Algorithms for Finding Nearest Neighbors (and Relatives)

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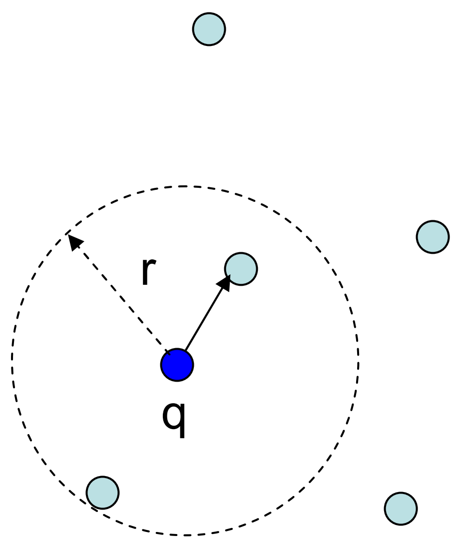
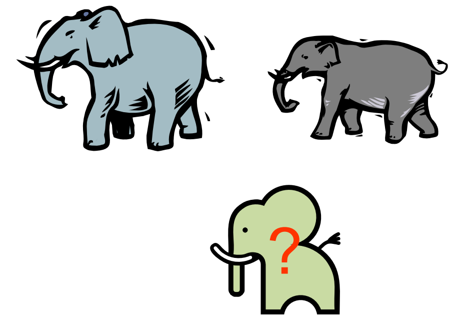
Definition

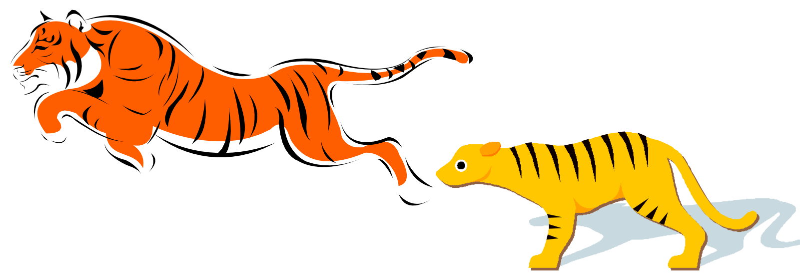
- Given: a set P of n points in R^d
- Nearest Neighbor: for any query q, returns a point $p \in P$ minimizing $||p-q||$
- r-Near Neighbor: for any query q, returns a point $p \in P$ s.t. $||p-q|| \leq r$ (if it exists)



