Scalable Nearest Neighbor Algorithms for High Dimensional Data

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https://qdata.github.io/deep2Read/

Roadmap

1. Background
2. Motivation
3. Scalable Nearest Neighbor Algorithms for High Dimensional Data
4. Results
5. Conclusion and Take-Aways

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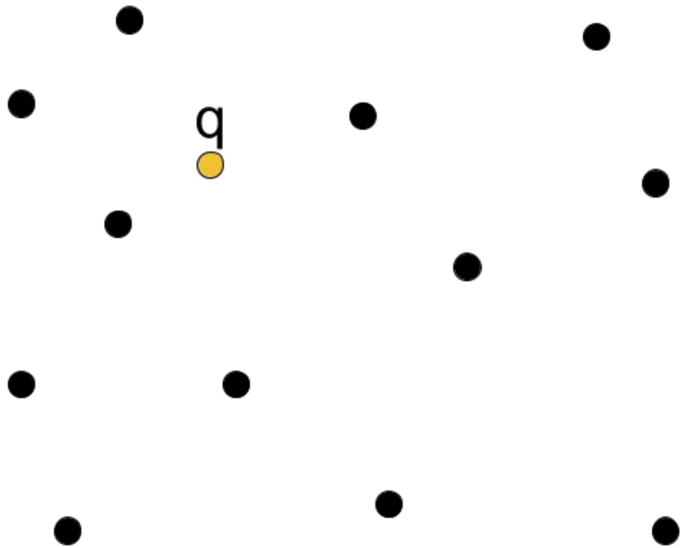
Nearest Neighbor Search



Input: Set of points P, d dimensions,
and query q

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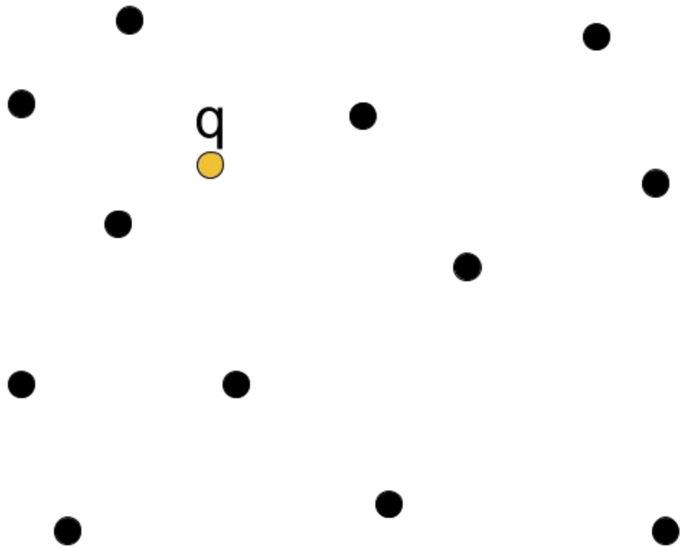

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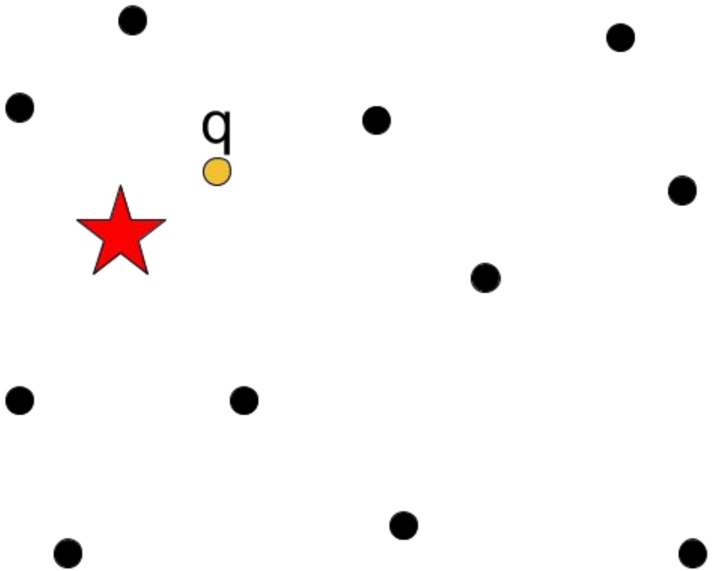

Output: Nearest neighbor p*

Exact Solutions

- Linear search: $O(nd)$, where $n = |P|$

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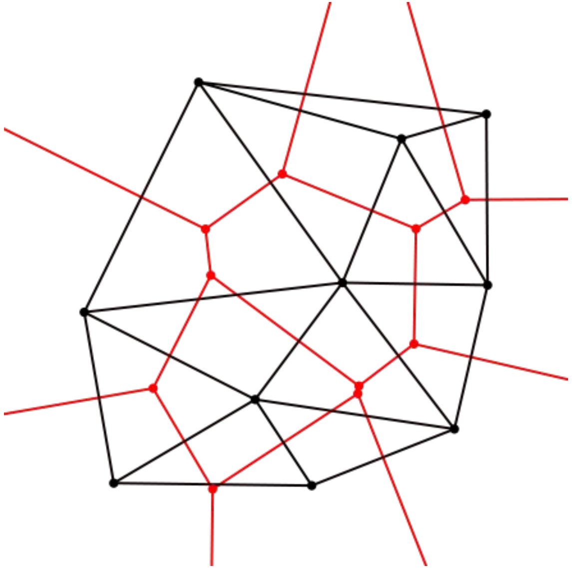

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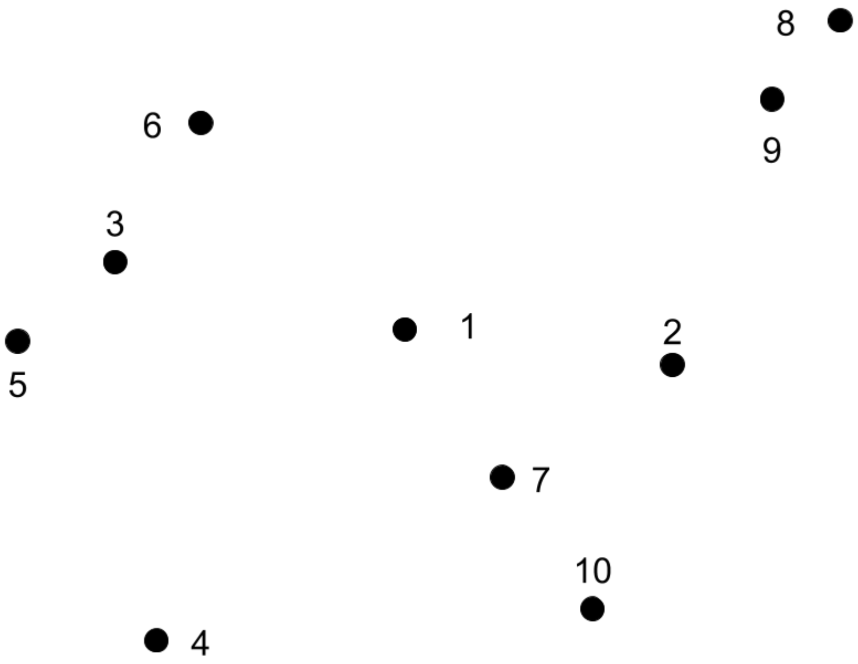
  - Ball trees (partition into hyperspheres)

