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



1/23

Chapter VI

Nearest Neighbors via Walking

Outline



- 2 Matrix-Based Techniques
- Basic Techniques for Euclidean Space

2 / 23

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 q p_{NN} p_5 p_1 p_2 p_4 p_3 p_7 p_6

Query processing:

- Start from some random *p_{NN}*
- Inspect members of $L(P_{NN})$ from left to right
- Whenever meet p' having $d(p',q) < d(p_{NN},q)$, set $p_{NN} := p'$
- Stopping condition: we reached p' having d(p', q) ≥ 2d(p_{NN}, q)

Hierarchical Orchard's Algorithm

- Randomly choose $S_1 \subset S_2 \subset \ldots S_k = S$ 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

Inspired by classic skip list technique Pugh'90

5 / 23

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?

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

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



Search algorithm:

- Start from a random point
- Check all Delaunay neighbors of current object *p*
- If some p' is closer to q, move to p' and repeat
- Otherwise return *p*

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)
- Recursively repeat

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 $d(q, s) < d(q, p_a(s)) + 2r_{NN}$

9 / 23

Chapter VII

Matrix-Based Techniques

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



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

10/23

Vidal'86

Approximating and Eliminating Search Algorithm

Preprocessing:

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

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') ≥ d(q, p) + d(p, p') inequality
 - Eliminating: delete all elements in *C* whose lower bounds exceeded *r_{NN}*

Linear AESA

Advantage of AESA: small number of distance computations Disadvantages: large storage and non-distance computation

Linear AESA:

Micó, Oncina, Vidal'94

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

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

13 / 23

Shapiro's Algorithm (1/2)

Data structure:

Shapiro'77

 $n \times m$ distance matrix (pivots p_1, \ldots, p_m) Non-pivot objects are sorted by there distances to first pivot $p_1 : o_1, \ldots, o_n$



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

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*:

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

14 / 23

Shapiro's Algorithm (2/2)



Query processing

Compute distances from query to pivots Start with o_i having $d(p_1, o_i) \approx d(p_1, q)$ Inspect other objects in order i - 1, i + 1, i - 2, i + 2, ...Whenever meet better candidate change the center of inspection Use flags to avoid double-check Use all pivots to skip some objects (similar to AESA) Stopping condition: $|d(p_1, o_i) - d(p_1, q)| \ge r_{NN}$

Actually, it's a mixture of LAESA and Orchard 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

18/23

Guttman, 1984

k-d Tree

Preprocessing:

Bentley, 1975

17 / 23

Top-down partitioning On level /: split the current set by hyperplane orthogonal to / mod k axis

Query processing:

Standard branch and bound



R-Tree

Preprocessing:

Bottom-up partitioning Keep bounding rectangles Every time: merge current rectangles and compute bounding rectangle for every group

Query processing:

Standard branch and bound

Insertions/delitions: similar to M-tree, B-tree



Exercises

Prove correctness of Delaunay graph stopping condition

Prove monotonicity of covering radii in SA-tree

Highlights

- Orchard: use local search around the current candidate, move whenever meet better option
- Spatial tree approximation: emulating Delaunay graph in general metric space
- AESA: use every inter-object distance to get a lower bound on unchecked distances
- Euclid space: use explicit boundaries in metric trees

Thanks for your attention! Questions?

21 / 23

References

http://simsearch.yury.name/tutorial.html **Course homepage** 9 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