Supervised Learning Approach to Approximate Nearest Neighbor Search

Ville Hyvönen,1,2 Elias Jaäsaari,3 Teemu Roos,1,2
1Department of Computer Science, University of Helsinki, Finland
2Helsinki Institute for Information Technology (HIIT), Finland
3Kvasir Analytics Ltd, Cambridge, UK
ville.o.hyvonen@gmail.com, elias@kvasira.com, teemu.roos@cs.helsinki.fi

Abstract

Approximate nearest neighbor search is a classic algorithmic problem where the goal is to design an efficient index structure for fast approximate nearest neighbor queries. We show that it can be framed as a classification problem and solved by training a suitable multi-label classifier and using it as an index. Compared to the existing algorithms, this supervised learning approach has several advantages: it enables adapting an index to the query distribution when the query distribution and the corpus distribution differ; it allows using training sets larger than the corpus; and in principle it enables using any multi-label classifier for approximate nearest neighbor search. We demonstrate these advantages on multiple synthetic and real-world data sets by using a random forest and an ensemble of random projection trees as the base classifiers.

Introduction

In \(k\)-nearest neighbor (\(k\)-nn) search, \(k\) points that are nearest to the query point are retrieved from the corpus. Approximate nearest neighbor search is used to speed up \(k\)-nn search in applications where fast response times are critical, such as in computer vision, robotics, and recommendation systems.

Traditionally, approximate nearest neighbor search is approached as a problem in algorithms and data structures. Space-partitioning methods—trees, hashing, and quantization—divide the space according to a geometric criterion. For instance, \(k\)-d trees (Bentley 1975) and principal component trees (McNames 2001) are grown by hierarchically partitioning the space along the maximum variance directions of the corpus. Graph methods, such as HNSW (Malkov and Yasamin 2018), approximate a \(k\)-nn graph of the corpus, and use greedy graph traversal to retrieve the approximate nearest neighbors of the query point.

In this paper, we propose a machine learning-based approach to approximate nearest neighbor search. The key idea is to fit a multi-label classification model to the set of training queries so that the classifier learns to predict the nearest neighbors among the corpus given the query point. This model is then used as an index structure to retrieve the nearest neighbor candidates for a new query point.

There are several advantages to our approach. First, current algorithms use unsupervised criteria, such as maximizing the variance (Bentley 1975; McNames 2001) or minimizing the reconstruction error (Jegou, Douze, and Schmid 2010), to optimize the index structure. Since there is a precisely defined correct output—the true nearest neighbors of a query point—we can use a supervised algorithm to learn the index. As expected, our experiments show that using supervised information results in a faster index.

Second, by explicitly formulating approximate nearest neighbor search as a statistical estimation problem, we can make the crucial distinction between the distributions of the query points and the corpus points. The corpus defines the correct output of the algorithm, and thus is a part of the problem definition. By adapting an index structure to the corpus, traditional approximate nearest neighbor algorithms implicitly assume that, in addition to defining the problem, the corpus is also a representative sample of the query distribution. However, we argue that in most use cases, this is actually an unrealistic assumption. For instance, Kvasir (Wang et al. 2016) recommends users web pages similar to the ones they are currently browsing. Its corpus consists of web pages only from certain domains, such as Wikipedia, whereas the query may be any website. The query distribution is sharply concentrated on the most popular pages, and has a long tail.

Modeling the query distribution separately from the corpus distribution enables learning a more efficient index structure when these distributions are different. If the query distribution is finite, constant time queries can be achieved by memorizing the true nearest neighbors of each possible query point. More realistically, as in Kvasir, the queries may have a continuous, but uneven, distribution. In this scenario, it seems natural that an index structure should adapt to the query distribution by concentrating most of the effort to its high density areas.

Another advantage of making the distinction between the corpus and the training set of the algorithm is that using a distinct training set drawn from the query distribution allows leveraging large training sets. If a new data point is added to the corpus, it changes the problem by adding a new potential nearest neighbor for the query points. This means that if we fit the model to the corpus, the training set size is fixed for the given approximate nearest neighbor problem. But if the model is fit to a set of training queries instead of the corpus,
it allows increasing the training set size even beyond the size of the corpus.