Exact Solutions: kd-Trees



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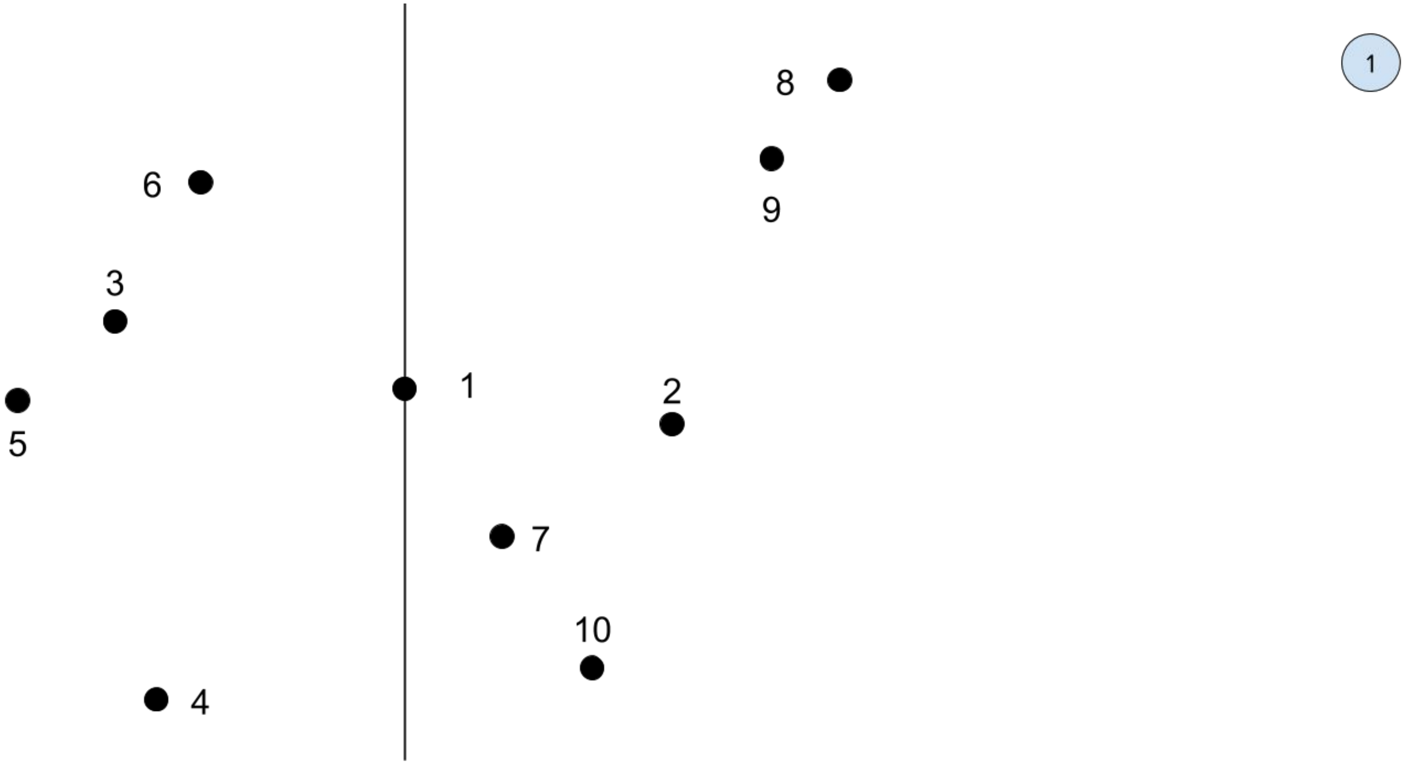

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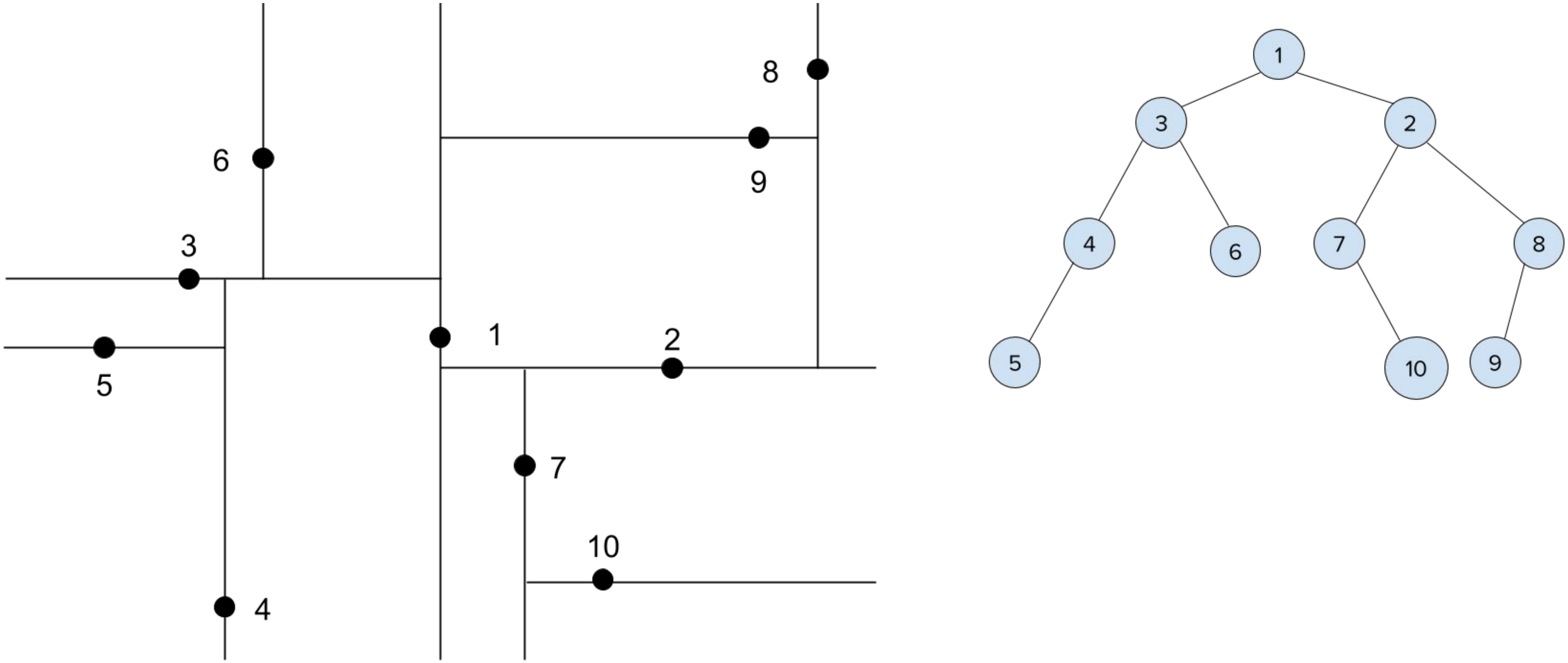

