

Algorithms for Nearest Neighbors

Classic Ideas, New Ideas

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University of Toronto, July 2007

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Outline

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 - Applications
 - Data Models
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 - Random Projections
 - Look-Up Methods
- 3 New Ideas
 - Proving Hardness of Nearest Neighbors
 - Probabilistic Analysis for NN
 - New Data Models

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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

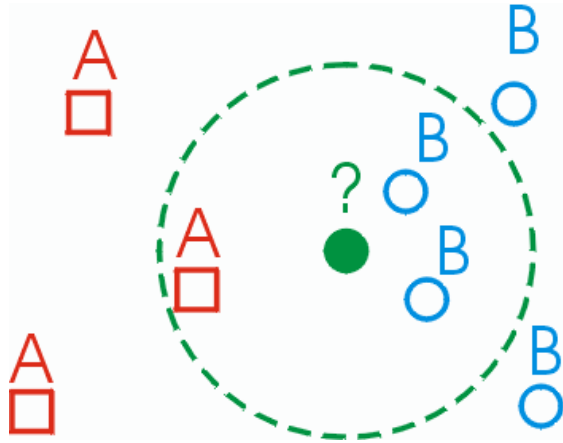
Part I Formulating the Problem

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First Application (1960s)

Nearest neighbors for classification:



Picture from <http://cgm.cs.mcgill.ca/~sooss/cs644/projects/perrier/Image25.gif>

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Applications

What applications of nearest neighbors do you know?

- Text classification
- Statistical data analysis, e.g. medicine diagnosis
- Pattern recognition: characters, faces
- Code plagiarism detection
- Coding theory
- Data compression
- **Web:** recommendation systems, on-line ads, personalized news aggregation, long queries in web search, near-duplicates detection

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Data Model in General

Formalization for nearest neighbors consists of:

- Representation format for objects
- Similarity function

Remark 1: Usually there is original and “reduced” representation for every object

Remark 2: Accuracy of NN-based algorithms depends solely on a data model, no matter what specific exact NN algorithm we use

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Data Models (1/2)

- Vector Model
 - Similarity: l^2 , scalar product, cosine
- String Model
 - Similarity: Hamming distance, edit distance
- Black-box model
 - Similarity: given by oracle
 - The only knowledge is triangle inequality

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Data Models (2/2)

- Set Model
 - Similarity: size of intersection
- Small graphs
 - Similarity: structure/labels matching

More data models?

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Part II Classic Ideas

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Variations of the Computation Task

- Range queries: retrieve all objects within given range from query object
- Approximate nearest neighbors
- Multiple nearest neighbors (many queries)
- Nearest assignment
- All over-threshold neighbor pairs
- Nearest neighbors in dynamically changing database: moving objects, deletes/inserts, changing similarity function

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Linear Scan

What is the most obvious solution for nearest neighbors?

Answer:

compare query object with every object in database

Advantages:

No preprocessing

Exact solution

Works in any data model

Directions for improvement:

order of scanning, pruning

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KD-Trees

Preprocessing:

Build a *kd-tree*: for every internal node on level l we make partitioning based on the value of $l \bmod d$ -th coordinate

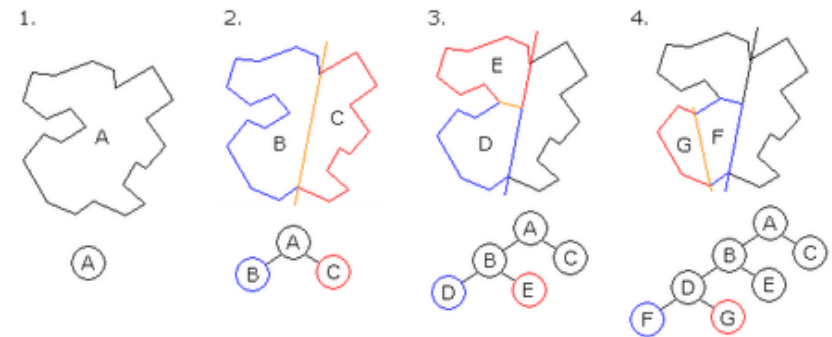
Query processing:

Go down to the leaf corresponding to the the query point and compute the distance;
(Recursively) Go one step up, check whether the distance to the second branch is larger than that to current candidate neighbor
if “yes” go up, else check this second branch

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BSP-Trees

Generalization: BSP-tree allows to use any hyperplanes in tree construction



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VP-Trees

Partitioning condition: $d(p, x) <? r$

Inner branch: $B(p, r(1 + \varepsilon))$

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 $d(p, q)$

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Kleinberg Algorithm (1/3)

Preprocessing

- 1 Choose l random vectors $V = \{v_1, \dots, v_l\}$ with unit norm
- 2 Precompute all scalar products between database points and vectors from V

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Kleinberg Algorithm (2/3)

Random Projection Test

Input: points x, y and q , vectors u_1, \dots, u_k

Question: what is smaller $|x - q|$ or $|y - q|$?

