Approximate Nearest Neighbor Search via Group Testing

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Contents

Nearest Neighbor Search

- Nearest neighbor search is a fundamental problem with many applications in machine learning systems.
- **Task:** Given a dataset $D = \{x_1, x_2, \ldots, x_N\}$, the goal is to build a data structure that can be queried with any point q to obtain a small set of points $x_i \in D$ that have high similarity (low distance) to the query. This structure is called an index.
- Such tasks frequently arise in genomics, web-scale data mining, machine learning, and other large-scale applications.

Group Testing

- We are given a set D of N items, with k positives ("hits") and $N - k$ negatives ("misses").
- **Goal:** Identify all positive items using fewer than N group tests.
- A *group test* is positive iff at least one item in the group is positive.
- **Testing Variants:** Can be *noisy* (with false positives/negatives), *adaptive* (tests depend on previous results), or *non-adaptive* (all tests run in parallel).
- The paper uses a **doubly regular design:** Each item appears in an equal number of tests; each test has an equal number of items.

Formal Problem Statement

- **(R, c)-Approximate Near Neighbor:** Given a dataset D, if there exists a point within distance R of a query y, return some point within distance $c \cdot R$, with high probability.
  - R is the distance threshold (radius).
  - $c > 1$ is the approximation factor.
- Any algorithm that solves the randomized nearest neighbor problem also solves the approximate near neighbor problem with $c = 1$ and any $R \geq$ distance to the nearest neighbor.
- (Definition) **Randomized Nearest neighbor:** Given a dataset D and a distance metric $d(\cdot, \cdot)$ and a failure probability $\delta \in [0, 1]$, construct a data structure which, given a query point y reports the point $x \in D$ with the smallest distance $d(x, y)$ with probability greater than $1 - \delta$.

Locality Sensitive Hashing

A hash function $h(x) \rightarrow \{1, \ldots, R\}$ is a function that maps an input x to an integer in the range $[1, R]$.
The two points x and y are said to collide if $h(x) = h(y)$.

$$s(x, y) = Pr_H(h(x) = h(y))$$

For now, we will assume that $s(x, y) = sim(x, y)$.
For any positive integer L, we may transform an LSH family H with collision probability $s(x, y)$ into a new family having $s(x, y)^L$ by sampling L hash functions from H and concatenating the values to obtain a new hash code $[h_1(x), h_2(x), ..., h_L(x)]$. If the original hash family had the range $[1, R]$, the new hash family has the range $[1, R^L]$.

Locality Sensitive Hashing

- **Locality Sensitive Hashing (LSH)** algorithms use an LSH function to partition the dataset into buckets.
- The hash function is selected so that the distance between points in the same bucket is likely to be small.
- To find the near neighbors of a query, we hash the query and compute the distance to every point in the corresponding bucket.
- **Count-Based LSH** identifies neighbors by simply counting how many times two points land in the same hash bucket across multiple hash functions.

Distance-Sensitive Bloom Filters

- (Definition) **Approximate Set Membership:** Given a set D of N points and similarity thresholds S_L and S_H, construct a data structure which, given a query point y, has:
  True Positive Rate: If there is $x \in D$ with $sim(x, y) > S_H$, the structure returns true w.p. $\geq p$
  False Positive Rate: If there is no $x \in D$ with $sim(x, y) > S_L$, the structure returns true w.p. $\leq q$
- The distance-sensitive Bloom filter solves this problem using LSH functions and a 2D bit array. The structure consists of m binary arrays that are each indexed by an LSH function. There are threeparameters: the number of arrays m, a positive threshold $t \leq m$, and the number of concatenated hash functions L used within each array.

Distance-Sensitive Bloom Filters

- To construct the filter, we insert elements $x \in D$ by setting the bit located at array index $[m, h_m(x)]$ to 1.
- To query the filter, we determine the m hash values of the query y. If at least t of the corresponding bits are set, we return true. Otherwise, we return false.
- (Theorem) Assuming the existence of an LSH family with collision probability $s(x,y) = sim(x,y)$, the distance-sensitive Bloom filter solves the approximate membership query problem with

$$p \geq 1 - exp\left(-2m(-t + S_H^L)^2\right)$$

$$q \leq exp\left(-2m(-t + NS_L^L)^2\right)$$

Index Construction

Input: Dataset D of size N, positive integers B and R, similarity threshold S
Output: A FLINNG search index consisting of membership sets $M_{r,b}$ and group tests $C_{r,b}$

