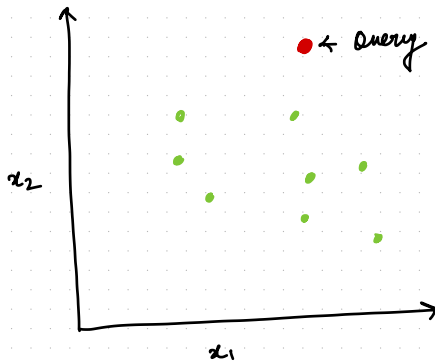


K-Nearest Neighbors Approximation

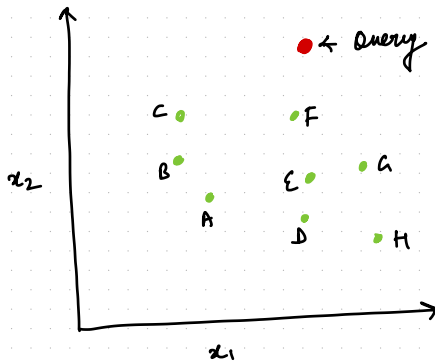
Nipun Batra

IIT Gandhinagar

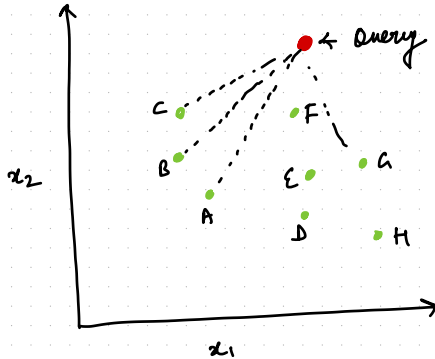
August 2, 2025



Find 1-NN for query point $\hat{q} \in \mathbb{R}^D$

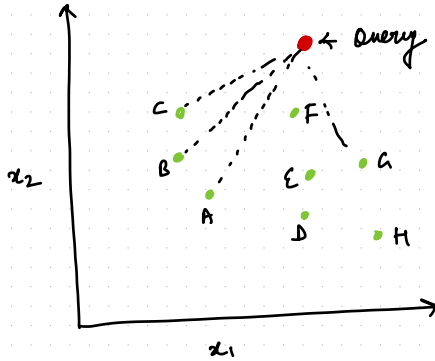


Find 1-NN for query point $q \in \mathbb{R}^D$
 TRAIN SET is $X \in \mathbb{R}^{N \times D}$



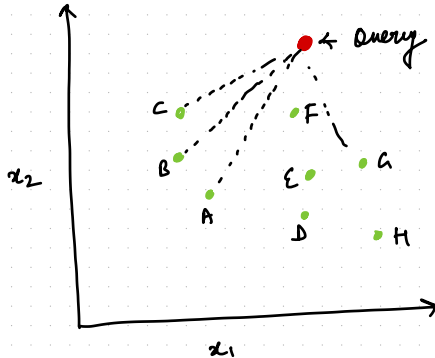
DISTANCE	
q-A	..
q-B	..
	..
	..
	..
	..
	..

Find 1-NN for query point $q \in \mathbb{R}^D$
 TRAIN SET is $X \in \mathbb{R}^{N \times D}$



DISTANCE	
$q-A$	..
$q-B$	..
	..
	..
	..
	..
	..

STEPS FOR FINDING $D(q, A)$



DISTANCE	
q-A	..
q-B	..
	..
	..
	..
	..
	..

STEPS FOR FINDING $D(q, A)$

$$D(q, A) = \sqrt{(q_1 - A_1)^2 + \dots (q_D - A_D)^2}$$

STEPS FOR FINDING $D(q, A)$

$$D(q, A) = \sqrt{(q_1 - A_1)^2 + \dots (q_D - A_D)^2}$$

SUBTRACTIONS

MULTIPLICATIONS

ADDITIONS

SQR

STEPS FOR FINDING $D(q, A)$

$$D(q, A) = \sqrt{(q_1 - A_1)^2 + \dots (q_D - A_D)^2}$$

SUBTRACTIONS D

MULTIPLICATIONS D

ADDITIONS D

SQR7 1

STEPS FOR FINDING $D(q, A)$

$$D(q, A) = \sqrt{(q_1 - A_1)^2 + \dots + (q_D - A_D)^2}$$

SUBTRACTIONS D

MULTIPLICATIONS D

ADDITIONS D

SQRT 1

Total time for $D(q, A)$ or
DISTANCE B/W 1 PAIR $= O(D)$

Q) Time required for
creating table

DISTANCE	
q-A	..
q-B	..
	..
	..
	..
	..
	..

Q) Time required for creating table

$O(ND)$

Dimensionality

samples

[illegible]

Q) Time required for
finding 1-NN?

DISTANCE	
q-A	20
q-B	30
.	2
.	8
.	9
.	..
.	..
.	34

Q) Time required for finding 1-NN?

$O(n)$: linear search

DISTANCE	
q-A	20
q-B	30
.	2
.	8
.	9
.	..
.	..
.	34

Q) Overall time complexity

$O(ND)$

Linear in # samples

(sometimes
millions of
samples)

DISTANCE	
q-A	20
q-B	30
.	2
.	8
.	9
.	..
.	34

Goal:

Reduce $O(ND)$
↑
Target

How?

