THE UNIVERSITY OF TEXAS AT AUSTIN
Department of Statistics and Data Sciences
College of Natural Sciences

SDS 385: Stat Models for Big Data

Lecture 9: KD trees

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https://psarkar.github.io/teaching

Background

- Has a long history–invented in 1970 by Jon Bentley
- k represents the number of dimensions
- Idea is to partition the data spatially, by using only one dimension at any level.
- While searching, this helps pruning most of the search space.

General idea

- Say you have some algorithm to decide which dimension to split on and which value to split on (call this cut-val).
- Call this cut-dim (cutting dimension)
- Node in tree is described by (cut-dim, cut-val)
- So, to find a point, only need to compare the cutting dimension.

Construct

- If there is one point, just form a leaf node
- Otherwise divide the points in half along the cutting axis
  - Find the axis with the widest spread
  - divide in alternative/round robin fashion
- recursively build kdtrees from each half
- Complexity $dn \log n$

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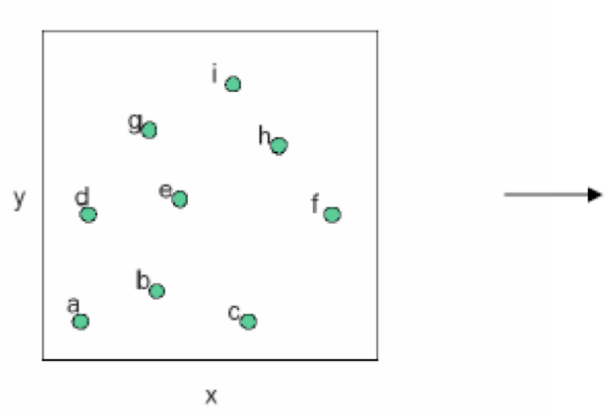
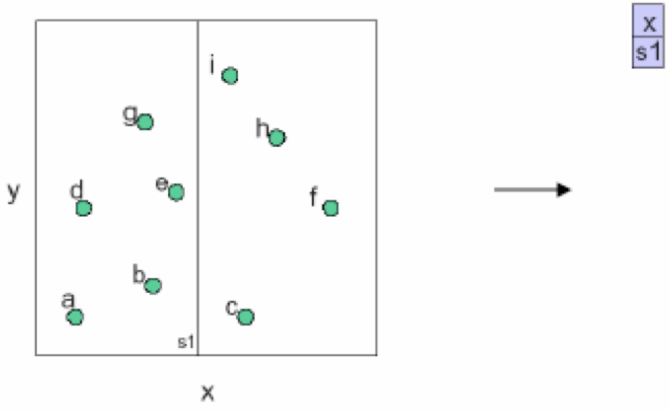
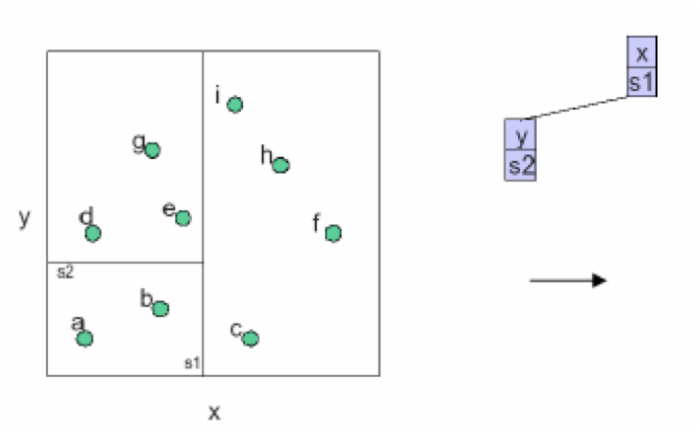
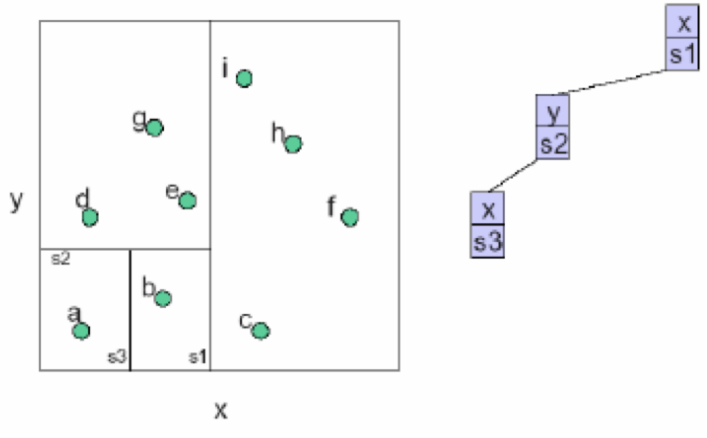


divide perpendicular to the widest spread.