- For $r = 0$ to $R - 1$:
  - Let $\pi(D)$ be a random permutation of D
  - For $b = 0$ to $B - 1$:
    - Define $M_{r,b} = \{\pi(D)_i \mid i \bmod B = b\}$
- For $r = 0$ to $R - 1$:
  - For $b = 0$ to $B - 1$:
    - Construct a classifier $C_{r,b}$ for membership set $M_{r,b}$ with true positive rate p and false positive rate q

Index Construction

- If we apply a similarity threshold to the dataset, we obtain a near neighbor set $K = \{x \in D | sim(x, y) \geq S\}$. We consider K to be the set of "positives" in the group testing problem.
- In order to do so, we split the dataset D into a set of groups, which we visualize as a $B \times R$ grid of cells. Each cell has a group of items $M_{r,b}$ and a corresponding group test $C_{r,b}$. To assign items to cells, we evenly distribute the N points among the B cells in each column of the grid, and we independently repeat this assignment process R times.

Index Query

Input: A FLINNG index and a query y
Output: Approximate set $\hat{K}$ of neighbors with similarity greater than the threshold S

- Initialize $\hat{K} = \{1, \ldots, N\}$
- For $r = 0$ to $R - 1$:
  - Initialize $Y = \emptyset$
  - For $b = 0$ to $B - 1$:
    - If $C_{r,b}(y) = 1$ then: $Y = Y \cup M_{r,b}$
  - $\hat{K} = \hat{K} \cap Y$

Index Query

- To query the index with a point y, we begin by querying each classifier. If $C_{r,b}(y) = 1$, then at least one of the points in $M_{r,b}$ has high similarity to y. We collect all of these "candidate points" by taking the union of the $M_{r,b}$ sets for which $C_{r,b}(y) = 1$.
- We repeat this process for each of the R repetitions to obtain R candidate sets, one for each column in the grid.
- With high probability, each candidate set contains the true neighbors, but it may also have some non-neighbors that were included in $M_{r,b}$ by chance. To filter out these points, we intersect the candidate sets to obtain our approximate near neighbor set $\hat{K}$.

Group Testing: Runtime and Accuracy

Lemma 1: Suppose we have a dataset D of points, where a subset $K \subseteq D$ is "positive" and the rest are "negative". Construct a $B \times R$ grid of tests, where each test has i.i.d true positive rate p and false negative rate q. Then the algorithm reports points as "positive" with probability:

$$Pr(\text{Report } x \mid x \in K) \geq p^R$$

$$\Pr(\text{Report } x \mid x \notin K) \leq \left[q \left(\frac{eN(B-1)}{B(N-1)} \right)^{|K|} + p \left(1 - \left(\frac{N(B-1)}{eB(N-1)} \right)^{|K|} \right) \right]^R$$

Group Testing: Runtime and Accuracy

The cost of group testing inference includes the cost to do all $B \times R$ tests, plus the cost of intersecting the positive groups.

Theorem: Under the assumptions in the previous lemma, let us suppose that each test runs in $\mathcal{O}(T)$. Then with probability $1 - \delta$:

$$t_{\text{query}} = \mathcal{O}\left(BRT + \frac{RN}{B}(p|K| + qB)log(\frac{1}{\delta})logN\right)$$

Bounding the Test Cost

To distinguish between the $|K|$ nearest neighbors and the rest of the dataset:

$$S_H = sim(x_{|K|}, y) = s_{|K|}$$

$$S_L = sim(x_{|K|+1}, y) = s_{|K|+1}$$

(Definition) γ-**Stable query:** We say that the query is γ-stable if $\frac{log(s_{|K|})}{log(s_{|K|}) - log(s_{|K|})} \leq \gamma$

Theorem: Given a true positive rate p, false negative rate qand stability parameter γ, it is possible to choose m, L and t so that the resulting distance-sensitive Bloom filter has true positive rate p and false negative rate q for all γ-stable queries. The query time is

$$\mathcal{O}(mL) = \mathcal{O}(-log(min(q, 1-p))N\gamma log(N))$$

Query Time Analysis

We will consider the query time of a $2\sqrt{N} \times R$ grid of Bloom filter classifiers and $T = mL$.