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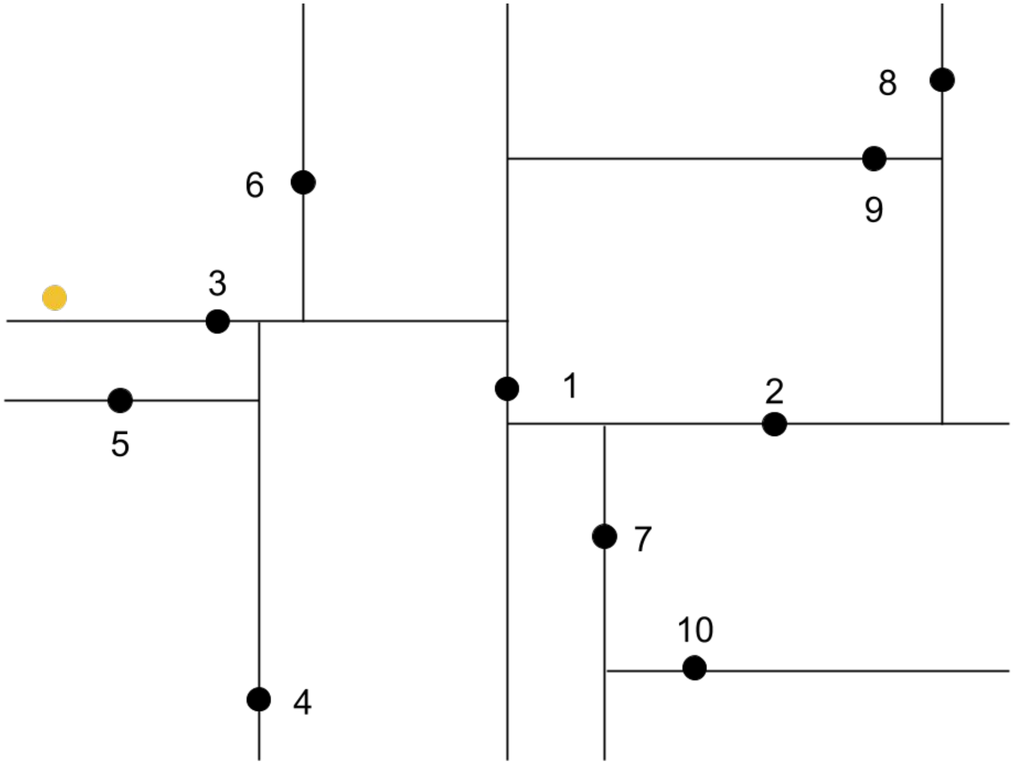
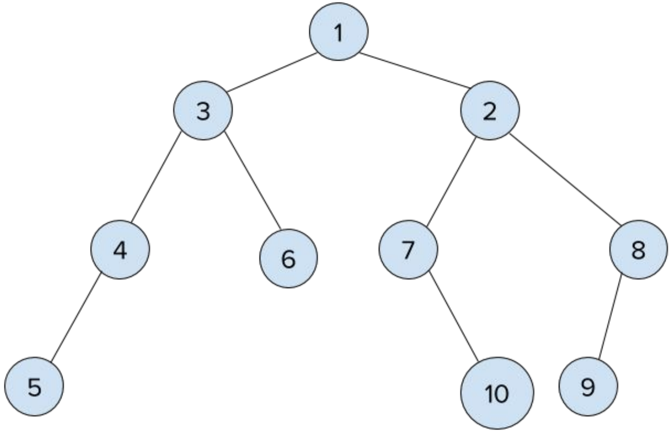
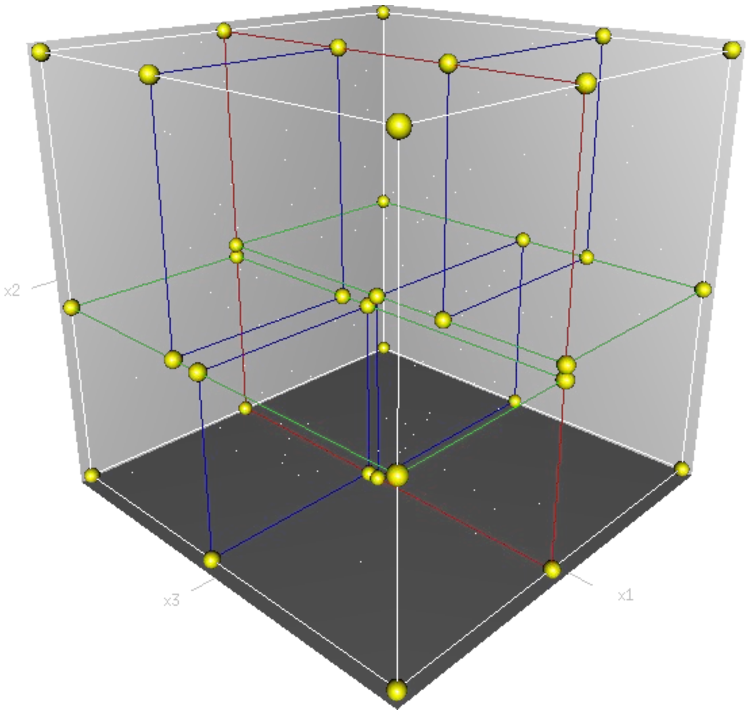




Exact Solutions: kd-Trees

- Linear once roughly d > 20



Approximate Nearest Neighbor (ANN)

