# Multidimensional Binary Search Trees

# Martin Rau

# October 13, 2025

#### Abstract

This entry provides a formalization of multidimensional binary trees, also known as k-d trees. It includes a balanced build algorithm as well as the nearest neighbor algorithm and the range search algorithm. It is based on the papers "Multidimensional binary search trees used for associative searching" [1] and "An Algorithm for Finding Best Matches in Logarithmic Expected Time" [2].

# Contents

1	Def	$\mathbf{finition}$ of the $k$ -d $\mathbf{Tree}$	2
	1.1	Definition of the $k$ -d Tree Invariant and Related Functions	2
	1.2	Lemmas adapted from $HOL-Library.Tree$ to $k$ -d Tree	4
	1.3	Lemmas adapted from $HOL-Library.Tree-Real$ to $k\text{-d}$ Tree .	8
2	Bui	llding a balanced k-d Tree from a List of Points	10
	2.1	Auxiliary Lemmas	11
	2.2	Widest Spread Axis	11
	2.3	Fast Axis Median	13
	2.4	Building the Tree	14
	2.5	Main Theorems	16
3	Range Searching		20
	3.1	Rectangle Definition	20
	3.2	Search Function	21
	3.3	Auxiliary Lemmas	21
	3.4	Main Theorem	21
4	Nearest Neighbor Search on the k-d Tree		22
	4.1	Auxiliary Lemmas about sorted-wrt	22
	4.2	Neighbors Sorted wrt. Distance	23
	4.3	The Recursive Nearest Neighbor Algorithm	24
	4.4	Auxiliary Lemmas	24
	4.5	The Main Theorems	25
	4.6	Nearest Neighbors Definition and Theorems	30
		<del>-</del>	

## 1 Definition of the k-d Tree

```
\begin{tabular}{ll} \textbf{theory} & \textit{KD-Tree} \\ \textbf{imports} \\ & \textit{Complex-Main} \\ & \textit{HOL-Analysis.Finite-Cartesian-Product} \\ & \textit{HOL-Analysis.Topology-Euclidean-Space} \\ \textbf{begin} \\ \end{tabular}
```

A k-d tree is a space-partitioning data structure for organizing points in a k-dimensional space. In principle the k-d tree is a binary tree. The leafs hold the k-dimensional points and the nodes contain left and right subtrees as well as a discriminator v at a particular axis k. Every node divides the space into two parts by splitting along a hyperplane. Consider a node n with associated discriminator v at axis k. All points in the left subtree must have a value at axis k that is less than or equal to v and all points in the right subtree must have a value at axis k that is greater than v.

Deviations from the papers:

The chosen tree representation is taken from [2] with one minor adjustment. Originally the leafs hold buckets of points of size b. This representation fixes the bucket size to b = 1, a single point per Leaf. This is only a minor adjustment since the paper proves that b = 1 is the optimal bucket size for minimizing the running time of the nearest neighbor algorithm [2], only simplifies building the optimized k-d trees [2] and has little influence on the search algorithm [1].

```
type-synonym 'k point = (real, 'k) vec

lemma dist-point-def:
    fixes p_0 :: ('k::finite) point
    shows dist p_0 p_1 = sqrt (\sum k \in UNIV. (p_0\$k - p_1\$k)^2)
    unfolding dist-vec-def L2-set-def dist-real-def by simp

datatype 'k kdt =

Leaf 'k point

| Node 'k real 'k kdt 'k kdt
```

# 1.1 Definition of the k-d Tree Invariant and Related Functions

```
fun set-kdt :: 'k kdt \Rightarrow ('k point) set where

set-kdt (Leaf p) = { p }

| set-kdt (Node - - l r) = set-kdt l \cup set-kdt r

definition spread :: ('k::finite) \Rightarrow 'k point set \Rightarrow real where

spread k P = (if P = {} then 0 else let V = (\lambdap. p$k) 'P in Max V - Min V)

definition widest-spread-axis :: ('k::finite) \Rightarrow 'k set \Rightarrow 'k point set \Rightarrow bool where
```

```
widest-spread-axis k \ K \ ps \longleftrightarrow (\forall k' \in K. \ spread \ k' \ ps \leq spread \ k \ ps)
\mathbf{fun} \ invar :: ('k::finite) \ kdt \Rightarrow bool \ \mathbf{where}
  invar\ (Leaf\ p) \longleftrightarrow True
|invar|(Node\ k\ v\ l\ r)\longleftrightarrow (\forall\ p\in set\text{-}kdt\ l.\ p\$k\leq v)\land (\forall\ p\in set\text{-}kdt\ r.\ v< p\$k)
    widest-spread-axis k UNIV (set-kdt l \cup set-kdt r) \land invar l \land invar r
fun size-kdt :: 'k \ kdt \Rightarrow nat \ \mathbf{where}
  size-kdt (Leaf -) = 1
| size-kdt (Node - - l r) = size-kdt l + size-kdt r
fun height :: 'k \ kdt \Rightarrow nat \ \mathbf{where}
  height (Leaf -) = 0
| height (Node - - l r) = max (height l) (height r) + 1
fun min-height :: 'k kdt \Rightarrow nat where
  min-height (Leaf -) = 0
| min-height (Node - - l r) = min (min-height l) (min-height r) + 1
definition balanced :: k k dt \Rightarrow bool where
  balanced\ kdt \longleftrightarrow height\ kdt - min-height\ kdt \le 1
fun complete :: 'k \ kdt \Rightarrow bool \ \mathbf{where}
  complete (Leaf -) = True
| complete (Node - - l r) \longleftrightarrow complete l \land complete r \land height l = height r
lemma invar-l:
  invar (Node \ k \ v \ l \ r) \Longrightarrow invar \ l
  by simp
lemma invar-r:
  invar (Node \ k \ v \ l \ r) \Longrightarrow invar \ r
  by simp
lemma invar-l-le-k:
  invar\ (Node\ k\ v\ l\ r) \Longrightarrow \forall\ p\in set\text{-}kdt\ l.\ p\$k \le v
  by simp
lemma invar-r-ge-k:
  invar\ (Node\ k\ v\ l\ r) \Longrightarrow \forall\ p\in set\text{-}kdt\ r.\ v< p\$k
  by simp
\mathbf{lemma}\ invar\text{-}set:
  set-kdt \ (Node \ k \ v \ l \ r) = set-kdt \ l \cup set-kdt \ r
  by simp
```

