CSE 589
Applied Algorithms
Spring 1999

Nearest Neighbor Search
k-d Trees

Nearest Neighbor Search

- Preprocess a set of n vectors V in d dimensions into a search data structure.
- Input: A query vector q.
- Ouput: The vector v in V that is nearest to q. That is, the vector v in V that minimizes

$$\|v-q\|^2 = \sum_{i=1}^{d} \left((v(i)-q(i)\right)^2$$

NNS in VQ

- Used in codebook design.
  - Used in GLA to partition the training set.
  - Since codebook design is seldom done then speed of NNS is not too big a issue.
- Used in VQ encoding.
  - Codebook size is commonly 1,000 or more.
  - Naive linear search would make encoding too slow.
  - Can we do better than linear search?

Naive Linear Search

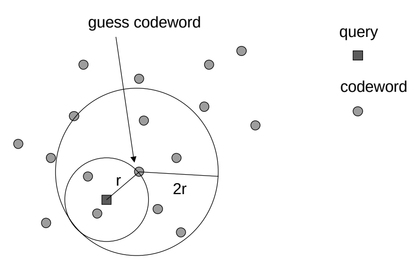
- Keep track of the current best vector, best-v, and best distance squared, best-squared-d.
  - For an unsearched vector v compute $||v - q||^2$ to see if it smaller than best-squared-d.
  - If so then replace best-v.
  - If d is moderately large it is a good idea not to compute the squared distance completely. Bail out when k < d and

$$\text{best}-\text{squared}-\text{d} \le \sum_{i=1}^{k} (v(i)-q(i))^2$$

Orchard's Method

- Invented by Orchard (1991)
- Uses a "guess codeword". The guess codeword is the codeword of an adjacent coded vector.
- Orchard's Principle.
  - if r is the distance between the guess codeword and the query vector q then the nearest codeword to q must be within a distance of 2r of the guess codeword.

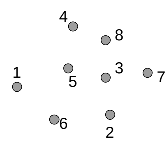
Orchard's Principle



Nearest codeword within distance r of guess codeword.

Orchard Data Structure

- For each codeword sort the other codewords by distance to the codeword.



A[1..8,1..7]

1	6	5	4	2	3	8	7	index
								distance
2	3	6	7	5	8	1	4	
3	5	2	7	8	6	4	1	

:
:

Basic Orchard Algorithm

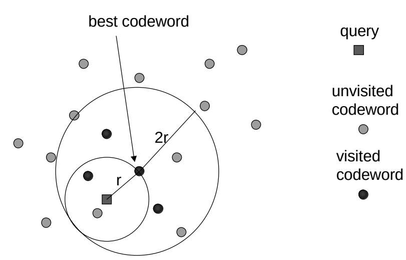
```
Let i be the index of initial guess codeword;
r := ||c_i - q||;
best-index := i;
j := 1;
while A[i,j].distance < 2 * r do
   if ||c_j - q|| < r then best-index := j;
   j := j + 1;
```

This algorithm searches all the codewords within a distance 2r of the guess codeword.

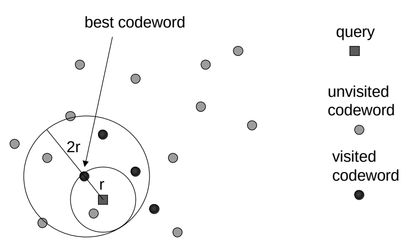
Orchard Improvements

- Early bailout using squared distance:
  - $||c_j - q|| < r$ is done by early bailout using the comparison $||c_j - q||^2 < r^2$.
- Switching Lists:
  - When a nearer codeword is found then switch the search to its list.
  - Care must be taken to avoid doing a distance computation the same codeword twice. Marking visited codewords solves this problem.

Switching Lists (1)



Switching Lists (2)



Orchard Notes

- Very fast.
  - Appears O(log n) average time per search, but there is no proof of this performance.
- Requires too much memory.
  - Requires $O(n^2)$ memory for the sorted lists.
  - Modification for large n. Just store the first m closest to make an n x m array. If the search runs off the array then revert to linear search.