The prevailing approach to assessing the performance of approximate nearest neighbor algorithms (see e.g. Aumüller, Bernhardsson, and Faithfull 2019) masks both of the advantages of using a distinct training set. A current practice is to split a data set into the corpus, on which the index is built, and the set of test queries, on which the performance of this index is measured. In this setting it makes sense to use the corpus as a training set of the algorithm, since both the corpus and the test set are random samples from the same data set, and thus draws from the same distribution. Furthermore, in this setting no separate set of training queries is available.

In the next section, we show how approximate nearest neighbor search can be formulated as a multi-label classification problem, and propose a generic algorithm, called an approximate nearest neighbor classifier (ANNC), for using any multi-label classifier as an index structure for the approximate nearest neighbor search. Then, as a specific example, we use a random forest (Breiman 2001) and an ensemble of random projection (RP) trees (Dasgupta and Freund 2008) as a classifier.

Finally, we test the performance of both the random forest version and the RP tree version of ANNC in three different scenarios: in the classical setting; when a separate set of training queries is available; and when the corpus and query distributions are different. Our experiments show that even when the corpus and the query points are drawn from the same distribution, the random forest version of ANNC is competitive with the state-of-the-art algorithms. With different corpus and query distributions, our proposed technique outperforms all other algorithms by a large margin. In addition, we find that the performance of ANNC improves as larger training sets are used.

**Related work**

The majority of index structures for approximate nearest neighbor search can be classified into one of four categories: locality-sensitive hashing (Andoni and Indyk 2008); graphs, such as hierarchical navigable small world (HNSW) graphs (Malkov and Yashunin 2018) and optimized nearest neighbor graphs (ONNG) (Iwasaki and Miyazaki 2018); quantizers, used for example in inverted file product quantization (IVF-PQ) (Jegou, Douze, and Schmid 2010), and space-partitioning trees, such as k-d trees (Bentley 1975) and random projection (RP) trees. According to a recent comparison (Aumüller, Bernhardsson, and Faithfull 2019), graphs currently achieve the best recall-query time trade-off of these options: HNSW and ONNG are the fastest algorithms with similar performance.

In a more general algorithmic context, Kraska et al. (2018) have recently suggested improving the performance of classic index structures, such as hash maps and B-trees, by considering them as models that can be estimated from training data. The applications include learned B-trees (Kraska et al. 2018), adaptive Bloom filters (Mitzenmacher 2018), and database systems that adapt to queries (Kraska et al. 2019).

In the context of the approximate nearest neighbor search, we are aware of only a few articles that suggest using supervised information to optimize the index structures. The use of training queries was first suggested by Maneewongvatana and Mount (2002). They used a sample from the query distribution to choose the optimal split points for a k-d tree. Later, Cayton and Dasgupta (2008), considered approximate nearest neighbor search as a learning problem, and applied learning techniques to improve the back-tracking search in a single k-d tree (Arya et al. 1998) and locality-sensitive hashing. However, k-d trees and LSH have since been superseded by the more efficient algorithms (see e.g. Aumüller, Bernhardsson, and Faithfull 2019 for performance comparisons).

More recently, Dong et al. (2019) have used logistic regression and shallow neural networks to grow trees that approximate balanced graph partitioning, but they do not present a concrete approximate nearest neighbor algorithm. Baranchuk et al. (2019) use a sample of training queries to approximate optimal routing in a nearest neighbor graph to reduce the number of distance computations required in the special case $k = 1$.

Jääsaari, Hyvönen, and Roos (2019) formulate hyper-parameter optimization of approximate nearest neighbor search as an estimation problem, and demonstrate how a statistical model can be used to automatically tune the hyper-parameters of a tree-based nearest neighbor index.

To summarize, the use of training queries to optimize index structures has been suggested earlier. However, we take the supervised learning approach further: instead of only using training queries to improve the performance of existing index structures, we formulate approximate nearest neighbor search as a multi-label classification problem, so that any classifier can be used as an index. This allows leveraging the vast existing literature on classification algorithms.

**Classification problem**

In this section we first review the classic formulation of approximate nearest neighbor search. We subsequently show how it can be framed as a supervised learning problem.