## 1.2 Lemmas adapted from HOL-Library. Tree to k-d Tree

```
lemma size-ge\theta[simp]:
  0 < size-kdt \ kdt
  by (induction kdt) auto
lemma eq-size-1[simp]:
  size-kdt \ kdt = 1 \longleftrightarrow (\exists \ p. \ kdt = Leaf \ p)
  apply (induction \ kdt)
  apply (auto)
  using size-ge0 nat-less-le apply blast+
  done
lemma eq-1-size[simp]:
  1 = size - kdt \ kdt \longleftrightarrow (\exists p. \ kdt = Leaf \ p)
  using eq-size-1 by metis
lemma neq-Leaf-iff:
  (\nexists p. \ kdt = Leaf \ p) = (\exists \ k \ v \ l \ r. \ kdt = Node \ k \ v \ l \ r)
  by (cases kdt) auto
lemma eq-height-0[simp]:
  height \ kdt = 0 \longleftrightarrow (\exists \ p. \ kdt = Leaf \ p)
  by (cases kdt) auto
lemma eq-\theta-height[simp]:
  0 = height \ kdt \longleftrightarrow (\exists \ p. \ kdt = Leaf \ p)
  by (cases kdt) auto
lemma eq-min-height-\theta[simp]:
  min-height \ kdt = 0 \longleftrightarrow (\exists \ p. \ kdt = Leaf \ p)
  by (cases kdt) auto
lemma eq-0-min-height[simp]:
  0 = min\text{-}height \ kdt \longleftrightarrow (\exists \ p. \ kdt = Leaf \ p)
  by (cases kdt) auto
lemma size-height:
  size-kdt \ kdt \leq 2 \ \hat{\ } height \ kdt
proof(induction \ kdt)
  case (Node k \ v \ l \ r)
  show ?case
  proof (cases height l \leq height r)
    case True
    have size-kdt (Node k \ v \ l \ r) = size-kdt \ l + size-kdt \ r \ by \ simp
    also have ... \leq 2 \ \hat{} \ height \ l + 2 \ \hat{} \ height \ r \ using \ Node.IH  by arith also have ... \leq 2 \ \hat{} \ height \ r + 2 \ \hat{} \ height \ r \ using  True by simp also have ... = 2 \ \hat{} \ height \ (Node \ k \ v \ l \ r)
      using True by (auto simp: max-def mult-2)
    finally show ?thesis.
```

```
next
   case False
   have size-kdt \ (Node \ k \ v \ l \ r) = size-kdt \ l + size-kdt \ r \ \mathbf{by} \ simp
   also have ... \leq 2 ^ height l + 2 ^ height r using Node.IH by arith
   also have ... \leq 2 ^ height l + 2 ^ height l using False by simp
   finally show ?thesis using False by (auto simp: max-def mult-2)
  qed
qed simp
lemma min-height-le-height:
  min-height \ kdt \leq height \ kdt
  by (induction kdt) auto
\mathbf{lemma} \ \mathit{min-height-size} :
  2 \cap min-height \ kdt < size-kdt \ kdt
proof(induction \ kdt)
  case (Node k \ v \ l \ r)
 have (2::nat) \widehat{\ } min-height (Node k \ v \ l \ r) \leq 2 \widehat{\ } min-height l + 2 \widehat{\ } min-height r
   by (simp add: min-def)
  also have \ldots \leq size\text{-}kdt \ (Node \ k \ v \ l \ r) using Node.IH by simp
  finally show ?case.
\mathbf{qed}\ simp
lemma complete-iff-height:
  complete \ kdt \longleftrightarrow (min-height \ kdt = height \ kdt)
  apply (induction kdt)
  apply simp
  apply (simp add: min-def max-def)
  by (metis le-antisym le-trans min-height-le-height)
lemma size-if-complete:
  complete \ kdt \Longrightarrow size-kdt \ kdt = 2 \ \hat{\ } height \ kdt
  by (induction kdt) auto
lemma complete-if-size-height:
  size-kdt \ kdt = 2 \ \hat{} \ height \ kdt \Longrightarrow complete \ kdt
proof (induction height kdt arbitrary: kdt)
  case \theta thus ?case by auto
\mathbf{next}
  case (Suc\ h)
  hence \nexists p. kdt = Leaf p
   by auto
  then obtain k \ v \ l \ r where [simp]: kdt = Node \ k \ v \ l \ r
   using neq-Leaf-iff by metis
  have 1: height l \leq h and 2: height r \leq h using Suc(2) by (auto)
  have 3: \neg height l < h
  proof
   assume \theta: height l < h
   have size-kdt \ kdt = size-kdt \ l + size-kdt \ r by simp
```

```
also have ... \leq 2 \hat{} height l + 2 \hat{} height r
     using size-height[of\ l] size-height[of\ r] by arith
   also have ... < 2 \hat{h} + 2 \hat{h} eight r using \theta by (simp)
   also have \dots \leq 2 \hat{h} + 2 \hat{h} using 2 by (simp)
   also have \dots = 2 \ \widehat{} (Suc \ h) by (simp)
   also have ... = size-kdt \ kdt \ using \ Suc(2,3) by simp
   finally have size-kdt \ kdt < size-kdt \ kdt.
   thus False by (simp)
  qed
  have 4: \neg height r < h
 proof
   assume \theta: height r < h
   have size-kdt \ kdt = size-kdt \ l + size-kdt \ r by simp
   also have . . . \leq 2 ^ height l + 2 ^ height r
     using size-height[of\ l] size-height[of\ r] by arith
   also have ... < 2 \hat{\ } height \ l + 2 \hat{\ } h \ using \ \theta \ by \ (simp)
   also have \dots \le 2 \ \hat{h} + 2 \ \hat{h} using 1 by (simp)
   also have \dots = 2 \ \widehat{} (Suc \ h) by (simp)
   also have ... = size-kdt \ kdt \ using \ Suc(2,3) by simp
   finally have size-kdt \ kdt < size-kdt \ kdt.
   thus False by (simp)
 \mathbf{qed}
  from 1 2 3 4 have *: height l = h height r = h by linarith+
 hence size-kdt\ l=2 ^ height\ l\ size-kdt\ r=2 ^ height\ r
   using Suc(3) size-height[of l] size-height[of r] by (auto)
  with *Suc(1) show ?case by simp
qed
\mathbf{lemma}\ \textit{complete-if-size-min-height}:
 size-kdt \ kdt = 2 \ \widehat{\ } min-height \ kdt \Longrightarrow complete \ kdt
proof (induct min-height kdt arbitrary: kdt)
 case 0 thus ?case by auto
next
  case (Suc\ h)
 hence \nexists p. kdt = Leaf p
   by auto
 then obtain k \ v \ l \ r where [simp]: kdt = Node \ k \ v \ l \ r
   using neg-Leaf-iff by metis
  have 1: h \leq min-height l and 2: h \leq min-height r using Suc(2) by (auto)
  have 3: \neg h < min-height l
 proof
   assume \theta: h < min-height l
   have size-kdt \ kdt = size-kdt \ l + size-kdt \ r by simp
   also note min-height-size[of l]
   also(xtrans) note min-height-size[of r]
   also(xtrans) have (2::nat) \widehat{\ } min-height l > 2 \widehat{\ } h
       using 0 by (simp add: diff-less-mono)
   also(xtrans) have (2::nat) \hat{} min-height r \geq 2 \hat{} h using 2 by simp
   also(xtrans) have (2::nat) \hat{h} + 2 \hat{h} = 2 \hat{such}  by (simp)
```

```
also have ... = size-kdt \ kdt \ using \ Suc(2,3) by simp
   finally show False by (simp add: diff-le-mono)
  qed
  have 4: \neg h < min-height r
  proof
   assume \theta: h < min-height r
   have size-kdt \ kdt = size-kdt \ l + size-kdt \ r by simp
   also note min-height-size[of l]
   also(xtrans) note min-height-size[of r]
   also(xtrans) have (2::nat) \hat{} min-height r > 2 \hat{} h
       using \theta by (simp add: diff-less-mono)
   also(xtrans) have (2::nat) \hat{} min-height l \geq 2 \hat{} h using 1 by simp
   also(xtrans) have (2::nat) \hat{h} + 2 \hat{h} = 2 \hat{Suc} \hat{h} by (simp)
   also have ... = size-kdt \ kdt \ using \ Suc(2,3) by simp
   finally show False by (simp add: diff-le-mono)
  qed
  from 1 2 3 4 have *: min-height l = h min-height r = h by linarith+
 hence size-kdt\ l=2 ^ min-height\ l\ size-kdt\ r=2 ^ min-height\ r
   using Suc(3) min-height-size[of l] min-height-size[of r] by (auto)
  with *Suc(1) show ?case
   by (simp add: complete-iff-height)
\mathbf{qed}
lemma complete-iff-size:
  complete \ kdt \longleftrightarrow size-kdt \ kdt = 2 \ \hat{} \ height \ kdt
 using complete-if-size-height size-if-complete by blast
lemma size-height-if-incomplete:
  \neg complete kdt \Longrightarrow size-kdt kdt < 2 \hat{\ } height kdt
 by (meson antisym-conv complete-iff-size not-le size-height)
lemma min-height-size-if-incomplete:
  \neg complete \ kdt \Longrightarrow 2 \ \widehat{} min-height \ kdt < size-kdt \ kdt
 by (metis complete-if-size-min-height le-less min-height-size)
\mathbf{lemma}\ balanced	ext{-}subtreeL:
  balanced (Node \ k \ v \ l \ r) \Longrightarrow balanced \ l
 by (simp add: balanced-def)
lemma balanced-subtreeR:
  balanced (Node \ k \ v \ l \ r) \Longrightarrow balanced \ r
 by (simp add: balanced-def)
lemma balanced-optimal:
 assumes balanced kdt size-kdt kdt \leq size-kdt kdt'
 shows height \ kdt \leq height \ kdt'
proof (cases complete kdt)
 case True
 have (2::nat) \hat{} height kdt \leq 2 \hat{} height kdt'
```

```
proof -
   have 2 \hat{\phantom{a}} height kdt = size-kdt kdt
     using True by (simp add: complete-iff-height size-if-complete)
   also have ... \le size - kdt \ kdt' using assms(2) by simp
   also have ... \leq 2 \hat{} height kdt' by (rule size-height)
   finally show ?thesis.
 qed
 thus ?thesis by (simp)
next
 case False
 have (2::nat) \hat{} min-height kdt < 2 \hat{} height kdt'
 proof -
   have (2::nat) \hat{} min-height kdt < size-kdt \ kdt
     by(rule min-height-size-if-incomplete[OF False])
   also have \dots < size-kdt \ kdt' using assms(2) by simp
   also have \dots \leq 2 height kdt' by (rule\ size-height)
   finally have (2::nat) \hat{} min-height kdt < (2::nat) \hat{} height kdt'.
   thus ?thesis.
 qed
 hence *: min-height kdt < height kdt' by simp
 have min-height\ kdt + 1 = height\ kdt
   using min-height-le-height[of kdt] assms(1) False
   by (simp add: complete-iff-height balanced-def)
 with * show ?thesis by arith
qed
       Lemmas adapted from HOL-Library. Tree-Real to k-d Tree
1.3
lemma size-height-log:
 log 2 (size-kdt kdt) < height kdt
 by (simp add: log2-of-power-le size-height)
lemma min-height-size-log:
 min-height \ kdt < log 2 \ (size-kdt \ kdt)
 by (simp add: le-log2-of-power min-height-size)
lemma size-log-if-complete:
 complete \ kdt \Longrightarrow height \ kdt = log \ 2 \ (size-kdt \ kdt)
 using complete-iff-size log2-of-power-eq by blast
lemma min-height-size-log-if-incomplete:
 \neg complete kdt \Longrightarrow min-height kdt < log 2 (size-kdt kdt)
 by (simp add: less-log2-of-power min-height-size-if-incomplete)
lemma min-height-balanced:
 assumes balanced kdt
 shows min-height kdt = nat(floor(log 2 (size-kdt kdt)))
proof cases
```

