New Trends in
High-D Vector Similarity Search
AI-driven, Progressive, and Distributed

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Questions This Tutorial Answers

- how important are high-dimensional (high-d) data nowadays?

- what types of analyses are performed on high-d data?
- how can we speed up such analyses?

- what are the different kinds of similarity search?
- what are the state-of-the-art high-d similarity search methods?
- how do methods designed for data series compare to those designed for general high-d vector similarity search?

- how do similarity search techniques support interactivity?
- how can AI help similarity search and vice versa?
- which similarity search techniques exploit modern hardware and distribution?

- what are the open research problems in this area?

Acknowledgements

- thanks for slides to
  - Michail Vlachos
  - Eamonn Keogh
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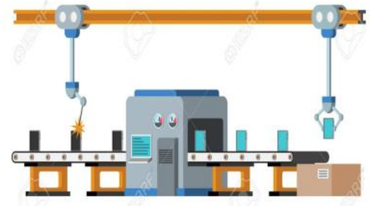
  - David Lowe
  - Walid Aref
  - John Paparrizos
  - Conglong Li
  - Saravanan Thirumuruganathan

Introduction, Motivation

High-d data are everywhere

Finance

Paleontology



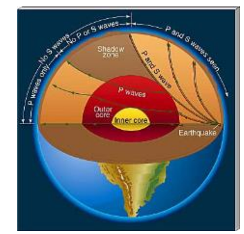
Manufacturing

Aviation

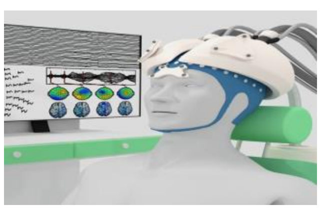
Agriculture

Astronomy

Criminology

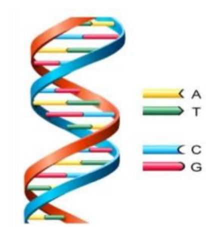


Seismology



Neuroscience

Medicine



Biology

High-d data are everywhere

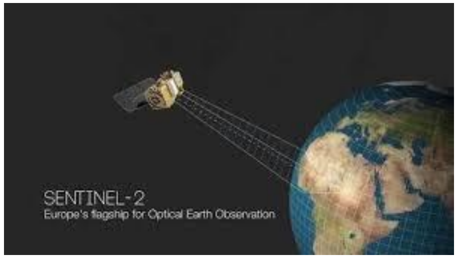
- operation health monitoring
  - classification, anomaly detection
- data integration
  - entity resolution, data discovery
- recommender systems
  - predict user interest
- information retrieval
  - similarity search
- software engineering
  - find software dependencies
- cybersecurity
  - network usage profiling, intrusion detection
- …

High-d collections are massive

≈ 500 ZB per year

≈ 130 TB

> 40 PB per day



> 5 TB per day

facebook

> 500 TB per day

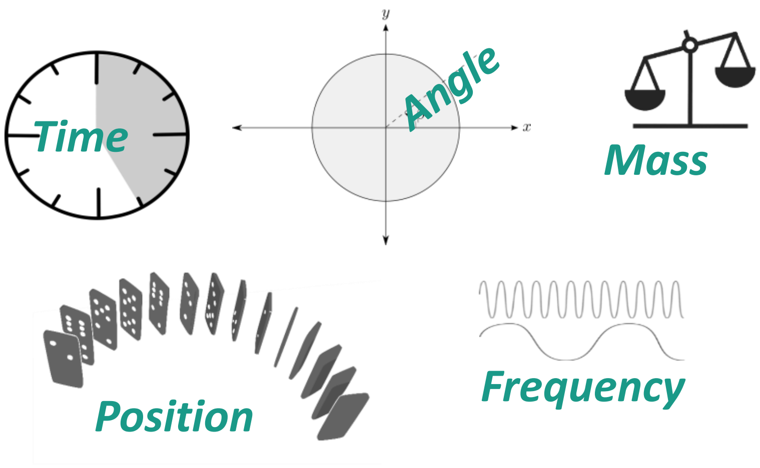
1 PB = 1 thousand TB

1 ZB = 1 billion TB

Popular High-d data

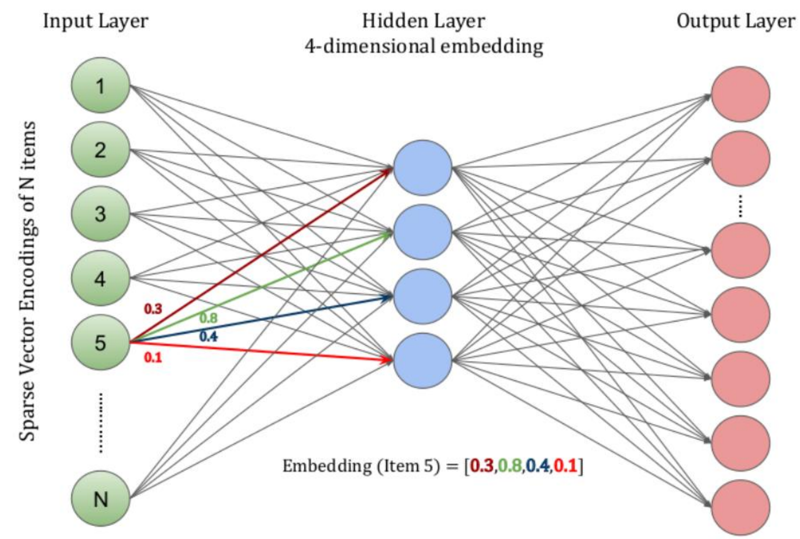
Data series

A collection of points ordered over a dimension



Deep Embeddings

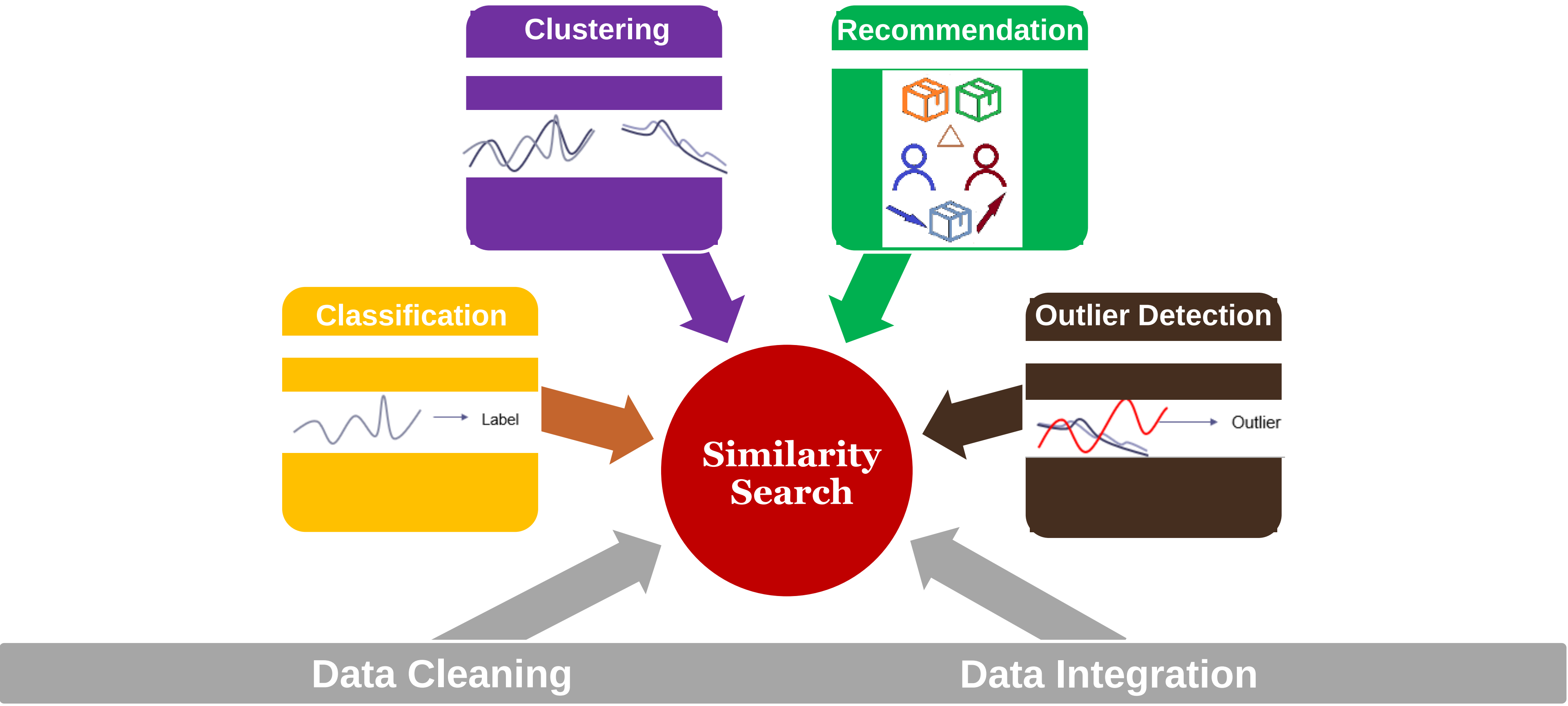
A high-d vector learned from data using a DNN



embedded
text, images, video, graphs, etc.

High-d data -> High-d vectors

Extracting value requires analytics



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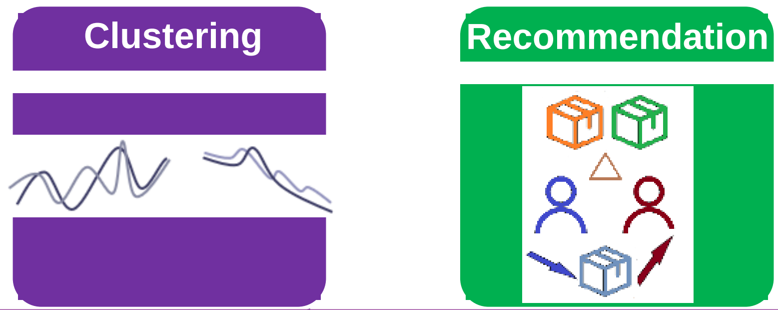


HARD, because of very high dimensionality:
each high-d vector has 100s-1000s of dimensions!

even HARDER, because of very large size:
millions to billions of high-d vectors (multi-TBs)!

Data Cleaning

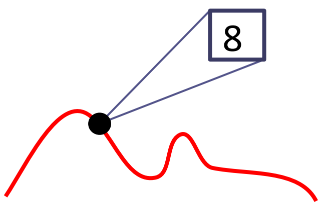
Data Integration

High-d Similarity Search

High-d Similarity Search Problem Variations

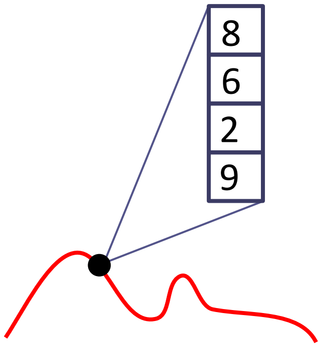
Problem Variations

Series



<u>Univariate</u>

each point represents one value (e.g., temperature)



<u>Multivariate</u>

each point represents many values (e.g., temperature, humidity, pressure, wind, etc.)

Problem Variations

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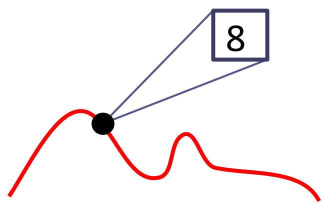

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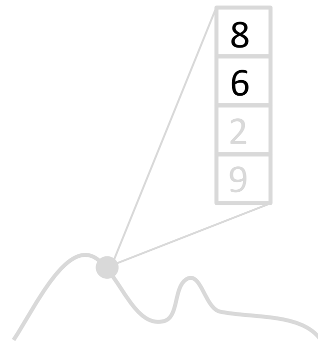

Multivariate

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Publications

Ding-PVLDB'08

Paparrizos-SIGMOD'20

Problem Variations

Data Series Distance Measures

- similarity search is based on measuring distance between sequences
- dozens of distance measures have been proposed
  - lock-step
    - Minkowski, Manhattan, Euclidean, Maximum, DISSIM, …
  - sliding
    - Normalized Cross-Correlation, SBD, …
  - elastic
    - DTW, LCSS, MSM, EDR, ERP, Swale, …
  - kernel-based
    - KDTW, GAK, SINK, …
  - embedding
    - GRAIL, RWS, SPIRAL, SEAnet, …

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Problem Variations

High-d Vectors Distance Measures

- similarity search is based on measuring distance between vectors
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  - L_p distances ($0<p\leq2, \infty$), (Euclidean for p = 2)
  - Cosine distance
  - Correlation
  - Hamming distance
  - …

Problem Variations

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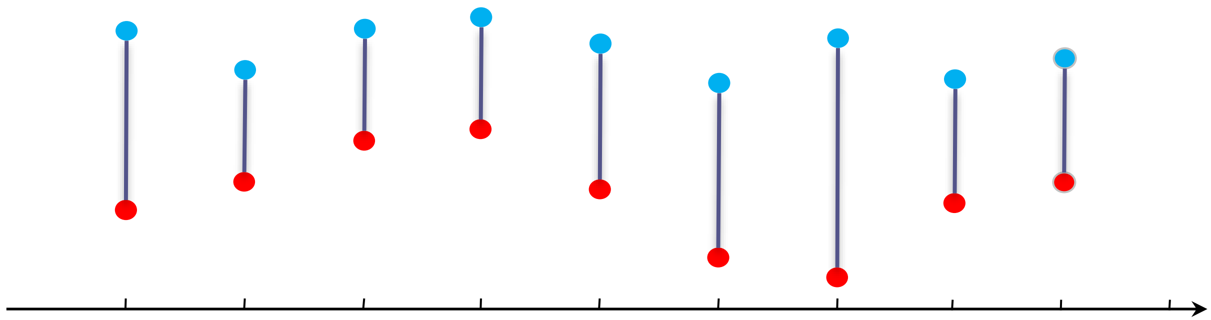
Euclidean Distance



- Euclidean distance
  - pair-wise point distance

$$ED(X,Y) = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$$

Correlation

- measures the degree of relationship between data series
  - indicates the degree and direction of relationship
- direction of change
  - positive correlation
    - values of two data series change in same direction
  - negative correlation
    - values of two data series change in opposite directions
- linear correlation
  - amount of change in one data series bears constant ratio of change in the other data series

- useful in several applications

Pearson's Correlation (PC) Coefficient

- used to see linear dependency between values of data series of equal length, n

$$PC = \frac{1}{n-1}\sum_{i=1}^{n}\left(\frac{x_i - \bar{x}}{s_x}\right)\left(\frac{y_i - \bar{y}}{s_y}\right)$$

- where $\bar{x}$ is the mean: $\bar{x} = \frac{1}{n-1}\sum_{i=1}^{n} x_i$
- and s_x is the standard deviation: $s_x = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2}$

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$$PC = \frac{1}{n-1}\sum_{i=1}^{n}\left(\frac{x_i - \bar{x}}{s_x}\right)\left(\frac{y_i - \bar{y}}{s_y}\right)$$

- takes values in [-1,1]
  - 0 – no correlation
  - -1, 1 – inverse/direct correlation
- there is a statistical test connected to PC, where null hypothesis is the no correlation case (correlation coefficient = 0)
  - test is used to ensure that the correlation similarity is not caused by a random process

PC and ED

- Euclidean distance: $$ED = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2},$$
- In case of Z-normalized data series (mean = 0, stddev = 1):

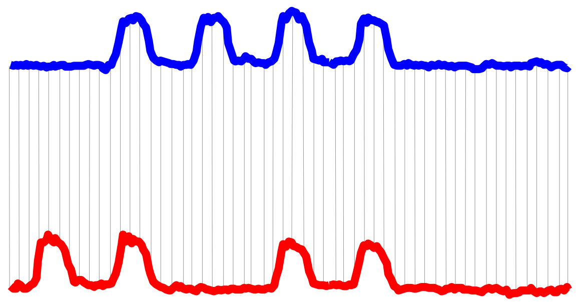
$$PC = \frac{1}{n-1}\sum_{i=1}^{n} x_i \cdot y_i$$ and $$ED^2 = 2n(n-1) - 2\sum_{i=1}^{n} x_i y_i$$

so the following formula is true: $$ED^2 = 2(n-1)(n - PC)$$

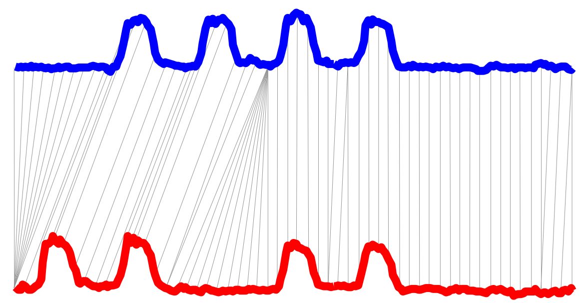
- direct connection between ED and PC for Z-normalized data series
  - if ED is calculated for normalized data series, it can be directly used to calculate the p-value for statistical test of Pearson's correlation instead of actual PC value.

Distance Measures: LCSS against Euclidean, DTW

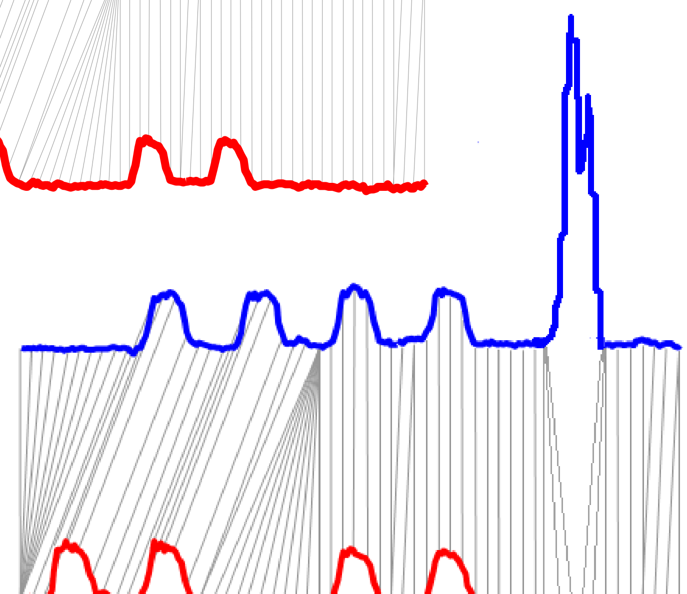
- Euclidean
  - rigid



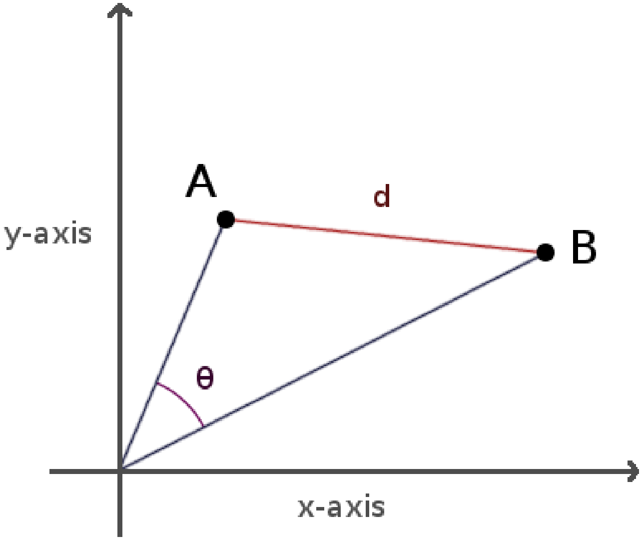
- Dynamic Time Warping (DTW)
  - allows local scaling



- Longest Common SubSequence (LCSS)
  - allows local scaling
  - ignores outliers



Distance Measures: Cosine Distance



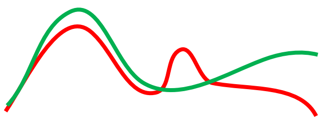
$$\text{similarity} = \cos(\theta) = \frac{\mathbf{A}\cdot\mathbf{B}}{\|\mathbf{A}\|\|\mathbf{B}\|} = \frac{\sum_{i=1}^{n} A_i B_i}{\sqrt{\sum_{i=1}^{n} A_i^2}\sqrt{\sum_{i=1}^{n} B_i^2}},$$

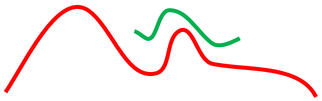
- Cosine distance = 1 - cosine similarity

- ED vs. Cosine similarity
  - If A and B are normalized to unit length in L_2, the square of ED is proportional to the cosine distance:
  - $||A||_2=||B||_2=1 \rightarrow ||A-B||_2=2-2\cos(A,B)$

Problem Variations

Queries





Whole matching

Entire query

Entire candidate

Subsequence matching

Entire query

A subsequence of a candidate

Problem Variations

Queries

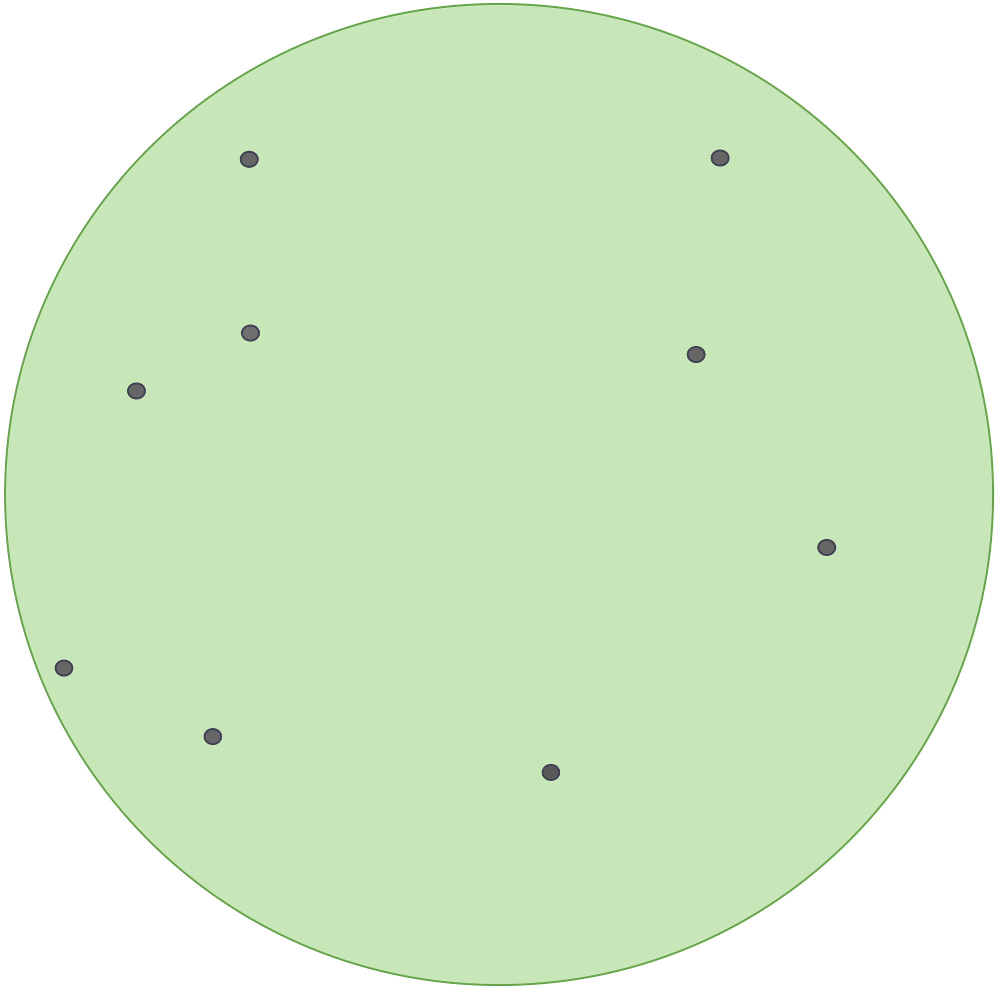
Nearest Neighbor (1NN)
k-Nearest Neighbor (kNN)
Farthest Neighbor
epsilon-Range

and more...

Nearest Neighbor (NN) Queries…

Publications

Echihabi et al. PVLDB'19



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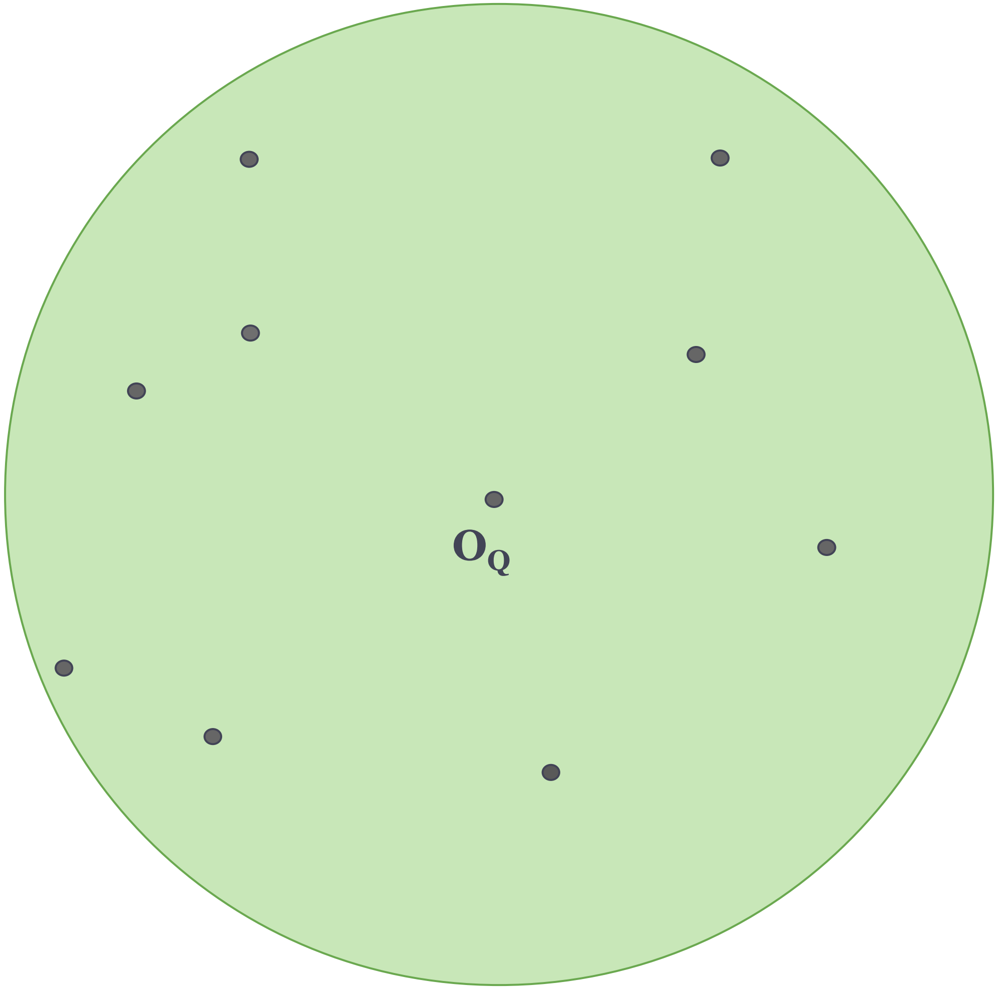

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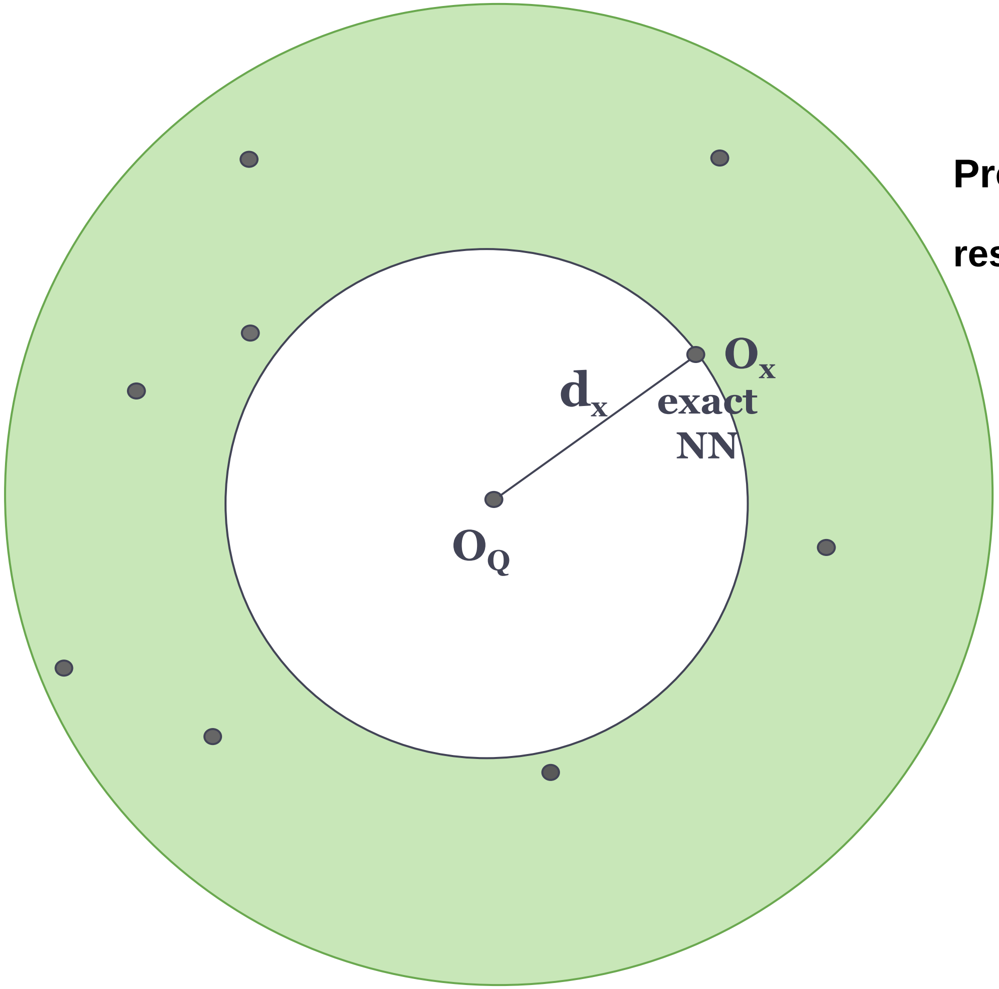

Prob($d_x = \min\{d_i\}$) = 1

result is exact NN

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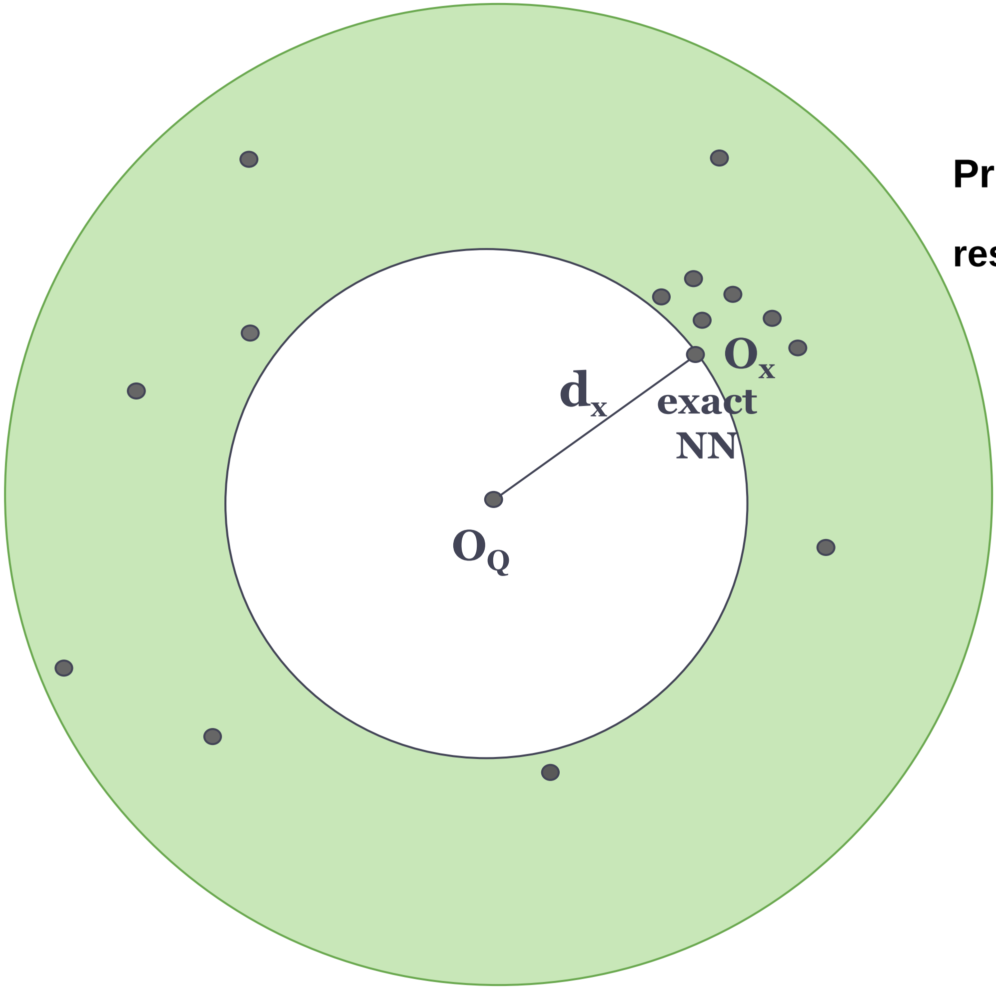

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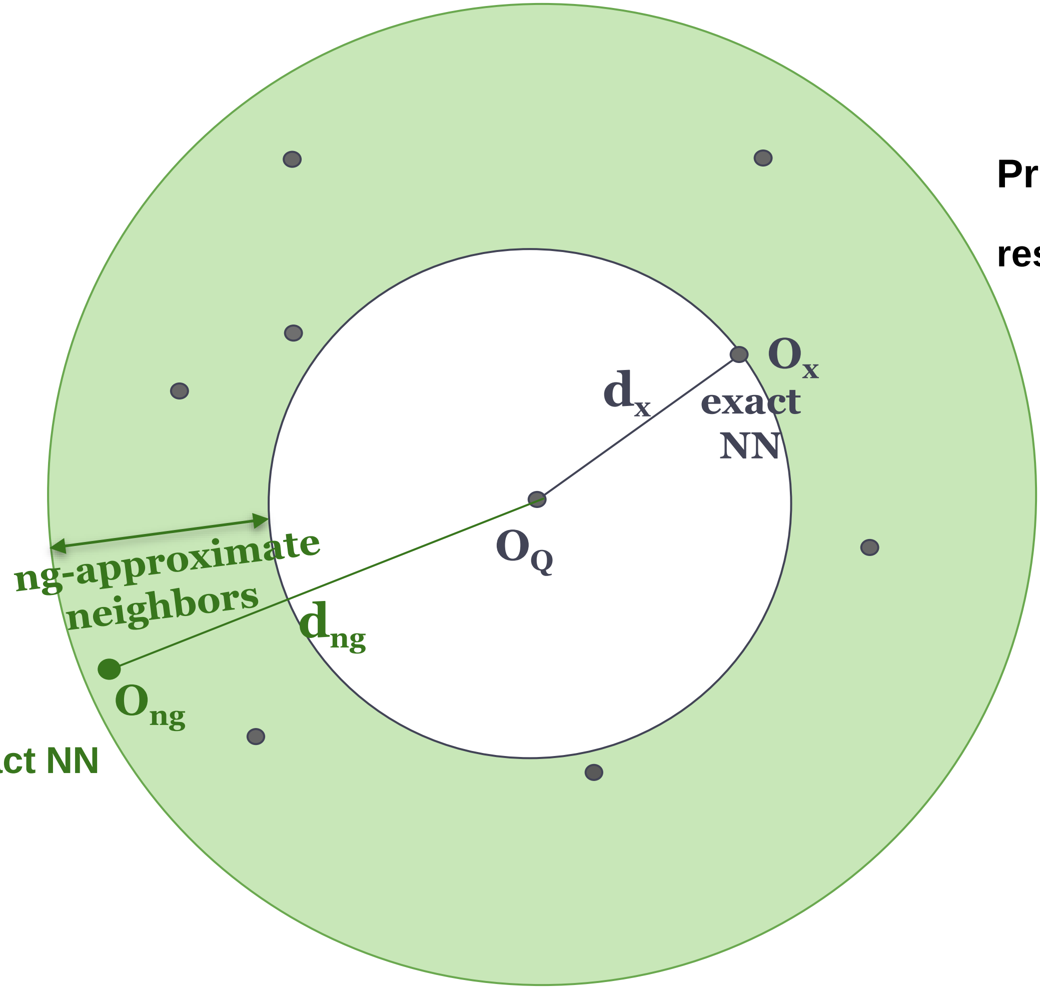

Prob($d_x = \min\{d_i\}$) = 1

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Prob(d_{ng} <>= ?) = ?

result within ? of exact NN

Nearest Neighbor (NN) Queries…

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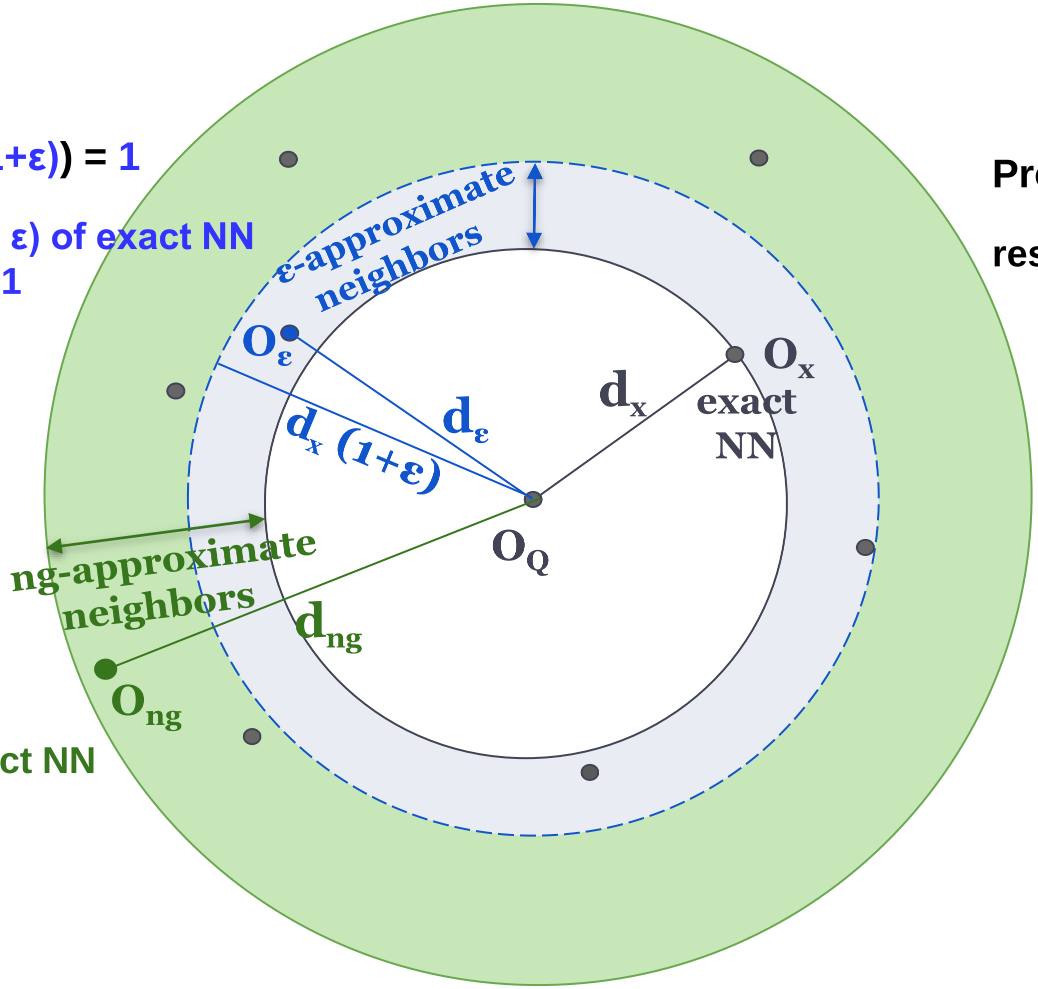
Prob(d_ε <= d_x (1+ε)) = 1

result within (1+ ε) of exact NN
with probability 1



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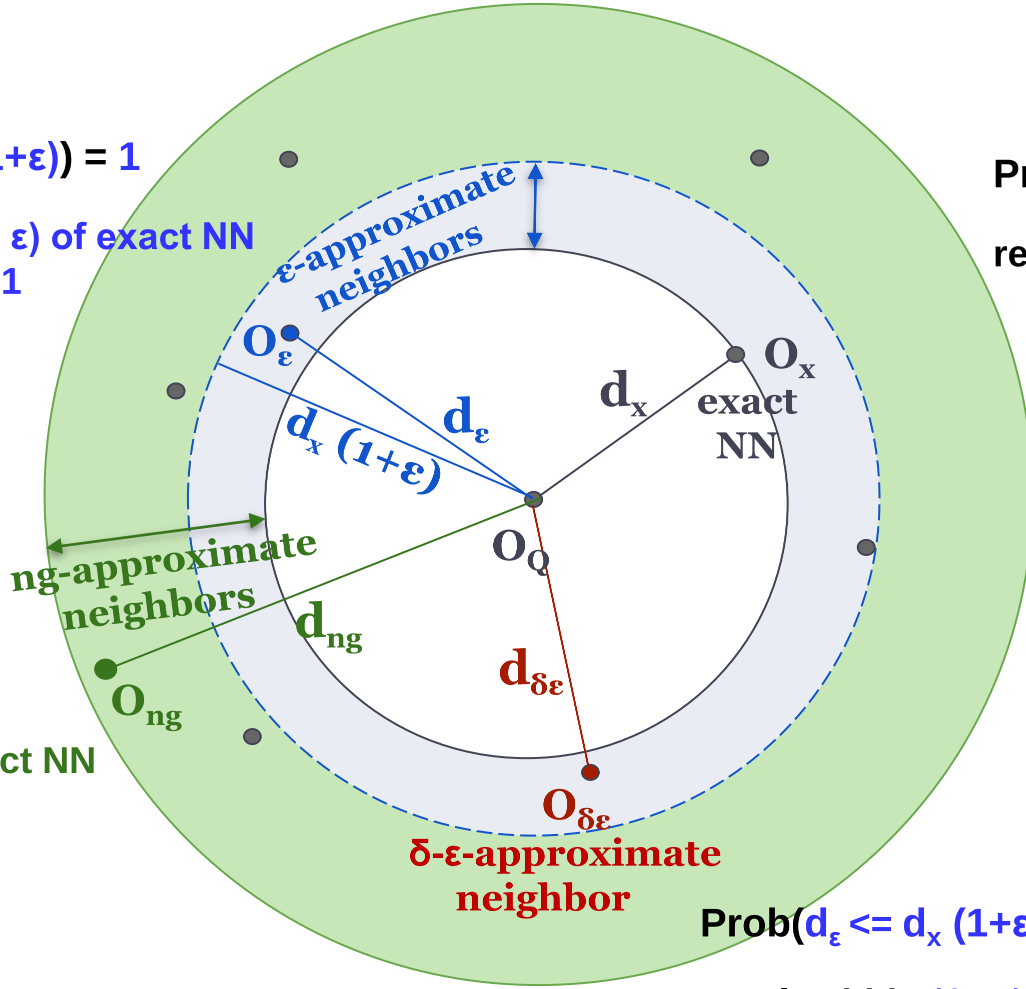

Prob(d_{ng} <>= ?) = ?

result within ? of exact NN

Prob(d_ε <= d_x (1+ε)) >= δ

result within (1+ ε) of exact NN
with probability at least δ

Nearest Neighbor (NN) Queries…

Publications

Echihabi et al. PVLDB'19

Prob(d_ε <= d_x (1+ε)) = 1

result within (1+ ε) of exact NN with probability 1

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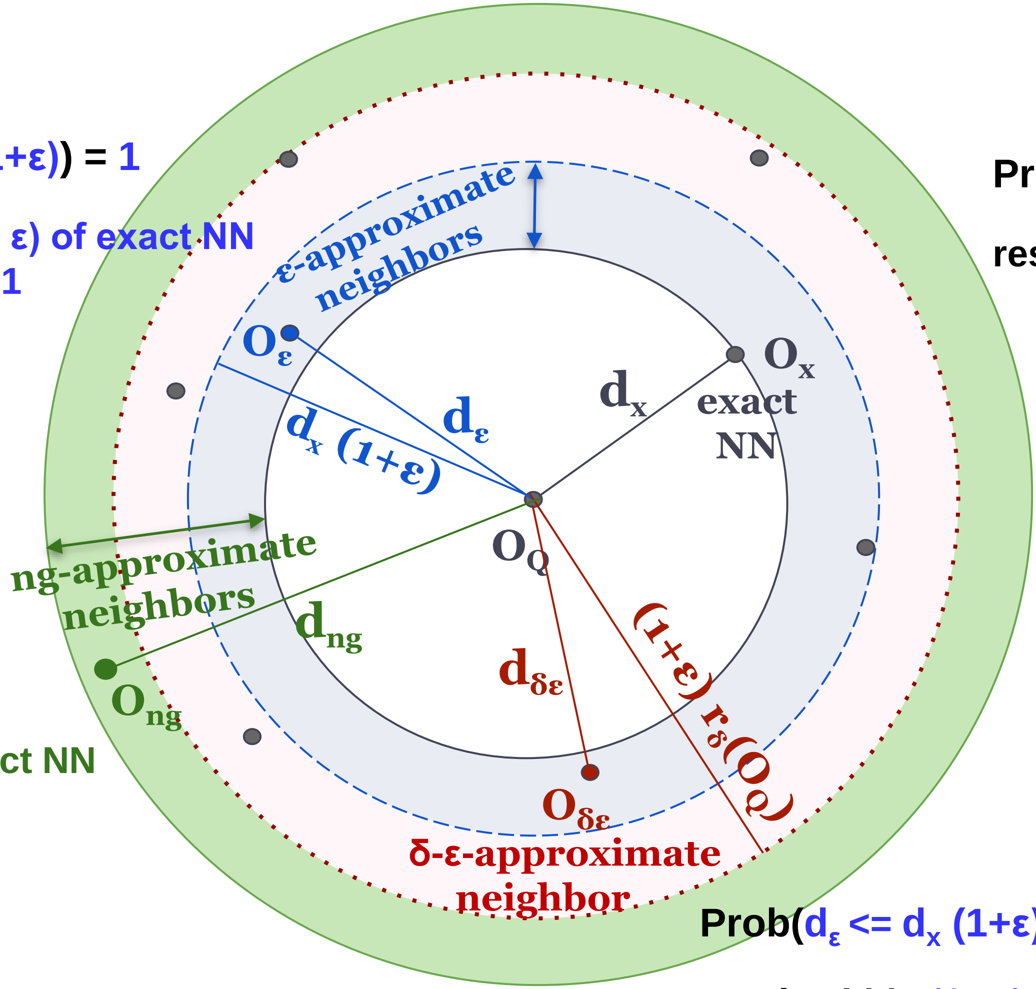

Prob(d_{ng} <>= ?) = ?

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Maximum Inner Product Search (MIPS)

- Problem Definition:
  - Given a collection of candidate vectors S and a query Q , find a candidate vector C maximizing the inner product with the query: :
    - Given $S \subset R^d$ and $Q \in R^d$, $C = \mathrm{argmax}_{X \in S}\, Q^T X$

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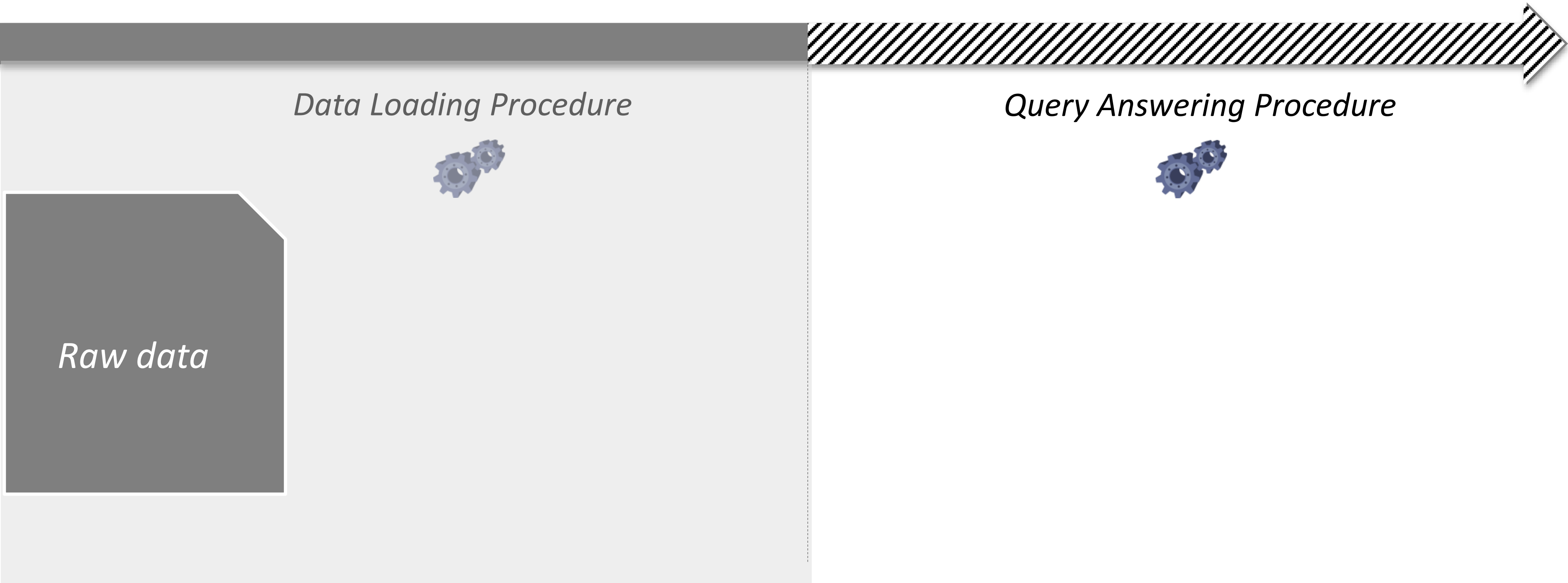
    - Given $S \subset R^d$ and $Q \in R^d$, $C = \text{argmax}_{X \in S}\, Q^T X$
  - MIPS is closely related to NN search:
    - If $\|Q\|_2 = 1$, $\|Q - X\|_2 = 1 + \|X\|_2 - 2Q^T X$
  - MIPS and NN search are equivalent when all vectors X in S have constant length c
  - Otherwise, MIPS can be converted to NN search with ED or Cosine similarity [1][2][3]

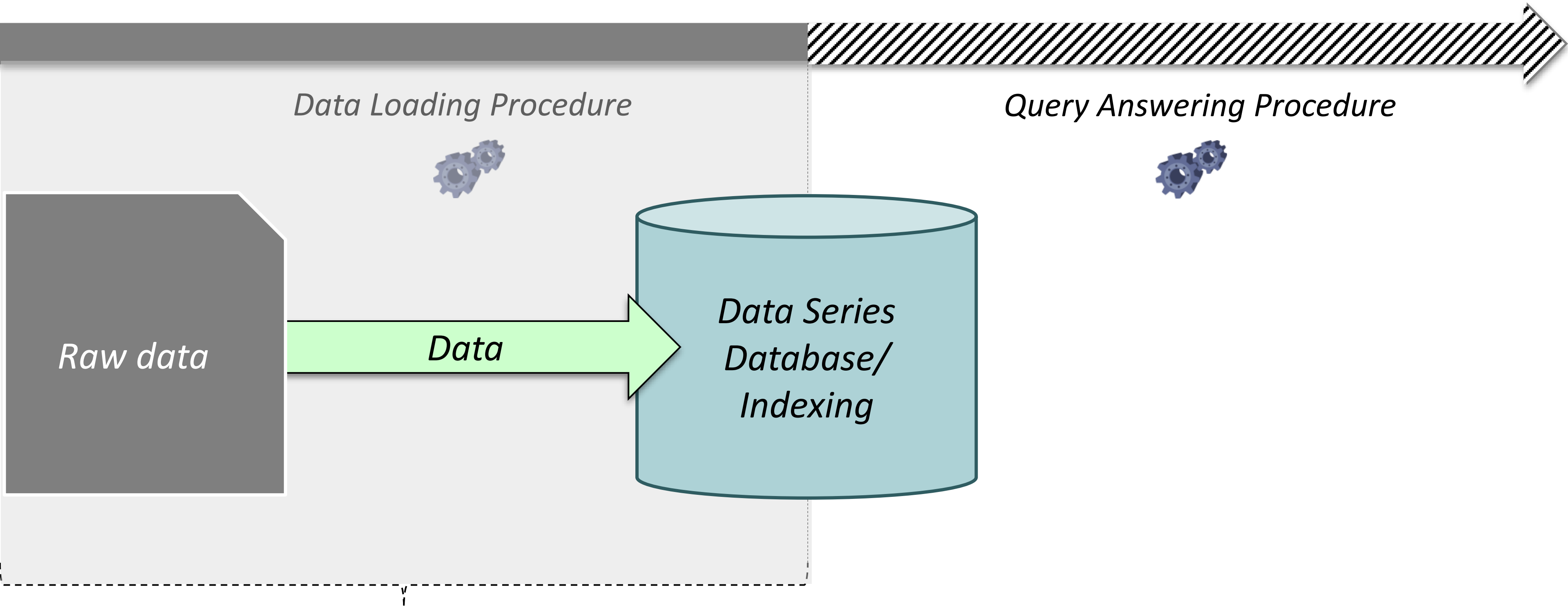
[1] Anshumali Shrivastava and Ping Li. 2014a. Asymmetric LSH (ALSH) for Sublinear Time Maximum Inner Product Search (MIPS). In NIPS. 2321–2329.
[2] Yoram Bachrach, Yehuda Finkelstein, Ran Gilad-Bachrach, Liran Katzir, Noam Koenigstein, Nir Nice, and Ulrich Paquet. 2014. Speeding Up the Xbox Recommender System Using a Euclidean Transformation for Inner-product Spaces. In RecSys. 257–264.
[3] B. Neyshabur and N. Srebro. 2014. On Symmetric and Asymmetric LSHs for Inner Product Search. ArXiv e-prints (Oct. 2014).