Goal:

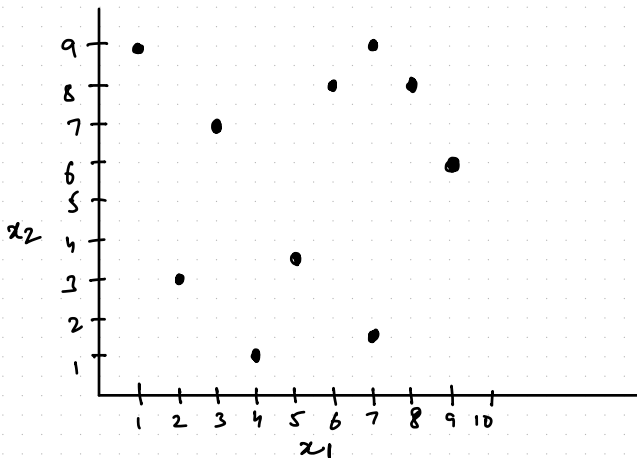
Reduce $O(ND)$
 $\uparrow$
 Target

How? (Hints)

- Decision trees
- Search for subset of examples
- Current algorithm does nothing at training time.

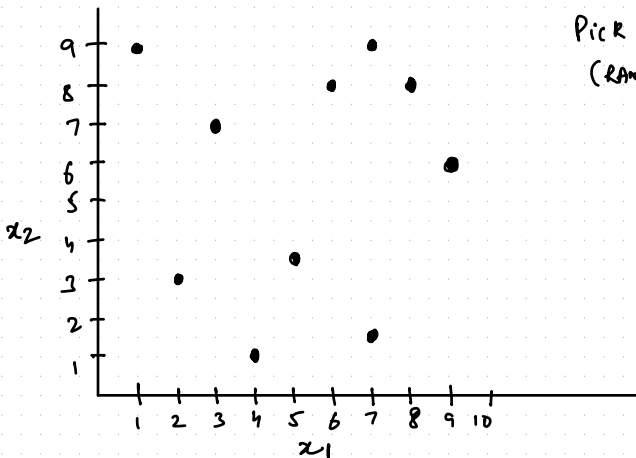
K-D trees (Victor Laranto slides)

$$- X = \{(1, 9), (2, 3), (4, 1), (3, 7), (5, 4), (6, 8), (7, 2), (8, 8), (7, 9), (9, 6)\}$$



K-D trees (Victor Laranto slides)

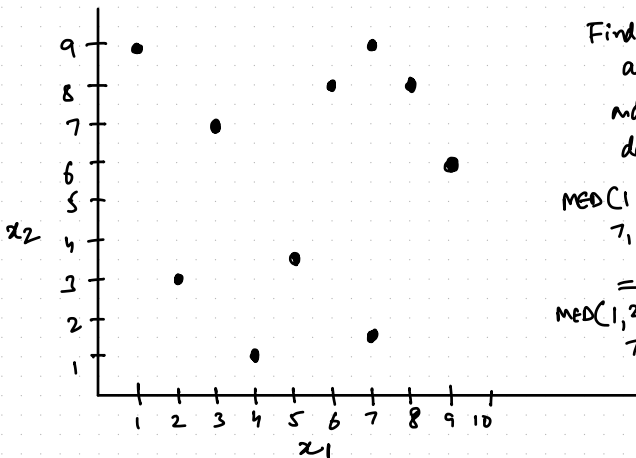
$$- X = \{(1, 9), (2, 3), (4, 1), (3, 7), (5, 4), (6, 8), (7, 2), (8, 8), (7, 9), (9, 6)\}$$



Pick dim x_1
(Random $\in x_1, x_2$)

K-D trees (Victor Laranto slides)