1. Partitioning Trees (kd-Trees, etc.)
2. Locality Sensitive Hashing
3. Nearest Neighbor Graphs

Partitioning Trees

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- Randomized forests, with trees searched in parallel

Kd-Tree Random Forests

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- Mitigates tendency of tree search to become linear as d increases

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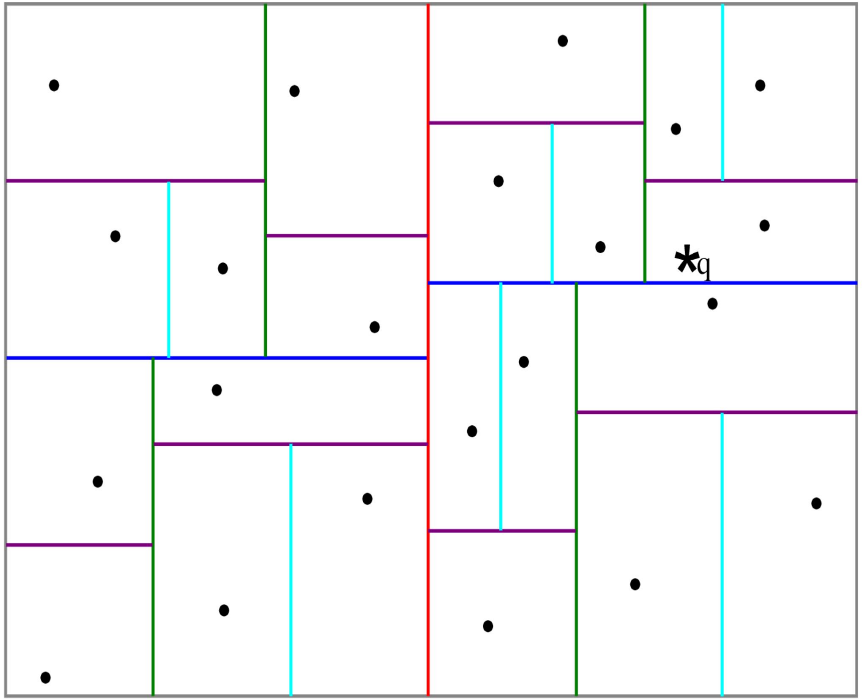

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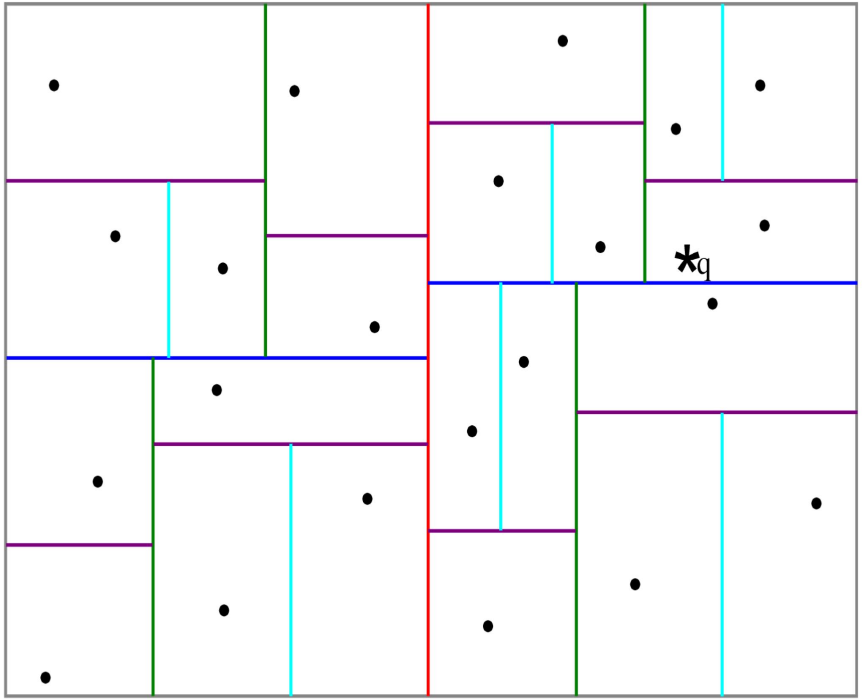
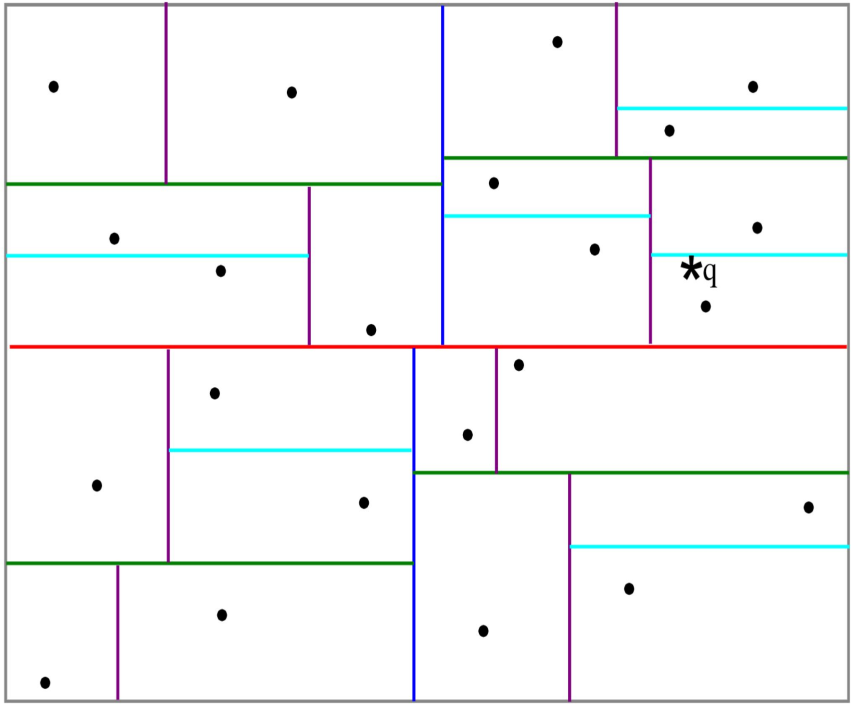
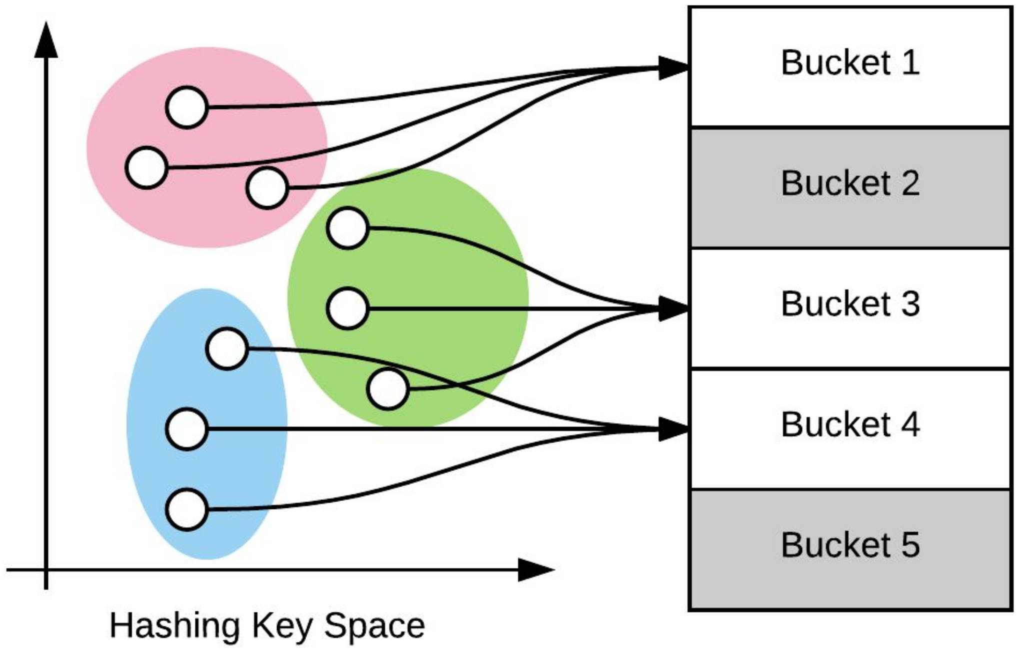
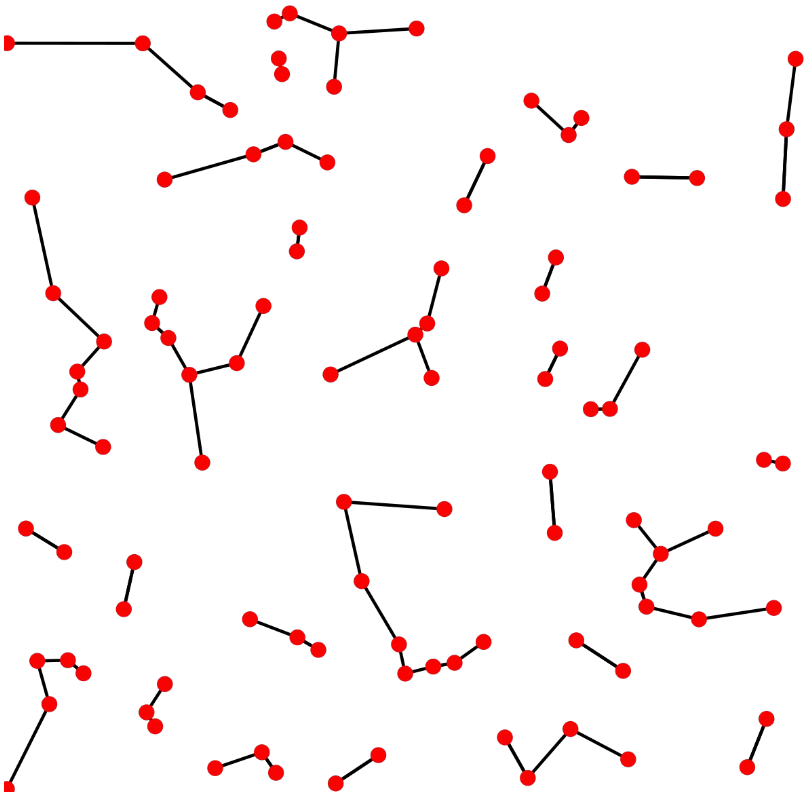




