## kd-Trees

- Invented in 1970s by Jon Bentley
- Name originally meant "3d-trees, 4d-trees, etc" where k was the \# of dimensions
- Now, people say "kd-tree of dimension d"
- Idea: Each level of the tree compares against 1 dimension.
- Let's us have only two children at each node (instead of $2^{d}$ )


## kd-trees

- Each level has a "cutting dimension"
- Cycle through the dimensions as you walk down the tree.
- Each node contains a point $\mathrm{P}=(\mathrm{x}, \mathrm{y})$
- To find ( $x^{\prime}, y^{\prime}$ ) you only compare coordinate from the cutting dimension

- e.g. if cutting dimension is $x$, then you ask: is $x^{\prime}<x$ ?


## kd-tree example

insert: $(30,40),(5,25),(10,12),(70,70),(50,30),(35,45)$


## kd-Trees vs. Quadtrees, another view

Consider a 3-d data set


Octtree

kd-tree
kd-tree splits the decision up over d levels don't have to represent levels (pointers) that you don't need

Quadtrees: one point determines all splits kd-trees: flexibility in how splits are chosen

## kd-tree Variants

- How do you pick the cutting dimension?
- kd-trees cycle through them, but may be better to pick a different dimension
- e.g. Suppose your 3d-data points all have same Z-coordinate in a give region:

- How do you pick the cutting value?
- kd-trees pick a key value to be the cutting value, based on the order of insertion
- optimal kd-trees: pick the key-value as the median
- Don't need to use key values $=>$ like PR Quadtrees $=>$ PR kd-trees
- What is the size of leaves?
- if you allow more than 1 key in a cell: bucket kd-trees
- kd-trees: discriminator = (hyper)plane;
quadtrees (and higher dim) discriminator complexity grows with $d$


## FindMin in kd-trees

- FindMin(d): find the point with the smallest value in the dth dimension.
- Recursively traverse the tree
- If cutdim(current_node) $=d$, then the minimum can't be in the right subtree, so recurse on just the left subtree
- if no left subtree, then current node is the min for tree rooted at this node.
- If cutdim(current_node) $\neq \mathrm{d}$, then minimum could be in either subtree, so recurse on both subtrees.
- (unlike in 1-d structures, often have to explore several paths down the tree)


## FindMin

FindMin(x-dimension):


## FindMin

FindMin(y-dimension):


## FindMin

FindMin(y-dimension): space searched


## Delete in kd-trees

Want to delete node A.
Assume cutting dimension of A is cd
In BST, we'd
findmin(A.right).
Here, we have to
findmin(A.right, cd)

Everything in Q has cd-coord $<\mathrm{B}$, and everything in P has cdcoord $\geq B$


## Nearest Neighbor Searching in kd-trees

- Nearest Neighbor Queries are very common: given a point $Q$ find the point $P$ in the data set that is closest to Q .
- Doesn't work: find cell that would contain Q and return the point it contains.
- Reason: the nearest point to $P$ in space may be far from $P$ in the tree:
- E.g. $\mathrm{NN}(52,52)$ :



## kd-Trees Nearest Neighbor

- Idea: traverse the whole tree, BUT make two modifications to prune to search space:

1. Keep variable of closest point $C$ found so far. Prune subtrees once their bounding boxes say that they can't contain any point closer than $C$
2. Search the subtrees in order that maximizes the chance for pruning

## Nearest Neighbor: Ideas, continued



> If $\mathrm{d}>\operatorname{dist}(\mathrm{C}, \mathrm{Q})$, then no point in $\mathrm{BB}(\mathrm{T})$ can be closer to Q than C . Hence, no reason to search subtree rooted at T .

Update the best point so far, if T is better: if $\operatorname{dist}(\mathrm{C}, \mathrm{Q})>\operatorname{dist}($ T.data, Q$), \mathrm{C}:=$ T.data

Recurse, but start with the subtree "closer" to Q:
First search the subtree that would contain Q if we were inserting Q below T .