$$- X = \{(1, 9), (2, 3), (4, 1), (3, 7), (5, 4), (6, 8), (7, 2), (8, 8), (7, 9), (9, 6)\}$$



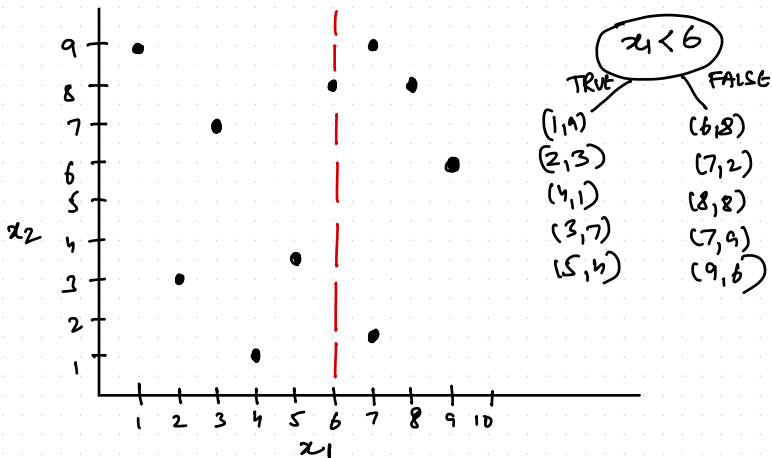
Find median
along x_1
and split
data

$$\text{MED}(1, 2, 4, 3, 5, 6, 7, 8, 7, 9)$$

$$= \text{MED}(1, 2, 3, 4, 5, \underline{6}, 7, 7, 8, 9)$$

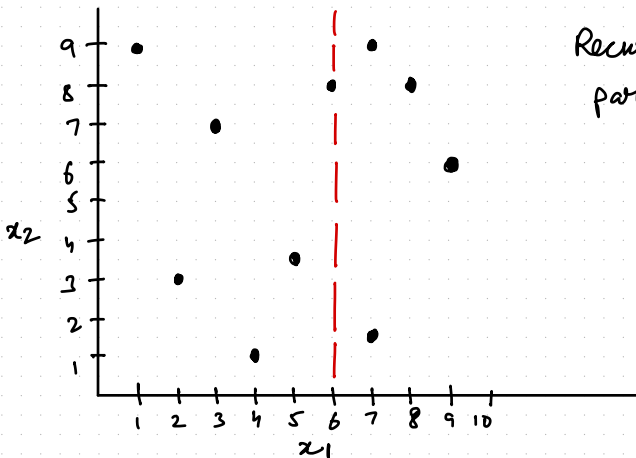
K-D trees (Victor Laranto slides)

- $X = \{(1, 9), (2, 3), (4, 1), (3, 7), (5, 4), (6, 8), (7, 2), (8, 8), (7, 9), (9, 6)\}$



K-D trees (Victor Laranto slides)

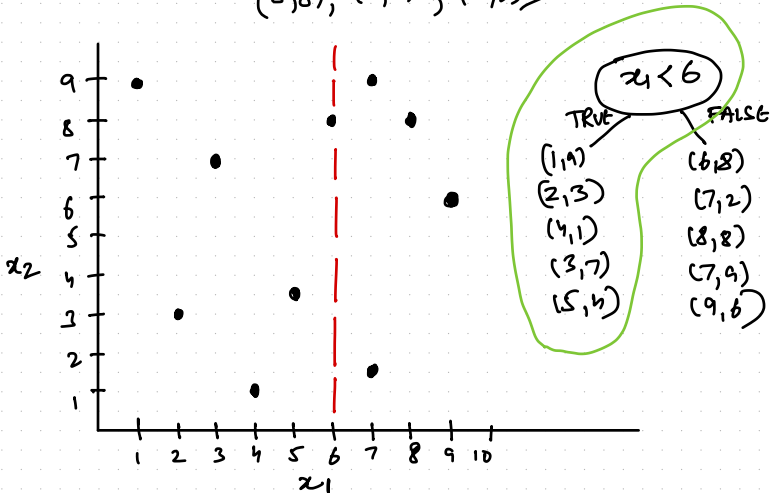
$$- X = \{(1, 9), (2, 3), (4, 1), (3, 7), (5, 4), (6, 8), (7, 2), (8, 8), (7, 9), (9, 6)\}$$



Recursive
partition

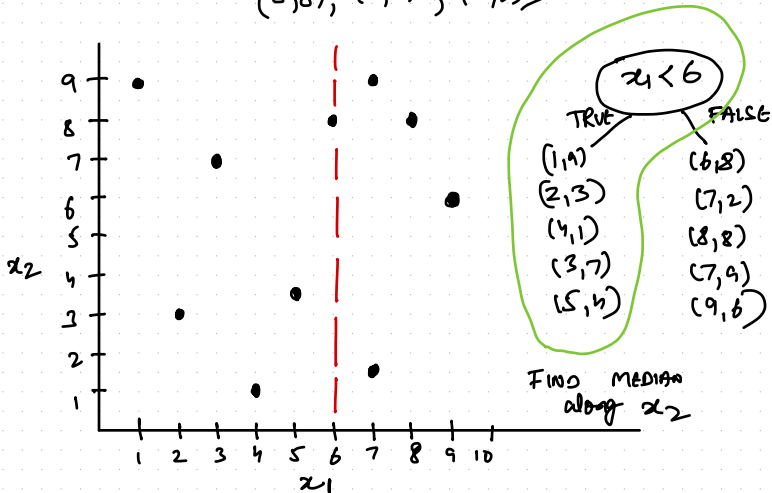
K-D trees (Victor Laranto slides)

- $X = \{(1, 9), (2, 3), (4, 1), (3, 7), (5, 4), (6, 8), (7, 2), (8, 8), (7, 9), (9, 6)\}$



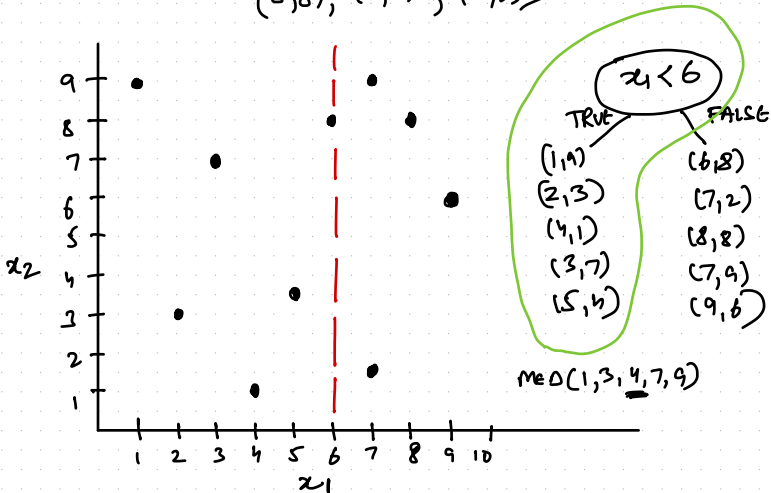
K-D trees (Victor Laranto slides)