High-d Similarity Search Process

Similarity Search Process

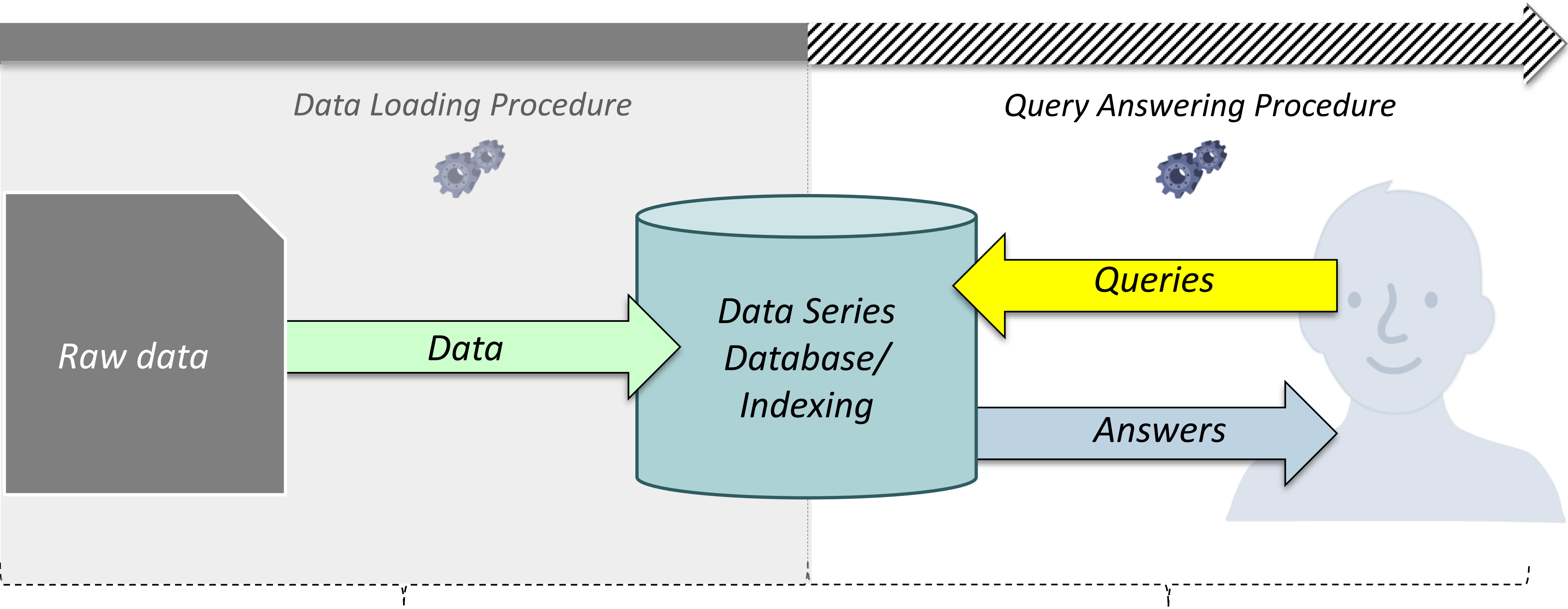


Similarity Search Process



data-to-query time

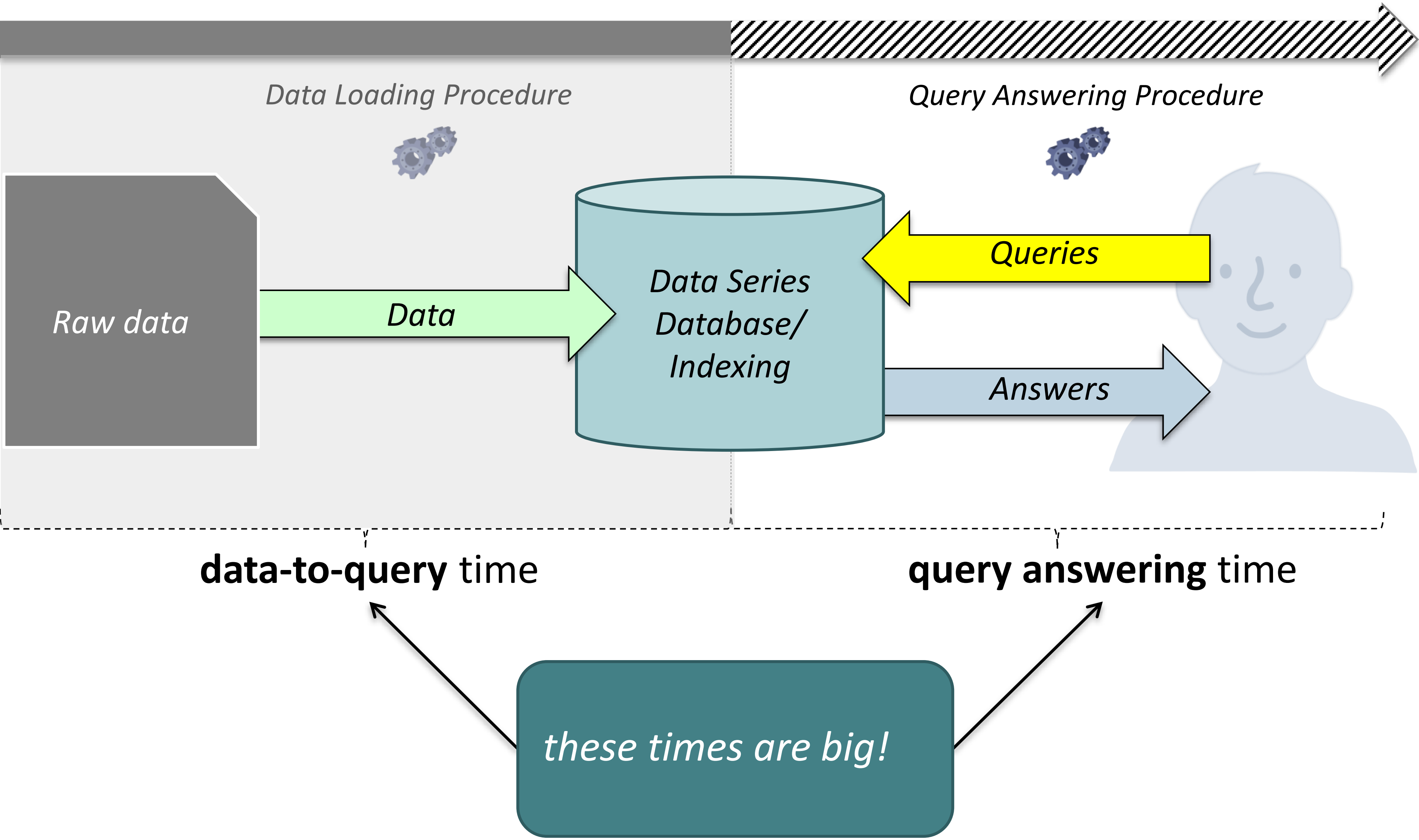
Similarity Search Process



data-to-query time

query answering time

Similarity Search Process



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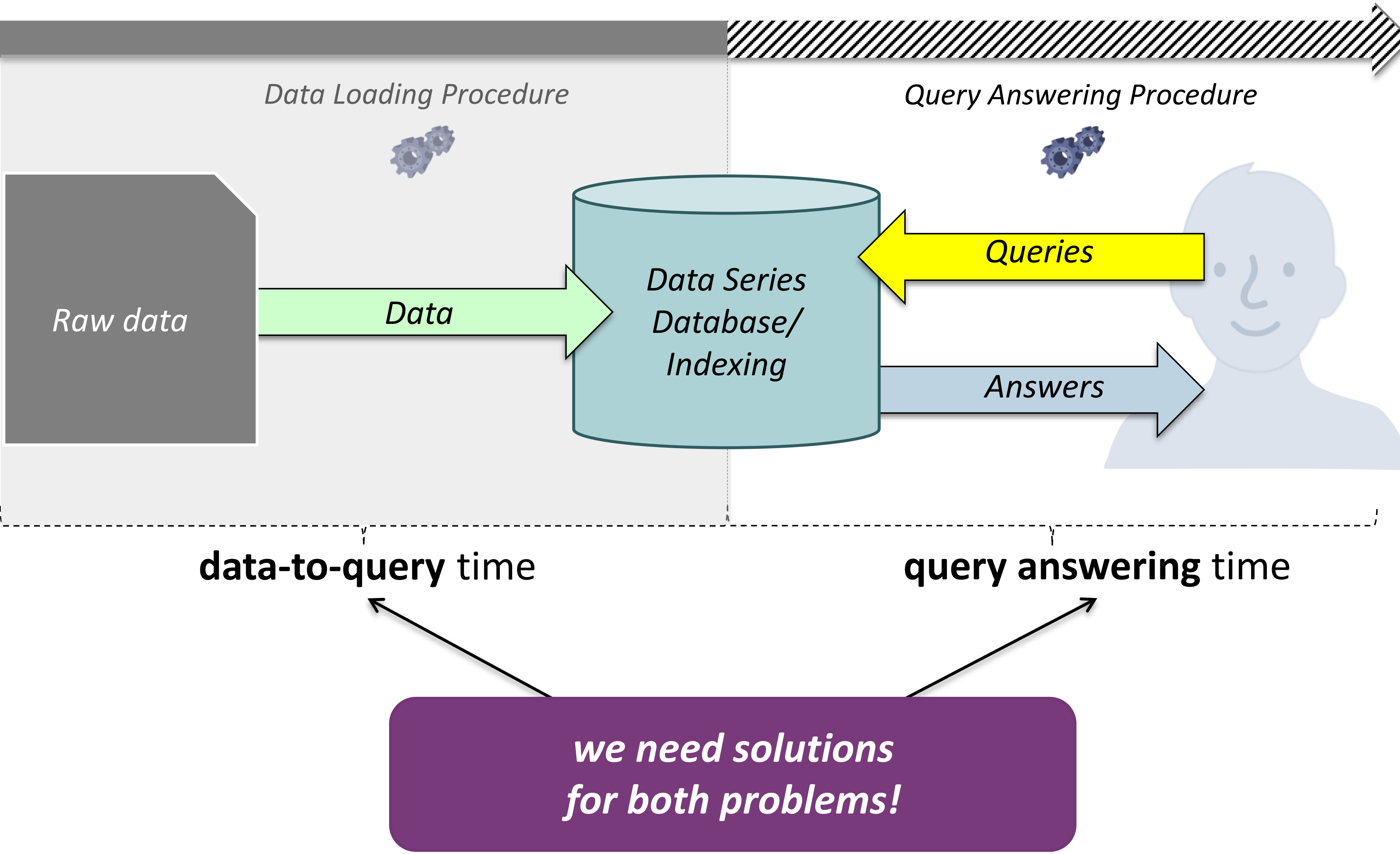
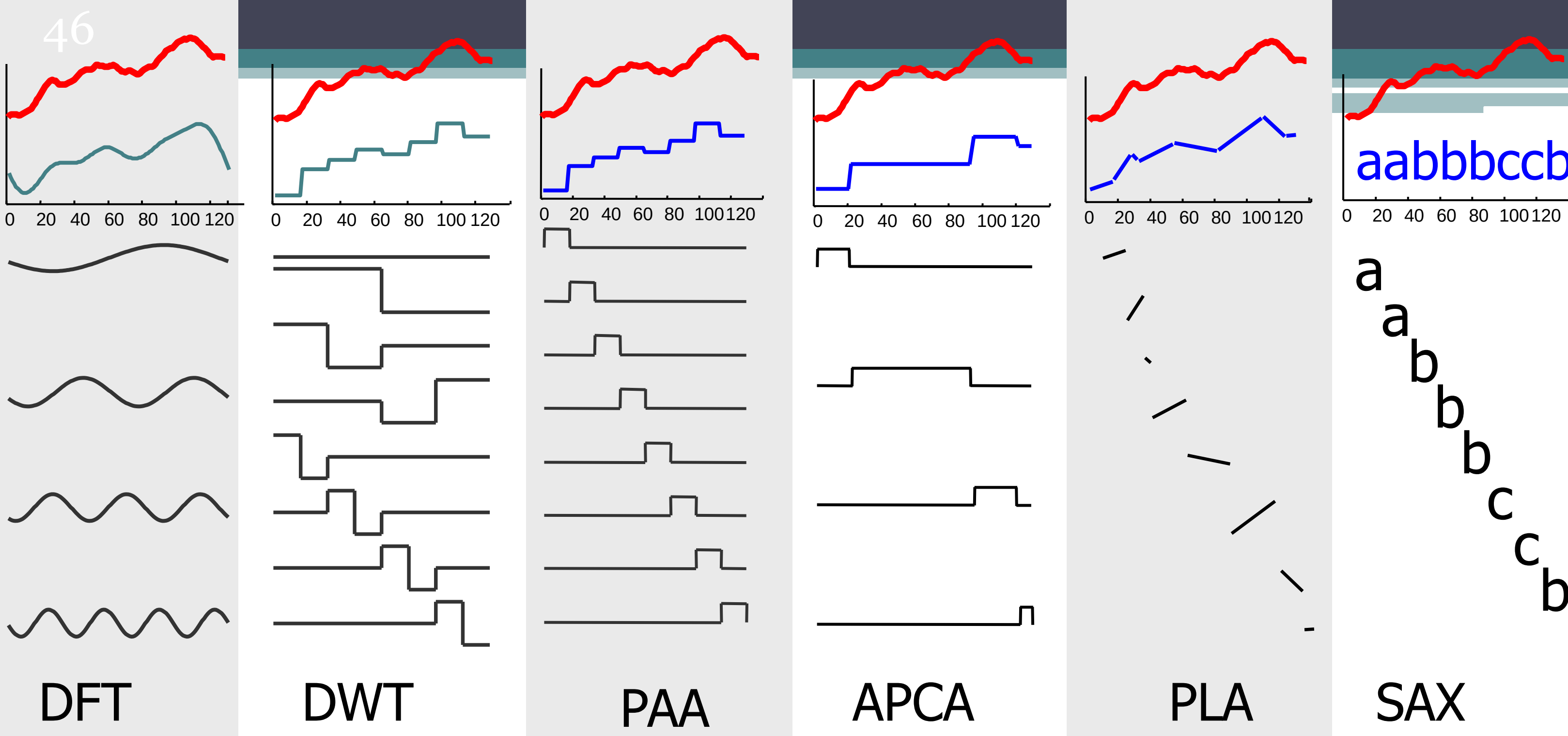


Questions?

Data Series Similarity Search



DFT: Agrawal, Faloutsos, &. Swami. FODO 1993
Faloutsos, Ranganathan, & Manolopoulos. SIGMOD 1994

DWT: Chan & Fu. ICDE 1999

PAA: Keogh, Chakrabarti, Pazzani & Mehrotra KAIS 2000
Yi & Faloutsos VLDB 2000

APCA: Keogh, Chakrabarti, Pazzani & Mehrotra SIGMOD 2001

PLA: Morinaka, Yoshikawa, Amagasa, & Uemura, PAKDD 2001

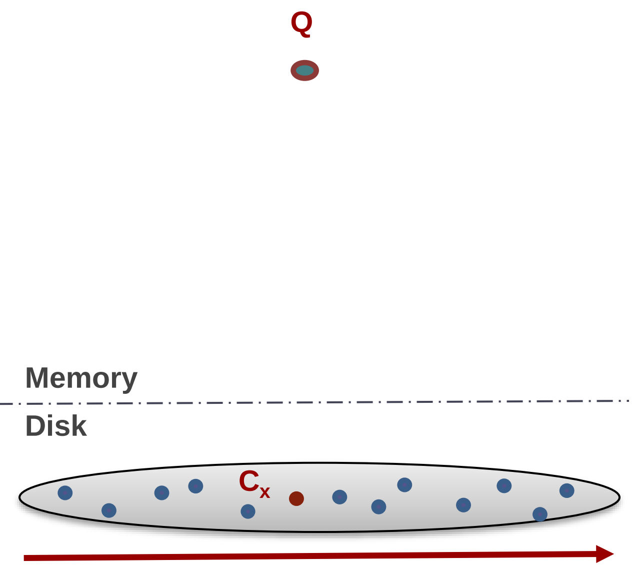
for a complete and detailed presentation, see tutorial:

Publications

Keogh - KDD‘04

Data Series Similarity Search
Classes of Methods

Similarity Matching
Serial Scan

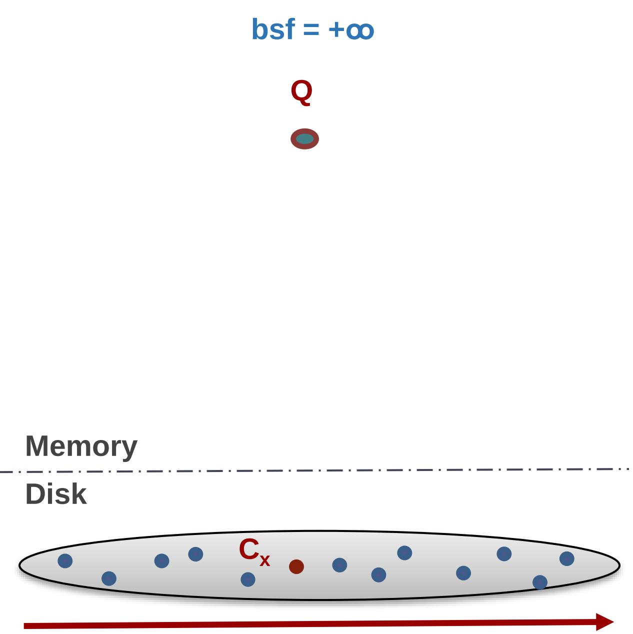


Q is compared to each raw candidate in the dataset before returning the answer C_x

(a) Serial scan

Answering a similarity search query using different access paths

Similarity Matching
Serial Scan



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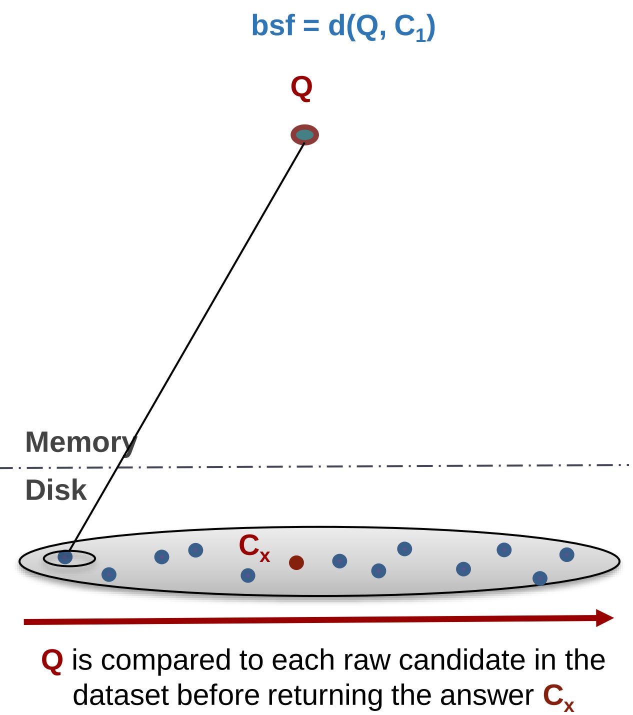

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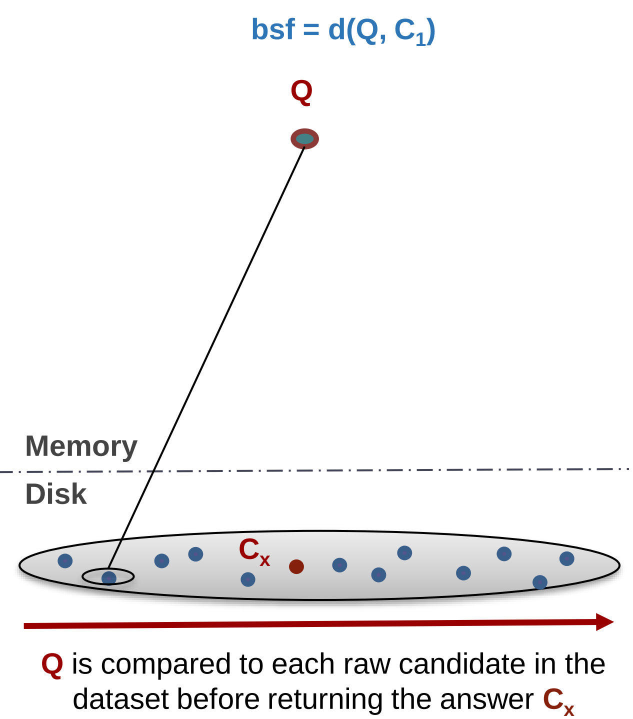

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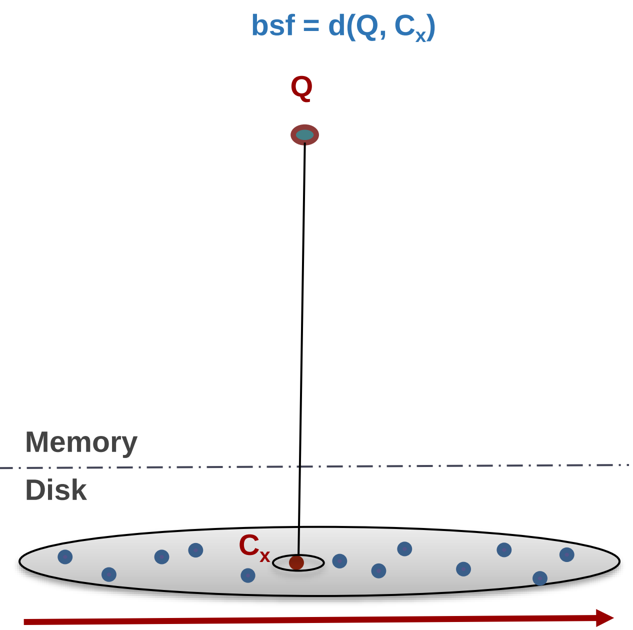

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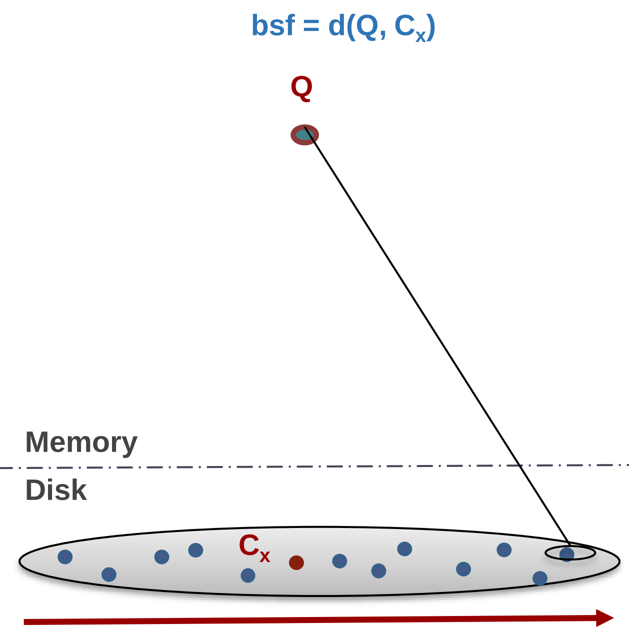
Similarity Matching
Serial Scan

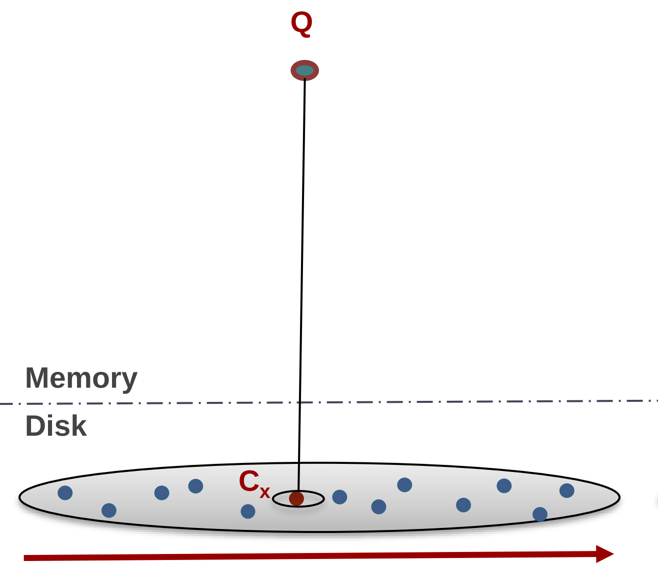


Q is compared to each raw candidate in the dataset before returning the answer **C_x**

(a) Serial scan

Answering a similarity search query using different access paths

Similarity Matching
Serial Scan



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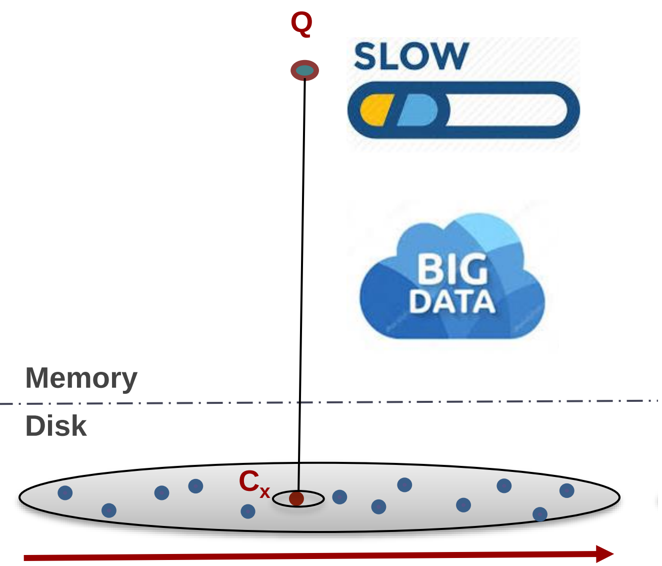
(a) Serial scan

Answering a similarity search query using different access paths

Similarity Matching
Serial Scan

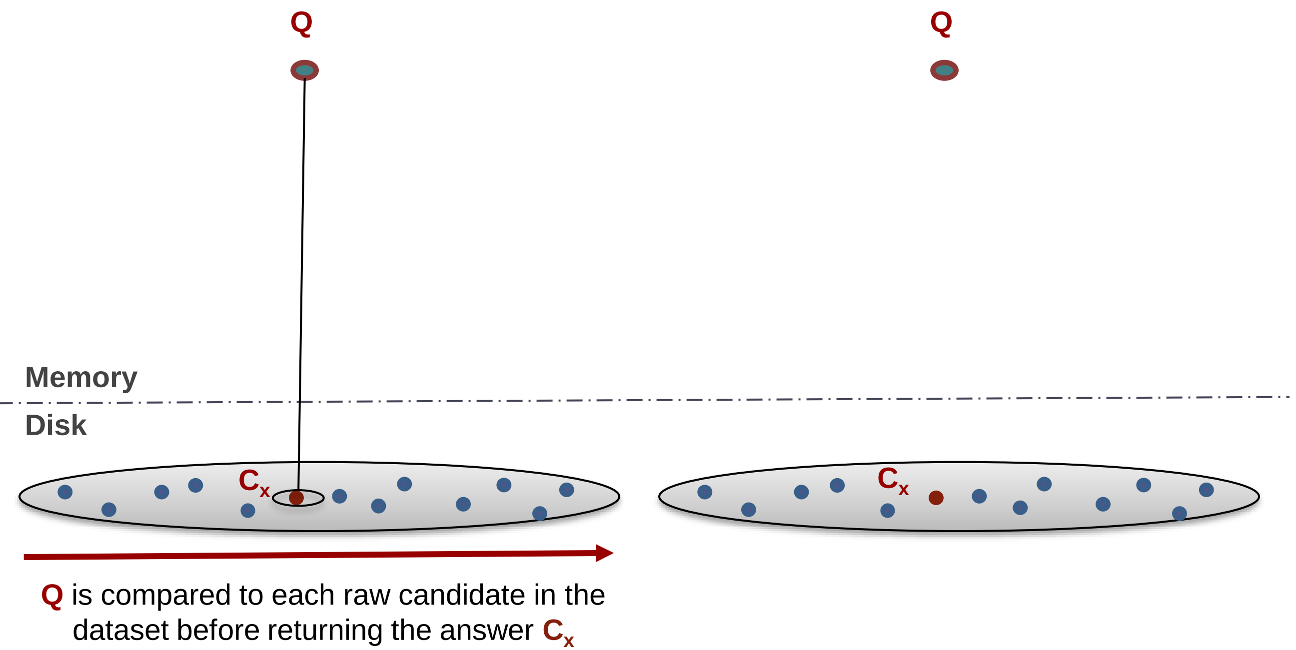


Q is compared to each raw candidate in the dataset before returning the answer C_x

(a) Serial scan

Answering a similarity search query using different access paths

Indexes vs. Scans

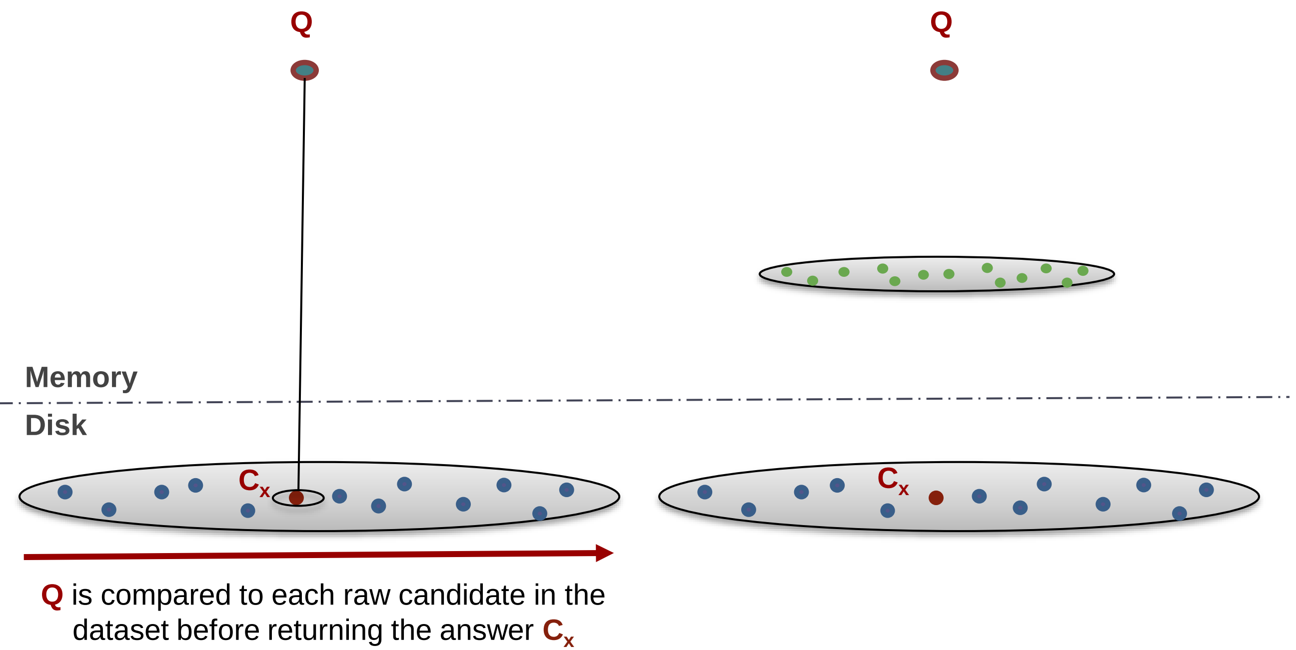


(a) Serial scan

(b) Skip-sequential scan

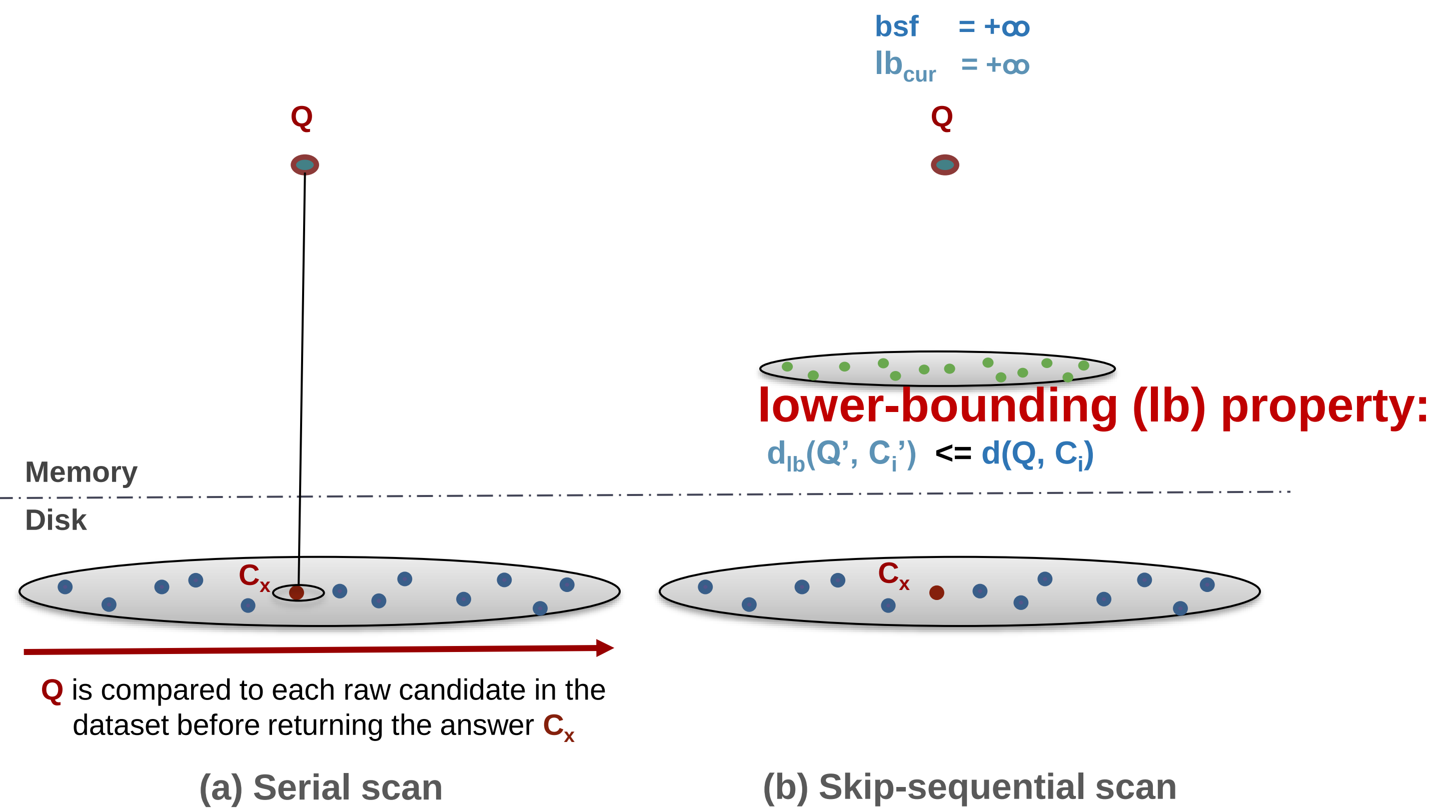
Answering a similarity search query using different access paths

Indexes vs. Scans



(a) Serial scan (b) Skip-sequential scan

Answering a similarity search query using different access paths

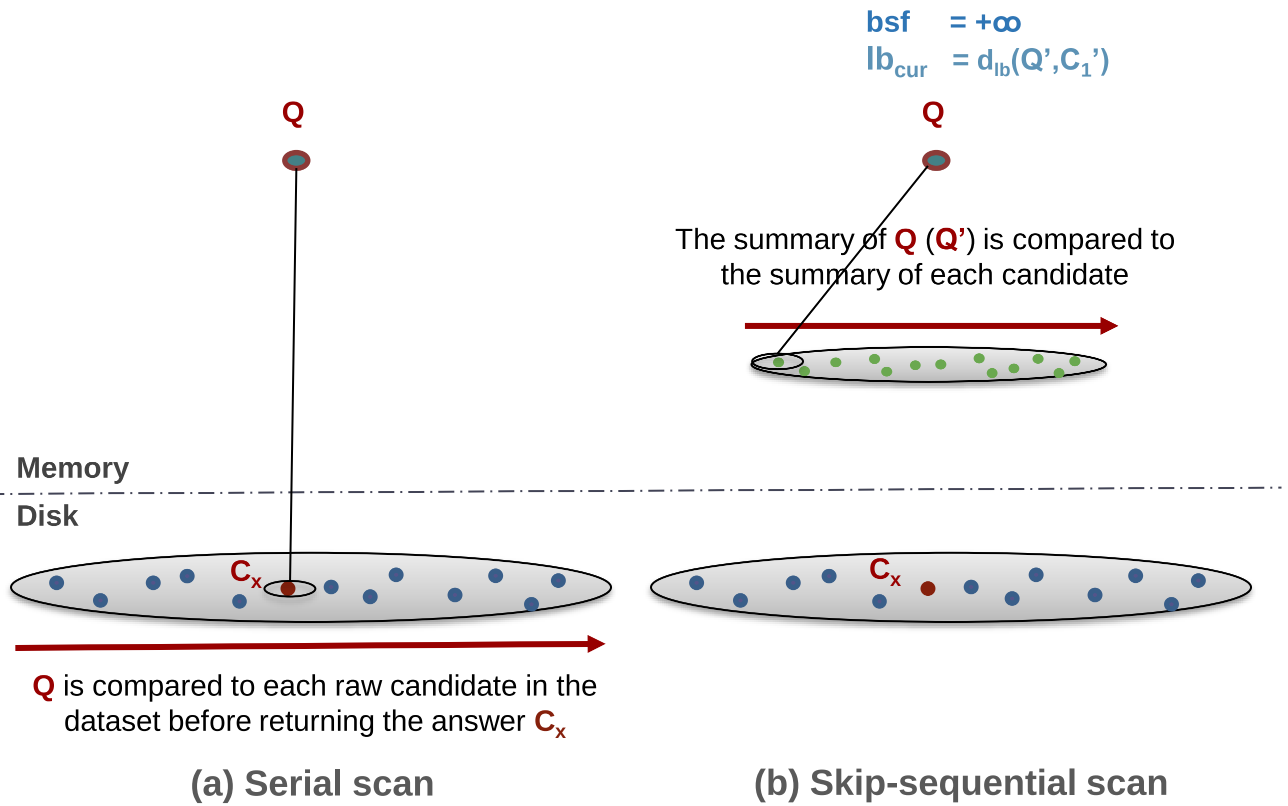


Publications

Faloutsos-SIGMOD'94

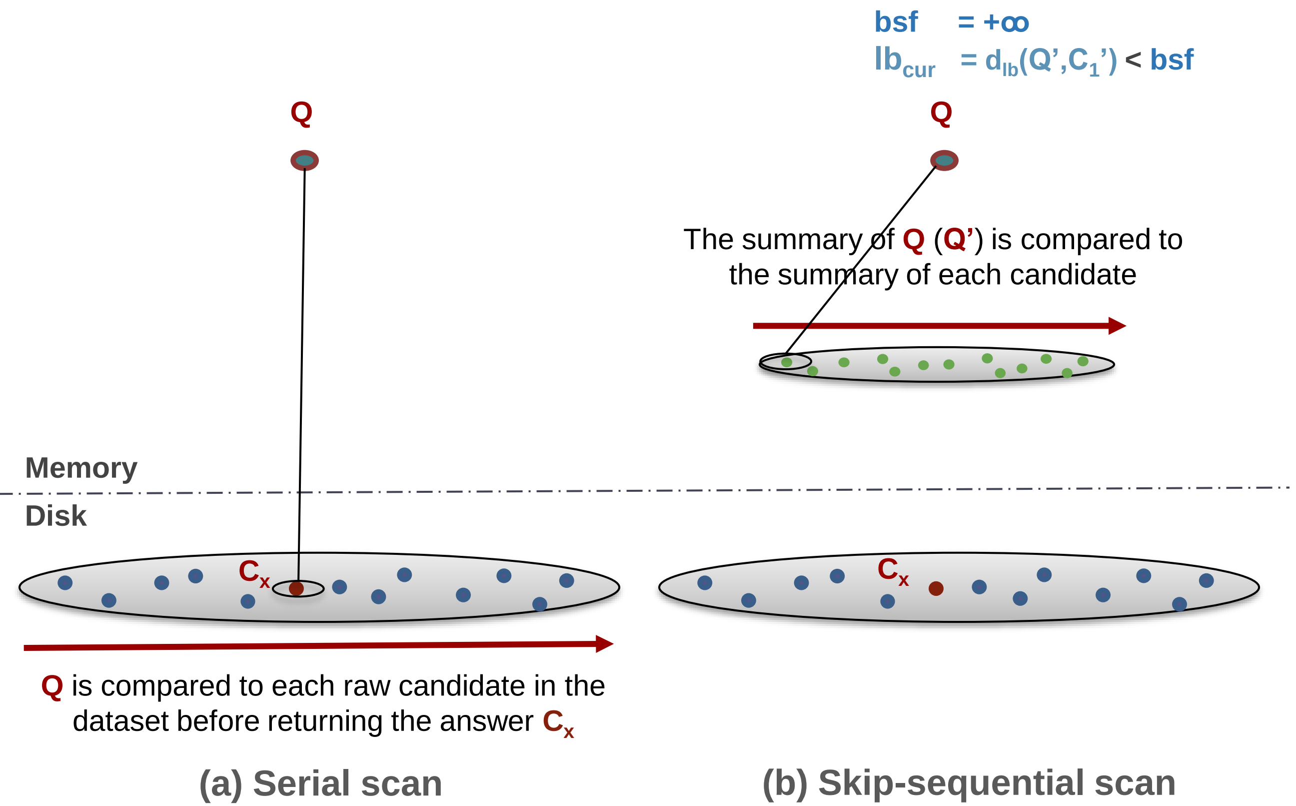
Answering a similarity search query using different access paths

Indexes vs. Scans



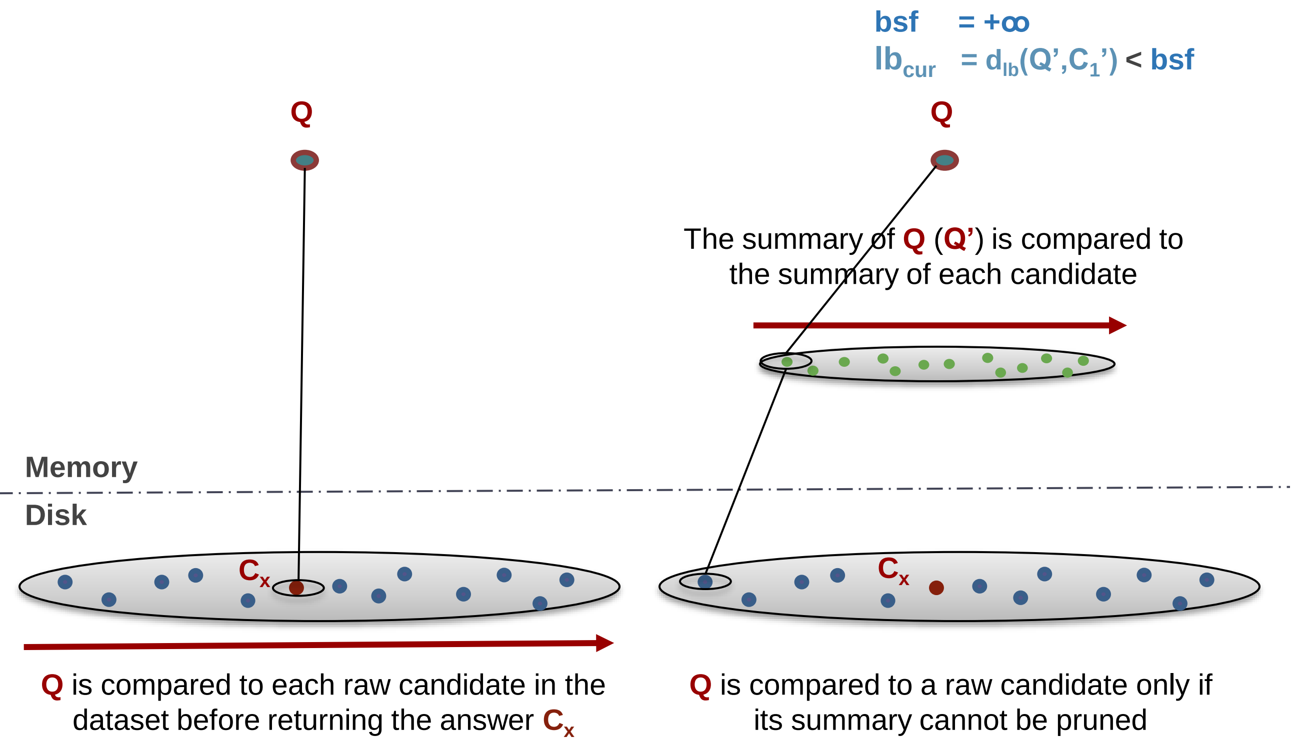
<u>**Answering a similarity search query using different access paths**</u>

Indexes vs. Scans



Answering a similarity search query using different access paths

Indexes vs. Scans

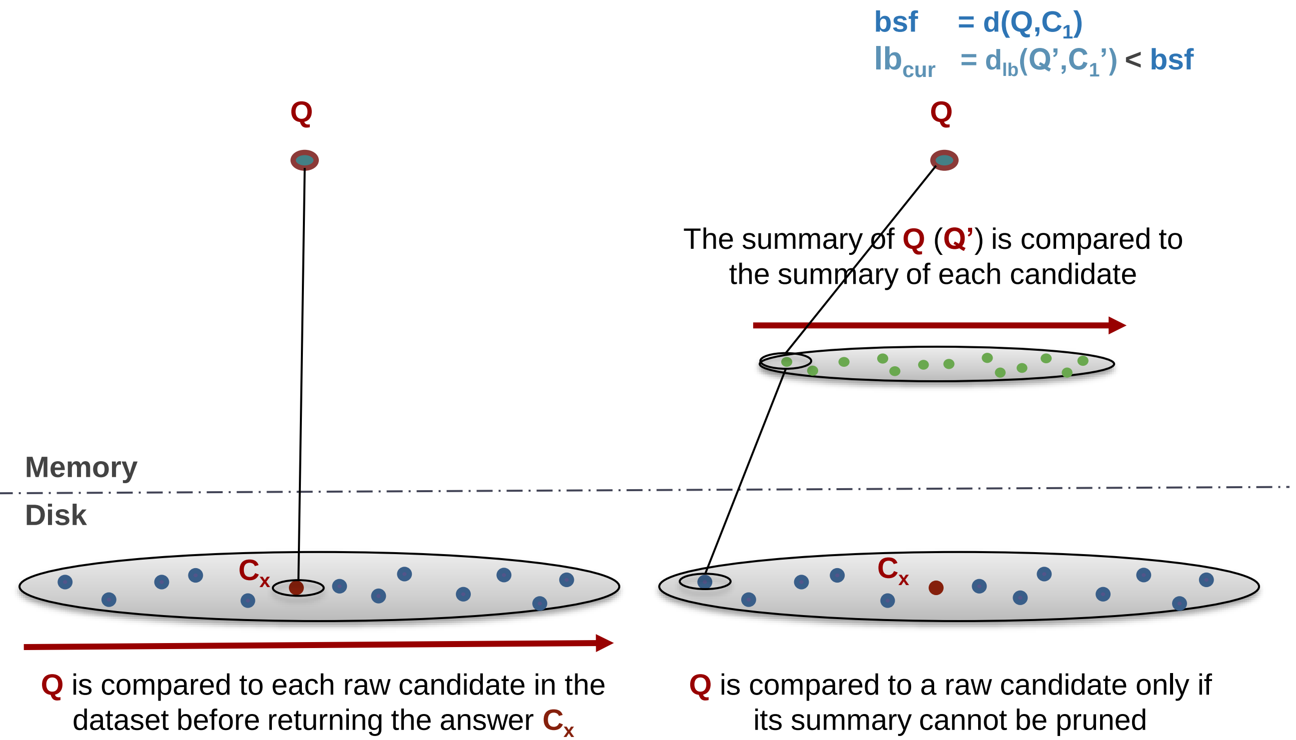


(a) Serial scan

(b) Skip-sequential scan

Answering a similarity search query using different access paths

Indexes vs. Scans



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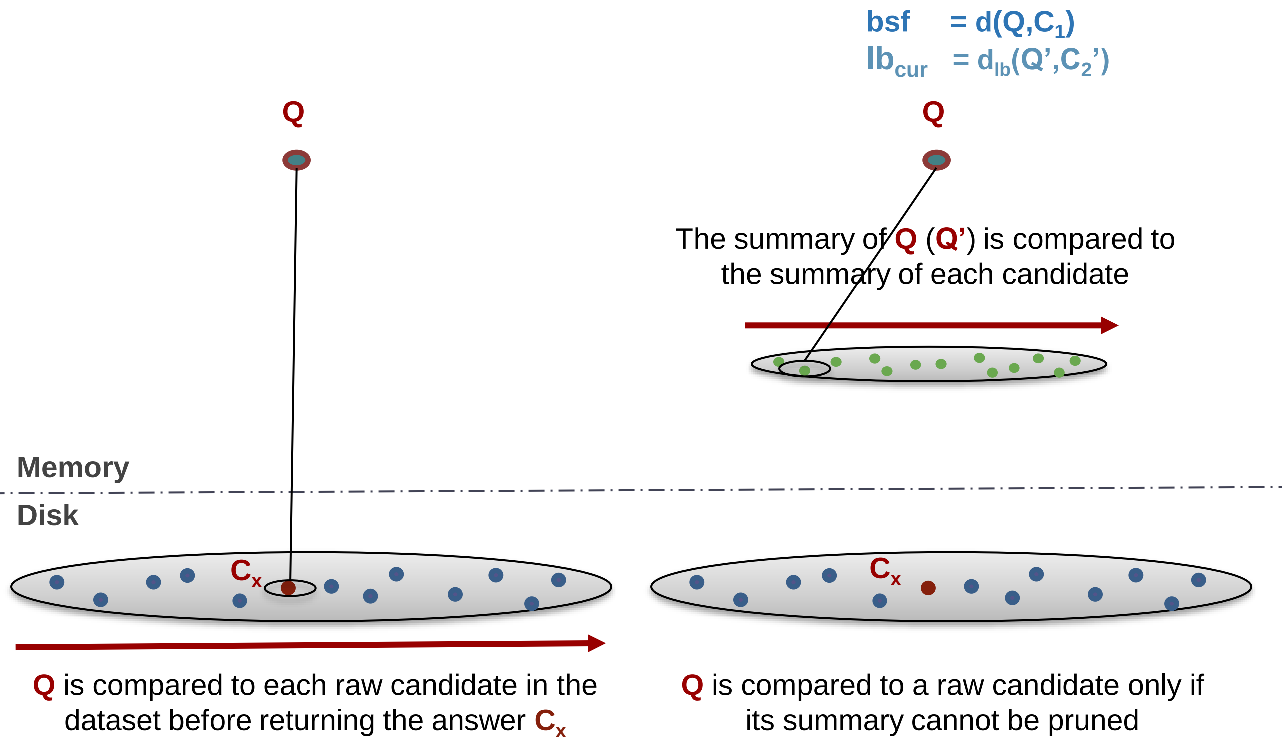
Answering a similarity search query using different access paths

Indexes vs. Scans



(a) Serial scan

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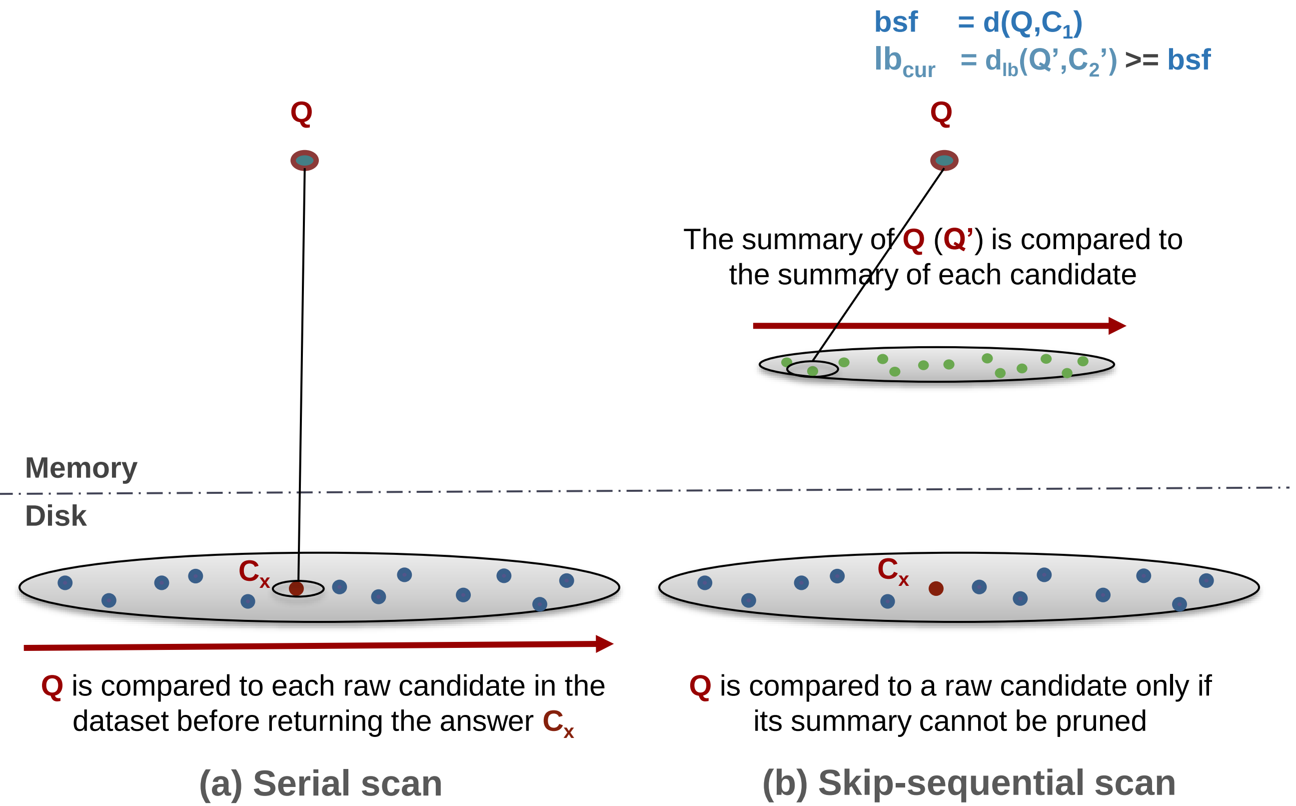
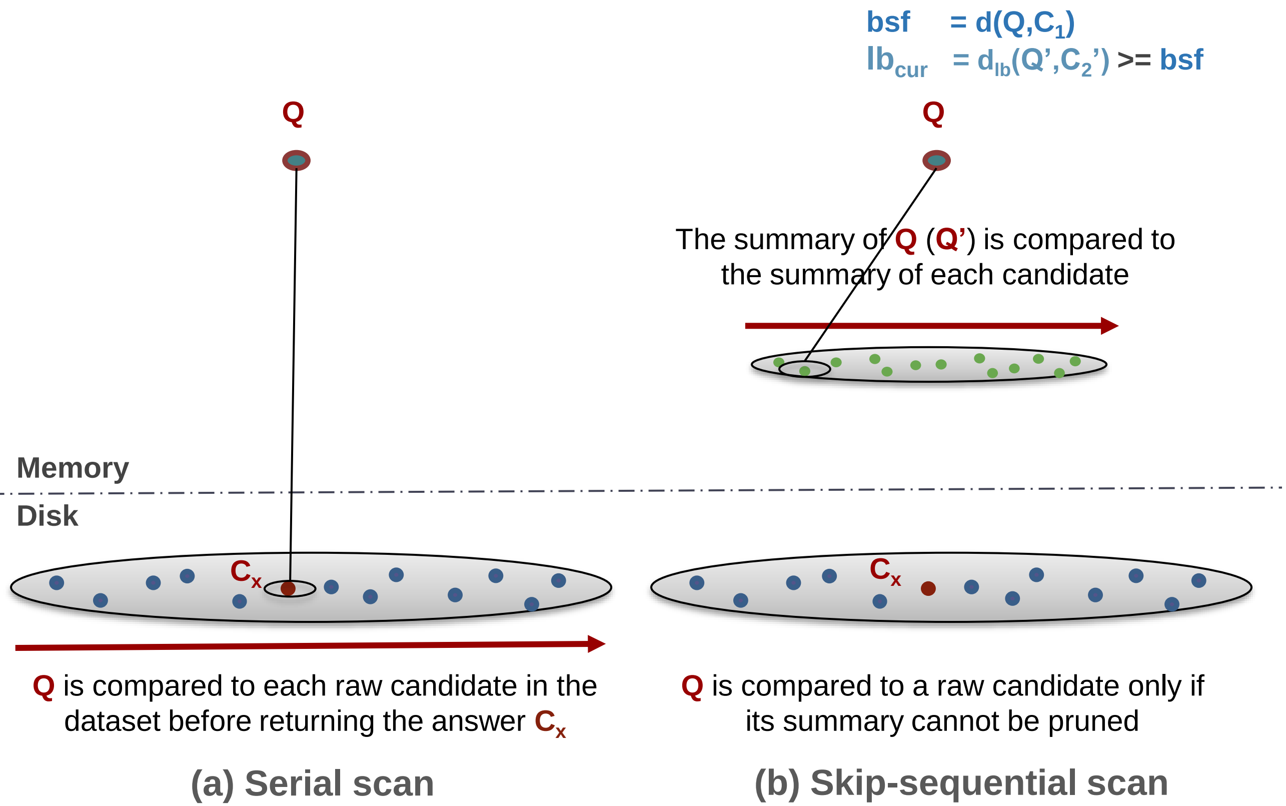
<u>Answering a similarity search query using different access paths</u>