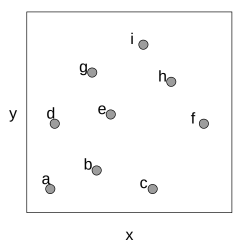
k-d Tree

- Jon Bentley, 1975
- Tree used to store spatial data.
  - Nearest neighbor search.
  - Range queries.
  - Fast look-up
- k-d tree are guaranteed $\log_2 n$ depth where n is the number of points in the set.
  - Traditionally, k-d trees store points in d-dimensional space which are equivalent to vectors in d-dimensional space.

k-d Tree Construction

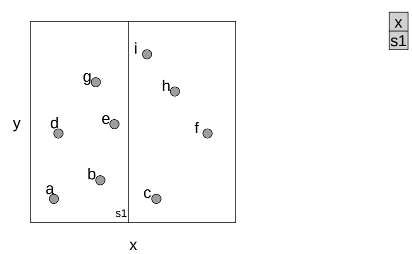
- If there is just one point, form a leaf with that point.
- Otherwise, divide the points in half by a line perpendicular to one of the axes.
- Recursively construct k-d trees for the two sets of points.
- Division strategies
  - divide points perpendicular to the axis with widest spread.
  - divide in a round-robin fashion.

k-d Tree Construction (1)



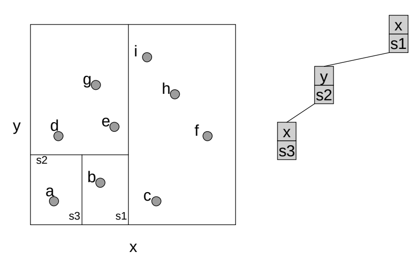
divide perpendicular to the widest spread.

k-d Tree Construction (2)

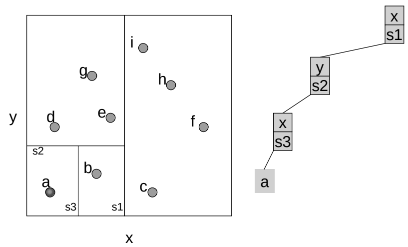


k-d Tree Construction (3)

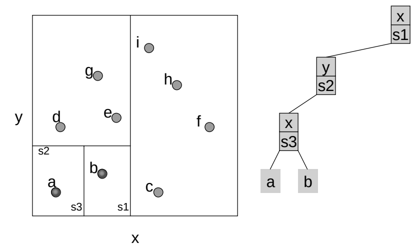
k-d Tree Construction (4)



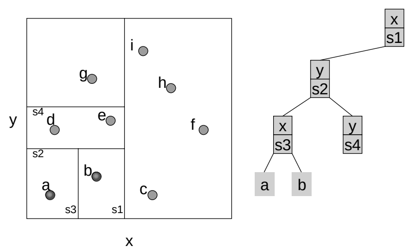
k-d Tree Construction (5)



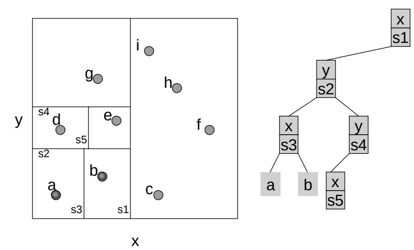
k-d Tree Construction (6)



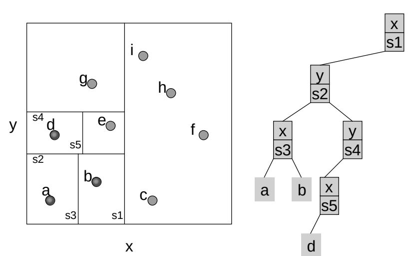
k-d Tree Construction (7)



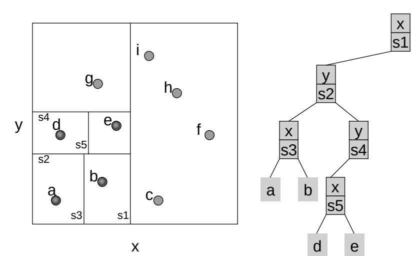
k-d Tree Construction (8)



