Proximity Searching and the Quest for the Holy Grail

David M. Mount

Department of Computer Science
University of Maryland, College Park

CG-APT 2012: Algorithms in the Field

Proximity Searching

Proximity searching:

A set of related geometric retrieval problems that involve finding the objects close to a given query object.

Given an n-element set P of points in a metric space. Will assume that the space is a vector space of low-dimension with a Minkowski norm.

- Nearest neighbor searching: Given a query point q, find the closest point of P to q
- (Bounded) Range searching: Given a bounded query range Q, count/report the points of $P \cap Q$

Proximity Searching: Variants

Variations and issues:

- Nearest-Neighbor Searching:
  - k-nearest neighbors
  - high dimensions (avoid exponential dependencies in dimension)
  - exploit properties of metric spaces (e.g., doubling dimension)
  - space-time tradeoffs
  - non-metric distances (e.g., Bregman Divergence)
- Range Searching:
  - range emptiness
  - more space-time tradeoffs
  - semigroup properties (integral: $x + y$, idempotent: $\max(x, y)$)

Proximity Searching: Applications

Applications:

- Pattern recognition and classification
- Object recognition in images (SIFT descriptors [Lowe 1999, 2004])
- Content-based retrieval:
  - Shape matching
  - Image retrieval
  - Document retrieval
  - Biometric identification (face/fingerprint/voice recognition)
- Clustering and phylogeny
- Data compression (vector quantization)
- Physical simulation (collision detection and response)
- Computer graphics: photon mapping and point-based modeling

. . . and many more

The problem that launched a thousand data structures

- 2-dimensions
  - Voronoi diagram + point location
- Low dimensional vector spaces
  - grids, kd-trees, quadtrees, R-trees, ...and variants
  - approximate Voronoi diagrams (AVD) [Har-Peled 2001, Arya *et al.* 2009]
- High dimensional vector spaces
  - locality sensitive hashing (LSH) [Gionis *et al.* 1999, Andoni and Indyk, 2008]
- Metric spaces
  - metric trees and ring separator trees [Indyk and Motwani 1998, Krauthgamer and Lee 2005] (...and variants)
  - pivot-based methods (AESA, LAESA, and others) [Brin 1995] [Chavéz *et al.* 2001]

Overview

- The Structureless Structure
- Enumerating Distances
- ANN via Polytope Membership

Overview

- The Structureless Structure
- Enumerating Distances
- ANN via Polytope Membership

The Structureless Structure

Motivation

- "Constant factors" can play a big role in query times. For example, in $O(\log n + (1/\varepsilon)^d)$ the term $(1/\varepsilon)^d$ is dominant
- Constant factors are often hidden by the memory model
- Tree-based data structures (if naively implemented) have notoriously poor memory access patterns

Morton Order

Morton Order

- Consider a point set P, lying within the unit hypercube $[0,1)^d$
- For each $p = (p_1, \ldots, p_d) \in \mathbb{R}^d$, assume its coordinates are given w-bit binary values $p_j = \langle 0.b_{j,1} \ldots b_{j,w} \rangle$
- Map p to an integer by shuffling the bits of its coordinates,

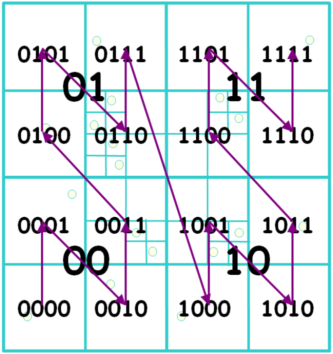
$$\sigma(p) \;=\; b_{1,1} \ldots b_{d,1} | b_{1,2} \ldots b_{d,2} | \cdots | b_{1,w} \ldots b_{d,w}$$

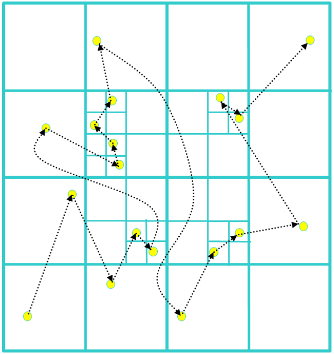
- This is called the Morton order or Z order.

