

Nearest Neighbor Search by Branch and Bound

Algorithmic Problems Around the Web #2

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Outline

- 1 Short Intro to Nearest Neighbors
- 2 Branch and Bound Methodology
- 3 Around Vantage-Point Trees
- 4 Generalized Hyperplane Trees and Relatives

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Part I

Short Intro to Nearest Neighbors

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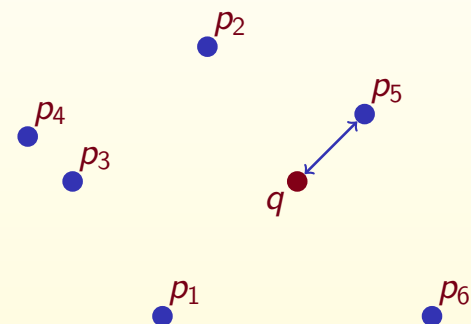
Problem Statement

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 $\operatorname{argmax}_{p_i} \sigma(p_i, q)$



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Applications (1/5) Information Retrieval

- Content-based retrieval (magnetic resonance images, tomography, CAD shapes, time series, texts)
- Spelling correction
- Geographic databases (post-office problem)
- Searching for similar DNA sequences
- Related pages web search
- Semantic search, concept matching

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Applications (2/5) Machine Learning

- kNN classification rule: classify by majority of k nearest training examples. E.g. recognition of faces, fingerprints, speaker identity, optical characters
- Nearest-neighbor interpolation

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Applications (3/5) Data Mining

- Near-duplicate detection
- Plagiarism detection
- Computing co-occurrence similarity (for detecting synonyms, query extension, machine translation...)

Key difference:

Mostly, off-line problems

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Applications (4/5) Bipartite Problems

- Recommendation systems (most relevant movie to a set of already watched ones)
- Personalized news aggregation (most relevant news articles to a given user's profile of interests)
- Behavioral targeting (most relevant ad for displaying to a given user)

Key differences:

Query and database objects have different nature
Objects are described by features and connections

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Applications (5/5) As a Subroutine

- Coding theory (maximum likelihood decoding)
- MPEG compression (searching for similar fragments in already compressed part)
- Clustering

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Variations of the Computation Task

Solution aspects:

- Approximate nearest neighbors
- Dynamic nearest neighbors: moving objects, deletes/inserts, changing similarity function

Related problems:

- Nearest neighbor: nearest museum to my hotel
- Reverse nearest neighbor: all museums for which my hotel is the nearest one
- Range queries: all museums up to 2km from my hotel
- Closest pair: closest pair of museum and hotel
- Spatial join: pairs of hotels and museums which are at most 1km apart
- Multiple nearest neighbors: nearest museums for each of these hotels
- Metric facility location: how to build hotels to minimize the sum of "museum — nearest hotel" distances

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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!

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Part II

Branch and Bound Methodology

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General Metric Space

Tell me definition of metric space

$M = (\mathbb{U}, d)$, distance function d satisfies:

Non negativity: $\forall s, t \in \mathbb{U} : d(s, t) \geq 0$

Symmetry: $\forall s, t \in \mathbb{U} : d(s, t) = d(t, s)$

Identity: $d(s, t) = 0 \Rightarrow s = t$

Triangle inequality: $\forall r, s, t \in \mathbb{U} : d(r, t) \leq d(r, s) + d(s, t)$

Basic Examples:

- Arbitrary metric space, oracle access to distance function
- k -dimensional Euclidean space with Euclidean, weighted Euclidean, Manhattan or L_p metric
- Strings with Hamming or Levenshtein distance

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Metric Spaces: More Examples

- Finite sets with Jaccard metric $d(A, B) = 1 - \frac{|A \cap B|}{|A \cup B|}$
- Correlated dimensions: $\bar{x} \cdot M \cdot \bar{y}$ distance
- Hausdorff distance for sets

Similarity spaces (no triangle inequality):

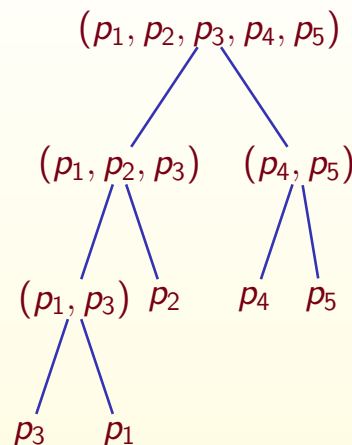
- Multidimensional vectors with scalar product similarity
- Bipartite graph, co-citations similarity for vertices in one part
- Social networks with “number of joint friends” similarity

