Algorithms for Nearest Neighbors

State-of-the-Art

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Outline

- Problem Statement
 - Applications
 - Data Models
 - Variations of the Computation Task

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- Overview of Algorithmic Techniques
 - Partitioning idea
 - Look-up idea
 - Embedding idea

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- Further Work

Part I

What are nearest neighbors about?

Short overview of applications

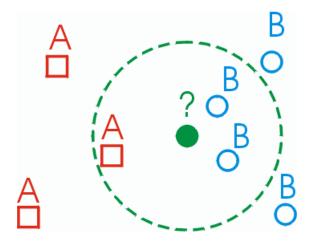
Variations of the problem

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:



Text classification (YaCa)

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- Semantic search

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Formalization for nearest neighbors consists of:

- Representation format for objects
- Similarity function

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Remark 2: Accuracy of NN-based classification, prediction or recommendations depends solely on a data model, no matter what specific exact NN algorithm we use.

Vector Model

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 - Similarity: Hamming distance

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More data models?

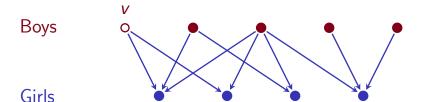
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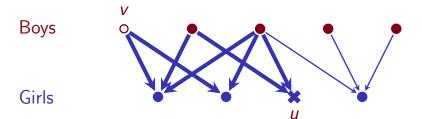
Boys

Girls

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Variations of the Computation Task

- Approximate nearest neighbors
- Multiple nearest neighbors
- Nearest assignment
- All over-threshold neighbor pairs
- Nearest neighbors in dynamically changing database: moving objects, deletes/inserts, changing similarity function

Part II Overview of Algorithmic Techniques

Partitioning, look-up and embedding-based approaches for **vector model**

New rare-point method (joint work with Hinrich Schütze)

Linear Scan

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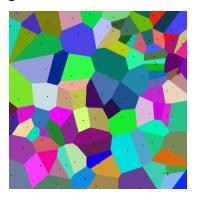
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Directions for improvement:

order of scanning, pruning

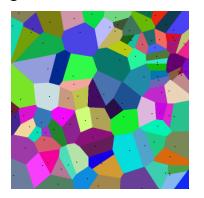
Voronoi diagrams

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Can we generalize one-dimensional binary search?

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Build a *k*d-tree: for every internal node on level *I* we make partitioning based on the value of *I* mod *d*-th coordinate

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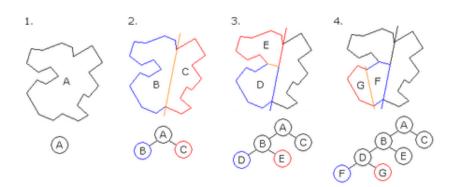
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Go down to the leaf corresponding to the the query point and compute the distance;

(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

BSP-Trees

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



VP-Trees

```
Partitioning condition: d(p,x) <? r
Inner branch: B(p,r(1+\varepsilon))
Outer branch: R^d/B(p,r(1-\delta))
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If d(p,q) < r go to inner branch
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return minimum between obtained result
and d(p,q)
```

Inverted Index

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For very coordinate store a list of all points in database with nonzero value on it

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

Locality-Sensitive Hashing

Desired hash family \mathcal{H} :

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

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Query processing:

Compute A(q);

Find its nearest neighbor in R^{I} ;

Part IV Further Work

Directions for Applied Research

Directions for Theoretical Research

Questions to Practitioners

Directions for Applied Research

Attractive goals: NN-based recommendation system, NN-based ads distribution system

- Choose reasonable data model, add some assumptions about the nature of database and queries
- Find (theoretically) the best solutions in the resulting formalization
- Perform experimental analysis of obtained solutions
- Develop a prototype product

Directions for Theoretical 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

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- Are you interested to apply NN approach in any of your future products?
- Give us benchmark data
- Give us names and contacts of potentially interested engineers

Summary

- Nearest neighbors is one of the key algorithmic problems for web technologies
- Key ideas: look-up tables, partitioning techniques, embeddings
- Further work: from algorithms to prototype products, from heuristics to theory, from canonical problem to new data models and new search tasks

Summary

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Thanks for your attention! Questions?

References (1/2)

Contact: http://logic.pdmi.ras.ru/~yura



B. Hoffmann, Y. Lifshits and D. Nowotka

Maximal Intersection Queries in Randomized Graph Models

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



P.N. Yianilos

 $\label{eq:decomposition} \mbox{Data structures and algorithms for nearest neighbor search in general metric spaces}$

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



J. Zobel and A. Moffat

Inverted files for text search engines

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



K. Teknomo

Links to nearest neighbors implementations

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

References (2/2)



J. Kleinberg

Two Algorithms for Nearest-Neighbor Search in High Dimensions

http://www.ece.tuc.gr/~vsam/csalgo/kleinberg-stoc97-nn.ps



P. Indyk and R. Motwani

Approximate nearest neighbors: towards removing the curse of dimensionality

 $\underline{\text{http://theory.csail.mit.edu/~indyk/nndraft.ps}}$



A. Andoni and P. Indyk

Near-Optimal Hashing Algorithms for Approximate Nearest Neighbor in High Dimensions

http://theory.lcs.mit.edu/~indyk/FOCSO6final.ps



P. Indvk

Nearest Neighbors Bibliography

http://theory.lcs.mit.edu/~indyk/bib.html