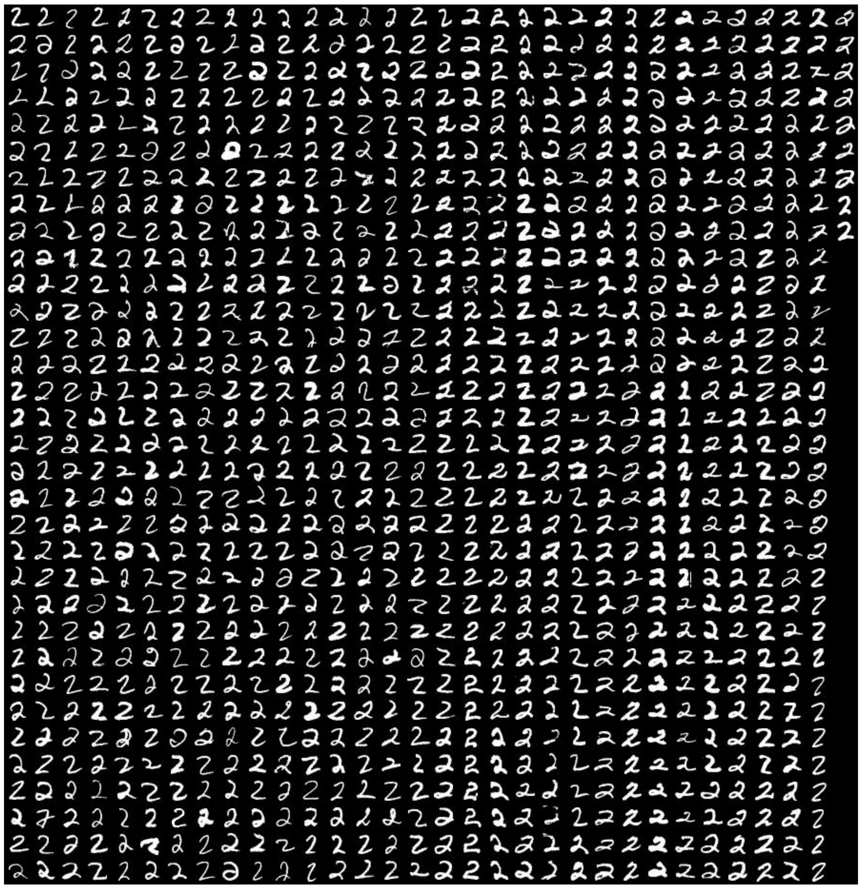
Nearest Neighbor: Motivation

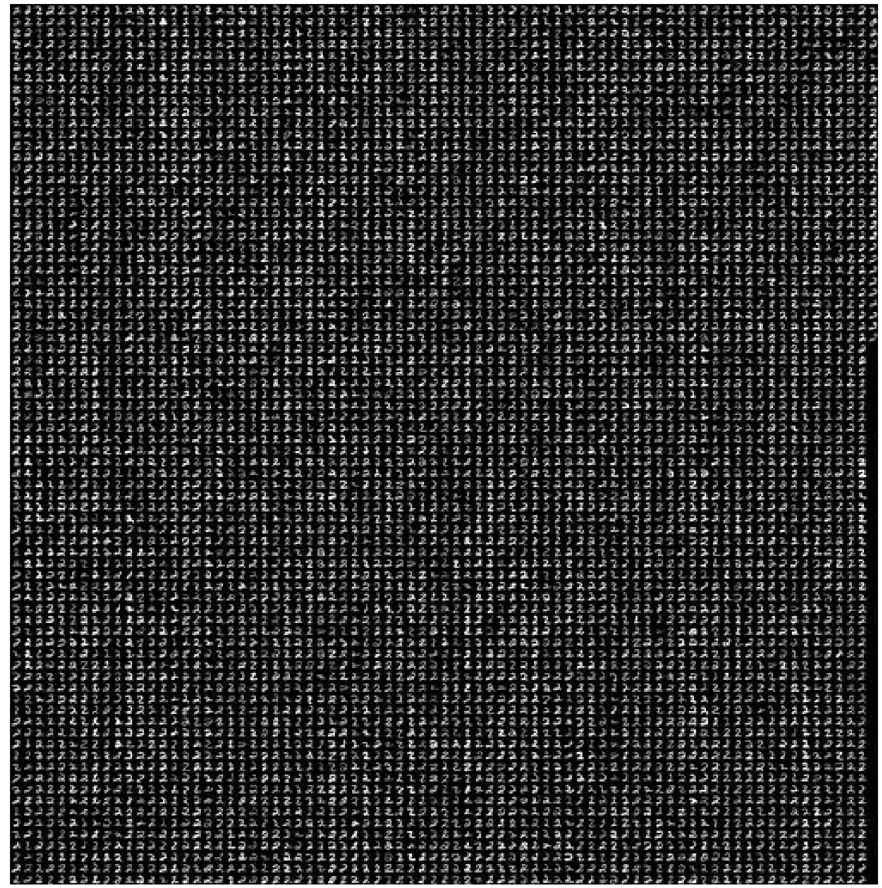
- Learning: nearest neighbor rule





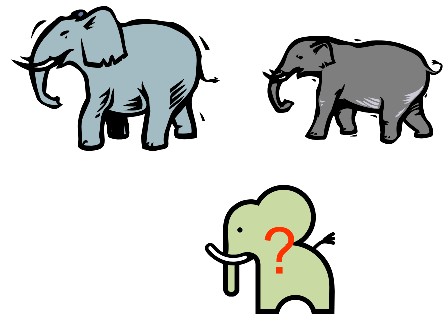
MNIST data set “2”