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Branch and Bound: Search Hierarchy

Database $S = \{p_1, \dots, p_n\}$ is represented by a tree:

- Every node corresponds to a subset of S
- Root corresponds to S itself
- Children's sets cover parent's set
- Every node contains a “description” of its subtree providing easy-computable lower bound for $d(q, \cdot)$ in the corresponding subset

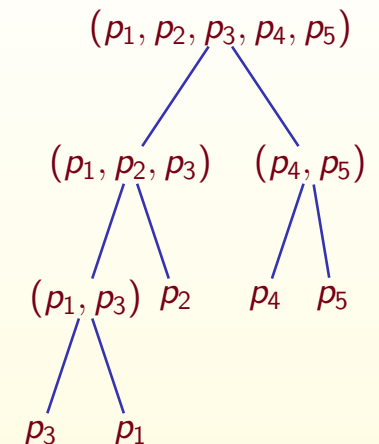


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Branch and Bound: Range Search

Task: find all i $d(p_i, q) \leq r$:

- 1 Make a depth-first traversal of search hierarchy
- 2 At every node compute the lower bound for its subtree
- 3 Prune branches with lower bounds above r



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B&B: Nearest Neighbor Search

Task: find $\operatorname{argmin}_{p_i} d(p_i, q)$:

- 1 Pick a random p_i , set $p_{NN} := p_i, r_{NN} := d(p_i, q)$
- 2 Start range search with r_{NN} range
- 3 Whenever meet p' such that $d(p', q) < r_{NN}$, update $p_{NN} := p', r_{NN} := d(p', q)$

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B&B: Best Bin First

Task: find $\operatorname{argmin}_{p_i} d(p_i, q)$:

- 1 Pick a random p_i , set $p_{NN} := p_i, r_{NN} := d(p_i, q)$
- 2 Put the root node into **inspection queue**
- 3 Every time: take the node with a smallest lower bound from inspection queue, compute lower bounds for children subtrees
- 4 Insert children with lower bound below r_{NN} into inspection queue; prune other children branches
- 5 Whenever meet p' such that $d(p', q) < r_{NN}$, update $p_{NN} := p', r_{NN} := d(p', q)$

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Part III

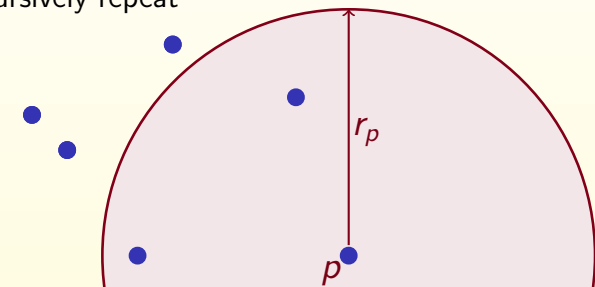
Vantage-Point Trees and Relatives

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Vantage-Point Partitioning

Uhlmann'91, Yianilos'93:

- 1 Choose some object p in database (called **pivot**)
- 2 Choose partitioning radius r_p
- 3 Put all p_i such that $d(p_i, p) \leq r$ into "inner" part, others to the "outer" part
- 4 Recursively repeat



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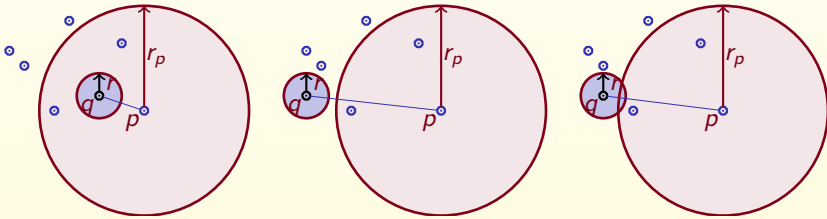
Pruning Conditions

For r -range search:

If $d(q, p) > r_p + r$ prune the inner branch

If $d(q, p) < r_p - r$ prune the outer branch

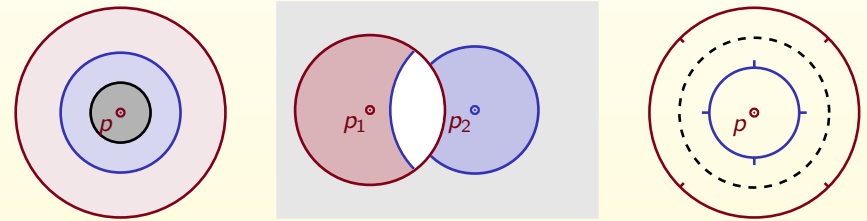
For $r_p - r \leq d(q, p) \leq r_p + r$ we have to inspect both branches