- $X = \{(1, 9), (2, 3), (4, 1), (3, 7), (5, 4), (6, 8), (7, 2), (8, 8), (7, 9), (9, 6)\}$



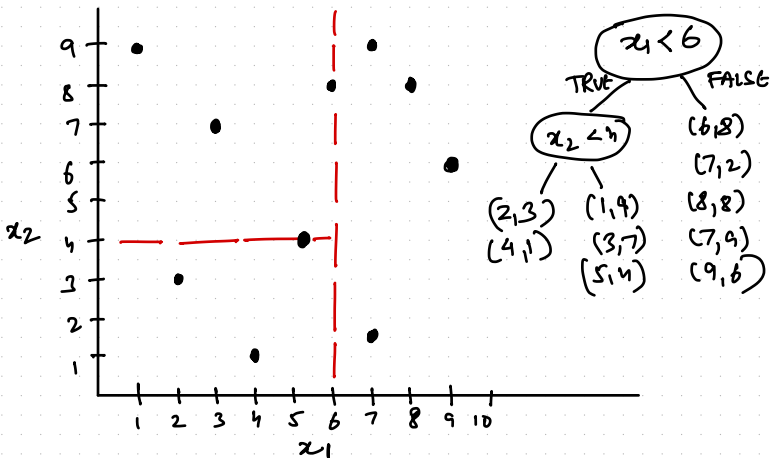
K-D trees (Victor Laranto slides)

- $X = \{(1, 9), (2, 3), (4, 1), (3, 7), (5, 4), (6, 8), (7, 2), (8, 8), (7, 9), (9, 6)\}$



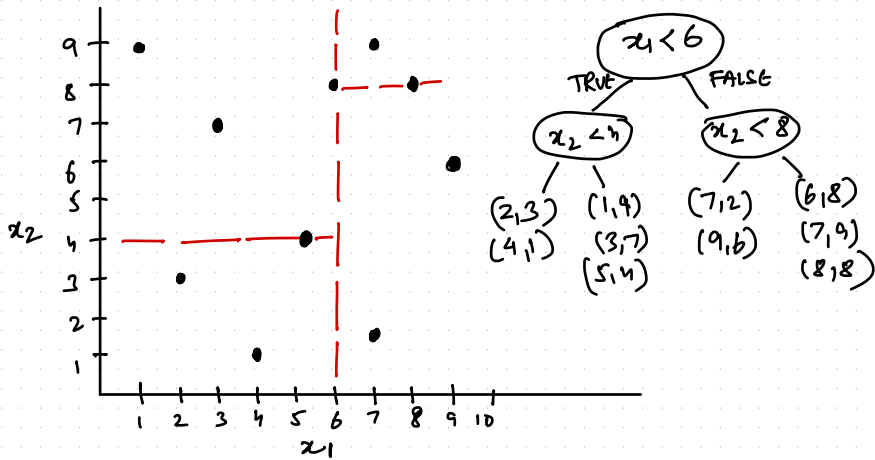
K-D trees (Victor Laranto slides)

- $X = \{(1, 9), (2, 3), (4, 1), (3, 7), (5, 4), (6, 8), (7, 2), (8, 8), (7, 9), (9, 6)\}$



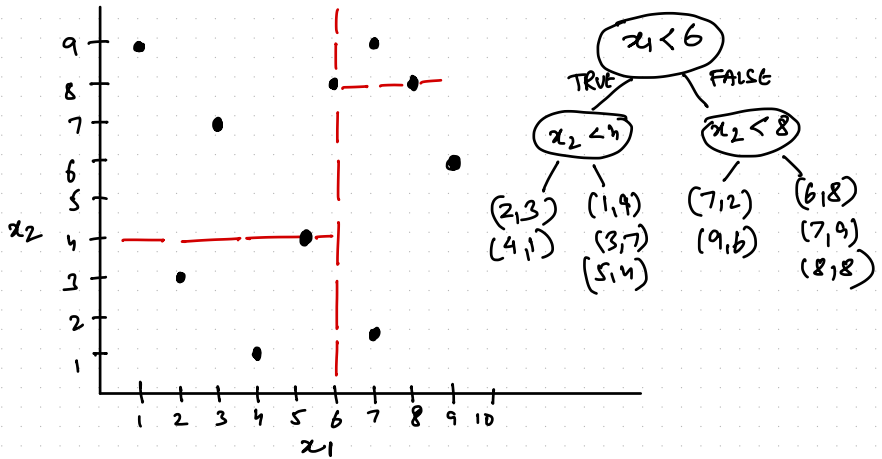
K-D trees (Victor Laranto slides)