Indexes vs. Scans



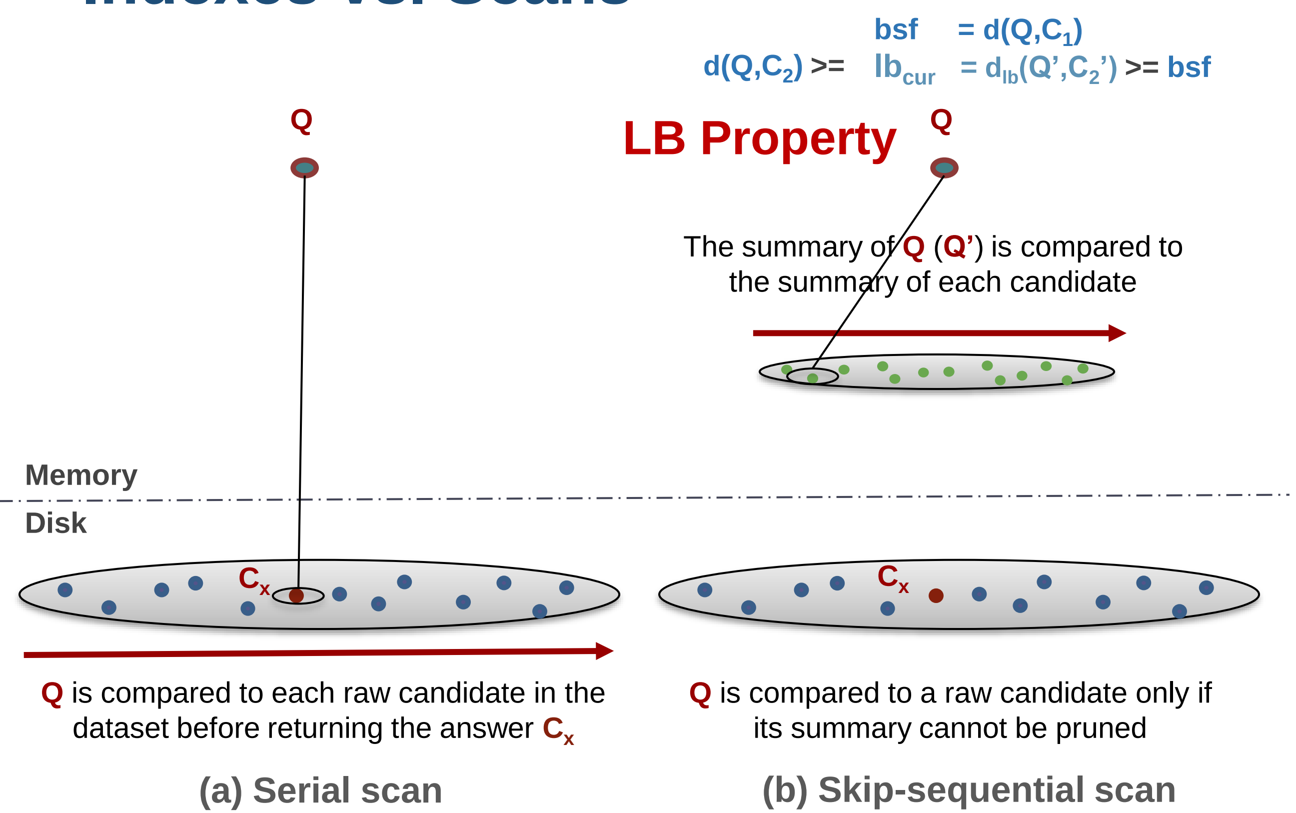
Answering a similarity search query using different access paths

Indexes vs. Scans



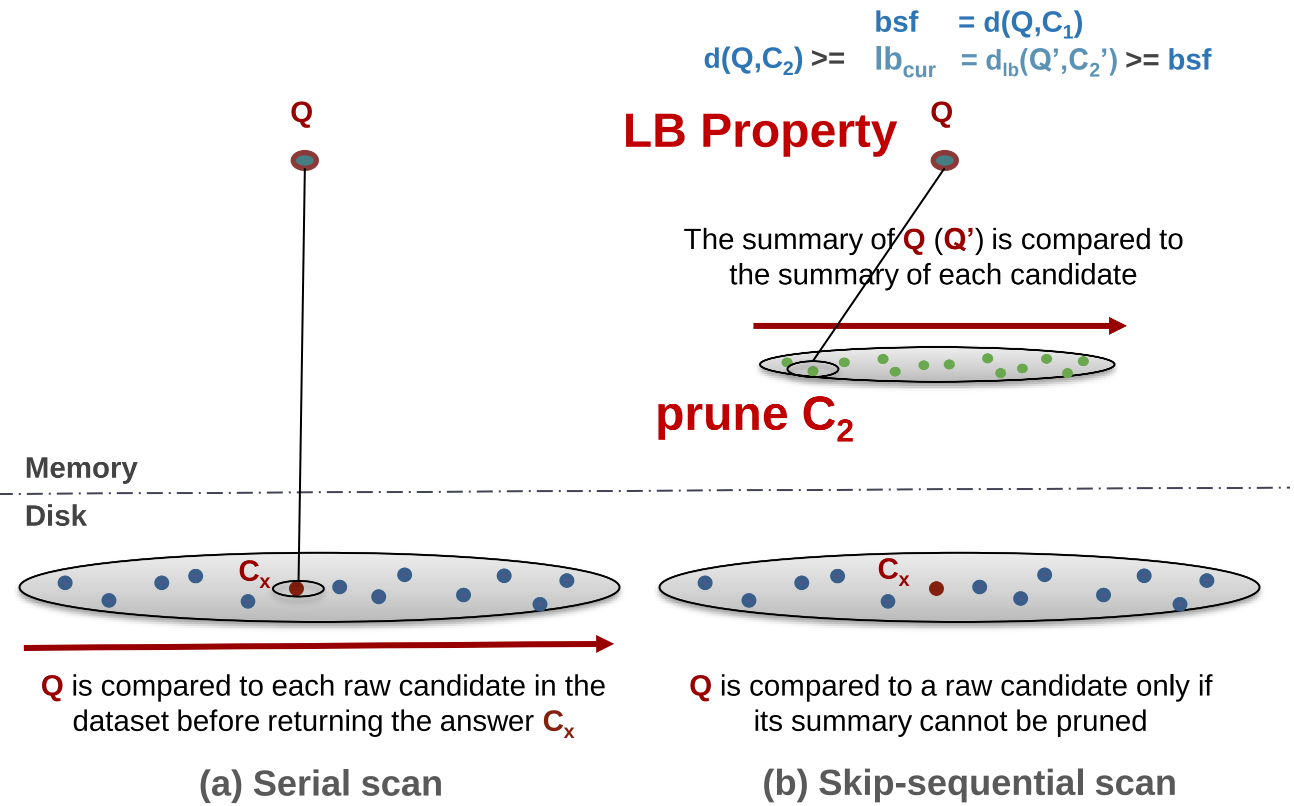
Answering a similarity search query using different access paths

Indexes vs. Scans



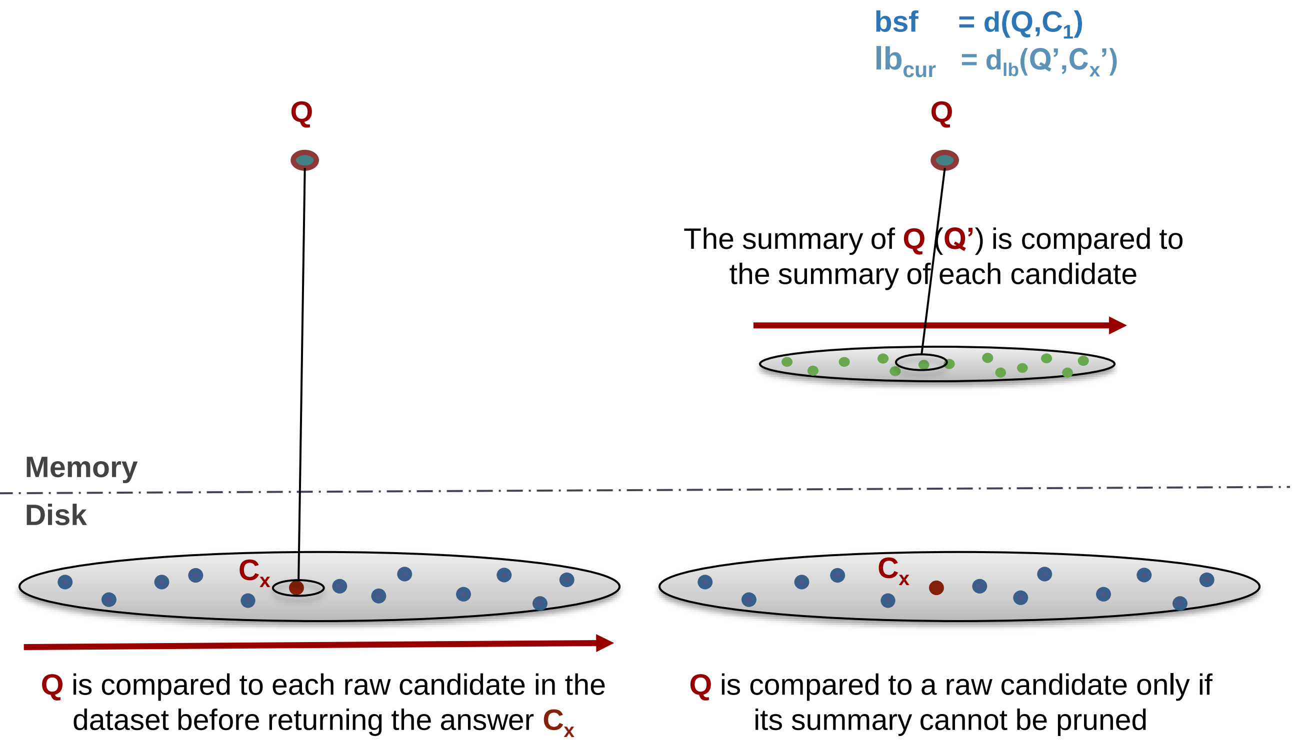
<u>**Answering a similarity search query using different access paths**</u>

Indexes vs. Scans



Answering a similarity search query using different access paths

Indexes vs. Scans



(a) Serial scan

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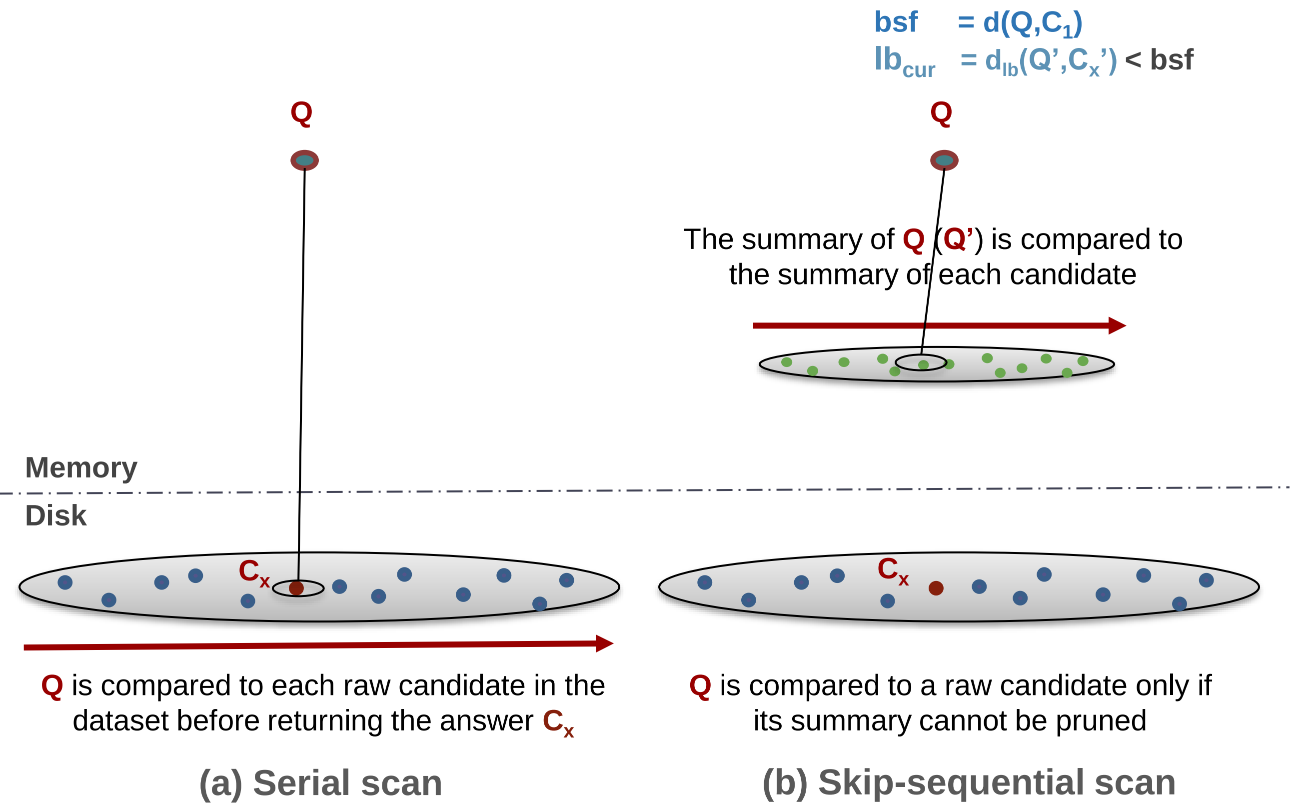
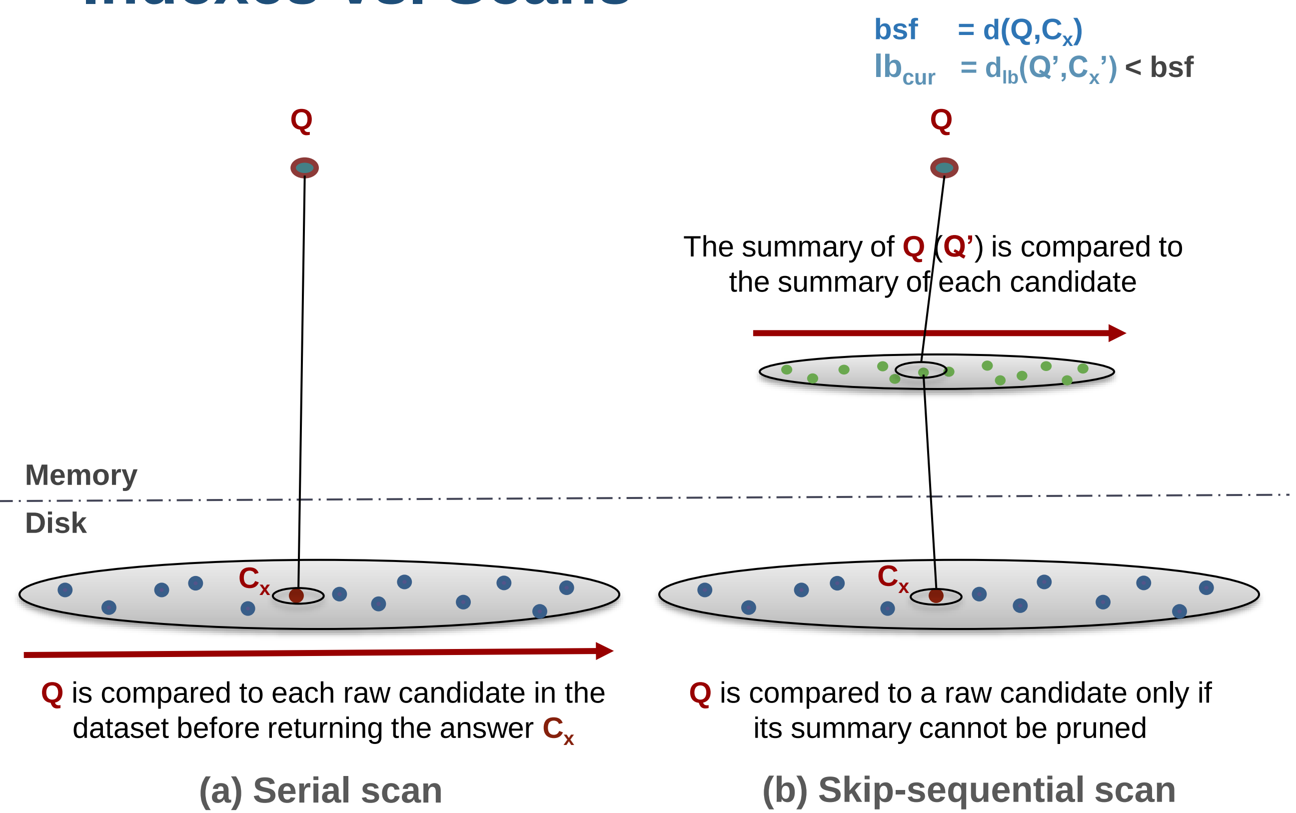
Answering a similarity search query using different access paths

Indexes vs. Scans



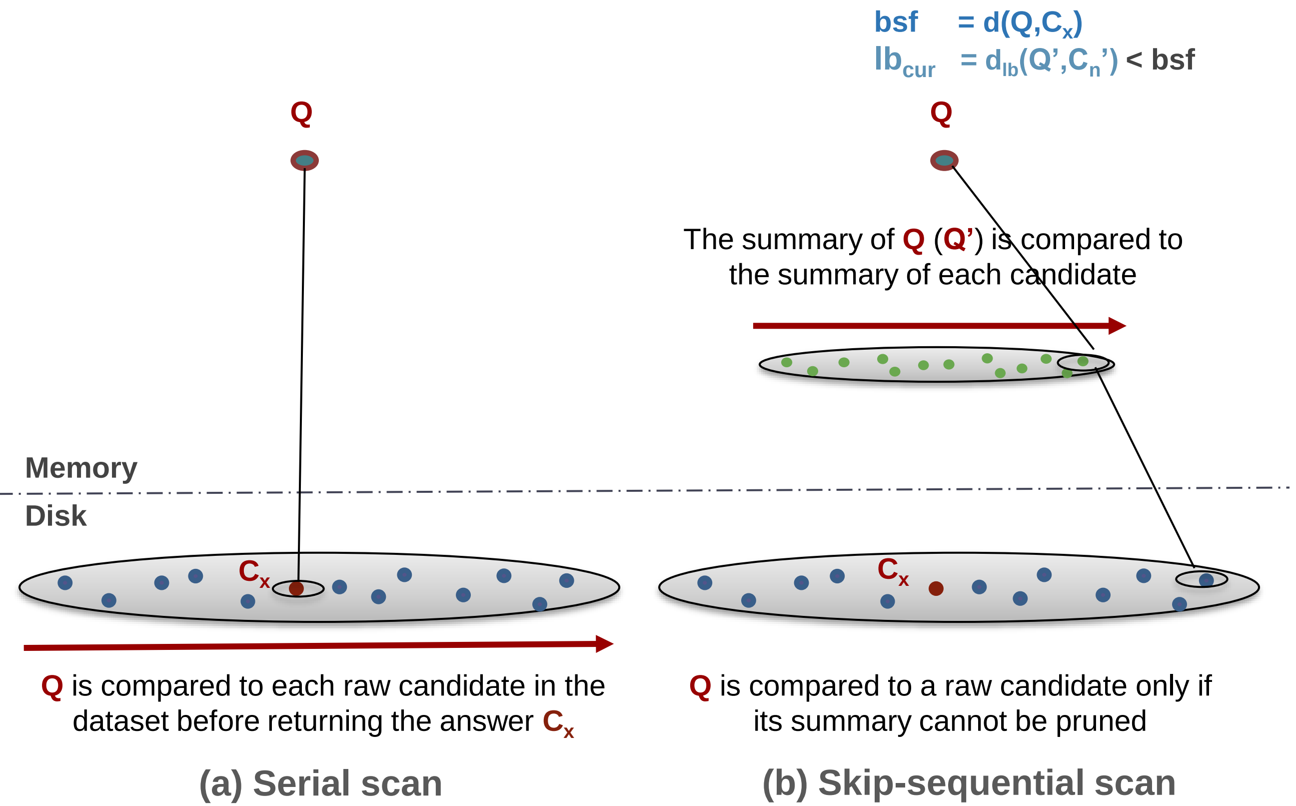
Answering a similarity search query using different access paths

Indexes vs. Scans



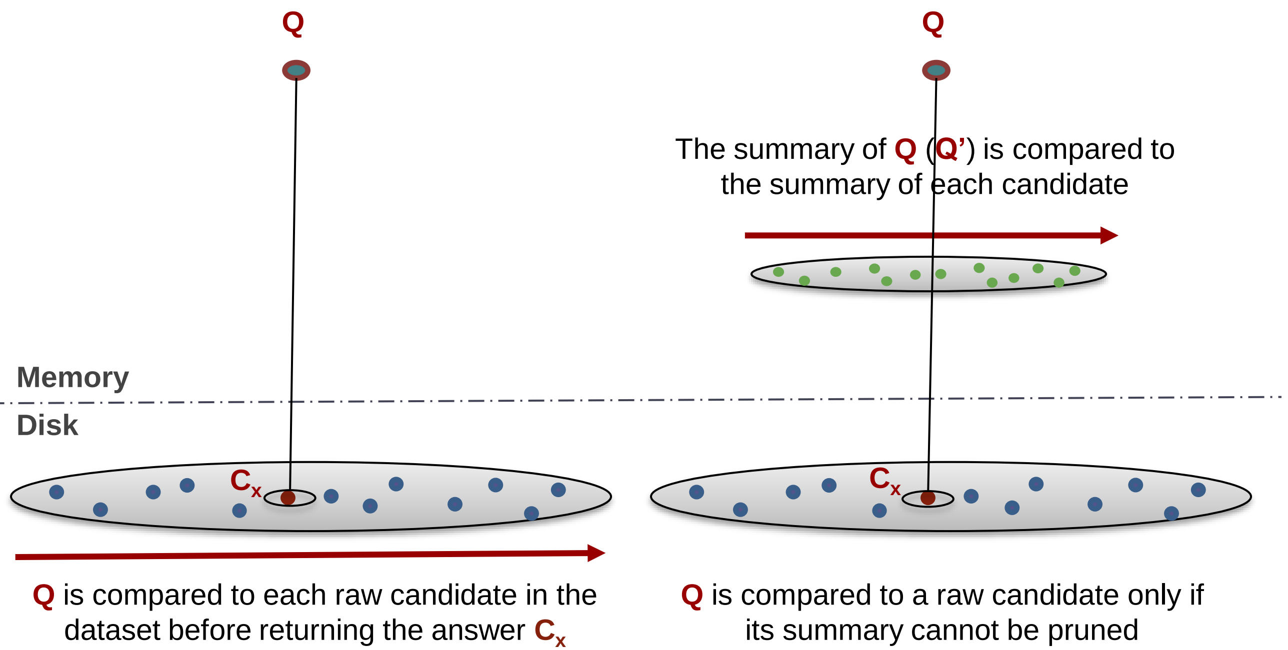
<u>**Answering a similarity search query using different access paths**</u>

Indexes vs. Scans



Answering a similarity search query using different access paths

Indexes vs. Scans

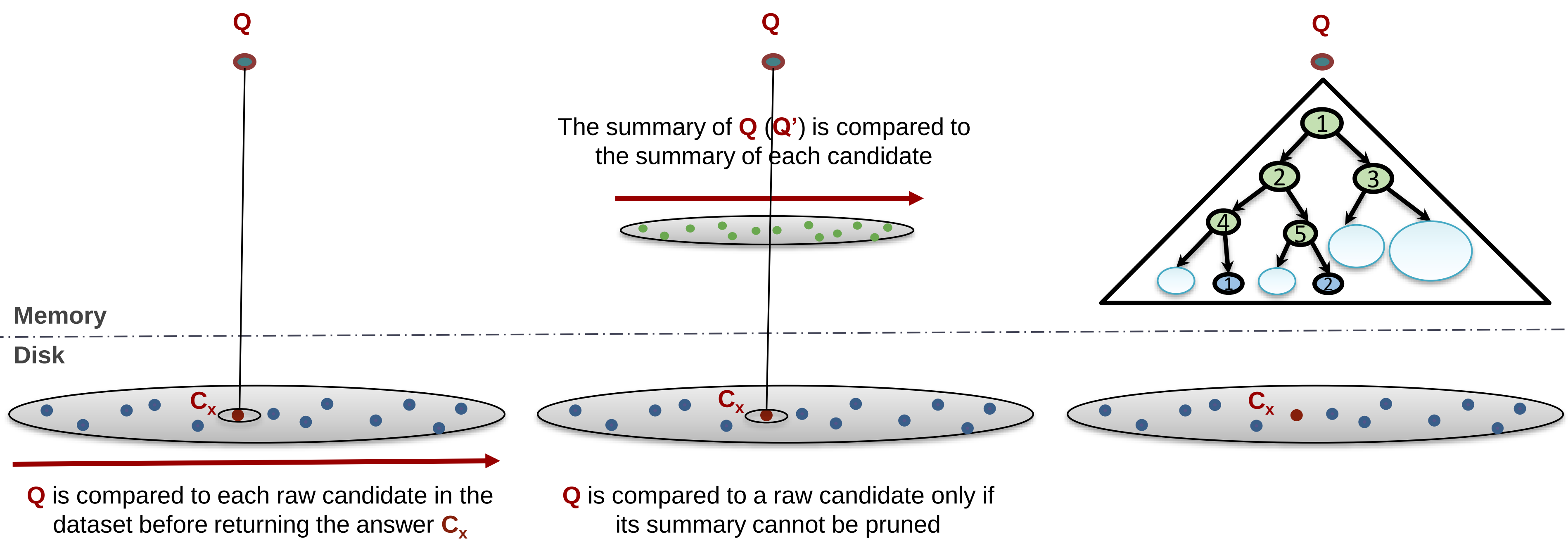


(a) Serial scan

(b) Skip-sequential scan

Answering a similarity search query using different access paths

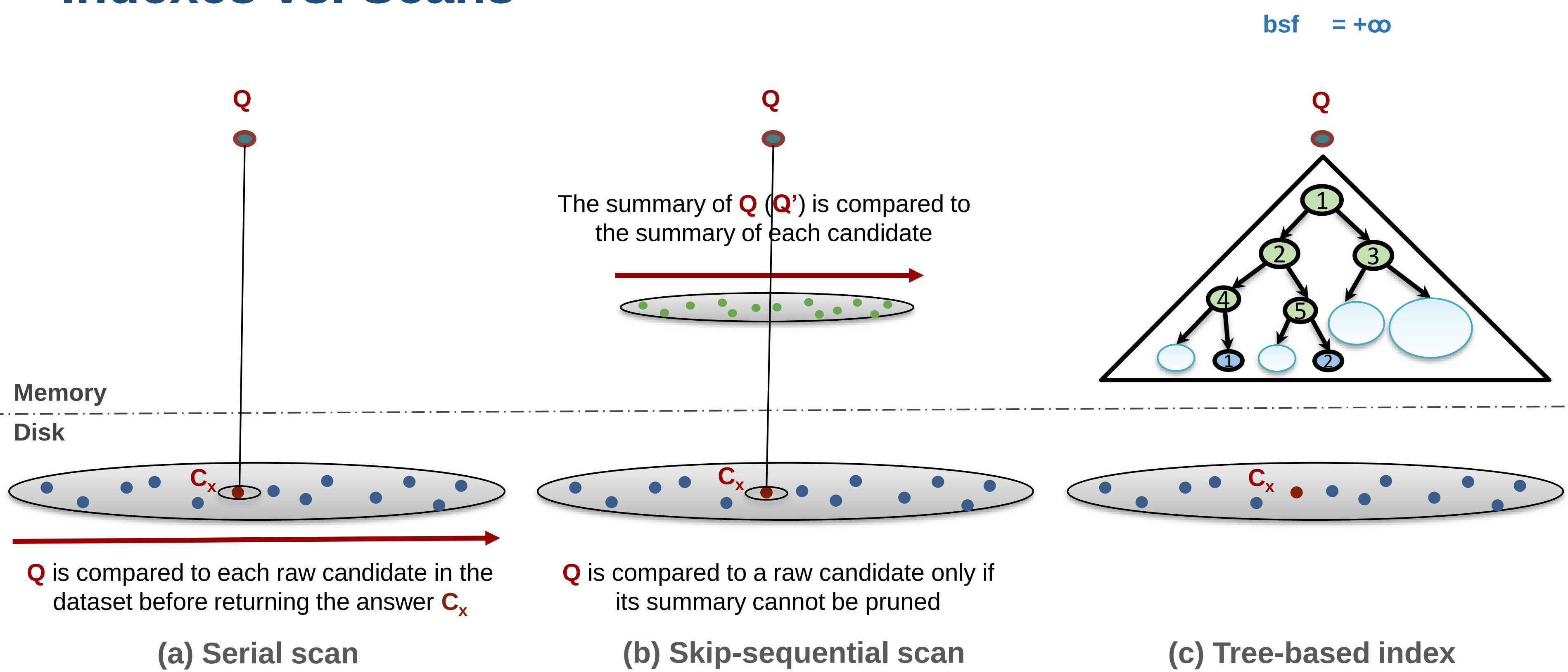
Indexes vs. Scans



(a) Serial scan (b) Skip-sequential scan (c) Tree-based index

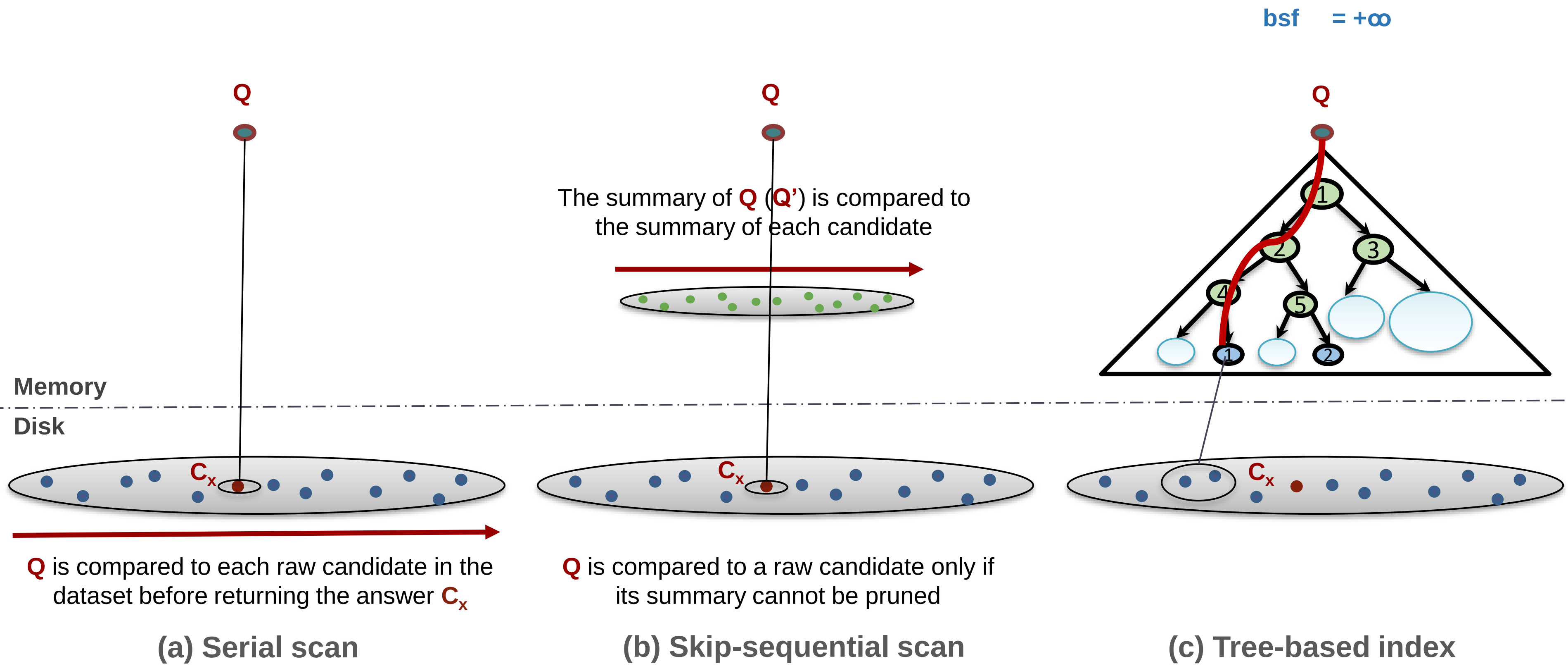
<u>Answering a similarity search query using different access paths</u>

Indexes vs. Scans



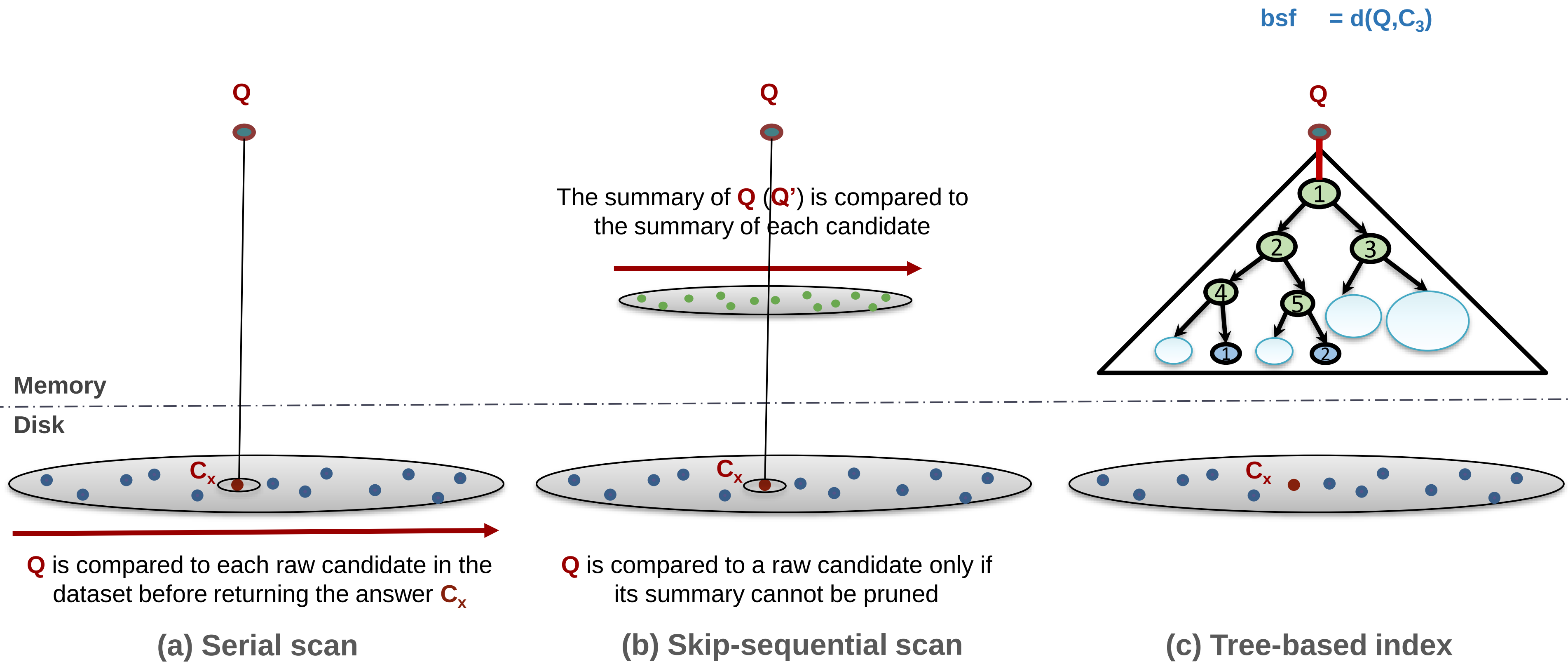
<u>**Answering a similarity search query using different access paths**</u>

Indexes vs. Scans



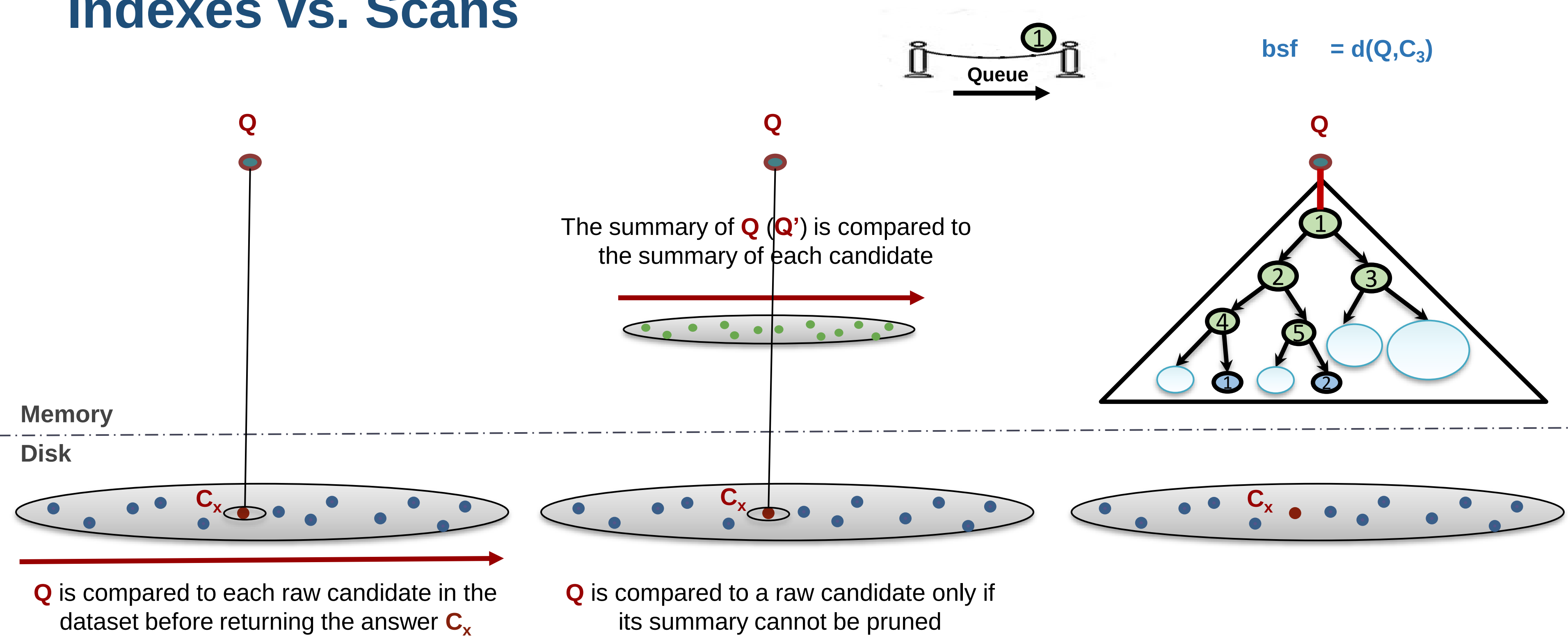
<u>**Answering a similarity search query using different access paths**</u>

Indexes vs. Scans



<u>Answering a similarity search query using different access paths</u>

Indexes vs. Scans



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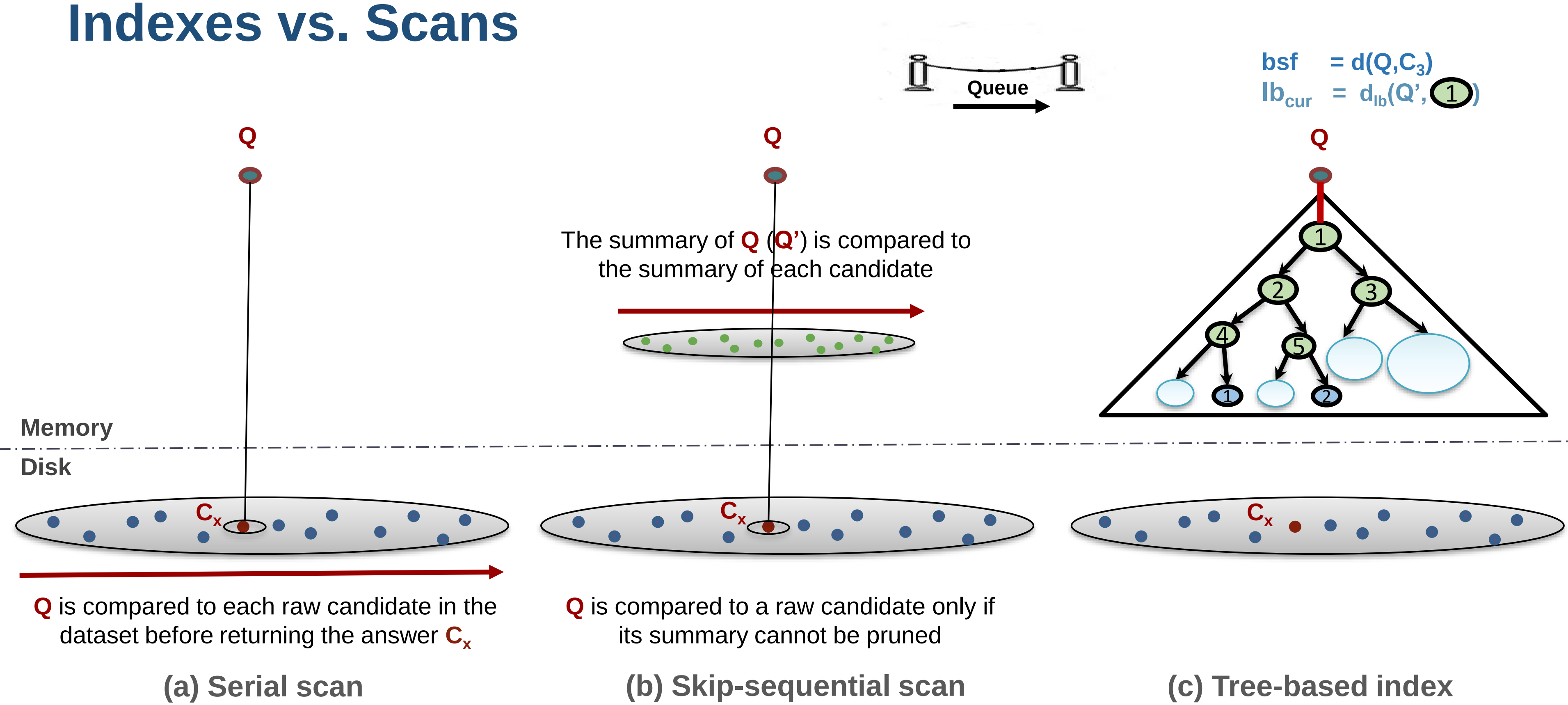
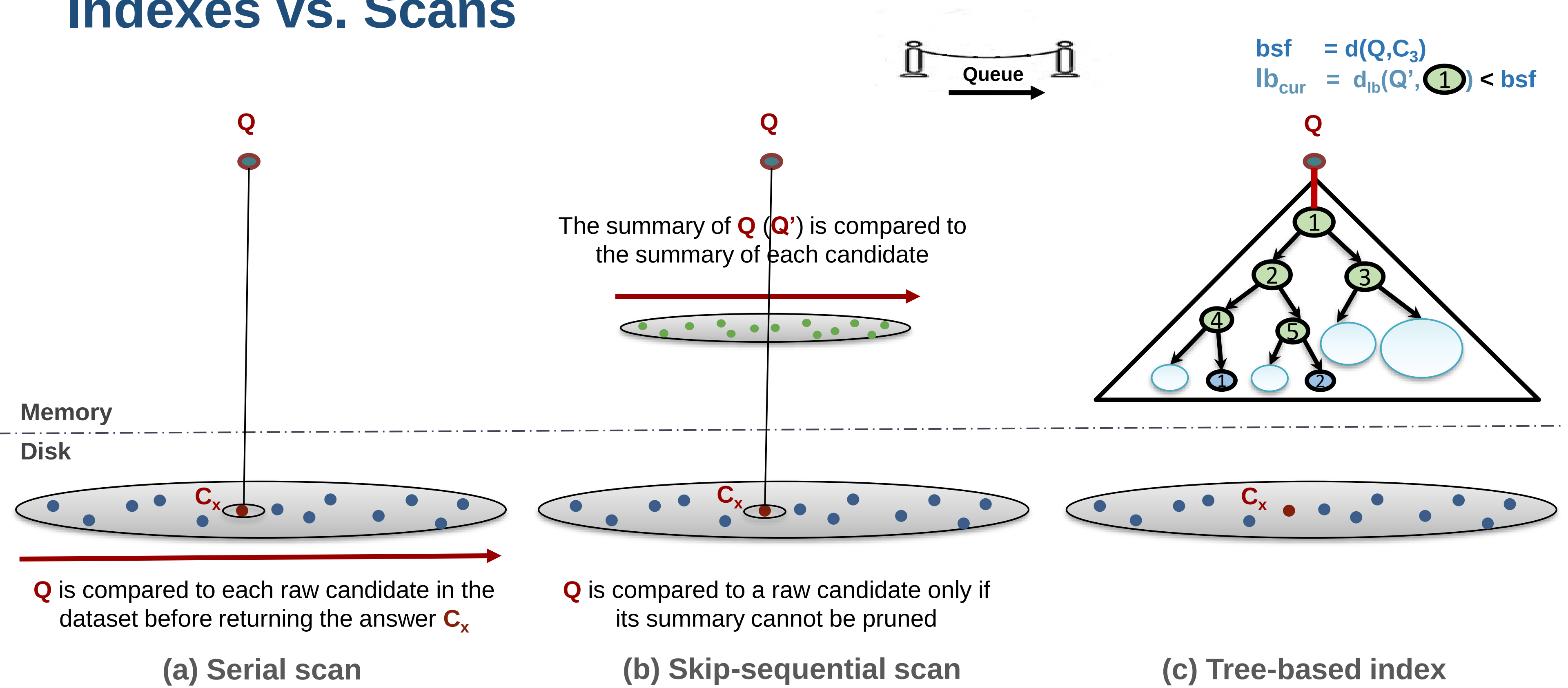
Answering a similarity search query using different access paths

Indexes vs. Scans



Answering a similarity search query using different access paths

Indexes vs. Scans



Answering a similarity search query using different access paths

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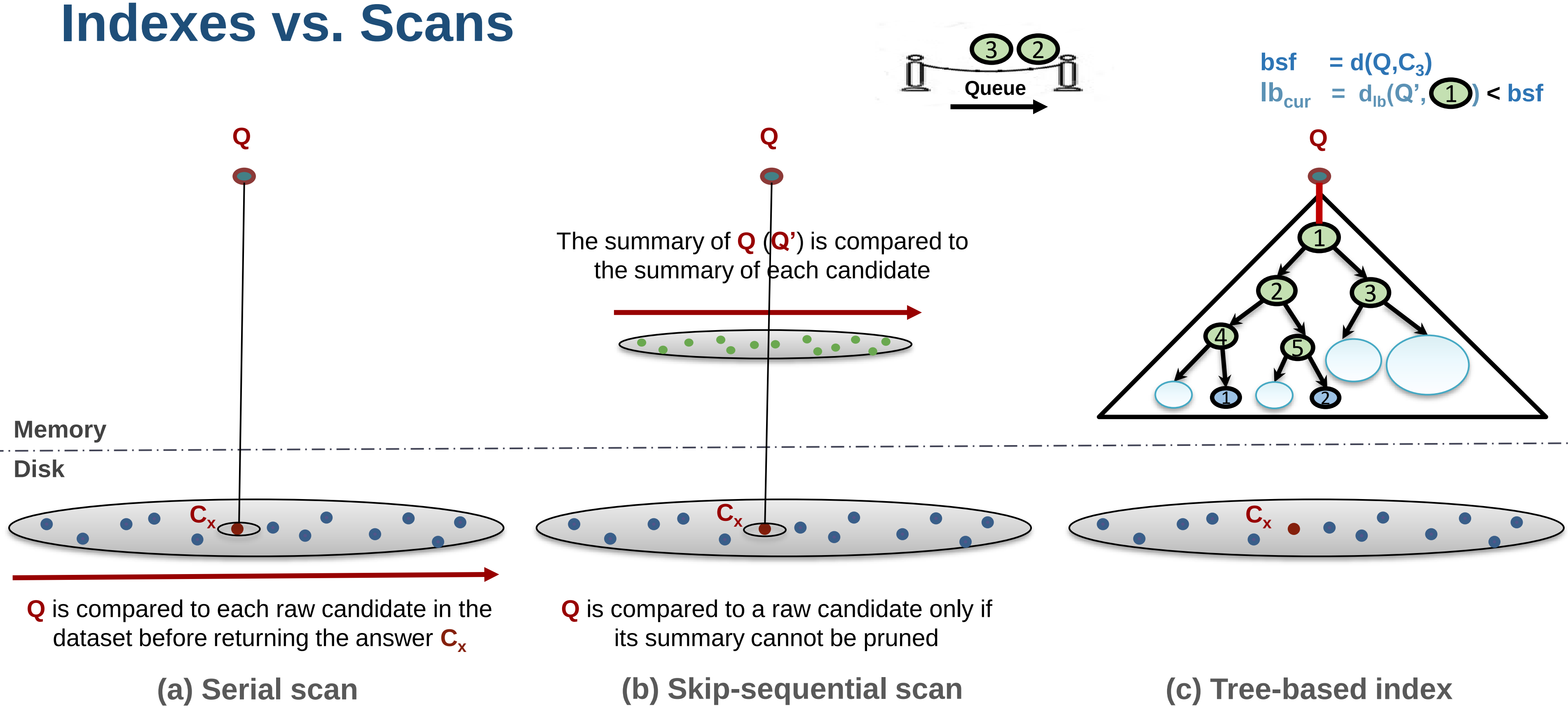

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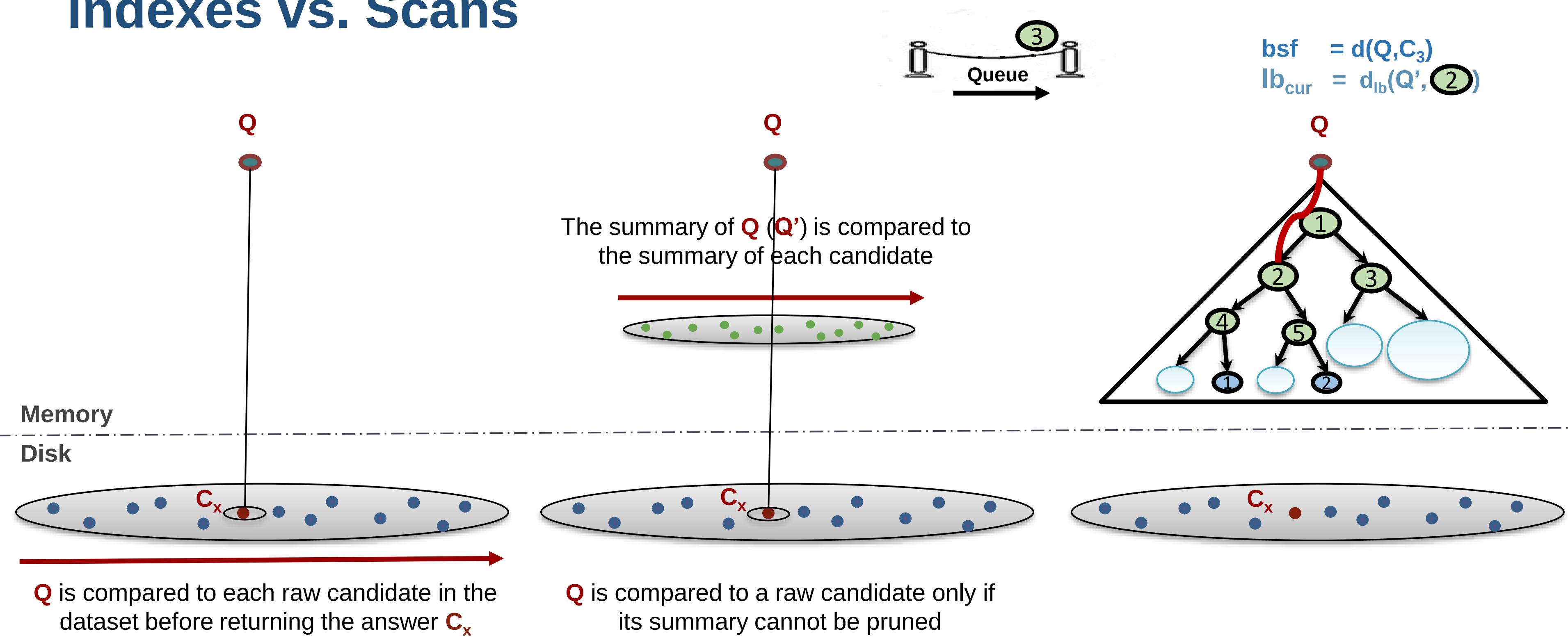
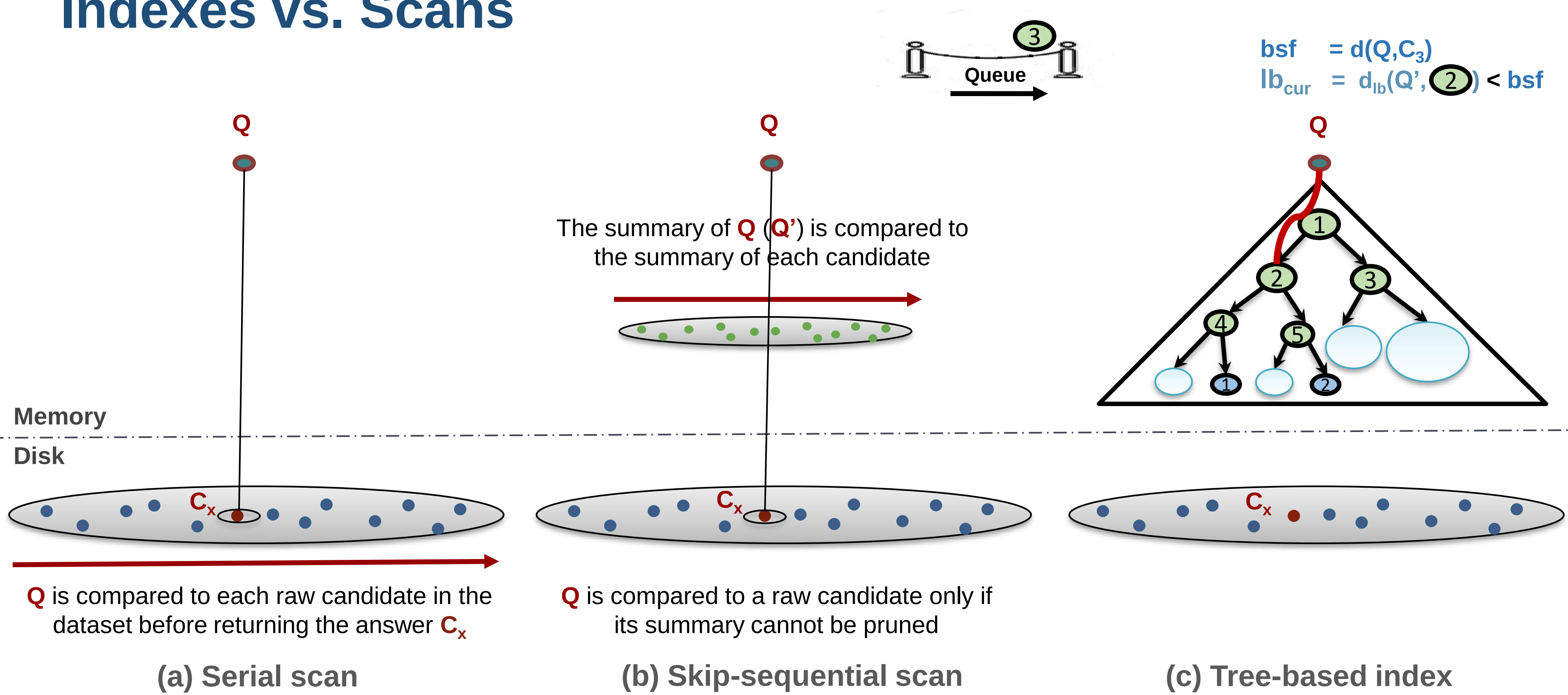
Indexes vs. Scans



(a) Serial scan (b) Skip-sequential scan (c) Tree-based index

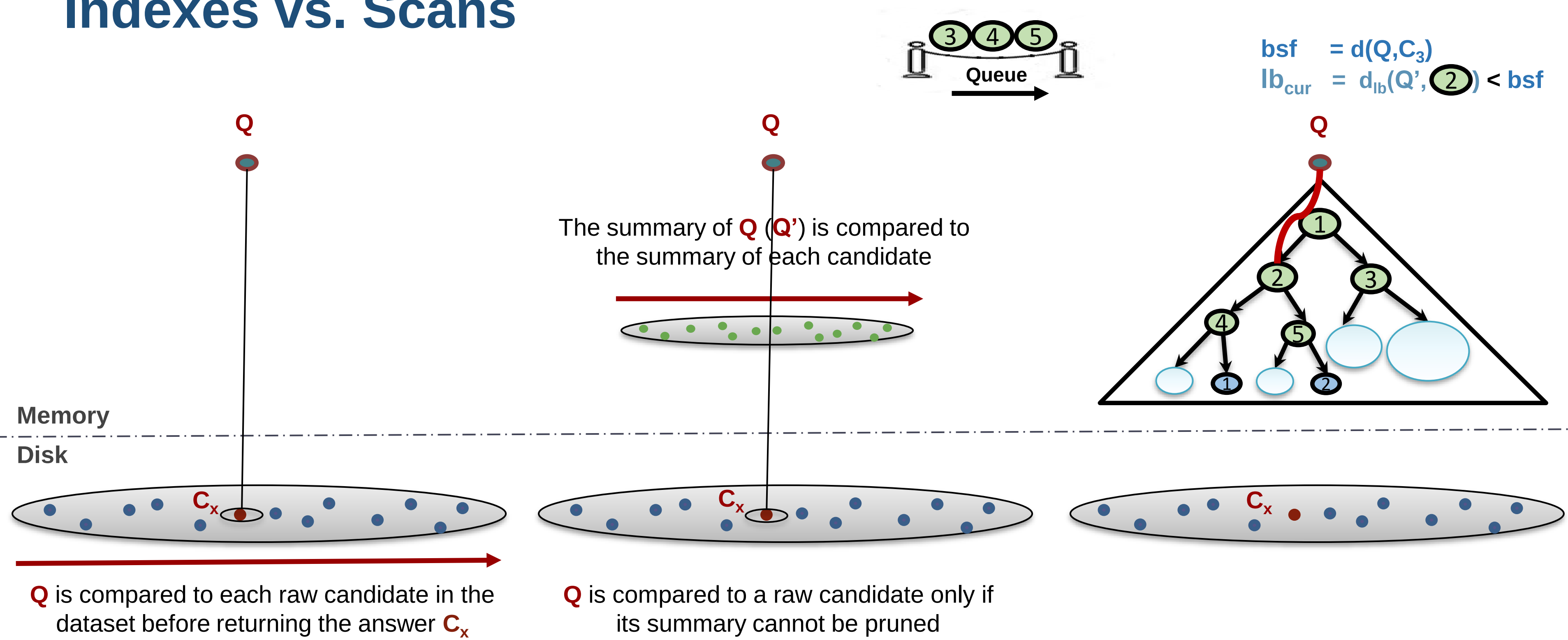
Answering a similarity search query using different access paths