**assume** \*: complete kdt

```
hence size-kdt \ kdt = 2 \ \widehat{\ } min-height \ kdt
   by (simp add: complete-iff-height size-if-complete)
  from log2-of-power-eq[OF this] show ?thesis by linarith
  assume *: \neg complete kdt
 hence height kdt = min-height kdt + 1
   using assms min-height-le-height[of kdt]
   by(auto simp add: balanced-def complete-iff-height)
  hence size-kdt \ kdt < 2 \ \widehat{\ } (min-height \ kdt + 1)
   by (metis * size-height-if-incomplete)
 hence log \ 2 \ (size-kdt \ kdt) < min-height \ kdt + 1
   using log2-of-power-less size-ge0 by blast
 thus ?thesis using min-height-size-log[of kdt] by linarith
qed
lemma height-balanced:
 assumes balanced kdt
 shows height kdt = nat(ceiling(log 2 (size-kdt kdt)))
proof cases
 assume *: complete kdt
 hence size-kdt \ kdt = 2 \ \hat{} height \ kdt
   by (simp add: size-if-complete)
  from log2-of-power-eq[OF this] show ?thesis
   by linarith
\mathbf{next}
 assume *: \neg complete kdt
 hence **: height kdt = min-height kdt + 1
   using assms min-height-le-height[of kdt]
   by(auto simp add: balanced-def complete-iff-height)
 hence size-kdt kdt \leq 2 (min-height kdt + 1) by (metis size-height)
  \textbf{from} \quad log 2-of\text{-}power\text{-}le[OF \ this \ size\text{-}ge0] \ min\text{-}height\text{-}size\text{-}log\text{-}if\text{-}incomplete}[OF \ *]
 show ?thesis by linarith
qed
lemma balanced-Node-if-wbal1:
 assumes balanced l balanced r size-kdt l = size-kdt r + 1
 shows balanced (Node k \ v \ l \ r)
proof -
  from assms(3) have [simp]: size-kdt \ l = size-kdt \ r + 1 by simp
 have nat \lceil log \ 2 \ (1 + size-kdt \ r) \rceil \ge nat \lceil log \ 2 \ (size-kdt \ r) \rceil
   \mathbf{by}(rule\ nat\text{-}mono[OF\ ceiling\text{-}mono])\ simp
 hence 1: height(Node\ k\ v\ l\ r) = nat\ \lceil log\ 2\ (1 + size-kdt\ r) \rceil + 1
   using height-balanced[OF assms(1)] height-balanced[OF assms(2)]
   by (simp del: nat-ceiling-le-eq add: max-def)
  have nat | log 2 (1 + size-kdt r) | \ge nat | log 2 (size-kdt r) |
   by(rule nat-mono[OF floor-mono]) simp
  hence 2: min-height(Node k \ v \ l \ r) = nat \ |log \ 2 \ (size-kdt \ r)| + 1
   using min-height-balanced [OF assms(1)] min-height-balanced [OF assms(2)]
```

```
by (simp)
 have size\text{-}kdt \ r \geq 1 by (simp \ add: Suc\text{-}leI)
  then obtain i where i: 2 \hat{i} \le size-kdt \ r \ size-kdt \ r < 2 \hat{i} + 1
   using ex-power-ivl1 [of 2 size-kdt r] by auto
 hence i1: 2 \hat{i} < size-kdt \ r+1 \ size-kdt \ r+1 \le 2 \hat{i} (i+1) by auto
 \mathbf{from} \ 1 \ 2 \ floor\text{-}log\text{-}nat\text{-}eq\text{-}if[OF \ i] \ ceiling\text{-}log\text{-}nat\text{-}eq\text{-}if[OF \ i1]
  show ?thesis by(simp add:balanced-def)
qed
lemma balanced-sym:
  balanced (Node \ k \ v \ l \ r) \Longrightarrow balanced (Node \ k' \ v' \ r \ l)
 by (auto simp: balanced-def)
lemma balanced-Node-if-wbal2:
  assumes balanced l balanced r abs(int(size-kdt\ l) - int(size-kdt\ r)) \le 1
 shows balanced (Node k \ v \ l \ r)
proof -
 have size-kdt\ l=size-kdt\ r\lor (size-kdt\ l=size-kdt\ r+1\lor size-kdt\ r=size-kdt
l + 1) (is ?A \lor ?B)
   using assms(3) by linarith
  thus ?thesis
 proof
   assume ?A
   thus ?thesis using assms(1,2)
     apply(simp add: balanced-def min-def max-def)
     by (metis assms(1,2) balanced-optimal le-antisym le-less)
 next
   assume ?B
   thus ?thesis
     by (meson assms(1,2) balanced-sym balanced-Node-if-wbal1)
 qed
qed
end
```

# 2 Building a balanced k-d Tree from a List of Points

```
\begin{tabular}{l} \textbf{theory } Build \\ \textbf{imports} \\ KD\text{-}Tree \\ Median\text{-}Of\text{-}Medians\text{-}Selection. Median\text{-}Of\text{-}Medians\text{-}Selection} \\ \textbf{begin} \\ \end{tabular}
```

Build a balanced k-d Tree by recursively partition the points into two lists. The partitioning criteria will be the median at a particular axis k. The left list will contain all points p with  $p \$   $k \le median$ . The right list will contain all points with median at axis median <math>k. The left and right list differ in length by one or none. The axis k will the widest spread axis.

#### 2.1 Auxiliary Lemmas

```
lemma length-filter-mset-sorted-nth:
 assumes distinct xs \ n < length \ xs \ sorted \ xs
 shows \{\# x \in \# mset xs. x \leq xs \mid n \#\} = mset (take (n + 1) xs)
 using assms
proof (induction xs arbitrary: n rule: list.induct)
  case (Cons \ x \ xs)
 thus ?case
 proof (cases n)
   case \theta
   thus ?thesis
     using Cons.prems(1,3) filter-mset-eq-mempty-iff by fastforce
 next
   case (Suc n')
   thus ?thesis
     using Cons by simp
 qed
qed auto
lemma length-filter-sort-nth:
 assumes distinct xs n < length xs
 shows length (filter (\lambda x. \ x \leq sort \ xs! \ n) \ xs) = n + 1
proof -
 have length (filter (\lambda x. \ x \leq sort \ xs! \ n) xs) = length (filter (\lambda x. \ x \leq sort \ xs! \ n)
(sort xs)
   by (simp add: filter-sort)
 also have ... = size (mset (filter (\lambda x. \ x \leq sort \ xs \ ! \ n) (sort xs)))
   using size-mset by metis
 also have ... = size (\{ \# x \in \# mset (sort xs). x \leq sort xs ! n \# \})
   using mset-filter by simp
 also have ... = size (mset (take (n + 1) (sort xs)))
   using length-filter-mset-sorted-nth assms sorted-sort distinct-sort length-sort by
metis
 finally show ?thesis
   using assms(2) by auto
qed
2.2
        Widest Spread Axis
definition calc-spread :: ('k::finite) \Rightarrow 'k point list \Rightarrow real where
  calc-spread k ps = (case ps of [] \Rightarrow 0 | ps \Rightarrow
   let ks = map (\lambda p. p\$k) (tl ps) in
   fold\ max\ ks\ ((hd\ ps)\$k) - fold\ min\ ks\ ((hd\ ps)\$k)
fun widest-spread :: ('k::finite) list \Rightarrow 'k point list \Rightarrow 'k \times real where
  widest-spread [] - = undefined
 widest-spread [k] ps = (k, calc-spread k ps)
 widest-spread (k \# ks) ps = (
```

```
let (k', s') = widest-spread ks ps in
   let \ s = calc-spread k ps in
   if s \leq s' then (k', s') else (k, s)
lemma calc-spread-spec:
  calc-spread k ps = spread k (set ps)
  using Max.set-eq-fold[of (hd ps)$k] Min.set-eq-fold[of (hd ps)$k]
 by (auto simp: Let-def spread-def calc-spread-def split: list.splits, metis set-map)
lemma widest-spread-calc-spread:
  ks \neq [] \Longrightarrow (k, s) = widest\text{-spread } ks \ ps \Longrightarrow s = calc\text{-spread } k \ ps
 by (induction ks ps rule: widest-spread.induct) (auto simp: Let-def split: prod.splits
if-splits)
lemma widest-spread-axis-Un:
 shows widest-spread-axis k \ K \ P \Longrightarrow spread \ k' \ P \le spread \ k \ P \Longrightarrow widest-spread-axis
k (K \cup \{k'\}) P
  and widest-spread-axis k \ K \ P \Longrightarrow spread \ k \ P \le spread \ k' \ P \Longrightarrow widest-spread-axis
k'(K \cup \{k'\}) P
 unfolding widest-spread-axis-def by auto
lemma widest-spread-spec:
  (k, s) = widest-spread ks ps \Longrightarrow widest-spread-axis k (set ks) (set ps)
proof (induction ks ps arbitrary: k s rule: widest-spread.induct)
  case (3 k_0 k_1 ks ps)
  obtain K' S' where K'-def: (K', S') = widest-spread (k_1 \# ks) ps
   by (metis surj-pair)
 hence IH: widest-spread-axis K' (set (k_1 \# ks)) (set ps)
   using 3.IH by blast
 hence \theta: S' = spread K' (set ps)
   using K'-def widest-spread-calc-spread calc-spread-spec by blast
  define S where S = calc-spread k_0 ps
 hence 1: S = spread k_0 (set ps)
   using calc-spread-spec by blast
 show ?case
 proof (cases S < S')
   case True
   hence widest-spread-axis K' (set (k_0 \# k_1 \# ks)) (set ps)
     using 0.1 widest-spread-axis-Un(1)[OF IH, of k_0] by auto
   thus ?thesis
     using True K'-def S-def 3.prems by (auto split: prod.splits)
  next
   case False
   hence widest-spread-axis k_0 (set (k_0 \# k_1 \# ks)) (set ps)
     using 0.1 widest-spread-axis-Un(2)[OF IH, of k_0] 3.prems(1) by auto
     using False K'-def S-def 3.prems by (auto split: prod.splits)
  qed
```

