RESEARCH STATEMENT

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1 PROJECT MOTIVATION

The past decade has seen significant advances in machine learning (ML) and a surge in ML applications to various domains, such as Natural Language Processing (Bubeck et al., 2023; Brown et al., 2020), Computer Vision (Radford et al., 2021; Krizhevsky et al., 2012), Graph Neural Networks (Kipf & Welling, 2017; Rossi et al., 2020). The core idea behind the success of these methods is the ability to construct a mapper $f(x)$ that maps raw data into embeddings high dimension vector. This embedding can be understood as a point in latent space. For example, to encode the semantics of words in the English vocabulary, models learn the representation and embedding of each word in the form of a vector, which can be represented in latent space, Figure 1.

To classify an image as a cat or dog, CNNs are trained to learn a meaningful presentation of an image in latent space. To predict a property of the chemical compound CH_4, GNNs are used to learn the entire structure and properties of a C, H in unified embeddings in latent space, which can be used to infer prediction. Given advanced representation learning, one can use ML models to learn representations of products in e-commerce markets and store these representations in the geometric database, which can later be used as a recommended system (Xu et al., 2020) Motivated by this, the goal of this project is to explore the practical time complexity of two geometric data structures in modeling high-dimensional data.

2 METHODOLOGY

We selected two well-known geometric data structures, the KD tree (Bentley, 1975) and the Ball tree (Dolatshah et al., 2015), to explore the practical time complexity of geometric structures in the modeling of high-dimensional data. Both are intended to organize points in higher-dimensional space, with their structure intended to speed up spatial queries such as nearest neighbors. A KD Tree is similar to a binary search tree but in multiple dimensions. At each node, the data is split by the median value of one of the points' dimensions, alternating dimensions with each level. This structure accelerates spatial queries by pruning branches that are too far away. The Ball Tree is similar in the goal of handling multidimensional points, but different in its implementation. It organizes points into nested hyper spheres (ie "balls). It begins by defining one ball around all the points, and then recursively splits the remaining points between two balls until it reaches the defined base case. By checking the ball's boundaries, spatial queries can quickly skip entire sub trees if their ball can not contain a closer point, speeding up traversals. They make sense to compare since they are trying to solve the same problem of efficient spatial searches but are making different trade-offs. The KD Tree works best in lower dimensions and when points are evenly spread out because their axis-aligned splits are easy to compute. However, they struggle in higher dimensions as the "curse of dimensionality" leads to the number of required splits growing exponentially with the number of dimensions. Ball Trees, on the other hand, are more capable of working with higher dimensional data as their sphere shape splits do not rely on-axis alignment. The trade-off to this is that constructing and querying ball trees is more computationally expensive because calculating distances with centroids is more difficult than the KD tree's straight line cuts. Overall, they are directly comparable data structures that are very different in terms of implementation.

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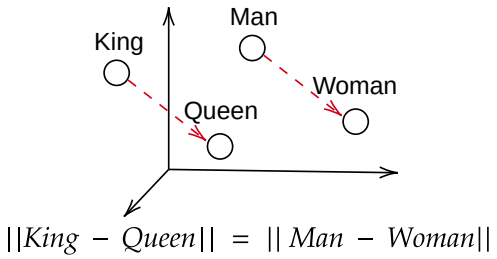

Figure 1: An example of representations of English words. Advancements in ML allow learning representations as high-dimension vectors (embeddings) that reserve semantic information for each word). In this example, the distance and direction of vector $\overrightarrow{KingQueen}$ is relatively the same as vector $\overrightarrow{ManWomman}$

We intend to fully implement KD-tree, Ball tree, and a simple brute force algorithm into a unified framework and test their insert, delete, range search, nearest neighbour, and construction operations. We plan on testing them with both low-dimension data (2D-5D) and higher-dimension data (50D-100D) as well as with sparse and non-sparse data to get a complete picture of their performance. We plan to obtain these data from synthetic data generated by us or from benchmark data used by Huang & Tung.

3 Expected outline

1. Abstract
2. Introduction
3. Related works
4. Notation and Preliminaries
5. Methodology
   (a) KD-tree
   (b) Ball tree
6. Results
7. Discussion

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