**Approximate nearest neighbor search**

Denote the corpus points by $c_1, \ldots, c_m$, $c_i \in \mathbb{R}^d$ for all $i = 1, \ldots, m$, and the query point by $x \in \mathbb{R}^d$. Given a dissimilarity measure $\text{dis}(u, v) : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$, denote the set of indices of the $k$ nearest neighbors of the query point in the corpus by $f(x) = \{f_1(x), \ldots, f_k(x)\}$.

The goal of approximate nearest neighbor search is to find $k$ corpus points that are not necessarily the $k$ nearest neighbors of the query point, but are close to the query point with a high probability; denote the indices of these approximate nearest neighbors by $\hat{f}(x) = \{\hat{f}_1(x), \ldots, \hat{f}_k(x)\}$.

The quality of the approximation can be measured by the error rate

$$\text{Err}(x) = \frac{1}{k} |f(x) \setminus \hat{f}(x)|,$$

which is the proportion of the true nearest neighbors missed, or equivalently, by the recall $\text{Rec}(x) = 1 - \text{Err}(x)$, which is the proportion of the true nearest neighbors found.

In addition to the error rate or recall, the query time $\text{Time}(x)$ has to be considered when assessing performance.
of an algorithm, since the aim is to find the approximate solution significantly faster compared to brute force search. Typically, the performance of an approximate nearest neighbor algorithm is measured by the trade-off between recall and query time on a set of test queries; see e.g. [Aumüller, Bernhardsson, and Faithfull (2019) or Li et al. (2019)].

Learning problem

For many approximate nearest neighbor algorithms, a query consists of two phases: candidate set generation and exact \( k \)-nn search in the candidate set. First, an index structure is used to choose a subset of the corpus points. Then the points of this candidate set, which we denote by \( S(x) \), are re-ranked according to their true distances from the query point \( x \), and the \( k \) closest points are returned.

For instance, locality-sensitive hashing (Andoni and Indyk 2008) hashes the corpus with several hash functions that have the property that the probability of collision is high for points that are near each other, and then uses the union of the buckets the query point is hashed into as a candidate set. The MRPT algorithm (Hyvönen et al. 2016) grows a forest of random projection trees using the corpus points; and then, for the vote threshold \( v \), chooses into the candidate set the corpus points that belong to the same leaf as the query point in at least \( v \) trees.

However, instead of partitioning the space guided by geometrical intuition, we take a more principled approach: we fit a statistical model that takes a query point as input, and outputs for each corpus point the estimated probability that it belongs to the \( k \) nearest neighbors of the query point. The candidate set then consists of the corpus points with the highest estimated probabilities.

The input variable of the model is the query point \( X \), which is a \( d \)-dimensional random vector. The output variable \( f(X) = \{f_1(X), \ldots, f_k(X)\} \subset \{1, \ldots, m\}^k \) is the set of the indices of the \( k \) nearest neighbors of the query point. This means that we have a multi-label classification problem with \( m \) labels and the additional constraint that there are always a fixed number \( k \) of correct labels. In the special case of 1-nn search, the problem reduces to multiclass classification with \( m \) classes.

Using dummy encoding, the output variable can be written as a \( m \)-dimensional random vector \( Y = (Y_1, \ldots, Y_m) \), where, for each \( j = 1, \ldots, m \),

\[
Y_j = \begin{cases} 
1, & \text{if } c_j \in f(X), \\
0, & \text{otherwise.}
\end{cases}
\]

In other words, the response variable is a \( m \)-component binary vector in which \( k \) bits are set.

To train the model, assume that we have an i.i.d. sample \( x_1, \ldots, x_n \) from the query distribution \( D \). If we do not have a separate training set of queries, we can use the corpus points \( c_1, \ldots, c_m \) as the training queries. However, by doing so, we make a strong assumption that the query points and the corpus are drawn from the same distribution.

The brute force search to find the correct labels \( y_1, \ldots, y_m \), where \( y_i = (y_{i1}, \ldots, y_{im}) \), can be done in linear time. We can then use \( (x_i, y_i), i = 1, \ldots, n \) as a training set.

After fitting the model, we can use it to predict the probabilities \( p_1, \ldots, p_m \), where

\[
p_j := P(Y_j = 1 \mid X = x),
\]

for a new query point \( x \). The estimated probabilities \( \hat{p}_1, \ldots, \hat{p}_m \) can then be used to pick the candidate set

\[
S(x) = \{ j \in 1, \ldots, m : \hat{p}_j > \tau \},
\]

for a threshold parameter \( \tau \in [0, 1] \).