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Variations of Vantage-Point Trees

- **Burkhard-Keller tree:** pivot used to divide the space into m rings [Burkhard&Keller'73](#)
- **MVP-tree:** use the same pivot for different nodes in one level [Bozkaya&Ozsoyoglu'97](#)
- **Post-office tree:** use $r_p + \delta$ for inner branch, $r_p - \delta$ for outer branch [McNutt'72](#)



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Part IV

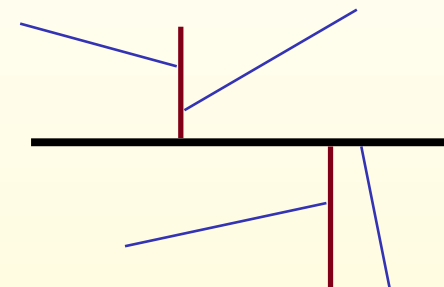
Generalized Hyperplane Trees and Relatives

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Generalized Hyperplane Tree

Partitioning technique ([Uhlmann'91](#)):

- Pick two objects (called pivots) p_1 and p_2
- Put all objects that are closer to p_1 than to p_2 to the left branch, others to the right branch
- Recursively repeat



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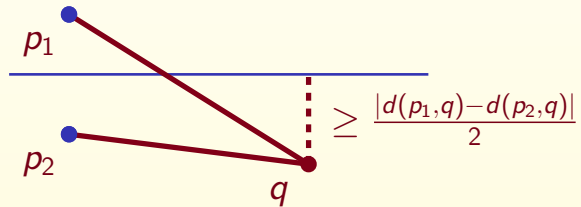
GH-Tree: Pruning Conditions

For r -range search:

If $d(q, p_1) > d(q, p_2) + 2r$ prune the left branch

If $d(q, p_1) < d(q, p_2) - 2r$ prune the right branch

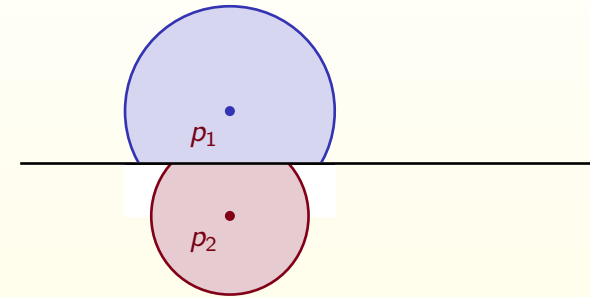
For $|d(q, p_1) - d(q, p_2)| \leq 2r$ we have to inspect both branches



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Bisector trees

Let's keep the covering radius for p_1 and left branch, for p_2 and right branch: useful information for stronger pruning conditions



Variation: monotonous bisector tree (Noltemeier, Verbag, Zirkelbach'92) always uses parent pivot as one of two children pivots

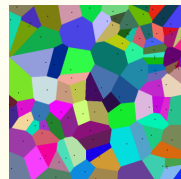
Exercise: prove that covering radii are monotonically decrease in mb-trees

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Geometric Near-Neighbor Access Tree

Brin'95:

- Use m pivots
- Branch i consists of objects for which p_i is the closest pivot
- Stores minimal and maximal distances from pivots to all "brother"-branches



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Exercises

Prove that Jaccard distance $d(A, B) = 1 - \frac{|A \cap B|}{|A \cup B|}$ satisfies triangle inequality

Prove that covering radii are monotonically decrease in mb-trees

Construct a database and a set of potential queries in some multidimensional Euclidean space for which **all described data structures** require $\Omega(n)$ nearest neighbor search time

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Highlights

- Nearest neighbor search is fundamental for information retrieval, data mining, machine learning and recommendation systems
- Balls, generalized hyperplanes and Voronoi cells are used for space partitioning
- Depth-first and Best-first strategies are used for search

Thanks for your attention! Questions?

References

Course homepage <http://yury.name/algoweb.html>



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/>



E. Chávez, G. Navarro, R. Baeza-Yates, J. L. Marroquín
Searching in Metric Spaces. ACM Computing Surveys, 2001.
<http://www.cs.ust.hk/~leichen/courses/comp630j/readings/acm-survey/searchinmetric.pdf>



G.R. Hjaltason, 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