Indexes vs. Scans



Answering a similarity search query using different access paths

Indexes vs. Scans



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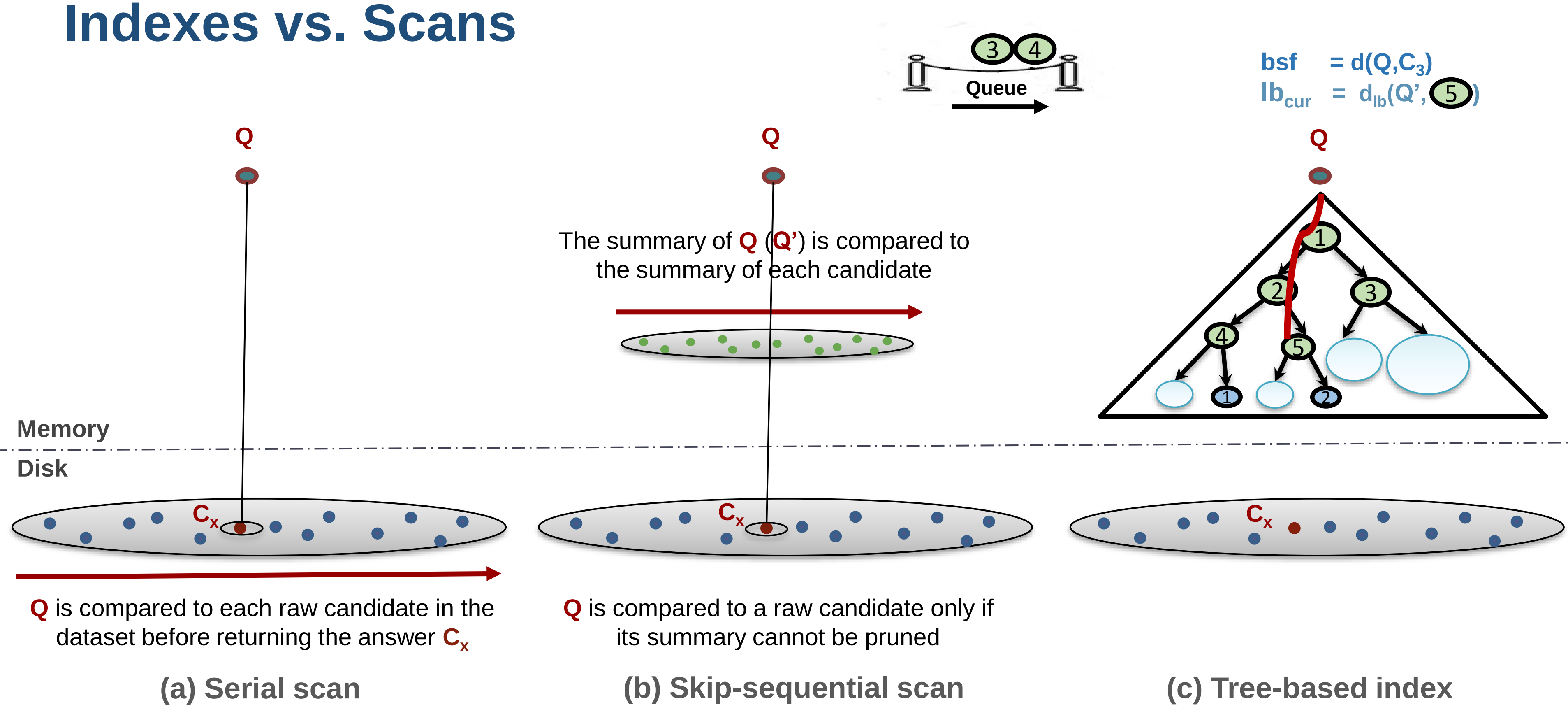
Indexes vs. Scans



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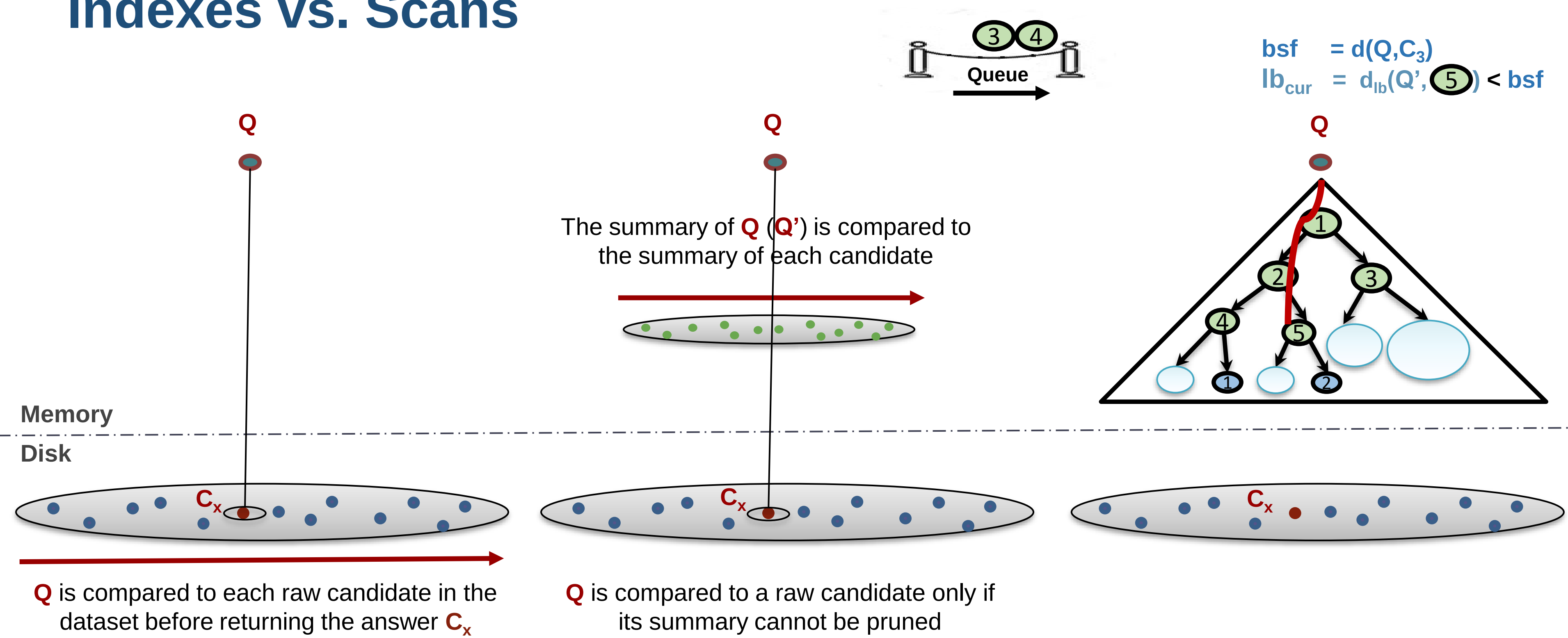
Indexes vs. Scans



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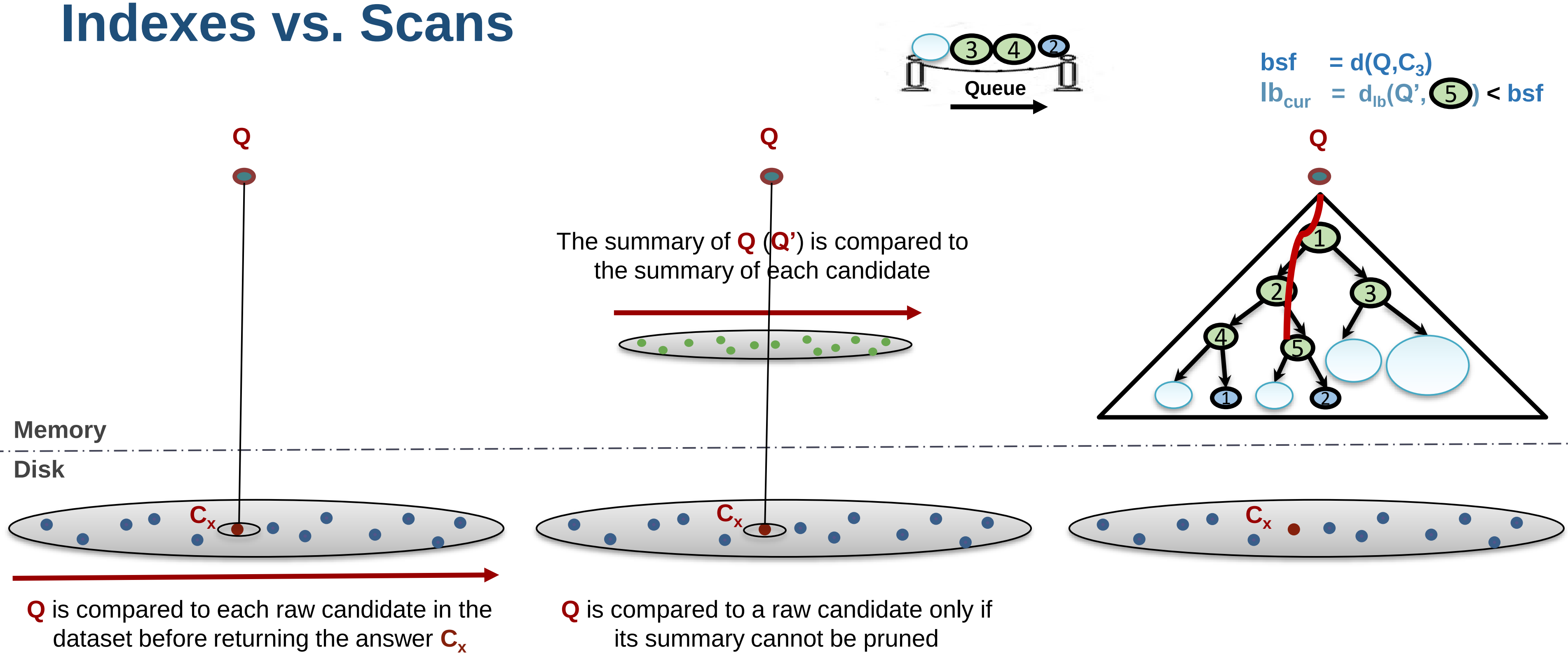

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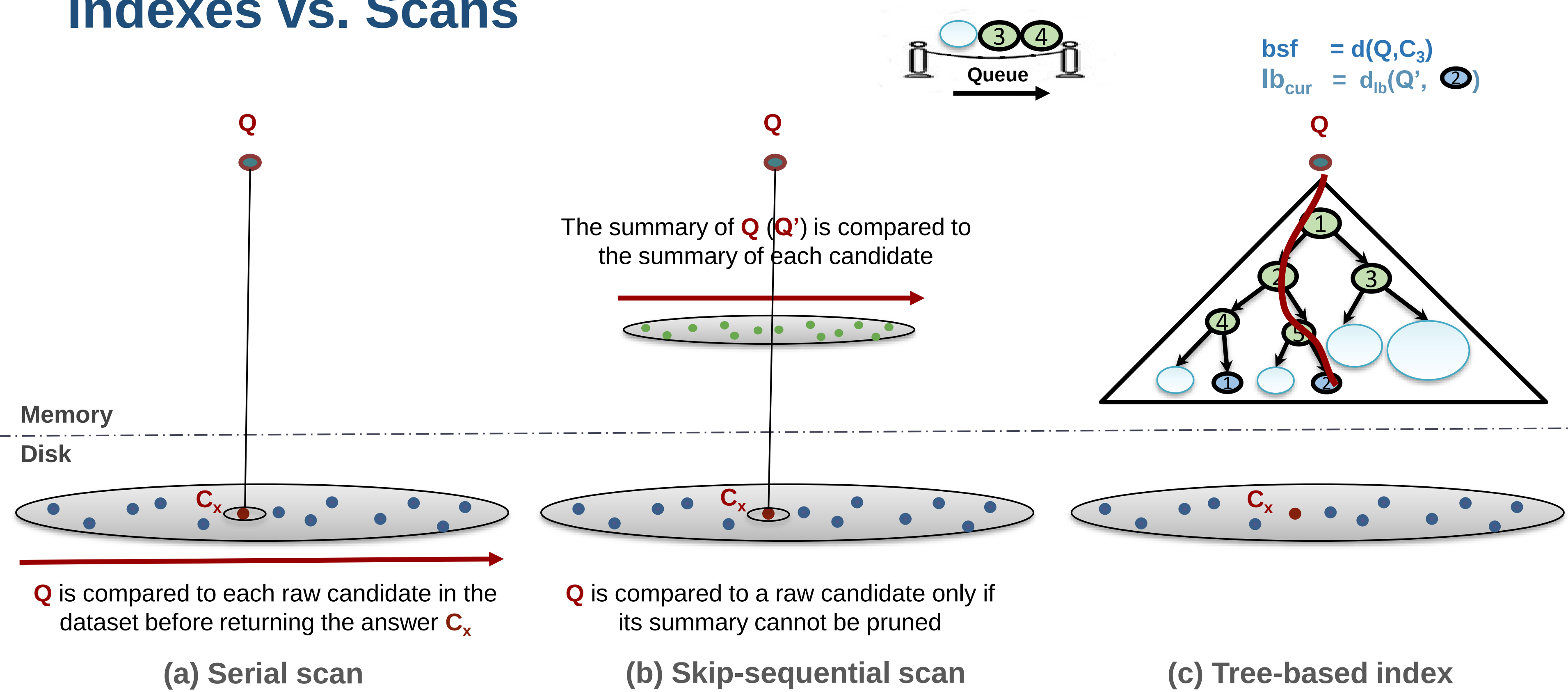

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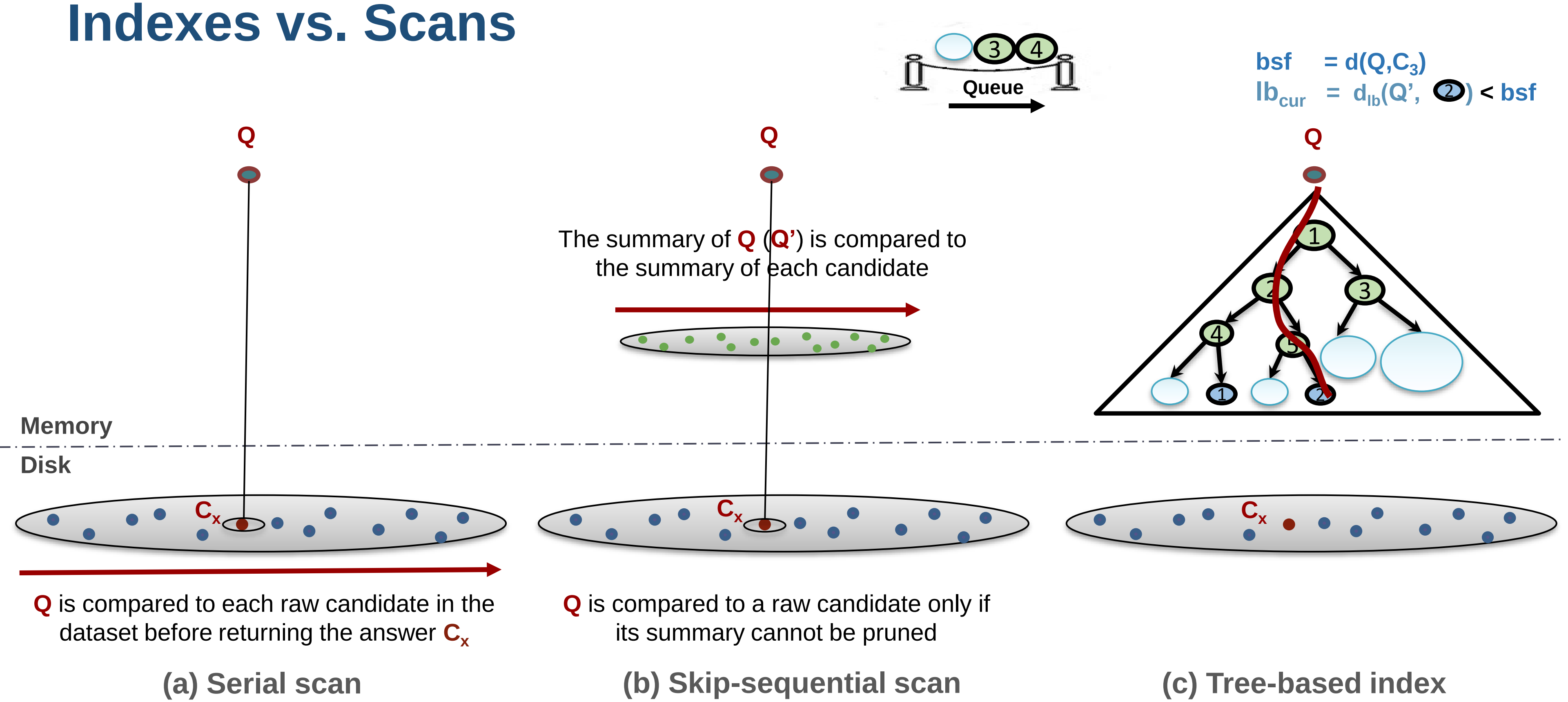
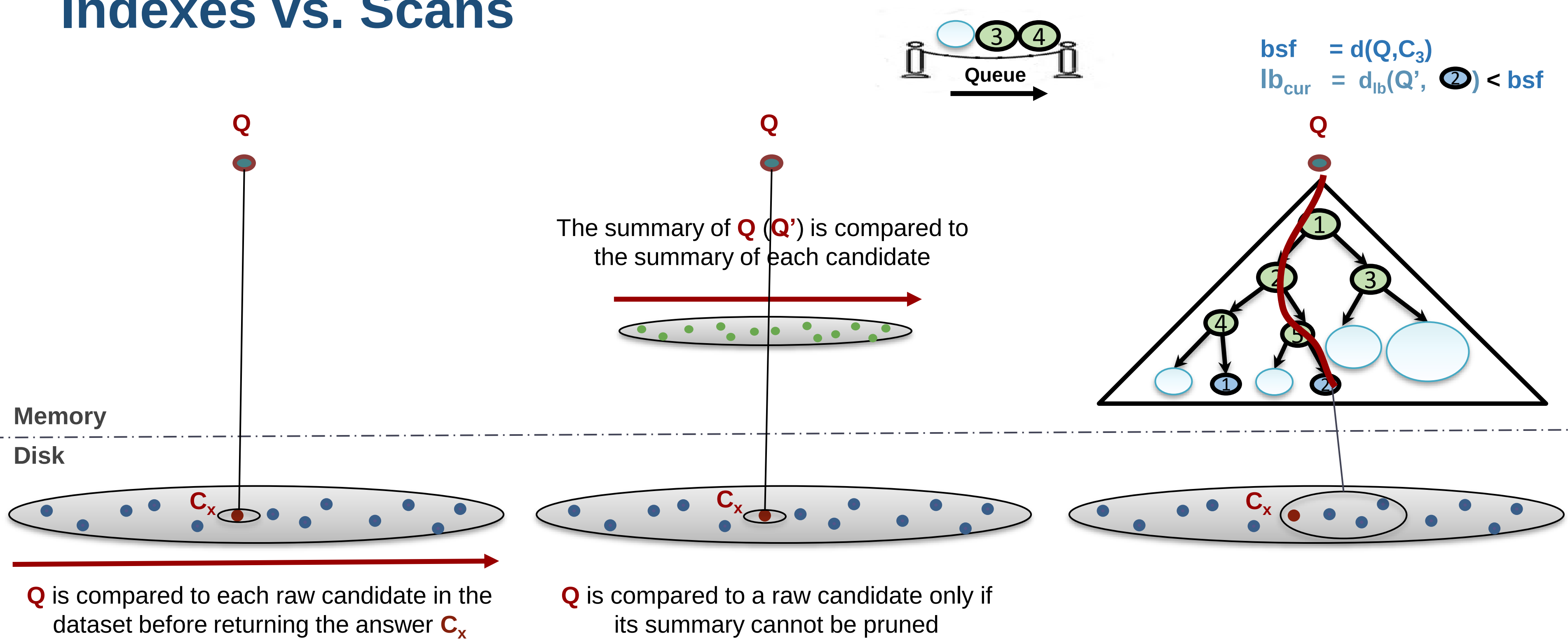


Answering a similarity search query using different access paths

Indexes vs. Scans



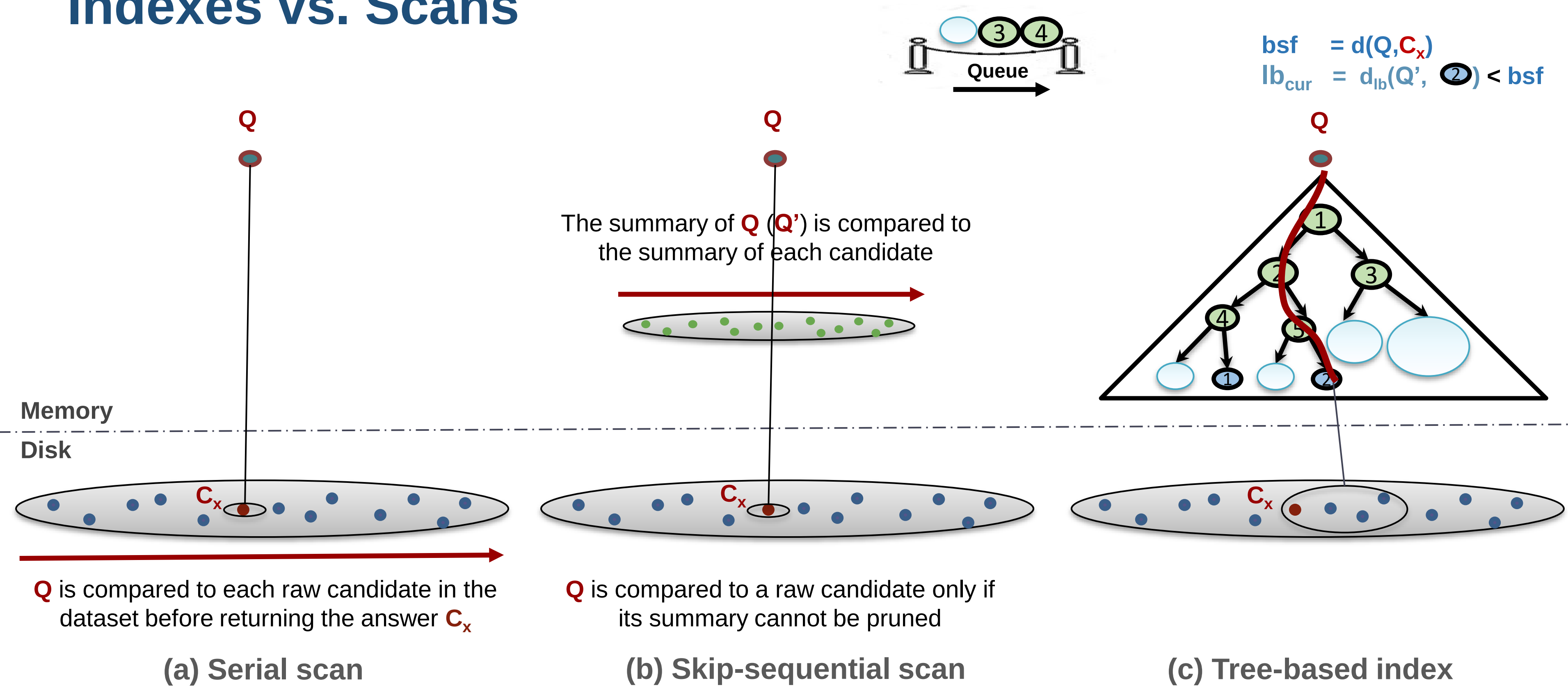
(a) Serial scan

(b) Skip-sequential scan

(c) Tree-based index

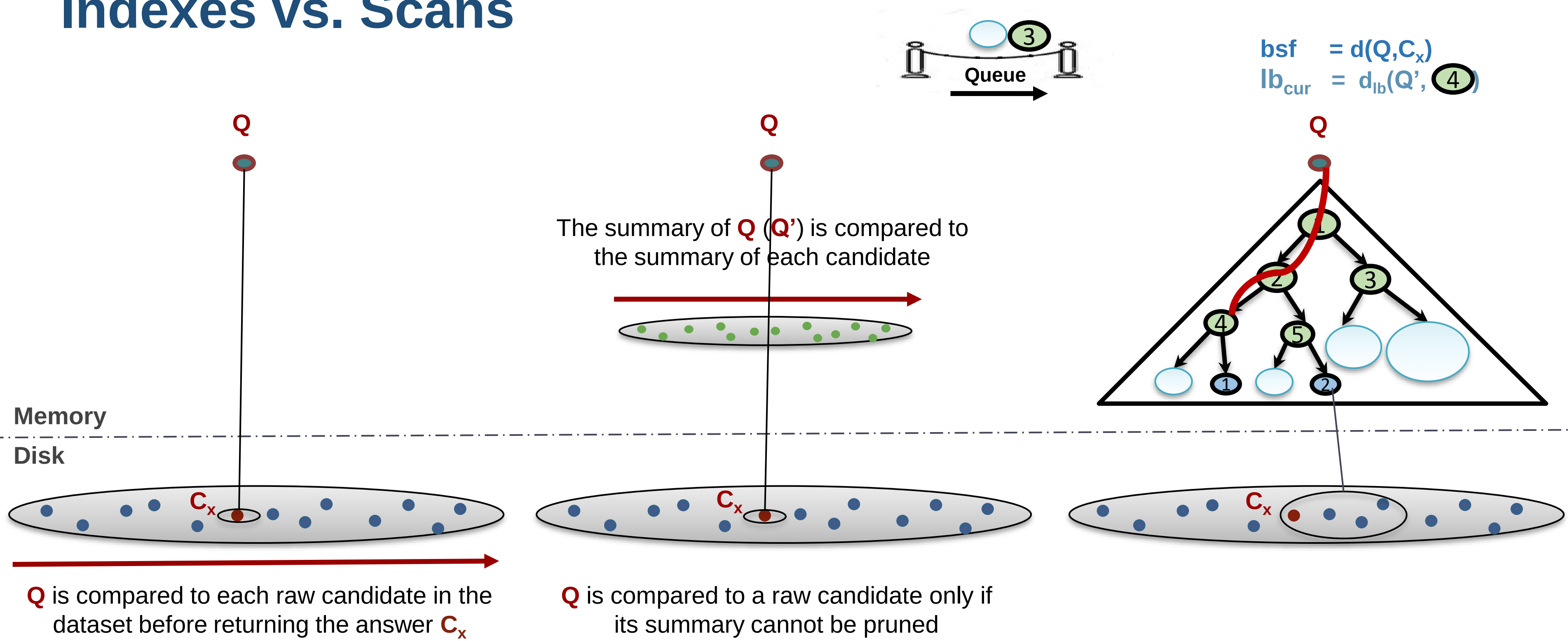
Answering a similarity search query using different access paths

Indexes vs. Scans



Answering a similarity search query using different access paths

Indexes vs. Scans



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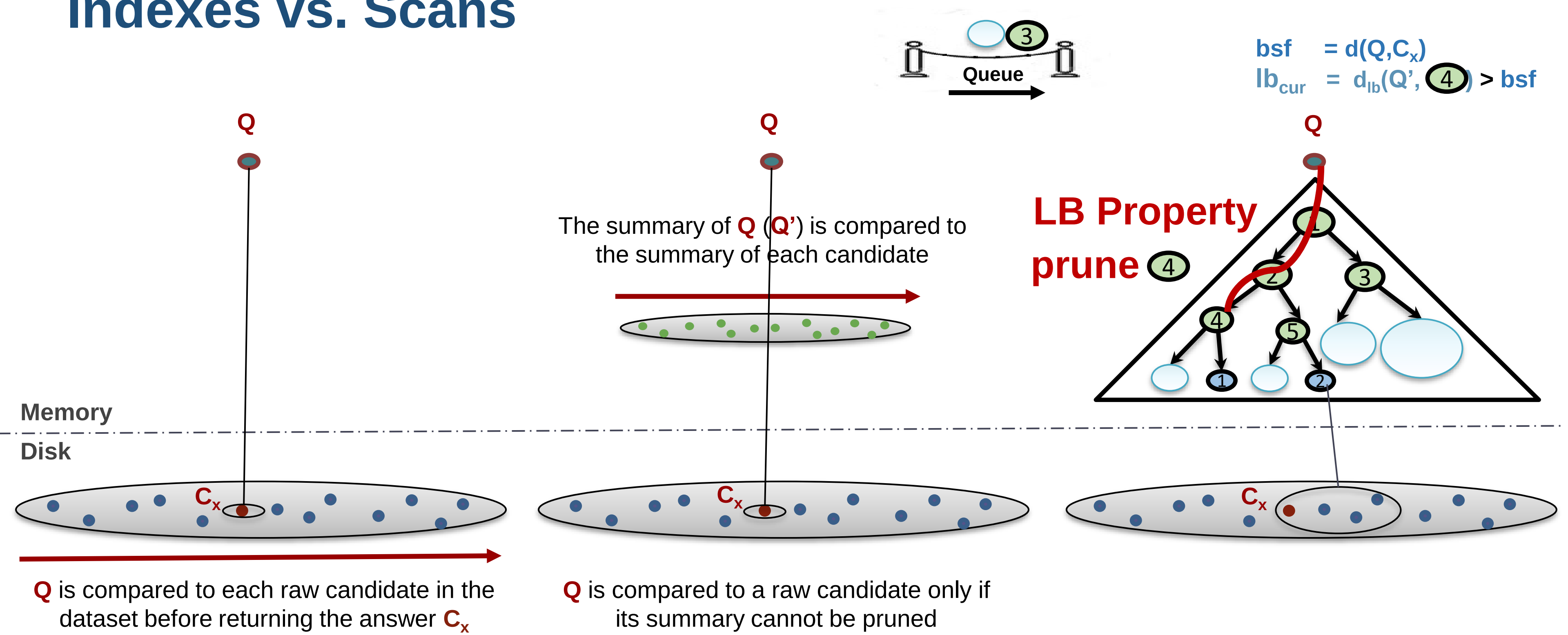
Answering a similarity search query using different access paths

Indexes vs. Scans



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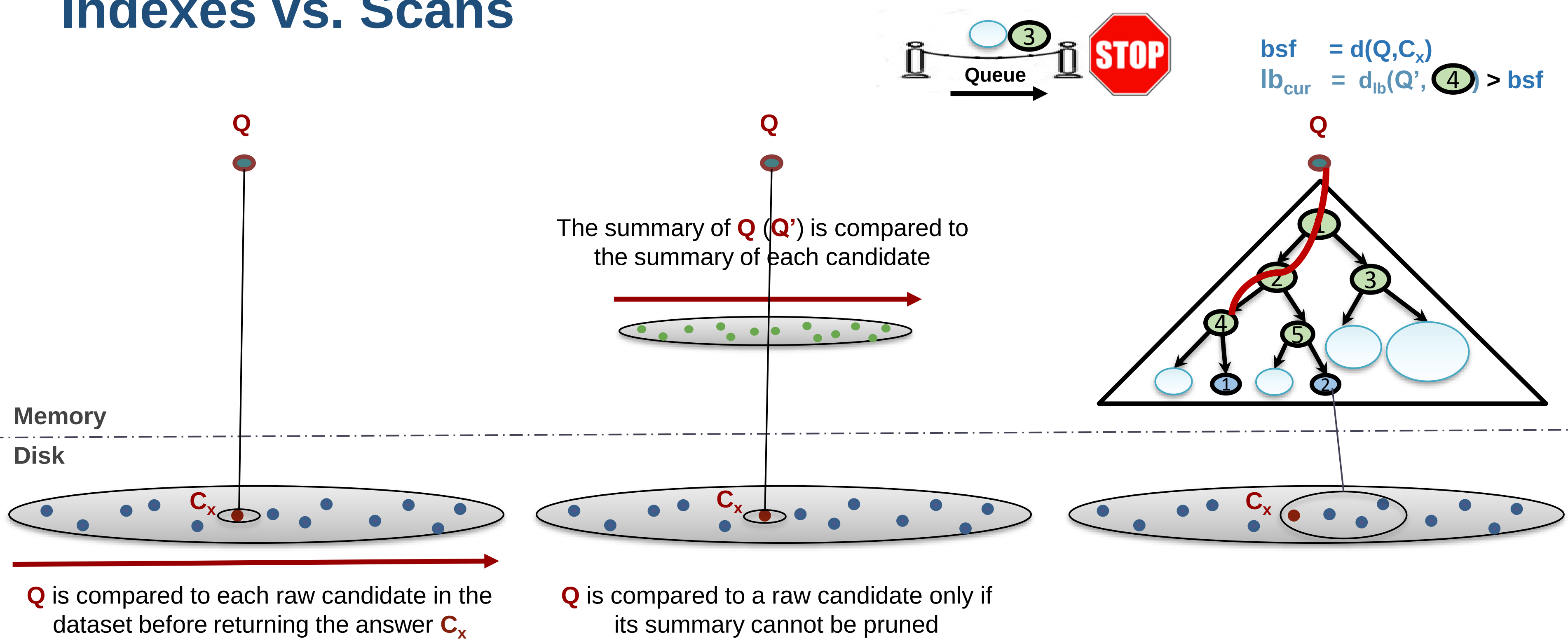
Answering a similarity search query using different access paths

Indexes vs. Scans



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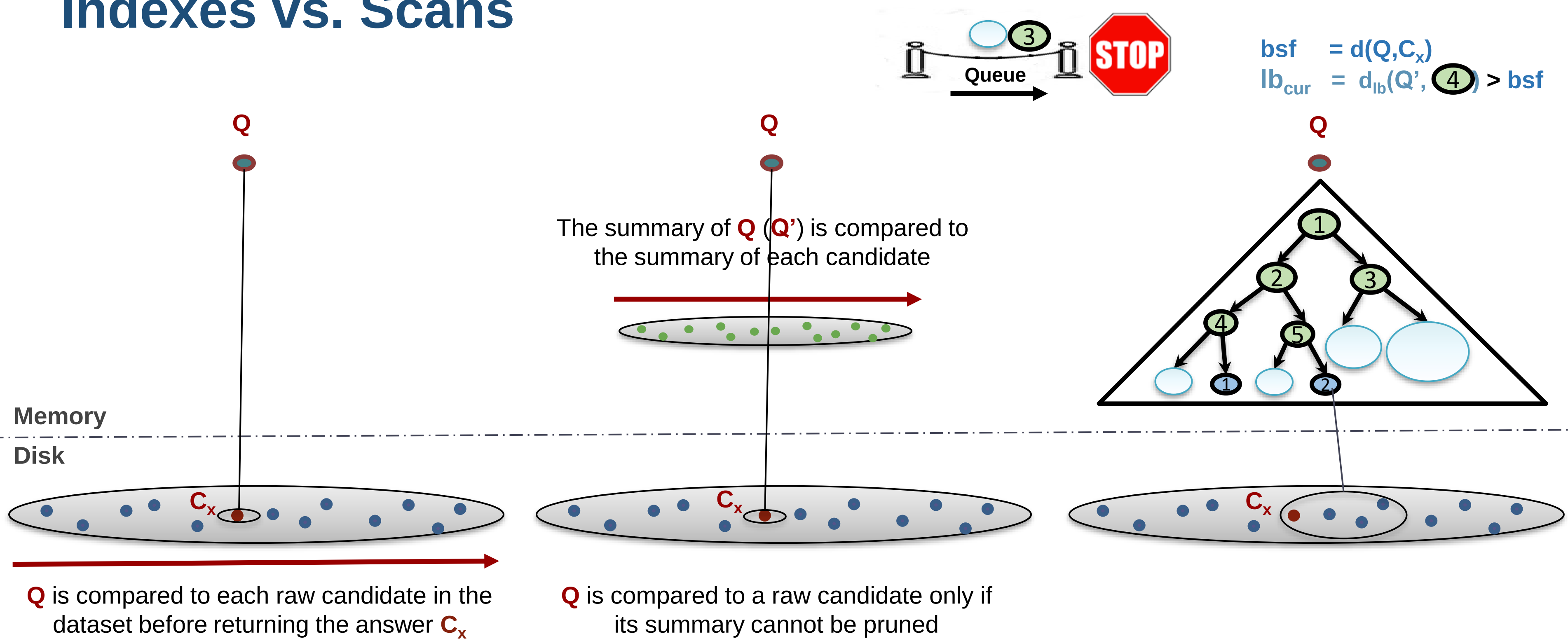
Answering a similarity search query using different access paths

Indexes vs. Scans

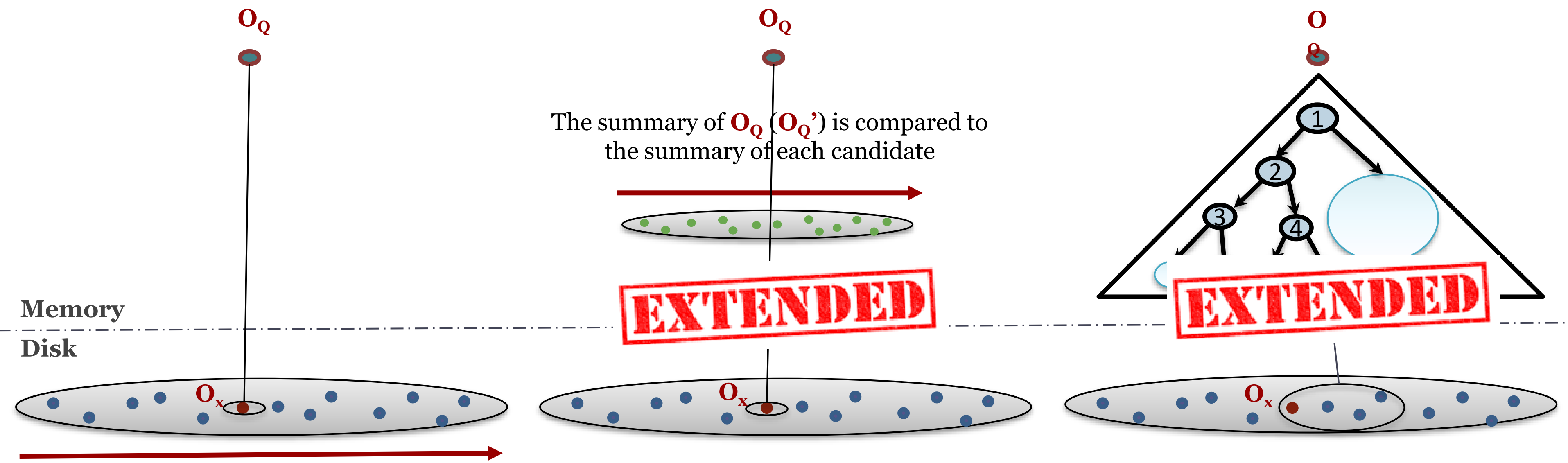


(a) Serial scan (b) Skip-sequential scan (c) Tree-based index

Answering a similarity search query using different access paths

Similarity Search
Data Series Extensions

Access Paths



O_Q is compared to each raw candidate in the dataset before returning the answer O_x

O_Q is compared to a raw candidate only if its summary cannot be pruned

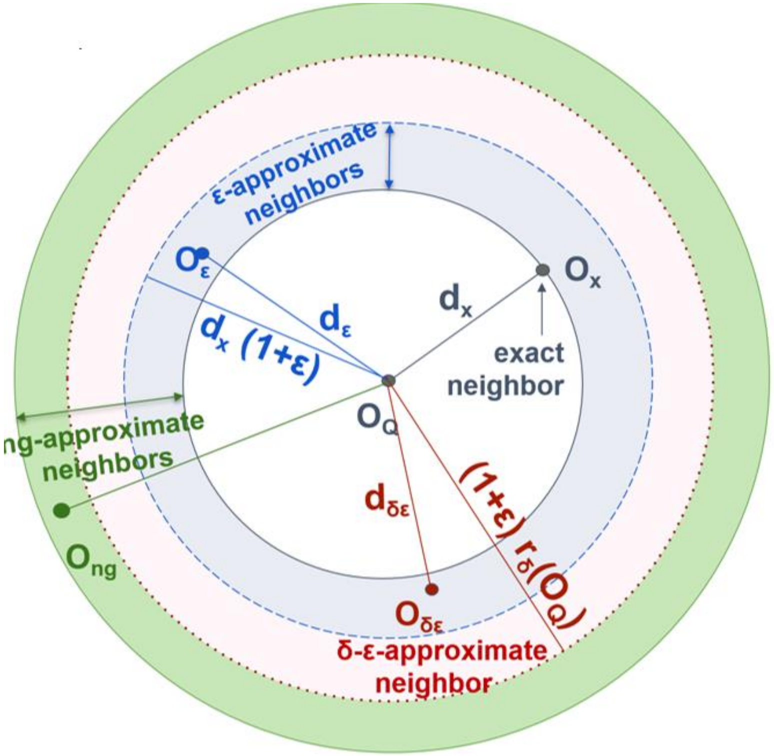
(a) Serial scan

(b) Skip-sequential scan

(c) Tree-based index

Answering a similarity search query using different access paths

Extensions: Skip-Sequential Scans

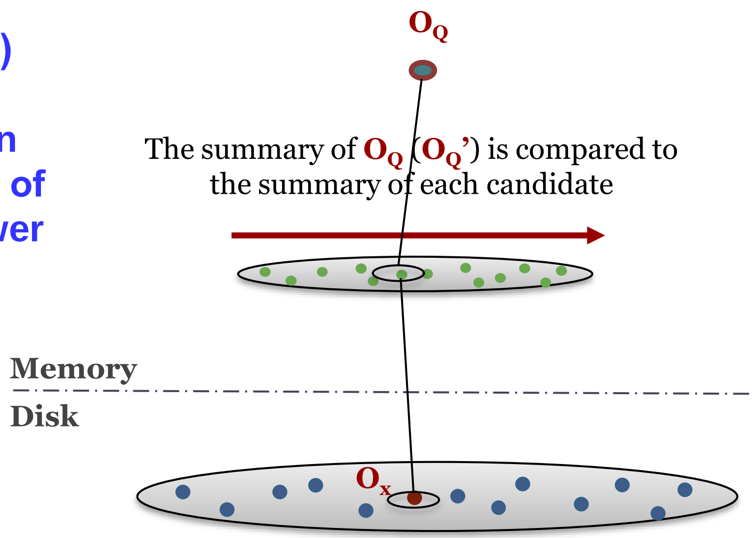


$d_\varepsilon <= d_x (1+\varepsilon)$

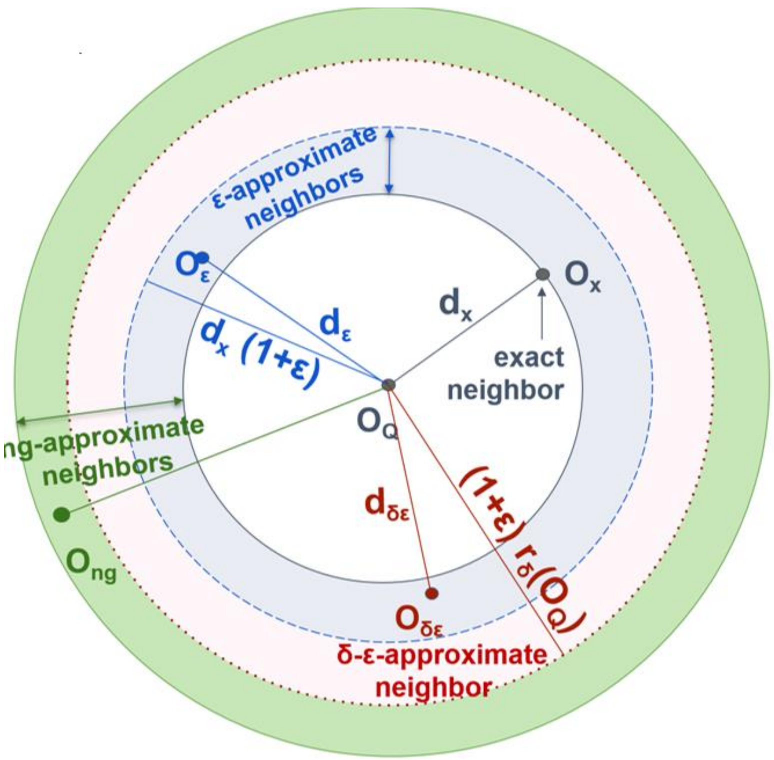
Result is within distance (1+ ε) of the exact answer

$bsf \quad = d(O_Q,O_1)$

$lb_{cur} \; = d_{lb}(O_Q', O_x') < bsf$



Extensions: Skip-Sequential Scans



$d_\varepsilon <= d_x (1+\varepsilon)$

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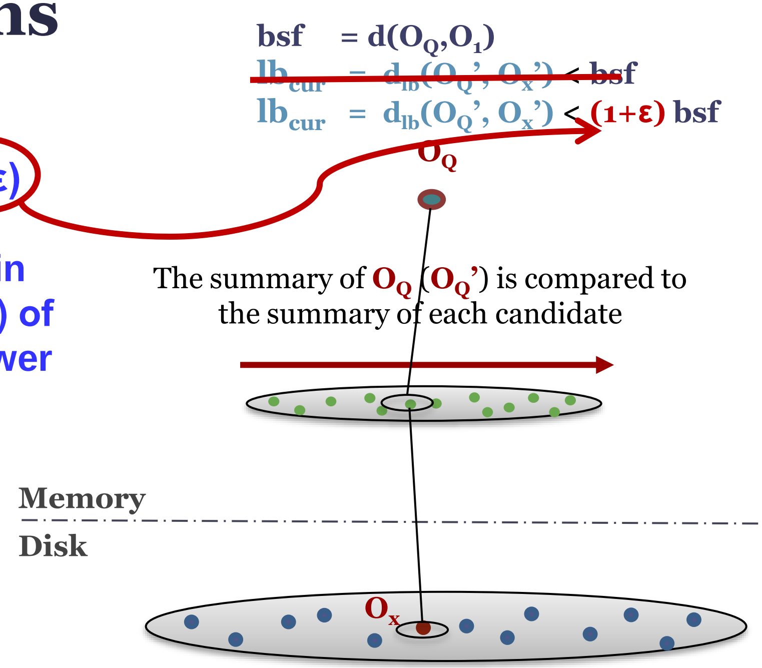
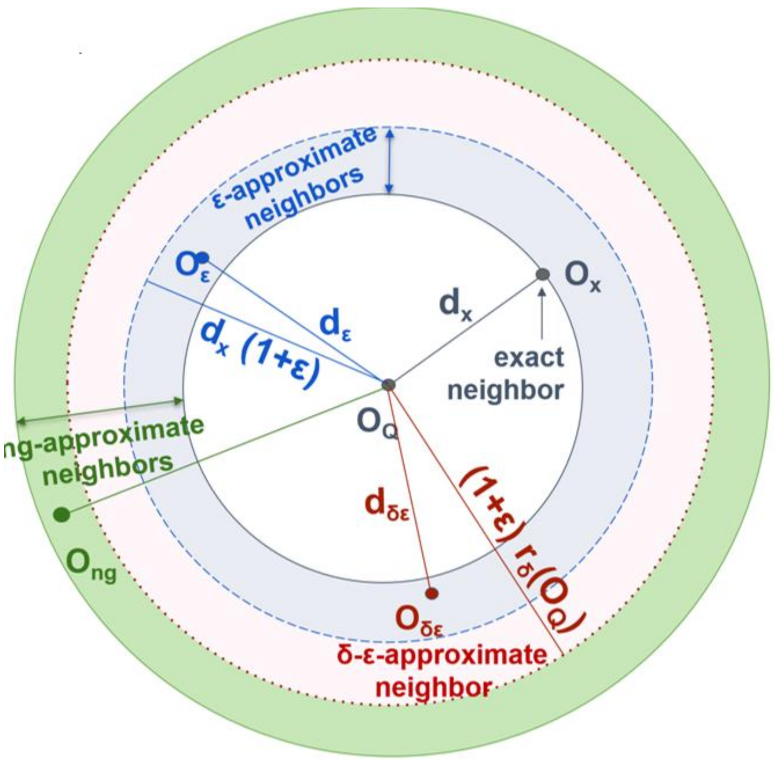


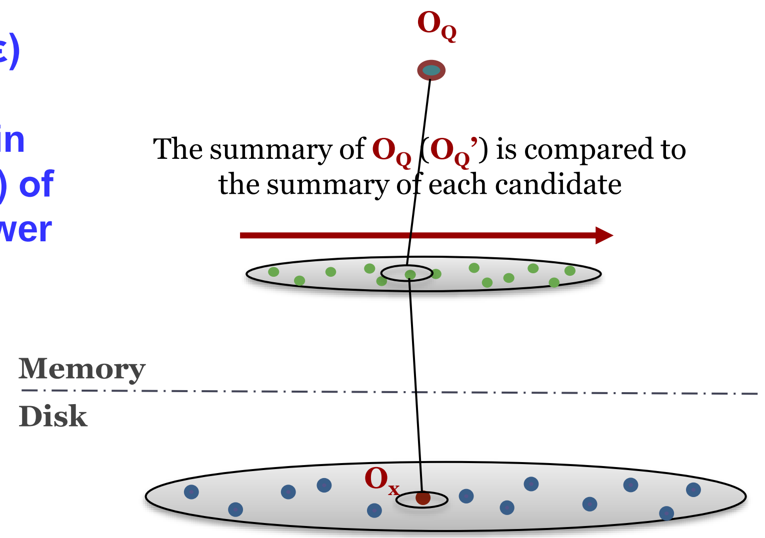
Extensions: Skip-Sequential Scans



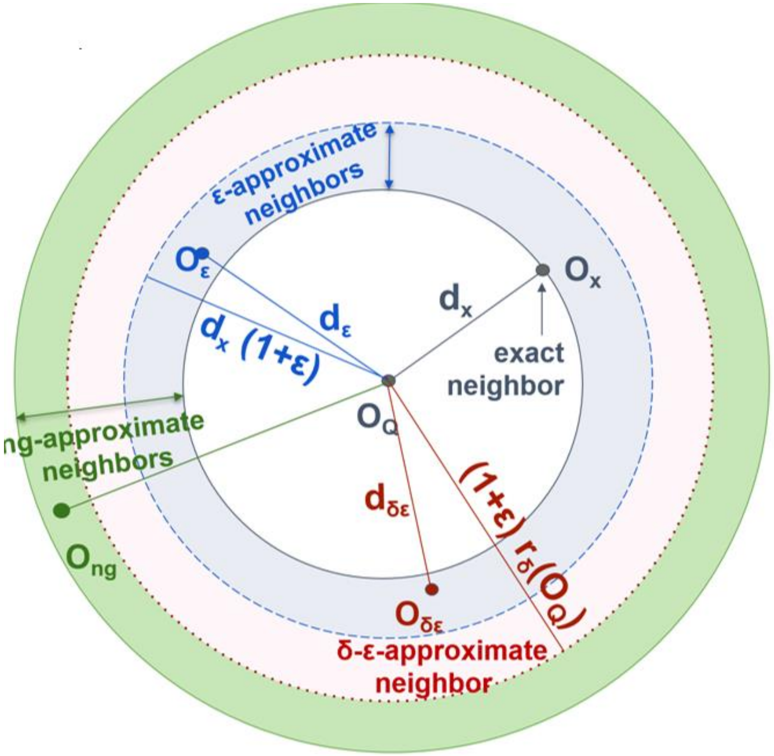
$d_ε$ <= d_x (1+ε)

Result is within distance (1+ ε) of the exact answer

bsf = $d(O_Q,O_1)$

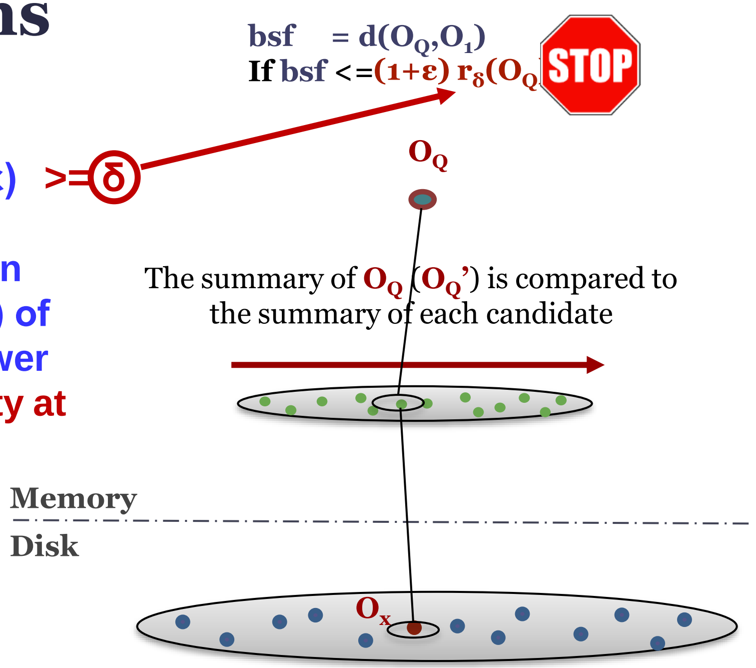


Extensions: Skip-Sequential Scans

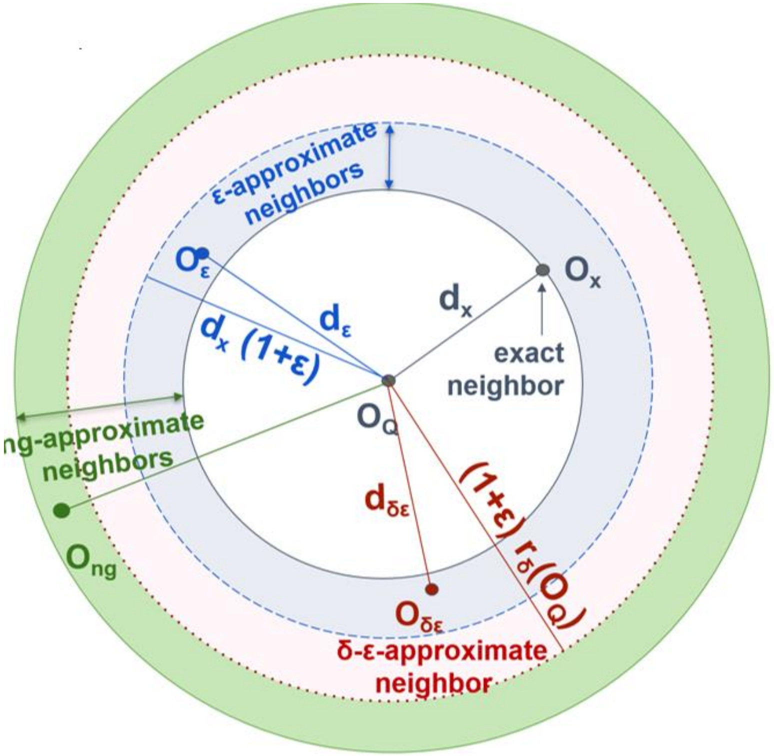


P{$d_ε$ <= d_x (1+ε) >= δ

Result is within distance (1+ ε) of the exact answer with probability at least δ

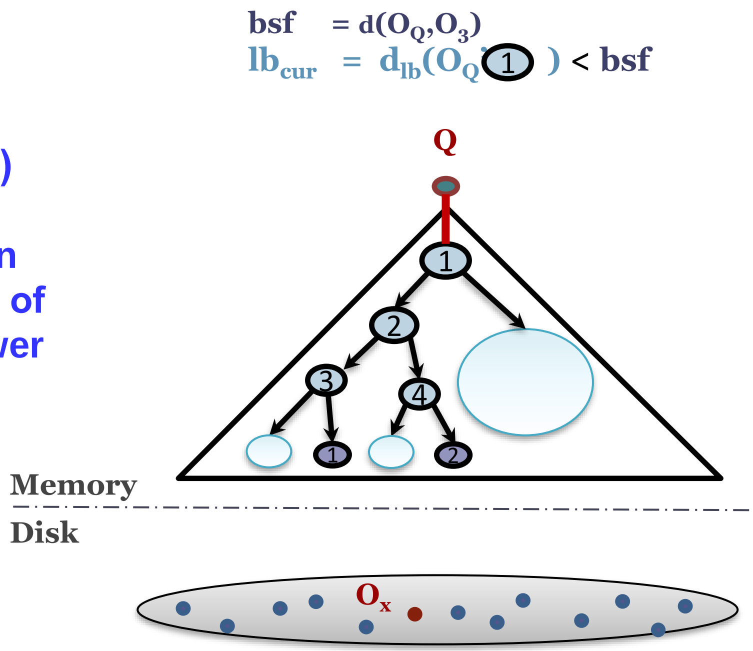


Extensions: Indexes

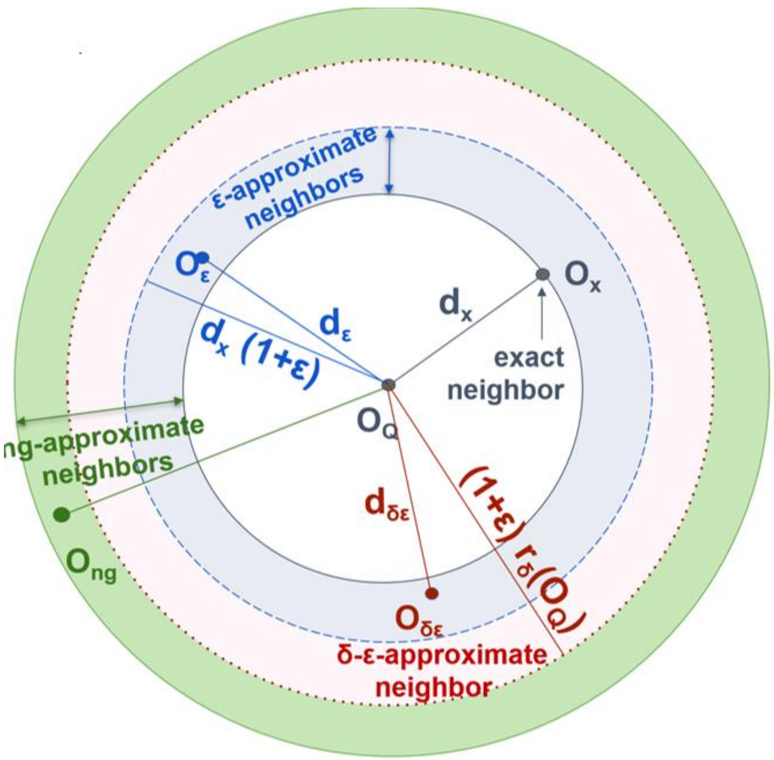


$d_\varepsilon <= d_x$ (1+ε)

