CMSC 420: KD Trees

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1 Introduction

All of the data we’ve stored so far has been premised on 1-dimensional keys. Essentially we’ve been using integers but any set which can be ordered would work just as well.

Now we’d like to investigate how we might construct a tree (or tree-like structure) to store keys which are in $n$-dimensional space. For example if the keys were things like $(40, 32)$ or $(81, 3)$ in the 2-dimensional case.

2 Initial Ideas

2.1 More Dimension Solution

A standard binary tree can be thought of as a layered collection of $x$-axis whereby each $x$-axis corresponds to a layer of the tree and each set of points is divided by the points above it:
In light of this we could store a collection of points using layers of planes. For example if the root node contains (5, 6) and the second level contains the points (2, 2), (7, 3), (2, 8), and (8, 7) we could draw the following. The dashed lines are just there to show how the points relate.

Note that the points are placed in the four quadrants relative to the root depending on how their x- and y-values relate to the parent node.

Then as a tree this would be the following, where the red lines are the ones connecting the root node to its four children and the planes and lines are just left for visual reference but of course are not part of the tree:
These stacked planes can also be simply drawn on top of each other. Here we have drawn dashed lines to show how each point has four related quadrants. Each point may have zero or one child in each quadrant, in our case we have exactly one in each.

Then if we wish to add further children we just add them in the sub-rectangles, for example let’s give (7, 3) two children (8, 1) and (9, 4), and (2, 2) one child (3, 5):

![Diagram showing the addition of children in sub-rectangles.](image-url)
2.2 Multi-Child Solution

The above picture may be pretty but it does little to instruct us on how to code it. One solution might be for each node to have up to four children, one for each combination of how their \(x\)- and \(y\)-values relate. For example a north-east (NE) child would have larger \(x\)- and \(y\)-values whereas a SE child would have smaller \(x\)- and \(y\)-values. For example the above picture would then become:

\[
\begin{align*}
(5,6) & \quad NW \quad NE \quad SW \quad SE \\
(2,8) & \quad (8,7) \quad (2,2) \quad (7,3) \\
& \quad NE \quad NE \quad SE \\
& \quad (3,5) \quad (9,4) \quad (8,1)
\end{align*}
\]

This isn’t a bad approach but we can easily see that it will become somewhat intractible if we add more dimensions. Moreover it’s not clear how we might implement some of our dictionary operations.

3 Standard Approach

3.1 Alternating Split Solution

Let’s head back to binary trees! We like binary trees because they’re easy to comprehend. But how can we store this sort of data in a binary tree?

In the 2D case, what we’ll do is this: When we go from the root level to the next level we will go left or right depending on the \(x\)-value. For the next level we will go left or right depending on the \(y\)-value. Then we switch back to \(x\), then \(y\), and so on.

Let’s insert all of the above points into such a tree in the order given here:

\[(5,6), (2,2), (7,3), (2,8), (8,7), (8,1), (9,4), (3,5)\]

The root node is \((5,6)\). The next level splits by \(x\)-value so when we insert \((2,2)\) we go left:
When we insert \((7, 3)\) we first ask how its \(x\)-value compares to \((5, 6)\). It’s larger, so we go right and place it there:

\[
\begin{array}{c}
(5, 6) \\
(2, 2) \quad (7, 3)
\end{array}
\]

Now when we insert \((2, 8)\) we first ask how its \(x\)-value compares to \((5, 6)\). It’s smaller so we go left and reach \((2, 2)\). Then we ask how its \(y\)-value compares to \((2, 2)\). It’s larger so we go right and place it there:

\[
\begin{array}{c}
(5, 6) \\
(2, 2) \quad (7, 3) \\
(2, 8)
\end{array}
\]

If we continue this process we get the final tree:

\[
\begin{array}{c}
(5, 6) \\
(2, 2) \quad (7, 3) \\
(2, 8) \quad (8, 1) \quad (8, 7) \\
(3, 5) \quad (9, 4)
\end{array}
\]

Traditionally in order to keep track of the splits we decorate the nodes. We put a vertical decoration to indicate that we’re splitting by \(x\)-coordinate and a horizontal decoration to indicate that we’re splitting by \(y\)-coordinate:

\[
\begin{array}{c}
(5, 6) \\
(2, 2) \quad (7, 3) \\
(2, 8) \quad (8, 1) \quad (8, 7) \\
(3, 5) \quad (9, 4)
\end{array}
\]

### 3.2 More than 2 Dimensions

One advantage to this approach is that it’s easy to generalize to more dimensions. For example when managing points in 3D we can rotate our splitting first by \(x\), then \(y\), then \(z\), then \(x\), then \(y\), and so on.

