DSC 190

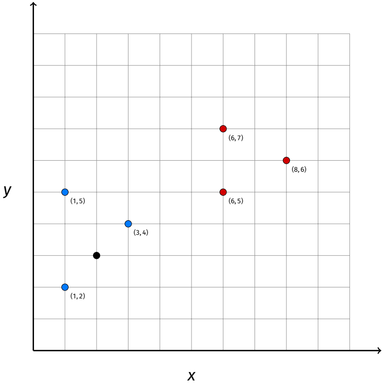
Data Structures & Algorithms

Today's Lecture

Nearest Neighbors

- Finding the closest data point to a query point is a common operation.
- In machine learning, at the core of the **nearest neighbor classifier**.

NN Classifier



NN Query

- **Given**: a data set X of n points in $\mathbb{R}^d$ and a **query** point, $p \in \mathbb{R}^d$.
- **Return**: the point in X that is nearest[1] to p

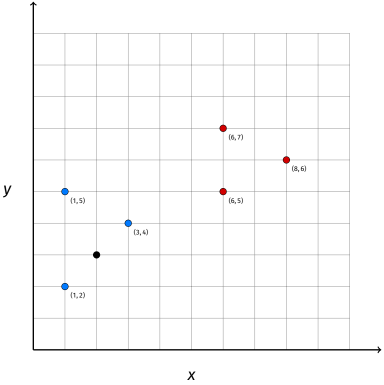
[1] In terms of Euclidean distance, though other distances can be considered.

Approach #1: Brute Force

- Compute distance between p and every point $x \in X$, keep closest.
- Time: $\Theta(nd)$

Intuitively...

- ...we can do better. We only need to look at region close to p.

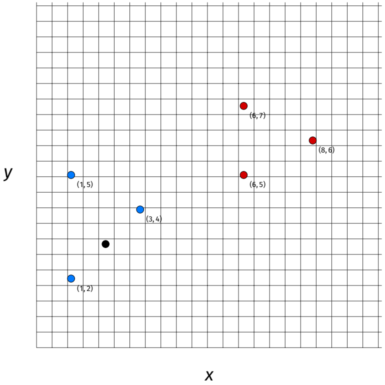


```python
def brute_force_nn_search(data, p):
    """Find nearest neighbor.

    Parameters
    ----------
    data : np.ndarray
        An n x d array of points.
    p : np.ndarray
        A d-array representing the query point.

    Returns
    -------
    nn : np.ndarray
        The closest point.
    nn_distance : float
        Distance to closest point.

    """
    distances = np.sqrt(np.sum((data - p)**2, axis=1))
    ix_of_nn = np.argmin(distances)
    nn = data[ix_of_nn]
    nn_distance = distances[ix_of_nn]
    return (nn, nn_distance)
```

Approach #2

- Build a grid.
- To query NN, find cell containing *p*.
- Start search in *p*'s cell, move outwards.

Intuitively...



Problems

- How do we choose grid cell size?
  - Too big: cells contain a lot of points = brute force.
  - Too small: Most of the cells are empty.
  - "Just right" for one region might be too big/small for another region.

- Number of cells grows **exponentially** with dimension.

Today

- We'll refine the idea of a grid.
- Adapt cell placement/size to the data.
- Result: **k-d trees**.

k-d Trees

- Will speed up NN queries in low dimensions (<10) from $\Theta(n)$ to $\Theta(\log n)$.
- But will be just as bad as brute force in high dimensions.

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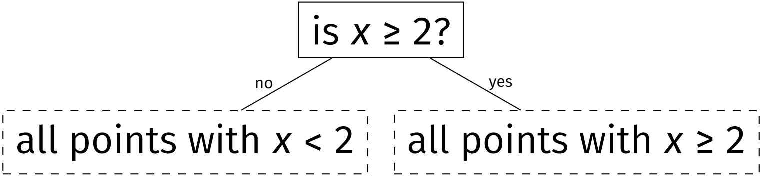
k-d Trees

k-d Trees

- **Binary search tree** for multidimensional data.
- Now: structure & properties.
- Next section: how to query them.
- Next next section: how to construct them.

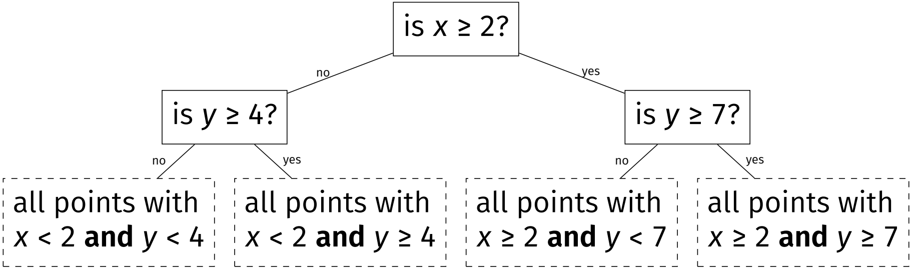
Internal Nodes

- Internal nodes are **threshold questions**.
  - can be of form $\boxed{x \geq 1?}$ or $\boxed{y \geq \tau?}$ in 2-d.
  - can be of form $\boxed{x \geq \tau?}$ or $\boxed{y \geq \tau?}$ or $\boxed{z \geq \tau?}$ in 3-d.
  - etc.



