2.5), whereas Spherical KMeans utilizes the cosine distance (Equation 2.7), which is more suitable for a MIPS-based problem. On the other hand, interesting results are obtained for Shallow KMeans which performs remarkably well, despite its intrinsic simplicity (see Algorithm 3).

To further validate the effectiveness of our proposed method, Table 5.3 presents additional results on top-1 accuracy using various embedding models, namely `Contriever`, `all-mpnet-base-v2`, and `all-distilroberta-v1`, on MS MARCO, with $\ell$ set to 0.1 and 1 percent of the total number of clusters.

The results in Table 5.3 reaffirm our previous findings, including the key point that the Learnt method consistently outperforms the Baseline across all experimental settings.

When comparing Tables 5.2 and 5.3, which employ 768-dimensional embeddings, the

Table 5.3: Top-1 accuracy of Baseline and Learnt methods on the MS MARCO dataset using `Contriever`, `all-mpnet-base-v2`, and `all-distilroberta-v1` embedding models. Results are reported for Standard, Spherical, and Shallow KMeans clustering algorithms, considering top-$\ell$ partitions with $\ell$ equal to 0.1% and 1% of $L$.

| Encoding | Method | Standard | | Spherical | | Shallow | |
|---|---|---|---|---|---|---|---|
| | | 0.1% | 1% | 0.1% | 1% | 0.1% | 1% |
| `Contriever` | Baseline | 0.602 | 0.895 | 0.756 | 0.938 | 0.640 | 0.909 |
| | Learnt | 0.790 | 0.952 | 0.780 | 0.946 | 0.690 | 0.927 |
| `all-mpnet-base-v2` | Baseline | 0.763 | 0.952 | 0.794 | 0.958 | 0.691 | 0.940 |
| | Learnt | 0.818 | 0.967 | 0.819 | 0.966 | 0.733 | 0.951 |
| `all-distilroberta-v1` | Baseline | 0.752 | 0.955 | 0.779 | 0.960 | 0.664 | 0.935 |
| | Learnt | 0.807 | 0.967 | 0.806 | 0.966 | 0.706 | 0.945 |

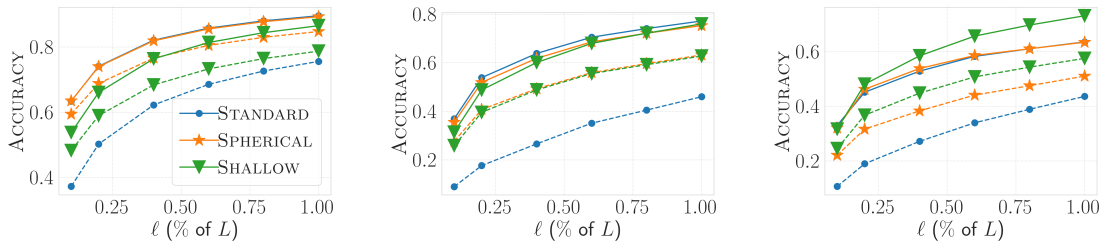
accuracy gap between Learnt and Baseline is less pronounced compared to Table 5.1, where 384-dimensional embeddings are used. This suggests that as the dimensionality of the embedding space increases, the Learnt method may face challenges in identifying significantly better representative points. A more in-depth investigation of this phenomenon is warranted in future research.

Finally, the McNemar's test [63] was conducted on all results, revealing a highly statistically significant difference between the Learnt and Baseline methods ($p$-value $< 0.001$), strongly supporting the superior performance of the learnt representative points.

### 5.4.2 Top-$k$ Retrieval

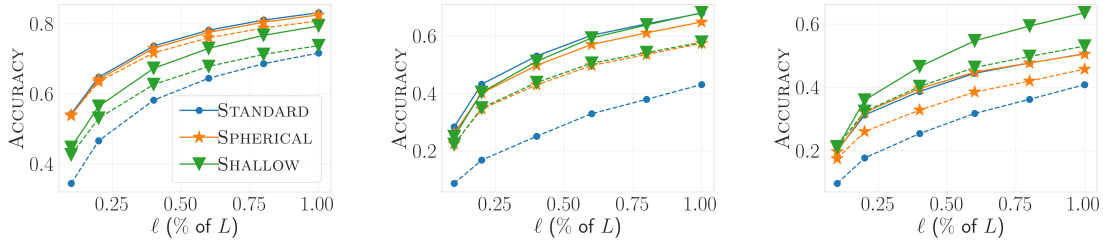
Until now, our analysis has focused on top-1 accuracy. We now turn our attention to top-$k$ accuracy, with $k > 1$. Figures 5.2 and 5.3 depict the obtained results for top-10 and top-100 accuracy, respectively, as a function of $\ell$.