Locality Sensitive Hashing



Nearest Neighbor Graphs



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- Create an ANN library for C++: FLANN
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- Distributing ANN with compute clusters and map reduce

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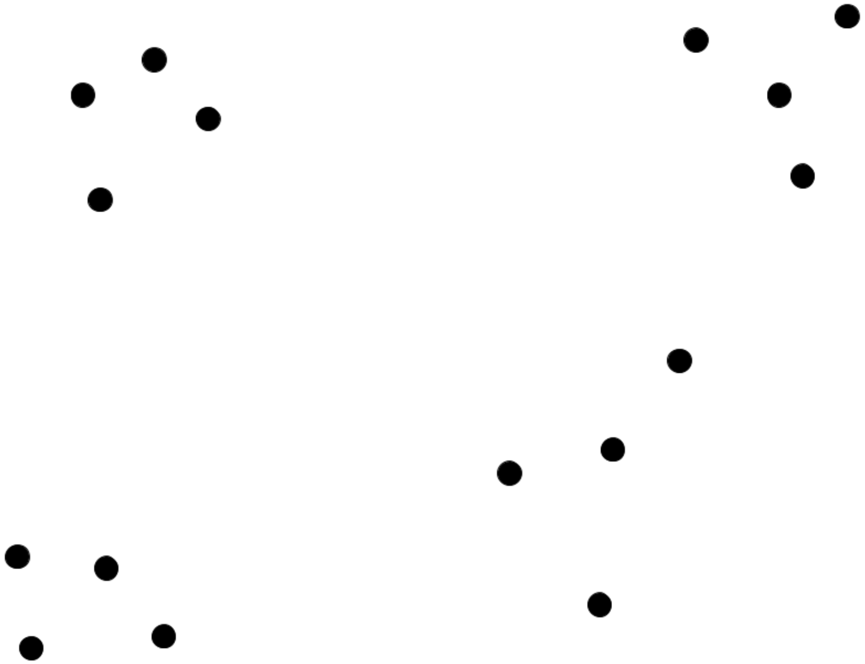
- Goal: better exploit distribution/structure of data points in P