Result is within distance (1+ ε) of the exact answer

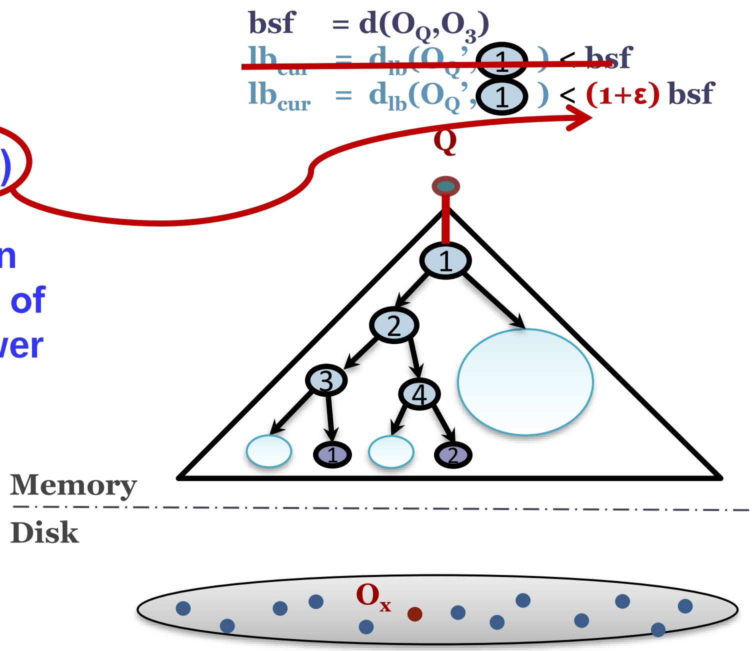


Extensions: Indexes

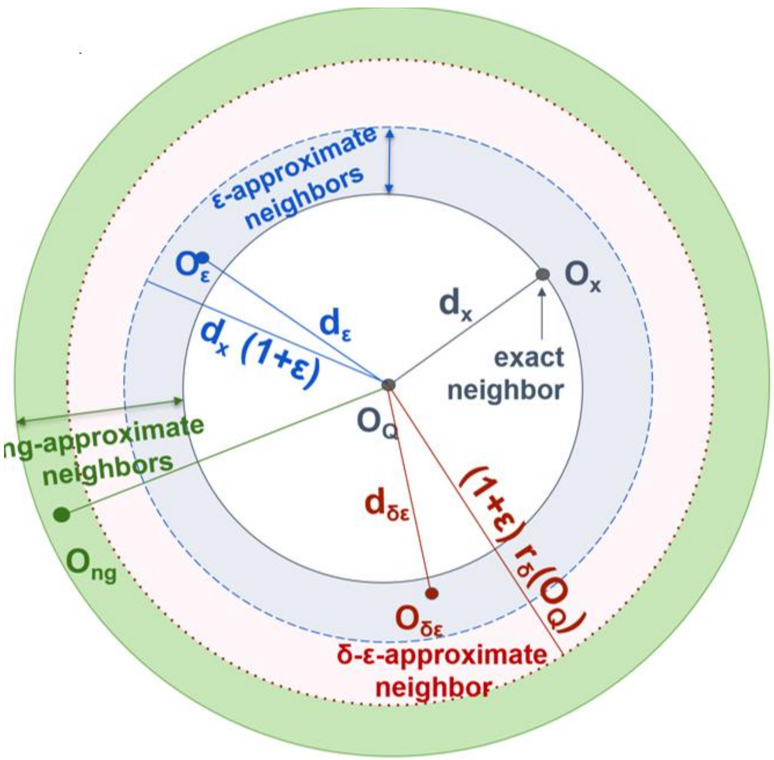


$d_\varepsilon \le d_x (1+\varepsilon)$

Result is within distance (1+ ε) of the exact answer

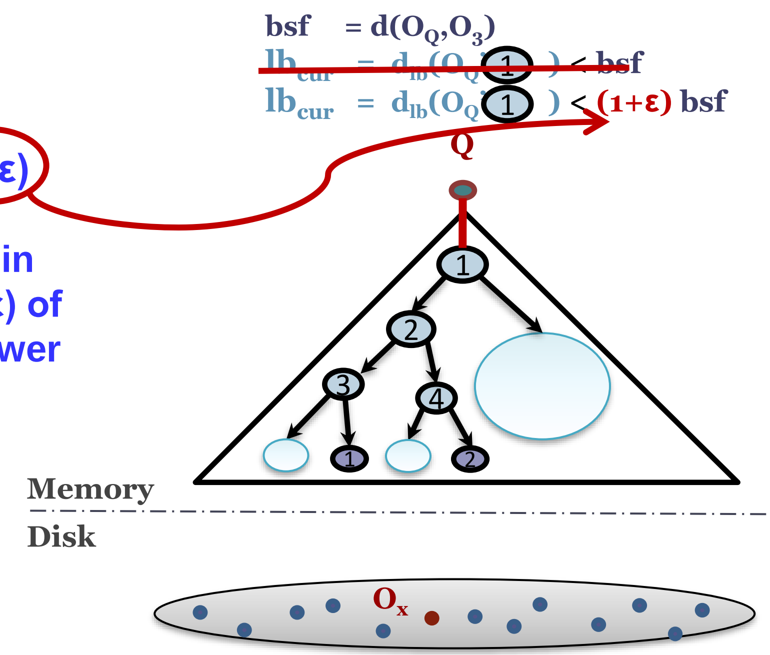


Extensions: Indexes

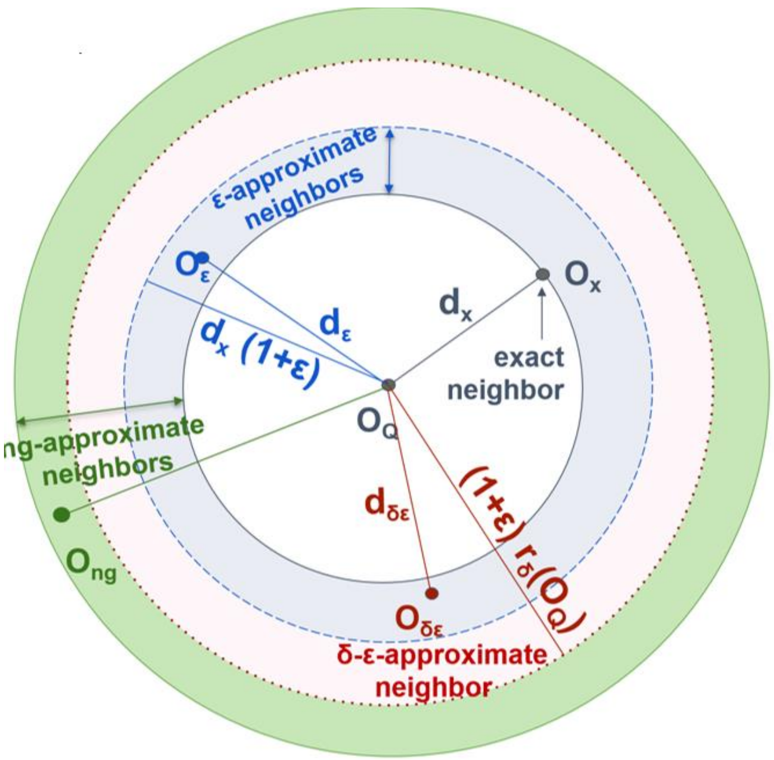


d_ε <= $d_x(1+\varepsilon)$

Result is within distance (1+ ε) of the exact answer

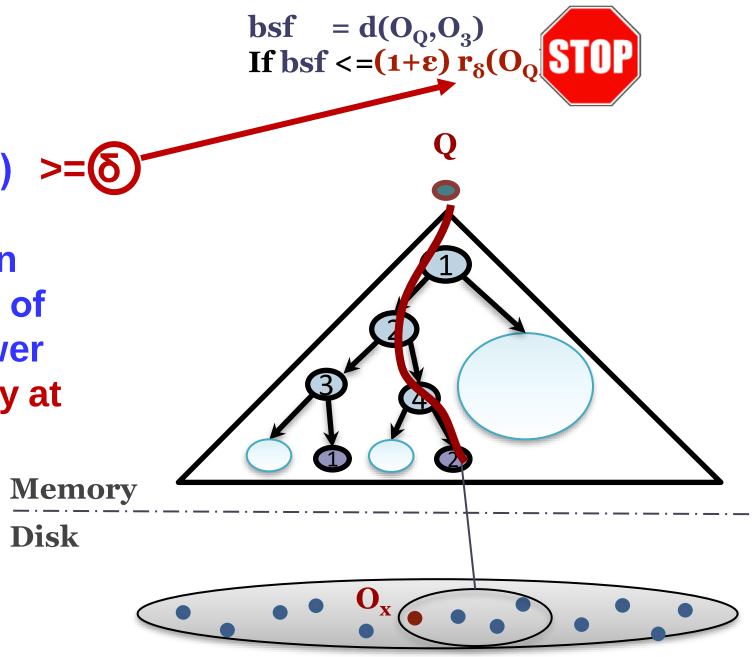


Extensions: Indexes



$P\{d_\varepsilon <= d_x\ (1+\varepsilon)\ >= \delta$

Result is within distance (1+ ε) of the exact answer with probability at least δ



Questions?

Data Series Similarity Search
State-of-the-Art Methods

Publications

Echihabi-EDBT'21

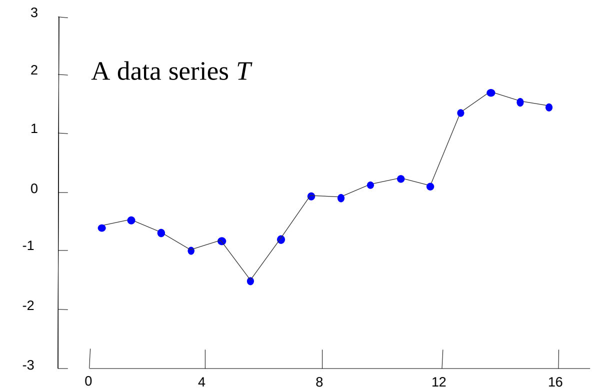
Data Series Similarity Search State-of-the-Art Methods

for a more complete and detailed presentation, see tutorial:

Karima Echihabi, Kostas Zoumpatianos, Themis Palpanas. Big Sequence Management: Scaling Up and Out. EDBT 2021
http://helios.mi.parisdescartes.fr/~themisp/publications.html#tutorials

iSAX Summarization

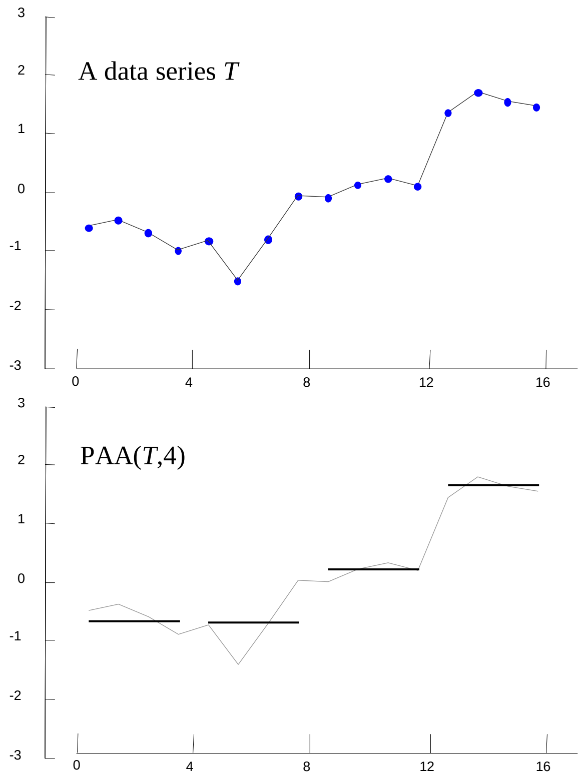
- **S**ymbolic **A**ggregate appro**X**imation (SAX)



iSAX Summarization

- **S**ymbolic **A**ggregate appro**X**imation (SAX)
  - **(1)** Represent data series *T* of length ***n*** with ***w*** segments using Piecewise Aggregate Approximation (PAA)
    - *T* typically normalized to $\mu = 0$, $\sigma = 1$
    - $\mathrm{PAA}(T,w) = \bar{T} = \bar{t}_1, \ldots, \bar{t}_w$

      where $\bar{t}_i = \frac{w}{n} \sum_{j=\frac{n}{w}(i-1)+1}^{\frac{n}{w}i} T_j$



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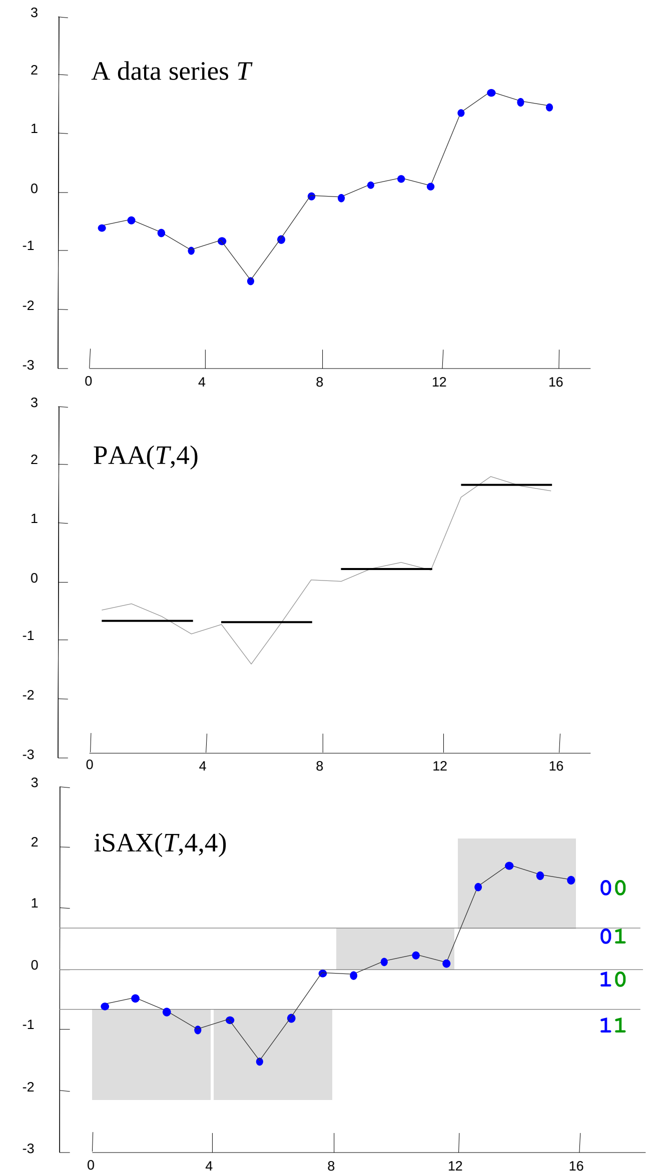
  - (2) Discretize into a vector of symbols
    - Breakpoints map to small alphabet $\boldsymbol{a}$ of symbols

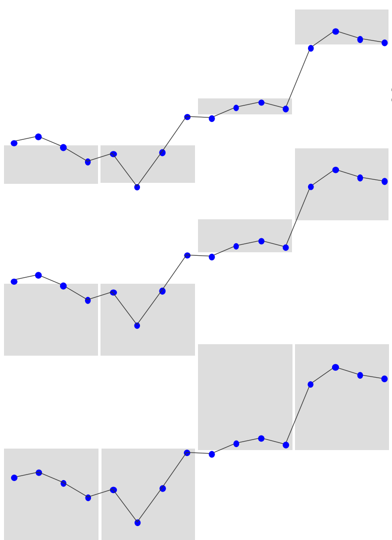


iSAX Summarization

Publications

Shieh-KDD'08

- *i*SAX representation offers a bit-aware, quantized, multi-resolution representation with variable granularity



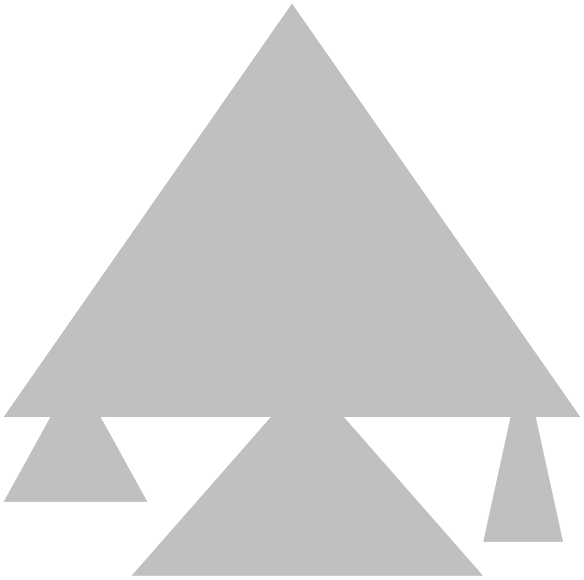
= { 6, 6, 3, 0} = {110 ,110 ,0111 ,000}

= { 3, 3, 1, 0} = {11 ,11 ,011 ,00 }

= { 1, 1, 0, 0} = {1 ,1 ,0 ,0 }

*i*SAX Index Family

- non-balanced tree-based index with non-overlapping regions, and controlled fan-out rate
  - base cardinality ***b*** (optional), segments ***w***, threshold ***th***
  - hierarchically subdivides SAX space until num. entries ≤ ***th***



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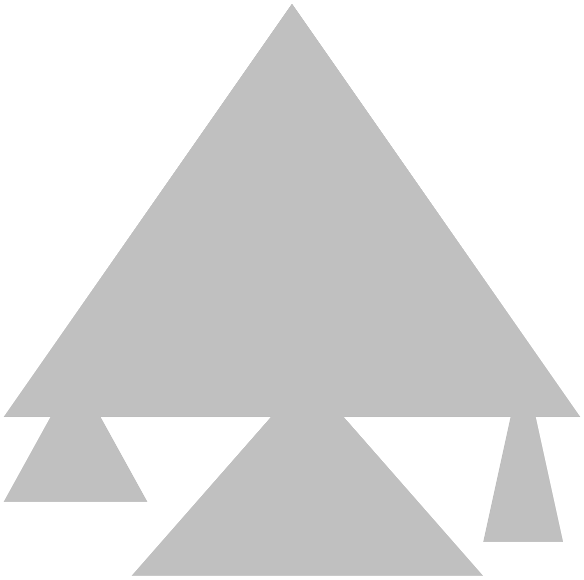
e.g., th=4, w=4, b=1

$$\begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$



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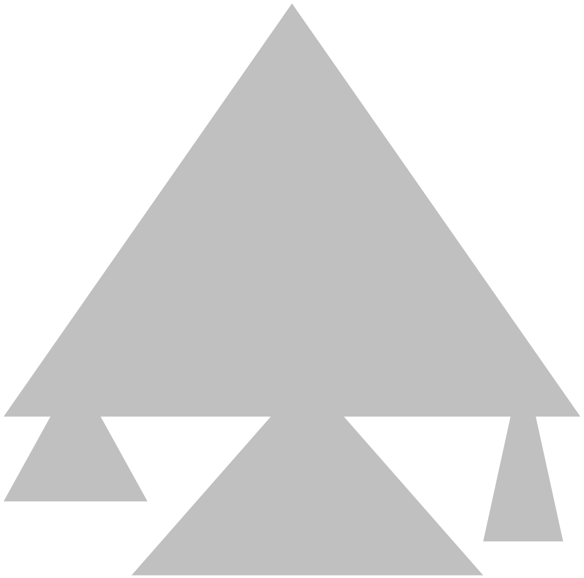
Insert:
1 1 1 0

$$\left[\begin{matrix}1 & 1 & 1 & 0\\ 1 & 1 & 1 & 0\\ 1 & 1 & 1 & 0\\ 1 & 1 & 1 & 0\end{matrix}\right.$$



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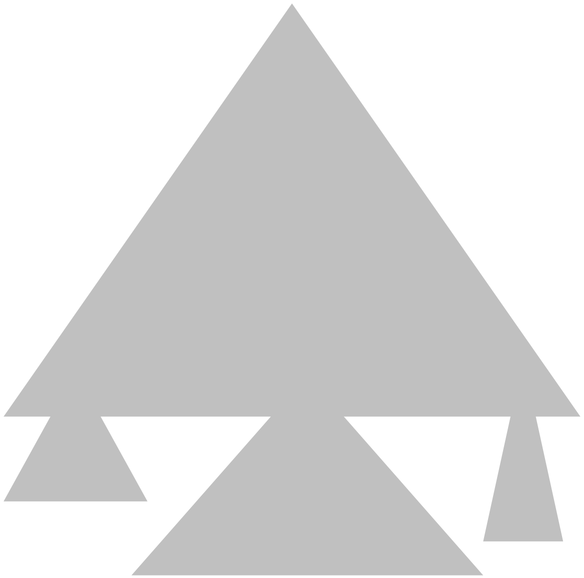
1 1 1**0** 0
1 1 1**0** 0

1 1 **1** 0

1 1 1**1** 0
1 1 1**1** 0
1 1 1**1** 0



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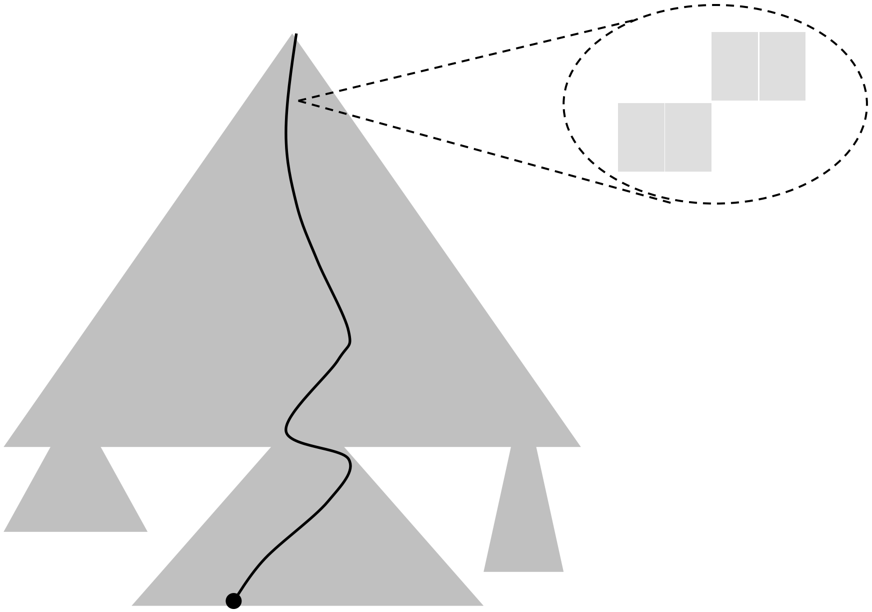

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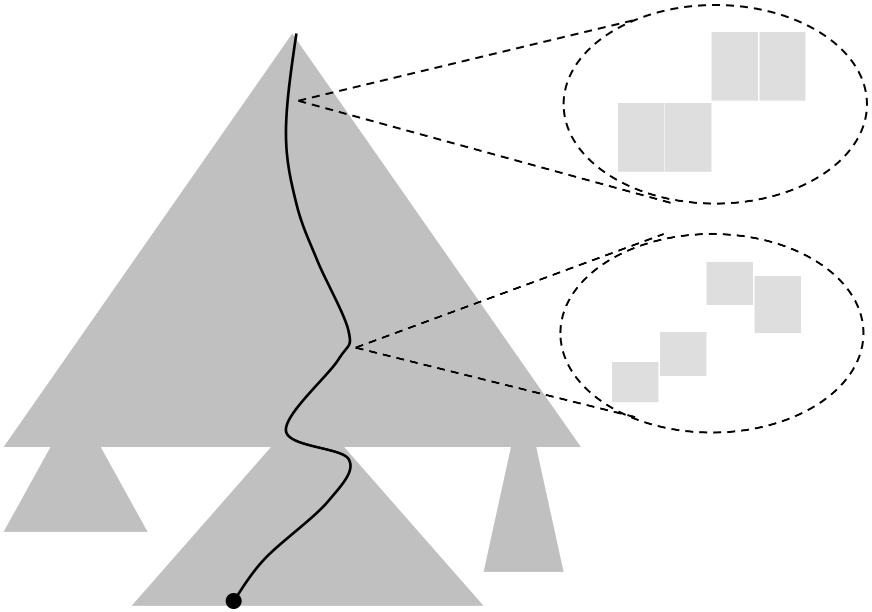

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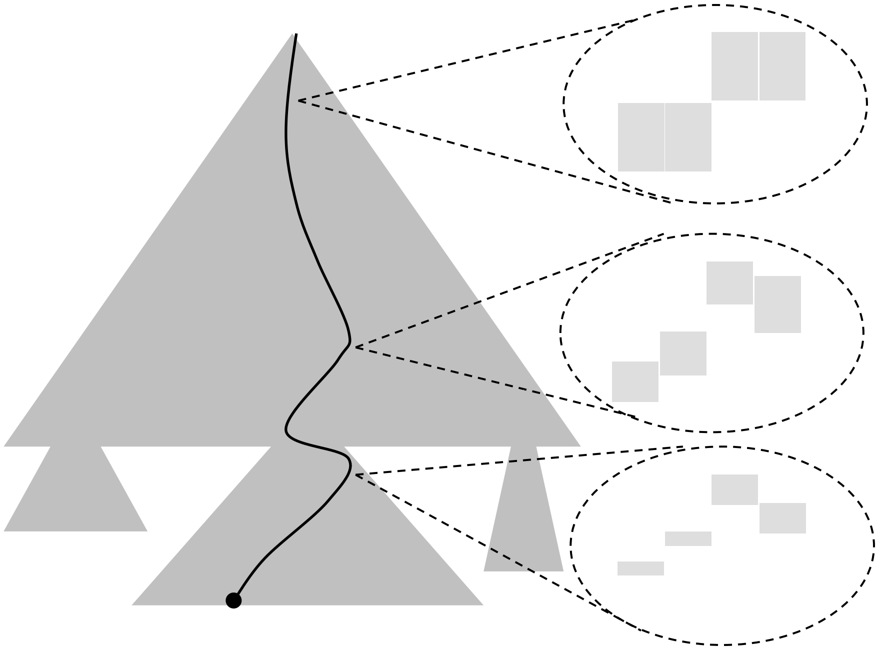

*i*SAX Index Family

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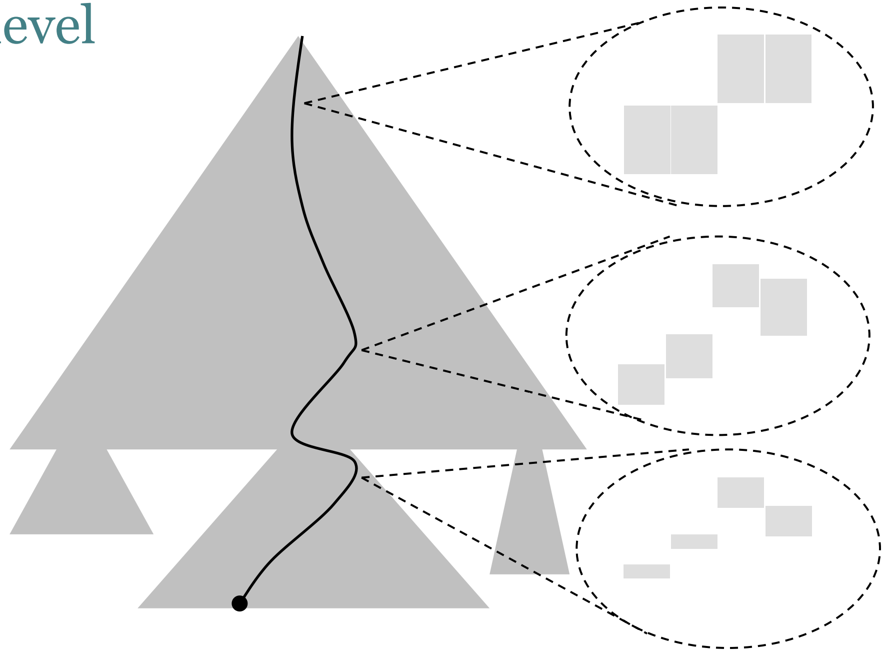
  - base cardinality ***b*** (optional), segments ***w***, threshold ***th***
  - hierarchically subdivides SAX space until num. entries ≤ ***th***
- Approximate Search
  - Match *i*SAX representation at each level
- Exact Search
  - Leverage approximate search
  - Prune search space
    - Lower bounding distance



Publications

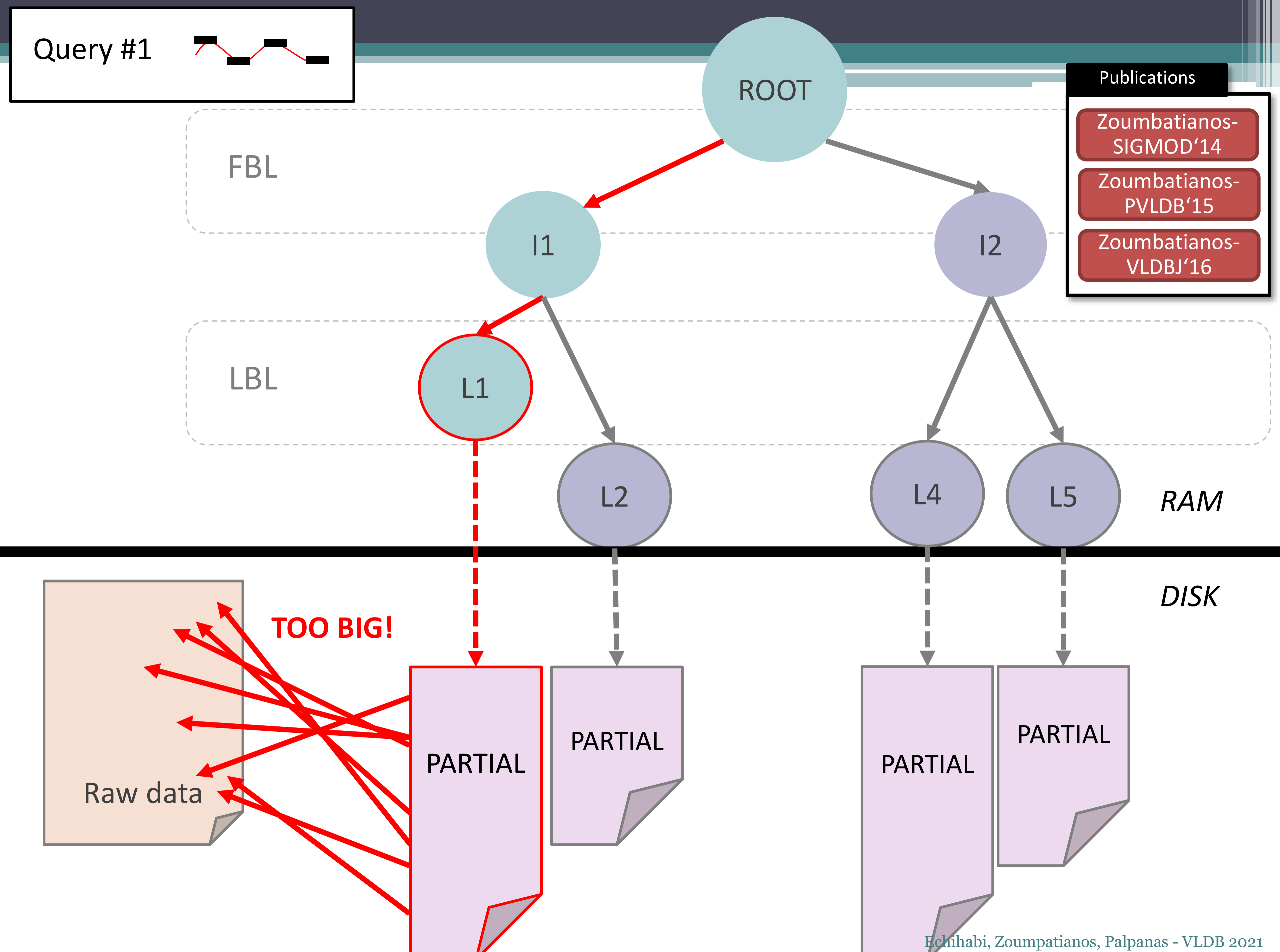
Zoumbatianos-SIGMOD‘14

Zoumbatianos-PVLDB‘15

Zoumbatianos-VLDBJ‘16

ADS+

- novel paradigm for building a data series index
  - does not build entire index and then answer queries
  - starts answering queries by building the part of the index needed by those queries
- still guarantees correct answers
- intuition for proposed solution
  - builds index using only *i*SAX summaries; uses large leaf size
  - postpones leaf materialization to query time
    - only materialize (at query time) leaves needed by queries
  - parts that are queried more are refined more
    - use smaller leaf sizes (reduced leaf materialization and query answering costs)



Query #1
ROOT
FBL
I1
I2
LBL
L1
L2
L4
L5
RAM
DISK
Raw data
TOO BIG!
PARTIAL
PARTIAL
PARTIAL
PARTIAL
Publications
Zoumbatianos-SIGMOD'14
Zoumbatianos-PVLDB'15
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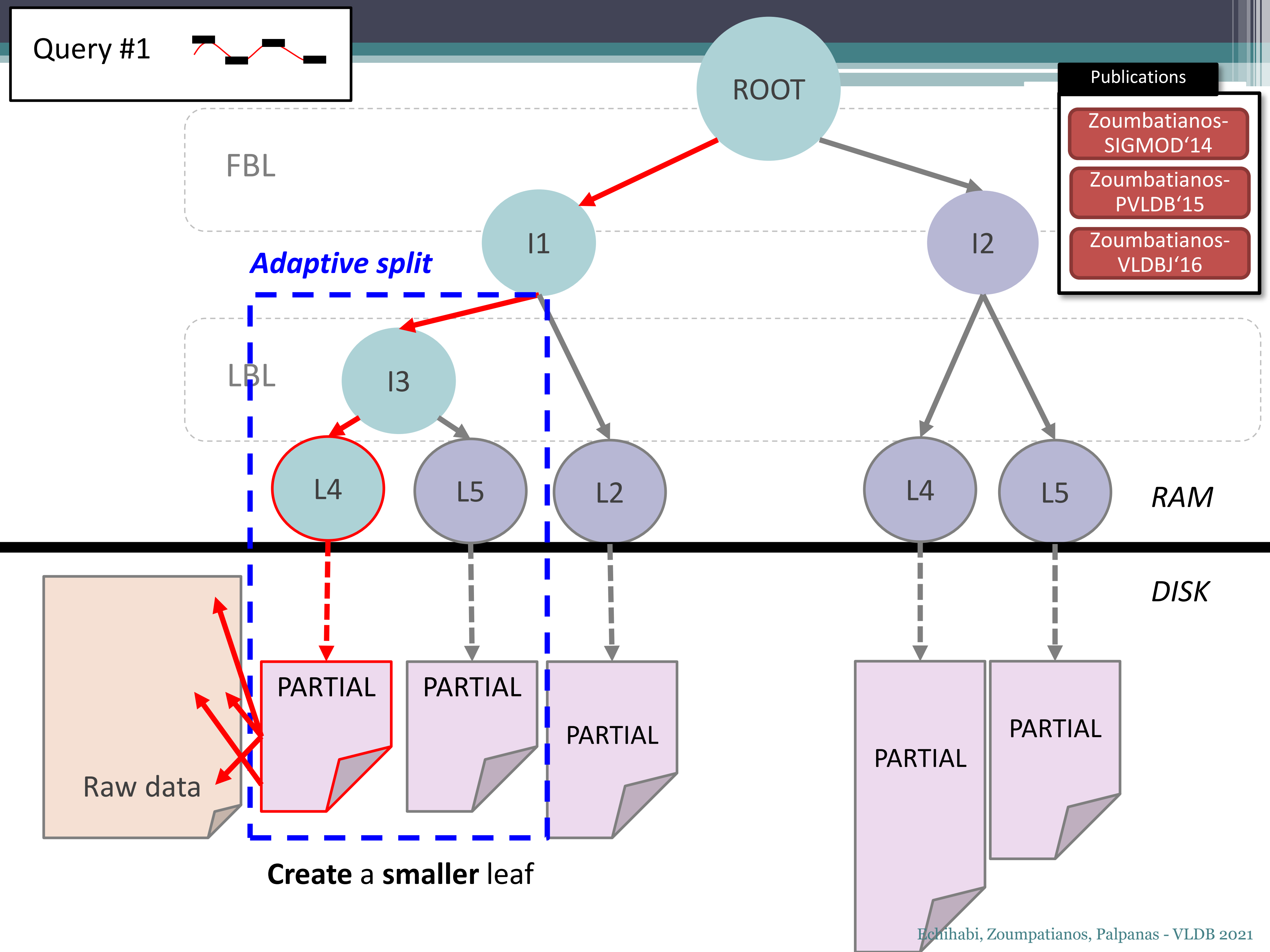
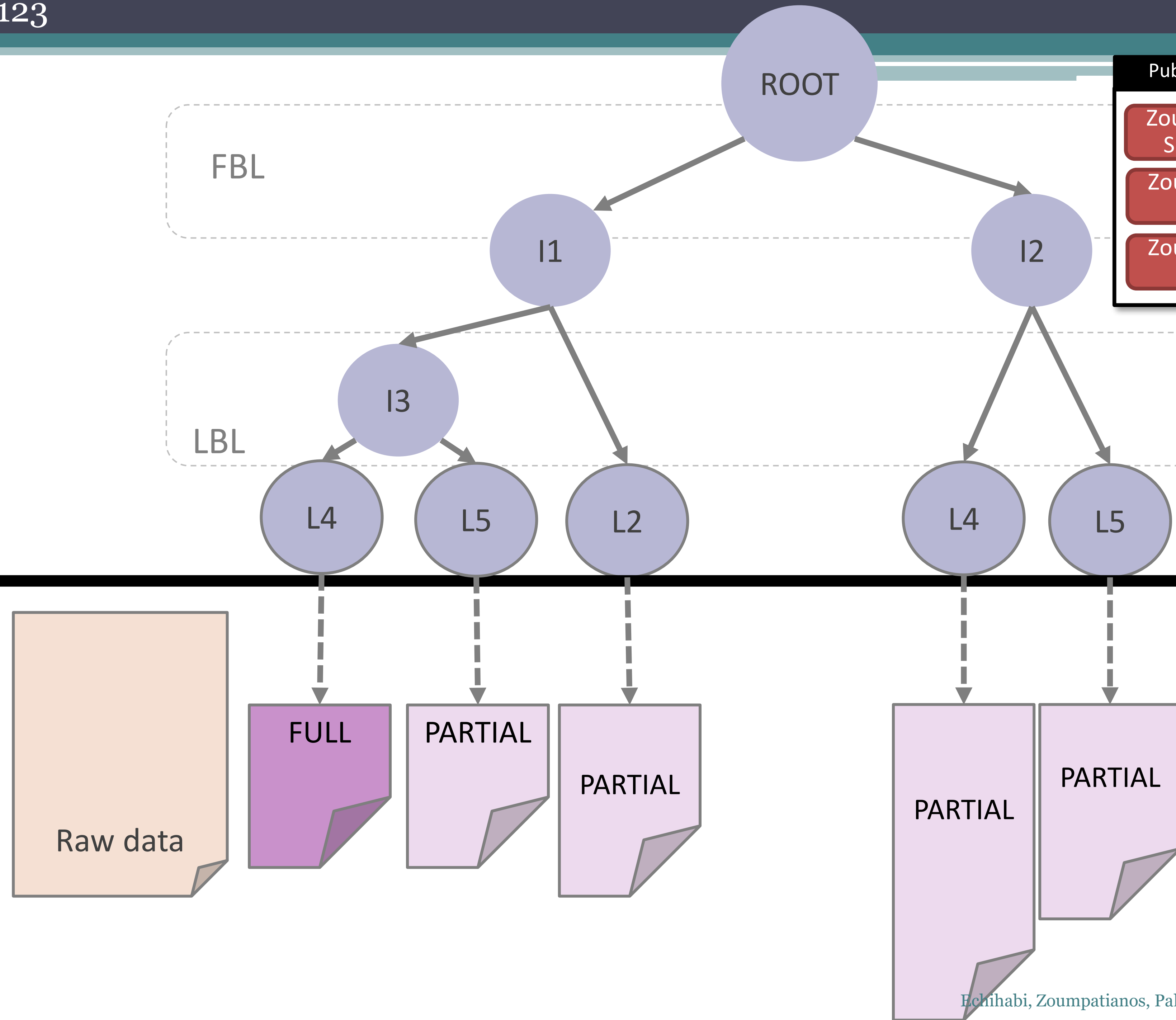


Create a **smaller** leaf



Publications

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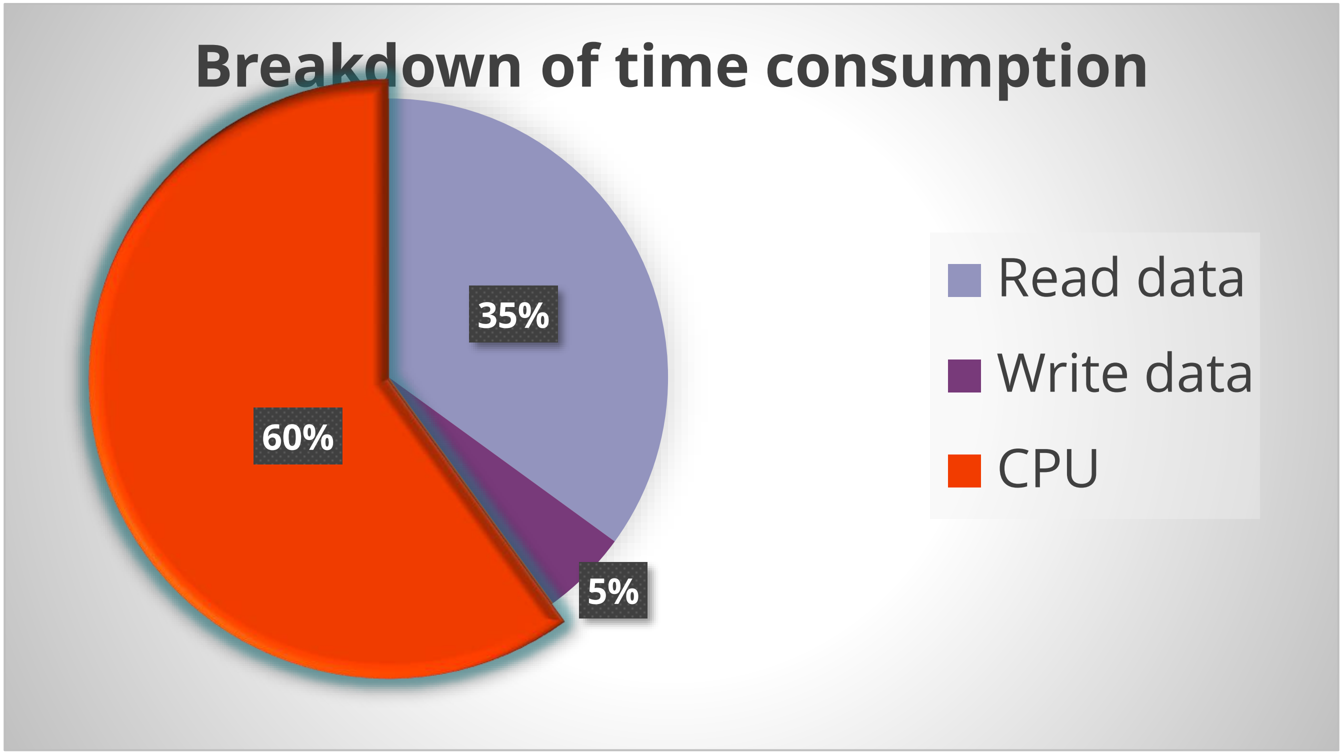
ADS Index creation



~60% of time spent in CPU: potential for improvement!

Publications

- Yagoubi-ICDM'17
- Yagoubi-TKDE'18
- Lavchenko-KAIS'20

Parallelization/Distribution

- DPiSAX: current solution for distributed processing (Spark)
  - balances work of different worker nodes

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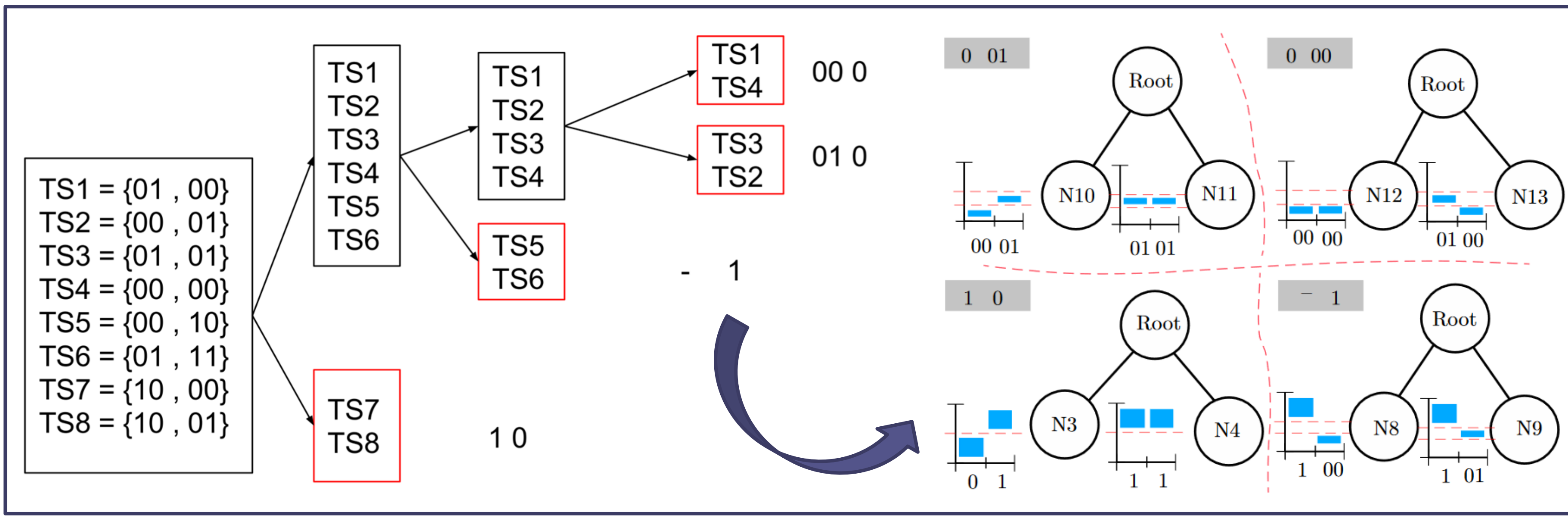

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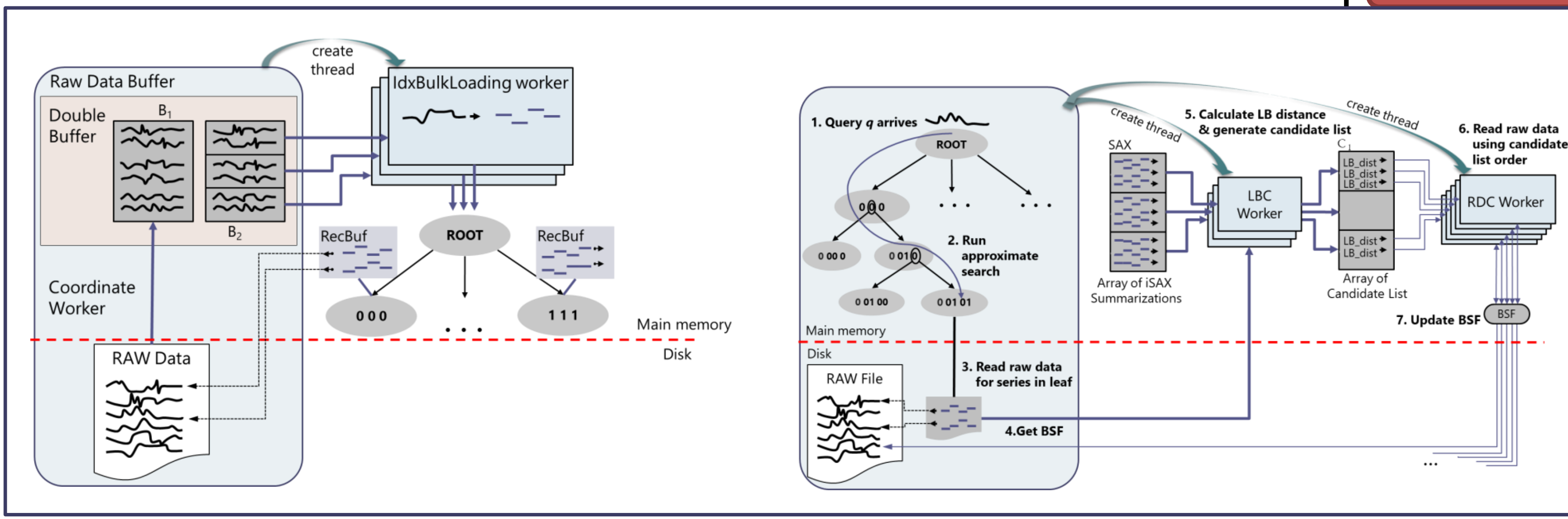

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  - answers exact queries in the order of a few secs
    - 3 orders of magnitude faster then single-core solutions

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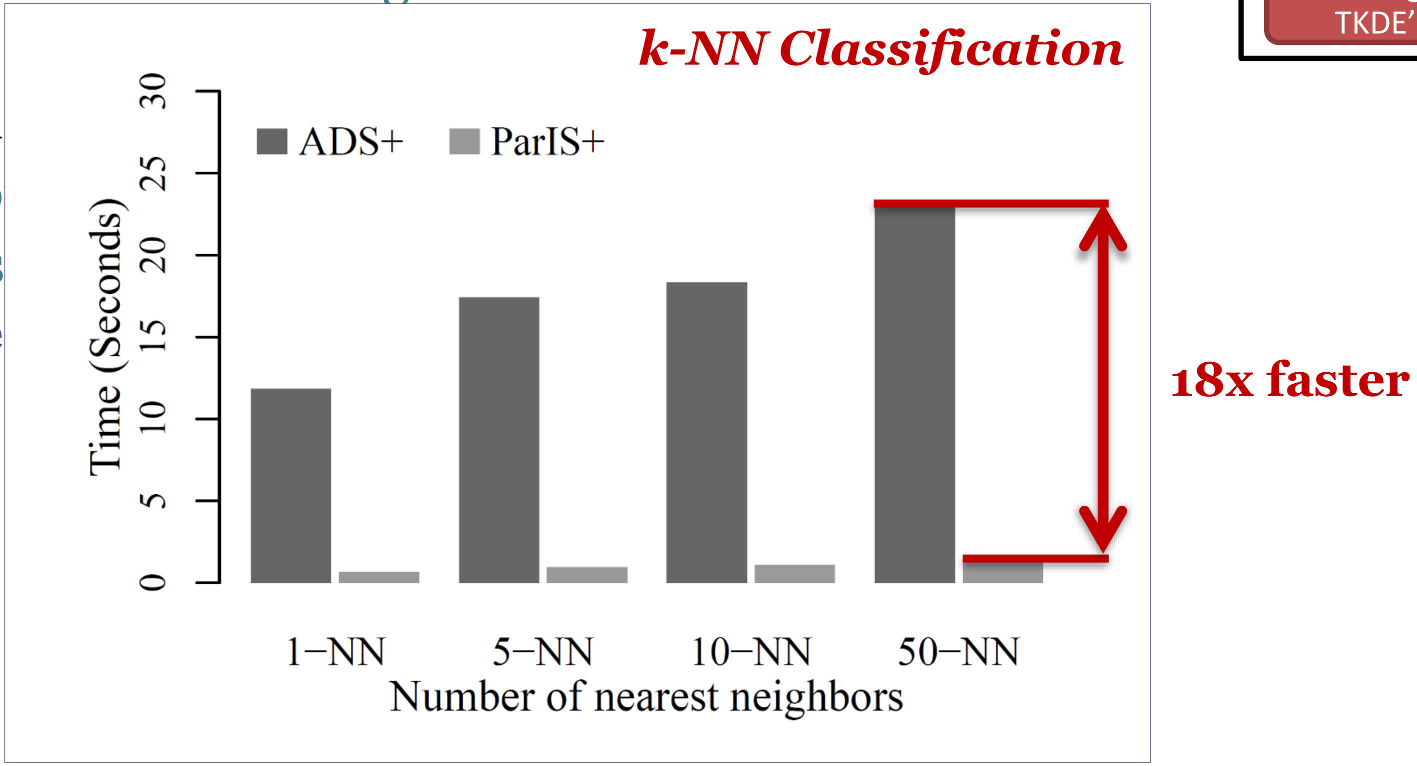

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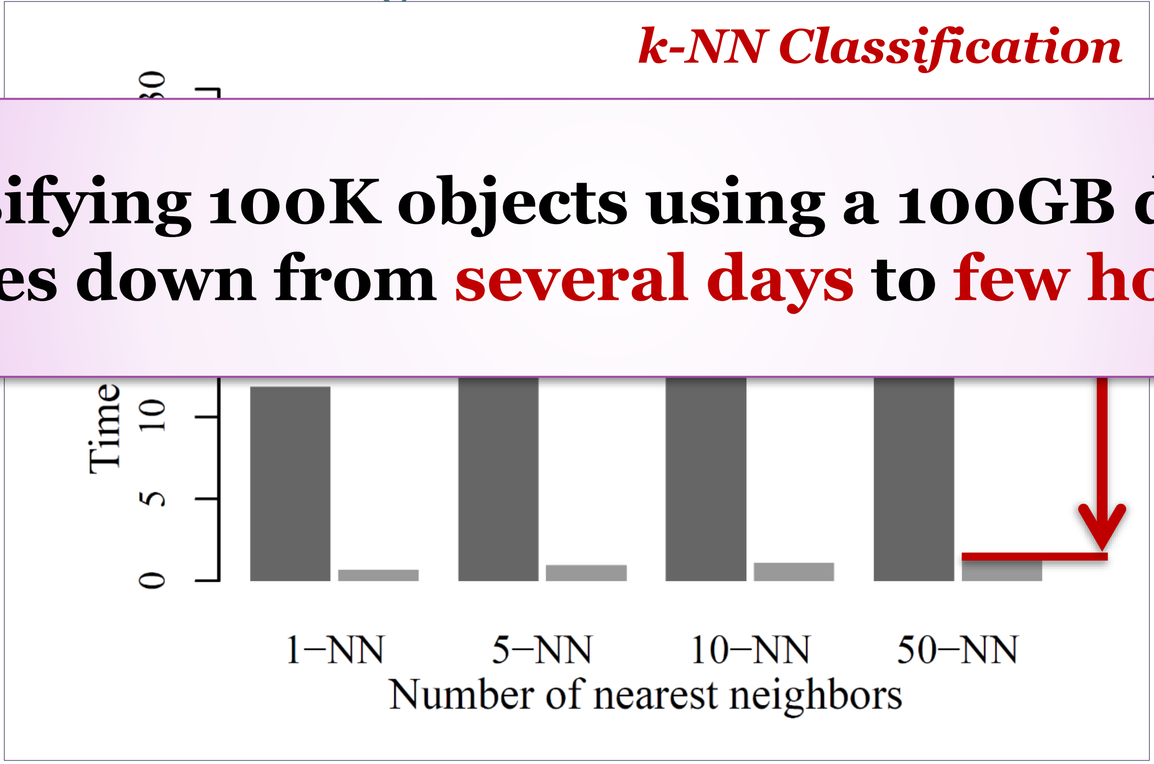

- P

classifying 100K objects using a 100GB dataset goes down from several days to few hours!

