Nearest Neighbor Search by Branch and Bound

Algorithmic Problems Around the Web #2

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Outline

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1. Short Intro to Nearest Neighbors
2. Branch and Bound Methodology

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2. Branch and Bound Methodology
3. Around Vantage-Point Trees

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Part I

Short Intro to Nearest Neighbors

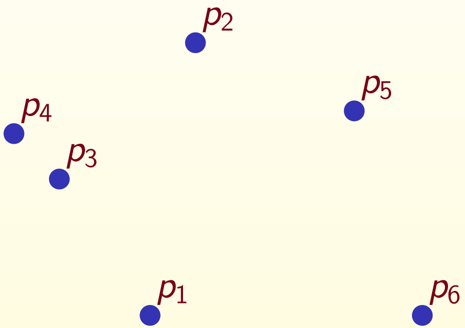
Problem Statement

Search space: object domain $\mathbb{U}$, similarity function σ

Input: database $S = \{p_1, \ldots, p_n\} \subseteq \mathbb{U}$

Query: $q \in \mathbb{U}$

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



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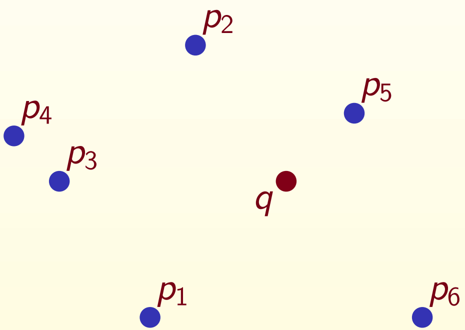

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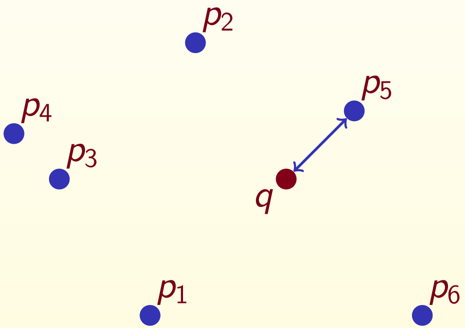

Applications (1/5) Information Retrieval

- 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

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

Applications (3/5) Data Mining

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

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Key difference:

Mostly, off-line problems

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)

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Key differences:

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

Applications (5/5) As a Subroutine

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

Variations of the Computation Task

Solution aspects:

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

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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

Brief History

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- **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!

Part II

Branch and Bound Methodology

General Metric Space

Tell me definition of metric space

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

Non negativity: $\forall s, t \in \mathbb{U}: \quad d(s,t) \geq 0$
Symmetry: $\forall s, t \in \mathbb{U}: \quad d(s,t) = d(t,s)$
Identity: $d(s,t) = 0 \Rightarrow s = t$
Triangle inequality: $\forall r, s, t \in \mathbb{U}: \quad d(r,t) \leq d(r,s) + d(s,t)$

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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

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

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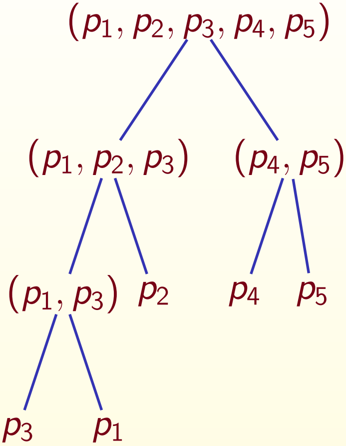
Similarity spaces (no triangle inequality):

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

Branch and Bound: Search Hierarchy

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

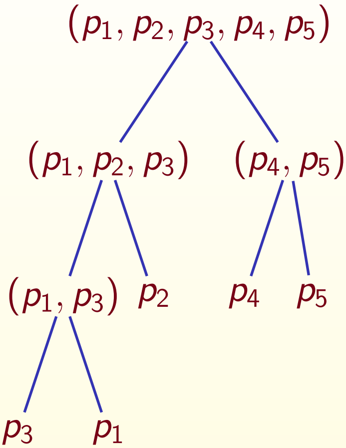
- Every node corresponds to a subset of S
- Root corresponds to S itself
- Children's sets cover parent's set
- Every node contains a "description" of its subtree providing easy-computable lower bound for $d(q, \cdot)$ in the corresponding subset



Branch and Bound: Range Search

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

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



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 $p_{NN} := p', r_{NN} := d(p', q)$

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 $p_{NN} := p', r_{NN} := d(p', q)$

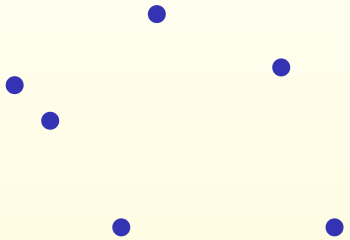
Part III

Vantage-Point Trees and Relatives

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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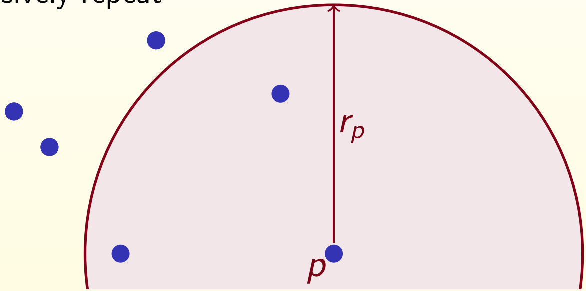
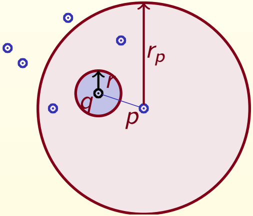