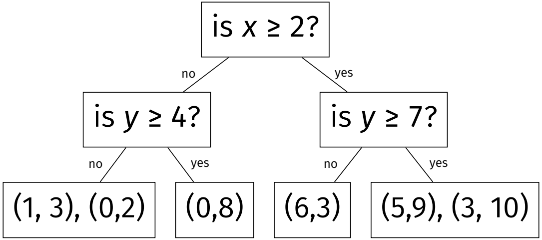
Internal Nodes

- A path forms a **conjunction**.



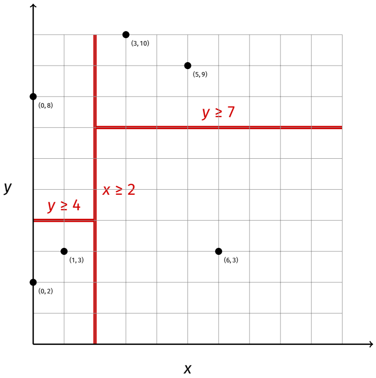
Leaf Nodes

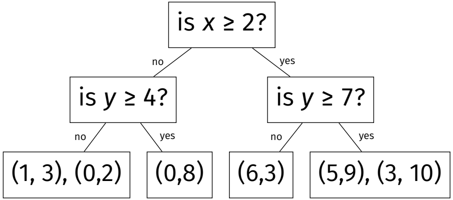
- Leaf nodes are (collections of) points.



Partitioning

- Each internal node **splits** space.





k-d Trees in Python

```python
from dataclasses import dataclass
from typing import Union, Optional
import numpy as np

@dataclass
class KDInternalNode:
    # the left and right children can be internal nodes
    # or numpy arrays of points (leaf nodes)
    left: Union['KDInternalNode', np.ndarray]
    right: Union['KDInternalNode', np.ndarray]

    # the threshold tau in the question
    threshold: float

    # the dimension used in the question
    dimension: int
```

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DATA STRUCTURES & ALGORITHMS

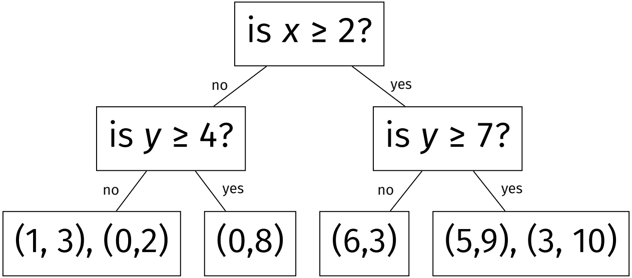
Queries on k-d Trees

Types of Queries

- Standard query:
  - Is $(1, 5)$ in the tree?
- Nearest neighbor query:
  - Return the nearest neighbor(s) of $(1, 5)$.

Standard Queries

- Is (6,3) in the tree? Is $(1, 5)$ in the tree?



Standard Queries

- Similar to BST query.
  - Recursively choose left/right by answering question.
  - Brute-force linear search on leaf (if needed).

- Takes $O(h)$ time, where h is height of the tree[2].

[2] Assuming each leaf has a bounded number of points.

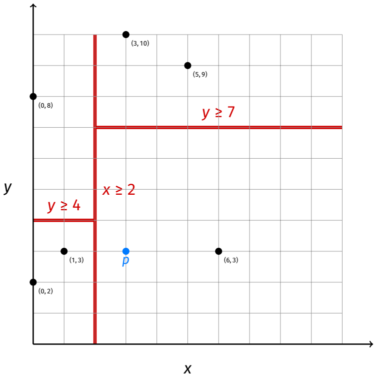
Nearest Neighbor Queries

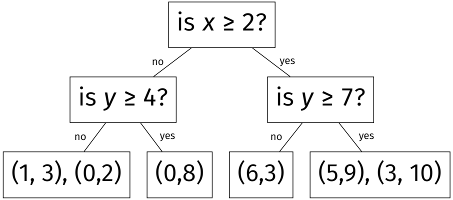
- Given query point $p = (x, y)$, find nearest neighbor in tree.

- Can we just do a standard query?
  - Find cell that *would* contain (x, y).
  - Return closest neighbor within that cell.

No

- Example: $p = (3, 3)$.





Main Idea

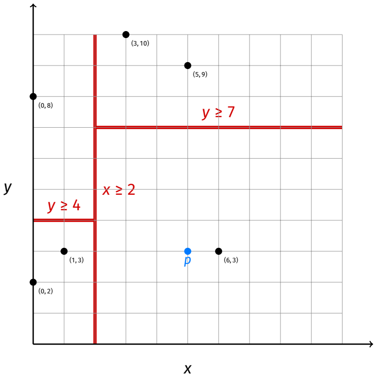
It is not sufficient to only check the cell that p *would* be placed in. You must also check neighboring cells (which can be very far away in the tree).

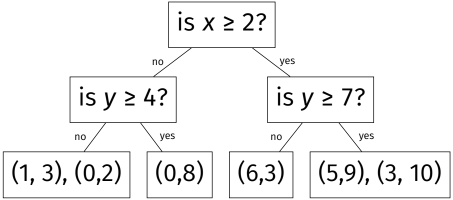
Brute Force?

- This suggests we need to traverse the whole tree.
- But we can actually do much better.
- Intuitively, some branches can be ruled out (**pruned**).