### 3.3 Duplicate Coordinates

Typically when keys consist of a single value they are unique, and in this case while the points will be unique, specific coordinates may not be. For example we must allow both \((20, 30)\) and \((20, 40)\) in the 2D-case.

By convention we will say that if we are traveling down the tree to insert a node and we are at a node where we split by the \(\alpha\)-coordinate and the node we wish to insert has the same coordinate value then we go right.
Note 3.3.1. $\alpha$ in this case represents any coordinate, think of it as a coordinate variable.

For example if we are inserting $(20, 30)$ and we encounter the node $(20, 40)$ where the split is by the $x$-coordinate then we go right.

We could just have well decided to go left, with some appropriate changes later, but the point is that we must make a choice so that we know how to handle search, insert, and as we’ll see, delete.

To simplify later discussion we’ll use the phrase identical coordinates split right.

4 Measurements

4.1 Space Requirements

Since we are storing $n$ points each with $d$ dimensions it takes $dn$ space to store all the coordinates and $O(dn)$ to store the pointers. Typically we just say $O(dn)$ overall.

4.2 Height

Much like a standard binary search tree the worst-case height is $O(n)$ and the best-case height is $O(\lg n)$.

Average-case is a little trickier. Our intuitive feeling in these situations, and perhaps our hope, is that average case is $O(\lg n)$, however this is not the case. Recalling when studying unbalanced binary trees that if we systematically choose an inorder successor when hunting for replacements that the height turns out to be $O(\sqrt{n})$. It turns out (as we’ll see) that deletion has the same issue here.

5 Search

5.1 Search Algorithm

Search in a k-d tree works exactly like a binary tree with the adjustment that we follow the branch according to the splitting coordinate for each node.

5.2 Worst-Case Time Complexity

Since the height of the tree could be $n$, the worst-case time complexity of search would be $O(n)$. 
6 Insert

6.1 Insertion Algorithm

Insertion in a k-d tree works exactly like a binary tree with the adjustment that we follow the branch according to the splitting coordinate for each node and we place the node as a leaf in the correct position with regards to the correct splitting coordinate at the end.

Example 6.1. For example the insertion of (9, 2) into our k-d tree from earlier would look proceed as shown. We start at the root and compare x-coordinates and go right. At (7, 3) we compare y-coordinates and go left. At (8, 1) we compare x-coordinates and insert right. Notice that the inserted node has its split direction set appropriately for the level it is on.

6.2 Worst-Case Time Complexity

Since the height of the tree could be $n$, the worst-case time complexity of insert would be $O(n)$.

7 Delete

7.1 Finding Replacements

With BSTs we regularly did replacements using a node’s inorder successor. This successor was easy to find - go right (if possible) then left as far as possible. However this algorithm is premised on the fact that we are always splitting by the single key and with a k-d tree this is no longer the case.

Let’s abstract the procedure and observe that when we are looking for a node’s inorder successor we are looking for the smallest key in the right subtree.

So let’s imagine we simply have a k-d tree and wish to find the node with smallest $\alpha$-coordinate. Here $\alpha$ could be $x$, or $y$, or whatever.

The following procedure is recursive:

- If we are at a node which splits by $\alpha$ then the target is in the left subtree.
  If that left subtree is NULL then just return the current node. Otherwise recurse to the root of the left subtree.
• If we are at a node which splits by something other than $\alpha$ then the target could be in any subtree or the node itself. We recurse to all, take the multiple results as well as the node itself and pick the one with minimum $\alpha$-coordinate. If there are several then we can pick any of them.

**Example 7.1.** Suppose in the most recent tree we wish to find the node with minimum $y$-coordinate. We start at (5,6) but since it splits by $x$-coordinate we have to check both subtrees.

We recurse to the subtree rooted at (2,2), note that (2,2) splits by $y$-coordinate and so we need to branch left. We cannot, however, so we simply return (2,2).

We recurse to the subtree rooted at (7,3), note that (7,3) splits by $y$-coordinate and so we need to branch left. We branch left to (8,1) but since it splits by $x$-coordinate we have to check both subtrees but there is only one, and that returns (9,2).

So the (8,1) subtree returns the minimum of (8,1) and (9,2), where minimum means minimum $y$-coordinate, so that’s (8,1). The (7,3) subtree returns this same value. The (5,6) subtree returns the minimum of (2,2), (8,1) and (5,6), so that’s (8,1).

This can be illustrated in the following diagram where we shade the nodes that we actually have to analyze. The recursive procedure takes the minimum up the tree:

![Diagram of a tree](image)

### 7.2 Deletion Algorithm

In the 1-D case the process was simple - go right then as far left as possible to find the inorder successor, replace the deleted node with that inorder successor, then either splice the tree (if the inorder successor was not a leaf) or just chop off the old inorder successor node (if it was).