Priority K-means Tree Construction



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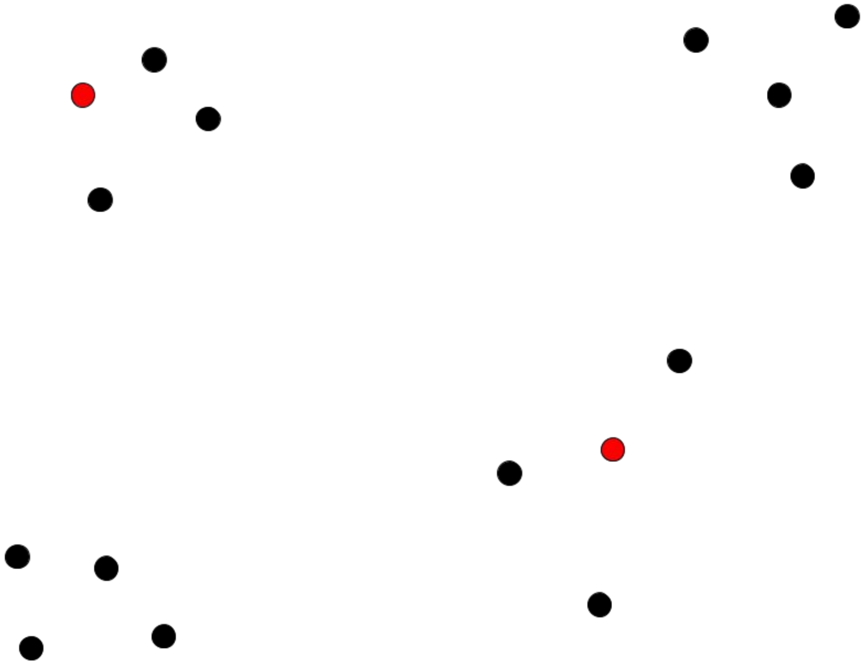

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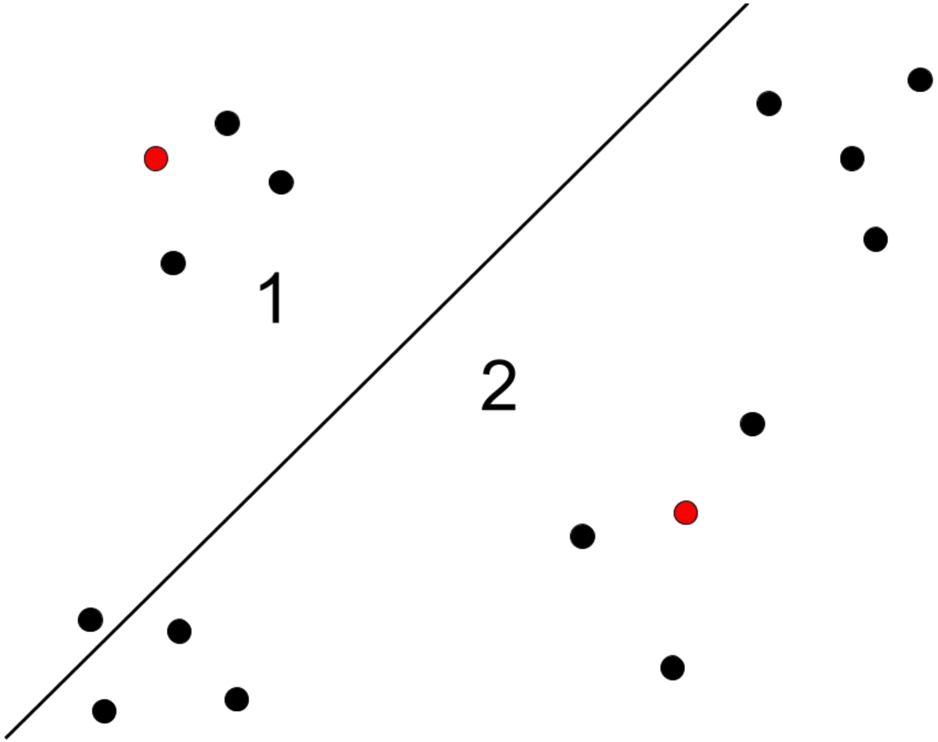

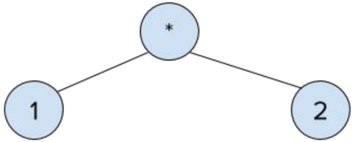

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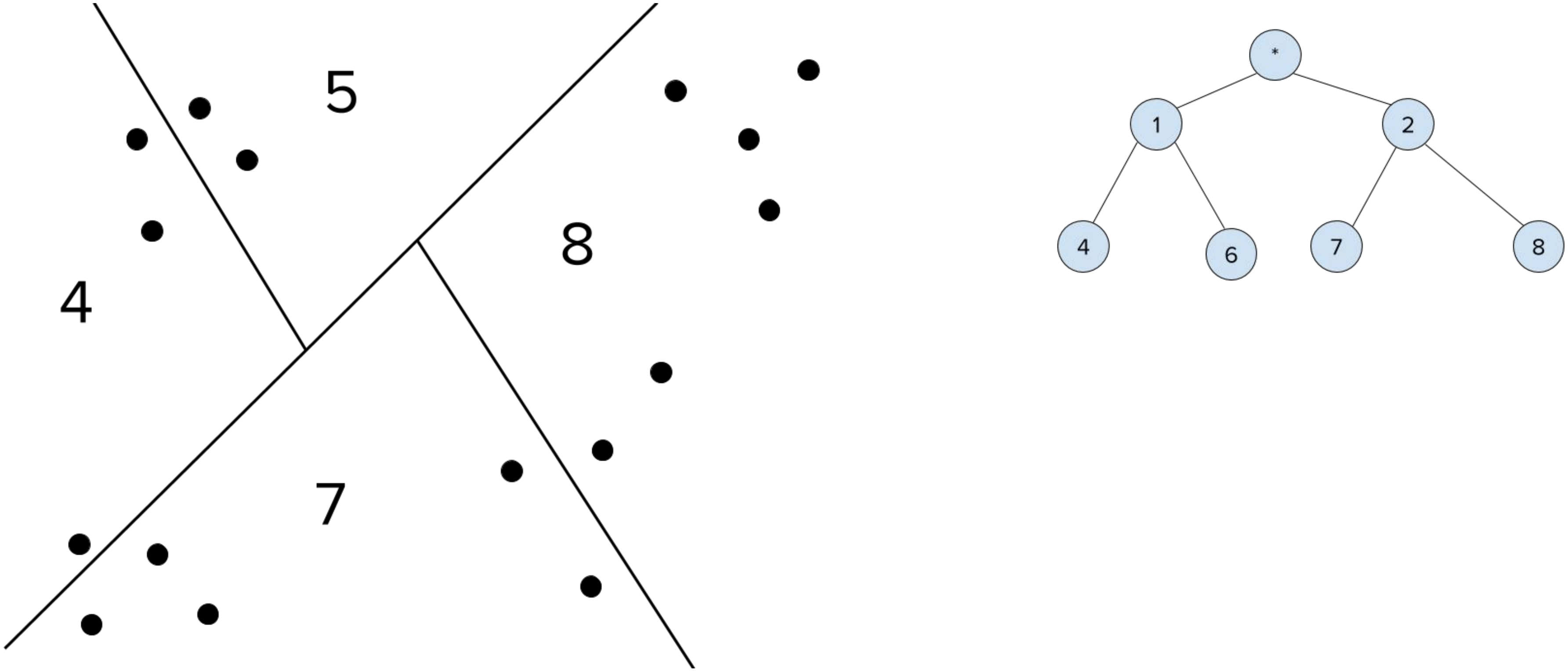