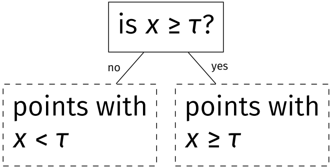
Example

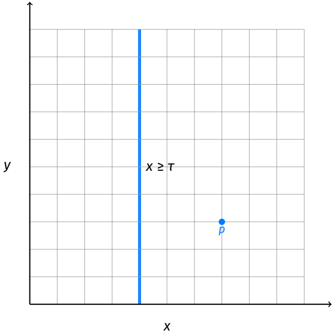
- Example: $p = (5, 3)$.





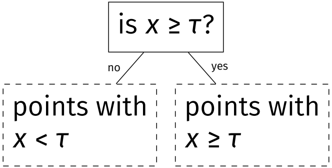
Bounding Branches

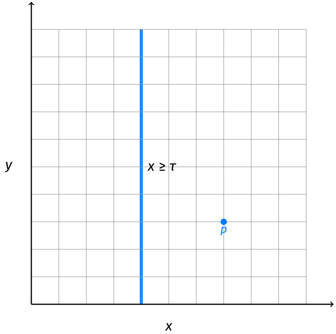




- **Observation**: let d_{bound} be distance from p to the boundary.
- Then the closest a point in the other branch can be to p is d_{bound}
- If we search and find a point whose distance to p is less than d_{bound}, **we do not need to search other branch**.

Bounding Branches





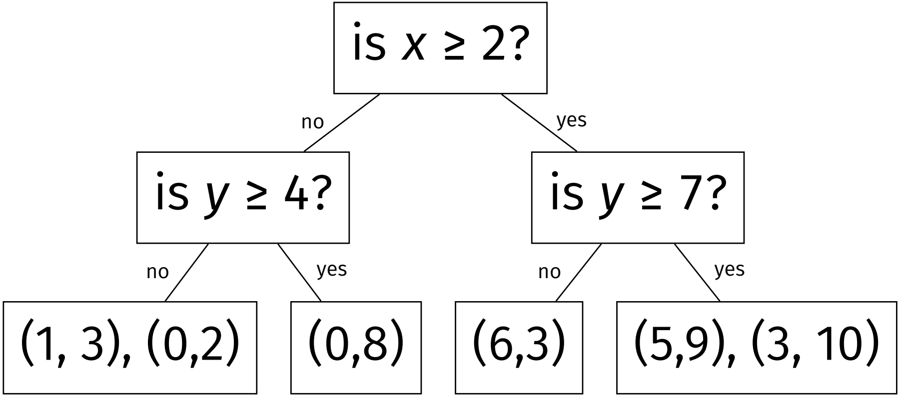
To query NN of (x, y):

- Search right branch first if $x \geq t$, otherwise search left branch first.
- Let d_{nn} be the distance from p to the closest point found.
- Let d_{bound} be the distance from p to boundary.
- Search other branch only if $d_{bound} < d_{nn}$.

Apply this idea recursively.

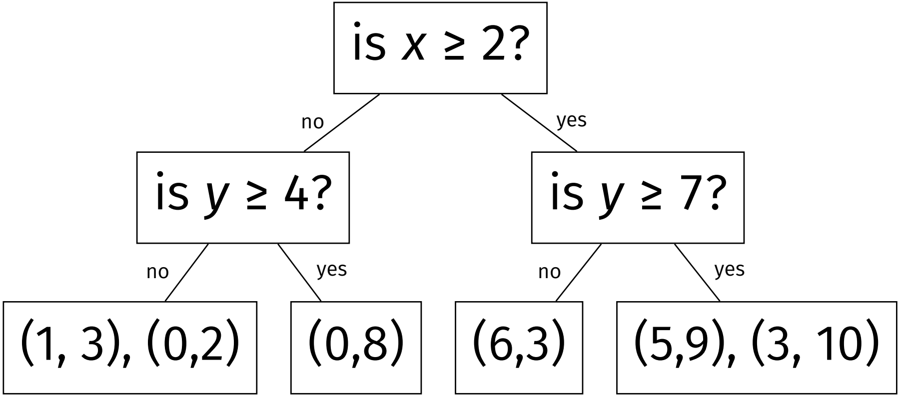
Example

- NN Query: $(5, 3)$



Example

- NN Query: $(3, 3)$



```python
def nn_query(node, p):
    if isinstance(node, np.ndarray):
        return brute_force_nn_search(node, p)
    else:
        # find the most likely branch
        if p[node.dimension] >= node.threshold:
            most_likely_branch, other_branch = node.right, node.left
        else:
            most_likely_branch, other_branch = node.left, node.right

        # compute distance to boundary
        distance_to_boundary = abs(p[node.dimension] - node.threshold)

        # find nn within most likely branch
        nn, nn_distance = nn_query(most_likely_branch, p)

        # check the other branch, but only if necessary
        if distance_to_boundary < nn_distance:
            nn_other, nn_other_distance = nn_query(other_branch, p)

            # check if the nn within this branch is closer
            if nn_other_distance < nn_distance:
                nn = nn_other
                nn_distance = nn_other_distance

        return nn, nn_distance
```

k-NN Search

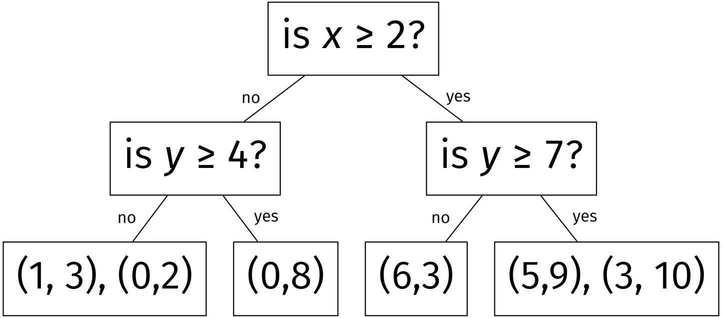
- Sometimes we want to find k nearest neighbors.
- Keep a max heap of best k so far.
- Check branch if distance to boundary < kth closest.