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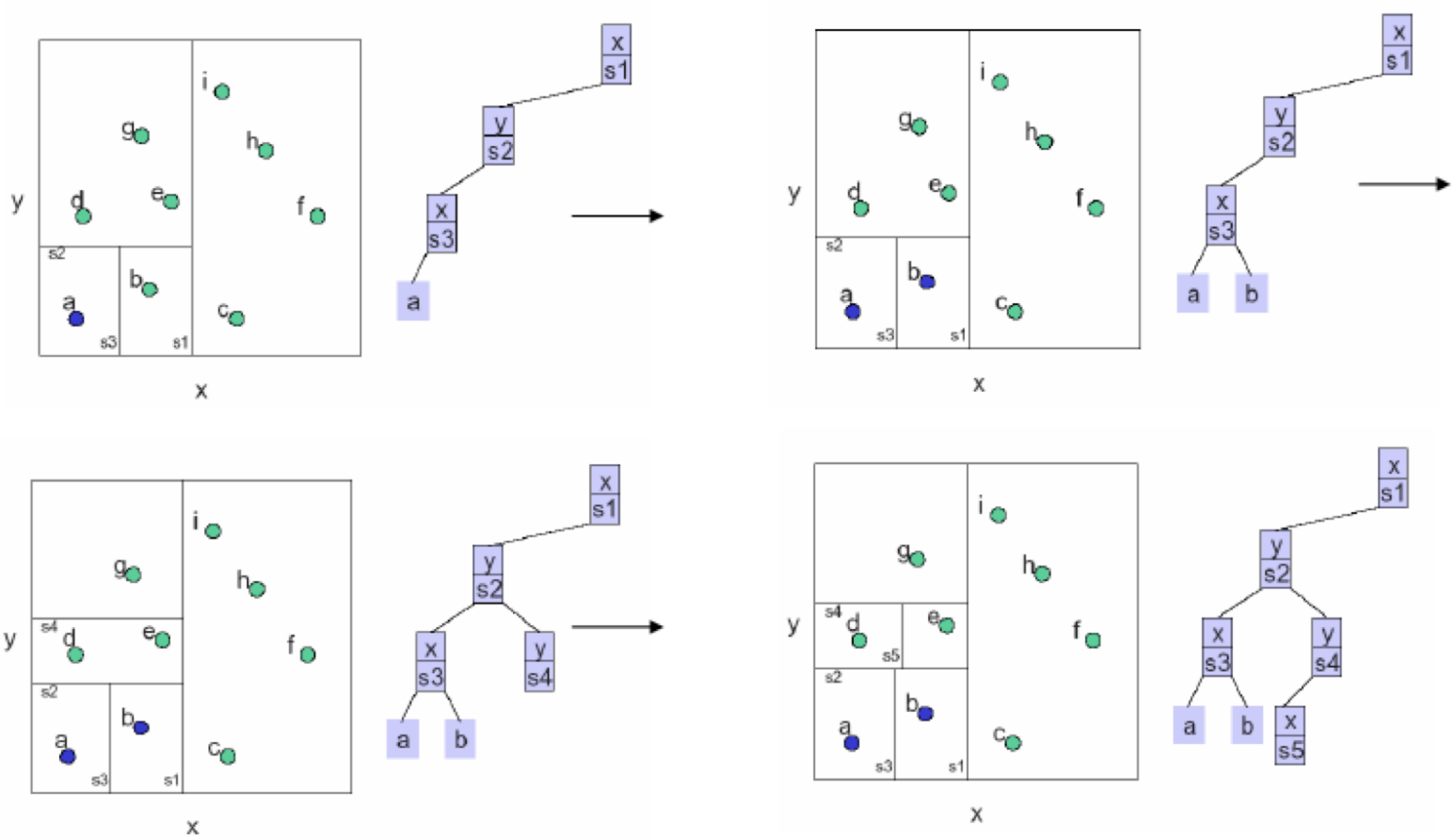
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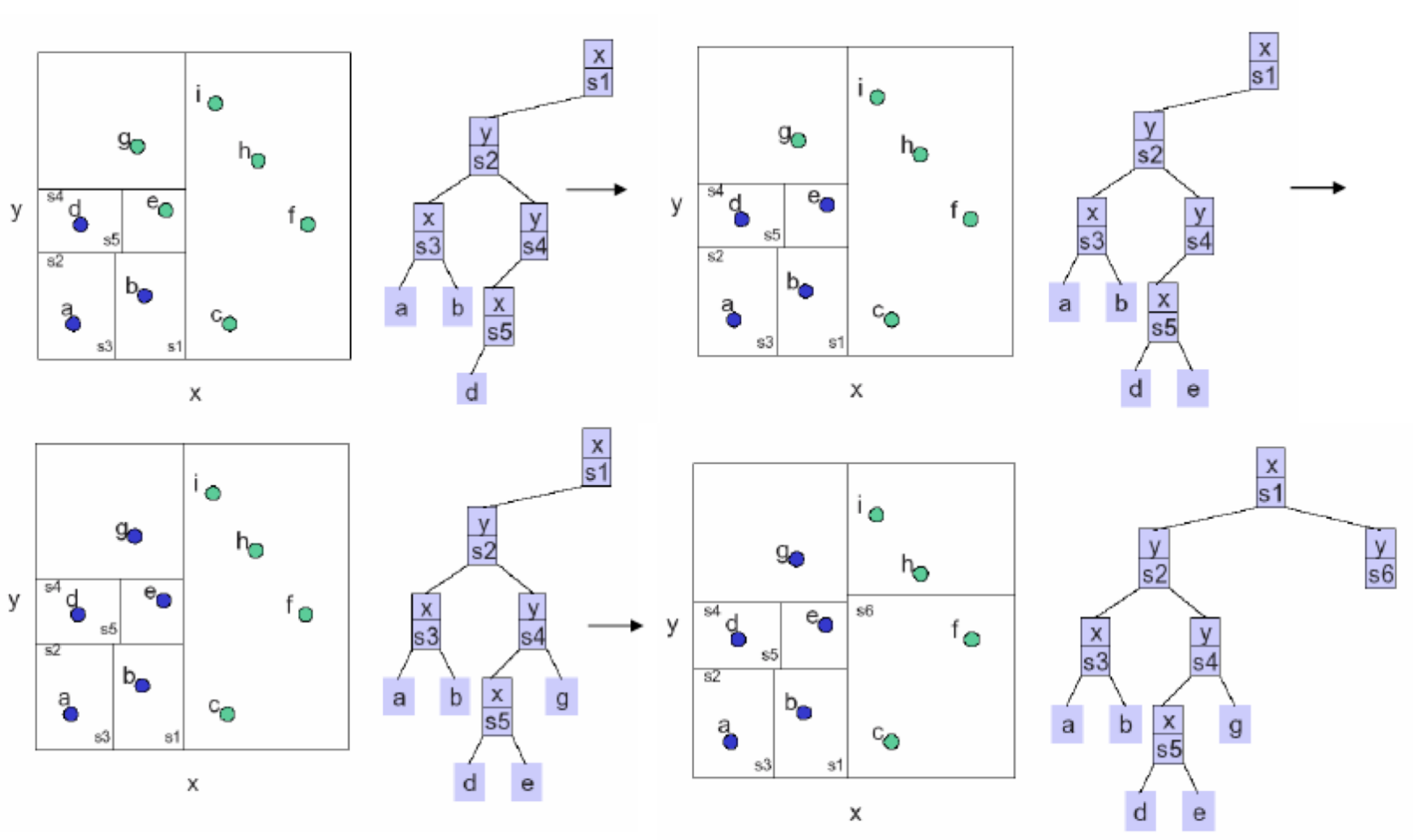
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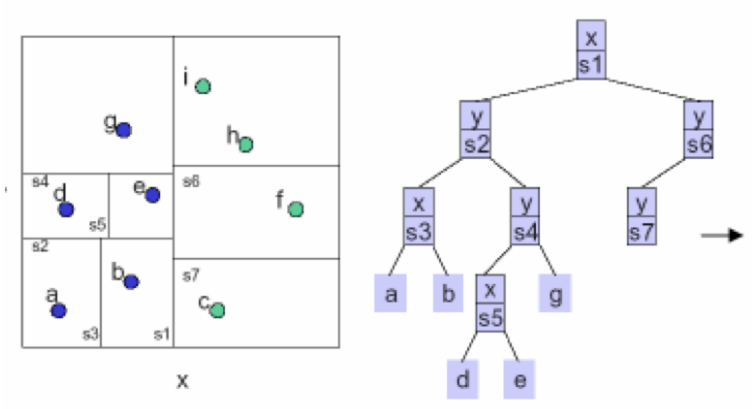
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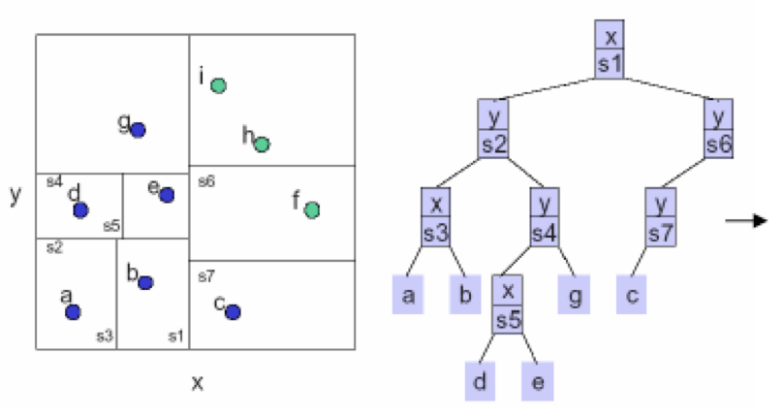
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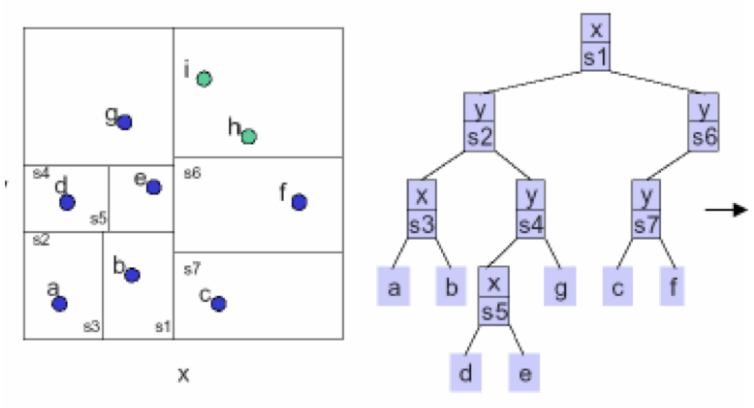
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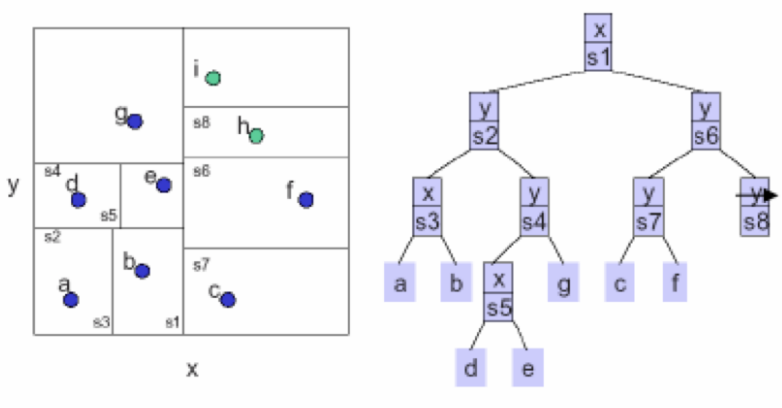
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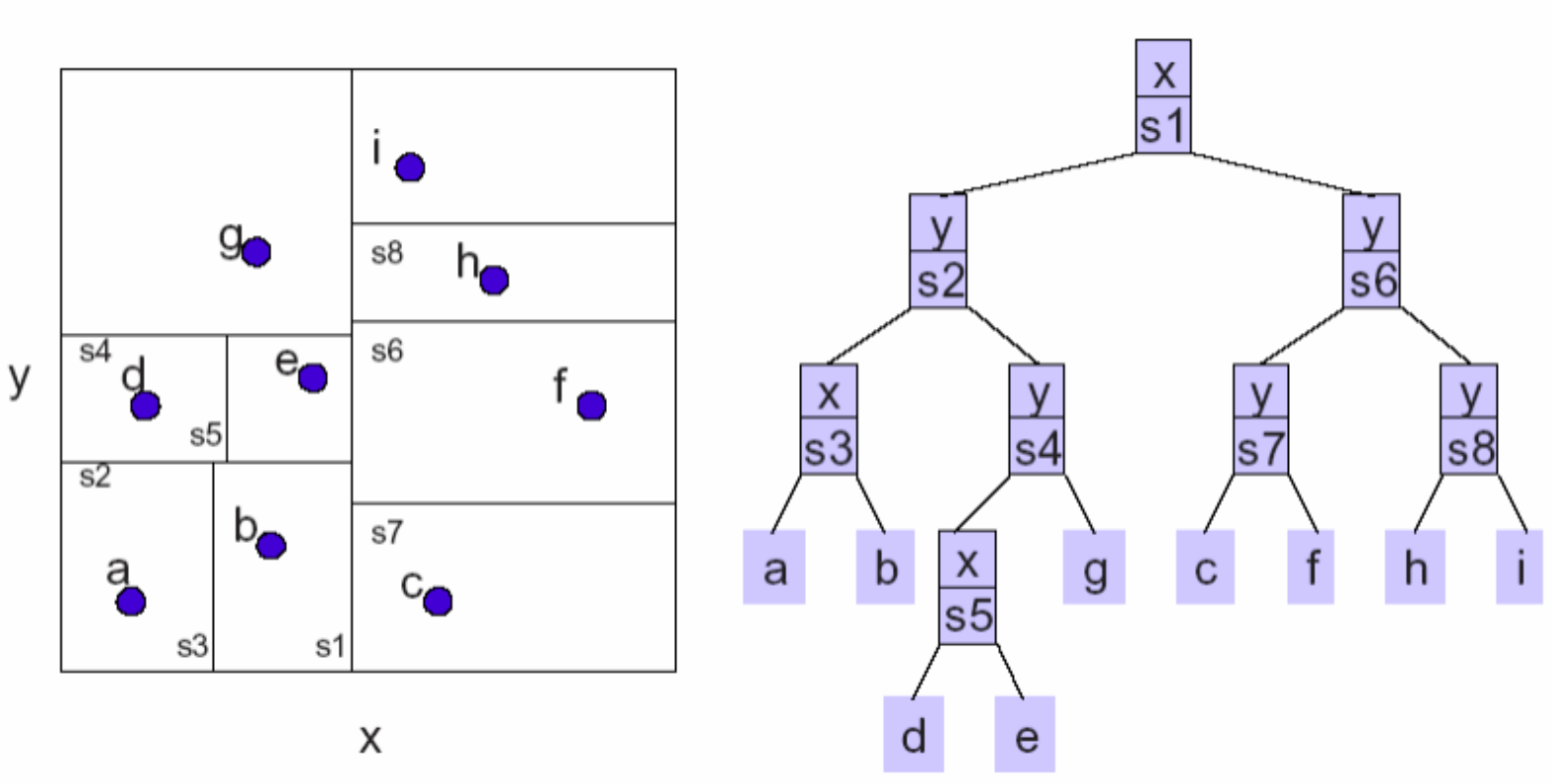
Find point with the smallest element in dimension a

