

# Other Use of Triangle Inequality

## Algorithms for Nearest Neighbor Search: Lecture 2

Yury Lifshits

<http://yury.name>

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



# Outline

- 1 Nearest Neighbors via Walking

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- 2 Matrix-Based Techniques

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- 3 Basic Techniques for Euclidean Space

# Chapter VI

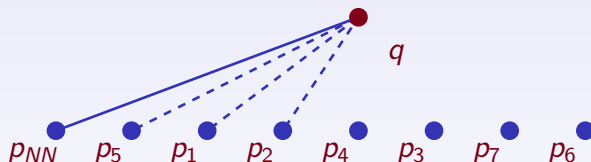
## Nearest Neighbors via Walking

# Orchard's Algorithm

## Preprocessing:

For every object  $p_i \in S$  construct a list  $L(p_i)$  of all other objects sorted by their similarity to  $p_i$

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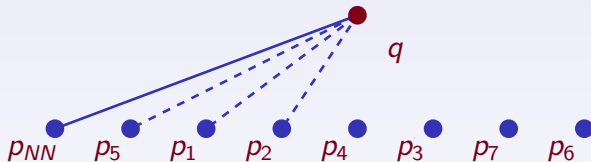


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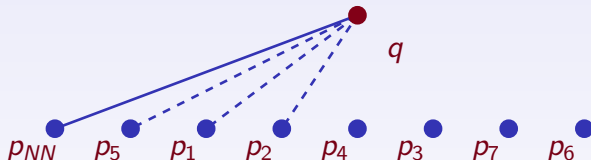
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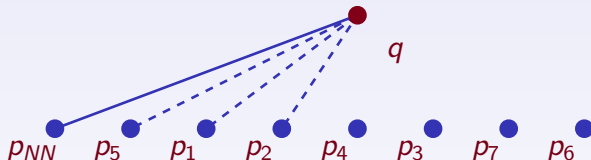


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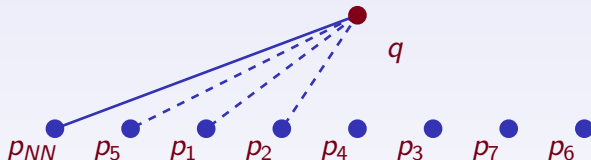
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- **Stopping condition:** we reached  $p'$  having  $d(p', q) \geq 2d(p_{NN}, q)$

# Hierarchical Orchard's Algorithm

- Randomly choose  $S_1 \subset S_2 \subset \dots S_k = S$  with  $|S_i|/|S_{i-1}| \approx \alpha > 1$
- Start with Orchard algorithm on  $S_1$
- For every  $i$  from 2 to  $k$  apply Orchard's algorithm for  $S_i$  using result of the previous step as a starting point

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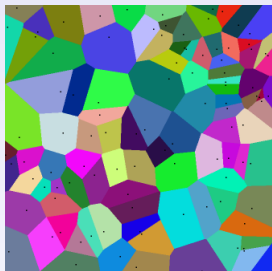
Inspired by classic skip list technique Pugh'90

# Delaunay Graph Algorithm

## **Delaunay Graph:**

Construct Voronoi diagram for set in Euclidean space.

Draw an edge between every two points whose Voronoi cells are adjacent

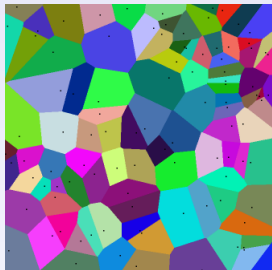


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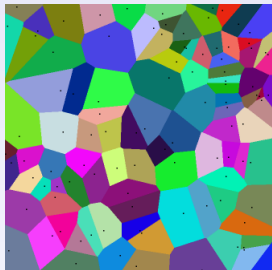
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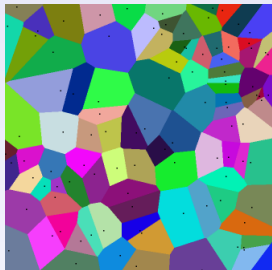
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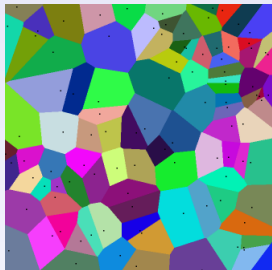
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- Otherwise return  $p$

# Delaunay Graph in General

**Exercise:** prove correctness of the above algorithm

Assume we have general metric space and full matrix of pairwise distances. How Delaunay graph should be defined?