Analysis

- Assume each leaf has bounded number of points.
- Best case: $\Theta(h) \to \Theta(\log n)$ if balanced
- Worst case: $\Theta(n)$.
  - We may be unable to rule out many of the branches.
  - Can occur even if tree is balanced.
  - Especially if query point far from data.
- Note: balancing is difficult, but possible.

Example of Worst Case

- NN Query: $(20, 20)$
- Closest point is $(5, 9)$ at distance ≈ 19



Performance Degradation

- In small dimensions, NN lookup usually takes $\Theta(\log n)$.
- We'll see performance **degrades** to $\Theta(n)$ (brute force) as dimensionality $\to \infty$.
- **Curse of Dimensionality**

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DATA STRUCTURES & ALGORITHMS

Constructing k-d Trees

Construction

- **Given**: a set of n data points in $\mathbb{R}^d$
- **Construct**: a k-d tree containing these points.

Caveats

- There are many variations on k-d tree construction.
- We'll describe one popular approach.
- **Assumption**: **offline** construction.
  - Have all of the data at once (no insert/delete).

Idea

- Starting with n points, either:
  - make internal node by splitting ($x \geq \tau$?)
  - make leaf node containing the points
- Apply this strategy recursively.
- Questions:
  - Do we split, or do we make a leaf?
  - If we split:
    - What dimension to split on?
    - What threshold to use?

Q1: Do we split?

- Take parameter M (max leaf size).
- If $n < M$, don't split.
- **Reason**: For small n, brute force is actually faster (less overhead).

Q2: Which dimension to split on?

- Choose dimension with largest **spread**.
  - Difference between largest and smallest values.
  - Calculated using only points in **this** subtree.

- **Alternatively**: round-robin. Split x, y, z, x, y, ...

Q3: What threshold to use?

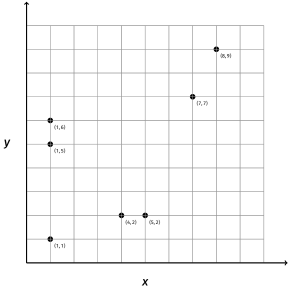
- Need threshold, τ.

- Use median value in splitting dimension.
  - Calculated using only points in **this** subtree.
  - Guaranteed to produce balanced tree.

- **Alternatively**: randomly-selected pivot, or median of random selection

Set $M = 2$, use median and spread for splitting. We start with data:

x	y
4	2
1	1
5	2
1	6
7	7
8	9
2	5



(1,1), (4,2), (5,2), (1,5), (1,6), (7,7), (8,9)

- Spread of x: 7
- Spread of y: 8
- Use y as splitting dimension.
- Median of y: 5.

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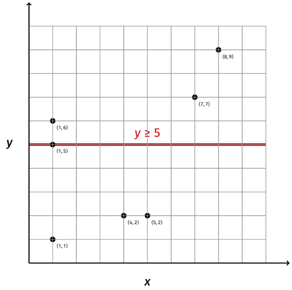
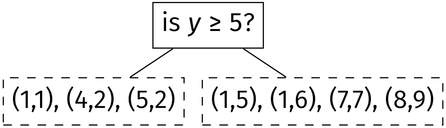
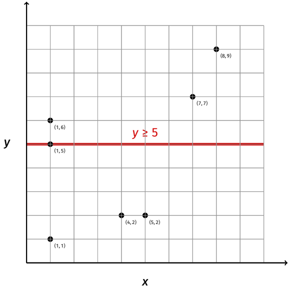
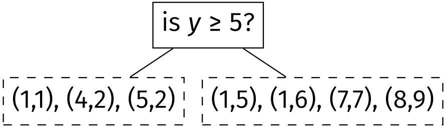




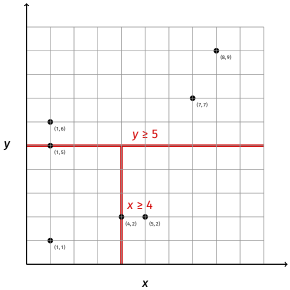


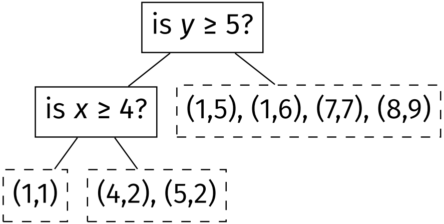


Recurse on left child. Data becomes:

x	y
4	2
1	1
5	2

- Spread of x: 4
- Spread of y: 1
- Use x as splitting dimension.
- Median of x: 4.