#### 2.3 Fast Axis Median

```
definition axis-median :: ('k::finite) \Rightarrow 'k \ point \ list \Rightarrow real \ where
 axis-median k ps = (let n = (length ps - 1) div 2 in fast-select n (map <math>(\lambda p. p\$k)
ps))
lemma length-filter-le-axis-median:
 assumes 0 < length ps \ \forall k. \ distinct \ (map \ (\lambda p. \ p\$k) \ ps)
 shows length (filter (\lambda p. p$k \le axis-median k ps) ps) = (length ps - 1) div 2 +
proof -
 let ?n = (length ps - 1) div 2
 let ?ps = map(\lambda p. p\$k) ps
 let ?m = fast\text{-}select ?n ?ps
 have \theta: ?n < length ?ps
   using assms(1) by (auto, linarith)
 have 1: distinct ?ps
   using assms(2) by blast
 have ?m = select ?n ?ps
   using fast-select-correct[OF\ 0] by blast
 hence length (filter (\lambda p. p\$k \leq axis\text{-median } k ps) ps) =
       length (filter (\lambda p. p\$k \leq sort ?ps ! ?n) ps)
     unfolding axis-median-def by (auto simp add: Let-def select-def simp del:
fast-select.simps)
 also have ... = length (filter (\lambda v. \ v \leq sort ?ps ! ?n) ?ps)
   by (induction ps) (auto, metis comp-apply)
 also have \dots = ?n + 1
   using length-filter-sort-nth[OF 1 0] by blast
 finally show ?thesis.
qed
definition partition-by-median :: ('k::finite) \Rightarrow 'k point list \Rightarrow 'k point list \times real
\times 'k point list where
 partition-by-median k ps = (
    let m = axis-median k ps in
    let (l, r) = partition (\lambda p. p\$k \le m) ps in
    (l, m, r)
lemma set-partition-by-median:
  (l, m, r) = partition-by-median \ k \ ps \Longrightarrow set \ ps = set \ l \cup set \ r
  unfolding partition-by-median-def by (auto simp: Let-def)
\mathbf{lemma}\ \mathit{filter-partition-by-median}:
 assumes (l, m, r) = partition-by-median k ps
 shows \forall p \in set \ l. \ p\$k \leq m
   and \forall p \in set \ r. \ \neg p\$k < m
```

```
using assms unfolding partition-by-median-def by (auto simp: Let-def)
\mathbf{lemma}\ \mathit{sum-length-partition-by-median}:
   assumes (l, m, r) = partition-by-median k ps
   shows length ps = length l + length r
   using assms sum-length-filter-compl[of (\lambda p. p \ \$ k \le axis-median \ k \ ps)]
   unfolding partition-by-median-def by (simp add: Let-def o-def)
lemma length-l-partition-by-median:
     assumes 0 < length ps \ \forall k. \ distinct \ (map \ (\lambda p. \ p\$k) \ ps) \ (l, \ m, \ r) = parti-
tion-by-median k ps
   shows length l = (length ps - 1) div 2 + 1
  using assms unfolding partition-by-median-def by (auto simp: Let-def length-filter-le-axis-median)
corollary lengths-partition-by-median-1:
     assumes \theta < length ps \ \forall k. \ distinct \ (map \ (\lambda p. \ p\$k) \ ps) \ (l, \ m, \ r) = parti-
tion-by-median k ps
   shows length l - length r \le 1
       and length r \leq length l
       and \theta < length l
       and length r < length ps
  \mathbf{using}\ length-l-partition-by-median [OF\ assms]\ sum-length-partition-by-median [OF\ assms]
assms(3)] by auto
corollary lengths-partition-by-median-2:
     assumes 1 < length ps \ \forall k. \ distinct \ (map \ (\lambda p. \ p\$k) \ ps) \ (l, \ m, \ r) = parti-
tion-by-median k ps
   shows \theta < length r
       and length \ l < length \ ps
proof -
   have *: \theta < length ps
       using assms(1) by auto
   show \theta < length \ r \ length \ l < length \ ps
      \textbf{using } length-l-partition-by-median [OF* assms(2,3)] \ sum-length-partition-by-median [OF*
assms(3)
       using assms(1) by linarith+
qed
lemmas length-partition-by-median =
    sum-length-partition-by-median length-l-partition-by-median
    lengths\mbox{-}partition\mbox{-}by\mbox{-}median\mbox{-}1\ lengths\mbox{-}partition\mbox{-}by\mbox{-}median\mbox{-}2
               Building the Tree
2.4
function (domintros, sequential) build :: ('k::finite) list \Rightarrow 'k point list \Rightarrow 'k kdt
where
    build - [] = undefined
   build - [p] = Leaf p
  build ks ps = 0
```

```
let(k, -) = widest-spread ks ps in
        let(l, m, r) = partition-by-median k ps in
        Node k m (build ks l) (build ks r)
    by pat-completeness auto
lemma build-domintros3:
    assumes (k, s) = widest\text{-}spread \ ks \ (x \# y \# zs) \ (l, m, r) = partition\text{-}by\text{-}median
k (x \# y \# zs)
    assumes build-dom\ (ks,\ l)\ build-dom\ (ks,\ r)
    shows build-dom (ks, x \# y \# zs)
proof -
    {
        \mathbf{fix}\ k\ s\ l\ m\ r
       assume (k, s) = widest-spread ks (x \# y \# zs) (l, m, r) = partition-by-median
k (x \# y \# zs)
        hence build-dom\ (ks,\ l)\ build-dom\ (ks,\ r)
            using assms by (metis Pair-inject)+
    thus ?thesis
        by (simp\ add:\ build.domintros(3))
\mathbf{qed}
lemma build-termination:
    assumes \forall k. distinct (map (\lambda p. p\$k) ps)
    shows build-dom (ks, ps)
    using assms
proof (induction ps rule: length-induct)
    case (1 xs)
    consider (A) xs = [ \mid \mid (B) \exists x. \ xs = [x] \mid (C) \exists x \ y \ zs. \ xs = x \# y \# zs
        by (induction xs rule: induct-list012) auto
     then show ?case
    proof cases
        case C
        then obtain x \ y \ zs where xyzs-def: xs = x \# y \# zs
        obtain k s where ks-def: (k, s) = widest-spread ks xs
             by (metis surj-pair)
        obtain l \ m \ r where lmr-def: (l, \ m, \ r) = partition-by-median \ k \ xs
             by (metis prod-cases3)
        note defs = xyzs\text{-}def ks\text{-}def lmr\text{-}def
        have \forall k. distinct (map (\lambda p. p \$ k) l) \forall k. distinct (map (\lambda p. p \$ k) r)
             using lmr-def unfolding partition-by-median-def
             by (auto simp: Let-def 1.prems distinct-map-filter)
        moreover have length l < length xs length r < length xs
         \textbf{using } \textit{length-partition-by-median} (8) [\textit{OF-1.prems}] \textit{ length-partition-by-median} (6) [\textit{OF-1.pre
- 1.prems
             using defs by auto
        ultimately have build-dom (ks, l) build-dom (ks, r)
```

```
using 1.IH by blast+
   thus ?thesis
     using build-domintros3 defs by blast
 qed (auto intro: build.domintros)
qed
lemma build-psimp-1:
  ps = [p] \Longrightarrow build \ k \ ps = Leaf \ p
 by (simp\ add:\ build.domintros(2)\ build.psimps(2))
lemma build-psimp-2:
 assumes (k, s) = widest-spread ks (x \# y \# zs) (l, m, r) = partition-by-median
k (x \# y \# zs)
 assumes build-dom\ (ks,\ l)\ build-dom\ (ks,\ r)
 shows build ks (x \# y \# zs) = Node k m (build ks l) (build ks r)
proof -
 have \theta: build-dom (ks, x \# y \# zs)
   using assms build-domintros3 by blast
 thus ?thesis
   using build.psimps(3)[OF 0] assms(1,2) by (auto split: prod.splits)
qed
\mathbf{lemma}\ \mathit{length}\text{-}\mathit{xs}\text{-}\mathit{gt}\text{-}\mathit{1}\text{:}
  1 < length \ xs \Longrightarrow \exists x \ y \ ys. \ xs = x \# y \# ys
 by (cases xs, auto simp: neq-Nil-conv)
lemma build-psimp-3:
 assumes 1 < length \ ps \ (k, s) = widest-spread \ ks \ ps \ (l, m, r) = partition-by-median
k ps
 assumes build-dom\ (ks,\ l)\ build-dom\ (ks,\ r)
 shows build ks ps = Node \ k \ m \ (build \ ks \ l) \ (build \ ks \ r)
 using build-psimp-2 length-xs-gt-1 assms by blast
lemmas \ build-psimps[simp] = build-psimp-1 \ build-psimp-3
       Main Theorems
2.5
theorem set-build:
 0 < length \ ps \Longrightarrow \forall k. \ distinct \ (map \ (\lambda p. \ p\$k) \ ps) \Longrightarrow set \ ps = set-kdt \ (build \ ks)
proof (induction ps rule: length-induct)
 case (1 ps)
 show ?case
 proof (cases 1 < length ps)
   case True
   obtain k s where ks-def: (k, s) = widest-spread ks ps
     by (metis surj-pair)
   obtain l \ m \ r where lmr-def: (l, \ m, \ r) = partition-by-median \ k \ ps