Test:

For all i compare $(x \cdot v_i - q \cdot v_i)$ with $(y \cdot v_i - q \cdot v_i)$

Return the point which has “smaller”

on majority of vectors

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Inverted Index

Data model: every object is a (weighted) set of terms from some dictionary

Preprocessing:

For very term store a list of all documents in database with nonzero weight on it

Query processing:

Retrieve all point that have at least one common term with the query documet;
Perform linear scan on them

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Kleinberg Algorithm (3/3)

Query Processing

- 1 Choose a random subset Γ of V , $|\Gamma| = \log^3 n$
- 2 Compute scalar products between query point q and vectors from Γ
- 3 Make a tournament for choosing a nearest neighbor:
 - 1 Draw a binary tree of height $\log n$
 - 2 Assign all database points to leafs
 - 3 For every internal point (say, x vs. y) make a random projection test using some vectors from Γ

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Locality-Sensitive Hashing

Desired hash family \mathcal{H} :

- If $\|p - q\| \leq R$ then $\Pr_{\mathcal{H}}[h(p) = h(q)] \geq p_1$
- If $\|p - q\| \geq cR$ then $\Pr_{\mathcal{H}}[h(p) = h(q)] \leq p_2$

Preprocessing:

Choose at random several hash functions from \mathcal{H}
Build inverted index for hash values of object in database

Query processing:

Retrieve all object that have at least one common hash value with query object;
Perform linear scan on them

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Part III

New Ideas

This section represents:

- Some of my own ideas
- Joint work with Benjamin Hoffmann and Dirk Nowotka (CSR'07)

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Inclusions with Preprocessing (1/2)

Input

Family \mathcal{F} of subsets of U

Query task

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

Constraints

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

Open problem: is there an algorithm satisfying given constraints?

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Inclusions with Preprocessing (2/2)

Reformulation in SAT style:

Input

Formula \mathcal{F} in DNF with n variables

Query task

Given an assignment x to evaluate $\mathcal{F}(x)$

Constraints

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

Open problem: is there an algorithm satisfying given constraints?

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“NP Analogue” for Search Problems

Every problem in **SEARCH class** is characterized by poly-time computable Turing Machine M :

Input

Strings x_1, \dots, x_n , $|x_i| = m$

Query task

Given string y of length m to answer whether $\exists i : M(x_i, y) = \text{yes}$

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Tractable problems in SEARCH

Input

Strings x_1, \dots, x_n , $|x_i| = m$

Query task

Given string y of length m to answer whether $\exists i : M(x_i, y) = \text{yes}$

Tractable solution

Preprocessing in $\text{poly}(m, n)$ space
Query processing in $\text{poly}(m, \log n)$ time
with RAM access to preprocessed database

Inclusions is in SEARCH. Is it tractable?

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Complete problems in SEARCH (1/2)

Program Search problem:

Input

Turing machines $P_1 \dots, P_n$

Query task

Given string y of length m to answer whether $\exists i : P_i(y) = \text{yes}$ after at most m steps

Open problem: is Program Search tractable?

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Complete problems in SEARCH (2/2)

Parallel Run problem:

Input

$x_1 \dots, x_n$

Query task

Given poly-time computable P to answer whether $\exists i : P(x_i) = \text{yes}$

Open problem: is Parallel Run tractable?

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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 “random” input/query

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Zipf Model

- Terms t_1, \dots, 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 $[e^i, e^{i+1}]$
- Similarity between documents is defined as the number of common terms

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Magic Level Theorem

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

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

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Sparse Vector Model

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

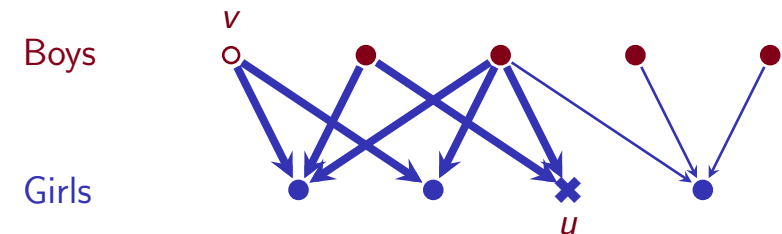
Similarity: scalar product

Constraints:
 $\text{poly}(n + d)$ for preprocessing time,
 $\text{poly}(k) \cdot \text{polylog}(n + d)$ for query

Open Problem: solve NN for sparse vector model
within given constraints

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Amazon Recommendations



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Amazon Nearest Neighbors

Database: Bipartite graph with n vertices,
every vertex of the first part
has out degree at most $k \ll n$

Query: Given a new vertex u in the first part
to find a vertex v in the second part
having maximal number of 3-step paths to v

Constraints:

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

Open Problem: solve NN for Amazon model within
given constraints

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Conclusions

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Directions for Further Research

- Extend classical NN algorithms to new data models and new search task variations
- Develop theoretical analysis of existing heuristics. Find subcases with provably efficient solutions
- Build complexity theory for problems with preprocessing

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Call for Feedback

- Any relevant work?
- How to improve this talk for the next time?
- **Give my open problems to your students!**

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Summary

- Classic ideas: search trees, random projections, locality-sensitive hashing, inverted index
- New ideas: SEARCH class, NN for random texts, Amazon and sparse vector models
- Open problems: lower bound for inclusions with preprocessing, algorithm for 3-step similarity

Thanks for your attention! Questions?

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<http://logic.pdmi.ras.ru/~yura/en/maxint-draft.pdf>



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<http://www.pnylab.com/pny/papers/vptree/vptree.ps>



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Inverted files for text search engines

<http://www.cs.mu.oz.au/~alistair/abstracts/zm06compsurv.html>



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Links to nearest neighbors implementations

<http://people.revoledu.com/kardi/tutorial/KNN/resources.html>

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