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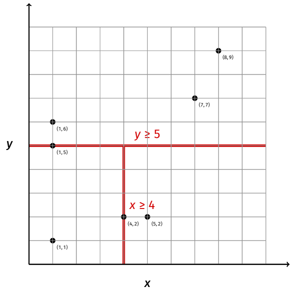
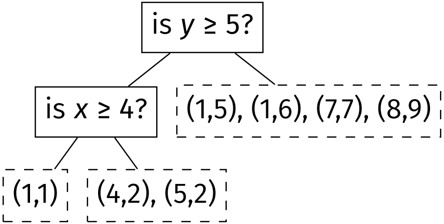
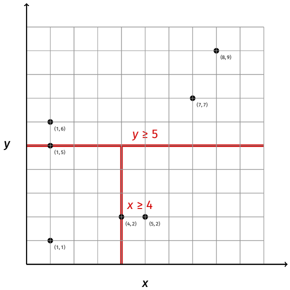
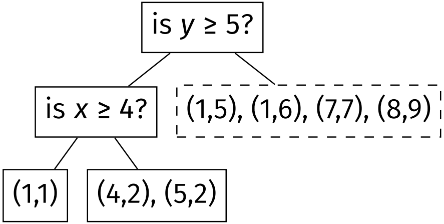




Recurse on children. Since size <= *M*, these become leaf nodes.





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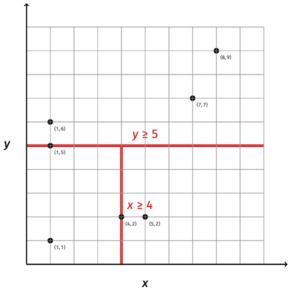
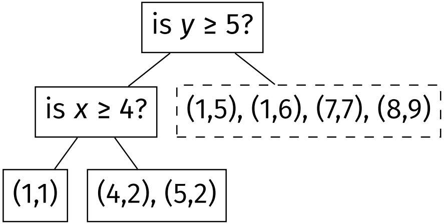
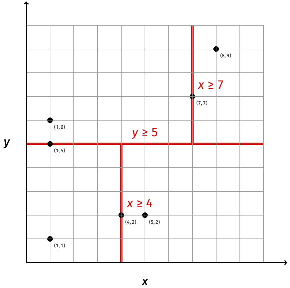


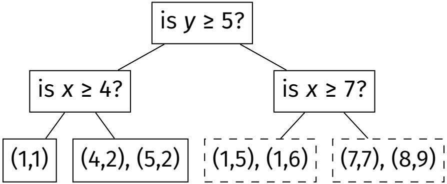


Unroll recursion, now recurse down right side of tree. Data becomes:

x	y
1	6
7	7
8	9
2	5

- Spread of x: 7
- Spread of y: 4
- Use x as splitting dimension.
- Median of x: 7 (or 2).





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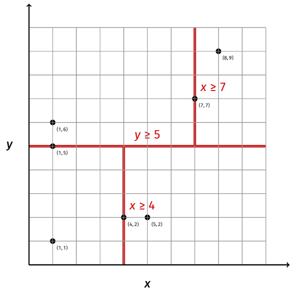
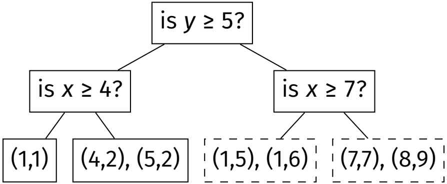
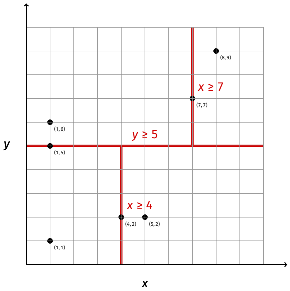
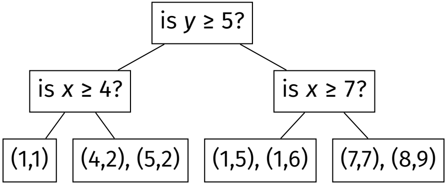




Make leaf nodes, since size ≤ M.





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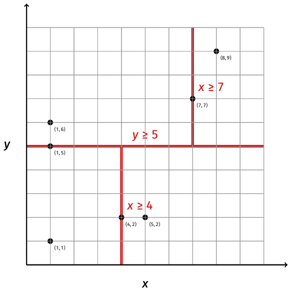
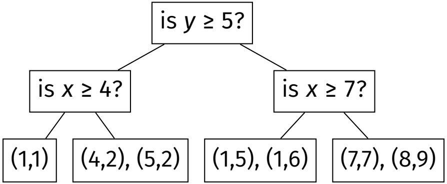




Tree complete!

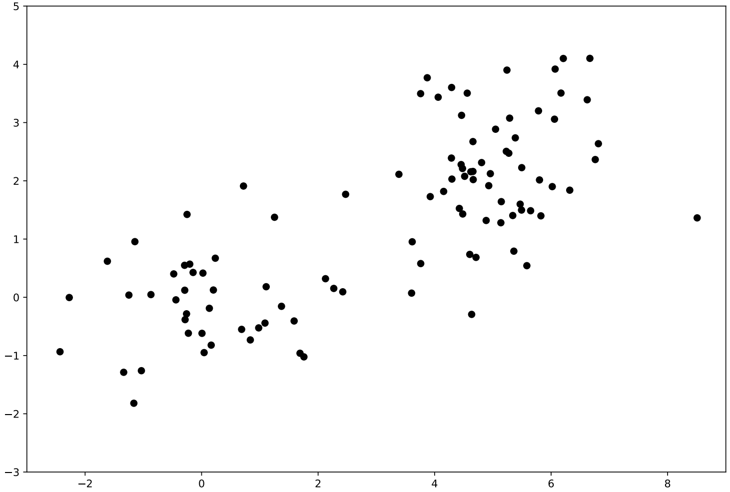
```python
def build_kd_tree(data, m=2):
    if len(data) <= m:
        return data

    # find the dimension with greatest spread
    spread = data.max(axis=0) - data.min(axis=0)
    splitting_dimension = np.argmax(spread)

    # find the median along this dimension
    median = np.median(data[:, splitting_dimension])

    # separate the data into new left and right sets
    # note that this isn't the most efficient since it will
    # produce a copy... better to do an in-place partition
    left_data = data[data[:, splitting_dimension] < median]
    right_data = data[data[:, splitting_dimension] >= median]

    left = build_kd_tree(left_data)
    right = build_kd_tree(right_data)

    return KDInternalNode(
        left=left, right=right, threshold=median,
        dimension=splitting_dimension
    )
```