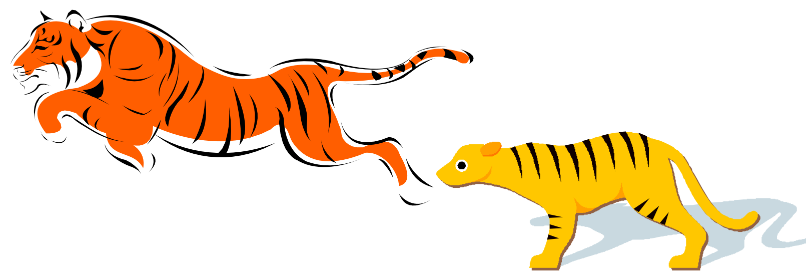




Nearest Neighbor: Motivation

- Learning: nearest neighbor rule
- Database retrieval
- Vector quantization, compression/clustering





Brief History of NN

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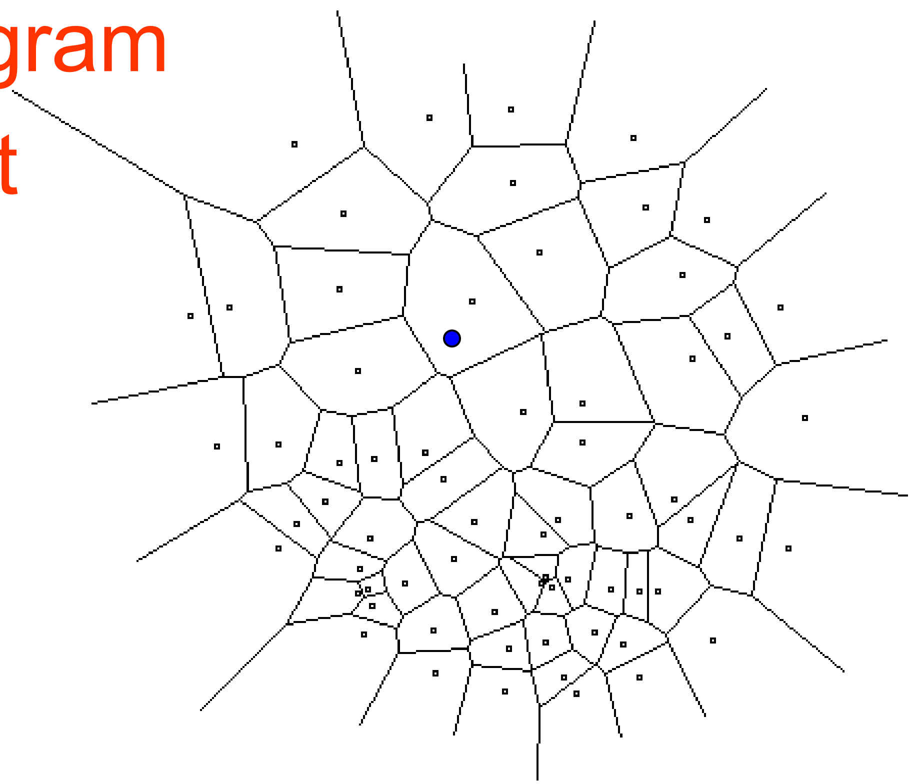
The case of d=2

- Compute Voronoi diagram
- Given q, perform point location
- Performance:
  - Space: O(n)
  - Query time: O(log n)