- If cutdim at current node equals a,
  - the min cannot be in the right subtree
  - recurse on the left subtree

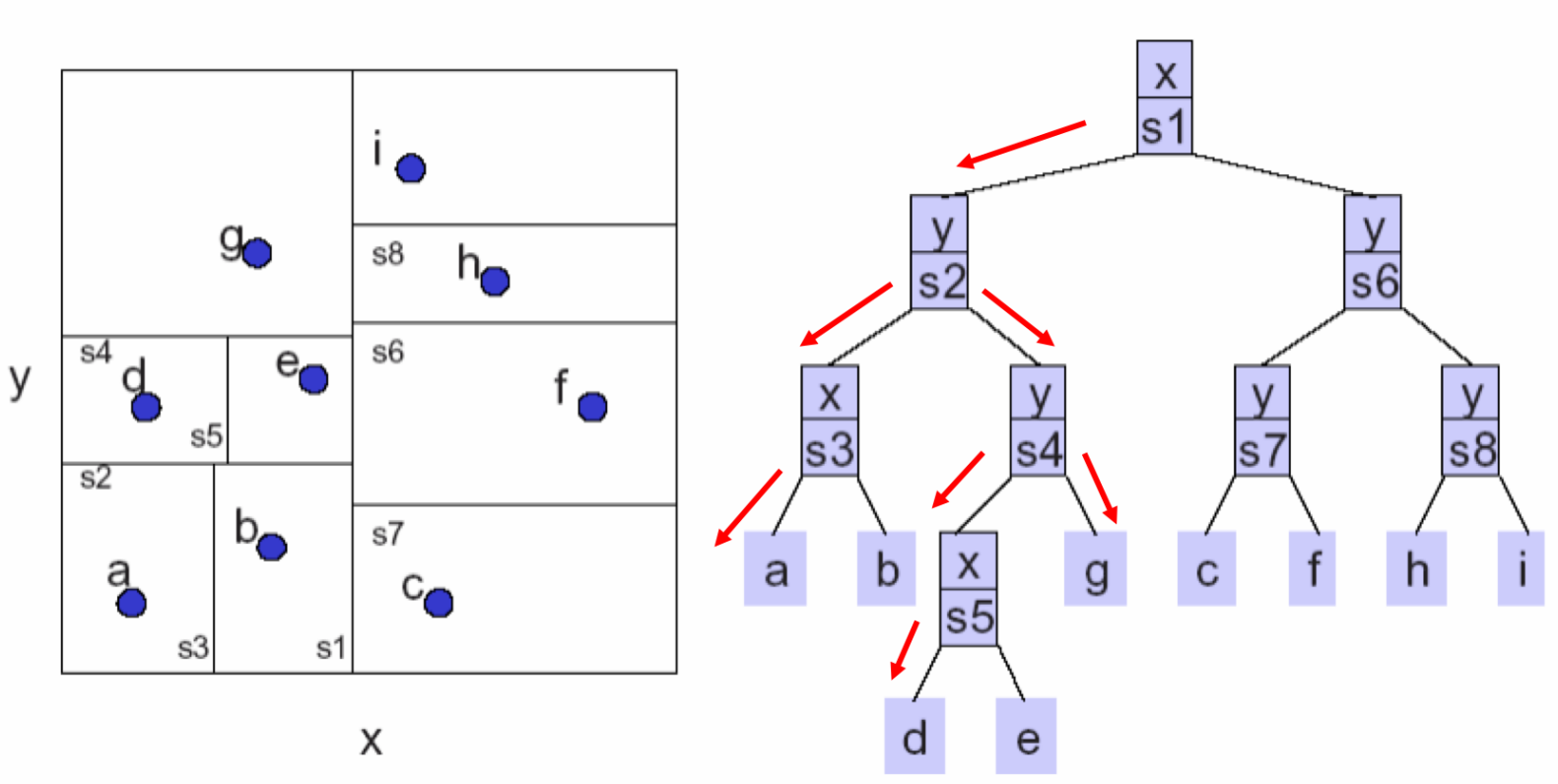
Base case: if there are no left children, stop and return current point.

