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 $D = \{x_1, x_2, \dots, x_N\}$, 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 $h(x) \rightarrow \{1, \dots, R\}$ 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: 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 false 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