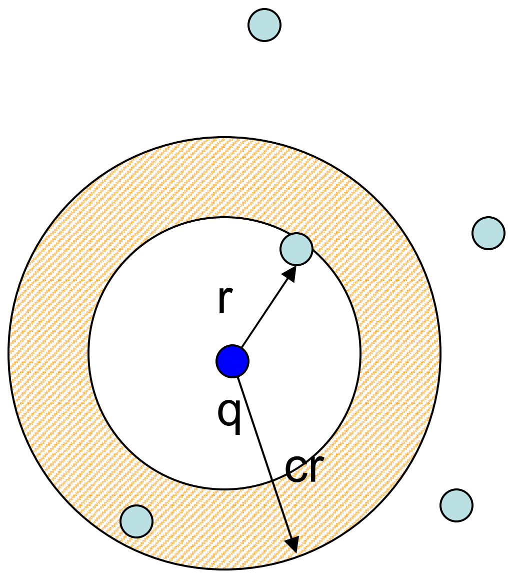


The case of d>2

- Voronoi diagram has size $n^{O(d)}$
- We can also perform a linear scan: $O(dn)$ time
- That is pretty much all what known for exact algorithms with theoretical guarantees
- In practice:
  - kd-trees work “well” in “low-medium” dimensions

Approximate Near Neighbor

- c-Approximate Nearest Neighbor: build data structure which, for any query q
  - returns $p' \in P$, $||p-q|| \leq cr$,
  - where r is the distance to the nearest neighbor of q



Plan

- Intro
- (Main memory) data structures:
  - Today: Kd-trees
    - Low-medium dimensions
    - A proud member of a (huge) family of tree-based data structures
  - Tomorrow: Locality Sensitive Hashing (LSH)
    - Dimensionality does not really matter
      (but other things do)

Kd-tree

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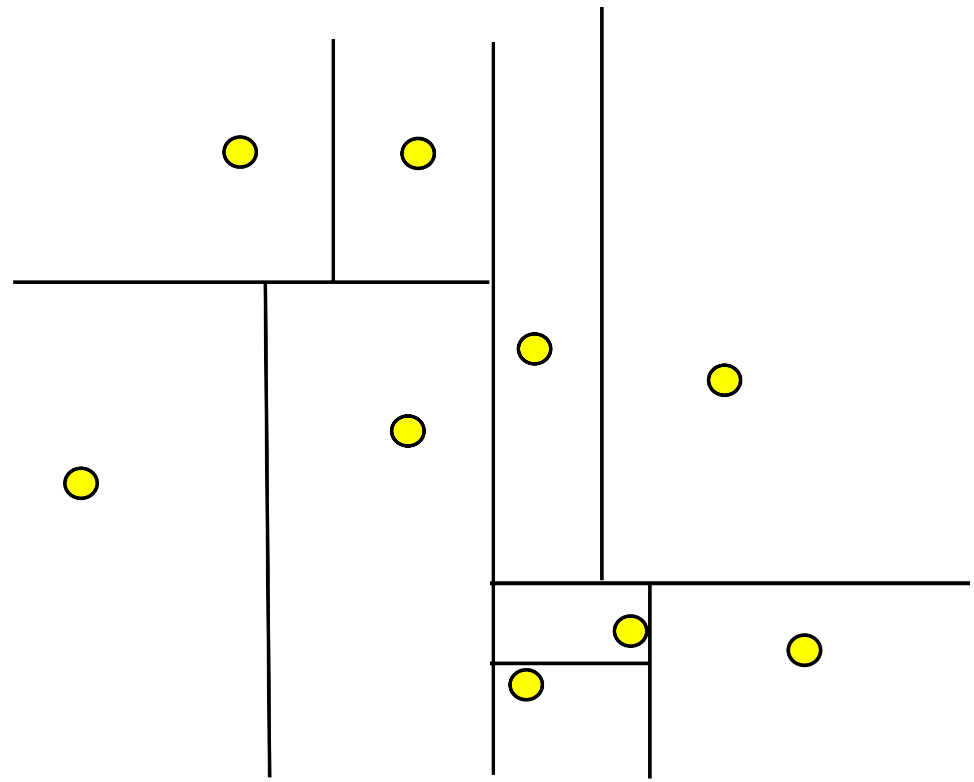
Kd-trees [Bentley'75]

- Not the most efficient solution in theory
- Everyone uses it in practice
- Algorithm:
  - Choose x or y coordinate (alternate)
  - Choose the median of the coordinate; this defines a horizontal or vertical line
  - Recurse on both sides
- We get a binary tree:
  - Size: $O(N)$
  - Depth: $O(\log N)$
  - Construction time: $O(N \log N)$