Instead of the probability estimates, we can also use the unnormalized probabilities, or, more generally, the values \( p_1^*, \ldots, p_m^* \) of a score function, to pick the candidate set

\[
S(x) = \{ j \in 1, \ldots, m : p_j^* > \tau^* \}
\]

for the corresponding threshold parameter \( \tau^* \).

The optimal threshold parameter \( \tau \) can be chosen based on desired properties. The exact form of the loss function depends on the application, but we assume that the decision problem is either maximizing recall for a given running time budget, or vice versa:

1. Bound expected query time \( E[\text{Time}(X)] < t \) for \( t \in (0, \infty) \), and maximize expected recall.
2. Bound expected recall \( E[\text{Rec}(X)] \geq r \) for \( r \in [0, 1] \), and minimize expected query time.

The expectations are over the query distribution \( D \); over the randomness of the algorithm, if a randomized algorithm is used; and, in the case of query time, also over the random variation that depends on the computing environment.

Recall for a query point \( x \) can be written as the proportion of the true nearest neighbors included the candidate set:

\[
\text{Rec}(x) = \frac{1}{k} |f(x) \cap S(x)|.
\]

Correspondingly, we define precision for a query point \( x \) as the proportion of the candidate set that belongs to the set of the true \( k \) nearest neighbors:

\[
\text{Prec}(x) = \frac{1}{|S(x)|} |f(x) \cap S(x)|.
\]

The running time of the first part of the query, that is, the time it takes to compute the model fit for a new query point, does not depend significantly on the query point. Thus, given the model, query time depends mainly only on the final brute force search time. The exact search time is dominated by the distance computation time that is linear on the candidate set size \( |S(x)| \). Hence, given the model, optimizing the recall-query time trade-off means optimizing the precision-recall trade-off on the candidate set; that is, picking the optimal threshold parameter \( \tau \) from the precision-recall curve.

**Algorithm 1** Query phase of the ANN C method

```
1: procedure QUERY(x, \tau)
2: \( \tilde{p}_1, \ldots, \tilde{p}_m \leftarrow \text{PREDICT}(x) \)
3: \( S(x) \leftarrow \{ j \in 1, \ldots, m \} : \tilde{p}_j \geq \tau \}
4: return \( k \)-nn of \( x \) from \( S(x) \)
```
The query phase for a new query point \( x \) is described in Algorithm 1. The threshold parameter \( \tau \) is a tunable hyper-parameter. The function \textsc{predict} is a classifier that has been trained offline. In principle, any multi-label classifier can be used; in practice, the classifier has to scale to a large set of labels and be able to classify a new point quickly. We will describe our choice of classifier in the next section.

Algorithm

In this section we describe the two specific models we use to solve the multi-label classification problem presented in the previous section. First we consider a random forest, that is, an ensemble of classification trees (Breiman et al. 1984). To speed up index building, instead of an ensemble of classification trees, we also consider an ensemble of random projection (RP) trees. The RP tree version is an intermediate step between the traditional approximate nearest neighbor algorithms and our classification approach: a distinct training set can be used to grow the trees instead of the corpus, but the trees are still grown in an unsupervised fashion.

Classification trees

Since the number of labels equals the corpus size, to be feasible for approximate nearest neighbor search, in addition to scaling with respect to the training set size and dimension, a classifier has to also scale to millions of labels. Therefore, instead of global parametric models—such as logistic regression or neural networks—that explicitly output the probability estimates for each of the labels, we consider classification trees. Classification trees have the advantage that they output only the non-zero probability estimates.

We grow a classification tree for multi-label classification in exactly the same way as a classification tree for multi-class classification; the only difference is in the final classification decision. Denote by \( N \) the set of indices of the training set points that belong to the current node. Starting from the root \( N = \{1, \ldots, n\} \), the node is split into the child nodes \( N_l := \{i \in N : x_{iw} \leq s\} \) and \( N_r := \{i \in N : x_{iw} > s\} \) by choosing the split dimension \( w \in \{1, \ldots, d\} \) and the split point \( s \) that minimize the combined node impurity measure \( Q \) of the child nodes. More precisely, we weight the impurities of the children by their sizes, add the weighted values, and subtract the sum from the impurity of the parent; this is called the gain of the split:

\[
\text{Gain}(w, s) = Q(N) - \left( \frac{|N_l|}{|N|} Q(N_l) + \frac{|N_r|}{|N|} Q(N_r) \right).
\]

We then choose the split \((\hat{w}, \hat{s})\) that maximizes the gain. The splitting process is continued recursively at each branch, until the maximum inner node size \( n_0 \) is met, or no split that further decreases node impurity is found.