Linear Quadtree

Linear Quadtree

- Sort P by Morton order
- Store the points in an array (or any 1-dimensional index)





Linear Quadtree – Easy Shuffling

Chan's Shuffle Trick [Chan 2002]

Compare Morton codes without bit manipulation, just exclusive-or!

```
// tests whether ⌊log₂ x⌋ < ⌊log₂ y⌋
f(x, y) { return (x > y ? false : x < (x ⊕ y)) }

// test whether σ(p) < σ(q)
compare(p, q) {
    i ← 1
    for j ← 2, ..., d do
        if (f(p_i ⊕ q_i, p_j ⊕ q_j)) i ← j
    return p_i < q_i
}
```

A Minimalist Approach to Nearest Neighbor Searching

Chan [Chan 2006] showed that it is possible to use a Morton-sorted array (no additional information) to answer approximate nearest neighbor queries

- Apply a random shift to the origin
- Query time is $O(\log n + (1/\varepsilon)^d)$ in expectation
- Space is $O(n)$, in fact, it is an in-place algorithm
- Preprocessing time is $O(n \log n)$
- Easily made dynamic (e.g., store in a skip list)

The program is absurdly short – less than 60 lines of C!

Competitive with ANN (my kd-tree implementation) in low dimensions

Overview

- The Structureless Structure
- Enumerating Distances
- ANN via Polytope Membership

Distance Enumeration

Motivations:

- Object-recognition: Want a sufficiently large number of high quality features [Lowe 1999]
- Global illumination: Want to collect a sufficiently large number of sampled photons near a point [Jensen 2001]

Want the k nearest neighbors of q, but want to pick k on the fly

Distance Enumeration

Distance Enumerator:

- Visit the points P in increasing order of distance from a point q
- Let $\Pi(q) = \langle \pi_1, \ldots, \pi_n \rangle$, where p_{π_k} is q's kth nearest neighbor
- Generate the elements of $\Pi(q)$ efficiently, one at a time

(c, ε)-Enumerator

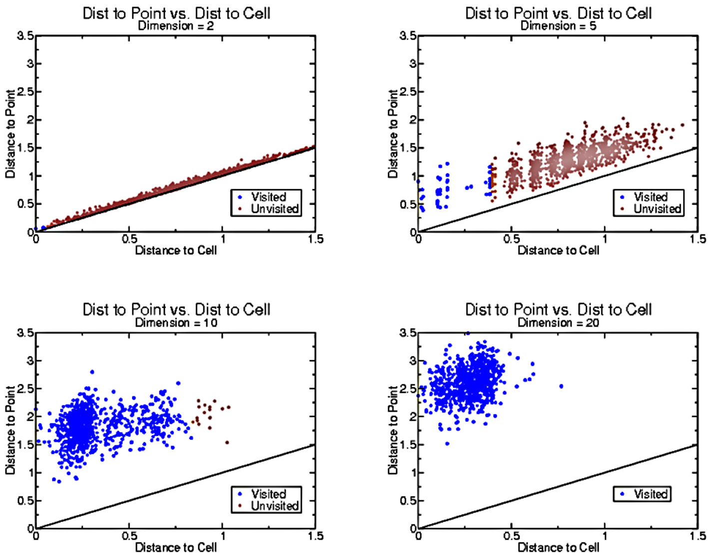
After preprocessing P, given a query point q, produces a generator for a $\Pi'(q)$ such that:

- Successive elements of $\Pi'(q)$ generated rapidly, e.g., $O(\log n)$ time
- For $1 \leq k \leq n$, a $(1 + \varepsilon)$ approximation to q's k-th nearest neighbor appears among the first $c \cdot k$ elements of Π'