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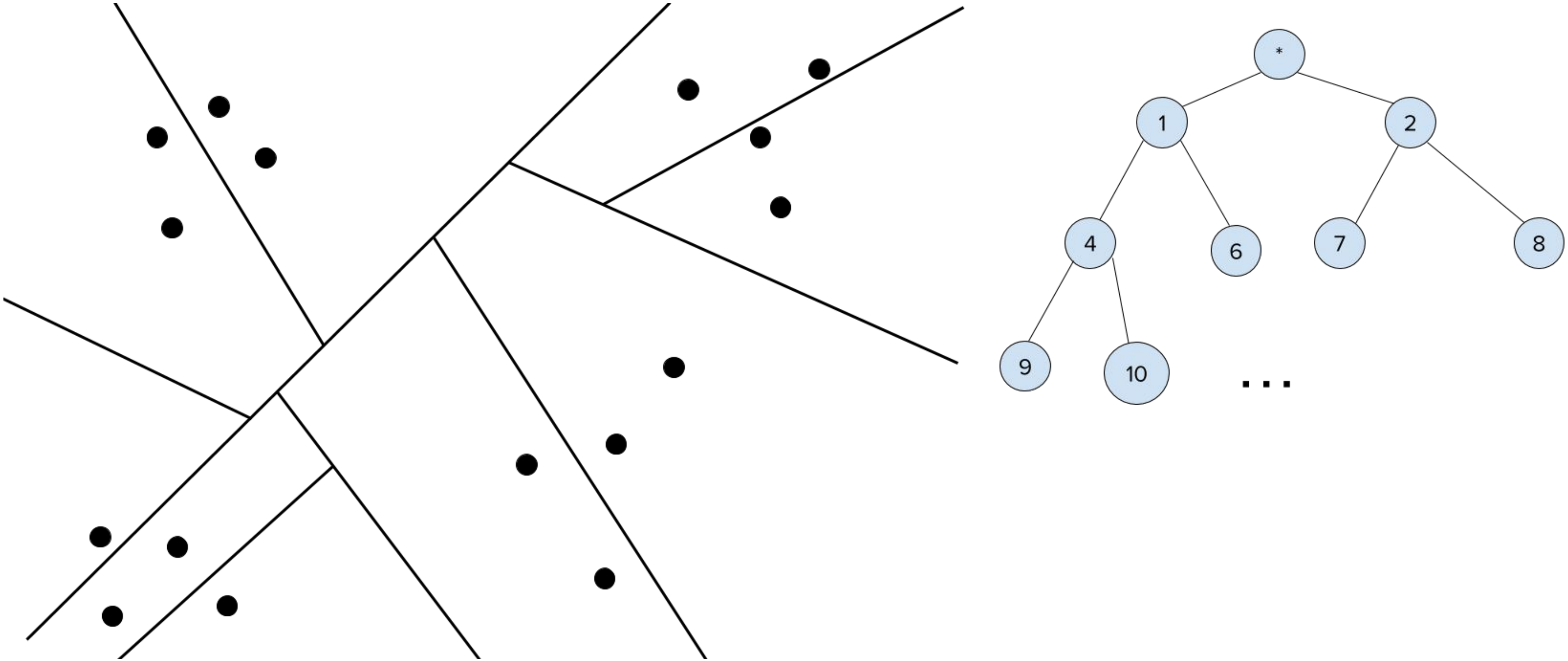
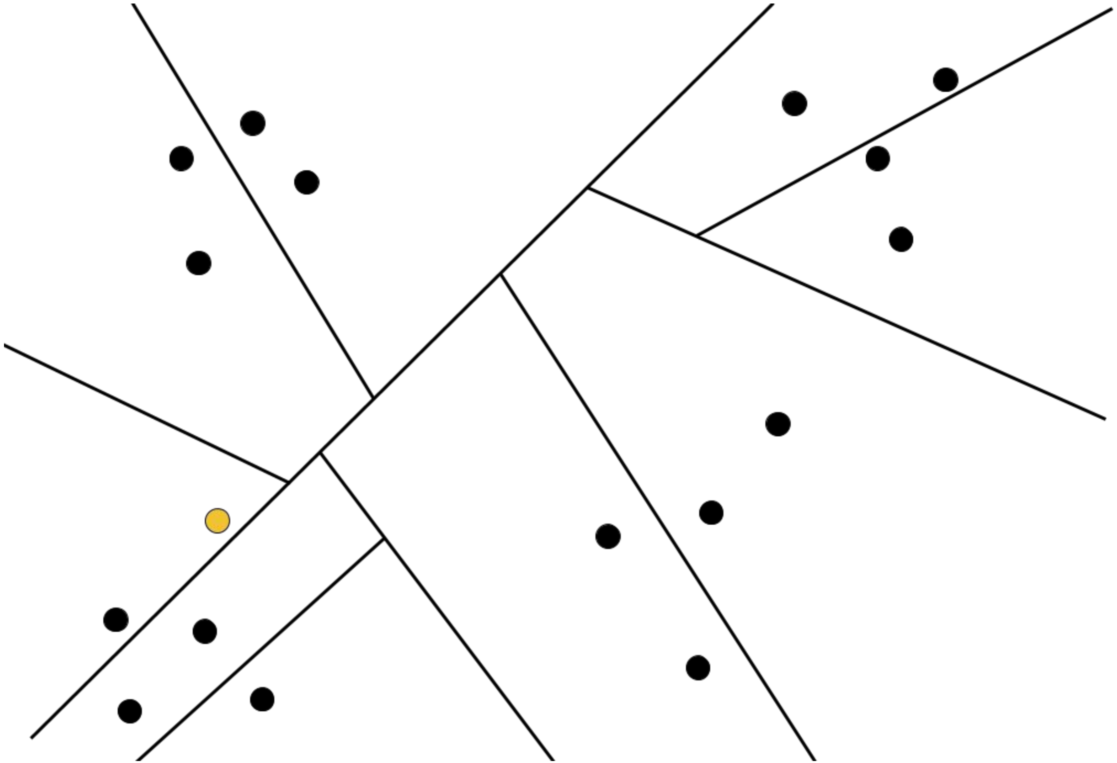
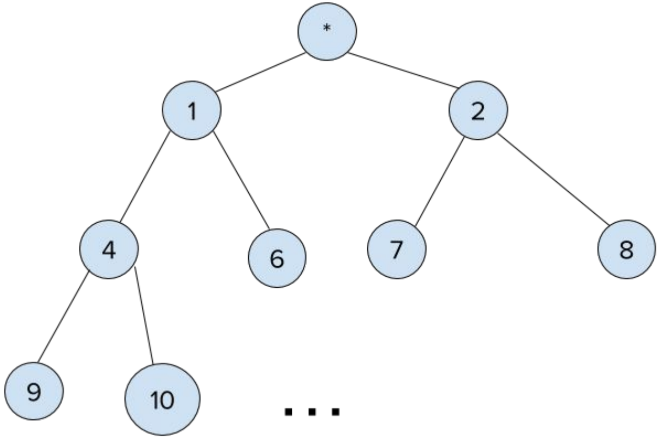


