## Algorithms for Nearest Neighbors: Theoretical Aspects

Yury Lifshits

Steklov Institute of Mathematics at St.Petersburg

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### Outline

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## Informal Problem Statement

Part I

What are nearest neighbors about?

Industrial applications

Three data models

To preprocess a database of *n* objects so that given a query object, one can effectively determine its nearest neighbors in database

## First Application (1960s)

### Nearest neighbors for classification:



#### Picture from http://cgm.cs.mcgill.ca/ soss/cs644/projects/perrier/Image25.gif

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### Data Model in General

Formalization for nearest neighbors consists of:

- Representation format for objects
- Similarity function

### Applications

What applications of nearest neighbors do you know?

- Statistical data analysis, e.g. medicine diagnosis
- Pattern recognition, e.g. for handwriting
- Code plagiarism detection
- Coding theory
- Future applications: recommendation systems, ads distribution, personalized news aggregation

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### Vector Model

**Database:** points in  $R^d$ 

Similarity: scalar product

### Constraints:

poly(n+d) for preprocessing time,  $d \cdot polylog(n+d)$  for query

### Sparse Vector Model

**Database:** points in  $\mathbb{R}^d$ , every point has at most  $k \ll d$  nonzero coordinates

Similarity: scalar product

### **Constraints:**

poly(n+d) for preprocessing time,  $poly(k) \cdot polylog(n+d)$  for query

### Set Model

**Database:** *n* subsets of *T*, having size at most k|T| = m

Similarity: size of intersection

**Constraints:** poly(n+m) for preprocessing time,  $poly(k) \cdot polylog(n+m)$  for query

More data models?

# Super-Nearest Neighbors

### Idea

We will search for nearest neighbors only within  $B(q, \tau)$ 

### Definition

p is nearest  $\tau$ -neighbor for q iff  $d(p,q) \leq \tau$  and p is in fact the nearest neighbor for q

## Part II

# Three Relaxed Versions of Nearest Neighbors

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## **Yianilos Theorem**

Consider some **nice** metric space S and probability distribution P over it

### Theorem (Nearest $\tau$ -Neighbors)

For any fixed database  $DB \subset S$  of size n and for any M > 1 there exists  $\tau > 0$  such that we can construct a binary tree for DB which answers nearest  $\tau$ -neighbor queries using at most  $M \cdot (\log n + 1)$  expected metric evaluations

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### VP-Trees for Approximate NN

Partitioning condition: 
$$d(p, x)  r</math  
Inner branch:  $B(p, r(1 + \delta))$ , where  $\delta = \frac{1}{1+\varepsilon}$   
Outer branch:  $R^d/B(p, r(1 - \delta))$$$

### Search:

If d(p,q) < r go to inner branch If d(p,q) > r go to outer branch and return minimum between obtained result and d(p,q)

## Approximate Nearest Neighbors

### Definition

<i>p</i> is $\varepsilon$ -approximate	nearest	neighbor for <i>q</i>
iff $\forall p' \in DB$ :	d(p,q)	$\leq (1+arepsilon) d(p',q)$

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## Rare Neighbors

### Definition

p is an r-rare neighbor for qiff p and q have common nonzero coordinate which is nonzero for at most r points in DB

### Cheating

We will search only for neighbors that have at least one common rare feature with query object

### Rare-Point Method

### **Preprocessing:**

For every rare feature store a list of all objects in database having it

### Query processing:

Retrieve all point that have at least one common rare feature with the query object; Perform linear scan on them

## Part III Probabilistic Analysis

Probabilistic assumptions about data collection can lead to provably efficient solutions for nearest neighbors

This section represents joint work with Benjamin Hoffmann and Dirk Nowotka

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## Probabilistic Analysis in a Nutshell

- We define a probability distribution over databases
- We define probability distribution over query objects
- We construct a solution that is efficient/accurate with high probability over input/query

## Zipf Model

- Terms  $t_1, \ldots, t_m$
- To generate a document we take every t<sub>i</sub> with probability <sup>1</sup>/<sub>i</sub>
- Database is *n* independently chosen documents
- Query document has exactly one term in every interval [e<sup>i</sup>, e<sup>i+1</sup>]
- Similarity between documents is defined as the number of common terms

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## Magic Level Theorem

**Magic Level**  $q = \sqrt{2 \log_e n}$ 

Theorem

- With very high probability there exists a document in database having q - ε top terms of query document
- With very small probability there exists a document in database having any  $q + \varepsilon$  overlap with query document

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## Part IV Further Work

Directions for Research

Three Specific Open Problems

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# Directions for Further Research

- Develop techniques for proving hardness of some computational problems with preprocessing. Find theoretical limits for some specific families of algorithms
- Extend classical NN algorithms to new data models and new task variations
- Develop theoretical analysis of existing heuristics. Average case complexity is particulary promising. Find subcases for which we can construct provably efficient solutions
- Compare NN-based approach with other methods for classification/recognition/prediction problems

## OP1: 3-Step NN

Construct an algorithm for solving nearest neighbors in bipartite graphs with 3-step similarity



## OP2: 1D Dynamic NN

### Input

Database of n points in one-dimensional space and their velocity vectors

### Query task

To find the nearest neighbor for a given query point at a given time point

### Constraints

Data storage after preprocessing  $n \cdot polylog(n)$ Time for query processing polylog(n)

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## Call for Feedback

- Any new ideas how to solve nearest neighbors?
- What kind of formalization should we consider?
- Any relevant work?
- How to improve this talk for the next time?

### **OP3:** Inclusions with Preprocessing

 $\begin{array}{l} \text{Input} \\ \text{Family } \mathcal{F} \text{ of subsets of } \mathcal{T} \end{array}$ 

Query task Given a set  $f_{new} \subseteq T$  to decide whether  $\exists f \in \mathcal{F} : f_{new} \subseteq f$ 

### Constraints

Data storage after preprocessing  $poly(|\mathcal{F}| + |T|)$ Time for query processing poly(|T|)

**Conjecture:** this problem CAN NOT be solved within such time/space constraints

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### Summary

- Nearest neighbors is one of the key algorithmic problems for web technologies
- Key ideas: relax search to approximately nearest neighbor, nearest *r*-rare neighbor or nearest neighbor in *τ*-neighborhood of query point
- Further work: theoretical analysis of heuristics, extending known solutions to new data models, lower bounds

## Thanks for your attention! Questions?

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Inverted files for text search engines

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Links to nearest neighbors implementations

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