Lemma 2: Under the assumptions of Lemma 1, we can use distance-sensitive Bloom filters as tests to achieve the following query time t_{query} of our Algorithm with probability $1 - \delta$

$$t_{\text{query}} = \mathcal{O}(RN^{\frac{1}{2}+\gamma}log(N)max(-log(q), -log(1-p)) + RN^{\frac{1}{2}}log^2(N)(|K| + qN^{\frac{1}{2}}log(\frac{1}{\delta}))$$

Lemma 3: Under the assumptions of Lemma 1,we can build a data structure that solves the randomized nearest neighbor problem for sufficiently large N and small δ, where

$p = 1 - \frac{\delta}{2R}$, $q = N^{-\frac{1}{2}}$, $R = \frac{log(\frac{1}{\delta})}{log(4.80N^{\frac{1}{2}}) - log(2e^2 + 3.44N^{\frac{1}{2}})}$

Query Time Analysis

Theorem: Under the assumptions of the previous Lemma, we solve the randomized nearest problem for γ-stable queries in time t_{query}:

$$t_{\text{query}} = \mathcal{O}(N^{\frac{1}{2}+\gamma} log^4(N) log^3(\frac{1}{\delta}))$$

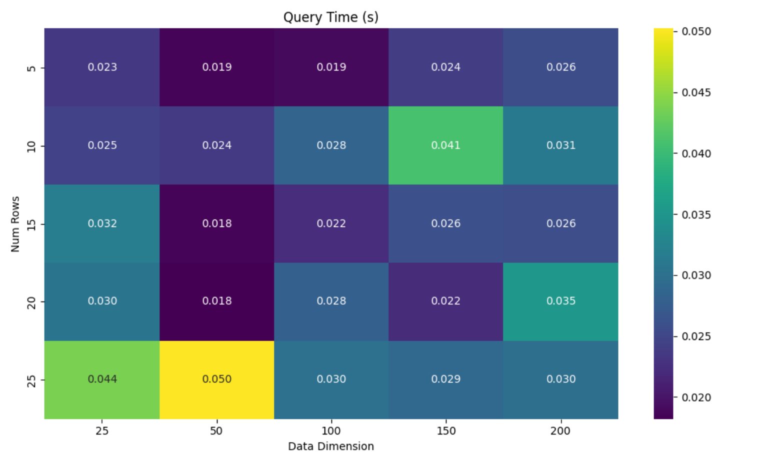
Metrics Used

- **Query Time (s)**: Measures the total time taken for FLINNG to process the queries. Lower values indicate faster retrieval times.
- **Average Precision**: The fraction of retrieved neighbors that are correct. High precision means most retrieved points are relevant.
- **Average Recall**: The fraction of true nearest neighbors that are retrieved. High recall means most true neighbors are found.
- **F1 Score**: Harmonic mean of precision and recall. A balanced metric that evaluates both correctness and completeness of retrieval.

Default Choice of Parameters

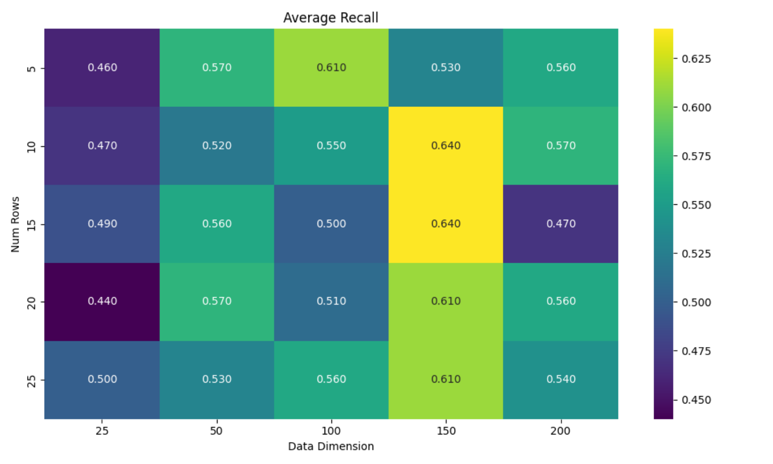
- **Dataset Size**: 10,000 points
- **Query Size**: 100 queries
- **Dataset Standard Deviation**: 1
- **Query Standard Deviation**: 0.5
- **Hashes per Table**: 16
- **Number of Hash Tables**: 20
- **k (Nearest Neighbors)**: 1

Heatmap for Query Time



Heatmap for Average Precision

Heatmap for Average Recall



Heatmap for Average F1 Score

Code and Report

The code and the report can be found at the following link:

https://github.com/sakshamrathi21/CS754-Project

Thank You