     by (metis prod-cases3)
```

```
have D: \forall k. \ distinct \ (map \ (\lambda p. \ p\$k) \ l) \ \forall k. \ distinct \ (map \ (\lambda p. \ p\$k) \ r)
     using lmr-def unfolding partition-by-median-def
     by (auto simp: 1.prems(2) Let-def distinct-map-filter)
   moreover have length l < length ps 0 < length l
                length r < length ps 0 < length r
     using length-partition-by-median(8)[OF True 1.prems(2)]
          length-partition-by-median(5)[OF\ 1.prems(1)\ 1.prems(2)]
          length-partition-by-median(6)[OF\ 1.prems(1)\ 1.prems(2)]
          length-partition-by-median(7)[OF True 1.prems(2)]
          lmr-def by blast+
   ultimately have set l = set\text{-}kdt (build ks l) set r = set\text{-}kdt (build ks r)
     using 1.IH by blast+
   moreover have set ps = set l \cup set r
     using lmr-def unfolding partition-by-median-def by (auto simp: Let-def)
   moreover have build ks ps = Node \ k \ m \ (build \ ks \ l) \ (build \ ks \ r)
     using build-psimp-3[OF True ks-def lmr-def] build-termination D by blast
   ultimately show ?thesis
     by simp
  next
   case False
   thus ?thesis
     using 1.prems by (cases ps) auto
  qed
qed
theorem invar-build:
 0 < length \ ps \Longrightarrow \forall k. \ distinct \ (map \ (\lambda p. \ p\$k) \ ps) \Longrightarrow set \ ks = UNIV \Longrightarrow invar
(build ks ps)
proof (induction ps rule: length-induct)
 case (1 ps)
 show ?case
 proof (cases 1 < length ps)
   case True
   obtain k s where ks-def: (k, s) = widest-spread ks ps
     by (metis surj-pair)
   obtain l \ m \ r where lmr-def: (l, m, r) = partition-by-median k \ ps
     by (metis prod-cases3)
   have D: \forall k. \ distinct \ (map \ (\lambda p. \ p\$k) \ l) \ \forall k. \ distinct \ (map \ (\lambda p. \ p\$k) \ r)
     using lmr-def unfolding partition-by-median-def
     by (auto simp: 1.prems(2) Let-def distinct-map-filter)
   moreover have length l < length ps 0 < length l
                length \ r < length \ ps \ 0 < length \ r
     using length-partition-by-median(8)[OF True 1.prems(2)]
          length-partition-by-median(5)[OF 1.prems(1) 1.prems(2)]
          length-partition-by-median(6)[OF\ 1.prems(1)\ 1.prems(2)]
          length-partition-by-median(7)[OF True 1.prems(2)]
          lmr-def bv blast+
   ultimately have invar (build ks l) invar (build ks r)
     using 1.IH 1.prems(3) by blast+
```

```
moreover have \forall p \in set \ l. \ p\$k \leq m \ \forall p \in set \ r. \ m < p\$k
     using filter-partition-by-median(1)[OF lmr-def]
          filter-partition-by-median(2)[OF\ lmr-def] by auto
   moreover have widest-spread-axis k UNIV (set l \cup set r)
      using widest-spread-spec[OF ks-def] 1.prems(3) set-partition-by-median[OF
lmr-def] by simp
   moreover have build ks ps = Node \ k \ m \ (build \ ks \ l) \ (build \ ks \ r)
     using build-psimp-3[OF True ks-def lmr-def] build-termination D by blast
   ultimately show ?thesis
      using set-build[OF \land 0 < length \ l \gt D(1)] set-build[OF \land 0 < length \ r \gt D(2)]
by simp
 \mathbf{next}
   case False
   thus ?thesis
     using 1.prems by (cases ps) auto
 qed
qed
theorem size-build:
  0 < length \ ps \Longrightarrow \forall k. \ distinct \ (map \ (\lambda p. \ p\$k) \ ps) \Longrightarrow size-kdt \ (build \ ks \ ps) =
length ps
proof (induction ps rule: length-induct)
 case (1 ps)
 show ?case
 proof (cases 1 < length ps)
   case True
   obtain k s where ks-def: (k, s) = widest-spread ks ps
     by (metis surj-pair)
   obtain l \ m \ r where lmr-def: (l, \ m, \ r) = partition-by-median \ k \ ps
     by (metis prod-cases3)
   have D: \forall k. \ distinct \ (map \ (\lambda p. \ p\$k) \ l) \ \forall k. \ distinct \ (map \ (\lambda p. \ p\$k) \ r)
     using lmr-def unfolding partition-by-median-def
     by (auto simp: 1.prems(2) Let-def distinct-map-filter)
   moreover have length l < length ps 0 < length l
                length \ r < length \ ps \ 0 < length \ r
     using length-partition-by-median(8)[OF True 1.prems(2)]
          length-partition-by-median(5)[OF\ 1.prems(1)\ 1.prems(2)]
          length-partition-by-median(6)[OF\ 1.prems(1)\ 1.prems(2)]
          length-partition-by-median(7)[OF True 1.prems(2)]
          lmr-def by blast+
   ultimately have size-kdt (build ks \ l) = length \ l \ size-kdt (build ks \ r) = length \ r
     using 1.IH by blast+
   moreover have build ks ps = Node \ k \ m \ (build \ ks \ l) \ (build \ ks \ r)
     using build-psimp-3[OF True ks-def lmr-def] build-termination D by blast
   ultimately show ?thesis
     using length-partition-by-median(1)[OF lmr-def] by simp
   case False
   thus ?thesis
```

```
using 1.prems by (cases ps) auto
 qed
qed
theorem balanced-build:
  0 < length \ ps \Longrightarrow \forall k. \ distinct \ (map \ (\lambda p. \ p\$k) \ ps) \Longrightarrow balanced \ (build \ ks \ ps)
proof (induction ps rule: length-induct)
 case (1 ps)
 show ?case
 proof (cases 1 < length ps)
   case True
   obtain k s where ks-def: (k, s) = widest-spread ks ps
     by (metis surj-pair)
   obtain l \ m \ r where lmr-def: (l, \ m, \ r) = partition-by-median \ k \ ps
     by (metis prod-cases3)
   have D: \forall k. \ distinct \ (map \ (\lambda p. \ p\$k) \ l) \ \forall k. \ distinct \ (map \ (\lambda p. \ p\$k) \ r)
     using lmr-def unfolding partition-by-median-def
     by (auto simp: 1.prems(2) Let-def distinct-map-filter)
   moreover have length l < length ps 0 < length l
                length \ r < length \ ps \ 0 < length \ r
     using length-partition-by-median(8)[OF True 1.prems(2)]
          length-partition-by-median(5)[OF\ 1.prems(1)\ 1.prems(2)]
          length-partition-by-median(6)[OF 1.prems(1) 1.prems(2)]
          length-partition-by-median(7)[OF True 1.prems(2)]
          lmr-def by blast+
   ultimately have IH: balanced (build ks l) balanced (build ks r)
     using 1.IH by blast+
   have build ks ps = Node \ k \ m (build ks l) (build ks r)
     using build-psimp-3[OF True ks-def lmr-def] build-termination D by blast
   moreover have length r + 1 = length \ l \lor length \ r = length \ l
     using length-partition-by-median(1)[OF lmr-def]
          length-partition-by-median(3)[OF\ 1.prems(1)\ 1.prems(2)\ lmr-def]
          length-partition-by-median(4)[OF 1.prems(1) 1.prems(2) lmr-def]
     by linarith
   ultimately show ?thesis
     using balanced-Node-if-wbal1 [OF IH] balanced-Node-if-wbal2 [OF IH]
          size-build[OF \langle 0 < length \ l \rangle \ D(1)] size-build[OF \langle 0 < length \ r \rangle \ D(2)]
     by auto
  next
   case False
   thus ?thesis
     using 1.prems by (cases ps) (auto simp: balanced-def)
 qed
qed
\mathbf{lemma}\ complete\text{-}if\text{-}balanced\text{-}size\text{-}2powh:
 assumes balanced kdt size-kdt kdt = 2 \hat{h}
 shows complete kdt
proof (rule ccontr)
```

```
\mathbf{assume} \, \neg \, \, complete \, \, kdt
 hence 2 ^ (min-height kdt) < size-kdt kdt size-kdt kdt < 2 ^ height kdt
   by (simp-all add: min-height-size-if-incomplete size-height-if-incomplete)
 hence height kdt - min-height kdt > 1
   using assms(2) by simp
 hence \neg balanced kdt
   using balanced-def by force
  thus False
   using assms(1) by simp
qed
theorem complete-build:
 length ps = 2 \ \hat{} \ h \Longrightarrow \forall k. distinct (map \ (\lambda p. \ p\$k) \ ps) \Longrightarrow complete \ (build \ k \ ps)
 by (simp add: balanced-build complete-if-balanced-size-2powh size-build)
corollary height-build:
 assumes length ps = 2 \hat{h} \forall k. distinct (map (\lambda p. p\$k) ps)
 shows h = height (build k ps)
 using complete-build[OF\ assms]\ size-build[OF\ -\ assms(2)] by (simp\ add:\ assms(1)
complete-iff-size)
```