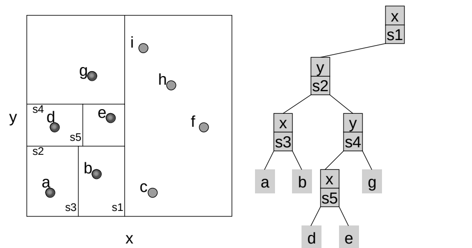
k-d Tree Construction (9)



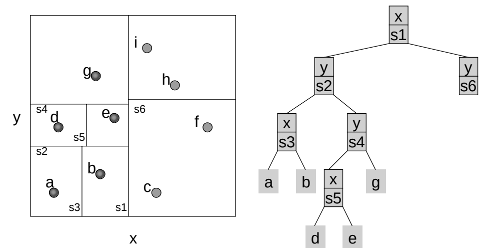
k-d Tree Construction (10)



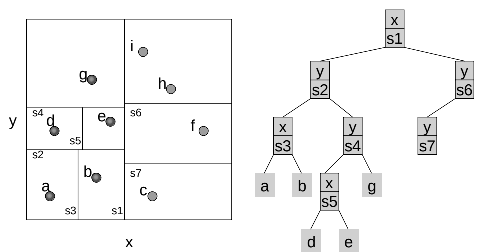
k-d Tree Construction (11)



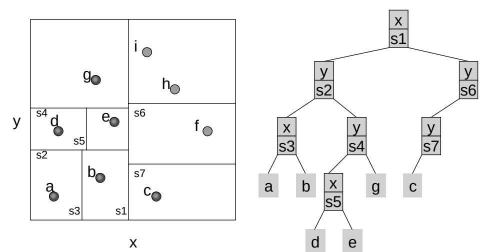
k-d Tree Construction (12)



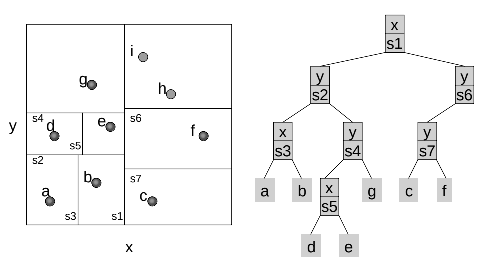
k-d Tree Construction (13)



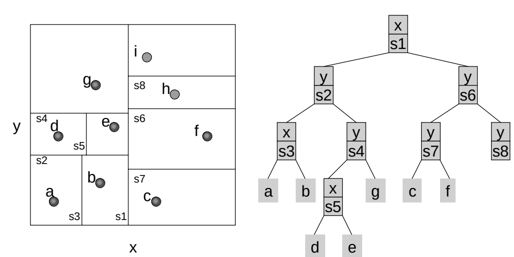
k-d Tree Construction (14)



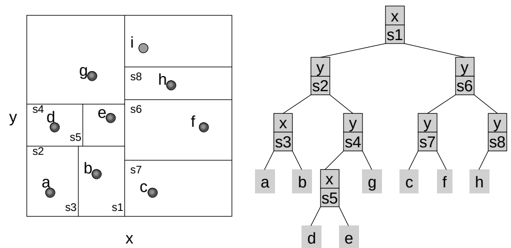
k-d Tree Construction (15)



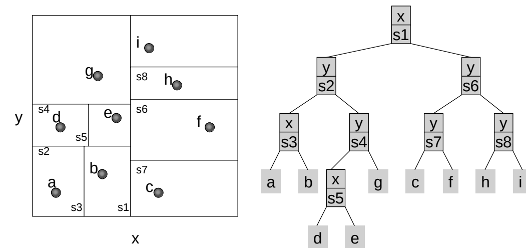
k-d Tree Construction (16)



k-d Tree Construction (17)



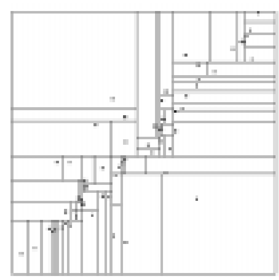
k-d Tree Construction (18)