Analysis

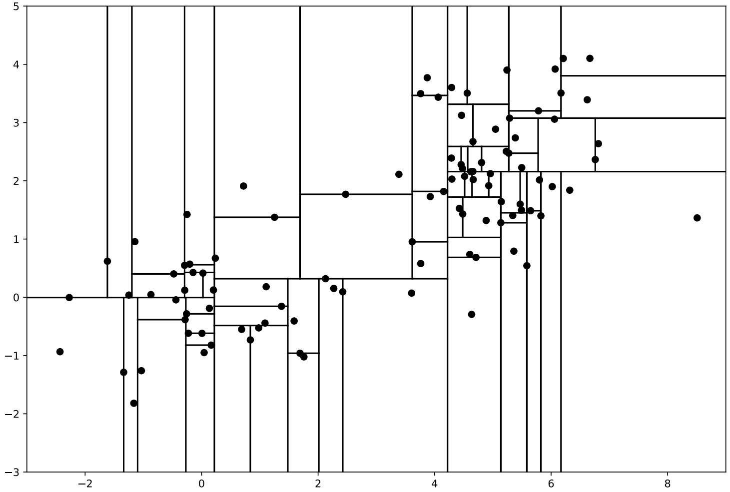
- $\Theta(k)$ to find median, perform copies, where k is number of points in subtree.
- Tree has $\Theta(\log n)$ levels (since it is balanced).
- Total time:

$$\underbrace{n}_{\text{level 1}} + \underbrace{(n/2 + n/2)}_{\text{level 2}} + \underbrace{(n/4 + n/4 + n/4 + n/4)}_{\text{level 3}} + \ldots = \Theta(n \log n)$$

Example



Example



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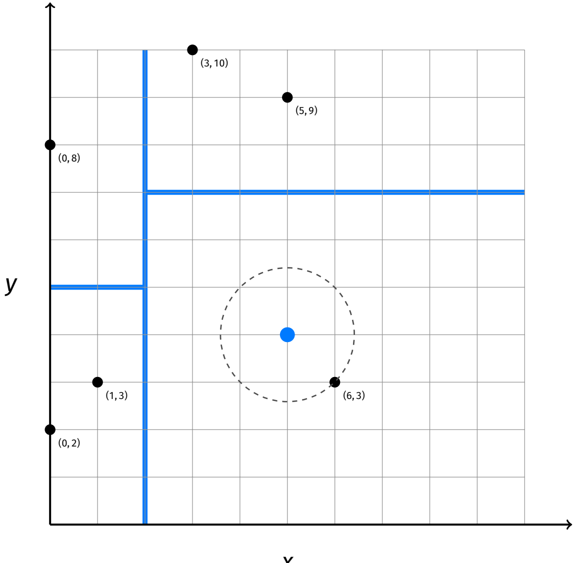
DATA STRUCTURES & ALGORITHMS

Curse of Dimensionality

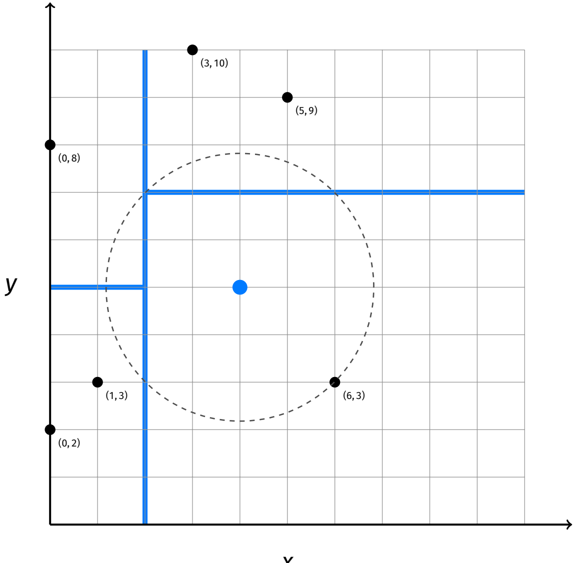
Performance Degradation

- Brute force NN search takes $\Theta(n)$ time.
- If dimensionality is small, k-d trees take $\Theta(\log n)$.
  - Great speedup!
- As dimensionality grows, performance **degrades**.
  - At worst, it is $\Theta(n)$.
  - Becomes just as bad as brute force!
- Why?

