## Algorithms for Nearest Neighbors: Theoretical Aspects

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## Outline

(1) Problem Statement

- Applications
- Three Data Models


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- Super-Nearest Neighbors
- Approximate Nearest Neighbors
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(3) Nearest Neighbors in Zipf Model


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(3) Nearest Neighbors in Zipf Model
(4) Further Work
- Three Open Problems


## Part I

What are nearest neighbors about?
Industrial applications
Three data models

## Informal Problem Statement

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

## Applications

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- 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


## Data Model in General

Formalization for nearest neighbors consists of:

- Representation format for objects
- Similarity function

Vector Model

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Similarity: scalar product

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## Set Model

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

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More data models?

## Part II

## Three Relaxed Versions of Nearest Neighbors

## 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 $q$

## Yianilos Theorem

Consider some nice metric space $\mathcal{S}$ and probability distribution $P$ over it

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

## Approximate Nearest Neighbors

Definition
$p$ is $\varepsilon$-approximate nearest neighbor for $q$ iff $\forall p^{\prime} \in D B$ : $d(p, q) \leq(1+\varepsilon) d\left(p^{\prime}, q\right)$

## VP-Trees for Approximate NN

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

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## Search:

If $d(p, q)<r$ go to inner branch If $d(p, q)>r$ go to outer branch

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## 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 $d(p, q)$

## Rare Neighbors

## Definition

$p$ is an $r$-rare neighbor for $q$
iff $p$ and $q$ have common nonzero coordinate which is nonzero for at most $r$ points in $D B$

## 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

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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

## Probabilistic Analysis in a Nutshell

- We define a probability distribution over databases


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- 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 $t_{i}$ with probability $\frac{1}{i}$
- Database is $n$ independently chosen documents
- Query document has exactly one term in every interval $\left[e^{i}, e^{i+1}\right]$
- Similarity between documents is defined as the number of common terms


## Magic Level Theorem

Magic Level $q=\sqrt{2 \log _{e} n}$
Theorem
(1) With very high probability there exists a document in database having $q-\varepsilon$ top terms of query document
(2) With very small probability there exists a document in database having any $q+\varepsilon$ overlap with query document

# Part IV Further Work 

Directions for Research

Three Specific Open Problems

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- Develop techniques for proving hardness of some computational problems with preprocessing. Find theoretical limits for some specific families of algorithms


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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

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Boys

Girls


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## 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( $n$ )

## OP3: Inclusions with Preprocessing

## Input

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

## Constraints

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

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## 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

## 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?


## 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 $\tau$-neighborhood of query point
- Further work: theoretical analysis of heuristics, extending known solutions to new data models, lower bounds


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- Nearest neighbors is one of the key algorithmic problems for web technologies
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Thanks for your attention! Questions?

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