Novel Approaches to Nearest Neighbors Random Walks, SEARCH Class,

Yury Lifshits http://yury.name

Steklov Institute of Mathematics at St.Petersburg California Institute of Technology

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Welcome to nearest neighbors!





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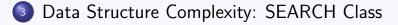
Nearest Neighbors via Random Walks





Welcome to nearest neighbors!

2 Nearest Neighbors via Random Walks

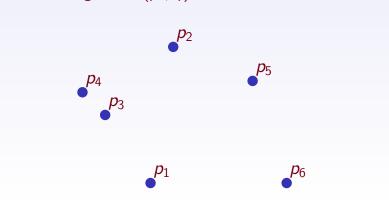


Chapter I

Welcome to Nearest Neighbors!

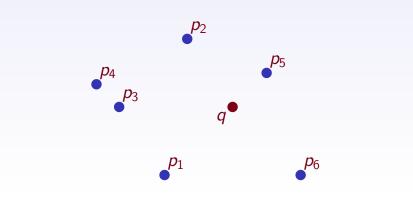
Problem Statement

Search space: object domain \mathbb{U} , similarity function σ Input: database $S = \{p_1, \dots, p_n\} \subseteq \mathbb{U}$ Query: $q \in \mathbb{U}$ Task: find $\operatorname{argmax} \sigma(p_i, q)$



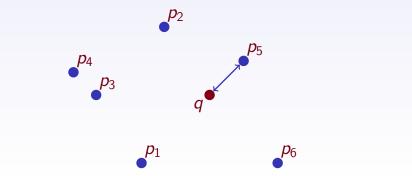
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Applications

Content-based retrieval Spelling correction Searching for similar **DNA** sequences Related pages web search Concept matching kNN classification rule Nearest-neighbor interpolation Near-duplicate Plagiarism detection detection Computing co-occurrence similarity Recommendation systems Personalized news aggregation Behavioral targeting Maximum likelihood decoding MPFG compression

Brief History

- 1908 Voronoi diagram
- 1967 kNN classification rule by Cover and Hart
- 1973 Post-office problem posed by Knuth
- 1997 The paper by Kleinberg, beginning of provable upper/lower bounds
- 2006 Similarity Search book by Zezula, Amato, Dohnal and Batko
- 2008 First International Workshop on Similarity Search. Consider submitting!

Some Nearest Neighbor Solutions

Orchard's Algorithm LAESA Sphere Rectangle Tree k-d-B tree Geometric near-neighbor access tree Excluded middle vantage point forest mvp-tree Fixed-height fixed-queries tree AESA Vantage-point tree R*-tree Burkhard-Keller tree BBD tree Navigating Nets Voronoi tree Balanced aspect ratio tree Metric tree vp^s-tree M-tree Locality-Sensitive Hashing SS-tree R-tree Spatial approximation tree Multi-vantage point tree Bisector tree mb-tree Generalized hyperplane tree Spill Tree Fixed queries tree X-tree k-d Hybrid tree Slim tree tree Balltree Quadtree Octree Post-office tree

Part II

Disorder Inequality

This section represents joint work with Navin Goyal and Hinrich Schütze

Concept of Disorder

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 $\forall p, r, s \in \{q\} \cup S$: $\operatorname{rank}_r(s) \leq D \cdot (\operatorname{rank}_p(r) + \operatorname{rank}_p(s))$

Minimal D providing disorder inequality is called disorder constant of a given set

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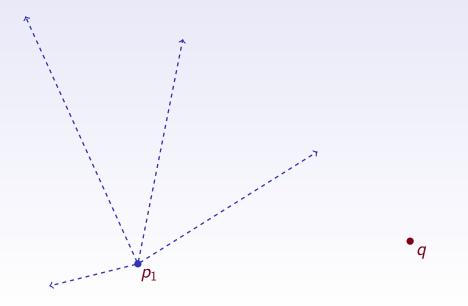
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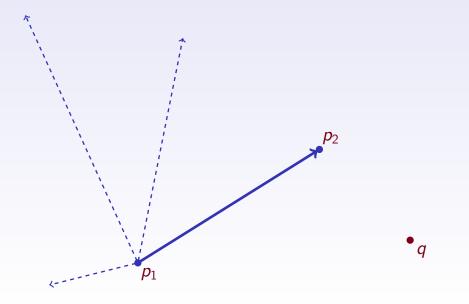
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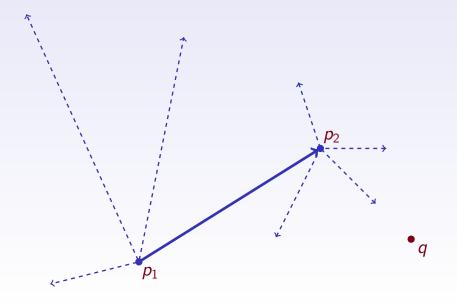
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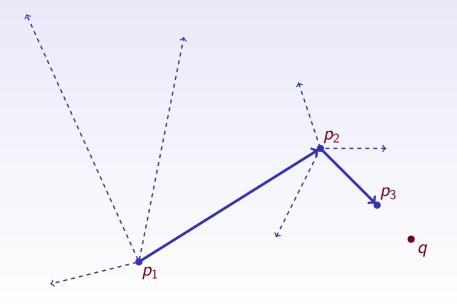
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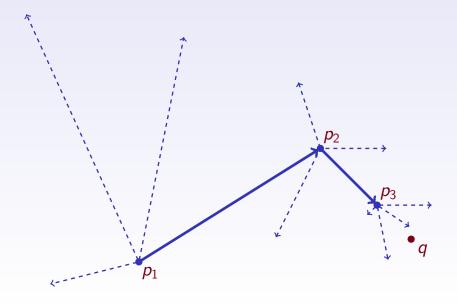
For "regular" sets in *d*-dimensional Euclidean space $D \approx 2^{d-1}$

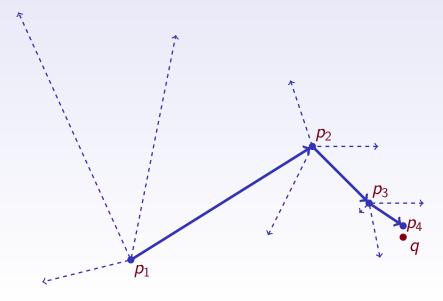












Hierarchical greedy navigation:

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Transport system: for level k choose c random arcs to $\frac{n}{2^k}$ neighborhood

Ranwalk Algorithm

Preprocessing:

• For every point *p* in database we sort all other points by their similarity to *p*

Data structure: *n* lists of n-1 points each.