- Otherwise
  - the min could be in either
  - recurse on both left and right subtrees

Find point with the smallest element in dimension x



Find point with the smallest element in dimension x



Nearest neighbor queries

- Given point Q, find the closest point R
- Have to be careful, because its possible that two points are far away in the tree but close in the Eucidean space.
- For each node store a bounding box

Nearest neighbor queries

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Nearest neighbor queries

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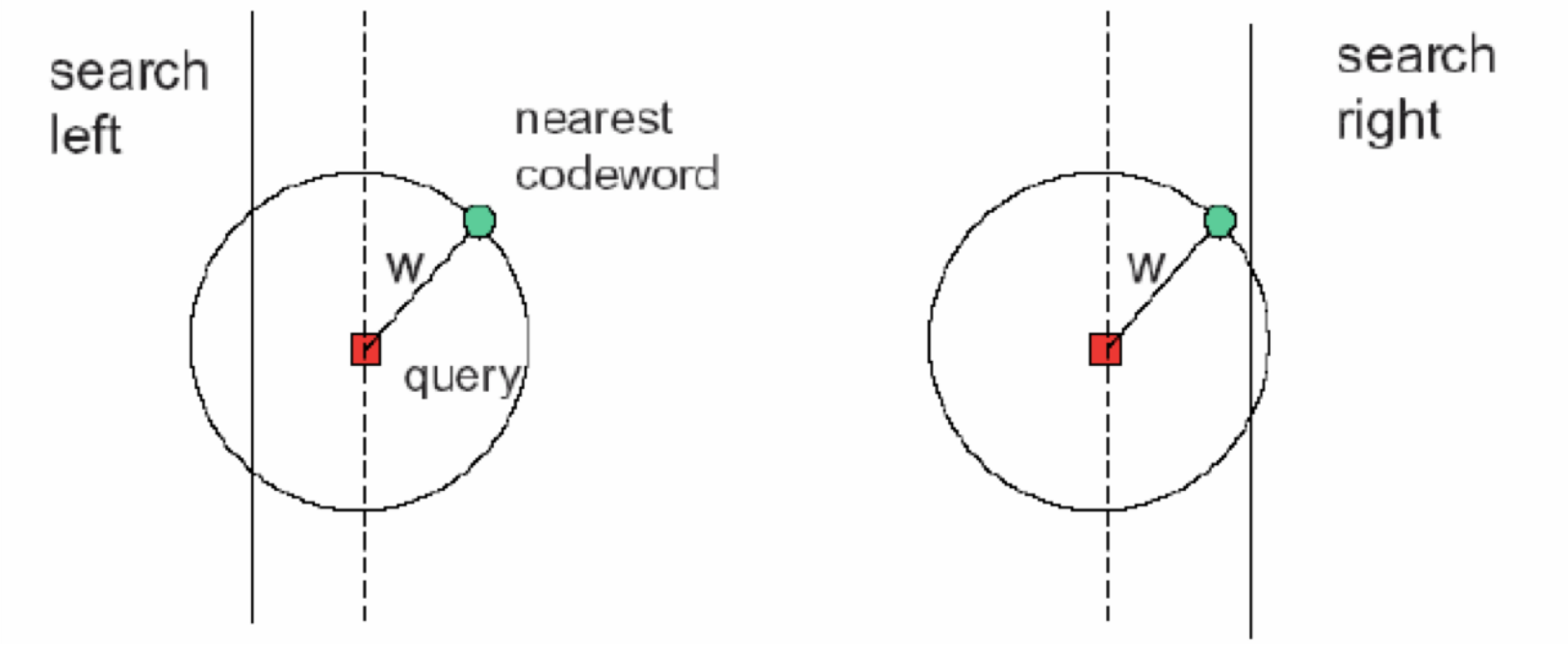
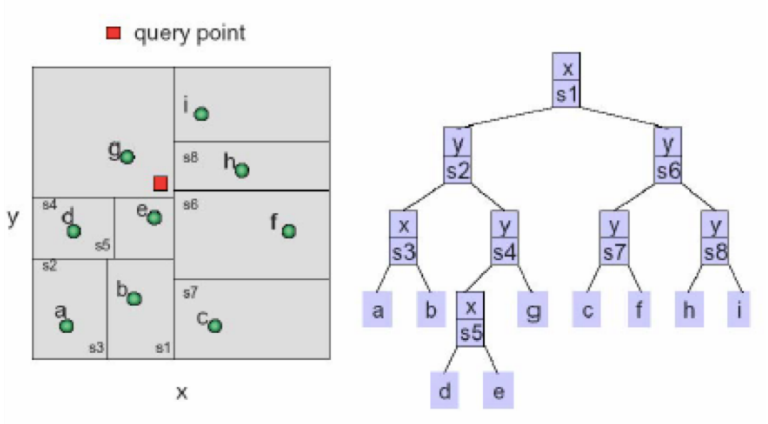
- Have to be careful, because its possible that two points are far away in the tree but close in the Eucidean space.
- For each node store a bounding box
- Remember the closest point to Q seen so far (call this R')
- Prune subtrees where bounding boxes cannot contain R'

Nearest neighbor queries



- If circle overlaps with left subtree, search left subtree
- If circle overlaps with right subtree search right subtree
- Has been shown to work in about $O(\log n)$ time.