The findings discussed in the previous subsection also hold for top-$k$ accuracy with $k > 1$: the Learnt method demonstrates superior performance compared to the Baseline,




(a) MS MARCO (b) HotpotQA (c) FEVER

Figure 5.2: Top-10 accuracy of Learnt and Baseline methods on MS MARCO, HotpotQA, and FEVER datasets using the `all-MiniLM-L6-v2` embedding model. The $x$-axis represents $\ell$, expressed as a percentage of $L$, while the $y$-axis represents the accuracy. Solid lines indicate the Learnt method, and dashed lines indicate the Baseline method.




(a) MS MARCO (b) HotpotQA (c) FEVER

Figure 5.3: Top-100 accuracy of Learnt and Baseline methods on MS MARCO, HotpotQA, and FEVER datasets using the `all-MiniLM-L6-v2` embedding model. The $x$-axis represents $\ell$, expressed as a percentage of $L$, while the $y$-axis represents the accuracy. Solid lines indicate the Learnt method, and dashed lines indicate the Baseline method.

especially for smaller values of $\ell$; and, the accuracy gap between the two methods is most pronounced for Standard, followed by Shallow, and finally, Spherical KMeans.

These results are particularly interesting given that our proposed method is specifically designed to optimize top-1 accuracy, where the goal is to identify the cluster associated with the top-1 document for a given query. Despite this, as is evident from Figures 5.2 and 5.3, our model demonstrates remarkable performance for top-$k$ accuracy as well.

These results, obtained for top-$k$ accuracy, are highly promising and point to a potential avenue for generalizing the loss function to the top-$k$ scenario, as detailed in Section 5.2.1, with the potential for further improved accuracy. A more in-depth exploration of this generalization is planned for future work.

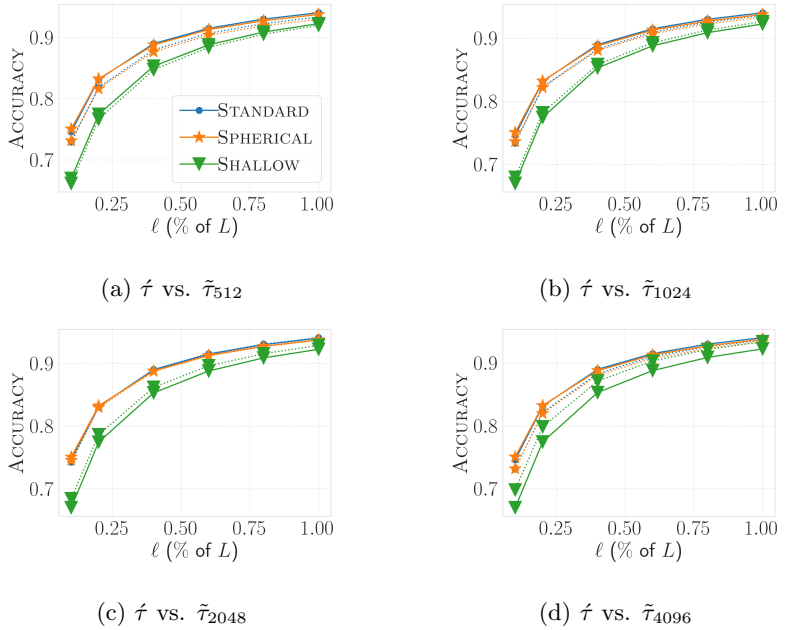
## 5.5 Further Analysis

Our objective was to learn a linear routing function, $\acute{\tau}$, to obtain representative points that best capture the content of the clusters. This allowed us to ensure that when a new query $q$, arrived, the inner product between the query and the learnt representative points would more accurately reflect the similarity between $q$ and the clusters. This, in turn, led to improved accuracy in retrieving the top-1 document or, more generally, the top-$k$ documents.

Let us now consider a scenario where our goal is not to learn new representatives but to focus solely on learning a routing function that, given a query, returns a score for each cluster corresponding to the likelihood of finding the top-1 document within that cluster. $\acute{\tau}$ emerges as a linear solution to this problem. However, what happens if we relax the assumption of linearity? By studying a nonlinear routing function, $\tilde{\tau}$, we will explore the impact of nonlinearity on solving this problem.

### 5.5.1 Nonlinearity

We explore and analyze the use of nonlinearity to solve the routing problem by defining a function, $\tilde{\tau}$, and comparing it to the linear routing function, $\acute{\tau}$.