We use the cross-entropy

\[
CE(N) = - \sum_{j=1}^{m} \hat{p}_j \log \hat{p}_j
\]

1The maximum of the number of split points with unique values of the impurity measure at each dimension is \(|N| - 1\), where \(|N|\) is the number of the training set points in the node.

as the impurity measure \( Q \) that is minimized greedily. Here

\[
\hat{p}_j := \frac{|\{i \in N : j \in f(x_i)\}|}{k|N|}
\]

is the proportion of the training set points of this node that belong into \( j \)-th class—in our application the proportion of the training set points for which the corpus point \( c_j \) belongs into their \( k \) nearest neighbors—normalized by the number of neighbors searched.

Random forest

A random forest is an ensemble of randomized classification trees. Different randomization methods can be used simultaneously: Breiman (2001) on the one hand grows each tree on its own bootstrap sample of the data, and on the other considers only randomly chosen \( p < d \) dimensions when choosing the optimal split dimension at each node. We use only the latter of these randomization methods and always choose \( p = \sqrt{d} \) in our experiments.

When classifying a new point \( x \), in our application a new query point, it is first routed into a leaf in all \( T \) trees. For the \( t \)-th tree, we denote the set of indices of the training set points of this leaf by \( N_t \). Then, for each class \( j = 1, \ldots, m \), we add the counts of the leaf points belonging into that class over the trees:

\[
p_j^* = \sum_{t=1}^{T} |\{i \in N_t : j \in f(x_i)\}|
\]

The counts could also be normalized into estimates for the class probabilities:

\[
\hat{p}_j = \frac{p_j^*}{k \sum_{t=1}^{T} |N_t|}.
\]

Finally, we label the new data point into the classes that have at least \( v \) counts, where the threshold \( v \) is a tuning parameter. In our application this translates into choosing the corresponding corpus points into the candidate set.

Random projection trees

At the root node of an RP tree the training set is projected onto a \( d \)-dimensional random vector. The training set is then split into two child nodes at the median of the projected training set points. The splitting process is continued recursively until the maximum inner node size \( n_0 \) is reached at each branch. We save the observed counts of the labels of the training set points in each leaf node. An ensemble of RP trees is used for classification exactly as a random forest.

In the original RP trees (Dasgupta and Freund 2008) the components of the random vectors are drawn from the standard normal distribution \( N(0, 1) \). We use the sparse variant (Hyvönen et al. 2016) where random vector components are non-zero with probability \( 1/\sqrt{d} \) (the non-zero components are drawn from \( N(0, 1) \)) and the same random vector is used for each branch at the same tree level.

RP trees have been used for approximate nearest neighbor search by Dasgupta and Sinha (2015) and Hyvönen et al.
Our version has two key differences. First, we partition the space using a set of training queries instead of the corpus points. Second, instead of the indices of leaf points itself, we store their labels, in this case the indices of their \( k \) nearest neighbors; thus using an ensemble of RP trees as a general purpose classifier instead of a specialized data structure for nearest neighbor search.

Both RP and classification trees can be grown using a different value of \( k \) than the number of neighbors searched; denote the value used for growing by \( k' \). In our experiments we noticed that it is sometimes beneficial to use a slightly higher value to grow the trees, for instance \( k' = 10 \) when \( k = 1 \), and \( k' = 50 \) when \( k = 10 \). Note that the MRPT algorithm introduced by [Hyvonen et al. (2016)] is a special case of the RP tree version of ANNC where the corpus is used as a training set and \( k' = 1 \).

