## Outline

- Introduction
- Exact Query Processing
- Approximate Query Processing
- Selectivity Estimation
- Open Problems

# Approximate Query Processing

- Space Partitioning-based
  - Tree
  - Encoding
  - Locality Sensitive Hashing
- Graph-based Methods

#### Notes:

- Recent works mainly in the Database area
- Prefer ease of exposition over rigor
- Categorization is not fixed/unique

# Space Partitioning-based

- Partition the whole space into partitions that cover the whole space
- Further divided into 3 sub-categories:
  - Tree-based
  - Encoding-based
  - Locality sensitive hashing-based

#### **Tree-based**

- Hierarchically partition the whole space into partitions that covers the whole space
- A natural idea in low-dimensional space
  - disjoint: kd-tree



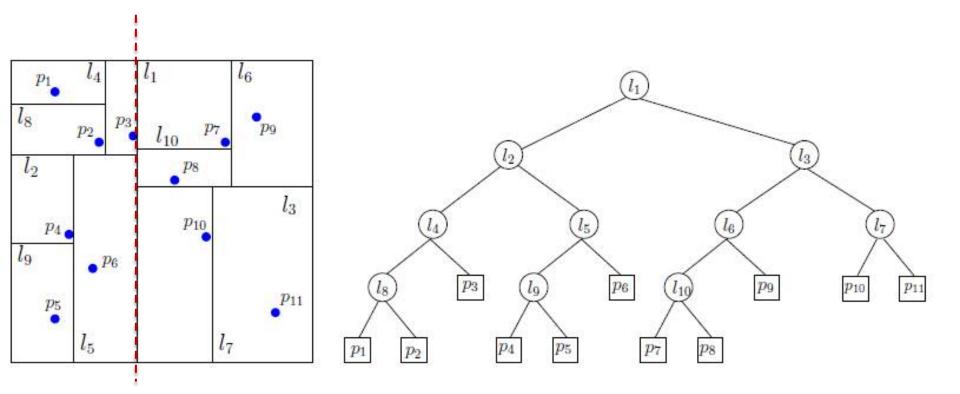
Randomized kd-trees and variants

overlapping: R-tree

M-tree, Cover Tree, Spill tree

Problem: Non-trivial modification needed to handle high-dimensional data

# kd-tree Examples (low dimensional space)



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# Step 1

- Mapping
  - Random top-k dimensions: Randomized kd-tree
  - PCA: PCA-tree
  - Random Rotation: NKD-Tree
  - Optimized Sparse Rotation: TP-Tree
  - Random Projection: RP-Tree

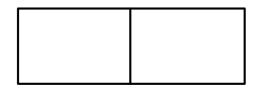
Main idea: maximize the variance before the split

# Step 2

#### Split

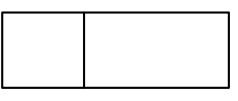
- Dim 1
  - Median split: (randomized) KD-tree, PCA-tree, ...
  - Perturbed split: RP-tree
  - Overlapping split: Spill Tree [DS15]
    - Virtual spill tree: "Spill" at query time
- **Dim 2:** 
  - Linear split
  - Non-linear split: [DIRW20]

median split



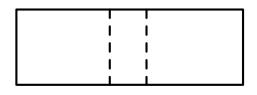


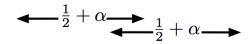
perturbed split



 $-\beta \rightarrow -1 - \beta -$ 

overlapping split



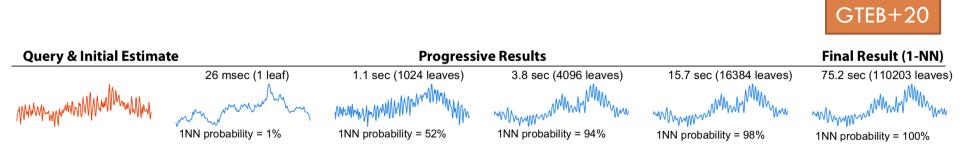


# Steps 3 & 4

#### Optional) Tree → Forest

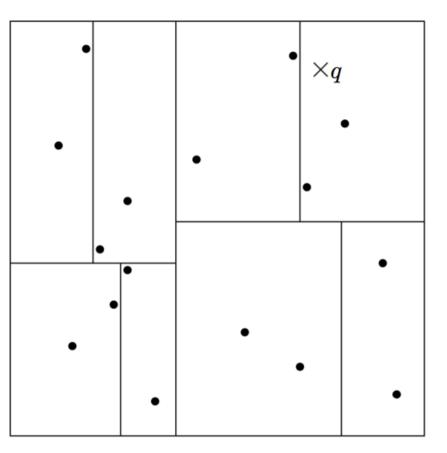
Can be applied to all kinds of trees

- Can use best-first search to coordinate the searches
- When to stop?
  - Guaranteed NN found
  - Bounded cost
  - Judged by a prediction model [LZAH20, GTEB+20]