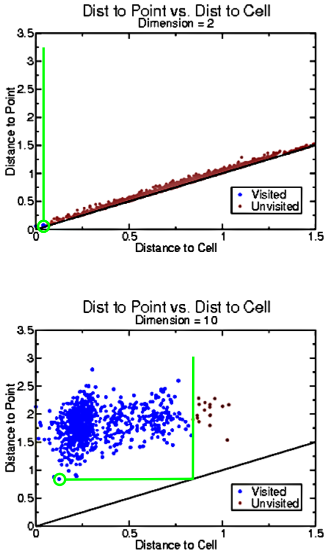
Priority Search

- Build a kd-tree T for P
- For each node u, let $C(u)$ be the cell associated with u
- Priority Search:
  - Store the root u of T in a priority queue based on $\mathrm{dist}(q, C(u))$
  - Repeat until queue is empty:
    - Extract closest node u from the queue
    - If u is a leaf then output the associate point
    - Otherwise, enqueue u's two children
- A (c, ε)-distance enumerator for $c = O(1/\varepsilon^d)$ [Arya *et al.* 1998]

Priority Search



Priority Search



Enhancing Robustness

Generate multiple “randomized” trees [Silpa-Anan and Hartley, 2008]

- Select splitting axis at random (after PCA)
- Rotate the points randomly: $O(d^2 n)$
- Project the points through a random hyperplane: $O(dn)$
- Generate m such trees and enumerate c points from each
- Total time $O(c \cdot m \log n)$

Cluster-based method [Muja and Lowe 2009]

- Preprocessing:
  - Perform k-means clustering for some k (depending on dimension)
  - Partition points into subtrees based on these clusters
  - Recurse
- Enumerate by visiting subtrees in order of distance of cluster center to query point

Overview

- The Structureless Structure
- Enumerating Distances
- ANN via Polytope Membership

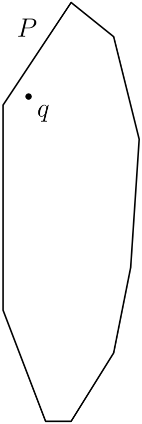
Polytope Membership Queries

Polytope Membership Queries

Given a polytope P in d-dimensional space, preprocess P to answer membership queries:

Given a point q, is $q \in P$?

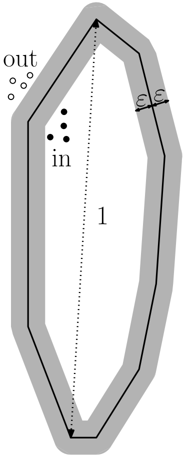
- Assume that dimension d is a constant and P is given as intersection of n halfspaces



Approximate Polytope Membership Queries

Approximate Version

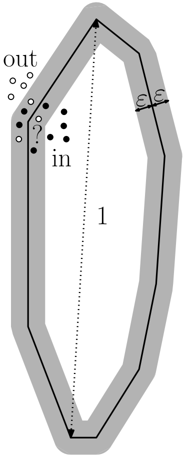
- An approximation parameter ε is given (at preprocessing time)
- Assume the polytope has diameter 1
- If the query point's distance from P's boundary:
  - $> \varepsilon$: answer must be correct
  - $\leq \varepsilon$: either answer is acceptable



Approximate Polytope Membership Queries

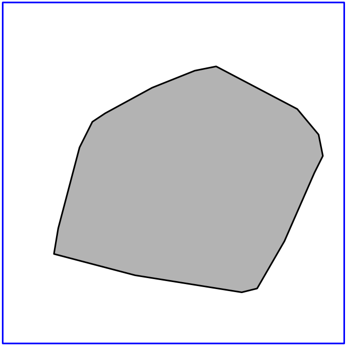
Approximate Version

- An approximation parameter ε is given (at preprocessing time)
- Assume the polytope has diameter 1
- If the query point's distance from P's boundary:
  - $> \varepsilon$: answer must be correct
  - $\leq \varepsilon$: either answer is acceptable



Split-Reduce

$t = 2$



Preprocess:

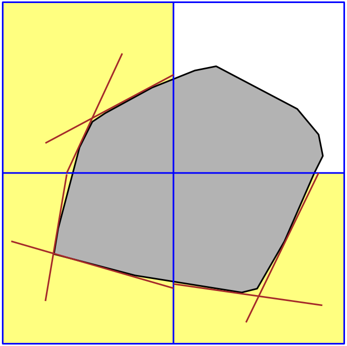
- Input P, ε, and desired query time t
- $Q \leftarrow$ unit hypercube
- Split-Reduce(Q)