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- MESSI: current single-node parallel solution + in-memory data
  - answers exact queries at interactive speeds: ~50msec on 100GB

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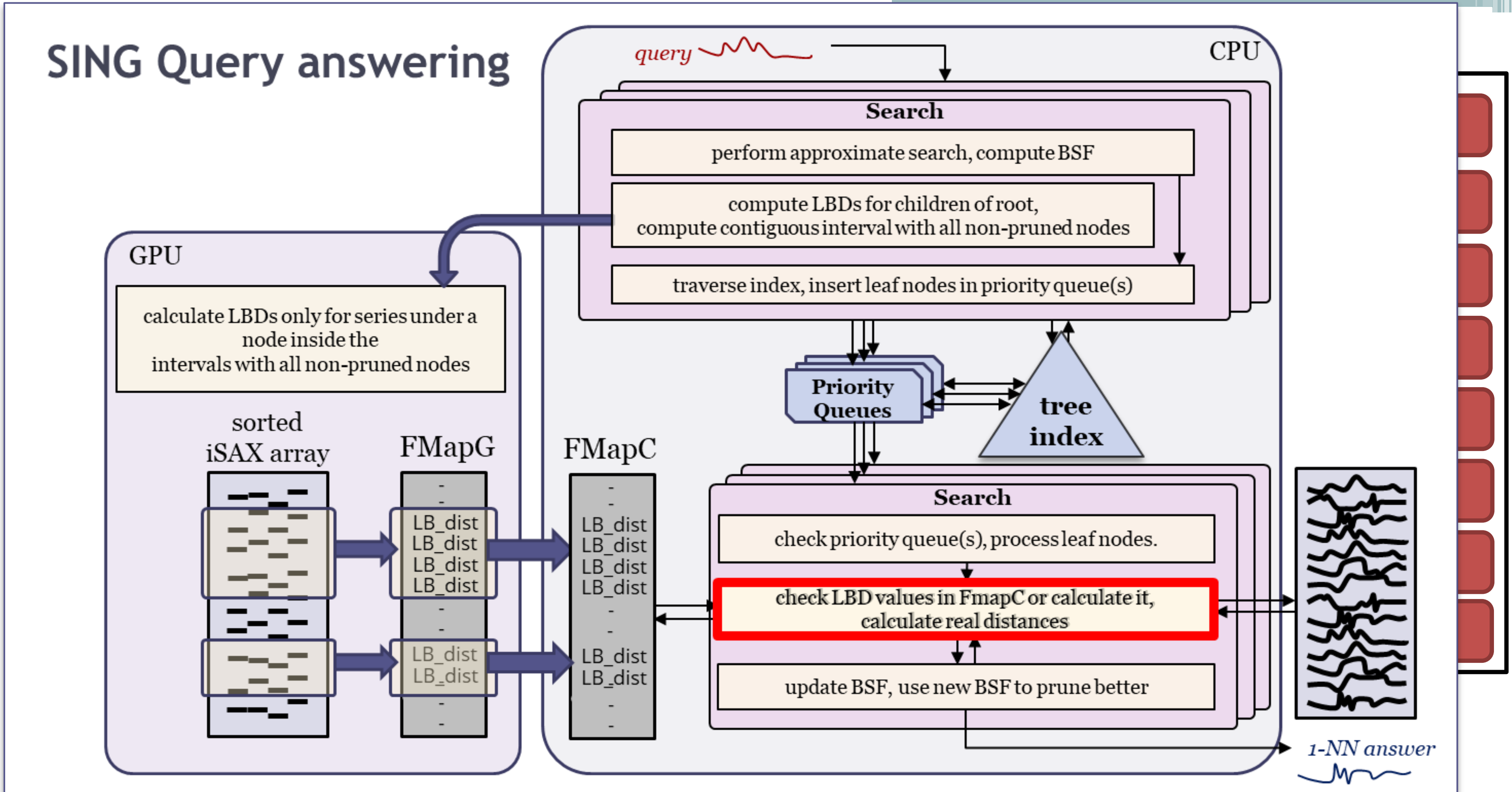
- SING: current single-node parallel solution + GPU + in-memory data
  - answers exact queries at interactive speeds: ~32msec on 100GB

SING Query answering



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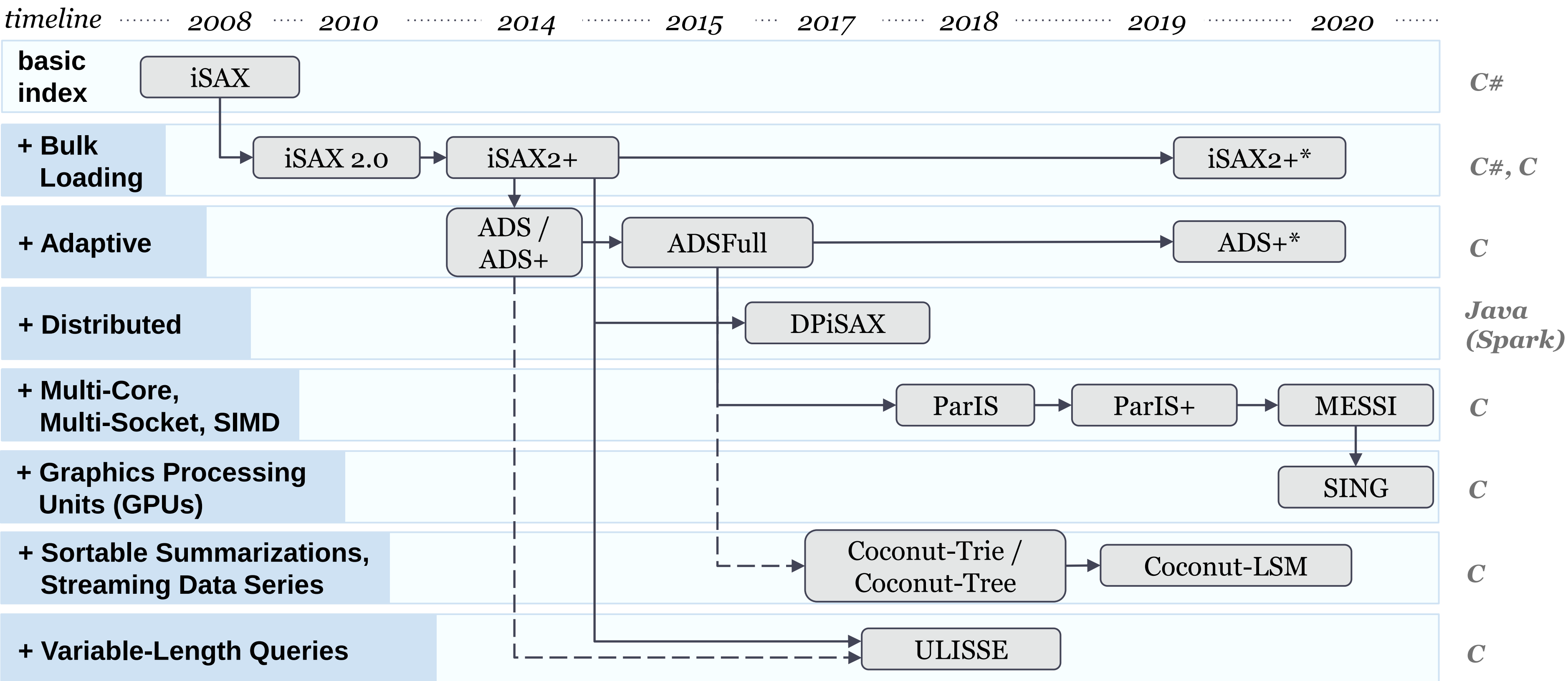
iSAX Index Family

Publications

Palpanas-ISIP'19

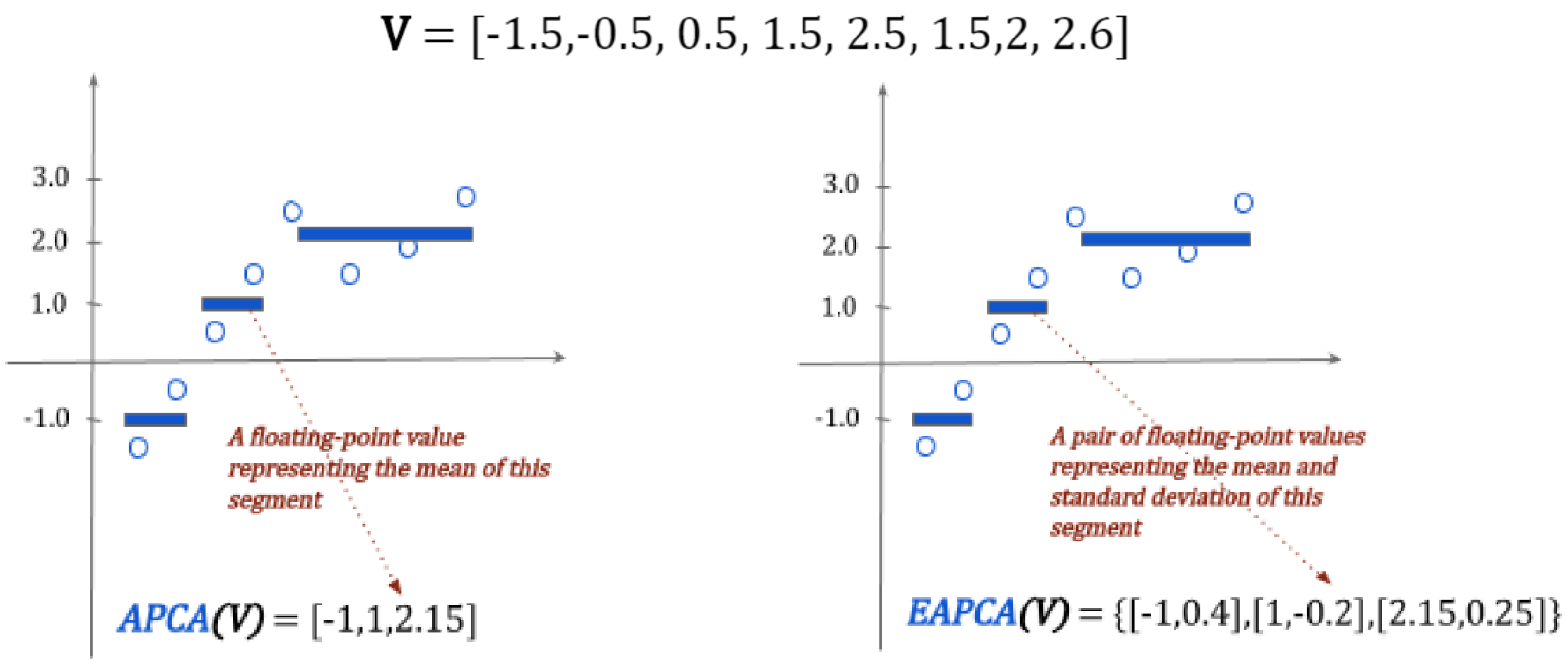


Timeline depicted on top; implementation languages marked on the right. Solid arrows denote inheritance of index design; dashed arrows denote inheritance of some of the design features; two new versions of iSAX2+/ADS+ marked with asterisk support approximate similarity search with deterministic and probabilistic quality guarantees.

DSTree
Summarization

Publications

Wang-PVLDB'13



(a) APCA

(b) EAPCA

Intertwined with indexing

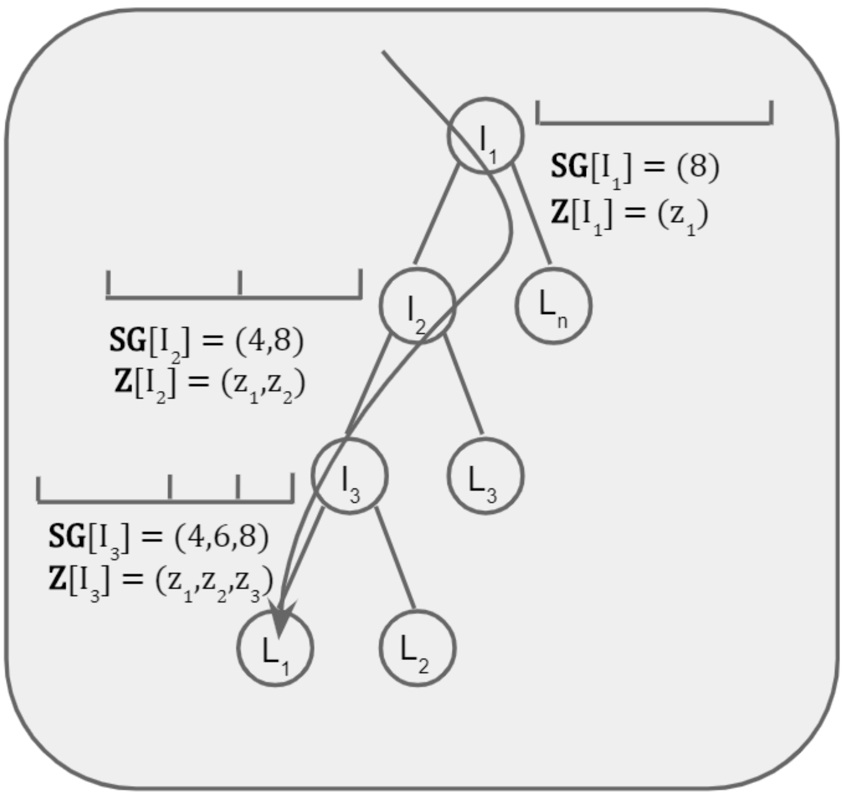
The APCA and EAPCA representations

DSTree
Indexing

Publications

Wang-PVLDB'13

$\mathbf{V} = [-1.5, -0.5, 0.5, 1.5, 2.5, 1.5, 2, 2.6]$



Each node contains
- ❑ # vectors
- ❑ segmentation **SG**
- ❑ synopsis **Z**

Each Leaf node also :
- ❑ stores its raw vectors in a separate disk file

ParSketch

Publications

Cole et al. KDD‘05

Yagoubi et al. DMKD‘18

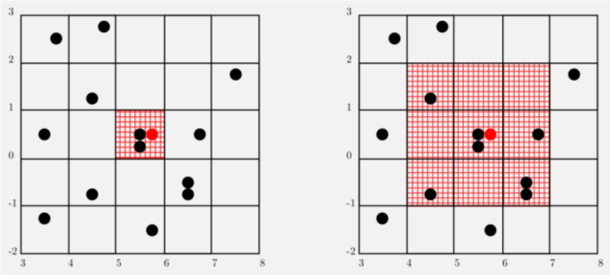
- solution for distributed processing (Spark)
  - represents data series using sketches
    - using a set of random vectors (Johnson-Lindenstrauss lemma)

$$x = (x_1, x_2, x_3, \dots x_n) \quad y = (y_1, y_2, y_3, \dots y_n) \quad z = (z_1, z_2, z_3, \dots z_n)$$

$$R1 = (r_1 1, r_1 2, r_1 3, \dots r_1 w) \quad R2 = (r_2 1, r_2 2, r_2 3, \dots r_2 w) \quad R3 = (r_3 1, r_3 2, r_3 3, \dots r_3 w) \quad R4 = (r_4 1, r_4 2, r_4 3, \dots r_4 w)$$

$$\Rightarrow (xsk1, xsk2, xsk3, xsk4) \quad (ysk1, ysk2, ysk3, ysk4) \quad (zsk1, zsk2, zsk3, zsk4)$$

  - define groups of dimensions in sketches
  - store the values of each group in a grid (in parallel)
    - each grid is kept by a node



node 1 **node 2**

  - for ng-approximate query answering (originally proposed for ε-range queries)
    - find in the grids time series that are close to the query
    - finally, check the real similarity of candidates to find the results
  - performs well for high-frequency series

Publications

- Zhang-ICDE'19
- Wu-ICDE'19
- Feng-IEEE Access'20
- Echihabi-EDBT'21

- other techniques, not covered here:
  - TARDIS
  - KV-Match (subsequence matching)
  - L-Match (subsequence matching)

- for a more complete and detailed presentation, see tutorial:
  - *Karima Echihabi, Kostas Zoumpatianos, Themis Palpanas. Big Sequence Management: Scaling Up and Out. EDBT 2021*

Questions?

High-d Vector Similarity Search State-of-the-Art Methods

High-d Vector Similarity Search Methods

- Tree-Based Methods
- Hash-Based Methods
- Quantization-Based Methods
- Graph-Based Methods

High-d Vector Similarity Search State-of-the-Art Methods

Tree-Based Methods

Tree-Based Methods

Publications

Bentley CACM'75

- A large body of work
- Some representative methods:
  - KD-tree

Tree-Based Methods

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Bentley CACM'75

Silpa-Anan CVPR'08

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Tree-Based Methods

Publications

- Bentley CACM'75
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- Muja et al. VISAPP'09

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- Ciaccia et al. VLDB'97
- Ciaccia et al. ICDE'00

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- Silpa-Anan CVPR'08
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- Arora et al. PVLDB'18

Tree-Based Methods

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- for a more complete and detailed presentation, see tutorial:
  - *Karima Echihabi, Kostas Zoumpatianos, Themis Palpanas. High-Dimensional Similarity Search for Scalable Data Science. ICDE 2021*

High-d Vector Similarity Search State-of-the-Art Methods

Hash-Based Methods

Locality Sensitive Hashing (LSH)

Publications

Indyk et al. STOC'98

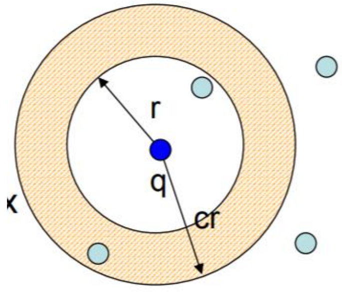
- Solution for δ-ε-approximate kNN search $\delta < 1$
- Random projections into a lower dimensional space using hashing
- Probability of collisions increases with locality

- c-Approximate r-Near Neighbor: build data structure which, for any query q:
  - If there is a point $p \in P$, $||p-q|| \le r$ Then return $p' \in P$, $||p-q|| \le c\,r$

- c-approximate nearest neighbor reduces to c-approximate near neighbor
  - Enumerate all approximate near neighbors

- Find a vector in a preprocessed set $S \subseteq \{0, 1\}\ d$ that has minimum Hamming distance to a query vector $y \in \{0, 1\}\ d$

(r_1, r_2, p_1, p_2)-sensitive [IM98]
- $\Pr[\, h(x) = h(y) \,] \ge p_1$, if $dist(x, y) \le r_1$
- $\Pr[\, h(x) = h(y) \,] \le p_2$, if $dist(x, y) \ge r_2$



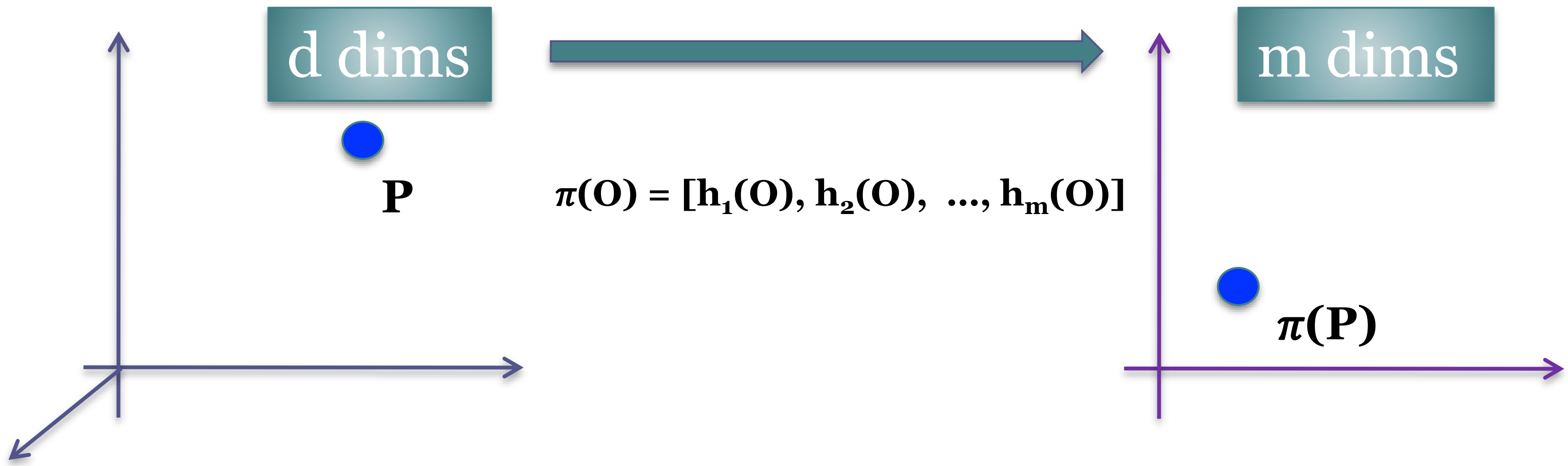
Locality Sensitive Hashing (LSH)

Publications

Andoni et al. CACM'08

- A large family
  - Different distance measures:
    - Hamming distance
    - L_p ($0 < p \leq 2$): use p-stable distribution to generate the projection vector
    - Angular distance (simHash)
    - Jaccard distance (minhash)
  - Tighter Theoretical Bounds
  - Better query efficiency/smaller index size

Probabilistic Mapping

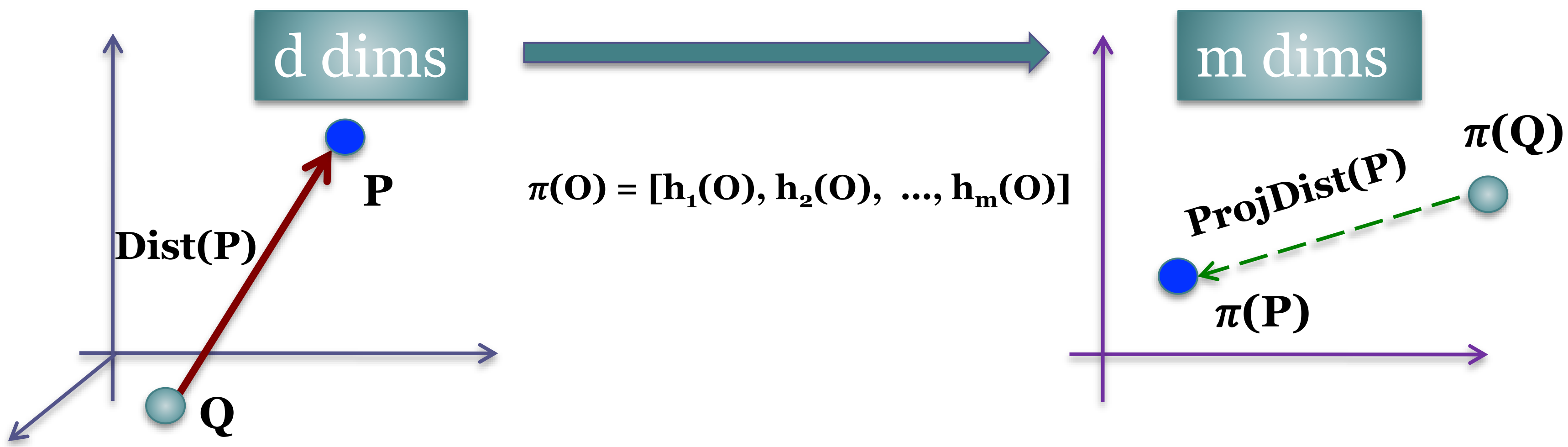


$\pi(O) = [h_1(O), h_2(O), \ldots, h_m(O)]$

- Probabilistic, linear mapping from the original space to the projected space

Slide by W. Wang

Probabilistic Mapping



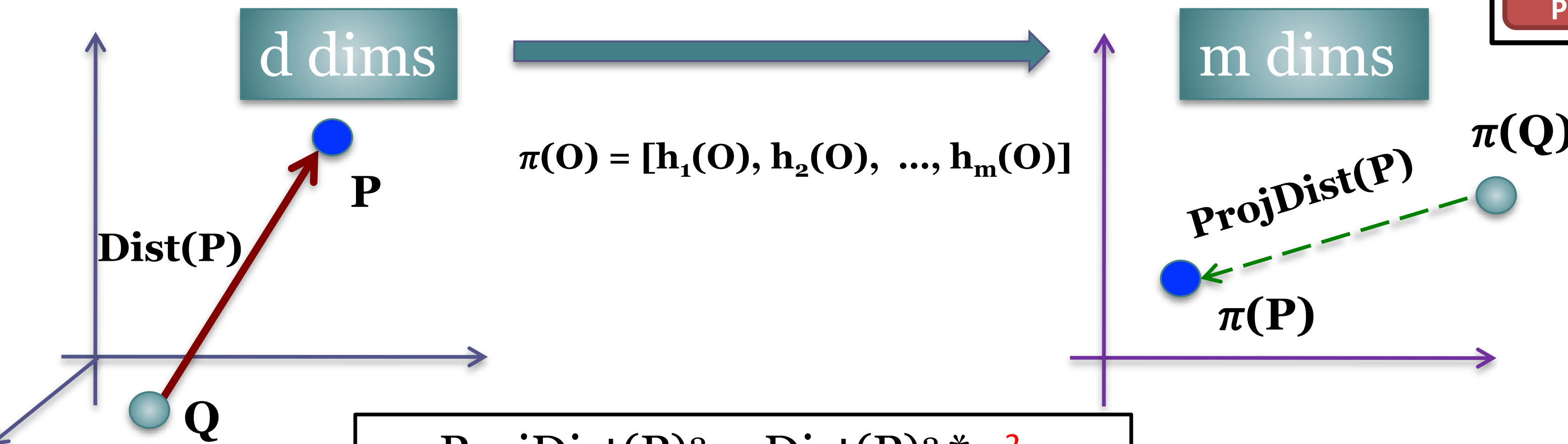
- Probabilistic, linear mapping from the original space to the projected space
- What about the distances (wrt Q or π(Q)) in these two spaces?

Slide by W. Wang

SRS

Publications

Sun et al. PVLDB' 14



$$\text{ProjDist}(P)^2 \sim \text{Dist}(P)^2 * \chi^2_m$$

- Given that ProjDist(P) ≤ r, what can we infer about Dist(P)?
  - If Dist(P) ≤ R, then Pr[ProjDist(P) ≤ r] ≥ $\Psi_m((r/R)^2)$
  - If Dist(P) > cR, then Pr[ProjDist(P) ≤ r] ≤ $\Psi_m((r/cR)^2)$ = t
  - (some probability) at most O(tn) points with ProjDist ≤ R
  - (constant probability) one of the O(tn) points has Dist ≤ R

- This solves the so-called (R, c)-NN queries ➔ returns a c^2 ANN
- Using another algorithm & proof ➔ returns a c-ANN

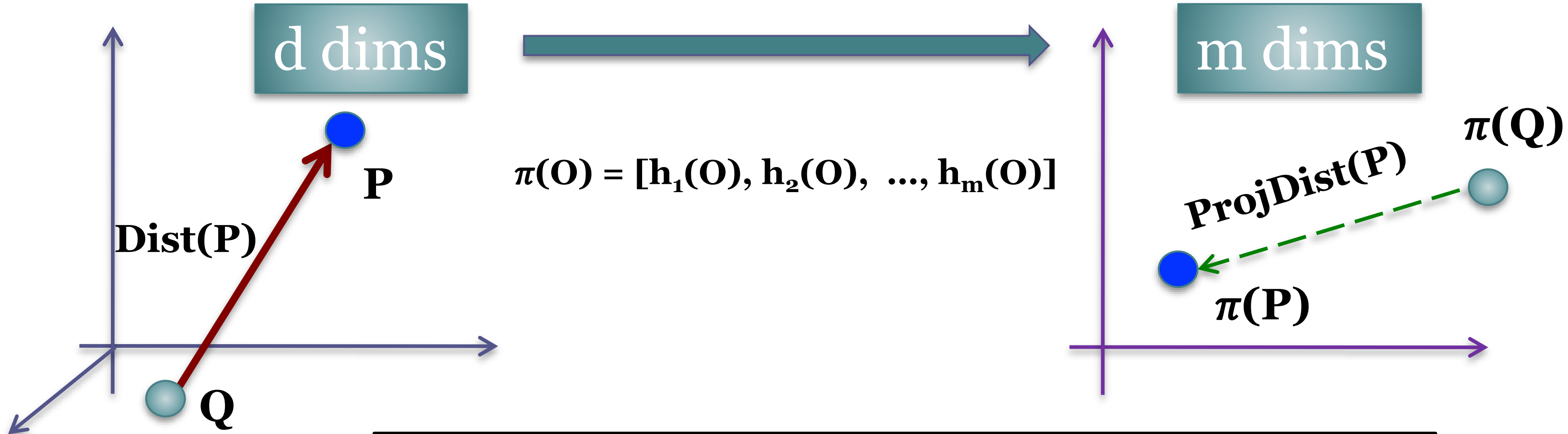
Slide by W. Wang

C2LSH/QALSH

Publications

Huang et al. PVLDB' 15

Gan et al. SIGMOD'12



Collision wrt w: if $|h_i(P) - h_i(Q)| \le w$

- Given that P's #collision $\ge \alpha m$, what can we infer about Dist(P)?
  - If Dist(P) ≤ R, then Pr[#collision $\ge \alpha m$] $\ge \gamma_1$
  - If Dist(P) > cR, then Pr[#collision $\ge \alpha m$] $\le \gamma_2$
  - (some probability) at most O(γ_2*n) points with #collision $\ge \alpha m$
  - (constant probability) one of the O(γ_2*n) points has #collision $\ge \alpha m$

Slide by W. Wang

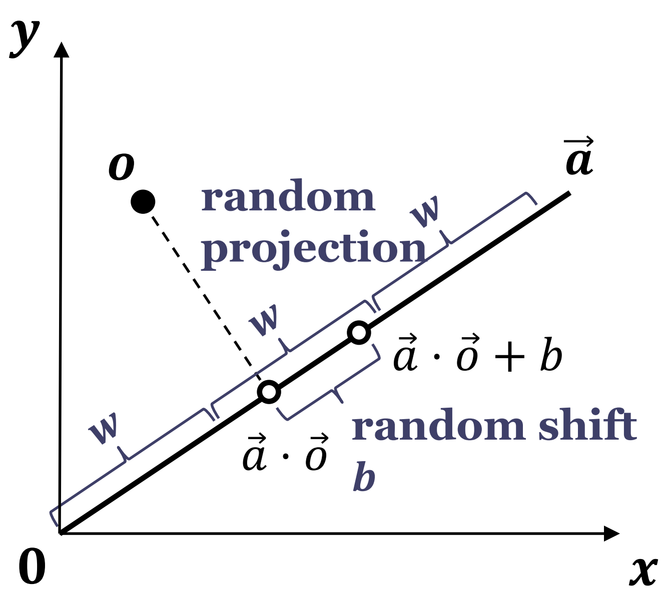
Query-oblivious LSH functions

Publications

Huang et al. PVLDB'15

- **The query-oblivious LSH functions for Euclidean distance:**

$$h_{\vec{a},b}(o) = \left\lfloor \frac{\vec{a}\cdot\vec{o}+b}{w} \right\rfloor$$



Query-Oblivious Bucket Partition:

- Buckets are ***statically*** determined before any query arrives;
- Use the **origin (i.e., "o") as anchor**;
- If $\boldsymbol{h_{\vec{a},b}(o) = h_{\vec{a},b}(q)}$, we say ***o* and *q* collide** under $h_{\vec{a},b}(\cdot)$.

Slide by Q. Huang

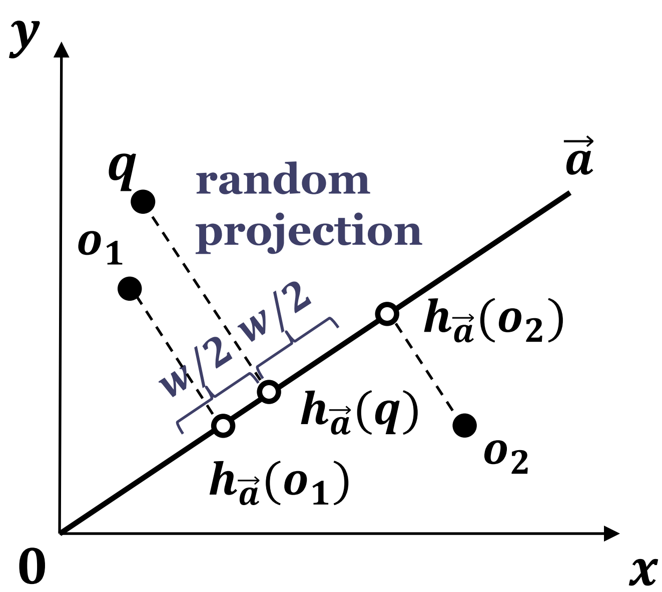
QALSH

Publications

Huang et al. PVLDB' 15

- **Query-aware LSH function = random projection + query-aware bucket partition**

$$h_{\vec{a}}(o) = \vec{a} \cdot \vec{o}$$



Query-Aware Bucket Partition:

- Buckets are **dynamically** determined when q arrives;
- Use "$h_{\vec{a}}(q)$" **as anchor** ;
- If an object o falls into the **anchor bucket**, i.e., $|h_{\vec{a}}(o) - h_{\vec{a}}(q)| \le \frac{w}{2}$, we say **$o$ and q collide** under $h_{\vec{a}}(\cdot)$.

Slide by Q. Huang

VHP

Publications

Lu et al. PVLDB’ 20

- Solution for δ-ε-approximate kNN search
  - Indexing:
    - Store LSH projections with independent B+ trees.
  - Querying
    - Impose a virtual hypersphere in the original high-d space
    - Keep enlarging the virtual hypersphere to accommodate more candidate until the success probability is met

Slide by W. Wang

Some Comparisons

Publications

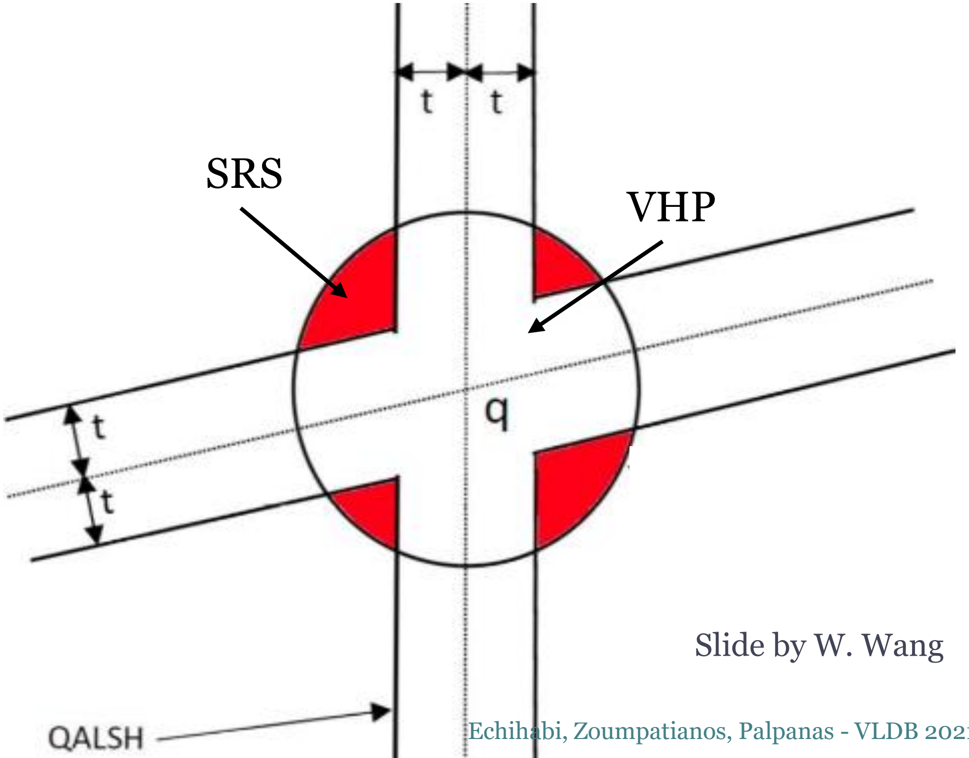
Huang et al. PVLDB' 15

Candidate Conditions

Method	Collision Count	(Observed) Distance	Max Candidates
SRS	= m	≤ r	T
QALSH	≥ αm	n/a	βn
VHP	≥ i (i = 1, 2, …, m)	≤ l_i	βn

Candidate Regions

VHP = SRS ∩ QALSH



Slide by W. Wang

High-d Vector Similarity Search
State-of-the-Art Methods

Quantization-Based Methods

Quantization

- A lossy compression process that maps a set of infinite numbers to a finite set of codewords that together constitute the codebook:
  - Scalar Quantization
    - Operates on the individual dimensions of the original vector independently
  - Vector Quantization
    - Considers the original vector as a whole
  - Product Quantization
    - Splits the original vector of dimension d into m smaller subvectors, on which a lower-complexity vector quantization is performed. The codebook consists of the cartesian product of the codebooks of the m subquantizers.
  - Scalar and vector quantization are special cases of product quantization, where m is equal to d and 1, respectively

VA-file

Publications

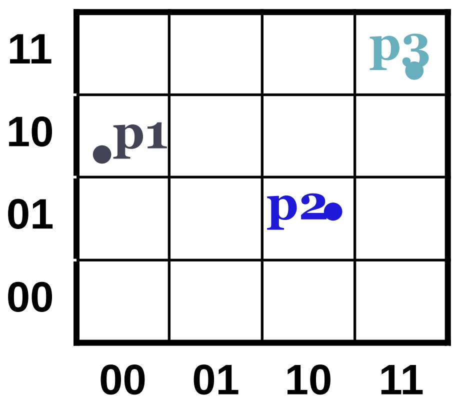
Blott et. al VLDB'98

- A solution for exact kNN search

- The basic idea of the VA-file is to speed-up the sequential scan by exploiting a "Vector Approximation"
- Each dimension of the data space is partitioned into 2^{b_i} intervals using b_i bits (scalar quantization)
  - E.g.: the 1st coordinate uses 2 bits, which leads to the intervals 00,01,10, and 11
- Thus, each coordinate of a point (vector) requires now b_i bits instead of 32

- The VA-file stores, for each point of the dataset, its approximation, which is a vector of $\sum_{i=1,D} b_i$ bits

Data space



Feature values

p1	0.1 0.6
p2	0.7 0.4
p3	0.9 0.3

VA-file

p1	00 10
p2	10 01
p3	11 11

Slides by M. Patella.

VA-file

Publications

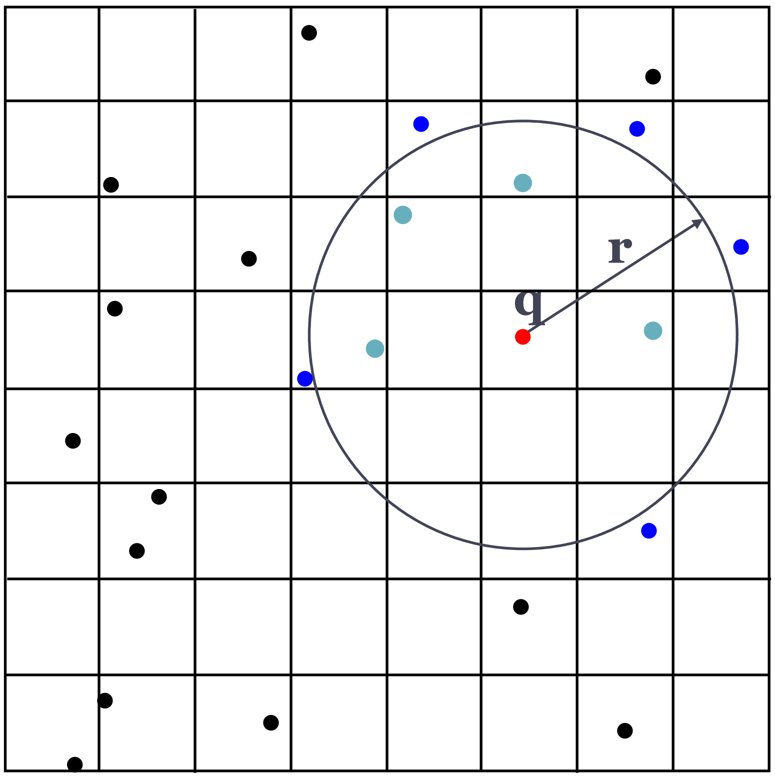
Blott et. al
VLDB'98

- Query processing with the VA-file is based on a filter & refine approach

- For simplicity, consider a range query

  Filter: the VA file is accessed and only the points in the regions that intersect the query region are kept

  Refine: the feature vectors are retrieved and an exact check is made



actual results
false drops
excluded points

Slides by M. Patella.

VA+file

Publications

Ferhatosmanoglu et al.
CIKM'00

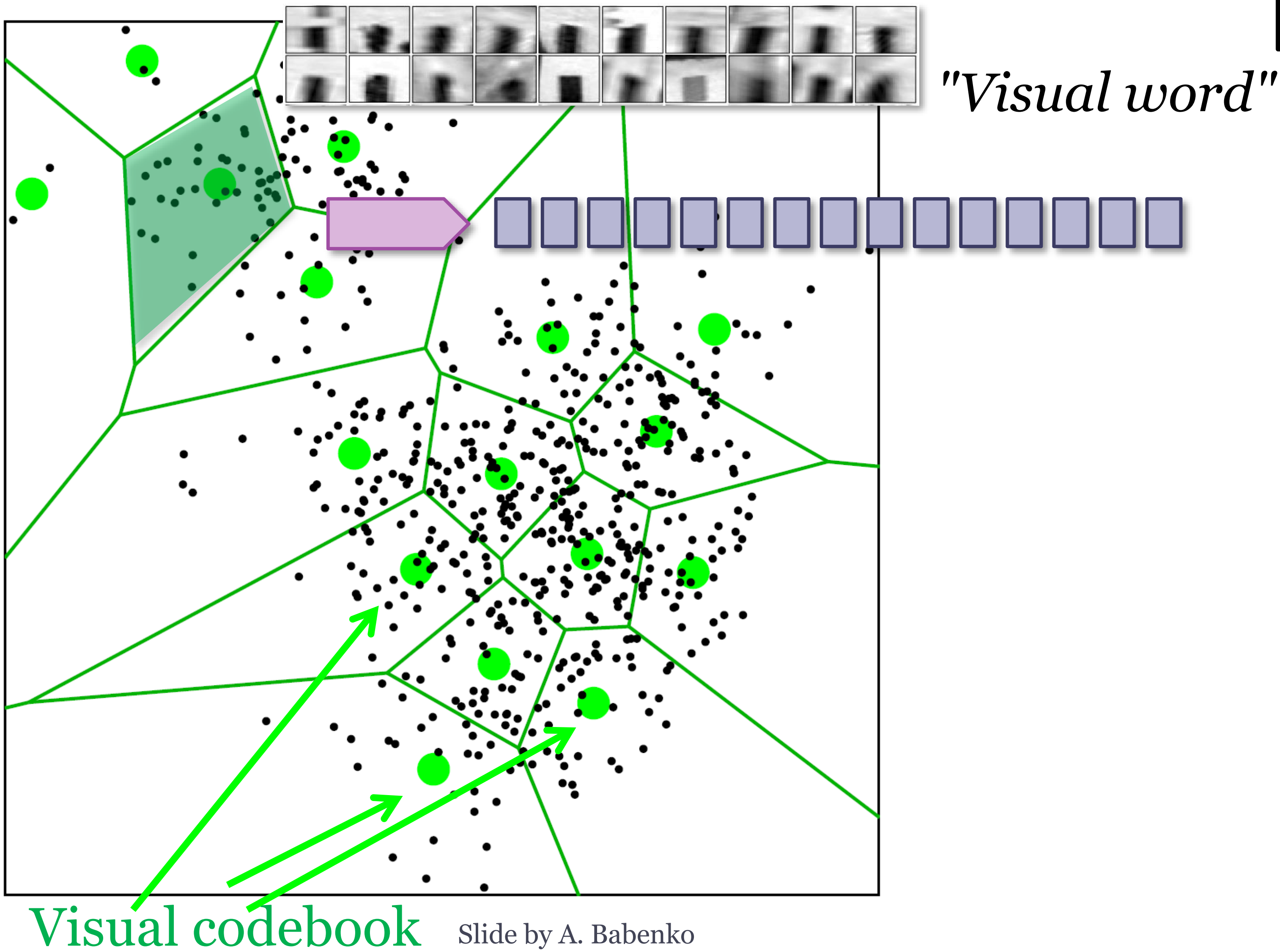
- Solution for exact kNN search

- An improvement of the VA-file method:
  - Does not assume that neighboring dimensions are uncorrelated
  - Decorrelates the data using KLT
  - Allocates bits per dimension in a non-uniform fashion
  - Partitions each dimension using k-means instead of equi-depth

The Inverted Index

Publications

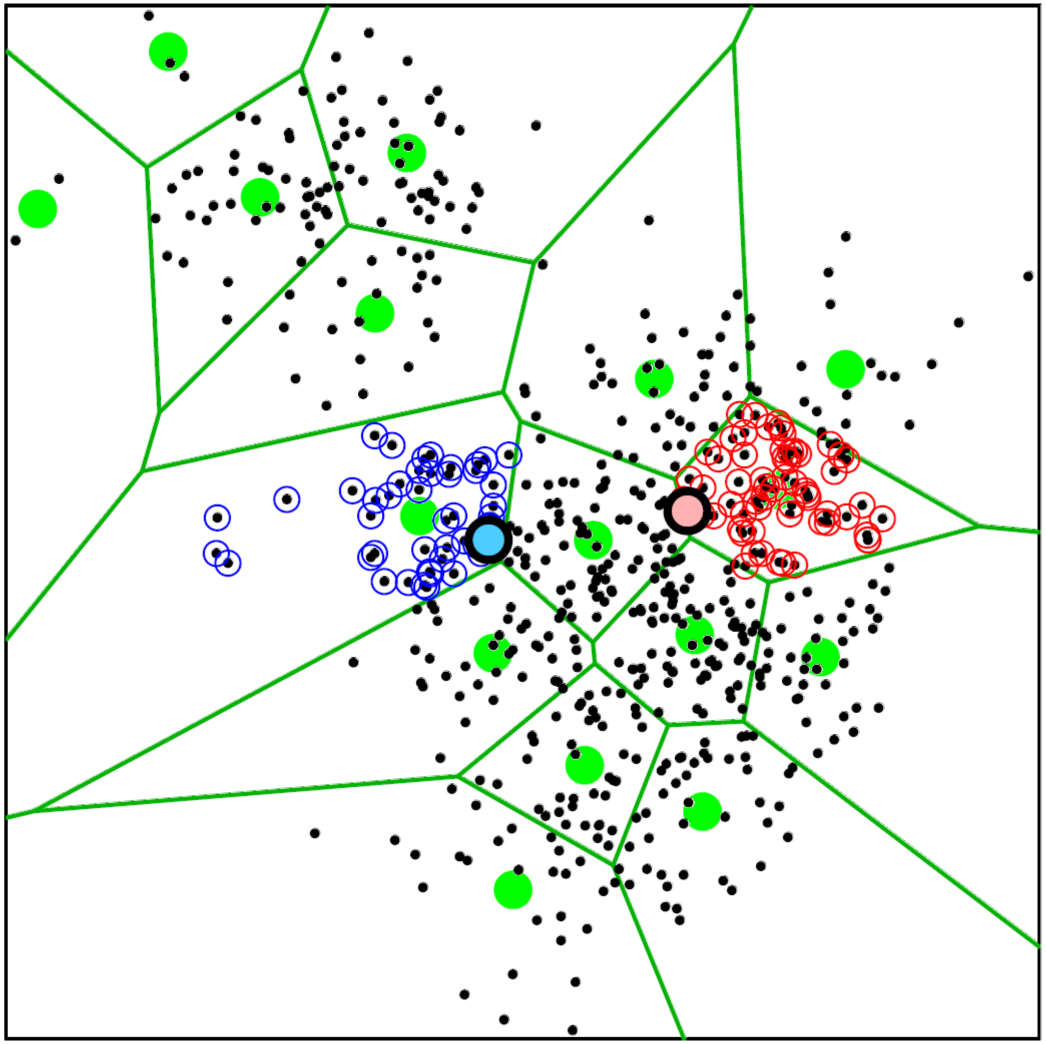
Sivic et al. ICCV' 03



Slide by A. Babenko

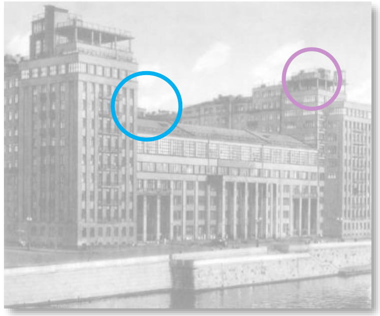
Querying the Inverted Index

Publications
Sivic et al. ICCV' 03



Slide by A. Babenko

Query:



- Have to consider several words for best accuracy
- Want to use as big codebook as possible

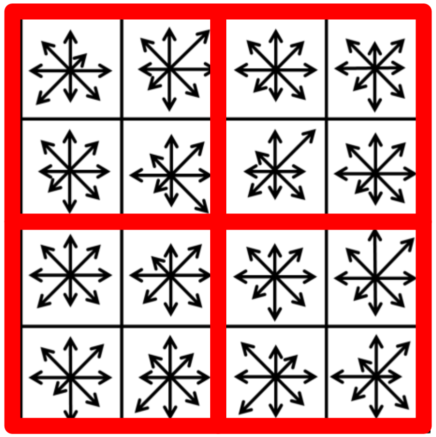
conflict

- Want to spend as little time as possible for matching to codebooks

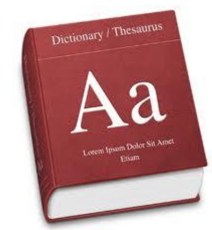
Product Quantization

Publications

Jegou et al. TPAMI' 11



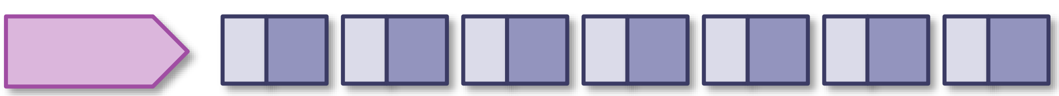
1. Split vector into correlated subvectors
2. use separate small codebook for each chunk



Quantization vs. Product quantization:

For a budget of 4 bytes per descriptor:

1. Can use a single codebook with 1 billion codewords
2. Can use 4 different codebooks with 256 codewords each



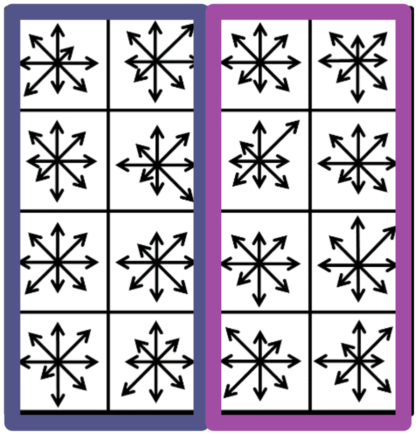
IVFADC+ variants (state-of-the-art for billion scale datasets) =
inverted index for indexing + product quantization for reranking

Slide by A. Babenko

The Inverted Multi-Index

Publications

Babenko et al. TPAMI' 12

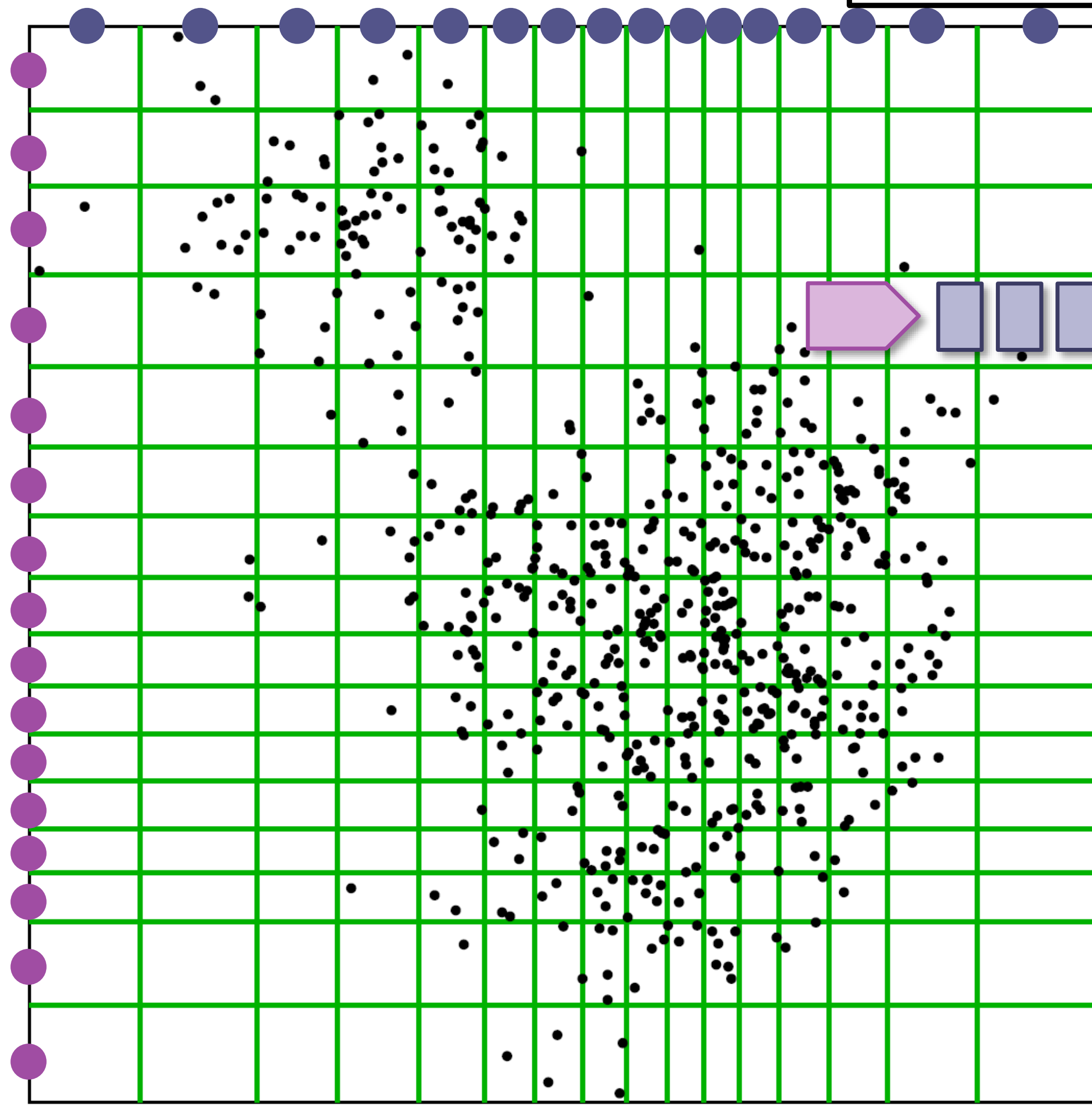


Idea: use product quantization for indexing

Main advantage:
For the same K, much finer subdivision achieved

Main problem:
Very non-uniform entry size distribution

Slide by A. Babenko



Querying the Inverted Multi-Index

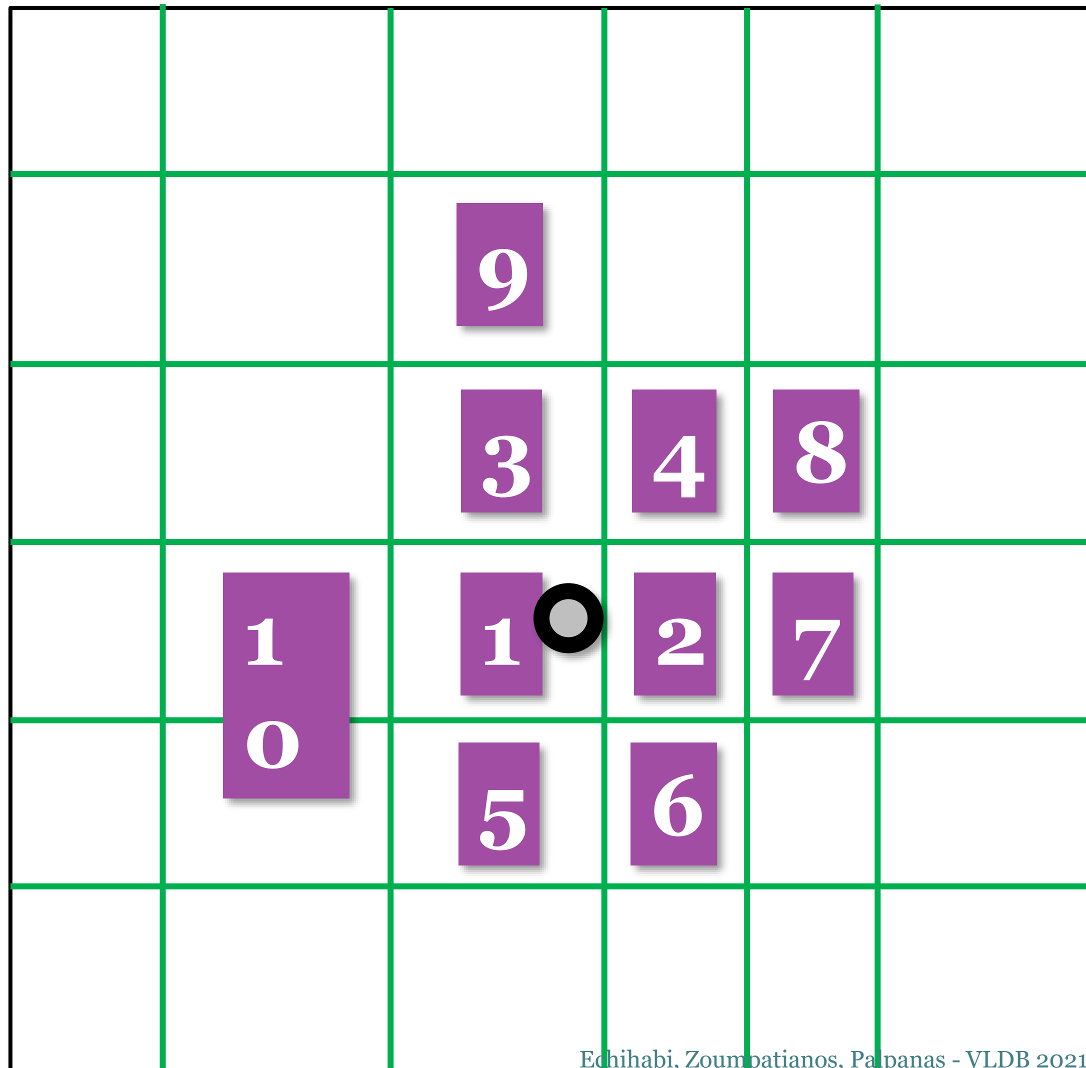
Publications

Babenko et al. TPAMI' 12

Answer to the query:

Input: query

Output: stream of entries



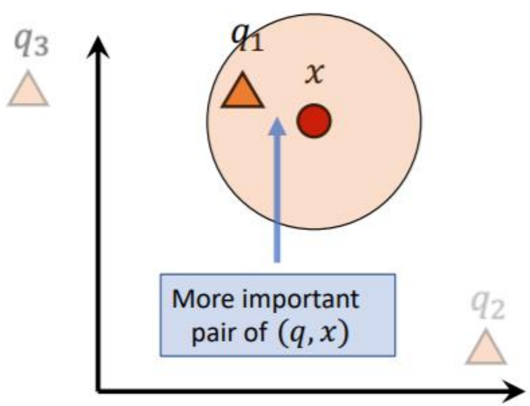
Slide by A. Babenko

Publications

Guo-ICML'20

Google ScaNN

- Quantization-based similarity search using MIPS
  - A novel score-aware loss function:
    - The approximation error on the pairs which have a high inner product is far more important than that of pairs whose inner product is low.