Query processing:

- **1** Step 0: choose a random point p_0 in the database.
- From k = 1 to k = log n do Step k: Choose D' := 3D(log log n + 1) random points from min(n, 3Dn/2^k)-neighborhood of p_{k-1}. Compute similarities of these points w.r.t. q and set p_k to be the most similar one.
- If $\operatorname{rank}_{p_{\log n}}(q) > D$ go to step 0, otherwise search the whole D^2 -neighborhood of $p_{\log n}$ and return the point most similar to q as the final answer.

Analysis of Ranwalk

Theorem

Assume that database points together with query point $S \cup \{q\}$ satisfy disorder inequality with constant D:

 $rank_x(y) \leq D(rank_z(x) + rank_z(y)).$

Then Ranwalk algorithm always answers nearest neighbor queries correctly. It uses the following resources: Preprocessing space: $O(n^2)$. Preprocessing time: $O(n^2 \log n)$. Expected query time: $O(D \log n \log \log n + D^2)$.

Arwalk Algorithm

Preprocessing:

• For every point *p* in database we sort all other points by their similarity to *p*. For every *level number k* from 1 to log *n* we store pointers to $D' = 3D(\log \log n + \log 1/\delta)$ random points within $\min(n, \frac{3Dn}{2^k})$ most similar to *p* points.

Query processing:

- **1** Step 0: choose a random point p_0 in the database.
- From k = 1 to k = log n do Step k: go by p_{k-1} pointers of level k. Compute similarities of these D' points to q and set p_k to be the most similar one.



Return $p_{\log n}$.

Analysis of Algorithm

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Then for any probability of error δ Arwalk algorithm answers nearest neighbor query within the following constraints:

Preprocessing space: $\mathcal{O}(nD \log n(\log \log n + \log 1/\delta))$. Preprocessing time: $\mathcal{O}(n^2 \log n)$. Query time: $\mathcal{O}(D \log n(\log \log n + \log 1/\delta))$.

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Average disorder. If disorder inequality does not hold for a small fraction of pairs, how should we modify our algorithm?

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Improving our algorithms. Is it possible to combine advantages of Ranwalk and Arwalk? Does there exist a deterministic algorithm with sublinear search time utilizing small disorder assumption? E.g., can we use expanders for derandomization?

Future of Disorder (2/2)

Disorder of random sets. Compute disorder values for some modelling examples. For example, consider *n* random points on *d*-dimensional sphere

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Lower bounds. Is it possible to prove lower bounds on preprocessing and query complexities in some "black-box" model of computation?

Part III

Data Structure Complexity: SEARCH Class

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|)

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Open problem: is there an algorithm satisfying given constraints?

Inclusions with Preprocessing (2/2)

Reformulation in SAT style:

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Formula \mathcal{F} in DNF with *n* variables

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

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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 $x_1, \ldots, x_n, \qquad |x_i| = m$

Query task

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

Tractable problems in SEARCH

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Tractable solution

Preprocessing in poly(m, n) space

Query processing in $poly(m, \log n)$ time with RAM access to preprocessed database

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Inclusions is in SEARCH. Is it tractable?

Complete problems in SEARCH (1/2)

Program Search problem:

Input

Turing machines $P_1 \ldots, P_n$

Query task

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

Complete problems in SEARCH (1/2)

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Input

Turing machines $P_1 \ldots, P_n$

Query task

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

Open problem: is Program Search tractable?

Complete problems in SEARCH (2/2)

Parallel Run problem:

Input

 $x_1 \ldots, x_n$

Query task

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

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Query task

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

Open problem: is Parallel Run tractable?

NN Proofs?

NN-proof system:

- Fix some family of basic statements about points in multidimensional space and some proof system
- Can we compute poly(|S|) statements about points of database S such that for any query q and any real nearest neighbor $p_{NN} \in S$ there is a logarithmic proof from precomputed statements that indeed p_{NN} is nearest point is S to q

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Do such an NN proof system exist?

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Thanks for your attention! Questions?

References

The Homepage of Nearest Neighbors and Similarity Search http://simsearch.yury.name

N. Goyal, Y. Lifshits, H.Schütze Disorder Inequality: A Combinatorial Approach to Nearest Neighbor Search. Submitted. http://yury.name/papers/goyal2008disorder.pdf

B. Hoffmann, Y. Lifshits, D.Novotka Maximal Intersection Queries in Randomized Graph Models. CSR'07. http://yury.name/papers/hoffmann2007maximal.pdf

P. Zezula, G. Amato, V. Dohnal, M. Batko Similarity Search: The Metric Space Approach. Springer, 2006. http://www.nmis.isti.cnr.it/amato/similarity-search-book/

G.R. Hjaltason and H. Samet

Index-driven similarity search in metric spaces. ACM Transactions on Database Systems, 2003 http://www.cs.utexas.edu/~abhinay/ee382v/Project/Papers/ft_gateway.cfm.pdf