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Navarro, 2002: for any distance matrix any two objects can be adjacent :-)

# Spatial Approximation Tree: Construction

Navarro'99:

- Set a random object  $p$  to be root
- Partitioning technique:
  - Inspect all other object in order by their similarity to  $p$
  - Whenever some  $p'$  is closer to  $p$  than to any of already chosen children  $Ch(p)$  add  $p'$  to children set
  - Put every other object  $p''$  to the subtree of closet member of  $Ch(p)$
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**Exercise:** prove that covering radius for children subtree is never exceeding covering radius of parent subtree

# SA-Tree: Search

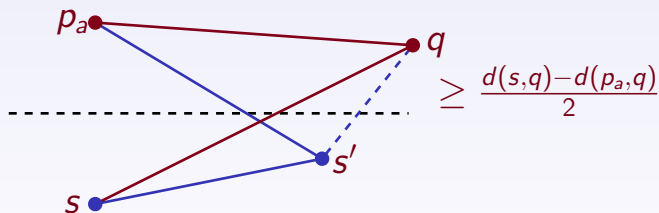
- Start from the root  $p$
- For every node to be inspected:
  - keep global candidate  $p_{NN}$   
(closest object to query visited so far)
  - and  $p_a$  — closest to  $q$  among  
all ancestors and brothers of current node
- Use usual depth-first or best-first tree traversal
- Processing current node  $t$ :
  - Compute distances from  $q$  to all children of  $t$
  - Go to child  $s$  whenever  $d(q, s) < d(q, p_a(s)) + 2r_{NN}$

# SA-Tree: Correctness

**Observation:** fix node  $s$ , let  $p_a$  be its ancestor/brother and  $s'$  be some objected in its subtree. Then  $s'$  is closer to  $s$  than to  $p_a$

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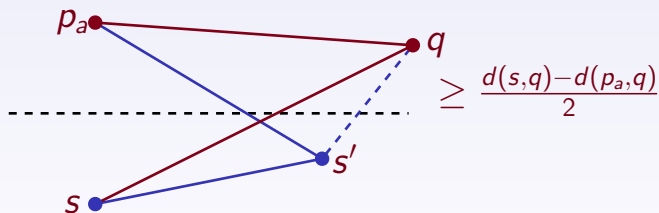
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If there exists  $s'$  such that  $d(s', q) < r_{NN}$  then  
 $d(s, q) < d(p_a, q) + 2r_{NN}$

# Chapter VII

## Matrix-Based Techniques

# Approximating and Eliminating Search Algorithm

## Preprocessing:

Vidal'86

Compute  $n \times n$  matrix of pairwise distances in  $S$

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## Query processing:

- Maintain a set  $C$  of candidate objects, initially  $C := S$
- For every  $p \in C$  keep the lower bound  $d_l(q, p)$
- Main loop:
  - Choose  $p \in C$  with smallest lower bound, compute  $d(q, p)$ , update  $p_{NN}, r_{NN} = d(q, p_{NN})$  if necessary
  - **Approximating:** update lower bounds in  $C$  using  $d(q, p') \geq d(q, p) + d(p, p')$  inequality
  - **Eliminating:** delete all elements in  $C$  whose lower bounds exceeded  $r_{NN}$

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Compute  $n \times m$  matrix choosing  $m$  objects as pivots

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**Range search:**

- Compute all query-pivot distances
- Compute lower bounds for all non-pivot objects
- Eliminate objects with lower bound exceeding search range
- Explicitly check remaining non-pivots

# TLAESA

A combination of bisector tree and LAESA

**Data structure:**

Micó, Oncina, Carrasco'96

Usual bisector tree

Additionally,  $m$  pivots

Distances from pivots to all objects are precomputed



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## Query processing

Compute distances from query to pivots

Depth-first/Best-first search in bisector tree

Additional condition to prune subtree of some object  $s$ :

$$\exists i : |d(p_i, s) - d(p_i, q)| \geq r_c(s) + r_{NN}$$

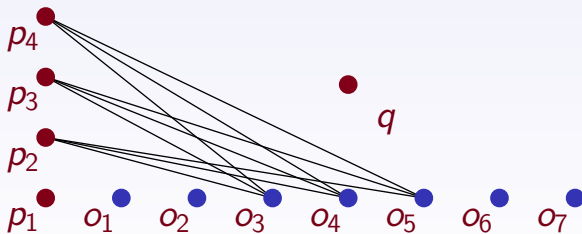
# Shapiro's Algorithm (1/2)

## Data structure:

Shapiro'77

$n \times m$  distance matrix (pivots  $p_1, \dots, p_m$ )

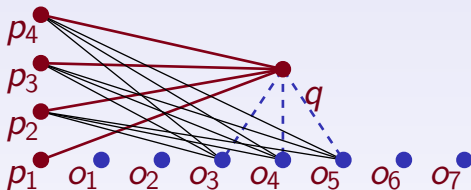
Non-pivot objects are sorted by their distances to first pivot  $p_1 : o_1, \dots, o_n$