NN search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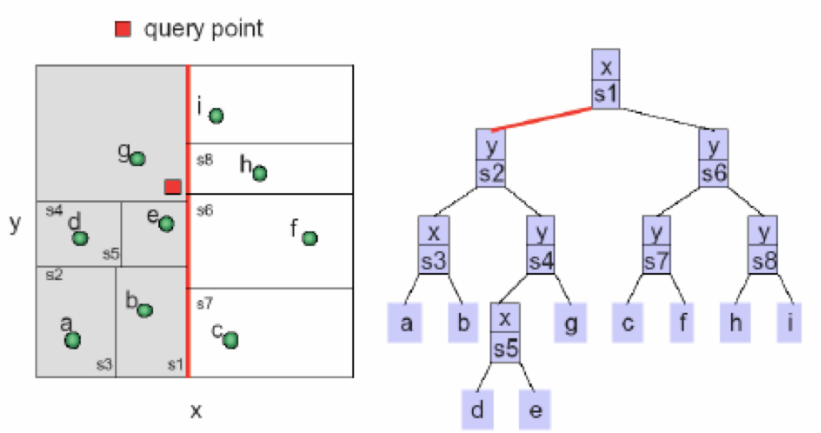
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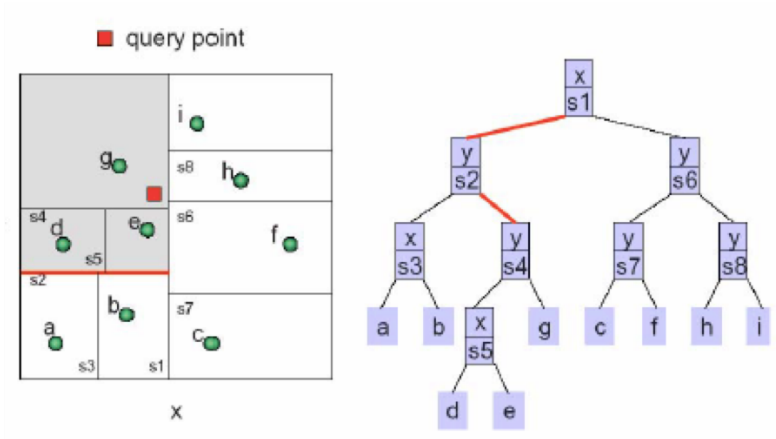
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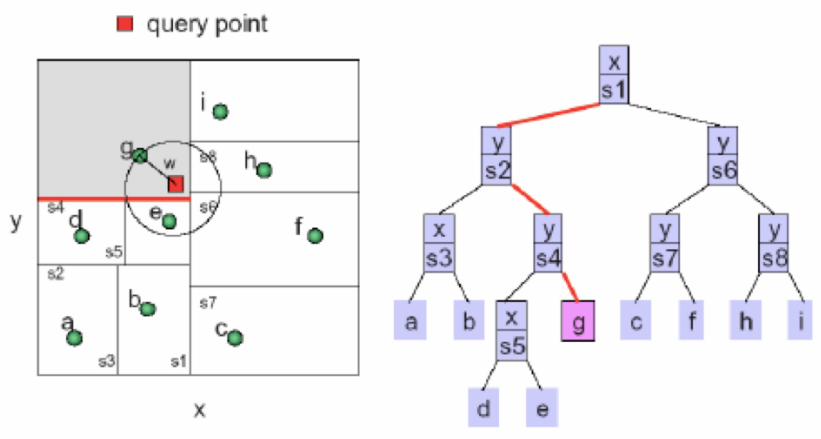
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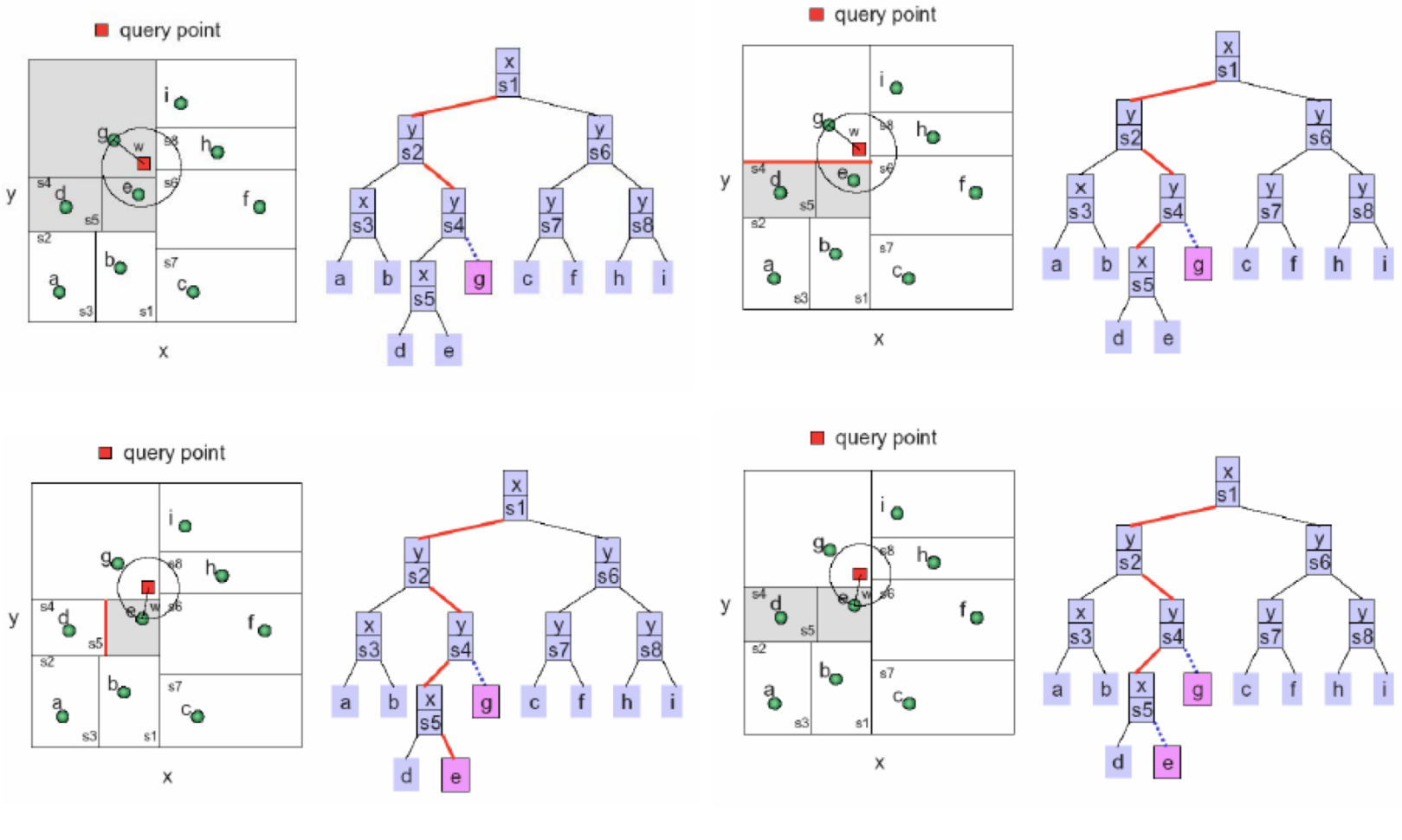

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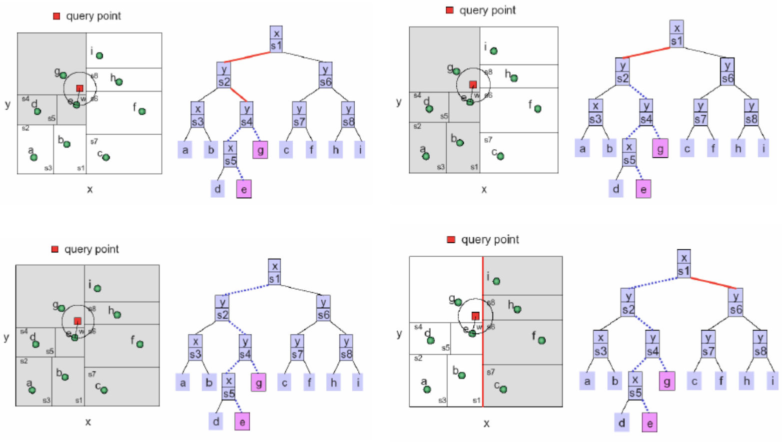

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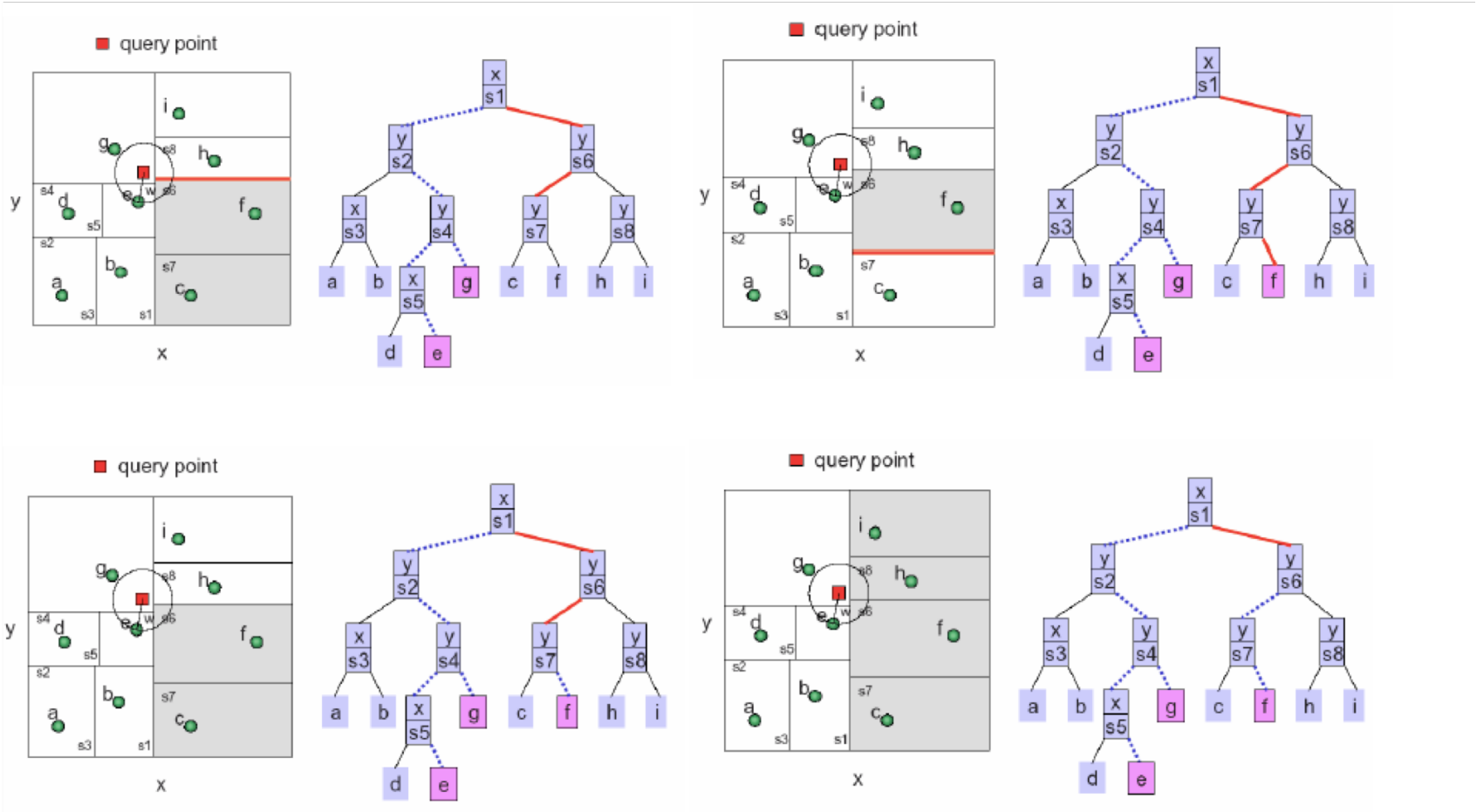