Both the random forest and random projection tree versions of ANNC require that the exact nearest neighbors for each training point are known before index construction. Finding these nearest neighbors using brute force in \( O(nmd) \) time can be costly on large data sets. However, a significant speedup can be achieved by using another approximate nearest neighbor search algorithm—such as MRPT—that has fast index construction and automatic hyperparameter tuning, to find these nearest neighbors. Our initial results suggest that using an index tuned to 95% recall to find the nearest neighbors decreases the index construction time significantly without affecting performance.

Experiments

We first compare ANNC to state-of-the-art approximate nearest neighbor algorithms in the classical setting, where the data set is randomly divided into a corpus and a set of test queries. Next, we test the effect of training set size on the performance of ANNC. Finally, we compare the algorithms in the setting where the corpus and the query points are drawn from different distributions.

The compared algorithms are HNSW, which according to an independent benchmarking project ANN-benchmarks[^5] (Aumüller, Bernhardsson, and Faithfull 2019) is currently (tied with ONNG) the fastest algorithm for ANN search; IVF-PQ, which is the fastest quantization-based algorithm; and MRPT[^6], which is (tied with Annoy[^7]) the fastest tree-based algorithm. For HNSW and IVF-PQ we use the implementations in the FAISS library[^8]. We use our own implementations of random forest and random projection trees for ANNC. The compared algorithms are all written in C++ and compiled with similar optimizations. All queries are performed using a single thread.

For brevity, we present results only for \( k = 10 \). We also ran all of the experiments with \( k = 1 \) and \( k = 100 \), and the results were similar to the ones shown here.

We use the query time-recall trade-off to measure the performance of the algorithms. The Euclidean distance is used as a dissimilarity measure to determine the true nearest neighbors on all the data sets. To optimize the hyperparameters, we run a grid search over the hyperparameter space (for algorithms other than our own, we use the same hyperparameters as those in ANN-benchmarks). We use a test set of 100 query points is used in all experiments.

### Table 1: Data sets used in the experiments

| Data set   | corpus size | dim | type      |
|------------|-------------|-----|-----------|
| MNIST      | 60000       | 784 | image     |
| Fashion    | 60000       | 784 | image     |
| STL-10     | 100000      | 9216| image     |
| GIST       | 100000      | 960 | image descriptors |
| Crawl      | 20000       | 300 | word embeddings |
| SIFT       | 100000      | 128 | image descriptors |
| Gaussian a-c | 100000  | 500 | synthetic |
| Clusters   | 100000      | 500 | synthetic |

#### Classical setting

We first compare the algorithms in a typical ANN performance evaluation setting by dividing the tested data set randomly into a corpus and a set of test queries, so that both the corpus and the test set are i.i.d. draws from the same distribution. This means that we train the classifiers using ANNC using the corpus as the training set since no other training set is available. We use four common benchmark data sets (MNIST[^2], Fashion[^3], GIST[^4], and STL-10[^1]) consisting of raw and preprocessed images and text. The specifications of the data sets of all the experiments are shown in Table 1.

The results for optimal parameters on the four data sets are shown in Figure 1. Even though no training set besides the corpus is used, the random forest version of ANNC (ANNC-RF) is faster than both IVF-PQ and MRPT. ANNC-RF is also faster than HNSW on STL-10, and close to HNSW on all of the other data sets.

In addition, on all four data sets, the random forest version is faster than the random projection tree version (ANNC-RP). This suggests that using the supervised approach indeed boosts the performance of the algorithm. However, the RP tree version is faster to train, so it can be used to approximate the random forest version on large data sets. Note that since MRPT is a special case of ANNC-RP, its performance should always be equal or worse than that of ANNC-RP.

#### Effect of training set size

Even if the query distribution matches that of the corpus, it is possible to exploit more training data drawn from the same distribution to create training sets that are even larger than the corpus. We expect that increasing the training set size makes the base classifier more accurate and thus improves the performance.

\[^2\]https://github.com/erikbern/ann-benchmarks
\[^3\]https://github.com/vioshyvo/mrpt
\[^4\]https://github.com/spotify/annoy
\[^5\]https://github.com/facebookresearch/faiss

[^1]: http://corpus-texmex.irisa.fr
[^2]: http://corpus-texmex.irisa.fr
[^3]: http://corpus-texmex.irisa.fr
[^4]: https://github.com/zalandoresearch/fashion-mnist
[^5]: http://yann.lecun.com/exdb/mnist
[^6]: https://github.com/vioshyvo/mrpt
[^7]: https://github.com/erikbern/ann-benchmarks
[^8]: https://cs.stanford.edu/~acoates/stl10
Figure 1: Recall vs. query time (log scale) in the classical setting.