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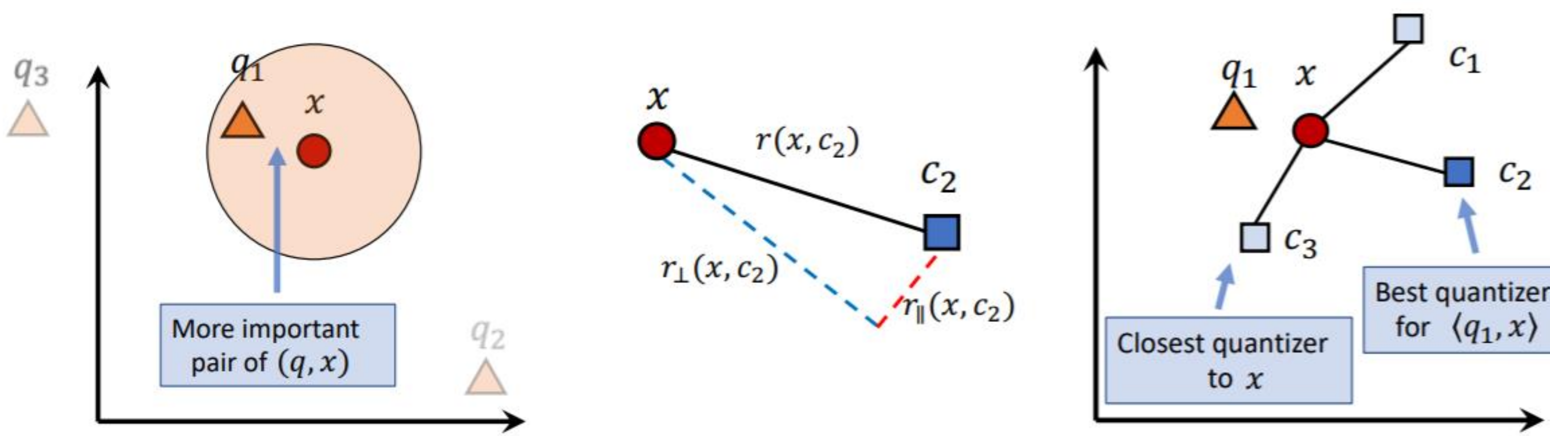


High-d Vector Similarity Search State-of-the-Art Methods

Graph-Based Methods

Conceptual Graphs

- Voronoi/Delaunay Diagrams
- kNN Graphs
- Navigable Small World Graphs
- Relative Neighborhood graphs

The Delaunay Diagram

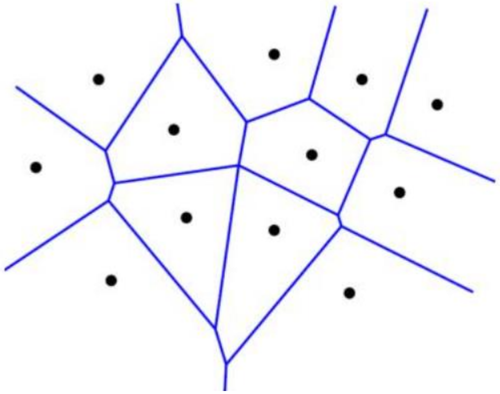
Publications

Delaunay
CSMN' 39

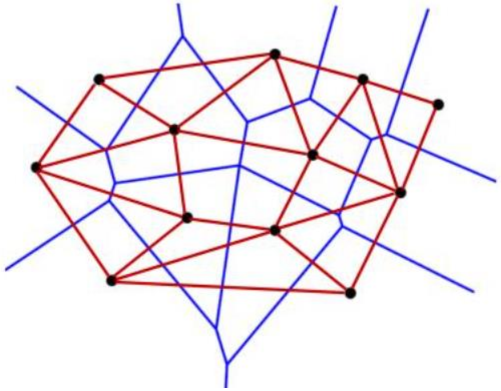
Delaunay Diagram – Dual of Voronoi Diagram

- The VD is constructed by decomposing the space using a finite number of points, called sites into regions, such that each site is associated to a region consisting of all points closer to it than to any other site.

- The DT is the dual of the VD, constructed by connecting sites with an edge if their regions share a side.



Voronoi Diagram



Delaunay Diagram

kNN Graphs

Publications

Anastasiu et al. CIKM' 15

Dong et al. WWW' 11

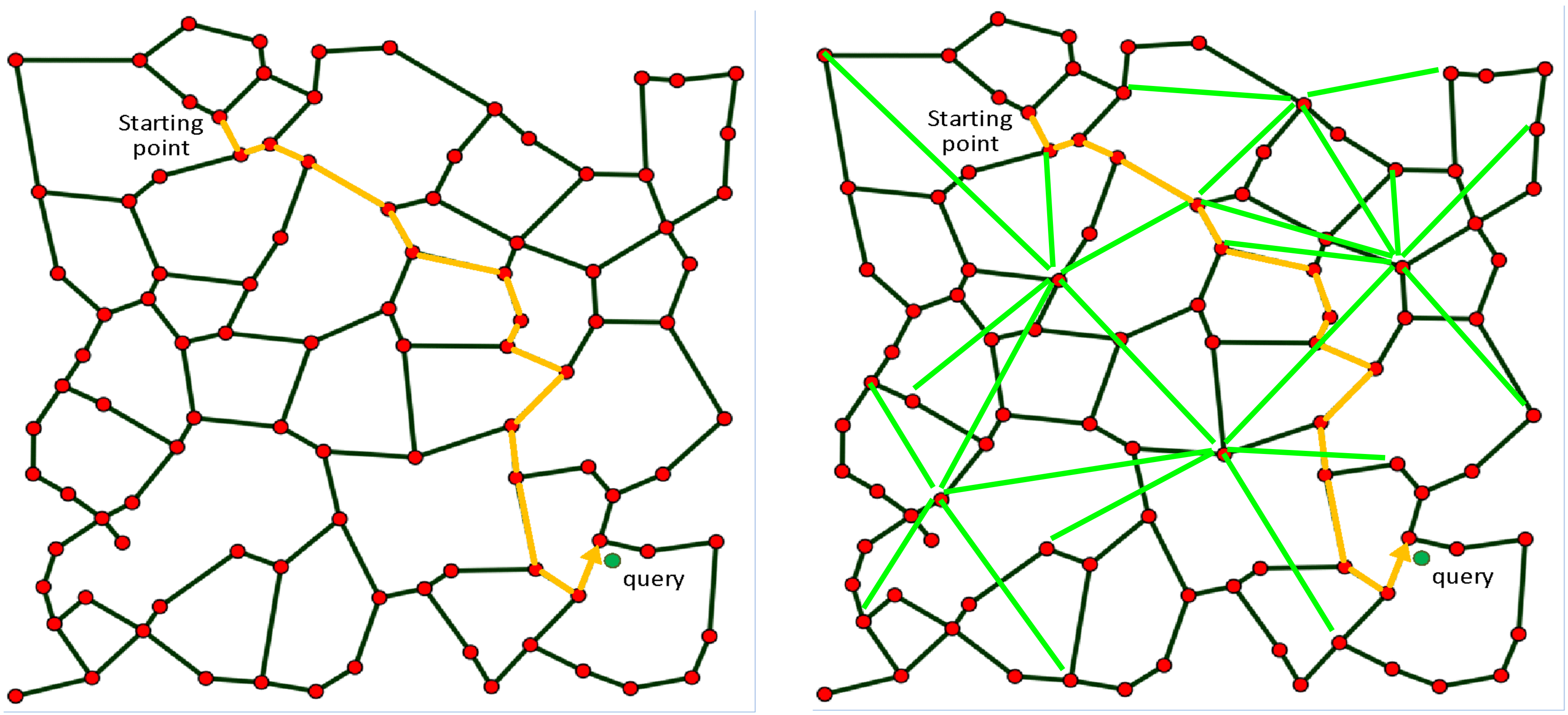
- Exact kNN graphs on n d-dimensional points:
  - Each point in the space is considered a node
  - A directed edge is added between nodes node A and B (A -=> B) if B is a kNN of A
  - $O(dn^2)$
  - Example: L2knng
- Approximate kNN Graphs:
  - LSH
  - Heuristics
    - Example: NN-Descent: "*a neighbor of a neighbor is also likely to be a neighbor*"

NSW Graphs

Publications

Kleinberg STOC' 00

- Augment approximate kNN graphs with long range links:
  - Milgram experiment
  - Shorten the greedy algorithm path to log(N)

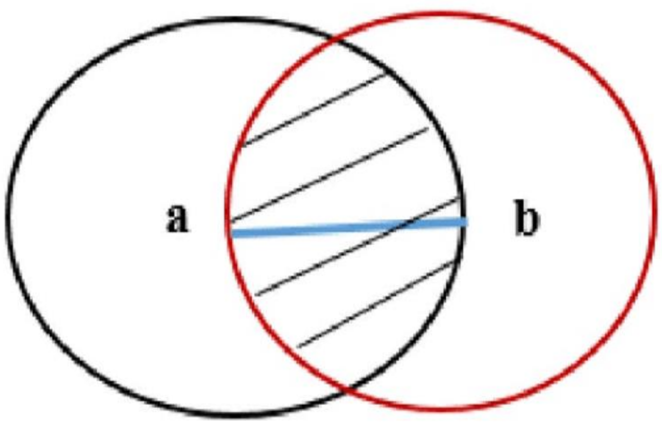


Publications

Toussaint
Pat. Recognit.'80

Relative Neighbourhood graph (RNG)

- A superset of the minimal spanning tree (MST) and a subset of the Delaunay Diagram.
- Two algorithms for obtaining the RNG of n points on the plane:
  - An algorithm for 1-d space in o(n2) time
  - Another algorithm for d-dimensional spaces running in o(n3).
- An edge is constructed between two vertices if there is no vertex in the intersection of the two balls

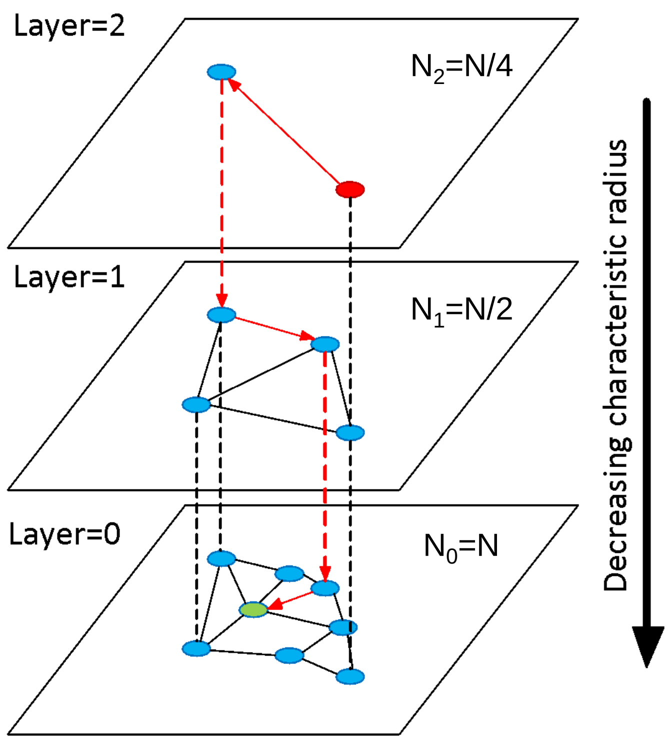


HNSW

Publications

Malkov et al. TPAMI' 20 Arxiv'16

- In HNSW we split the graph into layers (fewer elements at higher levels)
- Search starts for the top layer. Greedy routing at each level and descend to the next layer.
- Maximum degree is capped while paths ~ log(N) → log(N) complexity scaling.
- Incremental construction



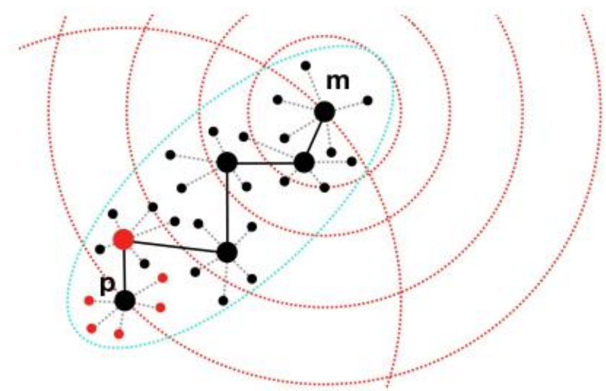
Slides by Malkov

Navigating Speading-out Graph (NSG)

Publications

Fu et al. PVLDB' 19

- RNGs do not guarantee monotonic search
  - There exists at least one monotonic path. Following this path, the query can be approached with the distance decreasing monotonically
- Propose a Monotonic RNG (MRNG)
- Build an approximate *k*NN graph.
- Find the <u>*Navigating Node*</u>. (All search will start with this fixed node – center of the graph).
- For each node p, find a relatively small candidate neighbour set. (*sparse*)
- Select the edges for p according to the definition of MRNG. (*low complexity*)
- leverage Depth-First-Search tree (*connectivity*)



Slides by Fu

Other tutorials

- for a more complete and detailed presentation, see tutorials:
  - Jianbin Qin, Wei Wang, Chuan Xiao, Ying Zhang: Similarity Query Processing for High-Dimensional Data. PVLDB. 13(12): 3437-3440 (2020).
  - *Karima Echihabi, Kostas Zoumpatianos, Themis Palpanas. High-Dimensional Similarity Search for Scalable Data Science. ICDE 2021*

High-d Vector Similarity Search State-of-the-Art Methods

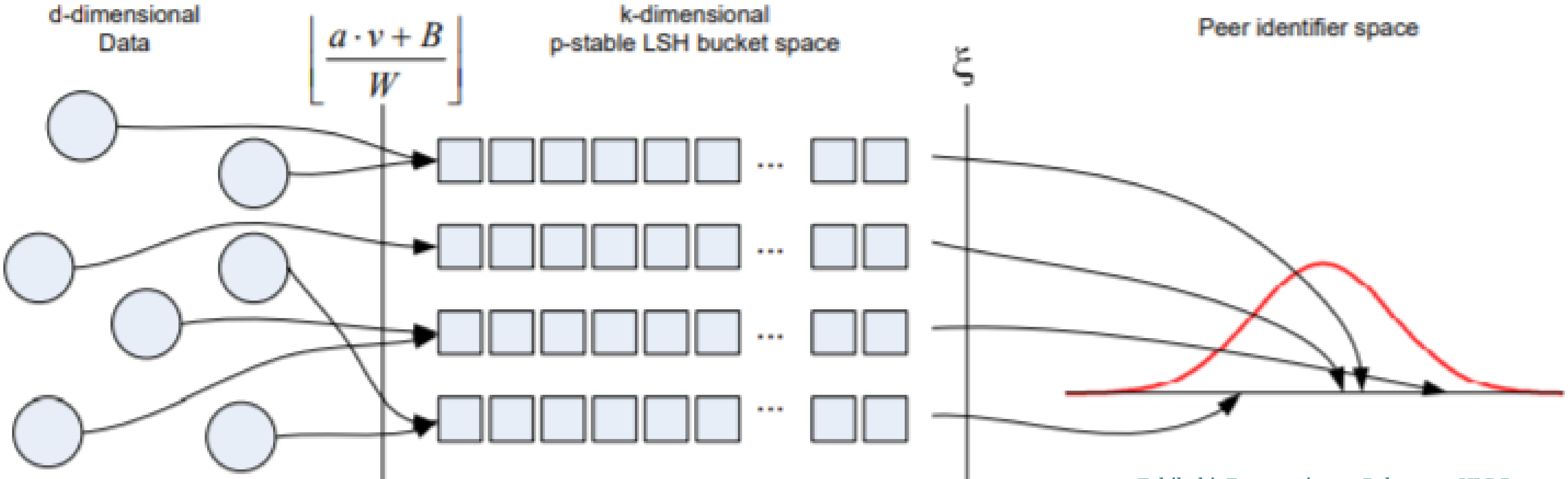
Modern Hardware & Distribution

Distributed LSH

Publications

Haghani-EDBT'09

- A two-level mapping strategy
  - Condition 1: assign buckets likely to hold similar data to the same peer.
  - Condition 2: have a predictable output distribution which fosters fair load balancing.
- Theoretical guarantees on locality preserving properties of the mapping
- Significant improvement over state-of-the-art



Layered LSH

Publications

Bahmani-CIKM'12

- One of the early works
- Entropy-based LSH in Euclidean space
- Apache Hadoop for disk-based version
- Twitter storm for in-memory version
- Theoretical guarantees
  - Only for the single hash tables setting

PLSH

Publications

Sundaram-PVLDB'13

- In-memory, multi-core, distributed LSH
  - Designed for text data (angular distance)
- Main idea
  - Use a caching strategy to improve online index construction
  - Insert-optimized delta tables to hold indexes of new data
    - Merge periodically with main index structures
  - Eliminate duplicate data using a bitmap-based strategy
  - Model to predict performance
- Experiments on a billion-tweet dataset on 100 nodes
  - 1-2.5 ms per query
  - Streaming 100 millions of tweets per day

RDH

Publications

Durmaz-PLR'19

- Distributed similarity search for images
- Main ideal:
  - Randomly splits and distributes the dataset over compute nodes
  - Each node builds an LSH index over its data subset
  - Same hash functions used in all nodes
  - No communication between nodes
  - Network used to send hash functions and
- 8x faster (with 10 nodes) than state-of-the-art while maintaining similar accuracy

FAISS

Publications

Johnson-ITBD'21

- Facebook's library for similarity search
  - CPU and GPU implementations
- FAISS GPU:
  - Quantization-based inverted index
  - kNN graph
- Experiments
  - Up to 8.5x faster than other GPU-based techniques
  - 5x-10x faster than corresponding CPU implementation on a single GPU
  - Near linear speedup with multiple GPUs over a single GPU
  - 95 million images in 35 minutes, and of a graph connecting 1 billion vectors in less than 12 hours on 4 Maxwell Titan X GPUs

Questions?

Experimental Comparisons: Similarity Search Methods

How do similarity search methods compare?

- several methods proposed in last 3 decades by different communities
  - never carefully compared to one another

- we now present results of extensive experimental comparison

Experimental Comparisons: A Taxonomy

Methods

Publications

Echihabi-PVLDB'18

Echihabi-PVLDB'19

Similarity Search Methods

Methods

Publications

Echihabi-PVLDB'18

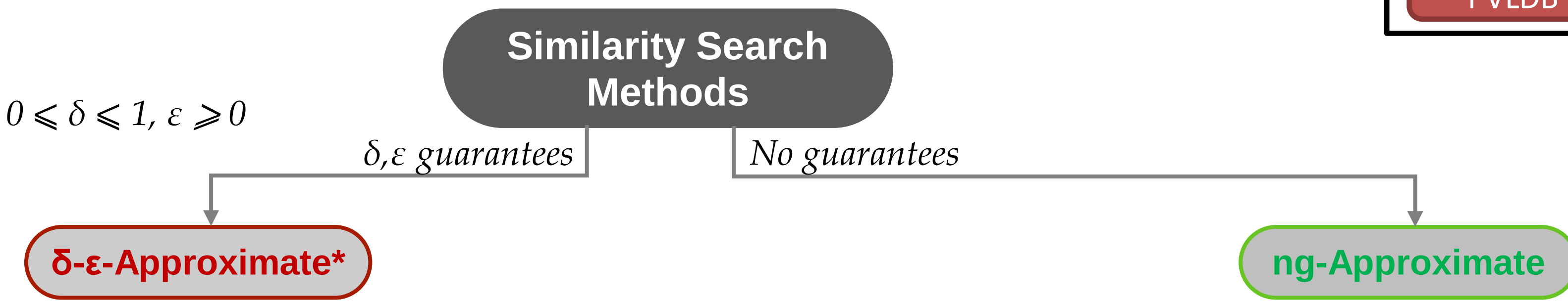
Echihabi-PVLDB'19

Methods

Publications

Echihabi-PVLDB'18

Echihabi-PVLDB'19



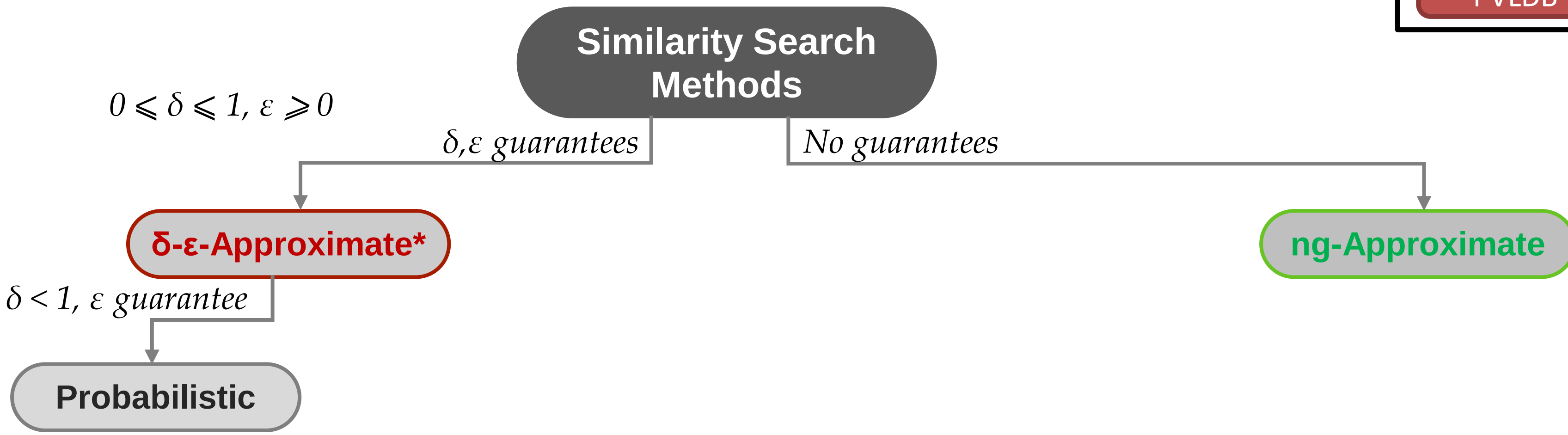
* result is within distance (1+ ε) of the exact answer with probability δ

Publications

Echihabi-PVLDB'18

Echihabi-PVLDB'19

Methods



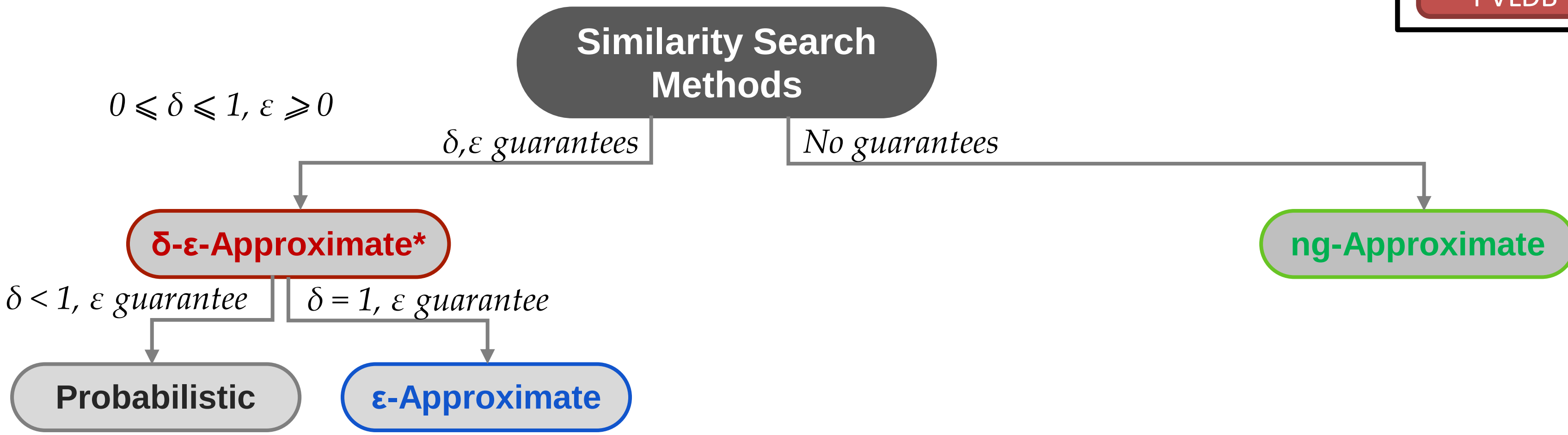
* result is within distance (1+ ε) of the exact answer with probability δ

Methods

Publications

Echihabi-PVLDB‘18

Echihabi-PVLDB‘19



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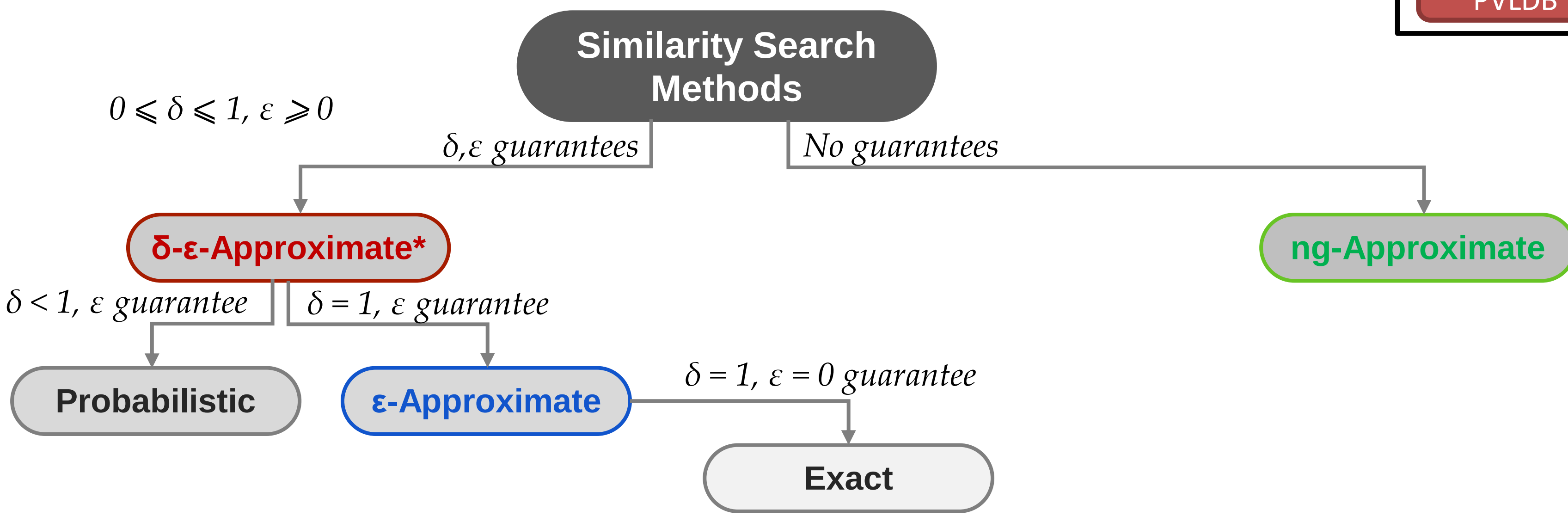
Methods

Publications

Echihabi-PVLDB'18

Echihabi-PVLDB'19

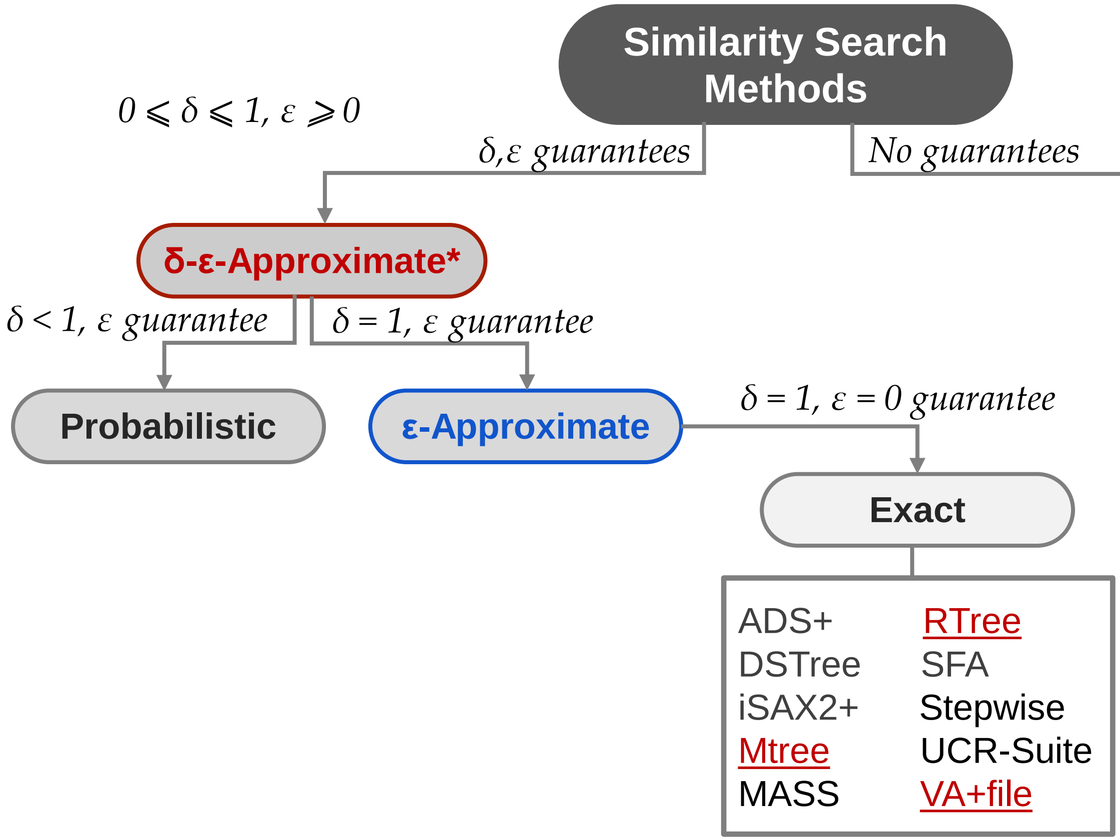


* result is within distance (1+ ε) of the exact answer with probability δ

Methods

Techniques for data Series
Techniques for High-D vectors

Publications
Echihabi-PVLDB‘18
Echihabi-PVLDB‘19



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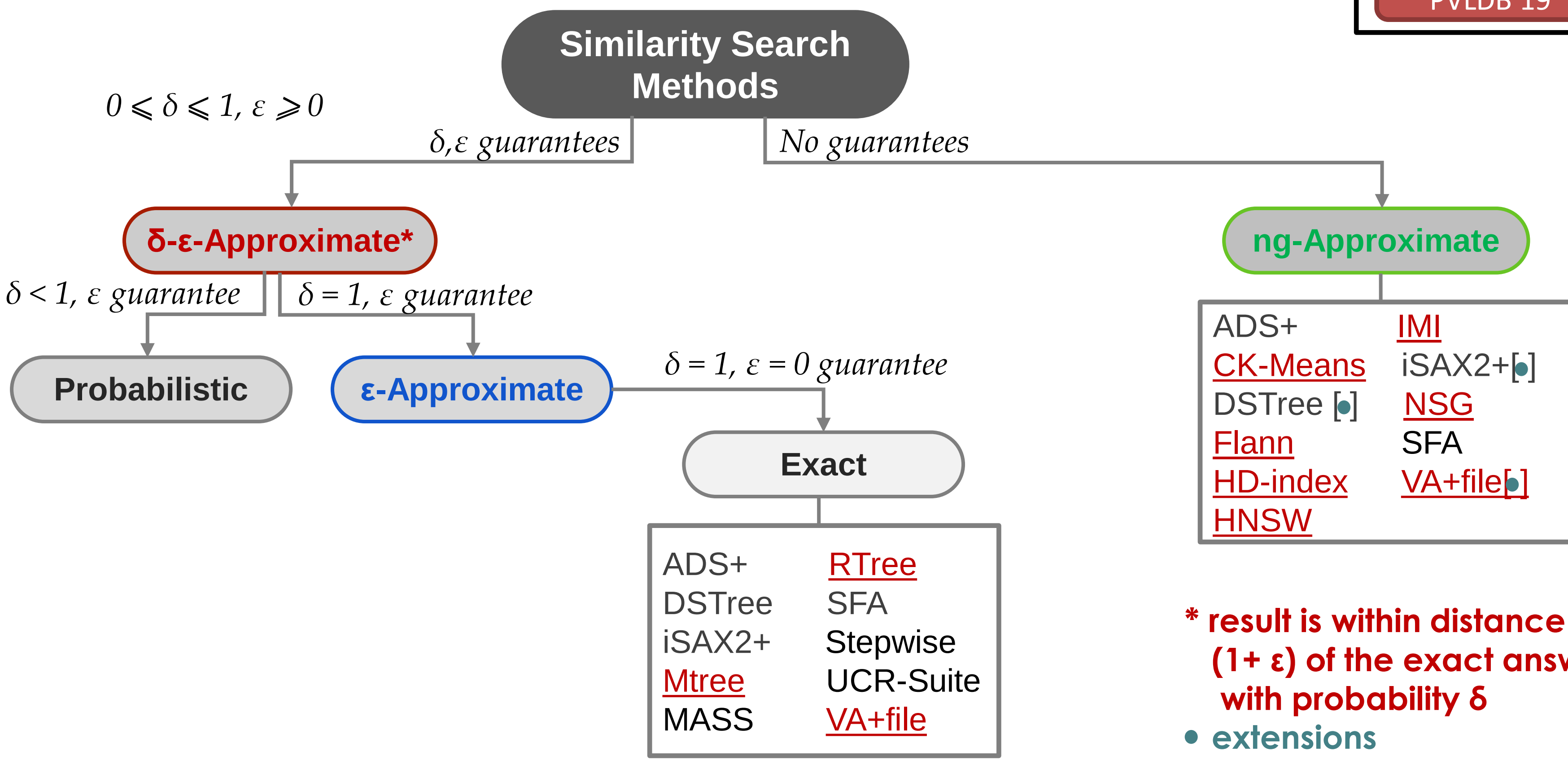
Methods

Techniques for data Series
Techniques for High-D vectors

Publications
Echihabi-PVLDB'18
Echihabi-PVLDB'19



*** result is within distance (1+ ε) of the exact answer with probability δ**

• extensions

Methods

Publications
- Echihabi-PVLDB'18
- Echihabi-PVLDB'19

Techniques for data Series
Techniques for High-D vectors

Similarity Search Methods

$0 \leqslant \delta \leqslant 1, \varepsilon \geqslant 0$

δ,ε guarantees → **δ-ε-Approximate***
- *δ < 1, ε guarantee* → **Probabilistic**
- *δ = 1, ε guarantee* → **ε-Approximate**
  - ADS+[•]
  - DSTree[•]
  - iSAX2+ [•]
  - Mtree
  - VA+file[•]
  - *δ = 1, ε = 0 guarantee* → **Exact**
    - ADS+
    - DSTree
    - iSAX2+
    - Mtree
    - MASS
    - RTree
    - SFA
    - Stepwise
    - UCR-Suite
    - VA+file

No guarantees → **ng-Approximate**
- ADS+
- CK-Means
- DSTree [•]
- Flann
- HD-index
- HNSW
- IMI
- iSAX2+[•]
- NSG
- SFA
- VA+file[•]

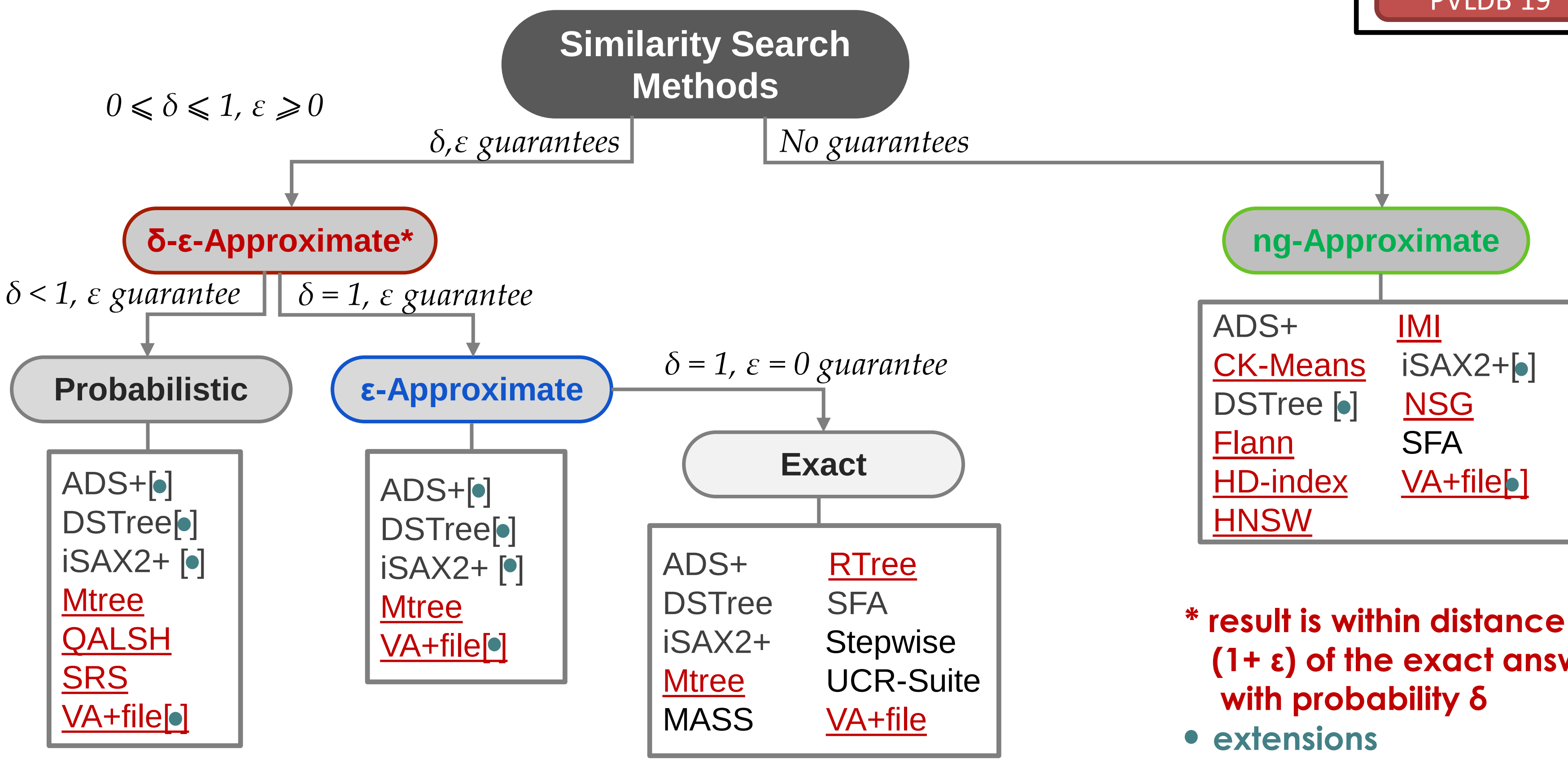
*** result is within distance (1+ ε) of the exact answer with probability δ**

• extensions

Methods

Techniques for data Series
Techniques for High-D vectors

Publications
- Echihabi-PVLDB'18
- Echihabi-PVLDB'19



*** result is within distance (1+ ε) of the exact answer with probability δ**
- **extensions**

Experimental Comparisons: Exact Query Answering

Experimental Framework

Publications

Echihabi-PVLDB'18

- Hardware
  - HDD and SSD
- Datasets
  - Synthetic (25GB to 1TB) and 4 real (100 GB)
- Exact Query Workloads
  - 100 – 10,000 queries
- Performance measures
  - Time, #disk accesses, footprint, pruning, Tightness of Lower Bound (TLB), etc.
- C/C++ methods (4 methods reimplemented from scratch)

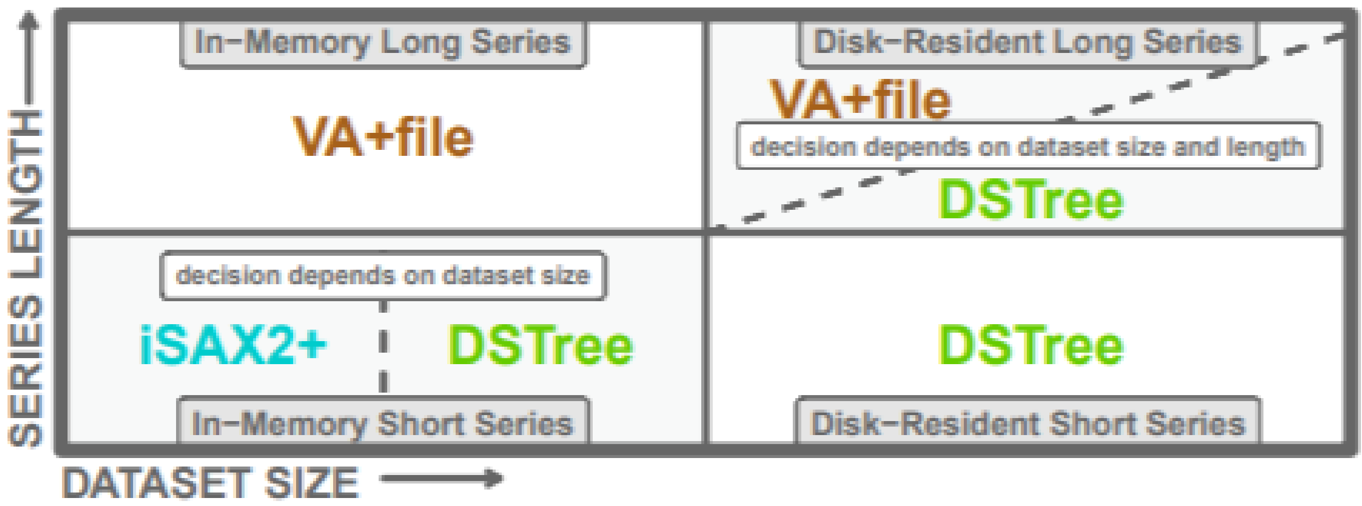
- Procedure:
  - Step 1: Parametrization
  - Step 2: Evaluation of individual methods
  - Step 3: Comparison of best methods

Recommendations

Publications

Echihabi-PVLDB'18

Scenario: Indexing and answering 10K exact queries on HDD



Unexpected Results

Publications

Echihabi-PVLDB'18

- Some methods do not scale as expected (or not at all!)
- Brought back to the spotlight two older methods VA+file and DSTree
  - New reimplementations outperform by far the original ones
- Optimal parameters for some methods are different from the ones reported in the original papers
- Tightness of Lower Bound (TLB) does not always predict performance

Insights

Publications

Echihabi-PVLDB'18

- Results are sensitive to:
  - Parameter tuning
  - Hardware setup
  - Implementation
  - Workload selection
- Results identify methods that would benefit from modern hardware

Experimental Comparisons: Approximate Query Answering

Experimental Framework

Publications

Echihabi-PVLDB'19

- Datasets
  - In-memory and disk-based datasets
  - Synthetic data modeling financial time series
  - Four real datasets from deep learning, computer vision, seismology, and neuroscience (25GB-250GB)
- Query Workloads
  - 100 – 10,000 kNN queries k in [1,100]
  - ng-approximate and δ-ε-approximate queries (exact queries used as yardstick)
- C/C++ methods (3 methods reimplemented from scratch)
- Performance measures
  - Efficiency: time, throughput, #disk accesses, % of data accessed
  - Accuracy: average recall, mean average precision, mean relative error
- Procedure:
  - Step 1: Parametrization
  - Step 2: Evaluation of indexing/query answering scalability in-memory
  - Step 3: Evaluation of indexing/query answering scalability on-disk
  - Step 4: Additional experiments with best-performing methods on disk

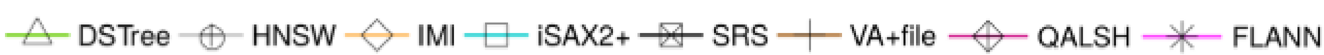
Approximate Methods Covered in Study

		Matching Accuracy				Representation		Implementation		
		exact	ng-appr.	ϵ-appr.	δ-ϵ-appr.	Raw	Reduced	Original	New	Disk-resident Data
Graphs	HNSW		[99]			✓		C++		
	NSG		[58]			✓		C++		
Inv. Indexes	IMI		[16, 60]				OPQ	C++		✓
LSH	QALSH				[69]		Signatures	C++		
	SRS				[136]		Signatures	C++		
Scans	VA+file	[55]	•	•	•		DFT	MATLAB	C	✓
Trees	Flann		[107]			✓		C++		
	DSTree	[146]	[146]	•	•		EAPCA	Java	C	✓
	HD-index		[11]				Hilbert keys	C++		✓
	iSAX2+	[30]	[30]	•	•		iSAX	C#	C	✓

- **Our extensions**

Unexpected Results

- New data series extensions are the overall winners even for general high-d vectors
  - perform the best for approximate queries with probabilistic guarantees (δ-ε-approximate search)



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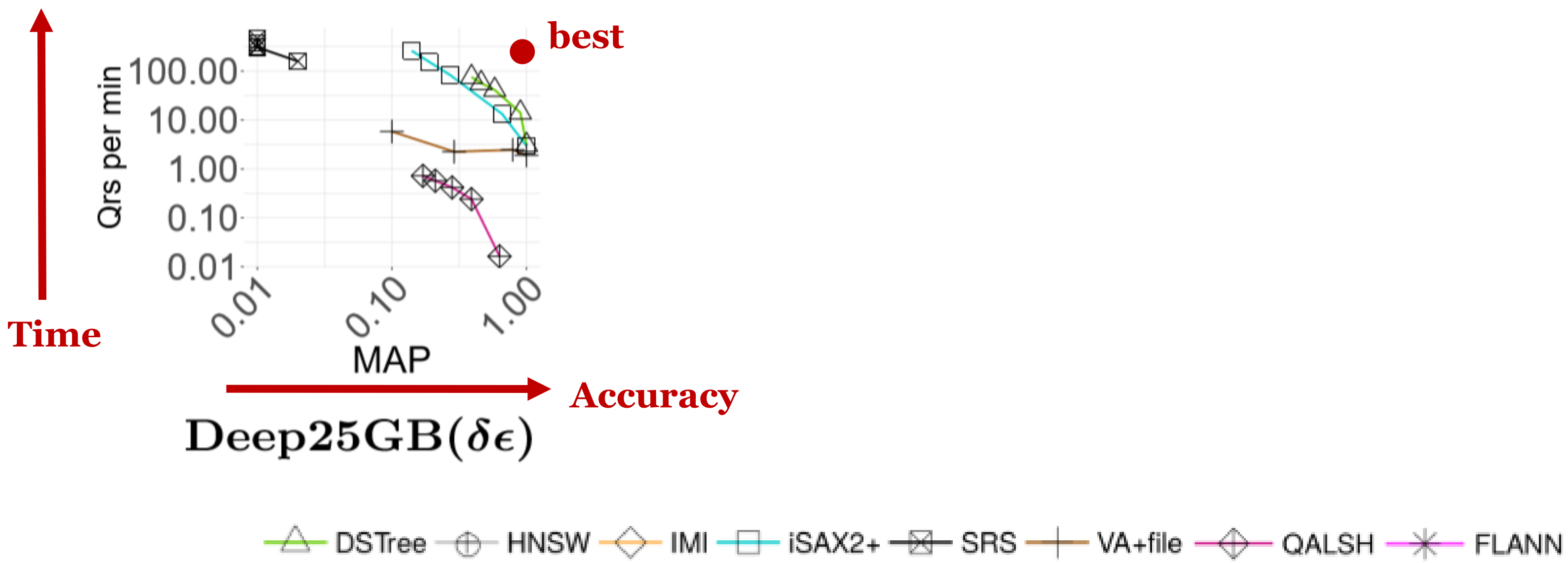
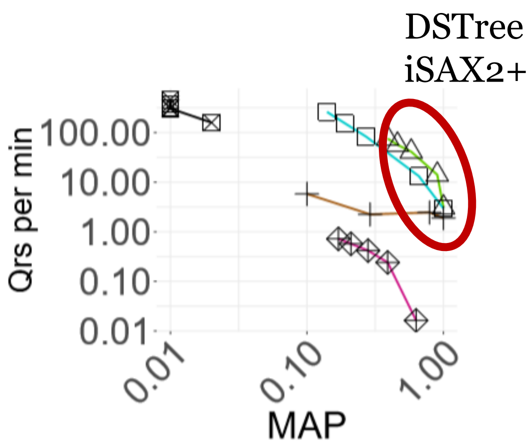
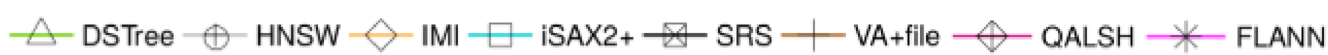


Unexpected Results

- New data series extensions are the overall winners even for general high-d vectors
  - perform the best for approximate queries with probabilistic guarantees (δ-ε-approximate search), in-memory

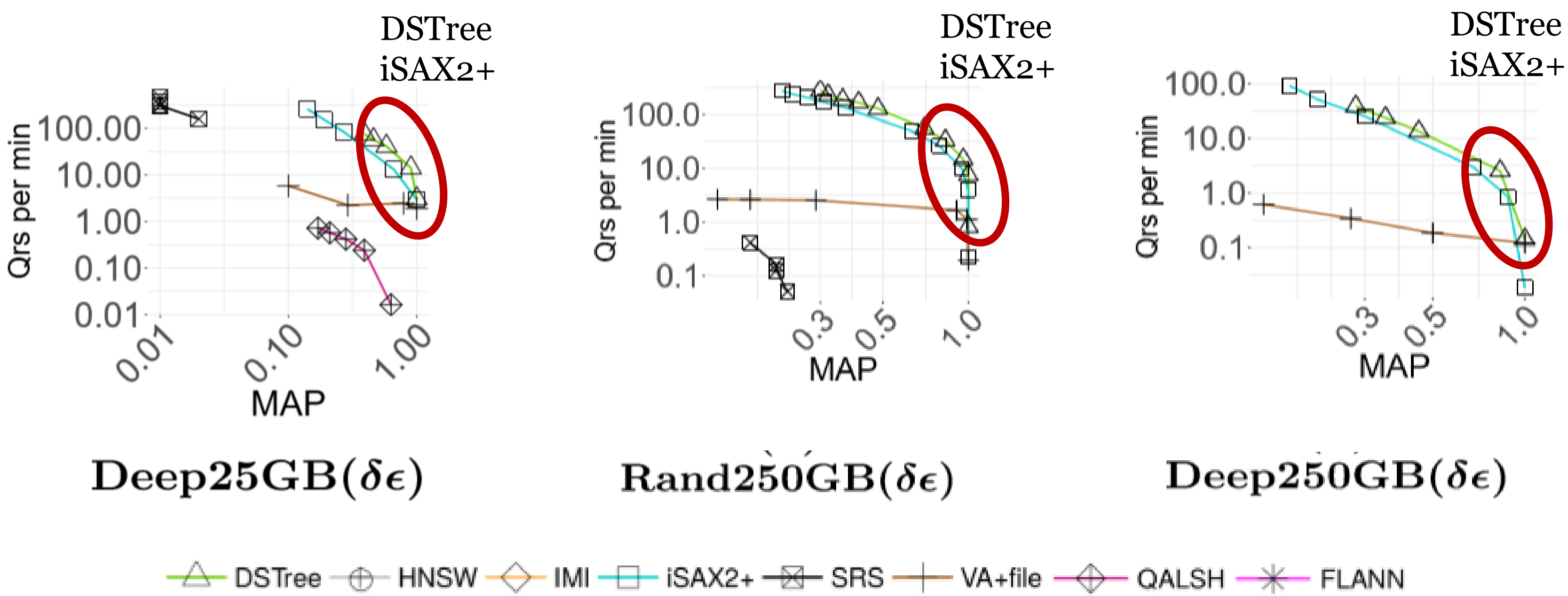


Deep25GB($\delta\epsilon$)