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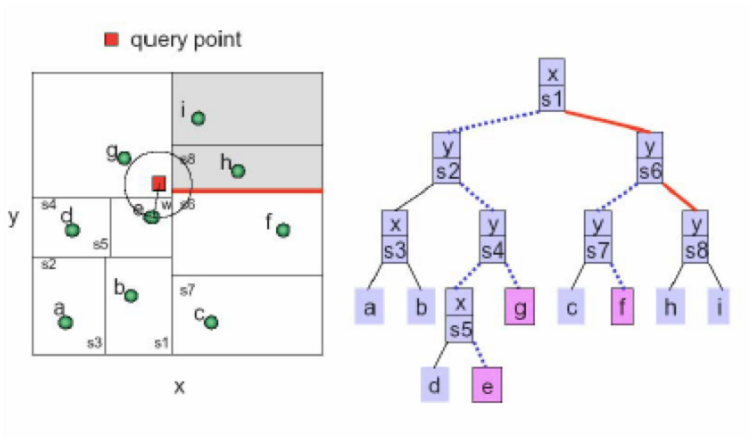
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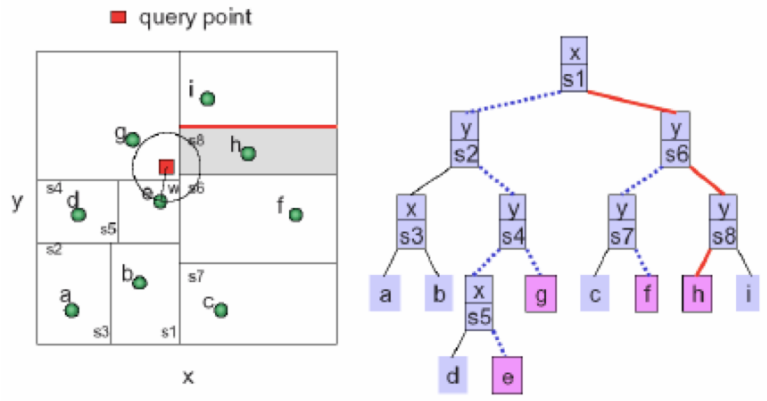
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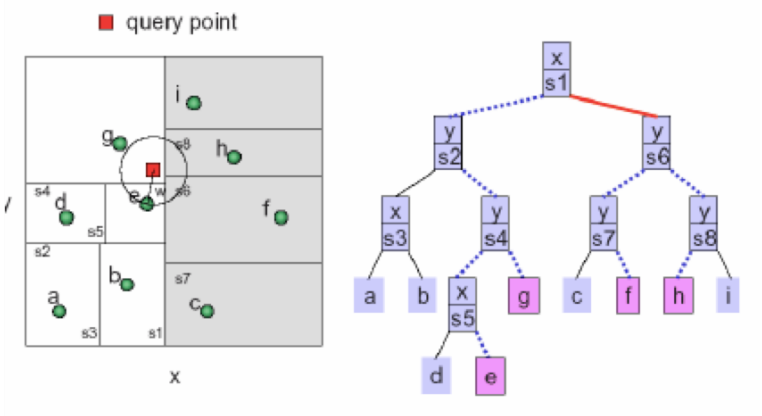
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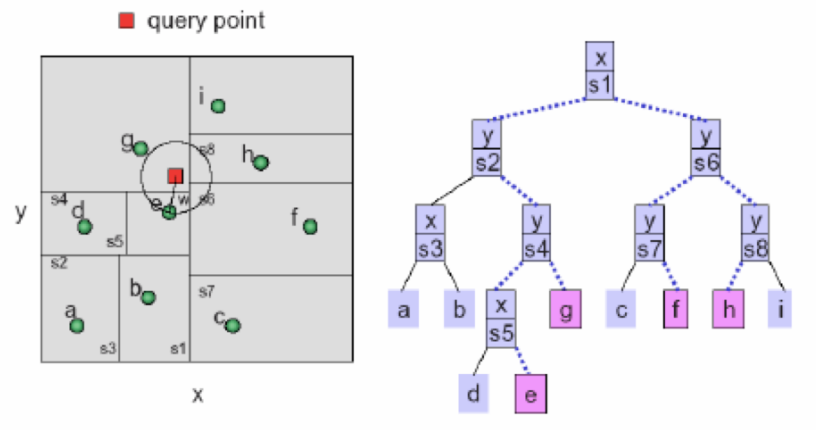
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NN search

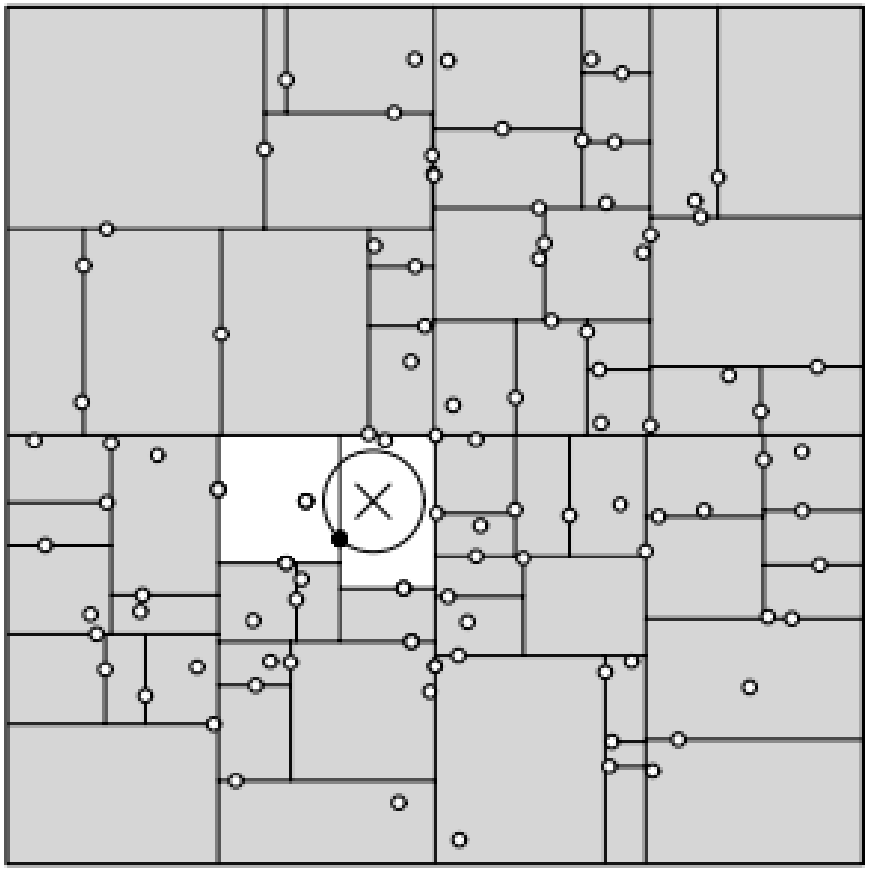


Figure 6.5

Generally during a nearest neighbour search only a few leaf nodes need to be inspected.

