

APPROXIMATE NEAREST NEIGHBOR SEARCH VIA GROUP TESTING

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Approximate Nearest Neighbor Search via Group Testing

Contents



Approximate Nearest Neighbor Search via Group Testing

Auth

Introduction

Locality Sensitive

Distance-Sensitive Bloom

Algorithm

..60......

....

Introduction

2 Locality Sensitive Hashing

3 Distance-Sensitive Bloom Filters

Algorithm

Theory

Nearest Neighbor Search



Approximate Nearest Neighbor Search via Group Testing

Introduction

Such tasks frequently arise in genomics, web-scale data mining,

- 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 gueried 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.
- machine learning, and other large-scale applications.

Group Testing



Approximate Nearest Neighbor Search via Group Testing

Introduction

Introduction

Locality Sensitive Hashing

Distance-Sensitive Bloom

Algorithm

Theory

- We are given a set D of N items, with k positives ("hits") and N-k negatives ("misses").
- ullet 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 > 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 $1 - \delta$.

Approximate Nearest Neighbor Search via Group Testing

Introduction

Locality Sensitive Hashing



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Locality Sensitive Hashing

A hash function $h(x) \to \{1, \dots, R\}$ 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



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Locality Sensitive

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Sensitive Bloom Filters

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Theory

- 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. < 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.

Approximate Nearest Neighbor Search via Group Testing

Introduction

Locality Sensitive

Distance-Sensitive Bloom Filters

Algorithm

Theony

Distance-Sensitive Bloom Filters



Approximate Nearest Neighbor Search via Group Testing

Introduction

Locality Sensitive Hashing

Distance-Sensitive Bloom Filters

Algorithr

Theory

Results

• 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

$$p \ge 1 - \exp\left(-2m(-t + S_H^L)^2\right)$$
$$q \le \exp\left(-2m(-t + NS_L^L)^2\right)$$

Index Construction



Approximate Nearest Neighbor Search via Group Testing

Introduction

Locality Sensitive Hashing

Distance-Sensitive Bloon Filters

Algorithm

Results

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:
 - ullet 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

Slide 10/27

Index Construction



• If we apply a similarity threshold to the dataset, we obtain a near neighbor set $K = \{x \in D | sim(x,y) \ge S\}$. 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.

Approximate Nearest Neighbor Search via Group Testing

Introduction

Locality Sensitive Hashing

Distance-Sensitive Bloom Filters

Algorithm

Index Query



Approximate Nearest Neighbor Search via Group Testing

Autno

Introduction

Locality Sensitiv Hashing

Distance-Sensitive Bloom Filters

Algorithm

Theory

Results

Input: A FLINNG index and a query y

 $\mbox{\bf Output:}$ Approximate set \hat{K} of neighbors with similarity greater than the threshold S

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

Index Query



Approximate Nearest Neighbor Search via Group Testing

r,b

Introduction

Hashing Distance-

Sensitive Bloom Filters

Algorithm

Theory

Results

• 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



Approximate Nearest Neighbor Search via Group Testing

Authors

Introduction

Locality Sensitiv Hashing

Distance-Sensitive Bloor Filters

Algorithn

Theory

Results

Results

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 positive q. Then the algorithm reports points as "positive" with probability:

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

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

Group Testing: Runtime and Accuracy



Approximate Nearest Neighbor Search via Group Testing

Authors

Introduction

Locality Sensitive Hashing

Distance-Sensitive Bloom Filters

Algorithr

...

Theory

Results

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 $1 - \delta$:

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

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 $\frac{\log(s_{|K|})}{\log(s_{|K|}) - \log(s_{|K|})} \le \gamma$

Theorem: Given a true positive rate p, false positive rate q and 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 positive rate q for all γ -stable queries. The query time is

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

Approximate Nearest Neighbor Search via Group Testing

Theory

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 $t_{\rm query}$ of our Algorithm with probability $1-\delta$

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

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

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

Approximate Nearest Neighbor Search via Group Testing

ntroduction

Locality Sensitive Hashing

Distance-Sensitive Bloom Filters

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Theory

Query Time Analysis



Approximate Nearest Neighbor Search via Group Testing

Introduction

Hashing

Sensitive Bloon

Algorithn

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Theory

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

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

Metrics Used



Approximate Nearest Neighbor Search via Group Testing

Authors

Introduction

Hashing

Distance-Sensitive Bloom

Algorithm

Theory

Results

 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



Approximate Nearest Neighbor Search via Group Testing

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Introduction

Locality Sensi Hashing

Distance-Sensitive Bloom

Algorithm

Theory

Results

• Dataset Size: 10,000 points

• Query Size: 100 queries

• Dataset Standard Deviation: 1

• Query Standard Deviation: 0.5

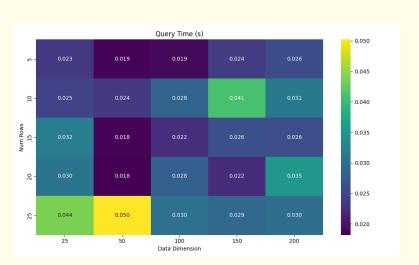
• Hashes per Table: 16

• Number of Hash Tables: 20

• k (Nearest Neighbors): 1

Heatmap for Query Time





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roduction

Locality Sensitive

Distance-Sensitive Bloom

Algorithm

Theory

Heatmap for Average Precision





Approximate Nearest Neighbor Search via Group Testing

troduction

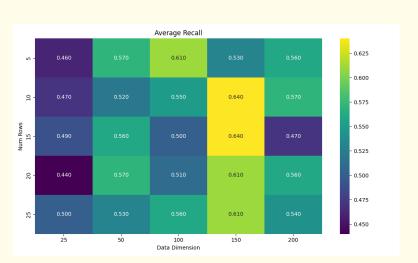
Locality Sensitive

Distance-Sensitive Bloom

Theory

Heatmap for Average Recall





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ntroduction

Locality Sensitive Hashing

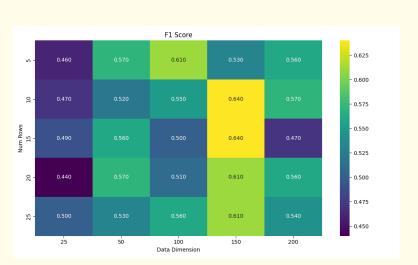
Distance-Sensitive Bloom Filters

.

Theory

Heatmap for Average F1 Score





Approximate Nearest Neighbor Search via Group Testing

troduction

Locality Sensitive

Distance-Sensitive Bloom

Algorithm

Theory

Individual Contributions



Approximate Nearest Neighbor Search via Group Testing

Authors

Introduction

Hashing

Distance-Sensitive Bloom

Algorithm

Theory

Results

 Saksham Rathi: Read through the paper, described the initial problem statement and the algorithms used in the paper in the report, code debugging, collection of results and adding them to the report.

- Kshitij Vaidya: Read through the paper, wrote the LSH, DSBF and FLINNG classes in Python and tested them for correct functionality, code debugging.
- **Ekansh Ravi Shankar**: Read through the paper, code debugging, wrote threshold relaxation algorithm.

Code and Report



Approximate Nearest Neighbor Search via Group Testing

Introduction

Locality Sensitive Hashing

Distance-Sensitive Bloor

Algorithm

Theory

Results

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

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



Approximate Nearest Neighbor Search via Group Testing

ntroduction

Locality Sensitive Hashing

Sensitive Bloon Filters

Algorithm

Theory

Results

Thank You