# Shapiro's Algorithm (2/2)

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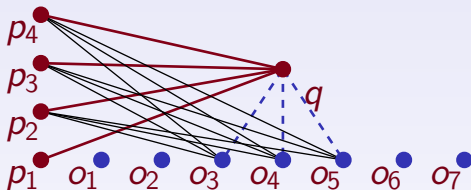
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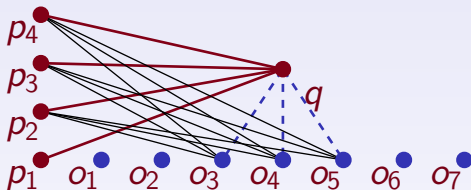
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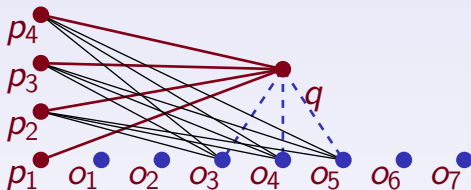
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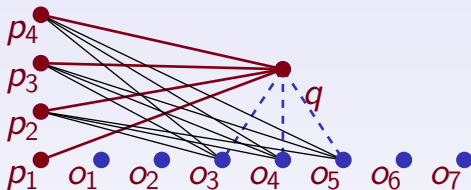
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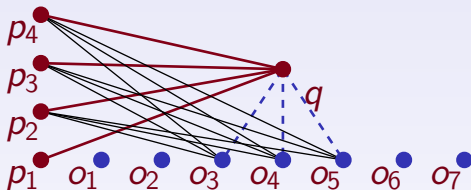
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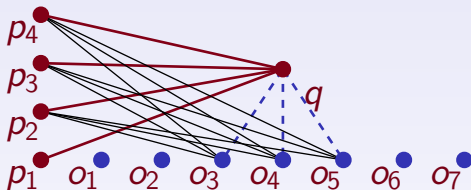
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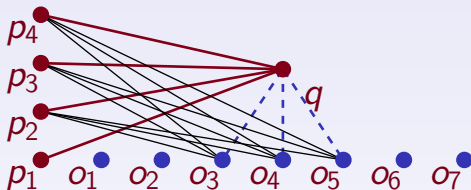
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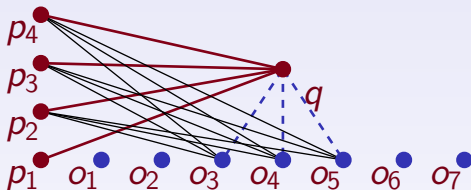
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But published before both: 1977 vs 1991 and 1992!

# Chapter VIII

## Basic Techniques for Euclidean Space

# Advantages of Euclidean Space

- Rich mathematical formalisms for defining a boundary of any set

**Examples:** rectangles, hyperplanes, polynomial curves

- Easy computation of lower bound on distance between query point and any set boundary
- (Tomorrow) Easy definable mappings to smaller spaces

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## Preprocessing:

Bentley, 1975

Top-down partitioning

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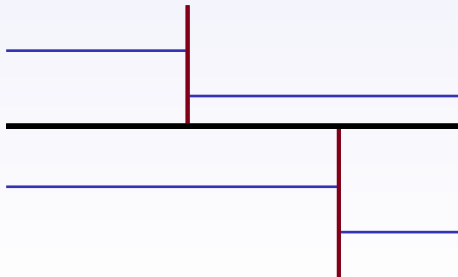
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Bottom-up partitioning

Keep bounding rectangles

Every time: merge current rectangles

and compute bounding rectangle for every group

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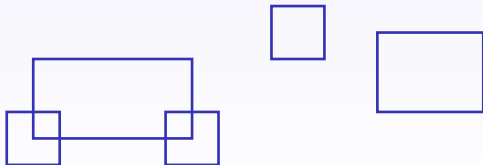
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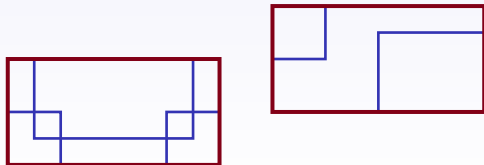
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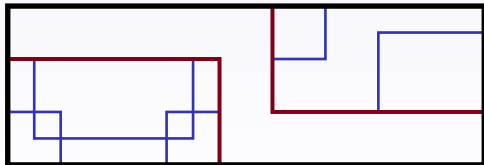
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# Exercises

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Prove monotonicity of covering radii in SA-tree

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Thanks for your attention! Questions?

# References

**Course homepage** <http://simsearch.yury.name/tutorial.html>



**Y. Lifshits**

The Homepage of Nearest Neighbors and Similarity Search

<http://simsearch.yury.name>



**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](http://www.cs.utexas.edu/~abhinay/ee382v/Project/Papers/ft_gateway.cfm.pdf)