Split-Reduce(Q)

- Find an ε-approximation of $Q \cap P$
- If at most t facets, then Q stores them
- Otherwise, subdivide Q and recurse

Split-Reduce

$t = 2$



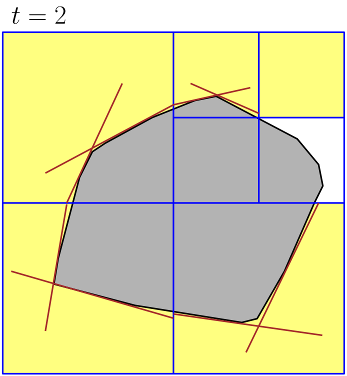
Preprocess:

- Input P, ε, and desired query time t
- $Q \leftarrow$ unit hypercube
- Split-Reduce(Q)

Split-Reduce(Q)

- Find an ε-approximation of $Q \cap P$
- If at most t facets, then Q stores them
- Otherwise, subdivide Q and recurse

Split-Reduce



Preprocess:

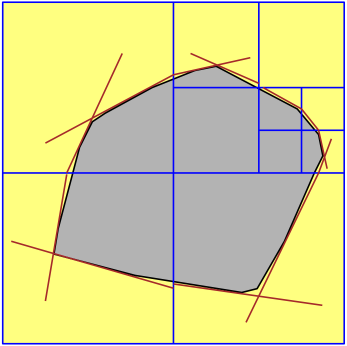
- Input P, ε, and desired query time t
- $Q \leftarrow$ unit hypercube
- Split-Reduce(Q)

Split-Reduce(Q)

- Find an ε-approximation of $Q \cap P$
- If at most t facets, then Q stores them
- Otherwise, subdivide Q and recurse

Split-Reduce

$t = 2$



Preprocess:

- Input P, ε, and desired query time t
- $Q \leftarrow$ unit hypercube
- Split-Reduce(Q)

Split-Reduce(Q)

- Find an ε-approximation of $Q \cap P$
- If at most t facets, then Q stores them
- Otherwise, subdivide Q and recurse

Space-Time Tradeoff

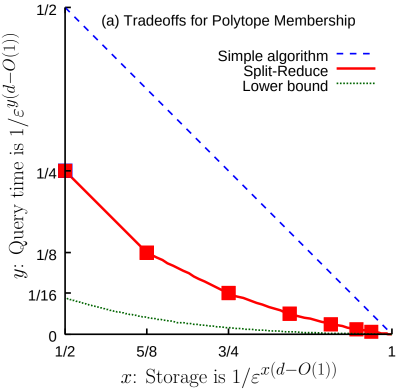
Arya *et al.* prove the following space-time tradeoff [Arya *et al.* 2011] for polytope membership queries

Theorem:

Split-Reduce can answer ε-approximate polytope membership queries with

Storage: $O(1/\varepsilon^{(d-1)/(1-k/2^k)})$

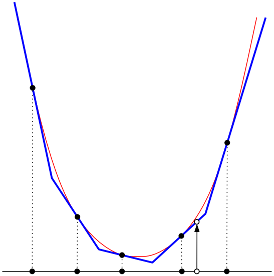
Query time: $O(1/\varepsilon^{(d-1)/2^k})$

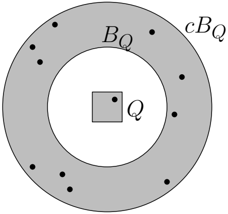


Approximate Nearest Neighbor (ANN) Searching

Approximate nearest neighbor searching can be reduced to approximate polytope membership:

- Lift: By lifting, we can reduce nearest neighbor search to ray shooting to a polytope
- Separate: Partition space into roughly $O(n)$ cells such that all nearest neighbors of each cell are of similar distance (AVD)

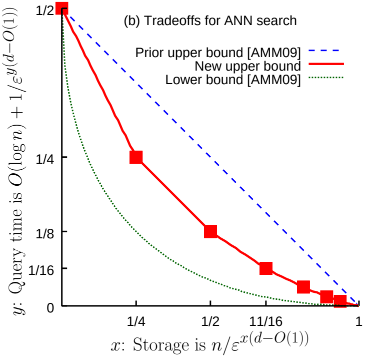




Approximate Nearest Neighbor (ANN) Searching

Space-Time Tradeoffs for ANN Search

- Arya, *et al.* [2009] showed that ANN queries could be answered in query time roughly $O(1/\varepsilon^{d/\alpha})$ with storage roughly $O(n/\varepsilon^{d(1-2/\alpha)})$, for $\alpha \geq 2$
- This is optimal in the extremes
- The reduction to polytope membership queries improves the tradeoff throughout the spectrum



Conclusions

Next steps on the quest?