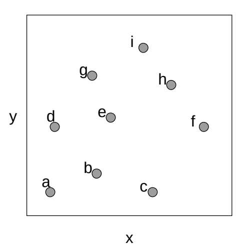
k-d Tree Construction Complexity

- First sort the points in each dimension.
  - O(dn log n) time and dn storage.
  - These are stored in A[1..d,1..n]
- Finding the widest spread and equally divide into two subsets can be done in O(dn) time.
- Constructing the k-d tree can be done in O(dn log n) and dn storage

k-d Tree Codebook Organizaton



k-d Tree Splitting



sorted points in each dimension

	1	2	3	4	5	6	7	8	9
x	a	d	g	b	e	i	c	h	f
y	a	c	b	d	f	e	h	g	i

• max spread is the max of $f_x - a_x$ an $i_y - a_y$.

• In the selected dimension the middle point in the list splits the data.

• To build the sorted lists for the other dimensions scan the sorted list adding each point to one of two sorted lists.

Node Structure for k-d Trees

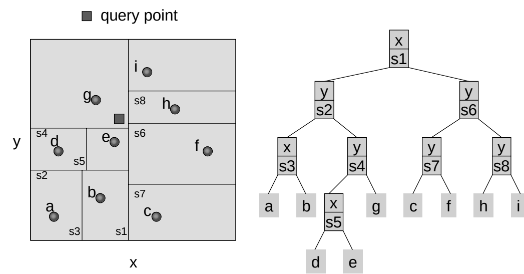
- A node has 5 fields
  - axis (splitting axis)
  - value (splitting value)
  - left (left subtree)
  - right (right subtree)
  - point (holds a point if left and right children are null)

k-d Tree Nearest Neighbor Search

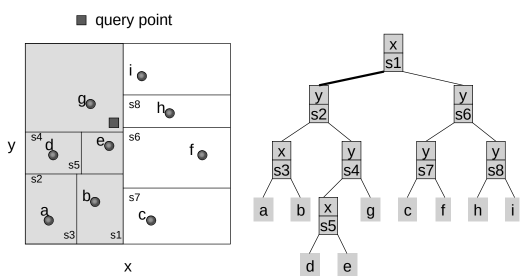
```
NNS(q: point, n: node, p: ref point w: ref distance)
if n.left = n.right = null then {leaf case}
    w' := ||q - n.point||;
    if w' < w then
        w := w';
        p := n.point;
else
    if q(n.axis) ≤ n.value then {query to left}
        NNS(q, n.left, p, w);
        if q(n.axis) + w > n.value then NNS(q, n.right, p, w);
    else {query to right}
        NNS(q, n.right, p, w);
        if q(n.axis) - w ≤ n.value then NNS(q, n.left, p, w)
```

initial call `NNS(q, root, p, infty)`

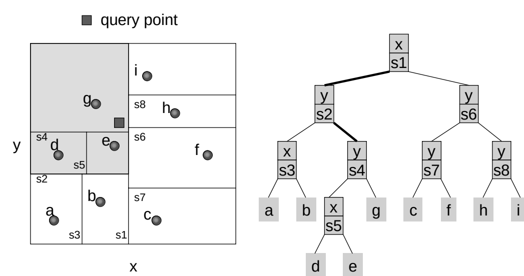
k-d Tree NNS (1)



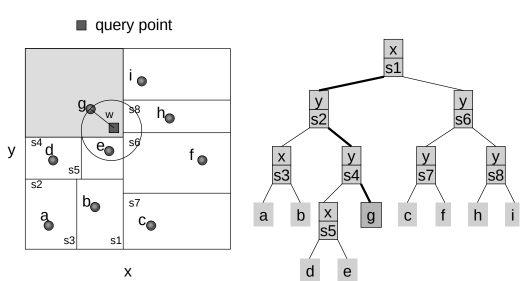
k-d Tree NNS (2)



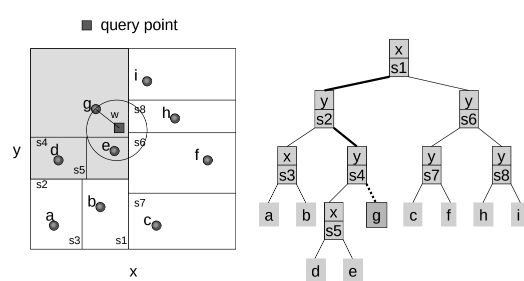
k-d Tree NNS (3)



k-d Tree NNS (4)