To test this hypothesis, we train all the algorithms using only the corpus, and in addition train ANNC-RF using two larger training sets. We use the SIFT corpus which has 100 000 points, with training sets of 1000 000 and 10 000 000 points, and the Crawl corpus which has 20 000 points, with training sets of 200 000 and 1 999 000 points.

The results, shown in Figure 2, seem to confirm the above hypothesis: using larger training sets improves the query time-recall trade-off for both data sets. It also seems that the performance could be further improved by using even larger training sets at the cost of increased training time and memory consumption.

**Different query distribution**

The most significant benefits of our approach are expected in situations where the query and corpus distributions are different. As the difference between the distributions grows larger, the performance difference between the traditional algorithms and our proposed method should become greater.

To test this hypothesis, we create three synthetic data sets (Gaussian a–c) with varying degrees of concentration of the query distribution. For all data sets the corpus of 100 000 points is drawn from the 500-dimensional uniform distribution on the interval (−10, 10). The training set of 100 000 query points and 100 test queries are drawn from the 500-dimensional normal distribution \(N(0, \sigma I)\), with standard deviations \(\sigma = 1, 2, 5, 5\), respectively. All query points are censored to the interval (−10, 10) to ensure the same support.

The results and the two-dimensional projections of the data sets are shown in Figure 3. Both versions of ANNC are

---

\[\text{http://corpus-texmex.irisa.fr}\]

---

Figure 2: Recall vs. query time (log scale) for SIFT and Crawl with different training set sizes for ANNC-RF.
faster than any of the other algorithms by a large margin, and as hypothesized, the performance difference is accentuated for the most concentrated query distributions.

We also test the effect of different distributions on a more complicated data set (Clusters), where the corpus is drawn from the same distribution as in the previous experiment, but the query distribution is a mixture of five 500-dimensional normal distributions with different means and variances. The results are shown in Figure 4. Again, both versions of ANNC are significantly faster than the other algorithms.

The performance of ANNC-RP and ANNC-RF is almost identical on these synthetic data sets. We believe that this is because the synthetic data sets do not have any structure that can be utilized to optimize the split points.

**Conclusion**

We have shown how approximate nearest neighbor search can be solved as a multi-label classification problem. The main advantages of this approach are that it allows leveraging large training sets drawn from the query distribution, and that it allows modeling the situation where the query and corpus distributions differ.

We demonstrated the efficiency of our approach by using a random forest and, alternatively, the more scalable but less performant ensemble of random projection trees to solve the classification task. Since any multi-label classifier can be used, we expect that the results can be improved by exploring other types of models.
References

[Andoni and Indyk 2008] Andoni, A., and Indyk, P. 2008. Near-optimal hashing algorithms for approximate nearest neighbor in high dimensions. Communications of the ACM 51(1):117.

[Arya et al. 1998] Arya, S.; Mount, D. M.; Netanyahu, N. S.; Silverman, R.; and Wu, A. Y. 1998. An optimal algorithm for approximate nearest neighbor searching in fixed dimensions. Journal of the ACM (JACM) 45(6):891–923.

[Aumüller, Bernhardtsson, and Faithfull 2019] Aumüller, Bernhardsson, and Faithfull 2019. Aumüller, M.; Bernhardtsson, E.; and Faithfull, A. 2019. ANN-benchmarks: A benchmarking tool for approximate nearest neighbor algorithms. Information Systems.

[Baranchuk et al. 2019] Baranchuk, D.; Persiyanov, D.; Persiyanov, A.; and Babenko, A. 2019. Learning to route in similarity graphs. arXiv preprint arXiv:1905.10987.

[Bentley 1975] Bentley, J. L. 1975. Multidimensional binary search trees used for associative searching. Communications of the ACM 18(9):509–517.

[Breiman et al. 1984] Breiman, L.; Friedman, J.; Olshen, R.; and Stone, C. 1984. Classification and Regression Trees. Wadsworth.

[Breiman 2001] Breiman, L. 2001. Random forests. Machine Learning 45(1):5–32.