(a) $\acute{\tau}$ vs. $\tilde{\tau}_{512}$ (b) $\acute{\tau}$ vs. $\tilde{\tau}_{1024}$

(c) $\acute{\tau}$ vs. $\tilde{\tau}_{2048}$ (d) $\acute{\tau}$ vs. $\tilde{\tau}_{4096}$

Figure 5.4: Top-1 accuracy of the learnt linear routing function, $\acute{\tau}$, and the learnt nonlinear routing function, $\tilde{\tau}$, on the MS MARCO dataset using the `all-MiniLM-L6-v2` embedding model. The $x$-axis represents $\ell$ as a percentage of $L$, while the $y$-axis represents the accuracy. Solid lines indicate $\acute{\tau}$, and dotted lines indicate $\tilde{\tau}$ variants with different hidden layer sizes: 512 (a), 1024 (b), 2048 (c), and 4096 (d).

$\tilde{\tau}$ is defined as a neural network with a structure similar to $\acute{\tau}$, but with some modifications: it includes a hidden layer, employs the ReLU activation function [2] in this layer, and incorporates biases in its neurons. For our analyses, we specifically consider four variants of $\tilde{\tau}$: one with 512 units in the hidden layer ($\tilde{\tau}_{512}$), one with 1024 units ($\tilde{\tau}_{1024}$), one with 2048 units ($\tilde{\tau}_{2048}$), and one with 4096 units ($\tilde{\tau}_{4096}$).

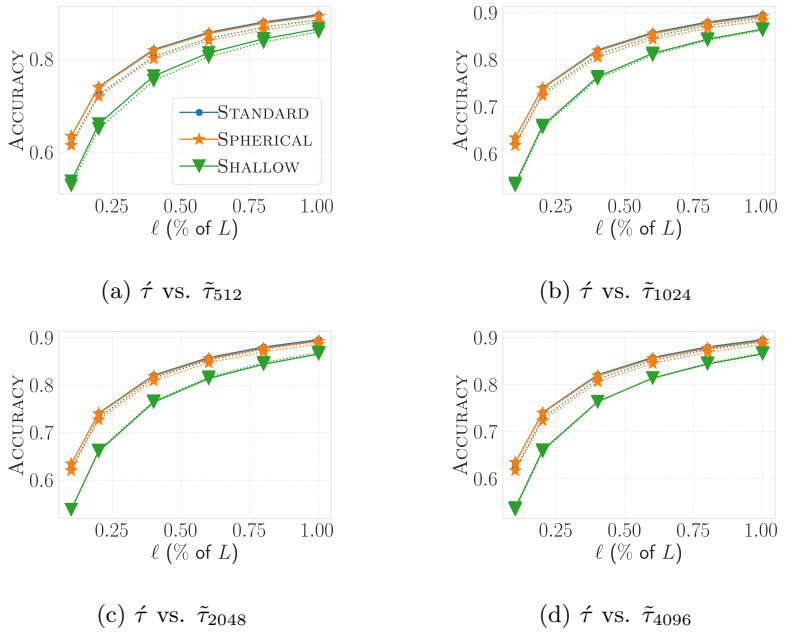
Figure 5.4 illustrates the top-1 accuracy for $\acute{\tau}$ and $\tilde{\tau}$ as a function of $\ell$, where $\ell$ varies between $0.1\% \times L$ and $1\% \times L$, on MS MARCO dataset using `all-MiniLM-L6-v2` as embedding model.

Figure 5.4 shows that, for the nonlinear routing function, considering both Standard and Spherical KMeans clustering algorithms, the best results are obtained with the $\tilde{\tau}_{2048}$ variant.

Focusing now on the comparison between $\tilde{\tau}_{2048}$ and $\acute{\tau}$ in terms of Standard and Spherical KMeans, it can be observed that despite the nonlinearity of $\tilde{\tau}_{2048}$, the two routing functions exhibit nearly identical accuracy results. Specifically, for lower values of $\ell$, $\acute{\tau}$ outperforms $\tilde{\tau}_{2048}$ by almost 1%.

For the Shallow KMeans clustering algorithm, however, the best performing variant of $\tilde{\tau}$ is $\tilde{\tau}_{4096}$. $\tilde{\tau}_{4096}$ achieves higher accuracy values compared to $\acute{\tau}$, with improvements of approximately 4.2% for $\ell = L/1000$ and 1.2% for $\ell = L/100$.