This won’t work here because splicing the tree will result in the lower part of the splice having all its splitting directions messed up. So what can we do?

Our deletion will work as follows:

• If the deleted node is a leaf, just delete it and we’re done.
• If the deleted node has a right subtree then if the deleted node is \( u \) then if \( u \) splits on the \( \alpha \)-coordinate then we find the node in the right subtree with minimal \( \alpha \) coordinate using the method above. This is our replacement node. We then recursively call delete on the old replacement node.

• If the deleted node does not have a right subtree then it has a left subtree. If the deleted node is \( u \) then if \( u \) splits on the \( \alpha \)-coordinate then we find the node in the left subtree of \( u \) for which \( \alpha \) is minimal. Call this node \( r \). We move \( r \) to \( u \) and then we take \( u \)’s original left subtree and make it \( u \)’s right subtree. We then recursively call delete on the old replacement node.

**Note 7.2.1.** It’s tempting to think that instead of the third bullet point above we could just find a replacement in the left subtree (maximum value). However this can mess up our insistence that identical coordinates branch right. You encouraged to draw an example.

The third bullet is funny. Why does it work? We need to ensure that the \( r \) we found is positioned correctly when we overwrite \( u \), meaning it works with all of \( u \)’s ancestors and children. In what follows we’ll use subscripts to denote coordinates, so \( x_\alpha \) will mean the \( \alpha \) coordinate of \( x \). e.g. \((17, 42, 100)_x = 17\) and so on.

Suppose \( u \) splits on the \( \alpha \)-coordinate. We find \( r \in u.left \) with minimal \( r_\alpha \) for all \( x_\alpha \in u.left \). In addition since we looked at the \( u.left \) and \( u \) splits on \( \alpha \) we know that \( r_\alpha < u_\alpha \).

Now then, for any coordinate \( \beta \) if \( u \) has an ancestor which splits on \( \beta \) then \( r_\beta \) was already positioned correctly with regards to that ancestor (since it’s lower than the ancestor) and this will not change when we move it.

In addition, since \( x_\alpha > r_\alpha \) for all \( x \in u.left \) we know that we can move the subtree \( u.left \) to \( u.right \) (which was empty) and since \( u = r \) at this point we know that what is now \( u.right \) is positioned correctly with regards to the splitting on \( \alpha \) occurring at \( u \).

**Example 7.2.** Let’s delete \((5, 6)\) from this tree:

```
    (5, 6)
   /    \
(2, 2)  (7, 3)
      /    \
(2, 8)  (8, 1)
     /    \
(3, 5)  (9, 2)
```

Since \((5, 6)\) splits on the \( x \)-coordinate and has a right subtree we pick the node in the right subtree with minimum \( x \)-coordinate, this is \((7, 3)\). We
replace. There are temporarily two copies of (7, 3), the red one below is next in line for replacement.

Since the red (7, 3) splits on the $y$-coordinate but has no right subtree we pick the node in the left subtree with minimum $y$-coordinate, this is (8, 1). We replace and then move the old left subtree to the right: There are now temporarily two copies of (8, 1), the red one below is next in line for replacement.

Since the red (8, 1) splits on the $x$-coordinate and has a right subtree we pick the node in the right subtree with minimum $x$-coordinate, this is (9, 2). We replace. There are temporarily two copies of (9, 2), the red one below is next in line for replacement.

Since the red (9, 2) is a leaf we chop it off and we are done:
7.3 Worst-Case Time Complexity

Since the height of the tree could be $n$, the worst-case time complexity of search would be $O(n)$. Notice that this is compounded by, but unaffected by, the fact that during delete we often need to run our algorithm to find a minimum coordinate. This procedure is recursive and visits every node in a subtree once and hence is $O(n)$ too.

8 Modifications

There are several ways that one could modify a k-d tree. Some examples are:

1. Trying to keep the tree balanced. This is tricky because we cannot use rotations since they ruin our splitting according to level. Theoretically it’s possible to take a scapegoat tree approach and rebuild subtrees.

2. Much like a B+ tree it not uncommon to modify a k-d tree so that the data is all in the leaf nodes and the internal nodes are used simply as guideposts to lead us to the data. The crucial benefit to this is that it makes it easier to insert and delete keys since we don’t have to go through the convoluted deletion process.

3. As a modification of the above we can permit a leaf node to contain several points, generally a small number, stored in some other method (a list, a linked list, etc.) which we simply work with in a more traditional manner.