[Cayton and Dasgupta 2008] Cayton, L., and Dasgupta, S. 2008. A learning framework for nearest neighbor search. In Proceedings of the 21st Conference on Advances in Neural Information Processing Systems, 233–240.

[Dasgupta and Freund 2008] Dasgupta, S., and Freund, Y. 2008. Random projection trees and low dimensional manifolds. In STOC, volume 8, 537–546.

[Dasgupta and Sinha 2015] Dasgupta, S., and Sinha, K. 2015. Randomized partition trees for nearest neighbor search. Algorithmica 72(1):237–263.

[Dong et al. 2019] Dong, Y.; Indyk, P.; Razenshteyn, I.; and Wagner, T. 2019. Learning sublinear-time indexing for nearest neighbor search. arXiv preprint arXiv:1901.08544.

[Ho 1995] Ho, T. K. 1995. Random decision forests. In Proceedings of 3rd International Conference on Document Analysis and Recognition, volume 1, 278–282. IEEE.

[Hyyönen et al. 2016] Hyyönen, V.; Pitkänen, T.; Tasoulis, S.; Jääsaari, E.; Tuomainen, R.; Wang, L.; Corander, J.; and Roos, T. 2016. Fast nearest neighbor search through sparse random projections and voting. In Proceedings of the 4th IEEE International Conference on Big Data, 881–888. IEEE.

[Iwasaki and Miyazaki 2018] Iwasaki, M., and Miyazaki, D. 2018. Optimization of indexing based on k-nearest neighbor graph for proximity search in high-dimensional data. arXiv preprint arXiv:1810.07355.

[Jääsaari, Hyyönen, and Roos 2019] Jääsaari, E.; Hyyönen, V.; and Roos, T. 2019. Efficient autotuning of hyperparameters in approximate nearest neighbor search. In Proceedings of the 25rd Pacific-Asia Conference on Knowledge Discovery and Data Mining, volume 2, 590–602. Springer.

[Jegou, Douze, and Schmid 2010] Jegou, H.; Douze, M.; and Schmid, C. 2010. Product quantization for nearest neighbor search. IEEE Transactions on Pattern Analysis and Machine Intelligence 33(1):117–128.

[Kraska et al. 2018] Kraska, T.; Beutel, A.; Chi, E. H.; Dean, J.; and Polyzotis, N. 2018. The case for learned index structures. In Proceedings of the 37th International Conference on Management of Data, 489–504. ACM.

[Kraska et al. 2019] Kraska, T.; Alizadeh, M.; Beutel, A.; Chi, E. H.; Kristo, A.; Leclerc, G.; Madden, S.; Mao, H.; and Nathan, V. 2019. SageDB: A learned database system. In Proceedings of the 9th Biennial Conference on Innovative Data Systems Research.

[Li et al. 2019] Li, W.; Zhang, Y.; Sun, Y.; Wang, W.; Li, M.; Zhang, W.; and Lin, X. 2019. Approximate nearest neighbor search on high dimensional data-experiments, analyses, and improvement. IEEE Transactions on Knowledge and Data Engineering.

[Malkov and Yashunin 2018] Malkov, Y. A., and Yashunin, D. A. 2018. Efficient and robust approximate nearest neighbor search using hierarchical navigable small world graphs. IEEE Transactions on Pattern Analysis and Machine Intelligence.

[Maneewongvatana and Mount 2002] Maneewongvatana, S., and Mount, D. M. 2002. Analysis of approximate nearest neighbor searching with clustered point sets. Data Structures, Near Neighbor Searches, and Methodology 59:105–123.

[McNames 2001] McNames, J. 2001. A fast nearest-neighbor algorithm based on a principal axis search tree. IEEE Transactions on Pattern Analysis and Machine Intelligence 23(9):964–976.

[Mitzenmacher 2018] Mitzenmacher, M. 2018. A model for learned Bloom filters and optimizing by sandwiching. In Proceedings of the 32nd Conference on Advances in Neural Information Processing Systems, 464–473.

[Wang et al. 2016] Wang, L.; Tasoulis, S.; Roos, T.; and Kangasharju, J. 2016. Kvasir: Scalable provision of semantically relevant web content on big data framework. IEEE Transactions on Big Data 2(3):219–233.