Pruning Conditions

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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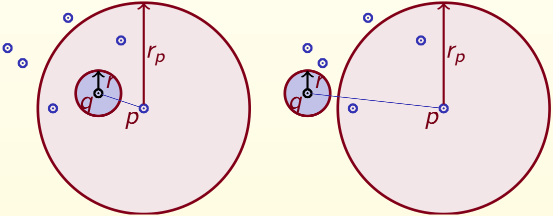

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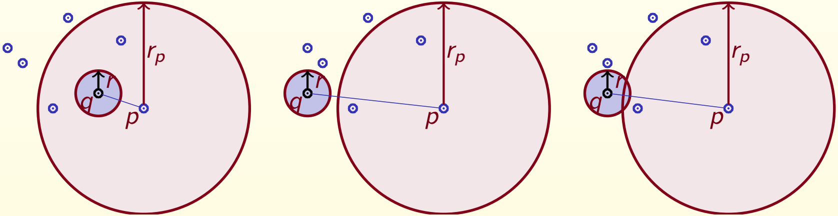
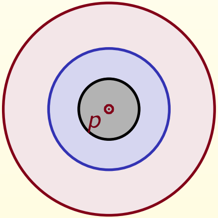


Variations of Vantage-Point Trees

- **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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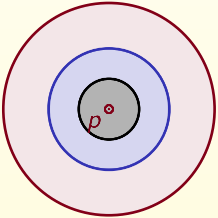

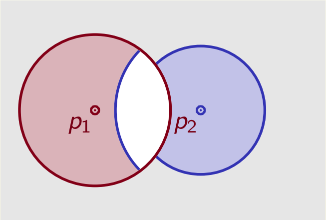

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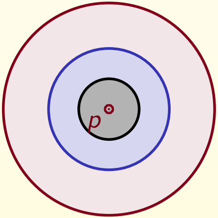

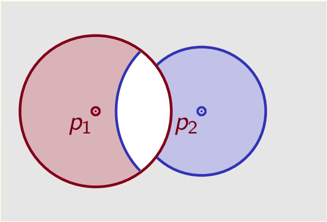

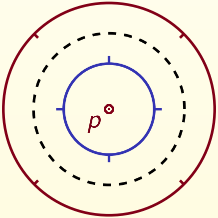

Part IV

Generalized Hyperplane Trees and Relatives

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
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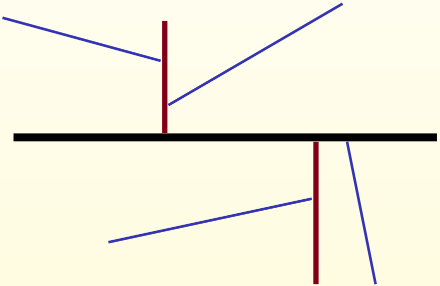

GH-Tree: Pruning Conditions

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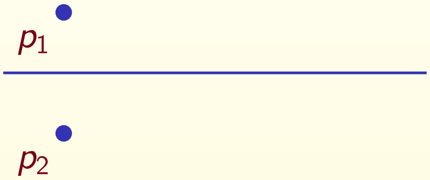

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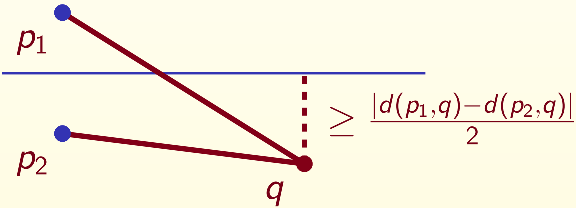
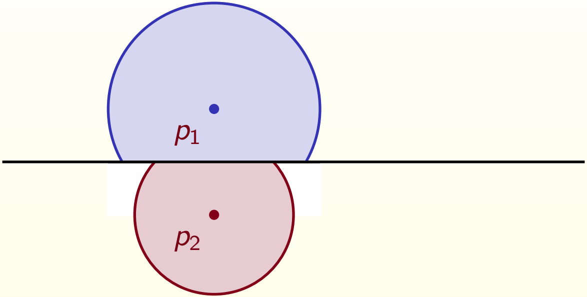


Bisector trees

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



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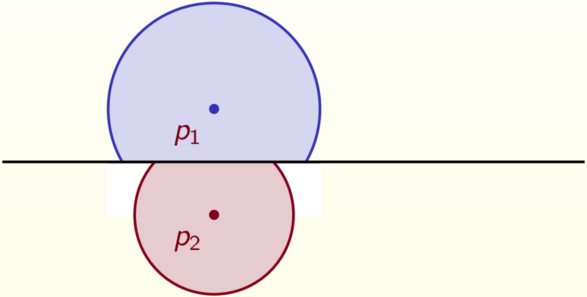

Variation: monotonous bisector tree (Noltemeier, Verbarg, Zirkelbach'92) always uses parent pivot as one of two children pivots

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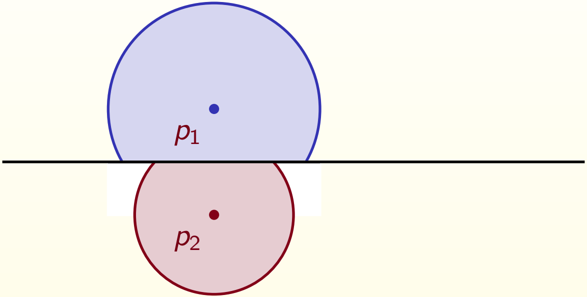

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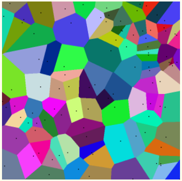
Exercise: prove that covering radii are monotonically decrease in mb-trees

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



Exercises

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

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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

Highlights

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Thanks for your attention! Questions?

References

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