## Nearest Neighbor Facts

- Might have to search close to the whole tree in the worst case. [O(n)]
- In practice, runtime is closer to:
- $O\left(2^{d}+\log n\right)$
- $\quad \log \mathrm{n}$ to find cells "near" the query point
- $\quad 2^{\mathrm{d}}$ to search around cells in that neighborhood
- Three important concepts that reoccur in range / nearest neighbor searching:
- storing partial results: keep best so far, and update
- pruning: reduce search space by eliminating irrelevant trees.
- traversal order: visit the most promising subtree first.


## Generalized Nearest Neighbor Search

- Saw last time: nearest neighbor search in kd-trees.
- What if you want the k-nearest neighbors?
- What if you don't know k?
- E.g.: Find me the closest gas station with price $<\$ 3.25$ / gallon.
- Approach: go through points (gas stations) in order of distance from me until I find one that meets the $\$$ criteria
- Need a NN search that will find points in order of their distance from a query point $q$.
- Same idea as the kd-tree NN search, just more general


## Generalized NN Search

- A feature of all spatial DS we've seen so far: decompose space hierarchically.
No matter what the DS, we get something like this:


Let the items in the hierarchy be e1,e2,e3...
Items may represent points, or bounding boxes, or ...
Let Type(e) be an abstract "type" of the object: we use the type to determine which distance function to use
E.g: if Type = "bounding box" then we'd use the point-to-rectangle distance function.

A concrete example: in a Quadtree: internal nodes have type "bounding box" Leaves would have type "point"

## Generalized, Incremental NN

Let IsLeaf(), Children(), and Type() represent the decomposition tree
Let $d_{t}\left(q, e_{t}\right)$ be the distance function appropriate to compare points with elements of type $t$.

Idea: keep a priority queue that contains all elements visited so far (points, bounding boxes)

Priority queue (heap) is ordered by distance to the query point
When you dequeue a point (leaf), it will be the next closest

```
HeapInsert(H, root, 0)
while not Empty(H):
    e := ExtractMin(H)
    if IsLeaf(e):
        output e as next nearest
    else
        foreach c in Children(e):
            t = Type(c)
            HeapInsert(H, c, dt(q,c))
```

$d_{t}(q, c)$ may be the distance to the bounding box represented by c, e.g.

## Incremental, Generalized NN Example

Some spatial data structure:

It's spatial decomposition (NOT the actual data structure)
HeapInsert(H, root, 0)
while not Empty(H):
e := ExtractMin(H)
if IsLeaf(e):
output e as next nearest
else
foreach $C$ in Children(e):
$t=$ Type(c)
HeapInsert( $H$, $c, d_{t}(q, C)$ )

## Incremental, Generalized NN Example

Some spatial data structure:


```
HeapInsert(H, root, 0)
while not Empty(H):
    e := ExtractMin(H)
    if IsLeaf(e) && IsPoint(e):
        output e as next nearest
    else
        foreach c in Children(e):
            t = Type(c)
            HeapInsert(H, c, dt(q,c))
HeapInsert(H, root, 0)
while not Empty(H):
e := ExtractMin(H)
if IsLeaf(e) \&\& IsPoint(e): output e as next nearest else
foreach \(c\) in Children(e):
\(t=\) Type(c)
HeapInsert( \(\left.H, ~ c, ~ d_{t}(q, c)\right)\)
```



Its spatial decomposition (NOT the actual data structure)
$\mathrm{H}=[]$
$\mathrm{H}=[\mathrm{T}]$
$\mathrm{H}=\left[\mathrm{L}_{\mathrm{T}} \mathrm{R}_{\mathrm{T}}\right]$
$H=\left[A_{Q} R_{T} B_{Q}\right]$
$H=\left[R_{T} B_{Q}\right]$
$\mathrm{H}=\left[\mathrm{B}_{\mathrm{S}} \mathrm{A}_{\mathrm{S}} \mathrm{B}_{\mathrm{Q}}\right]$
$\mathrm{L}, \mathrm{R}=$ left, right