- $X = \{(1, 9), (2, 3), (4, 1), (3, 7), (5, 4), (6, 8), (7, 2), (8, 8), (7, 9), (9, 6)\}$



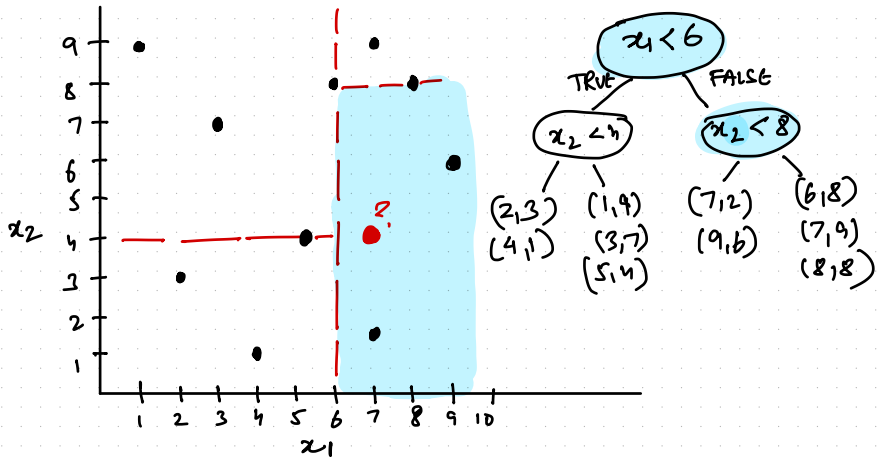
K-D trees (Victor Laranto slides)

- Query pt (7,4)



K-D trees (Victor Laranto slides)

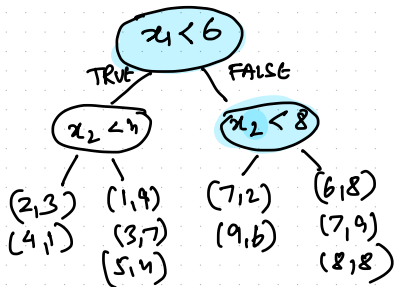
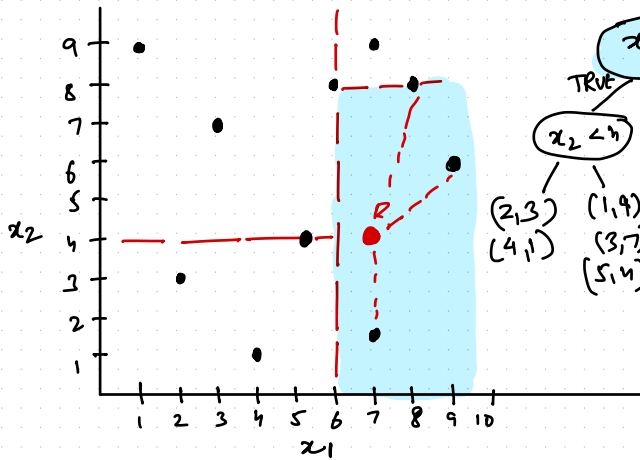
- Query pt (7,4)



K-D trees (Victor Laranto slides)

- Query pt (7,4)

For finding Nns, look
in subspace

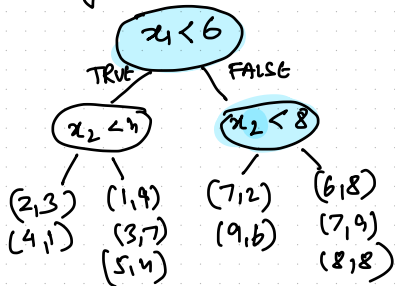
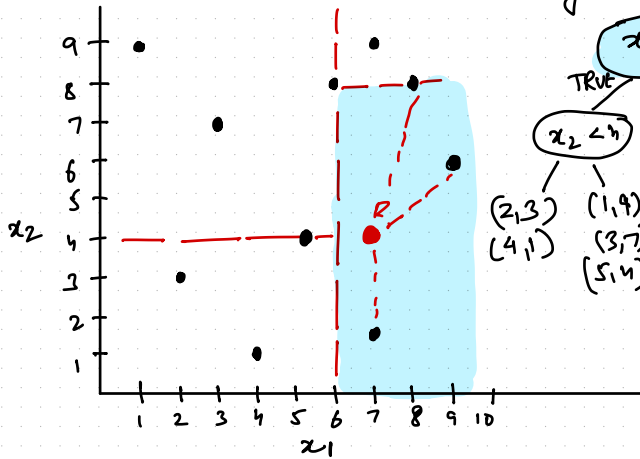


K-D trees (Victor Lammerto slides)

- Query pt (7,4)

For Finding Nns, look
in subspace

✓ way lesser comparisons

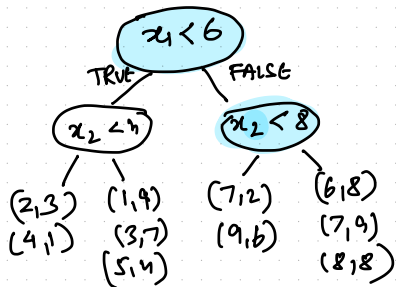
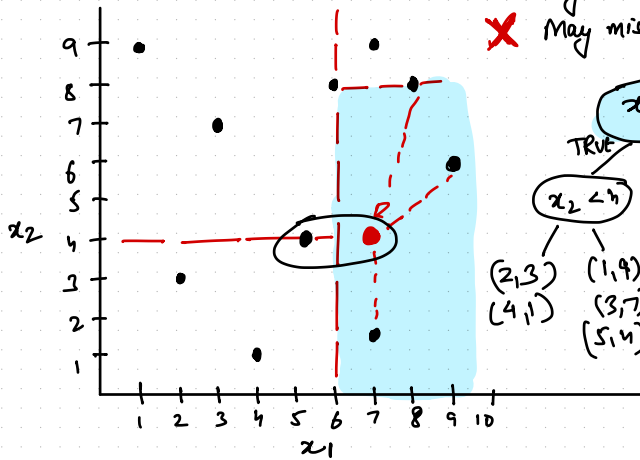