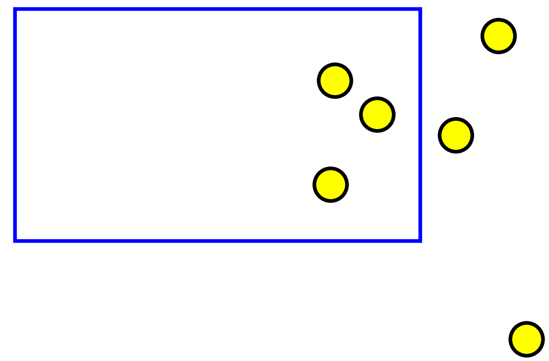
Kd-tree: Example



Each tree node v corresponds to a region Reg(v).

Searching in kd-trees

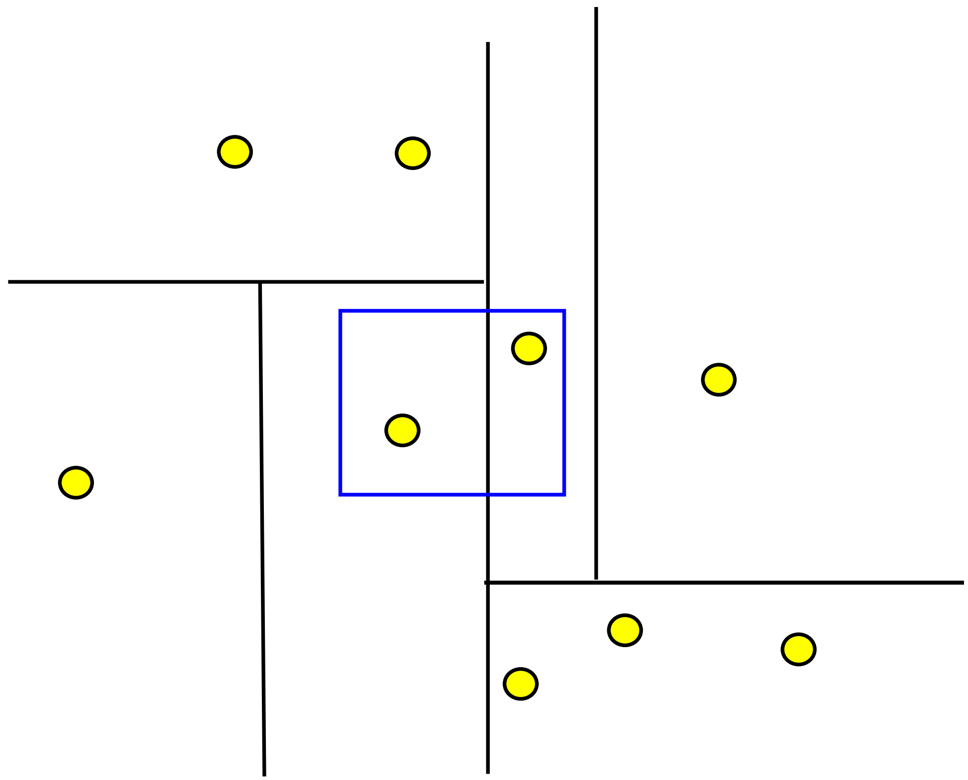
- Range Searching in 2D
  - Given a set of n points, build a data structure that for any query rectangle R, reports all points in R