# 3 Range Searching

```
theory Range-Search
imports
KD-Tree
begin
```

end

Given two k-dimensional points  $p_0$  and  $p_1$  which bound the search space, the search should return only the points which satisfy the following criteria:

For every point p in the resulting set:

```
For every axis k:

p_0 \ k \le p \ k \land p \ k \le p_1 \ k
```

For a 2-d tree a query corresponds to selecting all the points in the rectangle that has  $p_0$  and  $p_1$  as its defining edges.

#### 3.1 Rectangle Definition

```
lemma cbox\text{-}point\text{-}def: fixes p_0 :: ('k::finite) point shows cbox\ p_0\ p_1 = \{\ p.\ \forall\ k.\ p_0\$k \le p\$k \land p\$k \le p_1\$k\ \} proof - have cbox\ p_0\ p_1 = \{\ p.\ \forall\ k.\ p_0 \cdot axis\ k\ 1 \le p \cdot axis\ k\ 1 \land p \cdot axis\ k\ 1 \le p_1 \cdot axis\ k\ 1\ \}
```

```
unfolding cbox-def using axis-inverse by auto also have ... = { p. \forall k. p_0\$k \cdot 1 \leq p\$k \cdot 1 \wedge p\$k \cdot 1 \leq p_1\$k \cdot 1 } using inner-axis[of - - 1] by (metis (mono-tags, opaque-lifting)) also have ... = { p. \forall k. p_0\$k \leq p\$k \wedge p\$k \leq p_1\$k } by simp finally show ?thesis . qed
```

### 3.2 Search Function

```
fun search :: ('k::finite) point \Rightarrow 'k point \Rightarrow 'k kdt \Rightarrow 'k point set where search p_0 p_1 (Leaf p) = (if p \in cbox\ p_0 p_1 then \{\ p\ \} else \{\}\}) | search p_0 p_1 (Node k v l r) = (
    if v < p_0 \$k then
    search p_0 p_1 r
    else if p_1 \$k < v then
    search p_0 p_1 l
    else
    search p_0 p_1 l
    else
```

## 3.3 Auxiliary Lemmas

```
lemma l-empty:
 assumes invar (Node k \ v \ l \ r) v < p_0 \$ k
  shows set-kdt l \cap cbox p_0 p_1 = \{\}
proof -
 have \forall p \in set\text{-}kdt \ l. \ p\$k < p_0\$k
   using assms by auto
 hence \forall p \in set\text{-}kdt \ l. \ p \notin cbox \ p_0 \ p_1
   using cbox-point-def leD by blast
 thus ?thesis by blast
qed
lemma r-empty:
 assumes invar (Node k \ v \ l \ r) p_1 \$ k < v
 shows set-kdt r \cap cbox p_0 p_1 = \{\}
proof -
  have \forall p \in set\text{-}kdt \ r. \ p_1\$k < p\$k
   using assms by auto
  hence \forall p \in set\text{-}kdt \ r. \ p \notin cbox \ p_0 \ p_1
   using cbox-point-def leD by blast
  thus ?thesis by blast
qed
```

#### 3.4 Main Theorem

theorem search-cbox: assumes invar kdt

```
shows search p_0 p_1 kdt = set\text{-}kdt kdt \cap cbox p_0 p_1 using assms l\text{-}empty r\text{-}empty by (induction kdt) (auto, blast+)
```

end

# 4 Nearest Neighbor Search on the k-d Tree

```
theory Nearest-Neighbors
imports
KD-Tree
begin
```

Verifying nearest neighbor search on the k-d tree. Given a k-d tree and a point p, which might not be in the tree, find the points ps that are closest to p using the Euclidean metric.

## 4.1 Auxiliary Lemmas about sorted-wrt

```
lemma
 {\bf assumes}\ sorted\text{-}wrt\ f\ xs
 shows sorted-wrt-take: sorted-wrt f (take n xs)
 and sorted-wrt-drop: sorted-wrt f (drop n xs)
proof -
 have sorted-wrt f (take n xs @ drop n xs)
   using assms by simp
 thus sorted-wrt f (take n xs) sorted-wrt f (drop n xs)
   using sorted-wrt-append by blast+
qed
definition sorted-wrt-dist :: ('k::finite) point \Rightarrow 'k point list \Rightarrow bool where
 sorted\text{-}wrt\text{-}dist\ p \equiv sorted\text{-}wrt\ (\lambda p_0\ p_1.\ dist\ p_0\ p \leq dist\ p_1\ p)
lemma sorted-wrt-dist-insort-key:
  sorted-wrt-dist p ps \Longrightarrow sorted-wrt-dist p (insort-key (\lambda q. dist q p) q ps)
 by (induction ps) (auto simp: sorted-wrt-dist-def set-insort-key)
lemma sorted-wrt-dist-take-drop:
 assumes sorted-wrt-dist p ps
 shows \forall p_0 \in set \ (take \ n \ ps). \ \forall p_1 \in set \ (drop \ n \ ps). \ dist \ p_0 \ p \leq dist \ p_1 \ p
  using assms sorted-wrt-append unfolding sorted-wrt-dist-def by (metis ap-
pend-take-drop-id)
lemma sorted-wrt-dist-last-take-mono:
 assumes sorted-wrt-dist p ps n \le length ps 0 < n
 shows dist (last (take n ps)) p \leq dist (last ps) p
  using assms unfolding sorted-wrt-dist-def by (induction ps arbitrary: n) (auto
simp add: take-Cons')
```

```
lemma sorted-wrt-dist-last-insort-key-eq:
 assumes sorted-wrt-dist p ps insort-key (\lambda q. dist q p) q ps \neq ps @ [q]
 shows last (insort-key (\lambda q. dist q p) q ps) = last ps
 using assms unfolding sorted-wrt-dist-def by (induction ps) (auto)
\mathbf{lemma}\ sorted\text{-}wrt\text{-}dist\text{-}last\text{:}
 assumes sorted-wrt-dist p ps
 shows \forall q \in set \ ps. \ dist \ q \ p \leq dist \ (last \ ps) \ p
proof (cases \ ps = [])
 {f case}\ True
 thus ?thesis by simp
\mathbf{next}
 case False
 then obtain ps' p' where [simp]:ps = ps' @ [p']
   using rev-exhaust by blast
 hence sorted-wrt-dist p (ps' @ [p'])
   using assms by blast
 thus ?thesis
   unfolding sorted-wrt-dist-def using sorted-wrt-append[of - ps' [p']] by simp
qed
4.2
        Neighbors Sorted wrt. Distance
definition upd-nbors :: nat \Rightarrow ('k::finite) point \Rightarrow 'k point \Rightarrow 'k point list <math>\Rightarrow 'k
point list where
  upd-nbors n p q ps = take n (insort-key (<math>\lambda q. dist q p) q ps)
{f lemma} sorted\text{-}wrt\text{-}dist\text{-}nbors:
 assumes sorted-wrt-dist p ps
 shows sorted-wrt-dist p (upd-nbors n p q ps)
proof -
 have sorted-wrt-dist p (insort-key (\lambda q. dist q p) q ps)
   using assms sorted-wrt-dist-insort-key by blast
 thus ?thesis
   by (simp add: sorted-wrt-dist-def sorted-wrt-take upd-nbors-def)
qed
lemma sorted-wrt-dist-nbors-diff:
 assumes sorted-wrt-dist p ps
 shows \forall r \in set \ ps \cup \{q\} - set \ (upd\text{-}nbors \ n \ p \ q \ ps). \ \forall s \in set \ (upd\text{-}nbors \ n \ p \ q)
ps). dist s p \leq dist r p
proof -
 let ?ps' = insort\text{-}key (\lambda q. dist q p) q ps
 have set ps \cup \{ q \} = set ?ps'
   by (simp add: set-insort-key)
 moreover have set ?ps' = set (take n ?ps') \cup set (drop n ?ps')
   using append-take-drop-id set-append by metis
  ultimately have set ps \cup \{q\} - set \ (take \ n \ ?ps') \subseteq set \ (drop \ n \ ?ps')
   by blast
```

```
moreover have sorted-wrt-dist p ?ps'
   using assms sorted-wrt-dist-insort-key by blast
  ultimately show ?thesis
   unfolding upd-nbors-def using sorted-wrt-dist-take-drop by blast
qed
lemma sorted-wrt-dist-last-upd-nbors-mono:
 assumes sorted-wrt-dist p ps n \leq length ps 0 < n
 shows dist (last (upd-nbors n p q ps)) p \leq dist (last ps) p
proof (cases insort-key (\lambda q. dist q p) q ps = ps @ [q])
 {\bf case}\ {\it True}
 thus ?thesis
   unfolding upd-nbors-def using assms sorted-wrt-dist-last-take-mono by auto
\mathbf{next}
  case False
 hence last (insort-key (\lambda q. dist q p) q ps) = last ps
   using sorted-wrt-dist-last-insort-key-eq assms by blast
 moreover have dist (last (upd-nbors n p q ps)) p \leq dist (last (insort-key (\lambda q.
dist \ q \ p) \ q \ ps)) \ p
    unfolding upd-nbors-def using assms sorted-wrt-dist-last-take-mono[of p in-
sort-key (\lambda q. dist q p) q ps
   by (simp add: sorted-wrt-dist-insort-key)
  ultimately show ?thesis
   by simp
qed
       The Recursive Nearest Neighbor Algorithm
fun nearest-nbors :: nat \Rightarrow ('k::finite) point list \Rightarrow 'k point \Rightarrow 'k kdt \Rightarrow 'k point
list where
 nearest-nbors \ n \ ps \ p \ (Leaf \ q) = upd-nbors \ n \ p \ q \ ps
\mid nearest-nbors \ n \ ps \ p \ (Node \ k \ v \ l \ r) = (
   if p\$k \le v then
     let\ candidates = nearest-nbors\ n\ ps\ p\ l\ in
     if length candidates = n \wedge dist \ p \ (last \ candidates) \leq dist \ v \ (p\$k) \ then
       candidates\\
     else
       nearest-nbors n candidates p r
    else
     let\ candidates = nearest-nbors\ n\ ps\ p\ r\ in
     if length candidates = n \wedge dist \ p \ (last \ candidates) \leq dist \ v \ (p\$k) \ then
       candidates
     else
       nearest-nbors n candidates p l
```