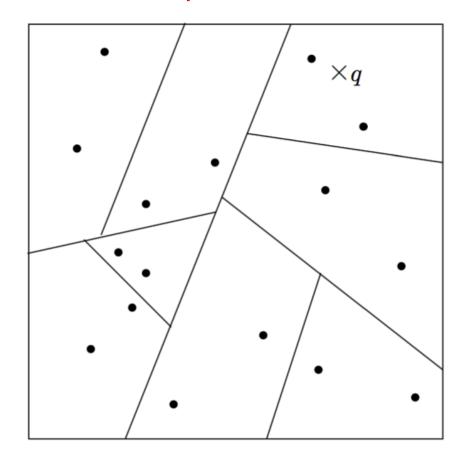


## **RP-tree Example**

#### kd-tree

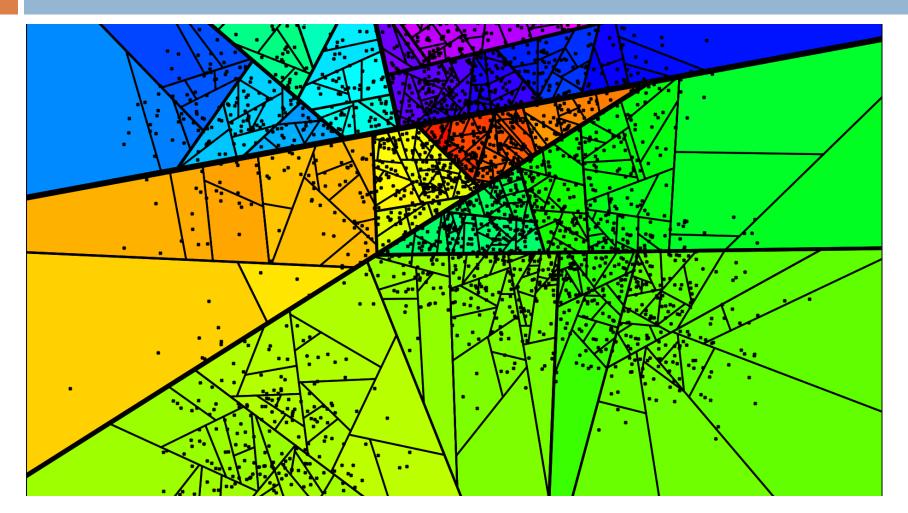


#### rp-tree



## Annoy Example





Erik Bernhardsson, "Approximate nearest neighbor methods and vector models", 2015

# Trees with Overlapping Partitions

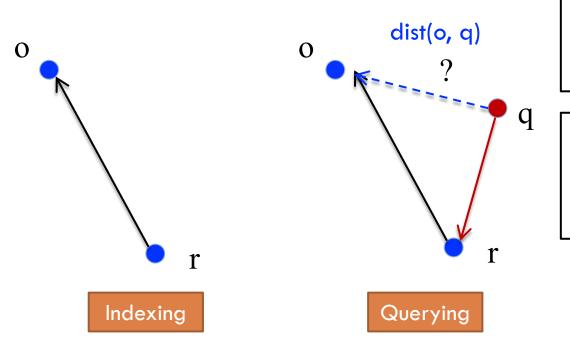
- Based on the metric property
  - (M)VP-tree, M-tree
- Based on intrinsic dimensionality
  - Cover Tree
- □ "Spill"
  - Spill for data: Spill Tree
  - Spill for query: Virtual Spill Tree

Able to index objects in a non-Euclidean space

## **Metric Property**

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- Inference on the lower & upper bound of dist(u, v)
  - Triangular inequality
  - Ptolemaic inequality



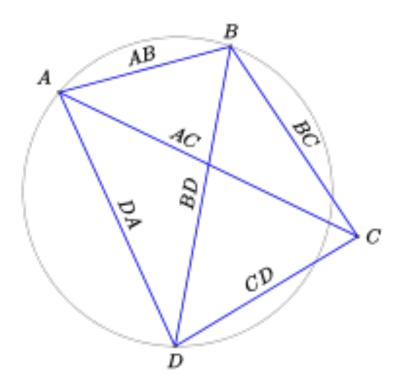
Triangular inequality:

 Lower and upper bounds of dist(o, q)

#### c.f., LSH (later)

 gives the full distribution of dist(o, q)