NN search

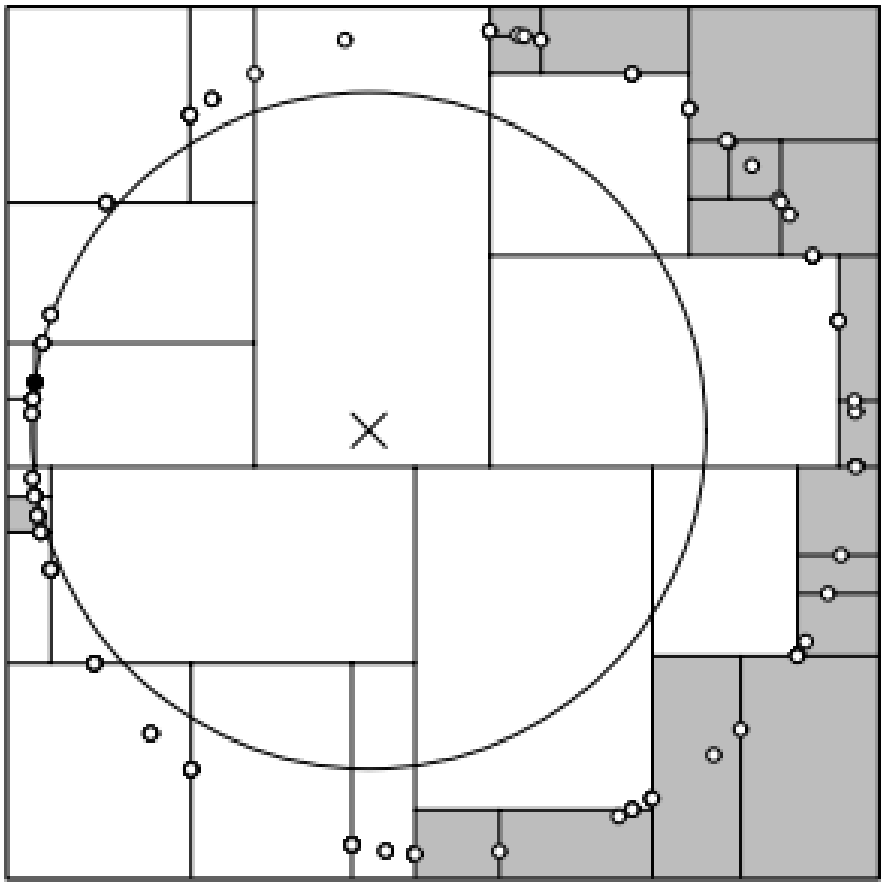


Figure 6.6

A bad distribution which forces almost all nodes to be inspected.

Timing vs tree size

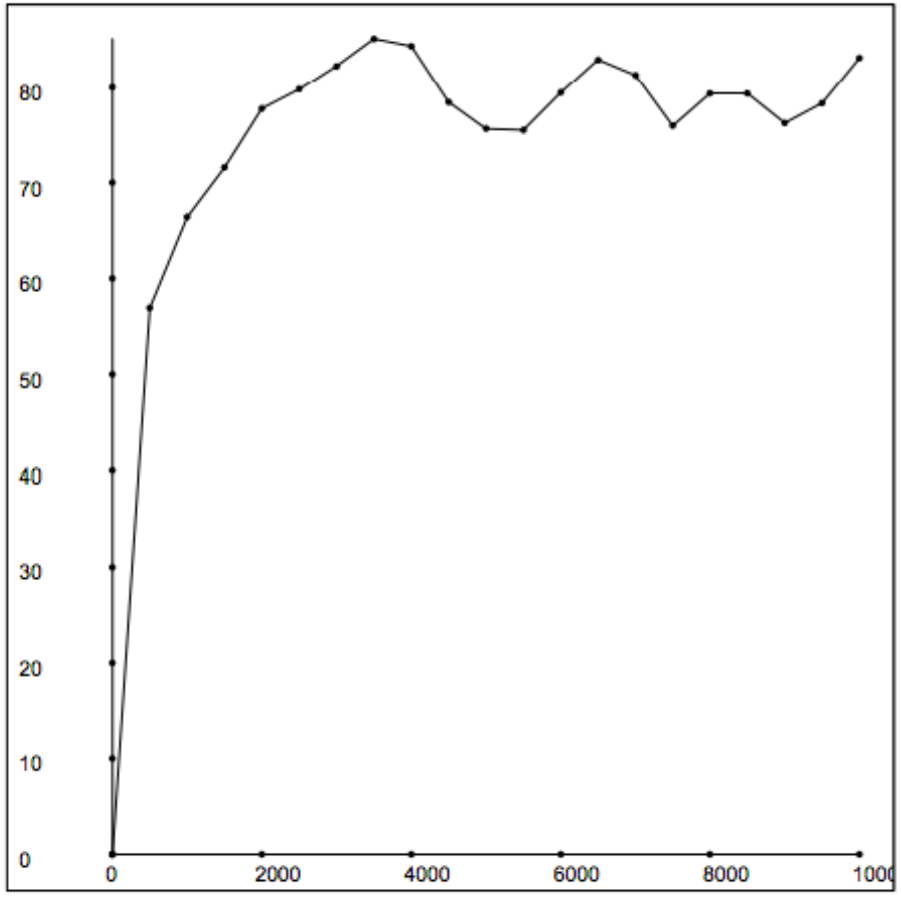


Figure 6.8

Number of inspections against kd-tree size for an eight-dimensional tree with an eight-dimensional underlying distribution.

Timing vs dimensions

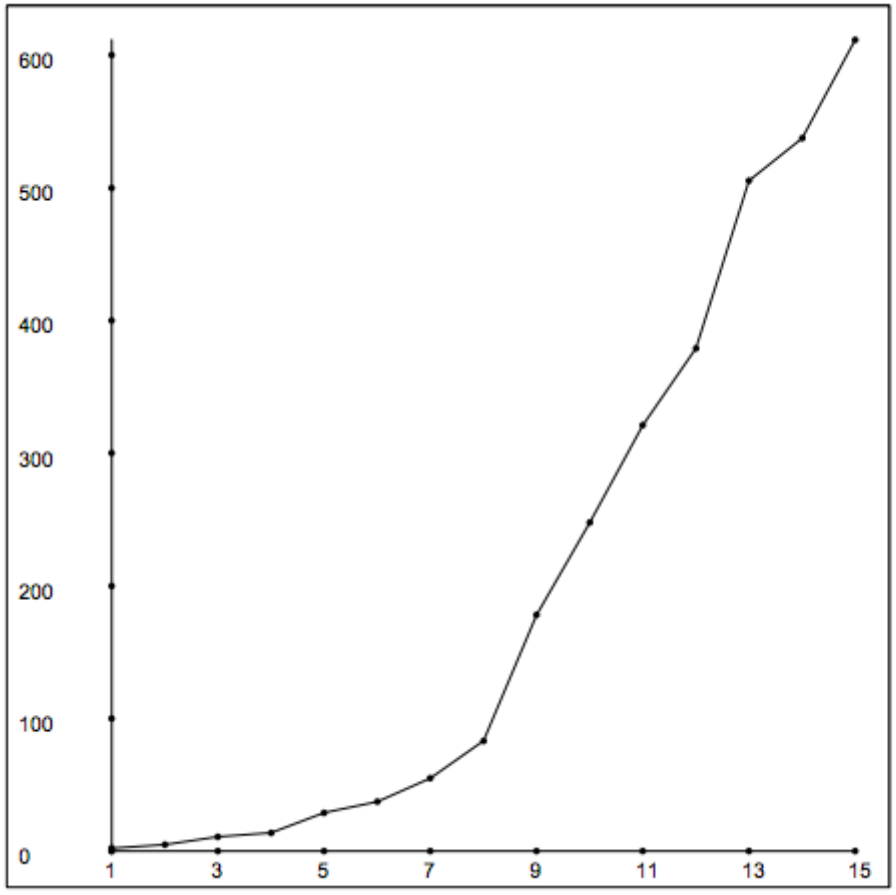


Figure 6.9

Number of inspections graphed against tree dimension. In these experiments the points had an underlying distribution with the same dimensionality as the tree.

k-nearest neighbor with kd trees

- Algorithm 1: find nearest neighbor with above approach, report label

k-nearest neighbor with kd trees

- Algorithm 1: find nearest neighbor with above approach, report label
    - Backtracking still takes time
- Algorithm 2: do approximate nearest neighbor, dont backtrack, report label
    - Still need to search brute force in the leaf node

k-nearest neighbor with kd trees

- Algorithm 1: find nearest neighbor with above approach, report label
    - Backtracking still takes time
- Algorithm 2: do approximate nearest neighbor, dont backtrack, report label
    - Still need to search brute force in the leaf node
- Algorithm 3: no brute force search. Can you tell me what to do?