Kd-tree: Range Queries

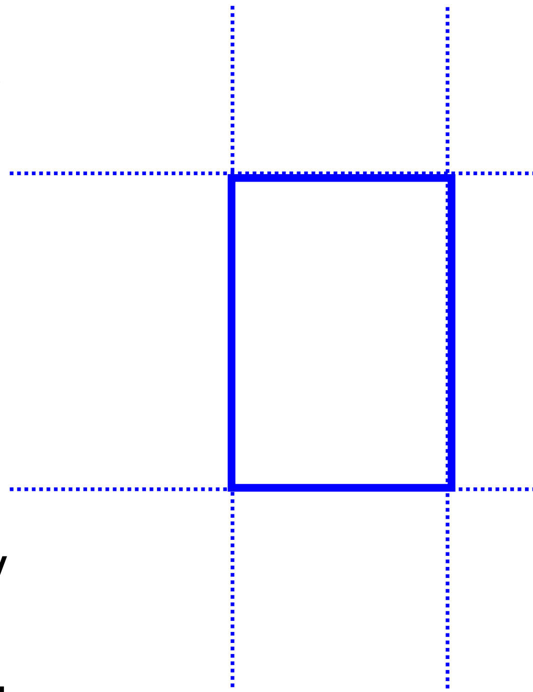
1. Recursive procedure, starting from v=root
2. Search (v,R):
   a) If v is a leaf, then report the point stored in v if it lies in R
   b) Otherwise, if Reg(v) is contained in R, report all points in the subtree of v
   c) Otherwise:
      - If Reg(left(v)) intersects R, then Search(left(v),R)
      - If Reg(right(v)) intersects R, then Search(right(v),R)

Query demo



Query Time Analysis

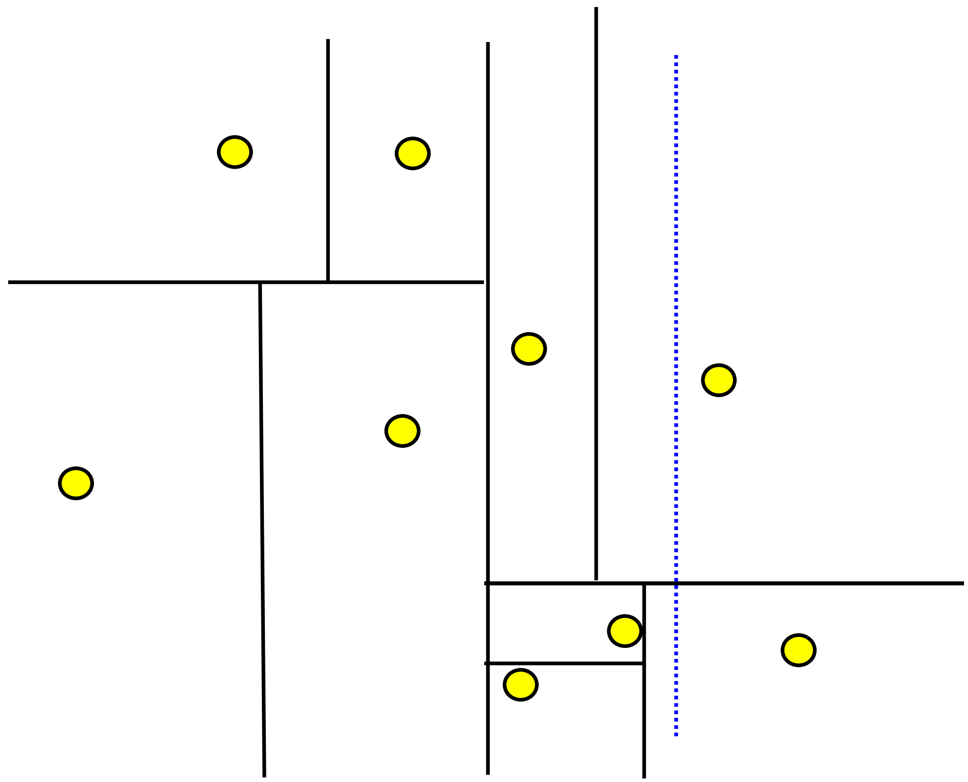
- We will show that Search takes at most $O(n^{1/2}+P)$ time, where P is the number of reported points
  - The total time needed to report all points in all sub-trees (i.e., taken by step b) is O(P)
  - We just need to bound the number of nodes v such that Reg(v) intersects R but is not contained in R. In other words, the boundary of R intersects the boundary of Reg(v)
  - Will make a gross overestimation: will bound the number of Reg(v) which are crossed by any of the 4 horizontal/vertical lines