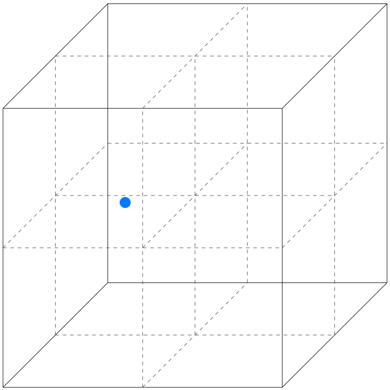
Explanation #1



Explanation #1



Explanation # 1

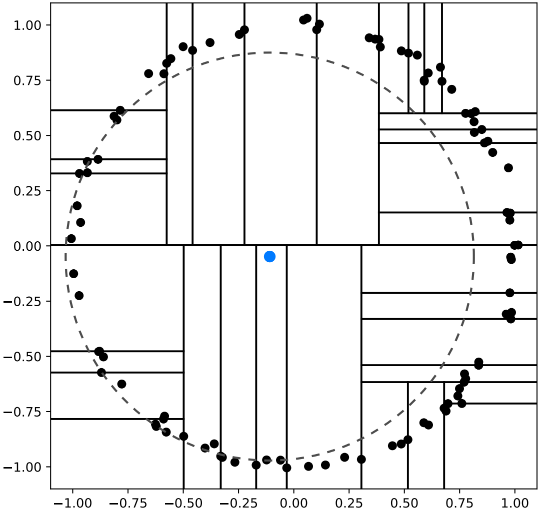


Main Idea

As d grows, the number of neighboring cells that we may need to check grows like 2^d.

Explanation #2

- We saw that if query point is far away, we cannot rule out branches.
- The reason? Distance from query to NN is not significantly different from distance between query and other points.


1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

Surprising Fact

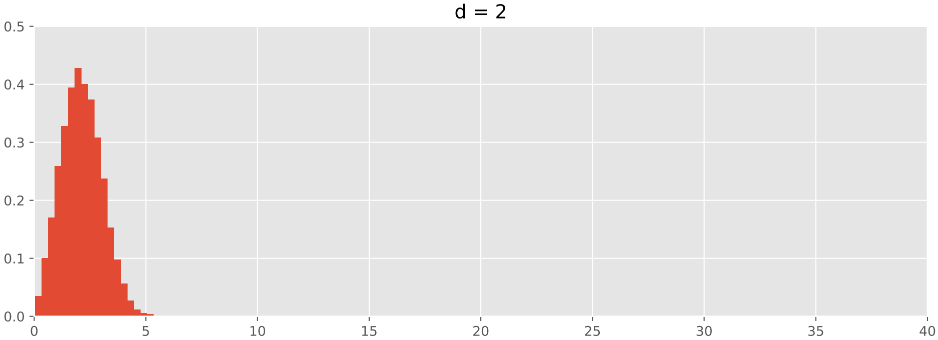
- In high dimensions[3], the ratio of the distance to nearest neighbor and distance to furthest neighbor $\to 1$.

[3] Under some assumptions on distribution of data.

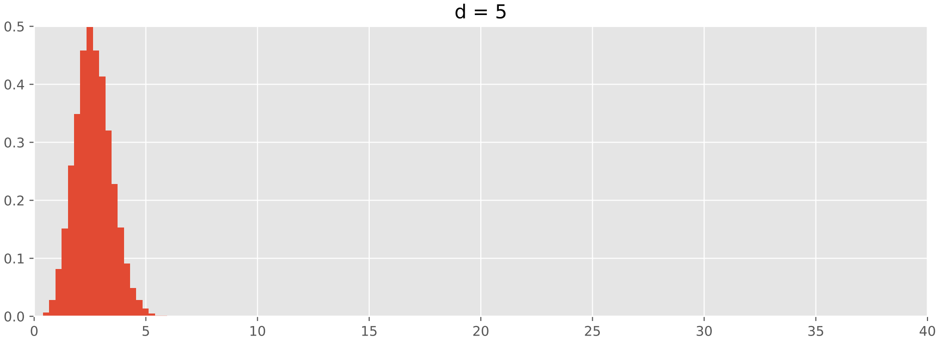
Experiment

- Generate random d-dimensional query vector from multivariate Gaussian.
- Generate 1000 d-dimensional data points from same Gaussian.
- Plot distribution of distances.