Curse of dimensionality

- What happens when you have high dimensional data?
- How about when data lies in a lower dimensional manifold?

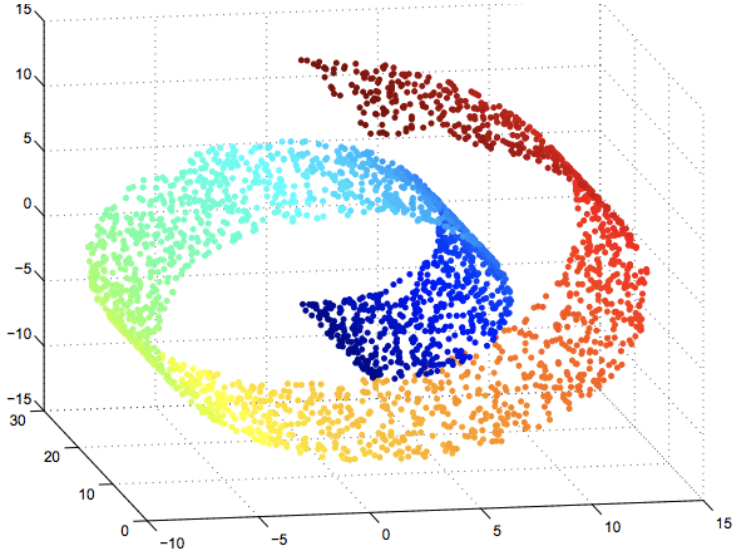


Figure 1: A curled plane: the swiss roll.

- How to fix this?
  - Projections?

Ball trees

- Pick direction of most variability

Ball trees

- Pick direction of most variability
- PCA?

Ball trees

- Pick direction of most variability
- PCA?
- Fast algorithm:
  - Pick point at random, call it X
  - Pick point far away from X, call it Y
  - Pick point far away from Y, call it Z
  - $Y - Z$ gives you a good proxy for the direction of most variability

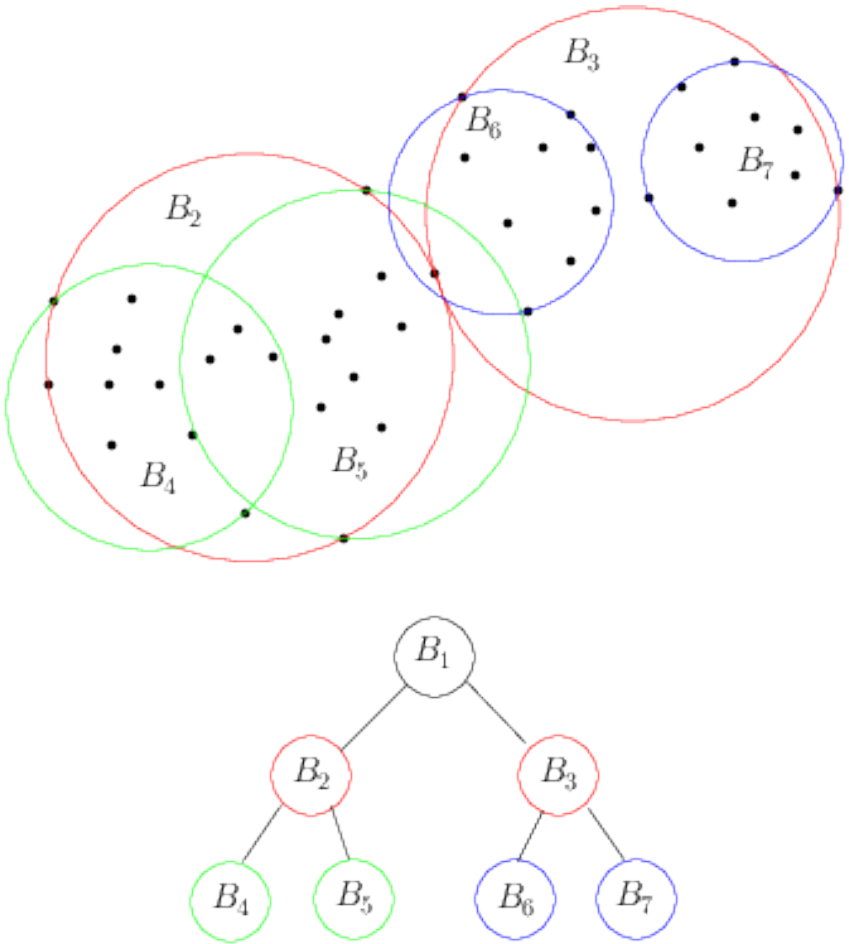
Ball trees

- Pick direction of most variability

Ball trees

- Pick direction of most variability
- Project all points on that direction
- Split by median
- In each split
  - Compute center
  - Compute distance of center to furthest point
  - Continue recursively

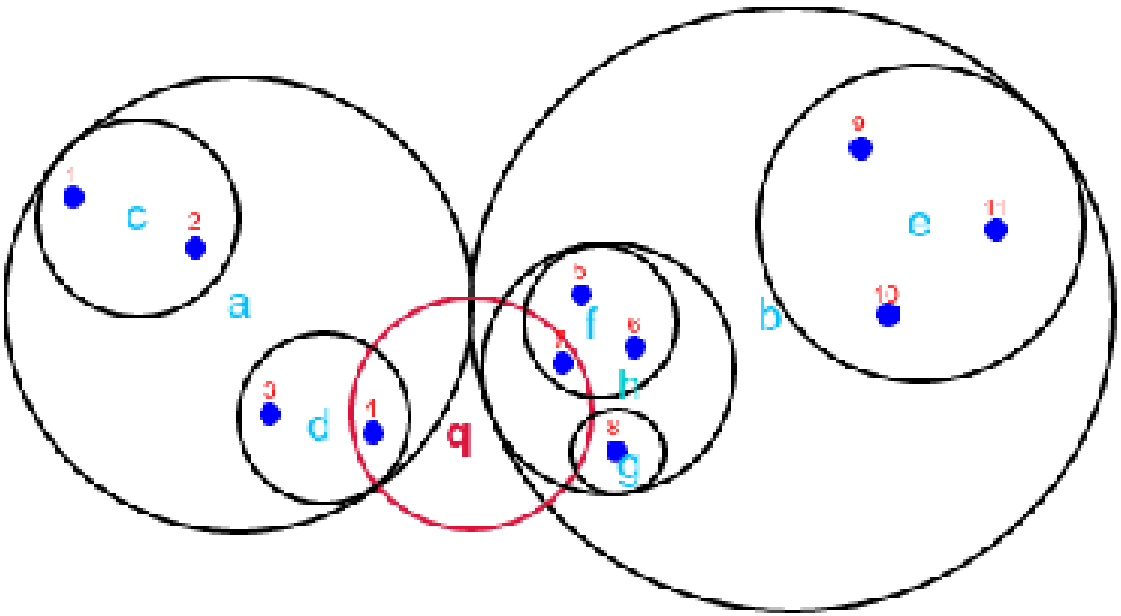
Ball trees



Ball tree search

- Traverse tree in depth first order
- Check if distance of point$x$ to current node B is smaller than distance to current nearest neighbor (call this n_x)
  - If no, move on.
  - If yes, and B is a leaf node, then find nearest neighbor in B, and update the nearest neighbor n_x
  - If yes, and B is an internal node, recursively search both children of node B. Search child whose center is closest, first.

Ball tree search



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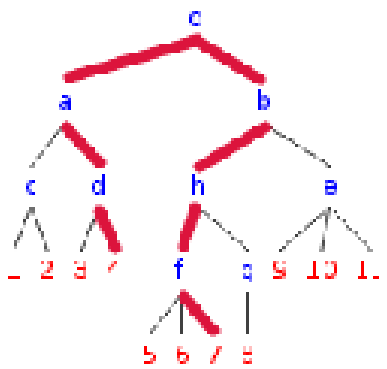

(b)

Acknowledgment

- The kdtrees animations were borrowed from
  - Thinh Nguyen's slides
  - Carl Kingsford's slides
- Andrew moore's tutorial