| $\mathrm{H}=[]$ | $\longrightarrow \mathrm{H}=\left[\mathrm{A}_{s}\right.$ a $\left.\mathrm{B}_{\mathrm{Q}}\right]$ |
| :---: | :---: |
| $\mathrm{H}=[\mathrm{T}]$ | $\mathrm{H}=\left[\begin{array}{llll}\mathrm{c} & \mathrm{B}\end{array}\right]$ |
| $\mathrm{H}=\left[\mathrm{L}_{\mathrm{T}} \mathrm{R}_{\mathrm{T}}\right]$ | $H=\left[\begin{array}{ccc}c & \mathrm{~b}\end{array}\right]$ |
| $\mathrm{H}=\left[\mathrm{A}_{\mathrm{Q}} \mathrm{R}_{\mathrm{T}} \mathrm{B}_{\mathrm{Q}}\right]$ | $\mathrm{H}=[\mathrm{ab}]$ |
| $H=\left[\mathrm{R}_{\mathrm{T}} \mathrm{B}_{\mathrm{Q}}\right]$ | $\mathrm{H}=[\mathrm{b}]$ |
| $\mathrm{H}=\left[\mathrm{B}_{S} \mathrm{~A}_{S} \mathrm{~B}_{\mathrm{Q}}\right]$ | $\mathrm{H}=[]$ |

## Range Searching in kd-trees

- Range Searches: another extremely common type of query.
- Orthogonal range queries:
- Given axis-aligned rectangle
- Return (or count) all the points inside it
- Example: find all people between 20 and 30 years old who are between $5^{\prime \prime} 8^{\prime \prime}$ and $6^{\prime}$ tall.



## Range Searching in kd-trees

- Basic algorithmic idea:
- traverse the whole tree, BUT
- prune if bounding box doesn't intersect with Query
- stop recursing or print all points in subtree if bounding box is entirely inside Query


## Range Searching Example



If query box doesn't overlap bounding box, stop recursion
If bounding box is a subset of query box, report all the points in current subtree If bounding box overlaps query box, recurse left and right.

## Expected \# of Nodes to Visit

- Completely process a node only if query box intersects bounding box of the node's cell:
- In other words, one of the edges of Q must cut through the cell.
- \# of cells a vertical line will pass through $\geq$ the number of cells cut by the left edge of Q .
- Top, bottom, right edges are the same, so bounding \# of cells cut by a vertical line is sufficient.



## \# of Stabbed Nodes $=\mathbf{O}(\sqrt{ } n)$

Consider a node $a$ with cutting dimension $=x$

Vertical line can intersect exactly one of $a^{\prime}$ s children (say c)

But will intersect both of c's children.

Thus, line will intersect at most 2 of $a^{\prime}$ s grandchildren.


## \# of Stabbed Nodes $=\mathbf{O}(\sqrt{ } n)$

So: you at most double \# of cut nodes every 2 levels

If kd-tree is balanced, has
O( $\log n$ ) levels
Cells cut

$$
\begin{aligned}
& =2^{(\log n) / 2} \\
& =2^{\log \sqrt{n}} \\
& =\sqrt{n}
\end{aligned}
$$



> Assuming random input, or all points known ahead of time, you'll get a balanced tree.

Each side of query rectangle stabs $<\mathrm{O}(\sqrt{n})$ cells. So whole query stabs at most $O(4 \sqrt{n})=O(\sqrt{n})$ cells.

## Suppose we want to output all points in region

- Then cost is $\mathrm{O}(\mathrm{k}+\sqrt{\mathrm{n}})$
- where k is \# of points in the query region.
- Why? Because: you visit every stabbed node $[\mathrm{O}(\sqrt{n})$ of them] + every node in the subtrees rooted in the contained cells.
- Takes linear time to traverse such subtrees
- Example of output sensitive running time analysis: running time depends on size of the output.