K-D trees (Victor Lammerto slides)

- Query pt (7,4)

For Finding Nns, look
in subspace

- ✓ Way lesser comparisons
- ✗ May miss closest neighbors



KD trees (time complexity)

TRAINING Time (Ref. Wikipedia KD trees)

KD trees (time complexity)

TRAINING Time

samples in subtrees

KD trees (time complexity)

TRAINING Time

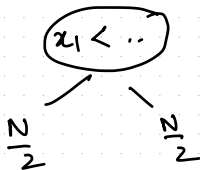
samples in subtrees

Depth 0
|
N

KD trees (time complexity)

TRAINING Time

samples in subtrees

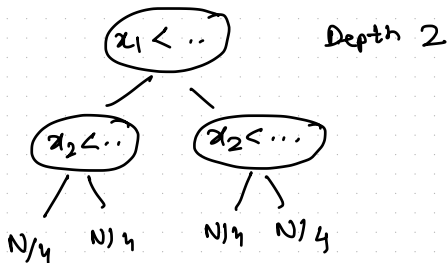


Depth 1

KD trees (time complexity)

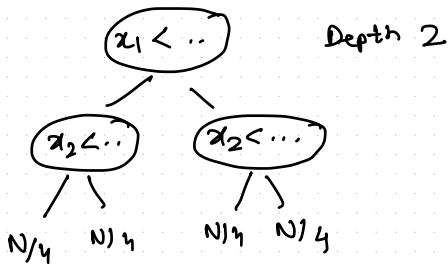
TRAINING Time

samples in subtrees



KD trees (time complexity)

TRAINING Time



Depth $O(\log_2 N)$

KD trees (time complexity)

TRAINING Time

- we have $O(\log_2 N)$ levels.
- For each level,
 - sort " N " examples to find median.
 - $O(N \log_2 N)$ time
- Total time to build data structure $O(N \log^2 N)$

KD trees (time complexity)

* let's assume 's' (≤ 40) is leaf size
(# samples at which
we stop partitioning)

* what is time complexity of query?

KD trees (time complexity)

* let's assume 'S' (≈ 40) is leaf size
(# samples at which
we stop partitioning)

* what is time complexity of query?

— How many levels
to reach leaf?

KD trees (time complexity)

* let's assume 's' (≈ 40) is leaf size
(# samples at which
we stop partitioning)

* what is time complexity of query?

- How many levels to reach leaf?

- $O(\log N)$

- How many computations per level?

KD trees (time complexity)

* let's assume 's' (≈ 40) is leaf size
(# samples at which we stop partitioning)

* what is time complexity of query?

- How many levels to reach leaf?

- $O(\log N)$

- How many computations per level?

- One KD comparison (e.g. $x_1 < b$)

KD trees (time complexity)

- * let's assume 's' (≈ 40) is leaf size
(# samples at which we stop partitioning)
- * what is time complexity of query?
 - How many levels to reach leaf?
 - $O(\log N)$
 - How many computations per level?
 - one KD comparison (e.g. $x_1 < b$)
 - How many computations at leaf?

KD trees (time complexity)

- * let's assume 's' (≈ 40) is leaf size
(# samples at which we stop partitioning)
- * what is time complexity of query?
 - How many levels to reach leaf?
 - $O(\log N)$
 - How many computations per level?
 - one KD comparison (e.g. $x_1 < b$)
 - How many computations at leaf?
 - $O(D * s)$

KD trees (time complexity)

* What is time complexity of query?

- How many levels to reach leaf?

- $O(\log N)$

- How many computatⁿs per level?

- One KD comparison (e.g. $x_1 < b$)

- How many computatⁿs at leaf?