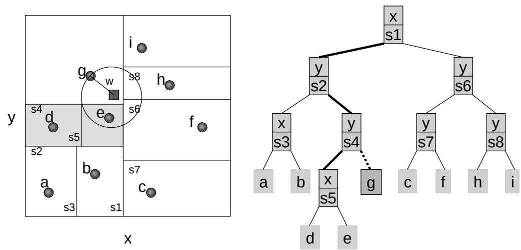


k-d Tree NNS (5)



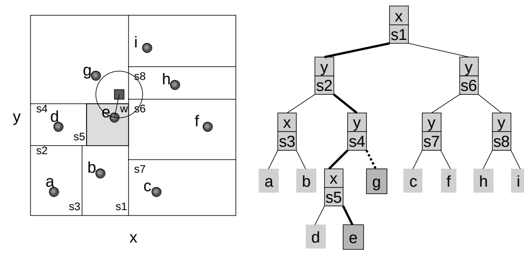
k-d Tree NNS (6)

■ query point



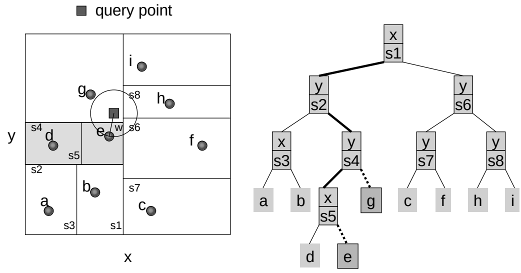
k-d Tree NNS (7)

■ query point



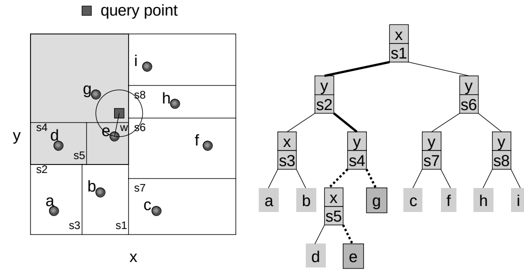
k-d Tree NNS (8)

■ query point



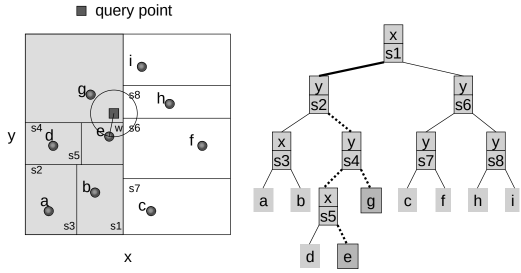
k-d Tree NNS (9)

■ query point



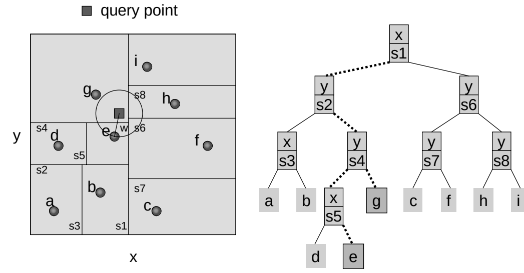
k-d Tree NNS (10)

■ query point

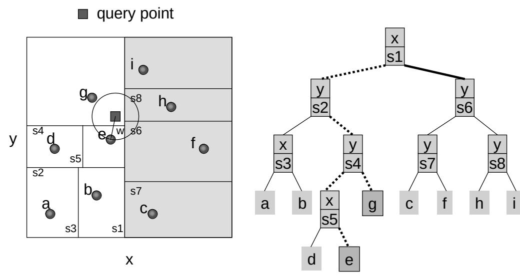


k-d Tree NNS (11)