## **Ptolemaic inequality**



#### $\overline{AB} \cdot \overline{CD} + \overline{BC} \cdot \overline{DA} \geq \overline{AC} \cdot \overline{BD}$

https://en.wikipedia.org/wiki/Ptolemy%27s\_inequality

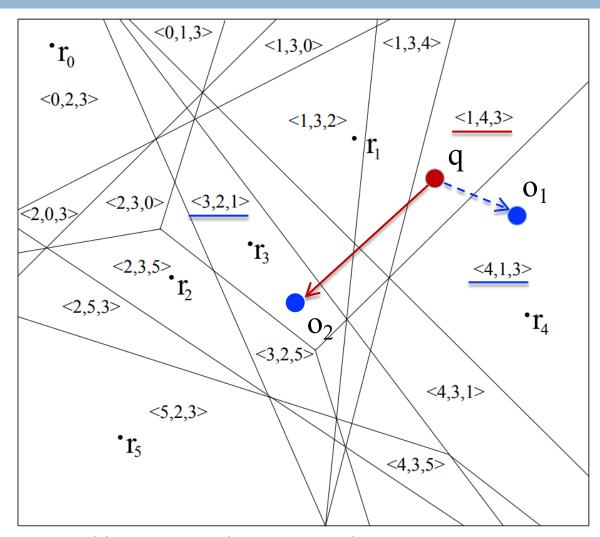
#### Variants

#### Reference points

- All DB objects: AESA
- Many work/heuristics to select a good subset
- [Diversion] Use rank() instead of dist() of reference points
  - Permutation index [NBN16, ...]
  - **dist**(v, v) is small  $\rightarrow d(perm(v), perm(v))$  is also small

#### **PP-Index**

#### Order-3 Voronoi Diagram

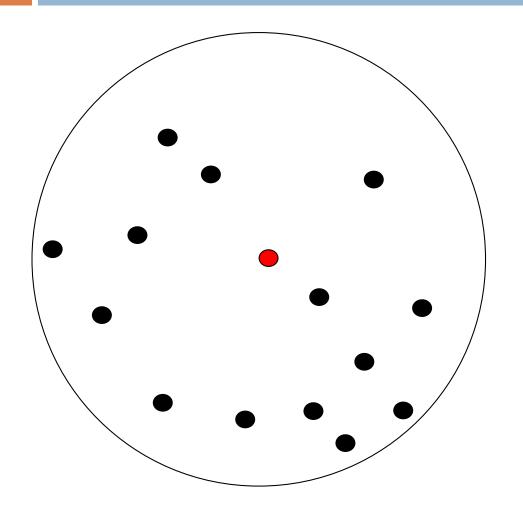


http://www.esuli.it/publications/PP-Index-slides.pdf

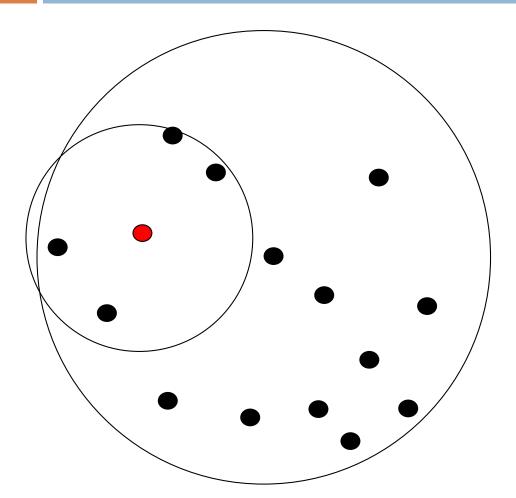
## Intrinsic Dimensionality

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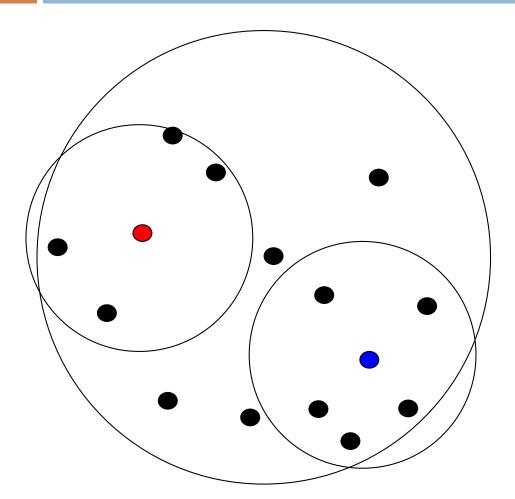
- One of the metrics is Expansion Constant
  - □ Smallest c such that  $|Ball(z, 2R)| \le c^* |Ball(z, R)|, \forall z$
- Cover Tree
  - O(n) space
  - O(c<sup>6</sup> \* nlog(n)) construction and update time
  - O(c<sup>12</sup> \* #log(n)) exact NN query time
  - $\label{eq:constraint} \square c^{O(1)} \log \Delta + (1/\epsilon)^{O(\log c)} \quad \textit{$\mathcal{E}$-NN query}$ 
    - Δ (aspect ratio): ratio between largest and smallest interpoint distance