4.4

**lemma** cutoff-r:

**Auxiliary Lemmas** 

assumes invar (Node  $k \ v \ l \ r$ )

```
assumes p\$k \le v \ dist \ p \ c \le dist \ (p\$k) \ v
  shows \forall q \in set\text{-}kdt \ r. \ dist \ p \ c \leq dist \ p \ q
proof standard
  \mathbf{fix} \ q
  assume *: q \in set\text{-}kdt \ r
  have dist p c \leq dist (p\$k) v
   using assms(3) by blast
  also have ... \leq dist (p\$k) v + dist v (q\$k)
   by simp
  also have ... = dist (p\$k) (q\$k)
   \mathbf{using} * assms(1,2) \ dist-real-def \ \mathbf{by} \ auto
  also have \dots \leq dist p q
   using dist-vec-nth-le by blast
 finally show dist p \ c \le dist \ p \ q.
qed
lemma cutoff-l:
 assumes invar (Node k \ v \ l \ r)
 assumes v \leq p\$k \ dist \ p \ c \leq dist \ v \ (p\$k)
  shows \forall q \in set\text{-}kdt \ l. \ dist \ p \ c \leq dist \ p \ q
proof standard
  \mathbf{fix} \ q
  assume *: q \in set\text{-}kdt \ l
  have dist p c \leq dist v (p\$k)
   using assms(3) by blast
  also have ... \leq dist \ v \ (p\$k) + dist \ (q\$k) \ v
   by simp
  also have ... = dist(p\$k)(q\$k)
   using * assms(1,2) dist-real-def by auto
 also have \dots \leq dist \ p \ q
   using dist-vec-nth-le by blast
  finally show dist p \ c \leq dist \ p \ q.
qed
        The Main Theorems
4.5
lemma set-nns:
  set\ (nearest-nbors\ n\ ps\ p\ kdt)\subseteq set-kdt\ kdt\cup set\ ps
  apply (induction kdt arbitrary: ps)
 apply (auto simp: Let-def upd-nbors-def set-insort-key)
  using in-set-takeD set-insort-key by fastforce
\mathbf{lemma}\ length\text{-}nns:
  length (nearest-nbors \ n \ ps \ p \ kdt) = min \ n \ (size-kdt \ kdt + length \ ps)
  by (induction kdt arbitrary: ps) (auto simp: Let-def upd-nbors-def)
lemma length-nns-gt-0:
  0 < n \Longrightarrow 0 < length (nearest-nbors n ps p kdt)
  by (induction kdt arbitrary: ps) (auto simp: Let-def upd-nbors-def)
```

```
lemma length-nns-n:
 assumes (set-kdt kdt \cup set ps) – set (nearest-nbors n ps p kdt) \neq {}
 shows length (nearest-nbors n ps p kdt) = n
  using assms
proof (induction kdt arbitrary: ps)
  case (Node k \ v \ l \ r)
 let ?nnsl = nearest-nbors \ n \ ps \ p \ l
 let ?nnsr = nearest-nbors n ps p r
 consider (A) p$k \le v \land length ?nnsl = n \land dist p (last ?nnsl) \le dist v (p$k)
         \mid (B) p\$k \leq v \land \neg (length ?nnsl = n \land dist p (last ?nnsl) \leq dist v (p\$k))
         (C) \ v < p\$k \land length ?nnsr = n \land dist \ p \ (last ?nnsr) \le dist \ v \ (p\$k)
        | (D) v < p\$k \land \neg (length ?nnsr = n \land dist p (last ?nnsr) \le dist v (p\$k))
   by argo
  thus ?case
  proof cases
   case B
   let ?nns = nearest-nbors \ n \ ?nnsl \ p \ r
   have length ?nnsl \neq n \longrightarrow (set-kdt l \cup set ps - set (nearest-nbors n ps p l) =
{})
     using Node.IH(1) by blast
   hence length ?nnsl \neq n \longrightarrow (set\text{-}kdt \ r \cup set ?nnsl - set ?nns \neq \{\})
     using B Node.prems by auto
   moreover have length ?nnsl = n \longrightarrow ?thesis
     using B by (auto simp: length-nns)
   ultimately show ?thesis
     using B Node.IH(2) by force
 next
   case D
   let ?nns = nearest-nbors \ n \ ?nnsr \ p \ l
   have length ?nnsr \neq n \longrightarrow (set\text{-}kdt \ r \cup set \ ps - set \ (nearest\text{-}nbors \ n \ ps \ p \ r)
     using Node.IH(2) by blast
   hence length ?nnsr \neq n \longrightarrow (set-kdt l \cup set ?nnsr - set ?nnsr \neq {})
     using D Node.prems by auto
   moreover have length ?nnsr = n \longrightarrow ?thesis
     using D by (auto simp: length-nns)
   ultimately show ?thesis
     using D Node.IH(1) by force
qed (auto simp: upd-nbors-def min-def set-insort-key)
lemma sorted-nns:
  sorted\text{-}wrt\text{-}dist\ p\ ps \Longrightarrow sorted\text{-}wrt\text{-}dist\ p\ (nearest\text{-}nbors\ n\ ps\ p\ kdt)
 using sorted-wrt-dist-nbors by (induction kdt arbitrary: ps) (auto simp: Let-def)
lemma distinct-nns:
 assumes invar kdt distinct ps set ps \cap set\text{-kdt } kdt = \{\}
 shows distinct (nearest-nbors n ps p kdt)
```

```
using assms
proof (induction kdt arbitrary: ps)
  case (Node k \ v \ l \ r)
 let ?nnsl = nearest-nbors \ n \ ps \ p \ l
 let ?nnsr = nearest-nbors n ps p r
 have set \ ps \cap set - kdt \ l = \{\} \ set \ ps \cap set - kdt \ r = \{\}
   using Node.prems(3) by auto
  hence DCLR: distinct ?nnsl distinct ?nnsr
   using Node invar-l invar-r by blast+
 have set ?nnsl \cap set-kdt r = \{\} set ?nnsr \cap set-kdt l = \{\}
   using Node.prems(1,3) set-nns by fastforce+
 hence distinct (nearest-nbors n ?nnsl p r) distinct (nearest-nbors n ?nnsr p l)
   using Node.IH(1,2) Node.prems(1,2) DCLR invar-l invar-r by blast+
 thus ?case
   using DCLR by (auto simp add: Let-def)
qed (auto simp: upd-nbors-def distinct-insort)
lemma last-nns-mono:
 assumes invar kdt sorted-wrt-dist p ps n \le length ps 0 < n
 shows dist (last (nearest-nbors n ps p kdt)) p \leq dist (last ps) p
  using assms
proof (induction kdt arbitrary: ps)
  case (Node \ k \ v \ l \ r)
  let ?nnsl = nearest-nbors \ n \ ps \ p \ l
 let ?nnsr = nearest-nbors n ps p r
 have n \leq length ?nnsl n \leq length ?nnsr
   using Node.prems(3) by (simp-all add: length-nns)
 hence dist (last (nearest-nbors n ?nnsl p r)) p \leq dist (last ?nnsl) p
       dist (last (nearest-nbors \ n \ ?nnsr \ p \ l)) \ p \leq dist (last \ ?nnsr) \ p
   using sorted-nns Node invar-l invar-r by blast+
 hence dist (last (nearest-nbors n ?nnsl p r)) p \leq dist (last ps) p
       dist (last (nearest-nbors n ?nnsr p l)) p \leq dist (last ps) p
   using Node.IH(1)[of\ ps]\ Node.IH(2)[of\ ps]\ Node.prems\ invar-l\ length-nns-gt-0
by auto
 thus ?case
   using Node by (auto simp add: Let-def)
qed (auto simp: sorted-wrt-dist-last-upd-nbors-mono)
theorem dist-nns:
 assumes invar kdt sorted-wrt-dist p ps set ps \cap set-kdt kdt = {} distinct ps 0 <
  shows \forall q \in set\text{-}kdt \ kdt \cup set \ ps - set \ (nearest\text{-}nbors \ n \ ps \ p \ kdt). \ dist \ (last
(nearest-nbors\ n\ ps\ p\ kdt))\ p \leq dist\ q\ p
 using assms
proof (induction kdt arbitrary: ps)
 case (Node k \ v \ l \ r)
 let ?nnsl = nearest-nbors n ps p l
 let ?nnsr = nearest-nbors n ps p r
```

```
have IHL: \forall q \in set\text{-}kdt \ l \cup set \ ps - set \ ?nnsl. \ dist \ (last \ ?nnsl) \ p \leq dist \ q \ p
   using Node.IH(1) Node.prems invar-l invar-set by auto
  have IHR: \forall q \in set\text{-}kdt \ r \cup set \ ps - set \ ?nnsr. \ dist \ (last \ ?nnsr) \ p \leq dist \ q \ p
   using Node.IH(2) Node.prems invar-r invar-set by auto
  have SORTED-L: sorted-wrt-dist p ?nnsl
    using sorted-nns Node.prems(2) by blast
  have SORTED-R: sorted-wrt-dist p ?nnsr
   using sorted-nns Node.prems(2) by blast
 have DISTINCT-L: distinct ?nnsl
   using Node.prems distinct-nns invar-set invar-l by fastforce
 have DISTINCT-R: distinct ?nnsr
   using Node.prems distinct-nns invar-set invar-r
   by (metis inf-bot-right inf-sup-absorb inf-sup-aci(3) sup.commute)
  consider (A) p\$k \le v \land length ?nnsl = n \land dist p (last ?nnsl) \le dist v (p\$k)
        | (B) p\$k \le v \land \neg (length ?nnsl = n \land dist p (last ?nnsl) \le dist v (p\$k))
        | (C) v < p\$k \land length ?nnsr = n \land dist p (last ?nnsr) \leq dist v (p\$k)
        \mid (D) \ v < p\$k \land \neg (length ?nnsr = n \land dist \ p \ (last ?nnsr) \le dist \ v \ (p\$k))
   by argo
  thus ?case
  proof cases
   case A
   hence \forall q \in set\text{-}kdt \ r. \ dist \ (last ?nnsl) \ p \leq dist \ q \ p
     using Node.prems(1,2) cutoff-r by (metis dist-commute)
   thus ?thesis
     using IHL A by auto
 next
   case B
   let ?nns = nearest-nbors \ n \ ?nnsl \ p \ r
   have set ?nnsl \subseteq set-kdt l \cup set ps set ps \cap set-kdt r = \{\}
    using set-nns Node.prems(1,3) by (simp add: set-nns disjoint-iff-not-equal)+
   hence set ?nnsl \cap set-kdt r = \{\}
     using Node.prems(1) by fastforce
   hence IHLR: \forall q \in set\text{-}kdt \ r \cup set ?nnsl - set ?nns. \ dist \ (last ?nns) \ p \leq dist
    using Node.IH(2)[OF - SORTED-L - DISTINCT-L Node.prems(5)] Node.prems(1)
invar-r by blast
   have \forall q \in set \ ps - set \ ?nnsl. \ dist \ (last \ ?nns) \ p \leq dist \ q \ p
   proof standard
     \mathbf{fix} \ q
     assume *: q \in set ps - set ?nnsl
     hence length ?nnsl = n
```

```
using length-nns-n by blast
     hence LAST: dist (last ?nns) p \leq dist (last ?nnsl) p
         using last-nns-mono SORTED-L invar-r Node.prems(1,2,5) by (metis
order-refl)
     have dist (last ?nnsl) p \leq dist q p
       using IHL * by blast
     thus dist (last ?nns) p \leq dist q p
       using LAST by argo
   qed
   hence R: \forall q \in set\text{-}kdt \ r \cup set \ ps - set ?nns. \ dist \ (last ?nns) \ p \leq dist \ q \ p
     using IHLR by auto
   have \forall q \in set\text{-}kdt \ l - set ?nnsl. \ dist (last ?nns) \ p \leq dist \ q \ p
   proof standard
     \mathbf{fix} \ q
     assume *: q \in set\text{-}kdt \ l - set \ ?nnsl
     hence length ?nnsl = n
       using length-nns-n by blast
     hence LAST: dist (last ?nns) p \leq dist (last ?nnsl) p
          using last-nns-mono SORTED-L invar-r Node.prems(1,2,5) by (metis
order-refl)
     have dist (last ?nnsl) p \leq dist q p
       using IHL * by blast
     thus dist (last ?nns) p \leq dist q p
       using LAST by argo
   hence L: \forall q \in set\text{-}kdt \ l - set ?nns. \ dist (last ?nns) \ p \leq dist \ q \ p
     using IHLR by blast
   show ?thesis
     using B R L by auto
 next
   case C
   hence \forall q \in set\text{-}kdt \ l. \ dist \ (last ?nnsr) \ p \leq dist \ q \ p
     using Node.prems(1,2) cutoff-l by (metis dist-commute less-imp-le)
   thus ?thesis
     using IHR C by auto
  next
   case D
   let ?nns = nearest-nbors \ n \ ?nnsr \ p \ l
   have set ?nnsr \subseteq set-kdt r \cup set ps set ps \cap set-kdt l = \{\}
    using set-nns Node.prems(1,3) by (simp add: set-nns disjoint-iff-not-equal)+
   hence set ?nnsr \cap set-kdt \ l = \{\}
     using Node.prems(1) by fastforce
   hence IHRL: \forall q \in set\text{-}kdt \ l \cup set ?nnsr - set ?nns. \ dist \ (last ?nns) \ p \leq dist
q p
```

```
using Node.IH(1)[OF - SORTED-R - DISTINCT-R Node.prems(5)] Node.prems(1)
invar-l by blast
   have \forall q \in set \ ps - set \ ?nnsr. \ dist \ (last \ ?nns) \ p \leq dist \ q \ p
   proof standard
     \mathbf{fix} \ q
     \mathbf{assume} *: q \in set\ ps - set\ ?nnsr
     hence length ?nnsr = n
       using length-nns-n by blast
     hence LAST: dist (last ?nns) p \le dist (last ?nnsr) p
         using last-nns-mono SORTED-R invar-l Node.prems(1,2,5) by (metis
order-refl)
     have dist (last ?nnsr) p \leq dist q p
       using IHR * by blast
     thus dist (last ?nns) p \leq dist q p
       using LAST by argo
   qed
   hence R: \forall q \in set\text{-}kdt \ l \cup set \ ps - set ?nns. \ dist \ (last ?nns) \ p \leq dist \ q \ p
     using IHRL by auto
   have \forall q \in set\text{-}kdt \ r - set ?nnsr. \ dist (last ?nns) \ p \leq dist \ q \ p
   proof standard
     \mathbf{fix} \ q
     assume *: q \in set\text{-}kdt \ r - set ?nnsr
     hence length ?nnsr = n
       using length-nns-n by blast
     hence LAST: dist (last ?nns) p \leq dist (last ?nnsr) p
         using last-nns-mono SORTED-R invar-l Node.prems(1,2,5) by (metis
order-refl)
     have dist (last ?nnsr) p \leq dist q p
       using IHR * by blast
     thus dist (last ?nns) p \leq dist q p
       using LAST by argo
   hence L: \forall q \in set\text{-}kdt \ r - set ?nns. \ dist (last ?nns) \ p \leq dist \ q \ p
     using IHRL by blast
   show ?thesis
     using D R L by auto
qed (auto simp: sorted-wrt-dist-nbors-diff upd-nbors-def)
```