## kd-tree Summary:

- Use $\mathrm{O}(\mathrm{n})$ storage [1 node for each point]
- If all points are known in advance, balanced kd-tree can be built in $O(n \log n)$ time
- Recall: sort the points by $x$ and $y$ coordinates
- Always split on the median point so each split divides remaining points nearly in half.
- Time dominated by the initial sorting.
- Can be orthogonal range searched in $O(\sqrt{n}+k)$ time.
- Can we do better than $O(\sqrt{n})$ to range search?
- (possibly at a cost of additional space)


## 1-Dimensional Range Trees

- Suppose you have "points" in 1-dimension (aka numbers)
- Want to answer range queries: "Return all keys between $x_{1}$ and $x_{2}$."
- How could you solve this?


## Balanced Binary Search Tree

## Range Queries on Binary Search Trees

Assume all data are in the leaves

Search for $x_{1}$ and $x_{2}$

Let $x_{\text {split }}$ be the node were the search paths diverge

Output leaves in the right subtrees of nodes on the path from $x_{\text {split }}$ to $x_{1}$

Output leaves in the left subtrees of nodes on the path from $x_{\text {split }}$ to $x_{2}$


## 1-D Query Time

- $\mathrm{O}(\mathrm{k}+\log \mathrm{n})$, where k is the number of points output.
- Tree is balanced, so depth is $\mathrm{O}(\log \mathrm{n})$
- Length of paths to $x 1$ and $x 2$ are $O(\log n)$
- Therefore visit $\mathrm{O}(\log n)$ nodes to find the roots of subtrees to output
- Traversing the subtrees is linear, $\mathrm{O}(\mathrm{k})$, in the number of items output.


## How would you generalize to $2 d$ ?

## 2d Range Trees

- Treat range query as 2 nested one-dimensional queries:
- [ $\left.\mathrm{x}_{1}, \mathrm{x}_{2}\right]$ by $\left[\mathrm{y}_{1}, \mathrm{y}_{2}\right]$
- First ask for the points with $x$-coordinates in the given range $\left[\mathrm{x}_{1}, \mathrm{x}_{2}\right]=>$ a set of subtrees $\triangle$
- Instead of all points in these subtrees, only want those that fall in $\left[y_{1}, y_{2}\right]$
$\mathrm{P}(\mathrm{u})$ is the set of points under $u$

We store those points in another tree $\mathrm{Y}(\mathrm{u})$, keyed by the $y$-dimension


## 2-D Range Trees, Cont.

Every node has a tree
associated with it:
multilevel data structure


Range Trees, continued.


## 2d-range tree space requirements

- Sum of the sizes of $Y(u)$ for $u$ at a given depth is $O(n)$
- Each point stored in the $\mathrm{Y}(\mathrm{u})$ tree for at most one node at a given depth
- Since main tree is balanced, has $\mathrm{O}(\log \mathrm{n})$ depth
- Meaning total space requirement is $\mathrm{O}(\mathrm{n} \log \mathrm{n})$


## 2d Range Tree Range Searches

1. First find trees that match the x -constraint;
2. Then output points in those subtrees that match the $y$ constraint (by 1-d range searching the associated $\mathrm{Y}(\mathrm{u})$ trees)

- Step 1 will return at most $O(\log n)$ subtrees to process.
- Step 2 will thus perform the following $O(\log n)$ times:
- Range search the $Y(u)$ tree. This takes $O\left(\log n+k_{u}\right)$, where $k_{u}$ is the number of points output for that $Y(u)$ tree.
- Total time is $\sum_{\mathrm{u}} \mathrm{O}\left(\log \mathrm{n}+\mathrm{k}_{\mathrm{u}}\right)$ where u ranges over $\mathrm{O}(\log \mathrm{n})$ nodes. Thus the total time is $\mathrm{O}\left(\log ^{2} \mathrm{n}+k\right)$.