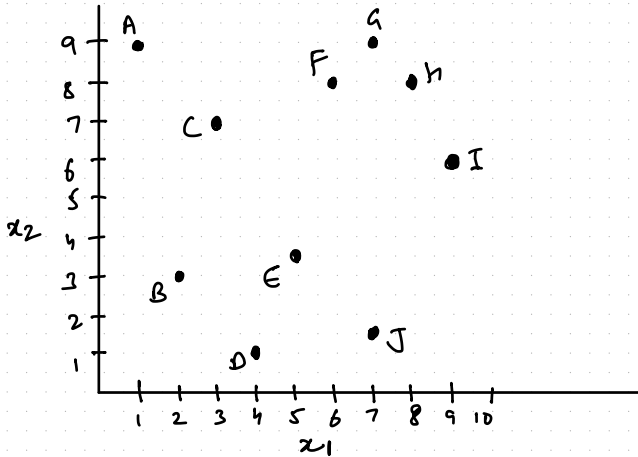
- $O(D * S)$

TOTAL QUERY $O(\log N + D * S)$

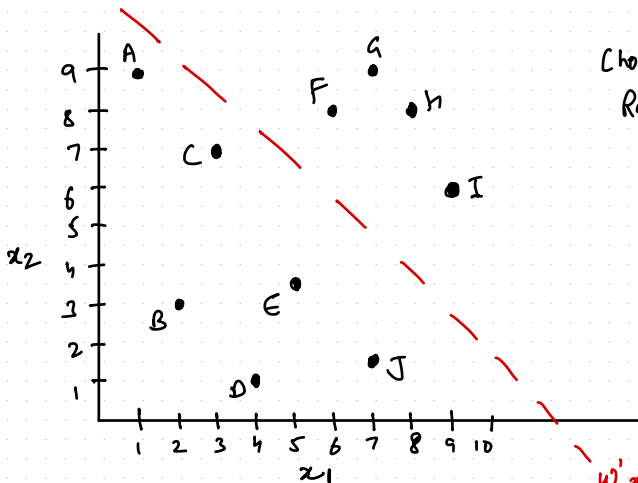
if $D \ll N$ and S is small

$O(\log N)$

Locality Sensitive Hashing (LSH) w/ Random Projection (Machine Learning Interview.com)



Locality Sensitive Hashing (LSH) w/ Random Projection

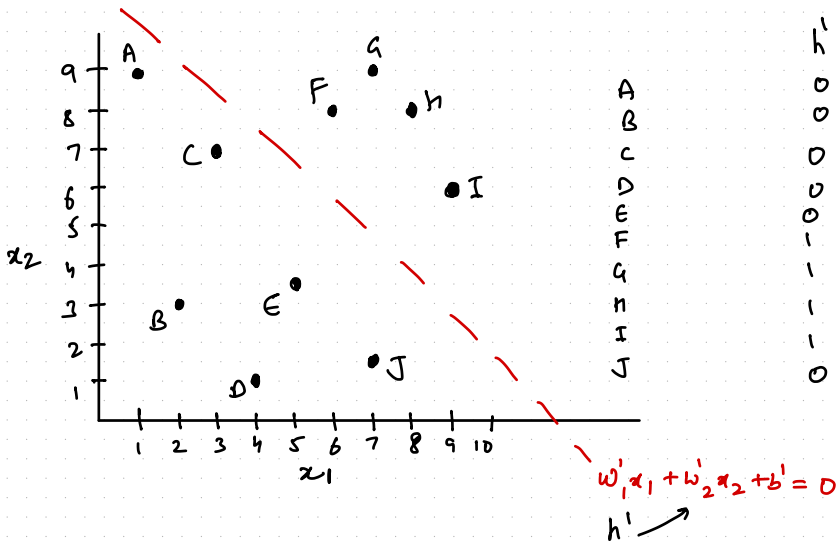


Choose h' :
Random hyperplane
in 'D' dim

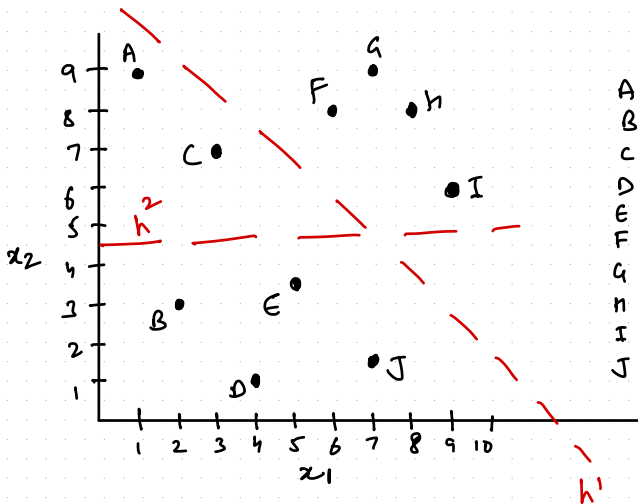
$$w'_1 x_1 + w'_2 x_2 + b' = 0$$

$h' \rightarrow$

Locality Sensitive Hashing (LSH) w/ Random Projection



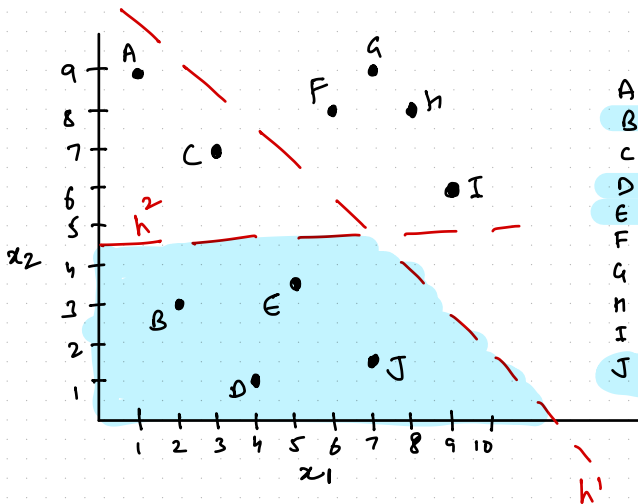
Locality Sensitive Hashing (LSH) w/ Random Projection