#### Nearest Neighbors Definition and Theorems

```
definition nearest-neighbors :: nat \Rightarrow ('k::finite) point \Rightarrow 'k kdt \Rightarrow 'k point list
where
```

nearest-neighbors n p kdt = nearest-nbors n p kdt

```
theorem length-nearest-neighbors:
  length (nearest-neighbors \ n \ p \ kdt) = min \ n \ (size-kdt \ kdt)
  by (simp add: length-nns nearest-neighbors-def)
{\bf theorem}\ sorted {\it -wrt-dist-nearest-neighbors}:
  sorted-wrt-dist p (nearest-neighbors n p kdt)
  using sorted-nns unfolding nearest-neighbors-def sorted-wrt-dist-def by force
theorem set-nearest-neighbors:
  set (nearest-neighbors \ n \ p \ kdt) \subseteq set-kdt \ kdt
  unfolding nearest-neighbors-def using set-nns by force
{\bf theorem}\ \textit{distinct-nearest-neighbors}:
  assumes invar kdt
  shows distinct (nearest-neighbors n p kdt)
  using assms by (simp add: distinct-nns nearest-neighbors-def)
theorem dist-nearest-neighbors:
 assumes invar\ kdt\ nns = nearest-neighbors\ n\ p\ kdt
  shows \forall q \in (set\text{-}kdt \ kdt - set \ nns). \ \forall r \in set \ nns. \ dist \ r \ p \leq dist \ q \ p
proof (cases 0 < n)
  case True
  have \forall q \in set\text{-}kdt \ kdt - set \ nns. \ dist \ (last \ nns) \ p \leq dist \ q \ p
     using nearest-neighbors-def dist-nns[OF\ assms(1),\ of\ p\ [],\ OF\ -\ -\ -\ True]
assms(2)
   by (simp add: nearest-neighbors-def sorted-wrt-dist-def)
  hence \forall q \in set\text{-}kdt \ kdt - set \ nns. \ \forall n \in set \ nns. \ dist \ n \ p \leq dist \ q \ p
  \mathbf{using}\ assms(2)\ sorted-wrt-dist-nearest-neighbors[of\ p\ n\ kdt]\ sorted-wrt-dist-last[of\ n\ kdt]
p nns] by force
  thus ?thesis
   using nearest-neighbors-def by blast
\mathbf{next}
  {\bf case}\ \mathit{False}
 hence length \ nns = 0
   using assms(2) unfolding nearest-neighbors-def by (auto simp: length-nns)
  thus ?thesis
   \mathbf{by} \ simp
qed
end
```

#### References

- [1] J. L. Bentley. Multidimensional binary search trees used for associative searching. *Commun. ACM*, 18(9):509–517, 1975.
- [2] J. H. Friedman, J. L. Bentley, and R. A. Finkel. An algorithm for finding

best matches in logarithmic expected time. ACM Trans. Math. Softw.,  $3(3):209-226,\ 1977.$