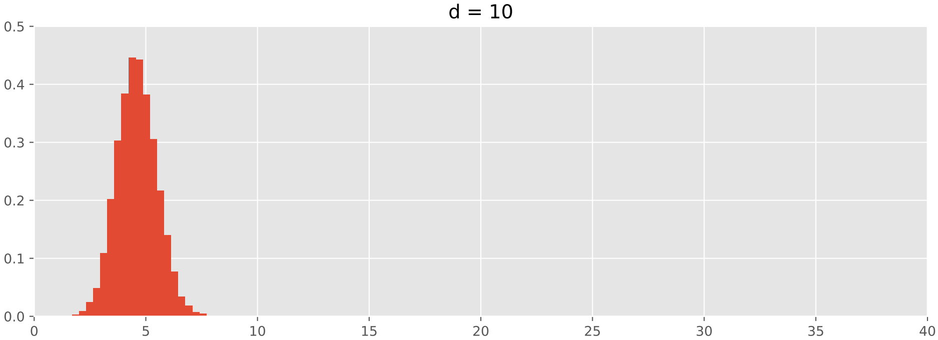
Experiment



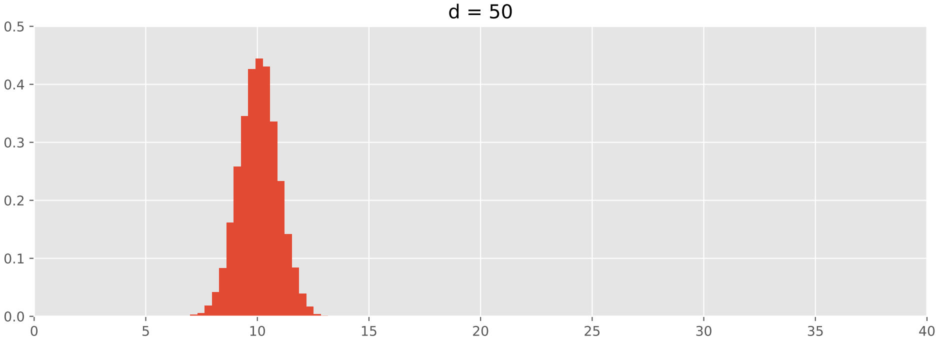
Experiment



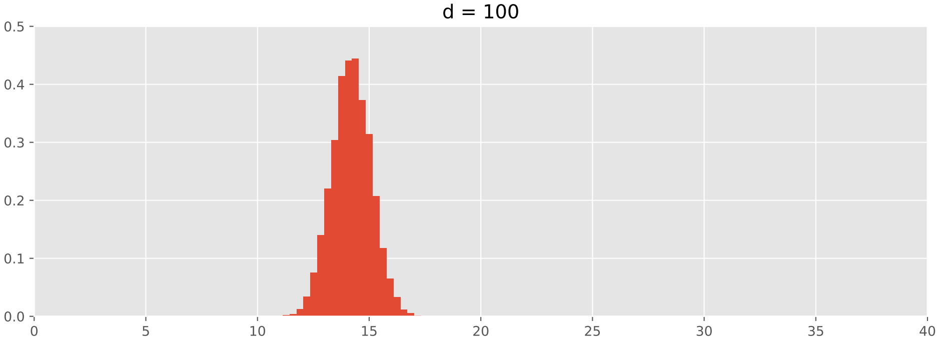
Experiment



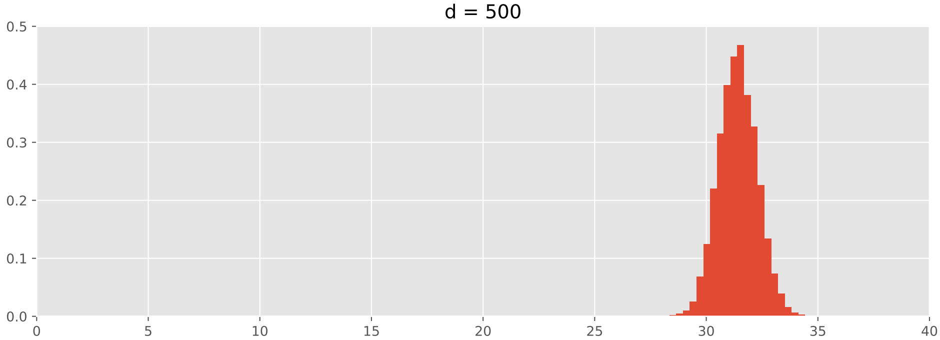
Experiment



Experiment



Experiment



Experiment

- Notice: width doesn't change, but center increases.

- So $\min = \max - \delta$, with δ constant.

$$\frac{\min}{\max} = 1 - \frac{\delta}{\max}$$

Explanation #2

- Every point in data set is approximately equidistant to query point.
- Can’t rule out branches.
- Have to perform a brute force search.

Main Idea

In high dimensions, every data point is approximately equidistant to the query point, meaning we can't rule out most branches.

Main Idea

Not only are k-d trees **inefficient** in high dimensions, Euclidean distance is **less meaningful** in high dimensions, and therefore so is the concept of NN search itself.

DSC 190

Data Structures & Algorithms

Approximate Nearest Neighbors

Why, exactly?

- Why do we need the **exact** NN?
- Often something close would do.
- Especially if not confident in distance measure.
  - As is the case in high dimensions.
- Maybe this can be done faster?

ANN

- **Given**: A set of points and a query point, p.
- **Return**: An **approximate nearest neighbor**.

k-D ANNs

- So far, our k-d trees find **exact** nearest neighbor.
- But there's a **very** simple way to do ANN query.
- Idea: prune more aggressively.

Before

- Let d_{nn} be distance from query point to best so far.
- Let d_{bound} be distance from query point to boundary.
- Search branch only if $d_{\text{bound}} < d_{\text{nn}}$.

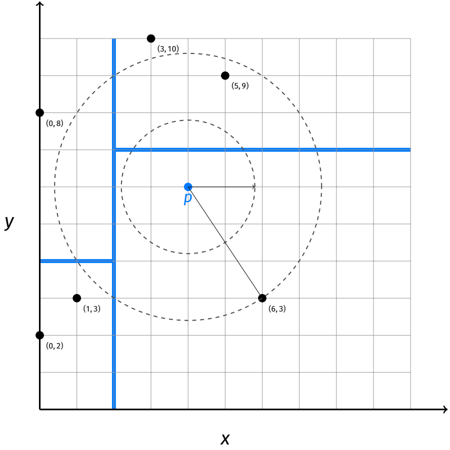
Now

- Take $\alpha \geq 1$ as a parameter.
- Search branch only if $d_{\text{bound}} < d_{\text{nn}}/\alpha$.
- **Idea**: make it easier to toss out branch.
- If $\alpha = 1$; exact search.
- If $\alpha > 1$; approximate, faster as α grows.

Theory

- Let q be exact NN, let q_{ann} be that found by this strategy.
- Then:

$$d(p, q_{\text{ann}}) \leq \alpha \cdot d(p, q)$$



Next Time

- ANNs via **Locality Sensitive Hashing**.