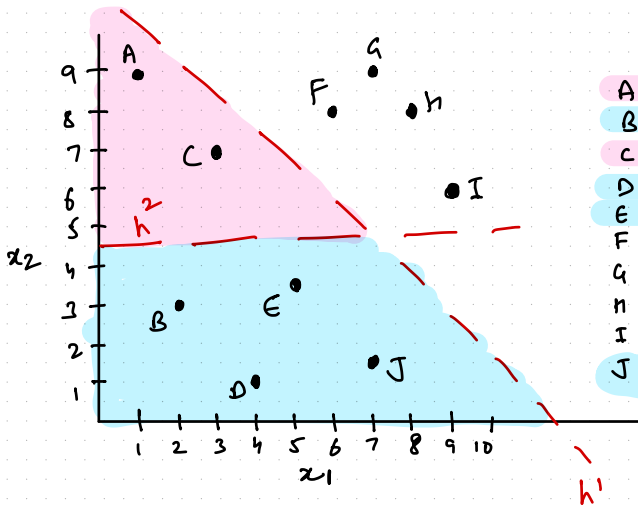
A
B
C
D
E
F
G
H
I
J

h^2	h^1
1	0
0	0
1	0
0	0
0	0
1	1
1	1
1	1
1	1
0	0

Locality Sensitive Hashing (LSH) w/ Random Projection

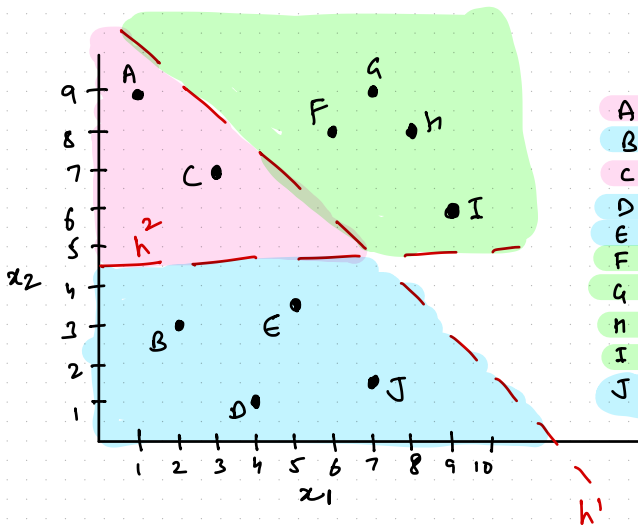


Locality Sensitive Hashing (LSH) w/ Random Projection



	h^2	h^1
A	1	0
B	0	0
C	1	0
D	0	0
E	0	0
F	1	1
G	1	1
H	1	1
I	1	1
J	0	0

Locality Sensitive Hashing (LSH) w/ Random Projection



Practical implementation

* How to sample hyperplane?

$i = 1 \dots D :$  sampled from
 $w_i \sim N(\dots, \dots)$
 $b \sim N(\dots, \dots)$

Practical implementation

* How to get $h^i(x) = 0$ or 1

$$h^i(x) = \text{SIGM}(b + w_1^i x_1 + w_2^i x_2 + \dots)$$

Practical implementation

* How to vectorize finding Hash Table

$$X = \begin{bmatrix} \end{bmatrix}$$

Practical implementation

* How to vectorize finding Hash Table

$$X = \begin{bmatrix} \vdots \end{bmatrix}_{N \times D}$$

$$X' = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}_{N \times D+1}$$

Practical implementation

* How to vectorize finding Hash Table

$$x^i = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}_{N \times D+1}$$

let # planes be 'p'

$$W = \begin{bmatrix} \text{---} \\ N(\text{---}, \text{---}) \\ \text{---} \\ \text{---} \end{bmatrix}_{D+1 \times p}$$

Practical implementation

* How to vectorize finding Hash Table

$$x' = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}_{N \times D+1}$$

$$H = \text{SGN}(x'w)_{N \times P}$$

let # planes be 'P'

$$w = \begin{bmatrix} \text{---} \\ N(\dots, \dots) \\ \text{---} \\ \text{---} \end{bmatrix}_{D+1 \times P}$$

Time complexity

Assuming one (1) set of hash functions

$$\rightarrow H_{N \times P} = \text{SGN}(X_{N \times D} \cdot R_{D \times P})$$

$$\text{Time} = O(N \times D \times P)$$

Time to generate $R = O(D \times P)$

Thus, at training time: $O(N \times D \times P)$

At testing time,

→ Computing hash on q_{ix} takes $O(DP)$

→ Assuming 'T' points in bucket:
 $O(T * D)$ to find
closest
neighbour

At testing time,

→ Computing hash on q_{ix} takes $O(DP)$

→ Assuming 'T' points in bucket:
 $O(T * D)$ to find
closest
neighbour

→ What is T in terms of N and P (on average)

At testing time,

→ Computing hash on q_{ix} takes $O(DP)$

→ Assuming 'T' points in bucket:
 $O(T * D)$ to find
closest
neighbour

→ What is T in terms of N and P (on average)

$$T \approx \frac{N}{2^P}$$

At testing time,

→ Computing hash on q_{ix} takes $O(DP)$

→ Assuming 'T' points in bucket:
 $O(T * D)$ to find
closest
neighbour

→ What is T in terms of N and P (on average)

$$T \approx \frac{N}{2^P}$$

→ Test Time = $O(DP + \frac{DN}{2^P})$