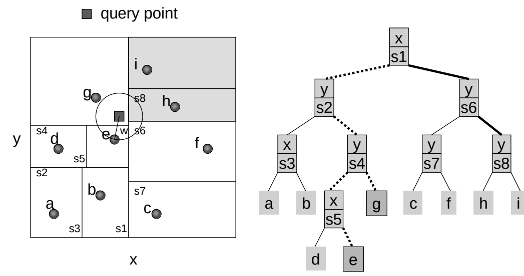
■ query point



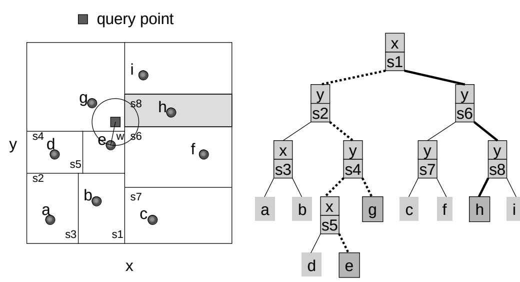
k-d Tree NNS (12)



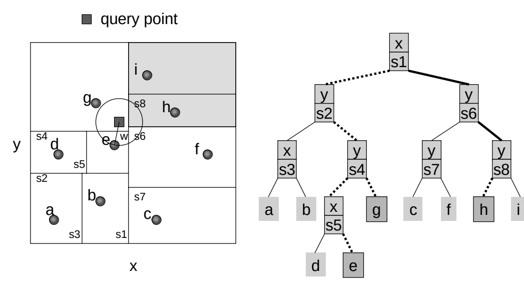
k-d Tree NNS (13)



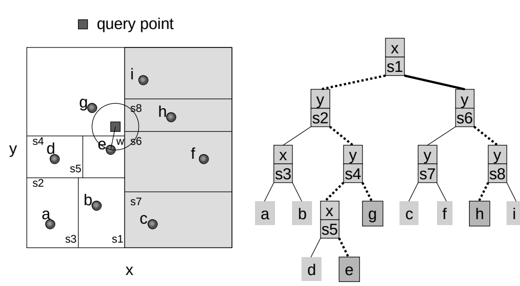
k-d Tree NNS (14)



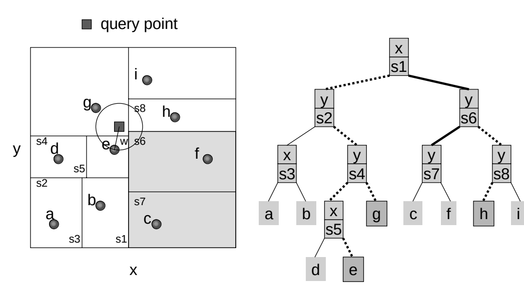
k-d Tree NNS (15)



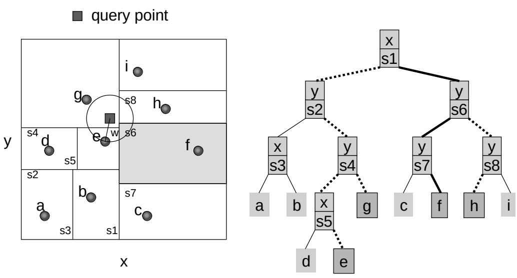
k-d Tree NNS (16)



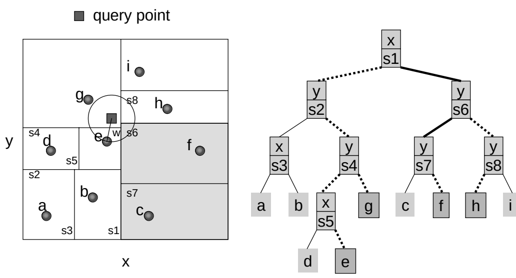
k-d Tree NNS (17)



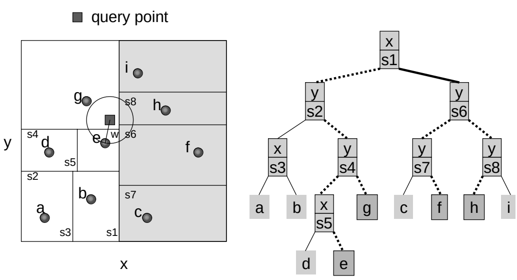
k-d Tree NNS (18)