## kd-tree vs. Range Tree

- 2d kd-tree:
- $\quad$ Space $=O(n)$
- $\quad$ Range Query Time $=O(k+\sqrt{n})$
- Inserts O(log n)
- 2d Range Tree:
- $\quad$ Space $=O(n \log n)$
- $\quad$ Range Query Time $=\mathrm{O}\left(\mathrm{k}+\log ^{2} \mathrm{n}\right)$
- Inserts O( $\log ^{2} n$ )


## How would you extend this to $>2$ dimensions?

## Range Trees for $\mathrm{d}>2$

- Now, your associated trees $\mathrm{Y}(\mathrm{u})$ themselves have associated trees $\mathrm{Z}(\mathrm{v})$ and so on:


Searching: find $\mathrm{O}(\log \mathrm{n})$ nodes in first tree for each of them, find another $\mathrm{O}(\log \mathrm{n})$ sets for each of them find another $\log \mathrm{n}$ sets

Leads to $O\left(k+\log ^{d} n\right)$ search time Space: $O\left(n \log ^{d-1} n\right)$ space

## Fractional Cascading Speed-up: Idea

- Suppose you had two sorted arrays $\mathrm{A}_{1} \mathrm{~A}_{2}$
- Elements in $\mathrm{A}_{2}$ are subset of those in $\mathrm{A}_{1}$
- Want to range search in both arrays with the same range: [ $\mathrm{x}_{1}, \mathrm{x}_{2}$ ]
- Simple:
- Binary Search to find $\mathrm{x}_{1}$ in both $\mathrm{A}_{1}$ and $\mathrm{A}_{2}$
- Walk along array until you pass $\mathrm{x}_{2}$
- O(log n) time for each Binary Search,
- have to do it twice though


## Can do better:

- Since $\mathrm{A}_{2}$ subset of $\mathrm{A}_{1}$ :
- Keep pointer at each element $u$ of $\mathrm{A}_{1}$ pointing to the smallest element of $\mathrm{A}_{2}$ that is $\geq u$.

| 3 | 7 | 11 | 12 | 15 | 18 | 30 | 32 | 41 | 49 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  |  |  |  |  |  |  |  |  |  |
|  |  | 15 | 30 | 32 | 41 | 49 |  |  |  |

- After Binary Search in $\mathrm{A}_{1}$, use pointer to find where to start in $\mathrm{A}_{2}$
- Can do similar in Range Trees to eliminate an $\mathrm{O}(\log \mathrm{n})$ factor (see next slides)


## Fractional Cascading in Range Trees

Instead of an aux. tree, we store an array, sorted by Y-coord. At $x_{\text {split, }}$ we do a binary search for $y_{1}$. As we continue to search for $x_{1}$ and $x_{2}$, we also use pointers to keep track of the result of a binary search for $\mathrm{y}_{1}$ in each of the arrays along the path.

(Only subset of pointers are shown)

## Fractional Cascading Search

- RangeQuery([x1,x2] by [y1,y2]):
- Search for $\mathrm{x}_{\text {split }}$
- Use binary search to find the first point in $\mathrm{A}\left(\mathrm{x}_{\text {split }}\right)$ that is larger that $\mathrm{y}_{1}$.
- Continue searching for $x_{1}$ and $x_{2}$, following the now diverged paths
- Let $u_{1}--u_{2}--u_{3}--u_{k}$ be the path to $x_{1}$. While following this path, use the "cascading" pointers to find the first point in each $\mathrm{A}\left(u_{\mathrm{i}}\right)$ that is larger than $\mathrm{y}_{1}$. [similarly with the path $\mathrm{v}_{1}-\mathrm{v}_{2}--\mathrm{v}_{\mathrm{m}}$ to $\mathrm{x}_{2}$ ]
- If a child of $u_{i}$ or $v_{i}$ is the root of a subtree to output, then use a cascading pointer to find the first point larger than $\mathrm{y}_{1}$, output all points until you pass $\mathrm{y}_{2}$.


## Fractional Cascading: Runtime

- Instead of $\mathrm{O}(\log \mathrm{n})$ binary searches, you perform just one
- Therefore, $\mathrm{O}\left(\log ^{2} \mathrm{n}\right)$ becomes $\mathrm{O}(\log \mathrm{n})$
- 2d-rectangle range queries in $\mathrm{O}(\log \mathrm{n}+\mathrm{k})$ time
- In d dimensions: $\mathrm{O}\left(\log ^{\mathrm{d}-1} \mathrm{n}+\mathrm{k}\right)$