- Better analyses of the performance of methods on realistic data sets
- Emphasis on general/flexibile methods (distance enumeration)
- More repositories of good test data
- How to explore/visualize/analyze the structure of multi-dimensional data sets

Acknowledgements

- The work on polytope approximation is joint with Sunil Arya and Guilherme da Fonseca
- I would also like to acknowledge the support of NSF grant CCR-0635099 and ONR grant N00014-08-1-1015

Bibliography

- M. Muja and D. G. Lowe, Fast approximate nearest neighbors with automatic algorithm configuration. *Int. Conf. on Computer Vision Theory and App.*, (VISSAPP'09), 2009, 331–340.
- C. Silpa-Anan and R. Hartley, Optimised KD-trees for fast image descriptor matching. *Proc. CVPR*, 2008, 1–8.
- A. Andoni and P. Indyk, Near-optimal hashing algorithms for approximate nearest neighbor in high dimensions. *Commun. ACM*, 51, 2008, 117–122.
- S. Arya, D. M. Mount, N. S. Netanyahu, R. Silverman, and A. Y. Wu. An optimal algorithm for approximate nearest neighbor searching in fixed dimensions. *J. ACM*, 45, 1998, 891-923.
- S. Arya, T. Malamatos, and D. M. Mount, Space-Time Tradeoffs for Approximate Nearest Neighbor Searching. *J. ACM*, 57, 2009, 1–54.
- S. Arya, G. D. da Fonseca, and D. M. Mount, Approximate Polytope Membership Queries. *Proc. 43rd Symp. on Theory of Comput.*, 2011, 579–586.
- S. Brin, Near neighbor search in large metric spaces. *Proc. 21st VLDB Conf.*, 1995, 574-584.

Bibliography

- T. M. Chan, Closest-point problems simplified on the RAM. *Proc. 13th ACM-SIAM SODA*, 2002, 472–473.
- T. M. Chan, A minimalist implementation of an approximate nearest neighbor algorithm in fixed dimensions. unpublished manuscript, 2006.
- E. Chávez, G. Navarro, R. Baeza-Yates, and J. L. Marroquín, Searching in Metric Spaces. *ACM Comput. Surveys*, 33, 2001, 273–321.
- A. Gionis, P. Indyk, R. Motwani. Similarity search in high dimensions via hashing. *Proc. 25th VLDB Conf.*, 1999, 518–529.
- S. Har-Peled. A replacement for Voronoi diagrams of near linear size. *Proc. 42nd Annu. IEEE Sympos. Found. Comput. Sci.*, 2001, 94–103.
- P. Indyk, and R. Motwani, Approximate nearest neighbors: towards removing the curse of dimensionality. *Proc. 30th Symp. on Theory of Comput.*, 1998, 604–613.
- H. W Jensen, *Realistic Image Synthesis Using Photon Mapping*. A.K. Peters, 2001

Bibliography

- R. Krauthgamer and J. R. Lee, The black-box complexity of nearest neighbor search. *Theoret. Comput. Sci.*, 348, 2005, 129–366.
- D. G. Lowe, Object recognition from local scale-invariant features. *Proc. Int. Conf. on Computer Vision*, 2, 1999, 1150–1157.
- D. G. Lowe, Distinctive image features from scale-invariant keypoints *Int. J. of Computer Vision*, 60, 2004, 91-110.
- M. L. Mico, J. Oncina, and E. Vidal, A new version of the nearest-neighbour approximating and eliminating search algorithm (AESA) with linear preprocessing time and memory requirements. *Pattern Recognition Letters*, 15, 1994, 9–17