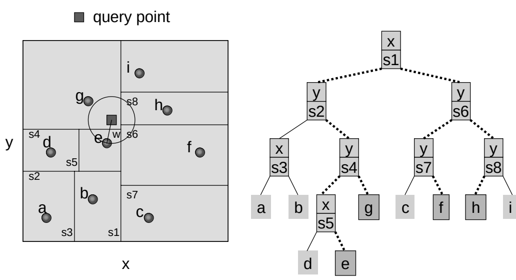
k-d Tree NNS (19)



k-d Tree NNS (20)



k-d Tree NNS (21)



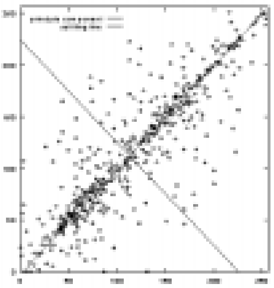
Notes on k-d NNS

- Has been shown to run in O(log n) average time per search in a reasonable model. (Assume d a constant)
- For VQ it appears that O(log n) is correct.
- Storage for the k-d tree is O(n).
- Preprocessing time is O(n log n) assuming d is a constant.

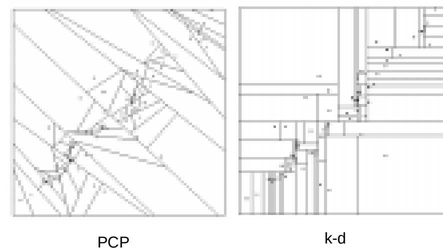
Alternative is PCP-Tree

- Zatloukal, Johnson, Ladner (1999)
- Organize a tree using principal components partitioning.
  - Partition the data perpendicular to the line that minimizes the sum of the distances of the points to the line. Eigenvector computation required.
- About is easy to construct as the k-d tree.
- In NNS processing per node in the PCP tree is more expensive than in the k-d tree, but fewer codewords are searched.

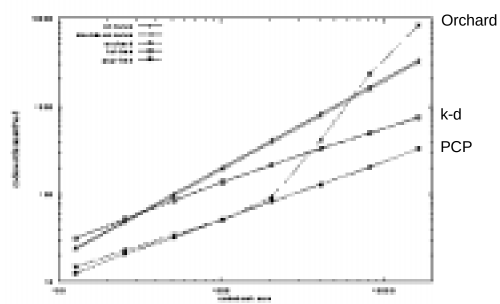
Principal Component Partition



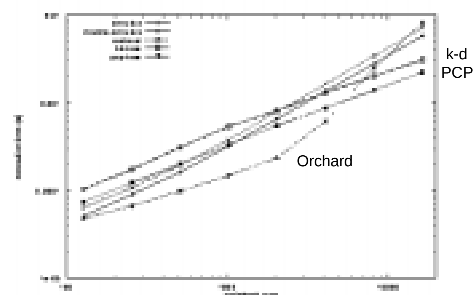
PCP Tree vs. k-d tree



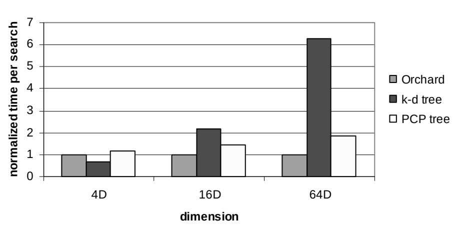
16D Codewords Searched



16D Execution Time



Comparison in Time per Search



4,096 codewords

NNS Summary

- Orchard
  - fastest
  - excessive memory
  - good guess codeword needed
- k-d tree
  - good in low dimension
  - small storage
  - no guess codeword
- PCP
  - best in high dimension
  - fewer codewords searched than k-d
  - small storage
  - no guess codeword

Notes on VQ

- Works well in some applications.
  - Requires training
- Has some interesting algorithms.
  - Codebook design
  - Nearest neighbor search
- Variable length codes for VQ.
  - PTSVQ - pruned tree structured VQ (Chou, Lookabaugh and Gray, 1989)
  - ECVQ - entropy constrained VQ (Chou, Lookabaugh and Gray, 1989)