Analysis of the results indicates that nonlinearity does not provide significant improvements in terms of top-1 accuracy. Consequently, the learnt linear routing function, $\acute{\tau}$, emerges as the optimal choice over the nonlinear functions examined. This conclusion is supported by the higher accuracy values achieved by $\acute{\tau}$ in Spherical and Standard KMeans




(a) $\acute{\tau}$ vs. $\tilde{\tau}_{512}$ (b) $\acute{\tau}$ vs. $\tilde{\tau}_{1024}$

(c) $\acute{\tau}$ vs. $\tilde{\tau}_{2048}$ (d) $\acute{\tau}$ vs. $\tilde{\tau}_{4096}$

Figure 5.5: Top-10 accuracy of the learnt linear routing function, $\acute{\tau}$, and the learnt nonlinear routing function, $\tilde{\tau}$, on the MS MARCO dataset using the `all-MiniLM-L6-v2` embedding model. The $x$-axis represents $\ell$ as a percentage of $L$, while the $y$-axis represents the accuracy. Solid lines indicate $\acute{\tau}$, and dotted lines indicate $\tilde{\tau}$ variants with different hidden layer sizes: 512 (a), 1024 (b), 2048 (c), and 4096 (d).

clustering algorithms, as well as by the fact that the additional complexity associated with $\tilde{\tau}_{4096}$ in Shallow KMeans does not justify the relatively small improvement in accuracy. Considering only the number of parameters, $\tilde{\tau}_{4096}$ has 13,867,960 parameters, significantly more than the 1,155,000 parameters of $\acute{\tau}$.

Similar trends can be observed for the top-10 accuracy, as depicted in Figure 5.5. The only exception pertains to Shallow KMeans: the best results are achieved with the $\tilde{\tau}_{2048}$ variant rather than $\tilde{\tau}_{4096}$; moreover, the accuracy difference between $\tilde{\tau}_{2048}$ and $\acute{\tau}$ is narrower compared to the previous case. This further supports the argument in favor of $\acute{\tau}$ over $\tilde{\tau}$.

In conclusion, in light of the findings presented in this section, it can be concluded that the learnt linear routing function, $\acute{\tau}$, is the most suitable choice compared to the nonlinear functions examined. $\acute{\tau}$ offers the best balance of efficiency and effectiveness that is essential in the field of ANN search.

# Chapter 6

# Conclusions and Future Work

In this work, we have presented a new state-of-the-art for clustering-based ANN search. Our proposed approach involves learning a linear routing function via LTR to generate learnt representative points. These points provide a more accurate and semantically rich representation of each cluster, significantly improving ANN search accuracy.

To facilitate a comprehensive understanding of our method, we first have provided a detailed overview of clustering-based ANN search, starting from the fundamental concepts such as vector search, ANN search, and clustering. Subsequently, we have introduced LTR, focusing on the essential ingredients for learning a ranking function.

Having established a solid foundation, encompassing all the necessary elements for a thorough understanding of our method, we then have proceed to present our approach in detail, first providing an intuitive explanation and then a formal definition.

Our proposed method is grounded in an intuitive observation: The routing function, which determines the most promising clusters for a given query, solves a ranking problem. In other words, the routing function ranks clusters based on their relevance to the query, specifically by ranking them according to their probability of containing the query's nearest neighbor.

This insight has led us to an innovative solution: Learning the routing function via LTR. In particular, we learn a simple linear function where the parameters of the function represent the new representative points for each cluster, more informative and discriminative than the standard representative points. It is noteworthy how straightforward it has been to prepare the necessary ingredients for learning the routing function, from the dataset to the loss function.

Through extensive experiments conducted on diverse datasets, embedding models, and clustering algorithms, we have empirically demonstrated that our proposed method consistently outperforms the baseline, significantly improving the accuracy of MIPS-based clustering-based ANN search. The learnt representative points, compared to standard representative points, enable the retrieval of top-$\ell$ partitions containing the top-1 or top-$k$ documents for a given query with significantly higher accuracy.

Furthermore, we have conducted additional investigations into learning the routing function by relaxing the linearity assumption and learning a nonlinear routing function, with the sole purpose of returning the top-$\ell$ partitions for a given query. Our findings have revealed that the learnt linear routing function emerged as the optimal choice, offering the

best balance between efficiency and effectiveness compared to the learnt nonlinear routing functions analyzed.

In summary, the proposed method emerges as a conceptually simple and the state-of-the-art approach for clustering-based ANN search. Moreover, by developing this method, we have demonstrated the potential of integrating two important fields of IR, LTR and ANN. Additionally, we have showcased the potential of learning representative points for groups of elements, an idea that can be extended to various domains.

Equally exciting is the fact that this work has also raised numerous questions for future research. These include generalizing the learning approach for the routing function to the top-$k$ problem, with $k > 1$, as discussed in Section 5.2.1; extending the method to other distance functions such as Euclidean distance, cosine distance, or Manhattan distance; investigating the influence of vector dimensionality of queries and documents on the accuracy of our method; and finally, exploring the new area of query-aware clustering for ANN search, where the document space is clustered using the query dataset.

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