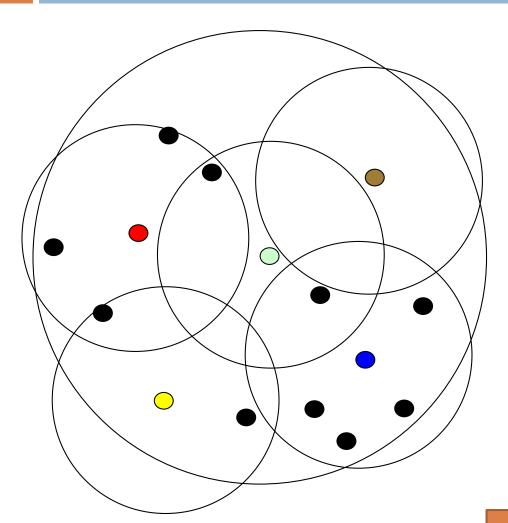
A node covered
 by a pivot data
 point (red) with
 radius R



Cover the points
 using a child pivot
 with radius R/2



 Repeat by picking the child pivot outside the previous covers



#### □ Nesting

- C<sup>(i)</sup>: C<sup>(i-1)</sup> U black nodes
- C<sup>(i-1)</sup>: colored nodes
- Covering
  - **dist**( $u^{(i)}$ ,  $v^{(i-1)}$ )  $\leq 2^{i}$
- Separation
  - **dist(** $u^{(i-1)}$ ,  $v^{(i-1)}$ )  $\geq 2^{i}$

fan-out of any node  $\leq c^4$ 

## **Encoding-based**

- Learning to hash
- Product Quantization
- Hierarchical k-means

# Learning to Hash

#### 🗆 Idea:

- Embed R<sup>d</sup> to a k-dimensional Hamming cube while minimizing some objective function (neighborhood preservation or distance distortion)
  - $\mathbf{x}_{i} \in \mathbb{R}^{d} \rightarrow z_{i} \in \{0, 1\}^{k}$

E.g., Spectral hashing:

**D** Minimize  $\sum_{ij} W_{ij} \|z_i - z_j\|$ 

 $\rightarrow$  Partition the space into 2<sup>k</sup> regions

Minimize avg Hamming distance between neighboring points

and other conditions (max utilization of bits + uncorrelatedness)

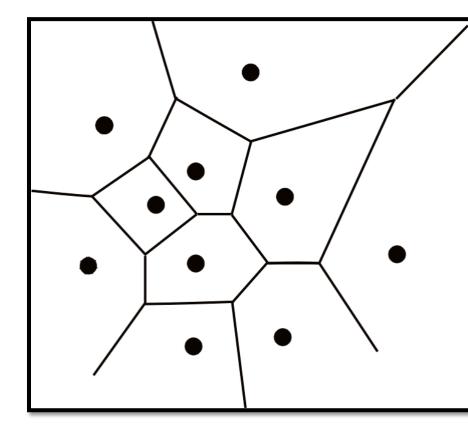
• Where 
$$W_{ij} = \exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / \varepsilon^2)$$

Many other variants

c.f., https://learning2hash.github.io\_and https://cs.nju.edu.cn/lwj/L2H.html

## Coding based on k-means

- Partition the whole space into n regions by nmeans → Voronoi
- Can be relaxed using k
  < n</p>
  - However, still cannot afford a very large k (why?)



## Solution 1: PQ (Product Quantization)

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#### Index:

- Tiny space consumption:  $\sim 1/32$  size of the data
  - if  $k = 2^8$

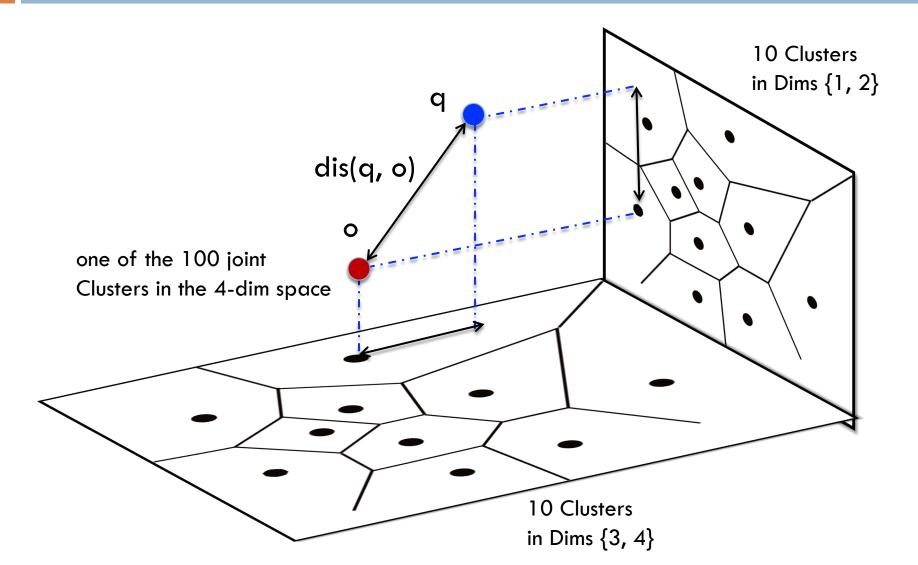
- Partition the d dims into L partitions
- k-means clustering within each partition
- $\blacksquare \{C_{1,j}\} X \{C_{2,j}\} X \dots \{C_{L,j}\} \text{ joint centers}$
- Each point encoded as the closest joint center
- Query Processing:
  - Repeat
    - Find the closest joint center
    - Compute the asymmetric distance (via table lookup)
  - Optimizations:
    - Multi-index-based (best with only 2 partitions)
    - PO Fast Scan [AKS15] POBE [[CC17]

Product

Quantization

## Illustration of PQ







	VA-File	PQ
#Partitions on dimensions	d	L = d/log(k)
Codebook	typically linear, equi- width partitioning of the domain	non-linear, "equi- width" partitioning of the domain
Query Processing	Brute-force on the encoded data	Best-first search on the encoded data

#### Solution 2: Hierarchical k-Means Tree

- PQ can be deemed as an approximate version of (L\*k)-means quantization
- Hierarchical k-Means Tree (as in FLANN) recursively partition the data using k-means clustering using a small k
  - Special case: hierarchical 2-means trees

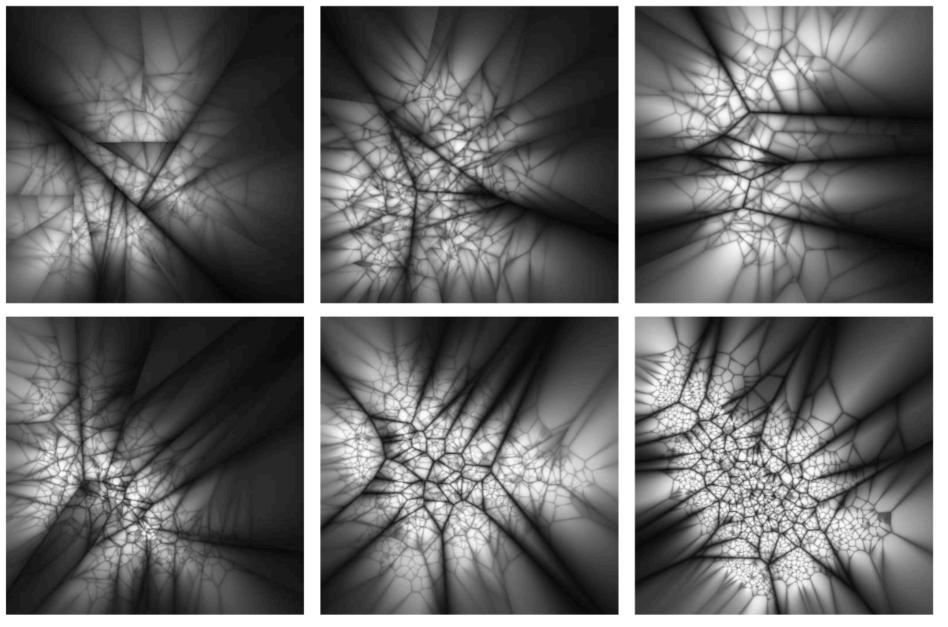


Figure 1: Projections of hierarchical k-means trees constructed using the same 100K SIFT features dataset with different branching factors: 2, 4, 8, 16, 32, 128. The projections are constructed using the same technique as in (Schindler et al., 2007). The gray values indicate the ratio between the distances to the nearest and the second-nearest cluster center at each tree level, so that the darkest values (ratio $\approx$ 1) fall near the boundaries between k-means regions.