Query Time Continued

- What is the max number $Q(n)$ of regions in an n-point kd-tree intersecting (say, vertical) line ?
  - If we split on x, $Q(n)=1+Q(n/2)$
  - If we split on y, $Q(n)=2*Q(n/2)+2$
  - Since we alternate, we can write $Q(n)=3+2Q(n/4)$
- This solves to $O(n^{1/2})$

Analysis demo



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Exercises

- Construct a set of n points, and a range query R such that:
  - R does not contain any of the points
  - The search procedure takes $\Omega(n^{1/2})$ time
- What happens if the query range is a circle, not a square?

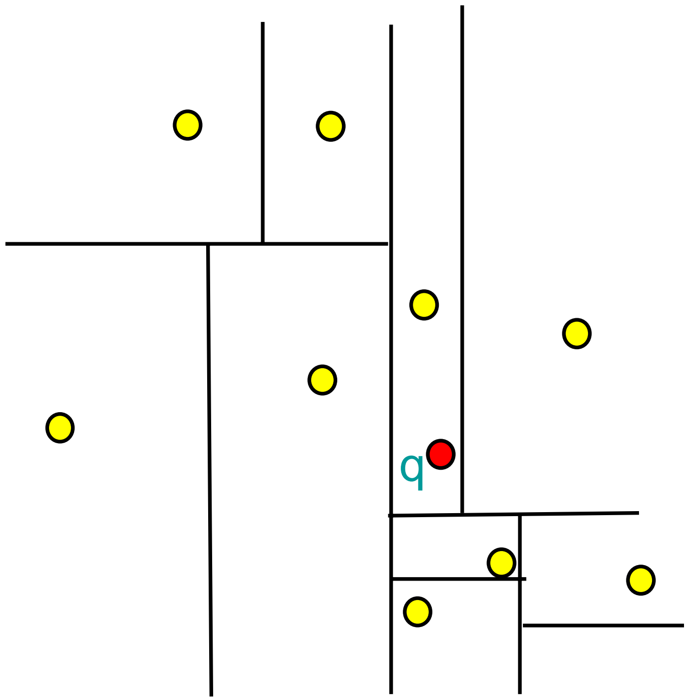
Back to $(1+\varepsilon)$-Nearest Neighbor

- We will solve the problem using kd-trees
- "Analysis"…under the assumption that all leaf cells of the kd-tree for P have bounded aspect ratio
- Assumption somewhat strict, but satisfied in practice for most of the leaf cells
- We will show
  - $O(\log n * O(1/\varepsilon)^d)$ query time
  - $O(n)$ space (inherited from kd-tree)

ANN Query Procedure

- Locate the leaf cell containing q
- Enumerate all leaf cells C in the increasing order of distance from q

  (denote it by r)
- Keep updating p' so that it is the closest point seen so far
  - Note: r increases, dist(q,p') decreases
- Stop if dist(q,p')<(1+ε)*r



Analysis

- Let R be the value of r before the last cell was examined
- Each cell C seen (except maybe for the last one) has diameter > εR
- …Because if not, then the point p in C would have been a $(1+\varepsilon)$-approximate nearest neighbor (by now), so we would have stopped earlier

$$\mathrm{dist}(q,p) \le \mathrm{dist}(q,C) + \mathrm{diameter}(C) \le R + \varepsilon R = (1+ \varepsilon)R$$

- The number of cells with diameter εR, bounded aspect ratio, and touching a ball of radius R is at most $O(1/\varepsilon)^d$
  - Ball of radius R has volume $O(R)^d$
  - Each cell has volume $\Omega(\varepsilon R/\mathrm{sqrt}\{d\})^d$

Refs

- JL Bentley, Binary Search Trees Used for Associative Searching, Communications of the ACM, 1975.
- S Arya, DM Mount, NS Netanyahu, R Silverman, AY Wu , An optimal algorithm for approximate nearest neighbor searching fixed dimensions, Journal of the ACM (JACM), 1998.
- D Lowe, 1992.