Priority K-means Tree Querying





Time Complexity

	Construction	Query
Randomized kd-tree	$O(ndK^*\log_k n)$	Expected $O(d\log n)$
Priority k-means tree	Single level: $O(ndKI)$ Total tree: $O(ndKI^*\log_k n)$, where I = max iterations for k-means clustering	At each level, finding closest centroid: $O(Kd)$ Traversal: $O(d\log_k n)$

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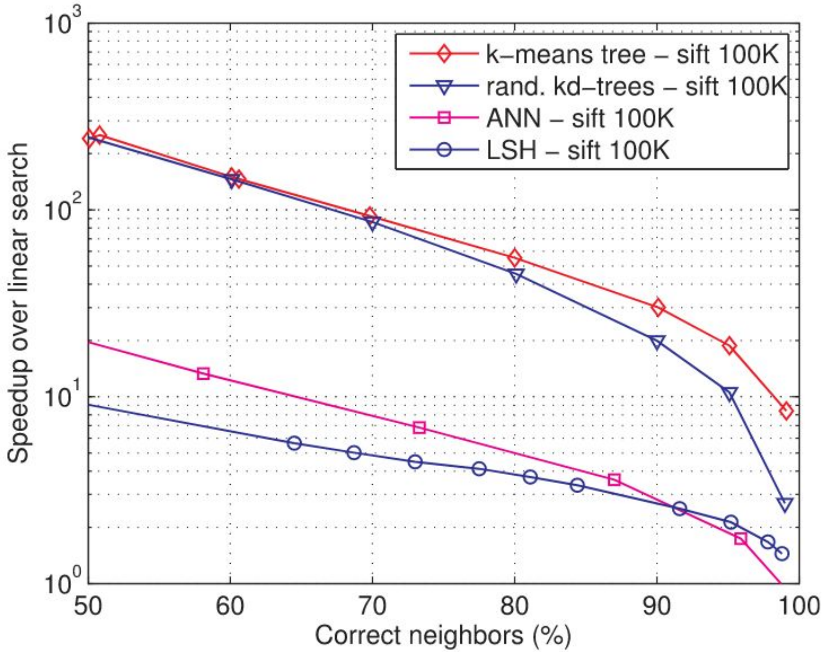
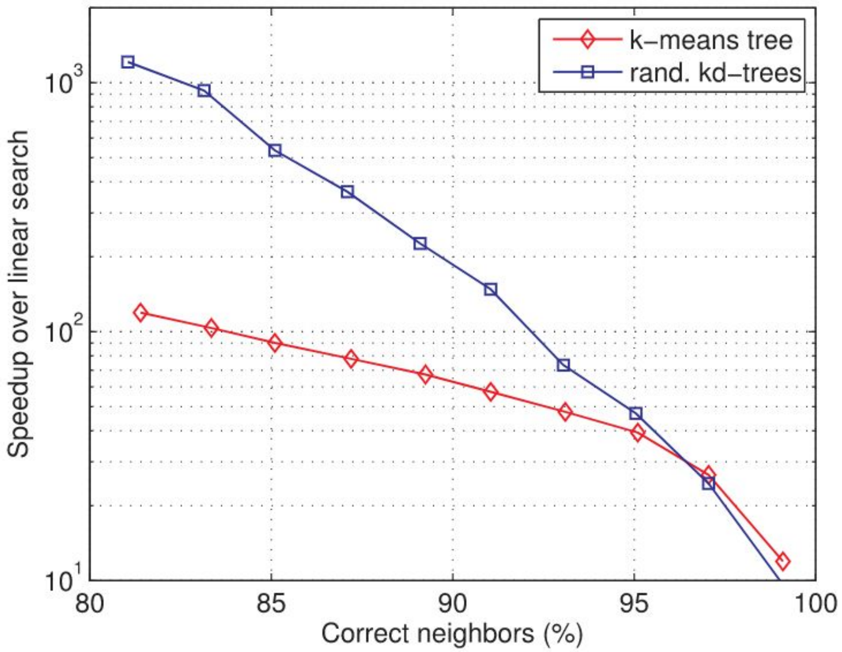


k–means tree – sift 100K
rand. kd–trees – sift 100K
ANN – sift 100K
LSH – sift 100K
Speedup over linear search
Correct neighbors (%)
10^0
10^1
10^2
10^3
50
60
70
80
90
100



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- Generally, search tree-based algos are the most scalable
- A lot of potential for LSH; difficult obtaining good hash functions
- Large scale ANN is a “big data” problem
    - Want good performance? Distribute with compute clusters and Map Reduce

FLANN

- Fast Library for Approximate Nearest Neighbor
- C++ source code
- Contains implementations of a bunch of nearest neighbor algos
- Included in the OpenCV package
- Very fast
- But has bugs, finicky, hard to use
- Annoy is more popular and is recommended by Radim Rehurek (Gensim creator)

Annoy

- Randomized forest of BSP-Trees
- Instead of splitting subsets based on a particular dimension it:
- Samples two points from the subset
- The boundary is chosen as the hyperplane equidistant from the two points
- Repeat the above k times (hyperparameter for making speed-precision tradeoffs)

What ANN Library Should We Use?

- See Gensim creator Radim Řehůřek's comparison
- FLANN is extremely fast (0.20-0.30 ms/query), but has bugs (reported 4 years ago but still unfixed), and is difficult to use
- Annoy is slower (6-7 ms/query), but much more usable; Radim declares it the “winner”
- LSH implementations (e.g., Yahoo, NearPy) very finicky; problem surrounding finding good hash functions; very low recall (~2 approx nearest neighbors per query)
- Important note: embedding spaces have clusters and
- ⇒ Trying out Annoy for the time being

Spotify