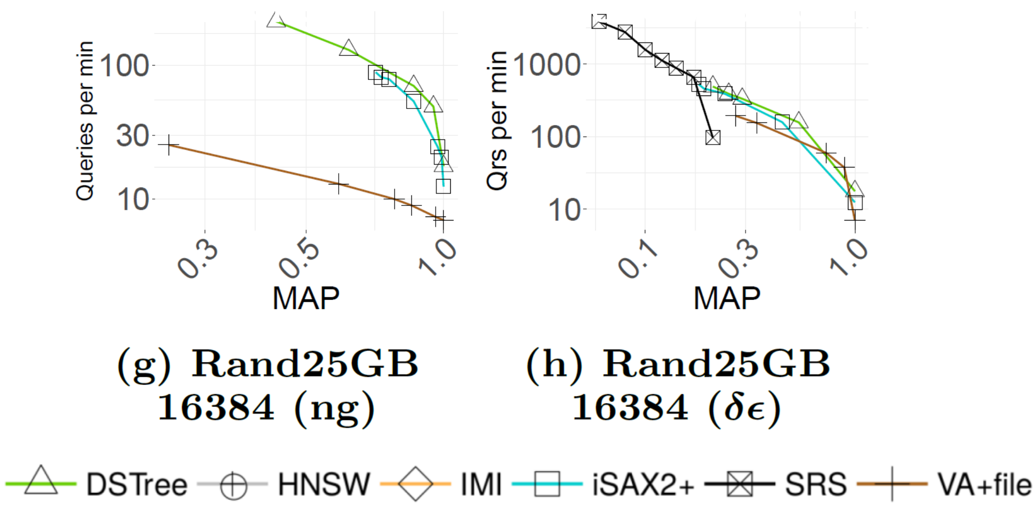
Unexpected Results

- New data series extensions are the overall winners even for general high-d vectors
  - perform the best for approximate queries with probabilistic guarantees (δ-ε-approximate search), in-memory and on-disk



Unexpected Results

- New data series extensions are the overall winners even for general high-d vectors
  - perform the best for approximate queries with probabilistic guarantees (δ-ε-approximate search), in-memory and on-disk
  - perform the best for long vectors



(g) Rand25GB 16384 (ng)

(h) Rand25GB 16384 ($\delta\epsilon$)

Unexpected Results

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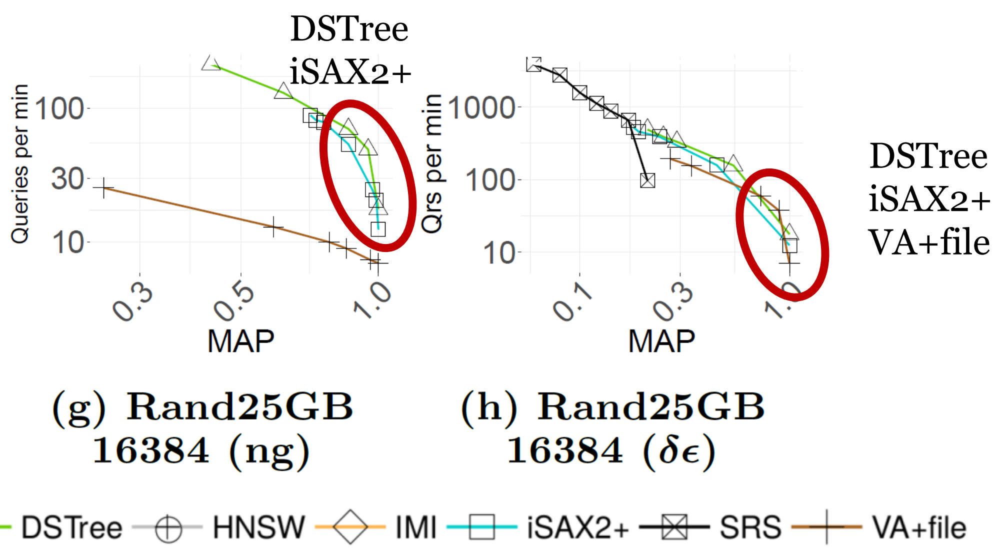

(g) Rand25GB 16384 (ng)

(h) Rand25GB 16384 (δϵ)

Unexpected Results

- New data series extensions are the overall winners even for general high-d vectors
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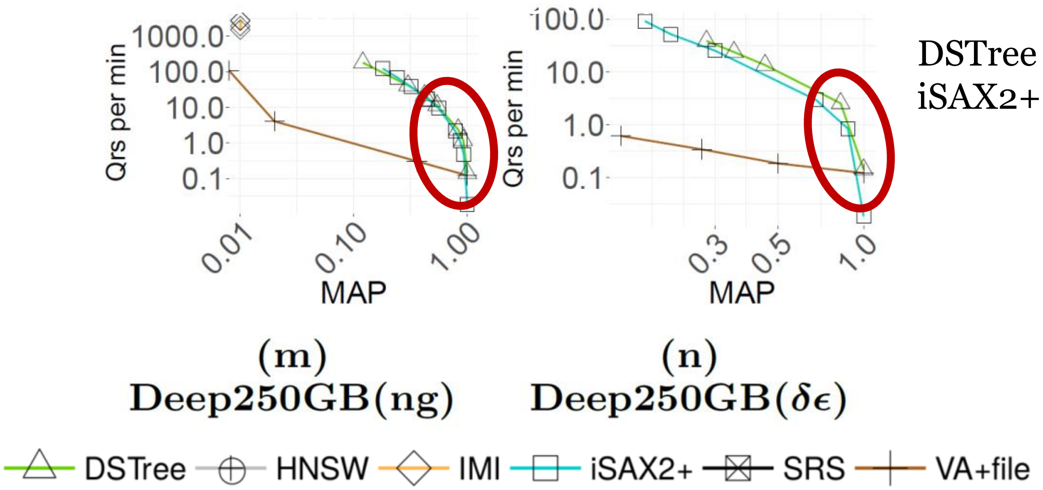
  - perform the best for disk-resident vectors



(m) Deep250GB(ng) (n) Deep250GB($\delta\epsilon$)

Unexpected Results

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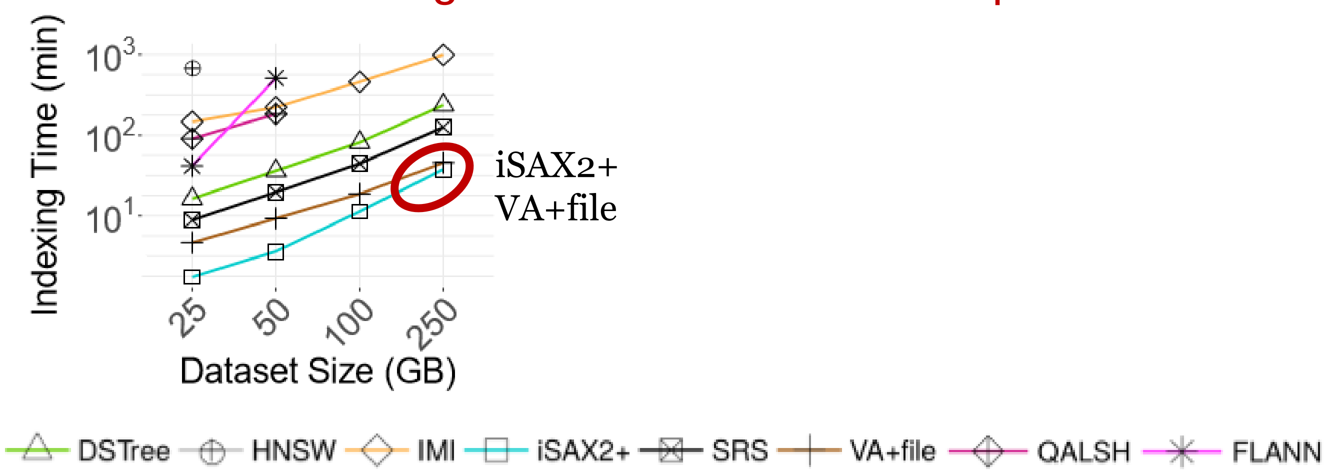
  - perform the best for long vectors, in-memory and on-disk
  - perform the best for disk-resident vectors
  - are fastest at indexing and have the lowest footprint



Unexpected Results

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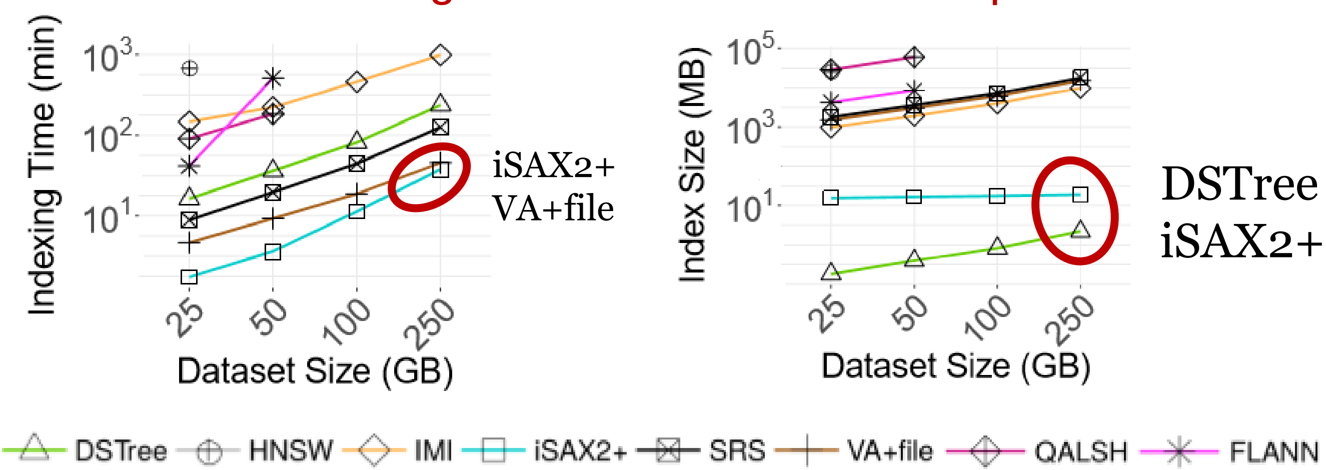

Insights

Exciting research direction for approximate similarity search in high-d spaces:

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Currently two main groups of solutions exist:

approximate search solutions
without guarantees
relatively efficient

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Exciting research direction for approximate similarity search in high-d spaces:

Currently two main groups of solutions exist:

approximate search solutions	approximate search solutions
without guarantees	with guarantees
relatively efficient	relatively slow

We show that it is possible to have efficient approximate algorithms with guarantees

Insights

Approximate state-of-the-art techniques for high-d vectors are not practical:

Insights

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- LSH-based techniques
  - slow, high-footprint, low accuracy (recall/MAP)

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slow, high-footprint, low accuracy (recall/MAP)

kNNG-based techniques

slow indexing, difficult to tune, in-memory, no guarantees

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- LSH-based techniques
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- kNNG-based techniques
  - slow indexing, difficult to tune, in-memory, no guarantees
- Quantization-based techniques
  - slow indexing, difficult to tune, no guarantees

Insights

Approximate state-of-the-art techniques for high-d vectors are not practical:

- LSH-based techniques
  - slow, high-footprint, low accuracy (recall/MAP)
- kNNG-based techniques
  - slow indexing, difficult to tune, in-memory, no guarantees
- Quantization-based techniques
  - slow indexing, difficult to tune, no guarantees

All suffer a serious limitation:
accuracy determined during index-building & query answering

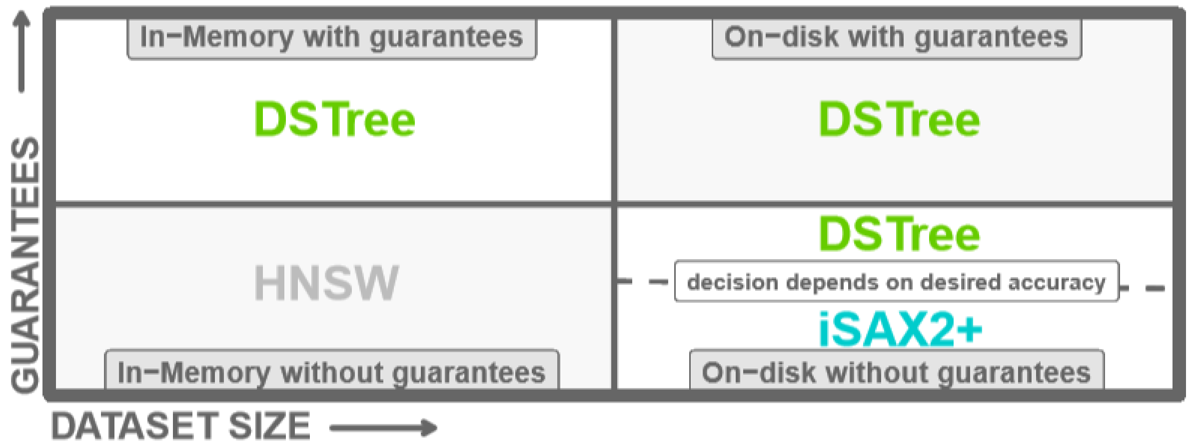
Recommendations for approx. techniques

Data series approaches are the overall winners!

The only exception is HNSW for in-memory ng-approximate queries using an existing index

Recommendations

Scenario: Answering a query workload using an existing index



Experimental evaluation of graph-based methods

Publications

Wang-PVLDB'2021

- A variety of evaluation criteria
  - Indexing:
    - Construction efficiency, index size, graph quality
  - Search
    - Efficiency, accuracy, candidate set size, query path length, memory overhead,
- 13 graph-based methods
- 8 real datasets and 12 synthetic datasets
  - Largest contains 2M vectors

Experimental evaluation of graph-based methods

Publications

Wang-PVLDB'2021

- Recommendations

Scenario	Algorithm
S1: A large amount of data updated frequently	NSG, NSSG
S2: Rapid construction of KNNG	KGraph, EFANNA, DPG
S3: Data is stored in external memory	DPG, HCNNG
S4: Search on hard datasets	HNSW, NSG, HCNNG
S5: Search on simple datasets	DPG, NSG, HCNNG, NSSG
S6: GPU acceleration	NGT
S7: Limited memory resources	NSG, NSSG

Questions?

Progressive Similarity Search

Interactive Analytics

- analytics over high-d data is computationally expensive
  - very high inherent complexity

- may not always be possible to remove delays
  - but could try to hide them!

Need for Interactive Analytics

- interaction with users offers new opportunities
  - progressive answers
    - produce intermediate results
      - iteratively converge to final, correct solution

Need for Interactive Analytics

- interaction with users offers new opportunities
  - progressive answers
    - produce intermediate results
      - iteratively converge to final, correct solution
        - Exact or approximate

Need for Interactive Analytics
Exact Search

Publications
- Gogolou-BigVis'19
- Gogolou-SIGMOD'20

- interaction with users offers new opportunities
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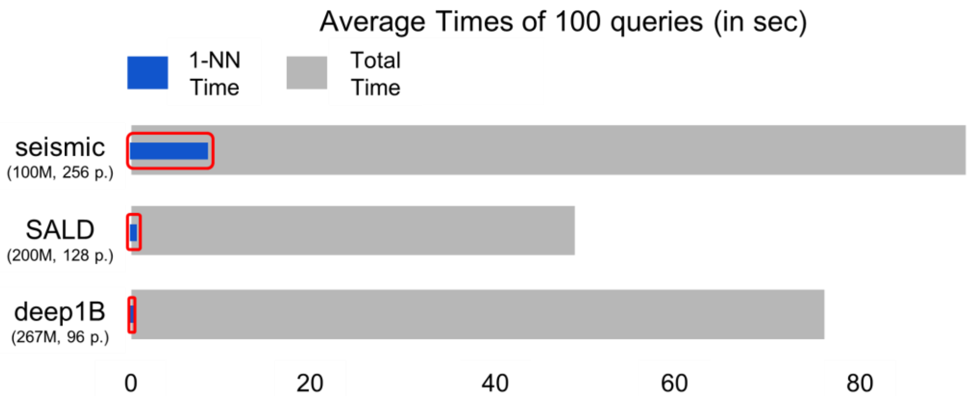
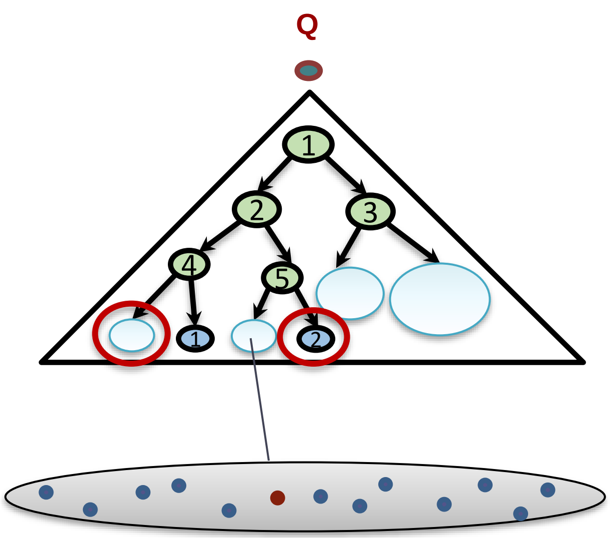
    - produce intermediate results
      - iteratively converge to final, correct solution
      - Tree-based indexes





Need for Interactive Analytics
Exact Search

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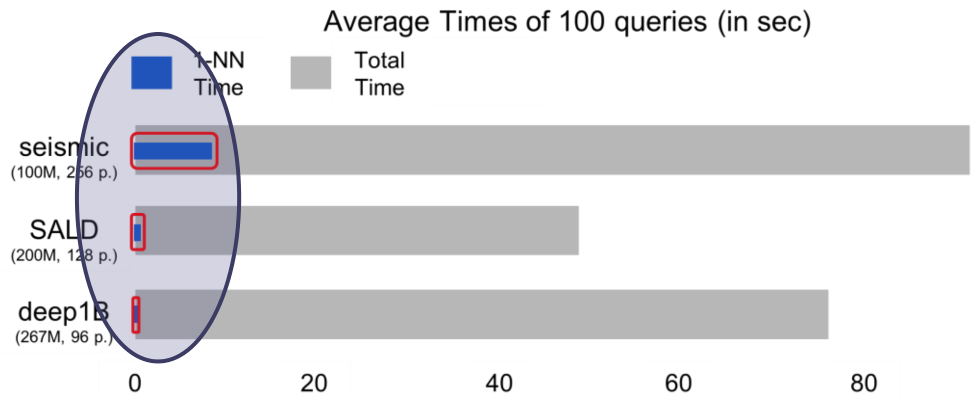

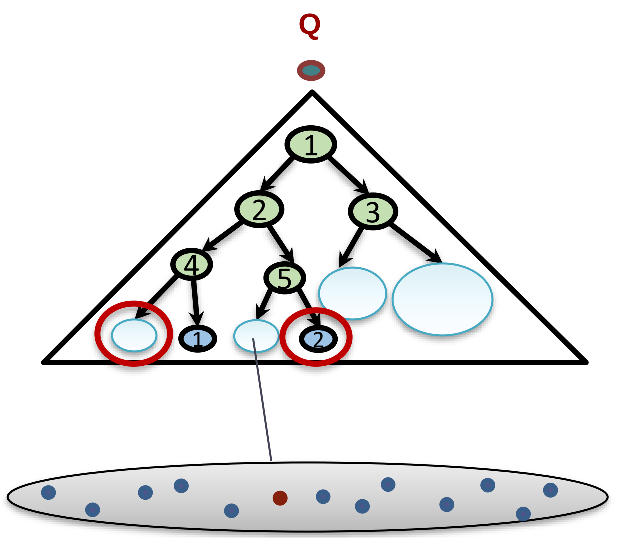

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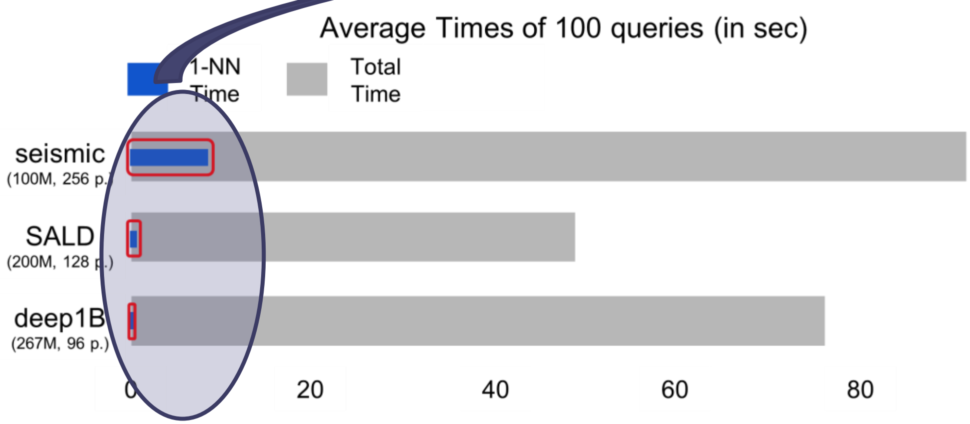

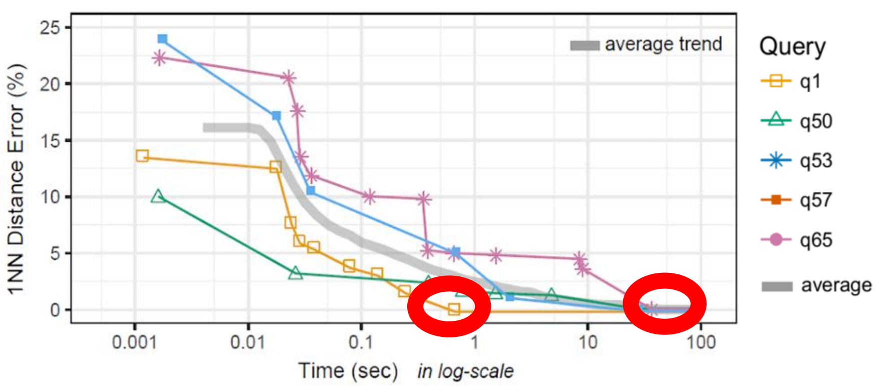

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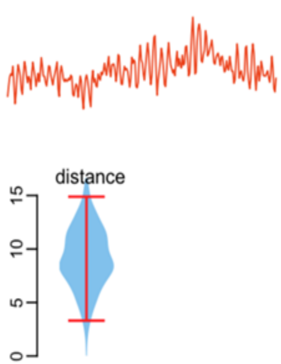
    - provide bounds on the errors (of the intermediate results) along the way

Publications
- Gogolou-BigVis‘19
- Gogolou-SIGMOD‘20

Query & Initial Estimate



Need for Interactive Analytics
Exact Search

Publications

Gogolou-BigVis'19

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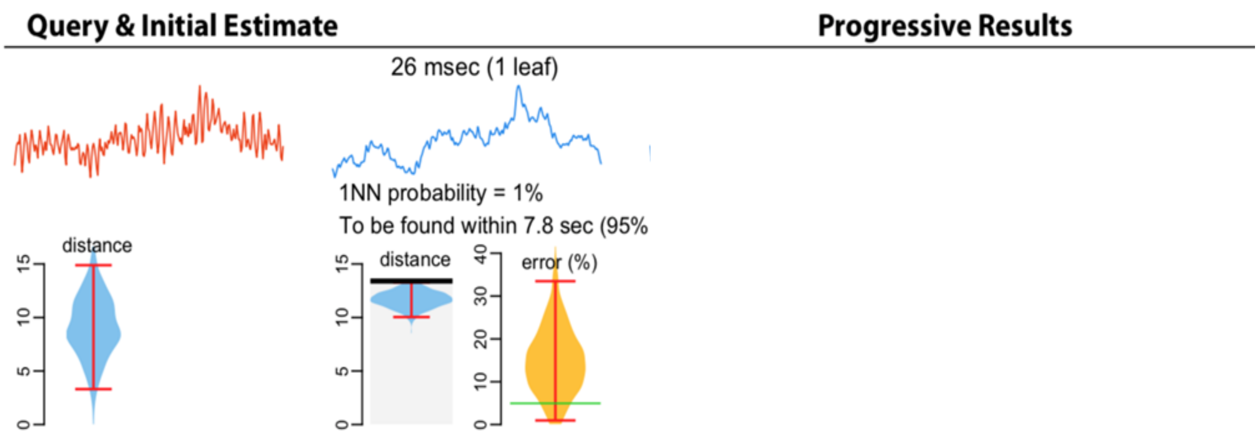

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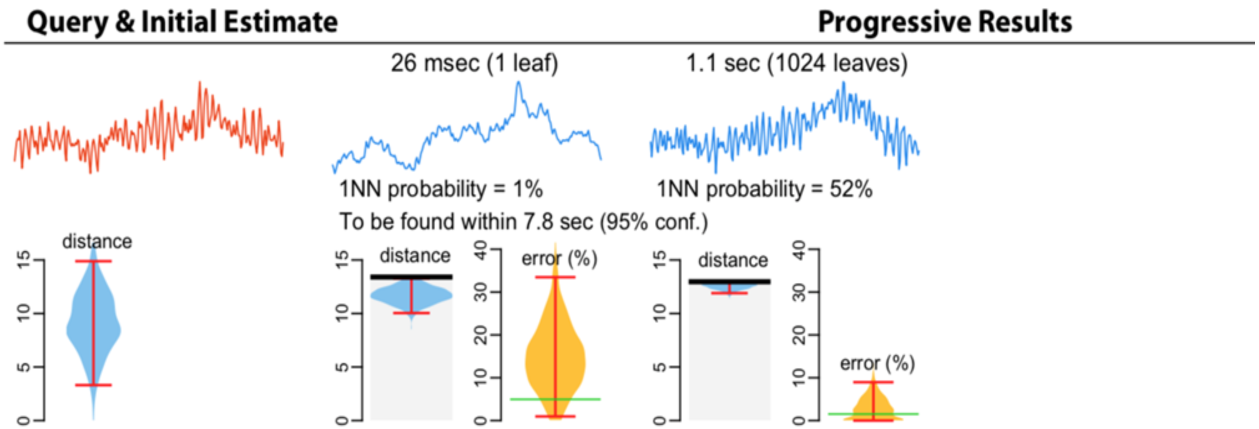

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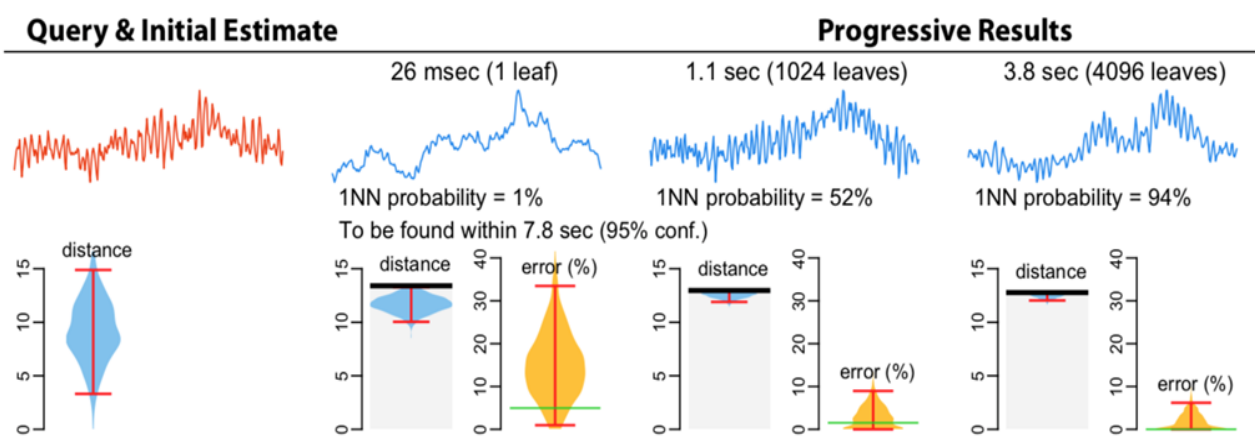

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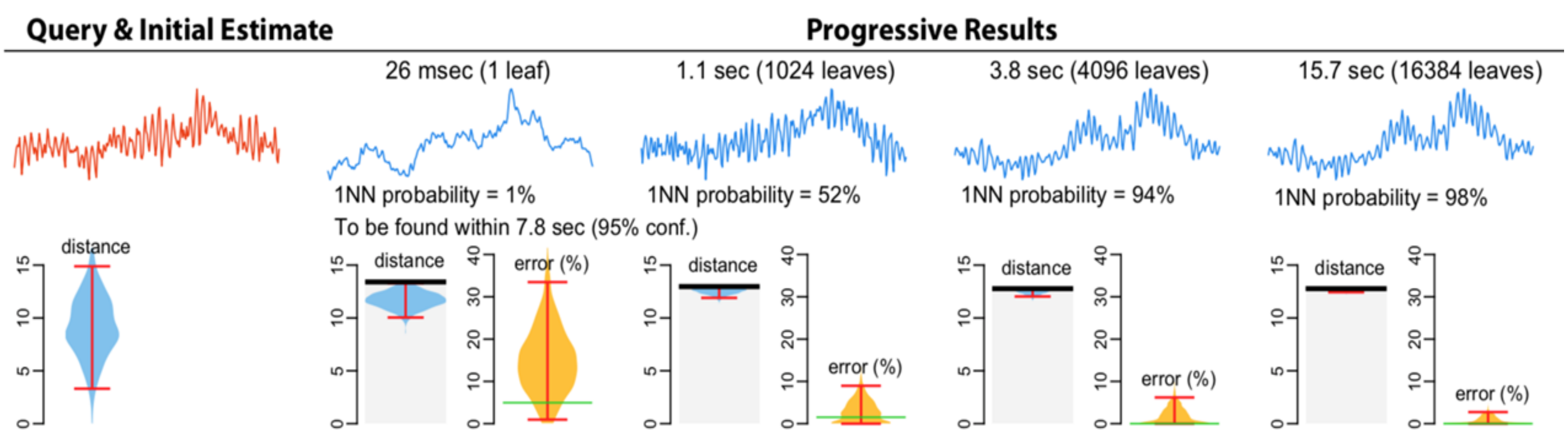

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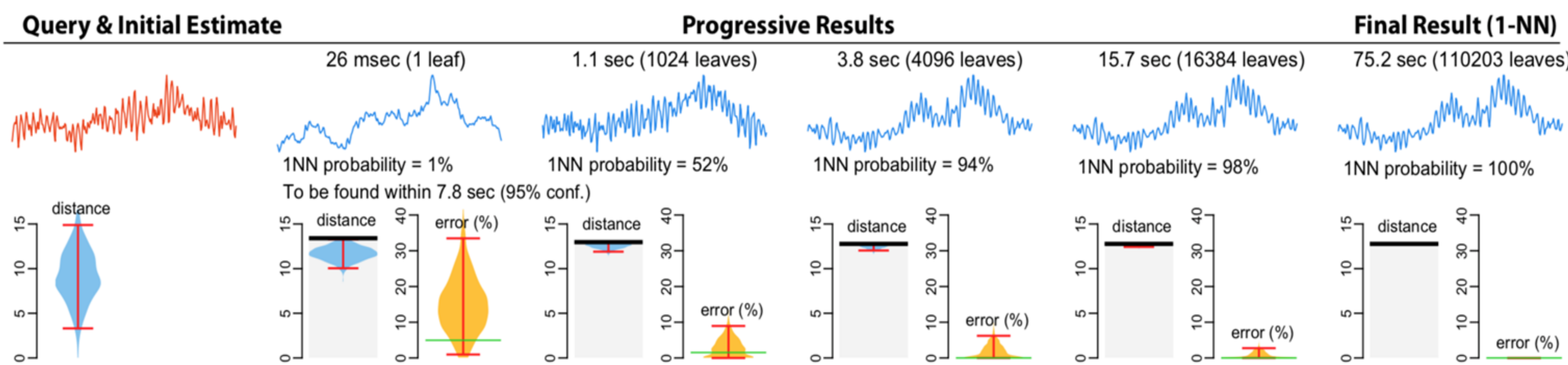

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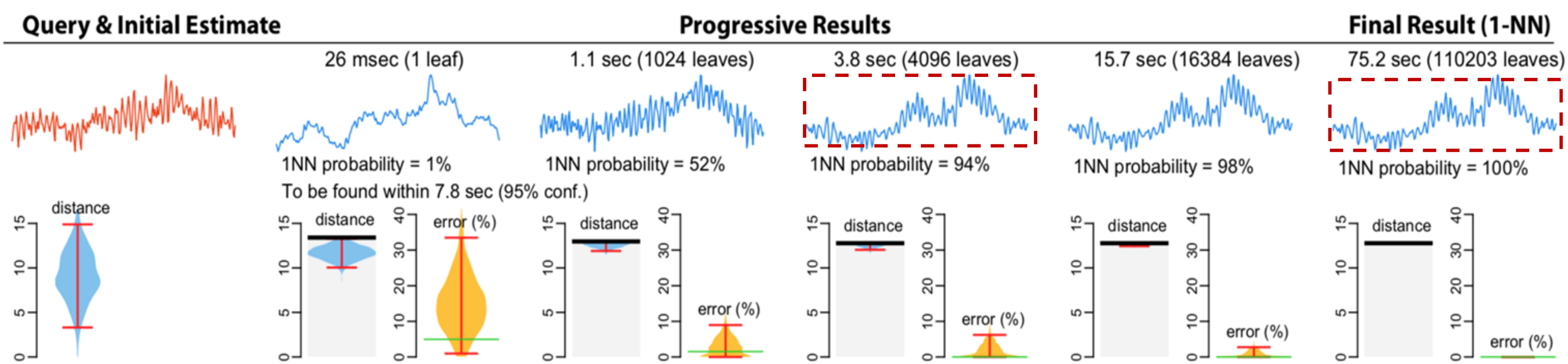


Need for Interactive Analytics
Exact Search

Publications

Gogolou-BigVis'19

Gogolou-SIGMOD'20

Contributions

Formalize **data series** **progressive similarity search** with **probabilistic quality guarantees** (wrt *exact* answers).

Propose **statistical models** (linear, quantile & logistic regression, and multivariate kernel density estimation) to support **reliable** **progressive estimation** with a **small** **number of training queries**.

Develop **stopping criteria** to stop a search **long before normal query execution ends**.

Need for Interactive Analytics
Exact Search

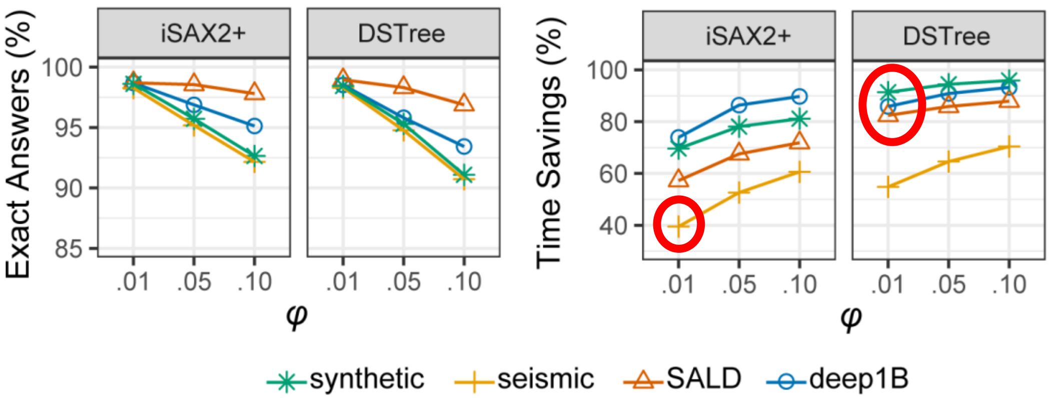
Publications

Gogolou-BigVis'19

Gogolou-SIGMOD'20

Time savings for 1NN queries

Early stopping when predicted **probability** that current answer is exact is higher than $1 - \varphi$



(n_r = 100 training queries)

time savings up to 90%

Need for Interactive Analytics
Exact Search

Publications

Gogolou-BigVis'19

Gogolou-SIGMOD'20

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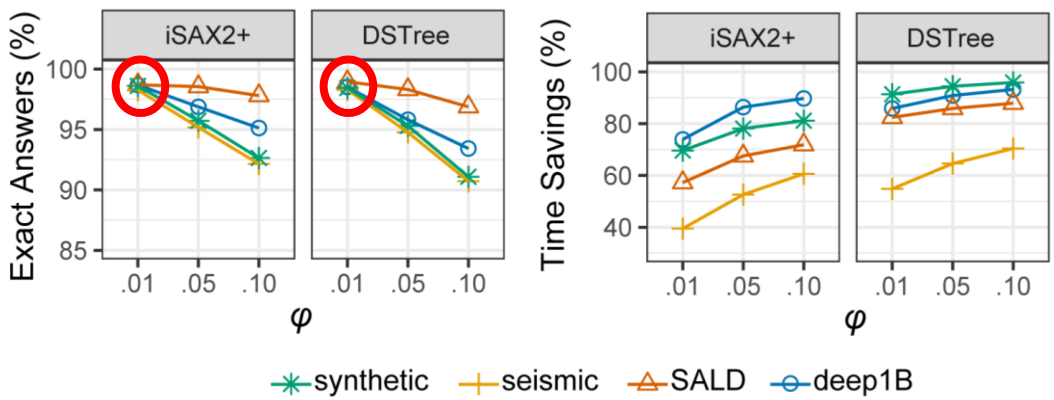


(n_r = 100 training queries)

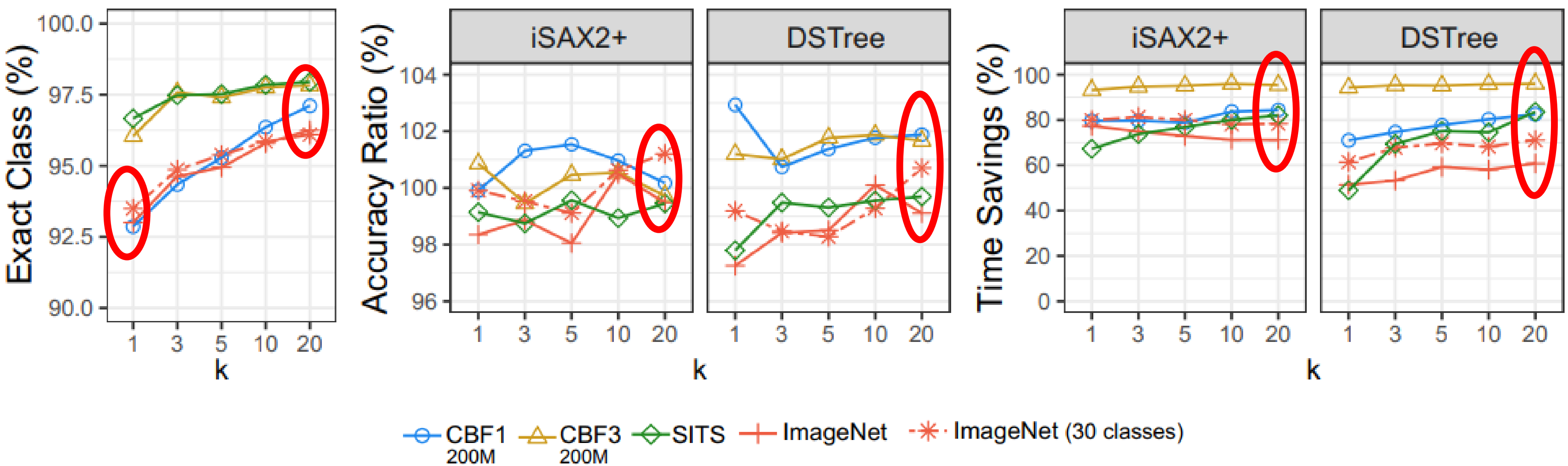
time savings up to 90%, with ~99% of the answers to be exact

Need for Interactive Analytics
Exact Search

Publications

Echihabi-submitted'21

Time savings for kNN classification



time savings up to 95% with ~99% of the answers to be exact

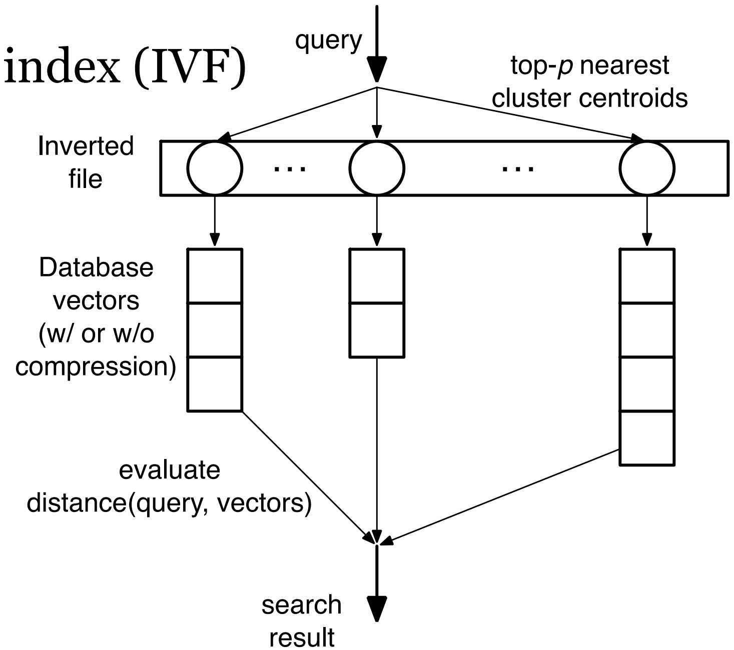
Need for Interactive Analytics
Approximate Search

Publications

Li-SIGMOD'20

- interaction with users offers new opportunities
  - progressive answers
    - produce intermediate results
      - iteratively converge to final, correct solution
      - Inverted files

Inverted file index (IVF)



Slide by C. Li

Need for Interactive Analytics
Approximate Search

Publications

Li-SIGMOD'20

- interaction with users offers new opportunities
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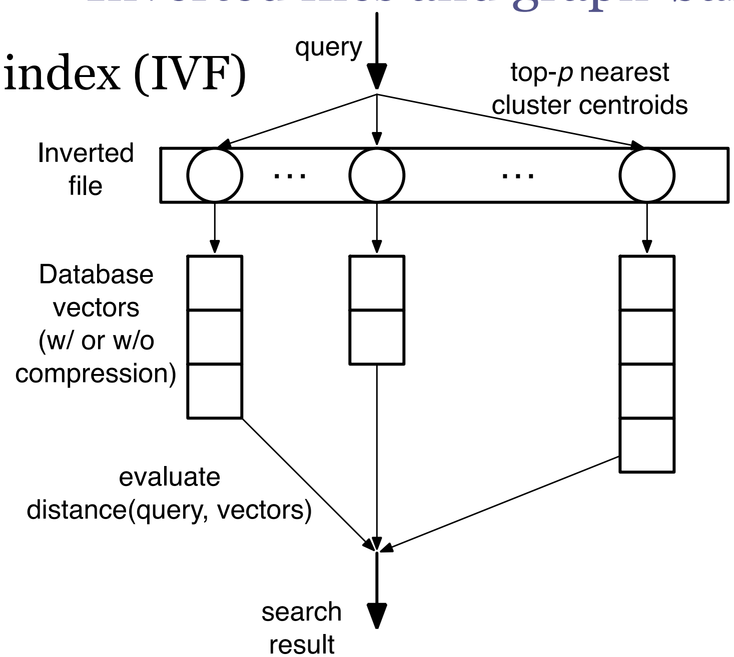
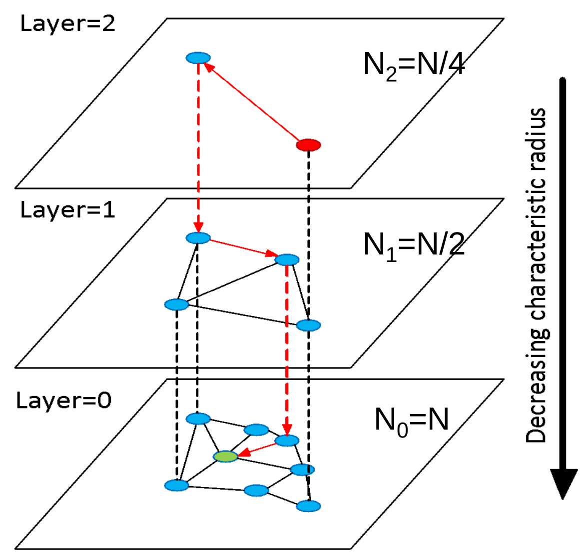
    - produce intermediate results
      - iteratively converge to final, correct solution
      - Inverted files and graph-based indexes

Inverted file index (IVF)



HNSW



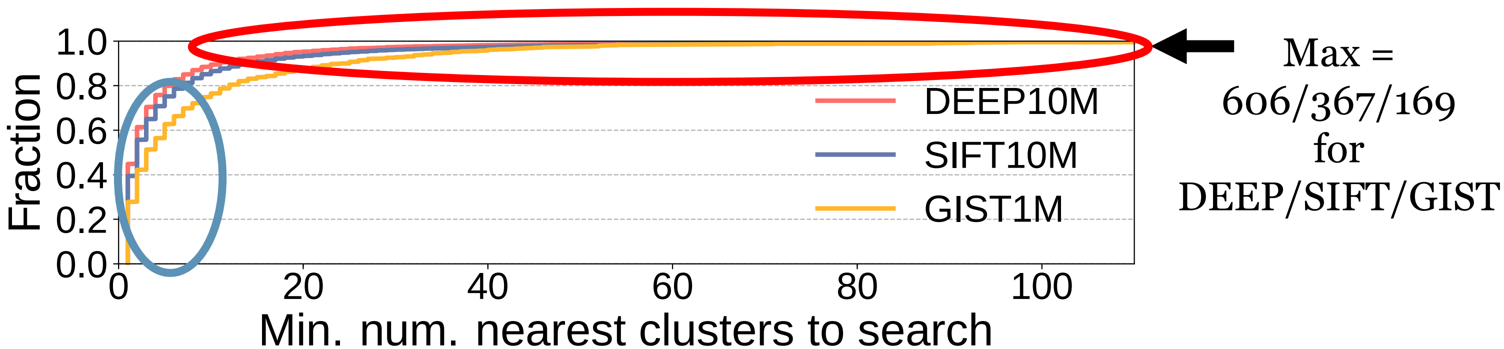
Slide by C. Li

Need for Interactive Analytics
Approximate Search

Publications

Li-SIGMOD'20

- Search termination condition varies greatly
  - Inverted indexes: number of nearest clusters
  - Graph-based indexes: Minimum number of distance evaluations.



IVF index: CDF of min. termination conditions among queries. DEEP10M and SIFT10M have 4000 clusters and GIST1M has 1000 clusters in total.

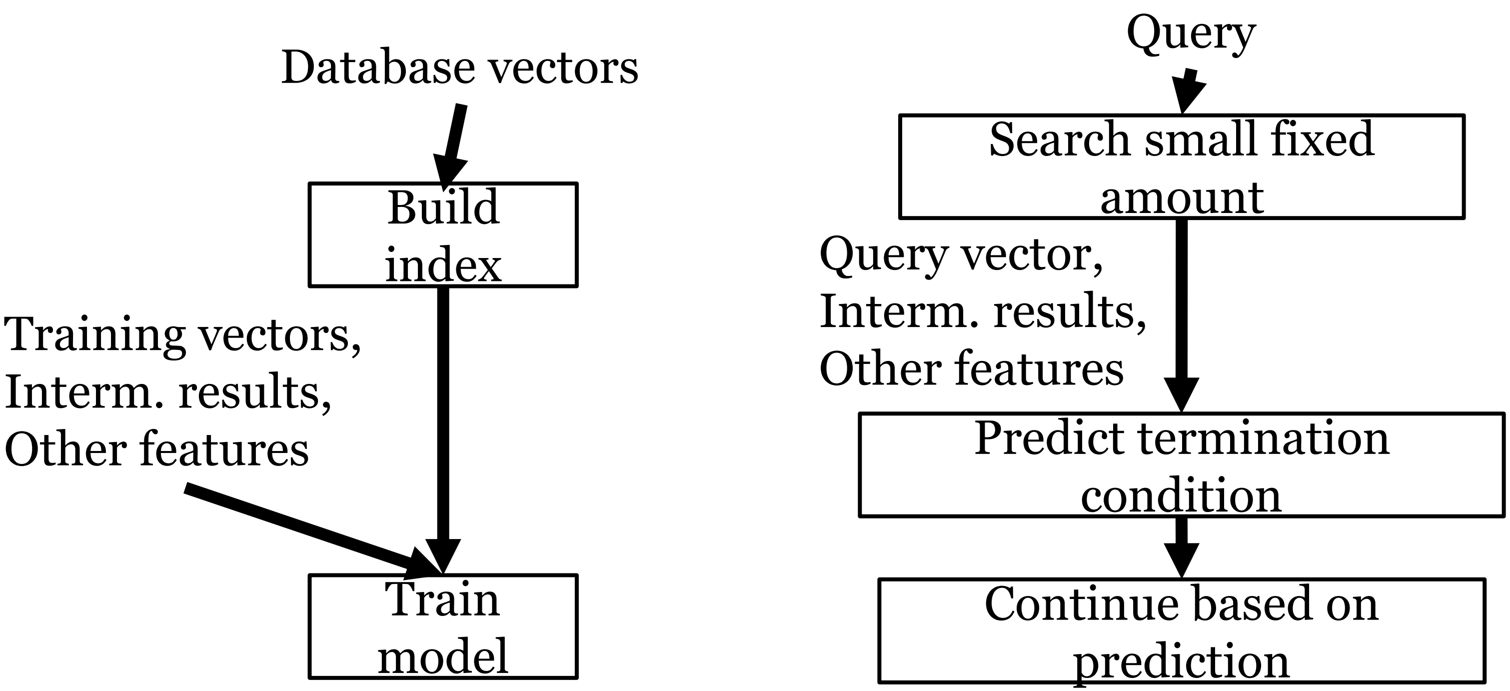
Need for Interactive Analytics
Approximate Search

Publications

Li-SIGMOD'20

- Learned Adaptive Early Termination

At index construction: At online search:



On average, end-to-end latency is improved by up to 7.1x under the same accuracy targets

Slide by C. Li

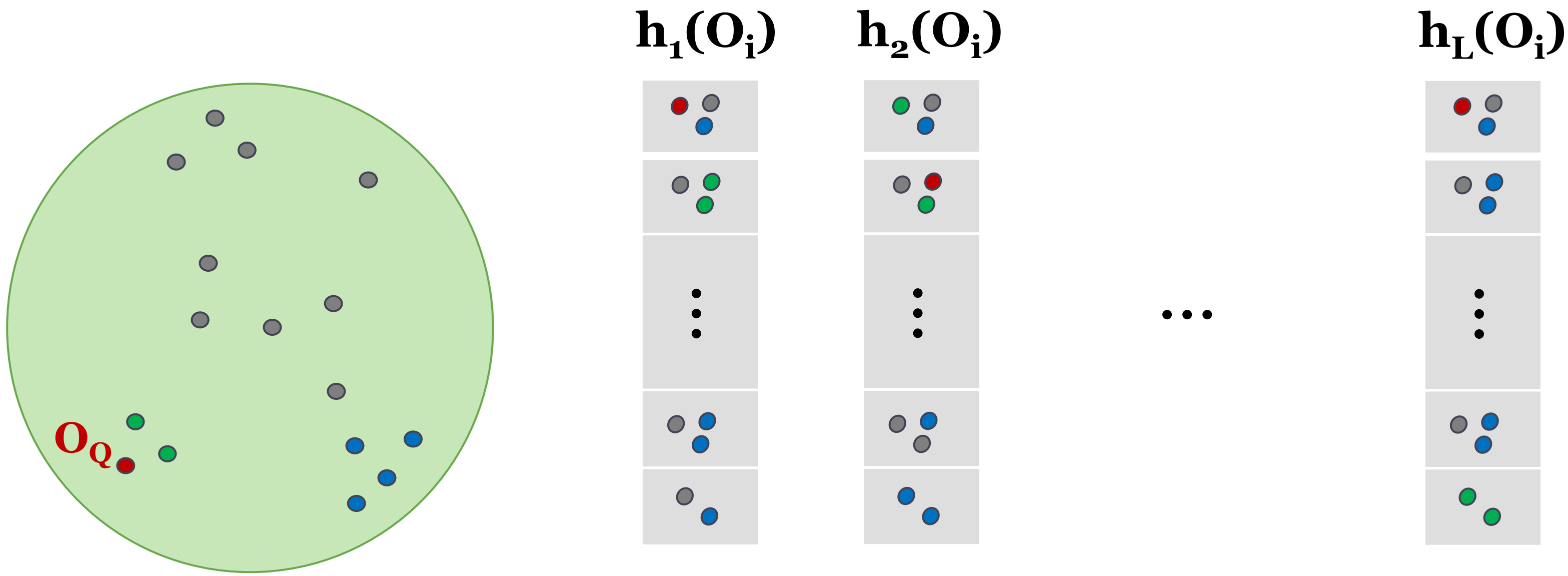
AI and Similarity Search

AI and Similarity Search

- Representation Learning
  - Learned hashing
  - Learned quantization
  - Learned summarizations for data series
- Search and Indexing
  - Learned indexes
  - Similarity search on deep network embeddings

AI and Similarity Search
Representation Learning

- Learned Hashing
  - Prior works:
    - Classical locality sensitive hashing. Typically data insensitive



Each object O is mapped to a single bucket in each of the L hash tables using hash function $h_j(O)$

AI and Similarity Search
Representation Learning

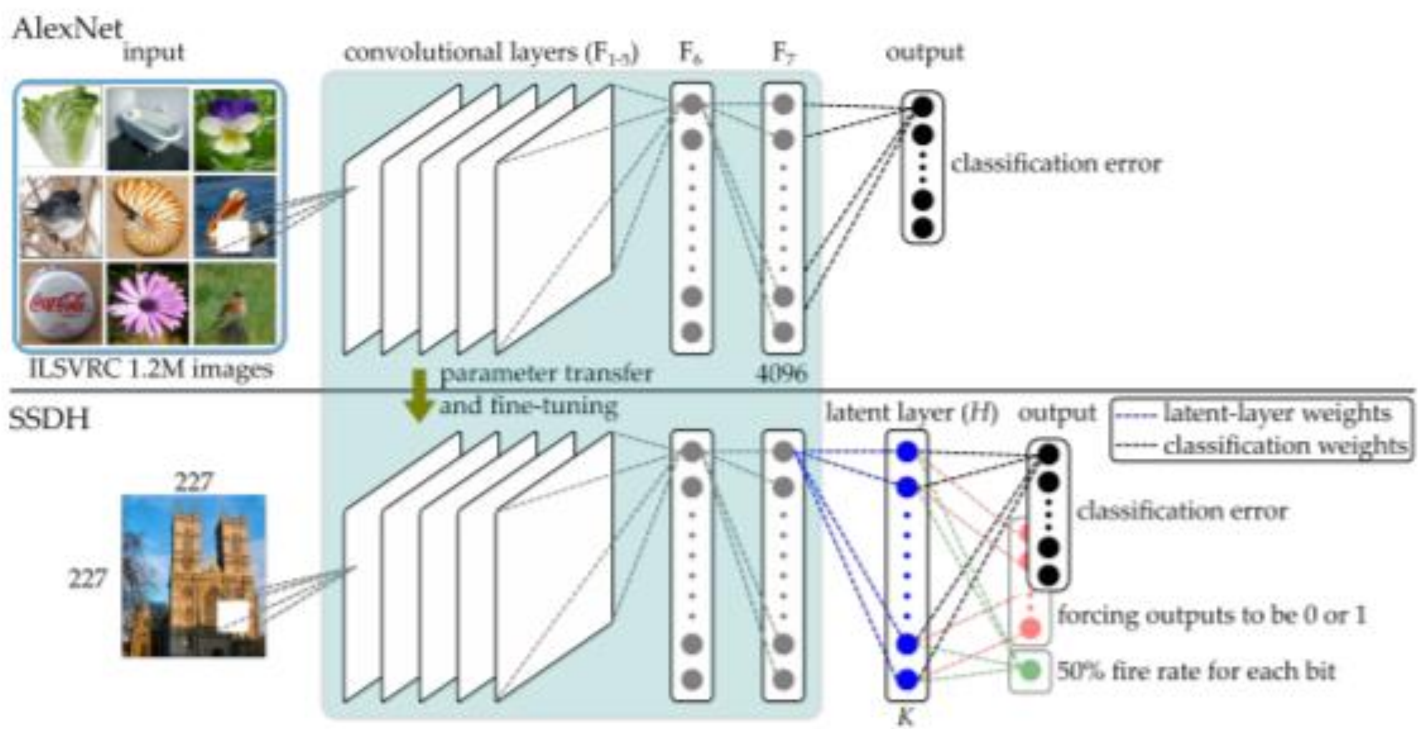
Publications
- Salakhutdinov-IJAR'09
- Weiss-NIPS'09

- Learned Hashing
  - Main goal: learn compact encodings that preserve similarity
  - Early works: semantic hashing, spectral hashing
    - Learn projection vectors instead of the random projections
  - A large body of follow-up work on data-sensitive approaches
    - http://cs.nju.edu.cn/lwj/slides/L2H.pdf
    - https://learning2hash.github.io/
  - Deep-learning approaches

AI and Similarity Search
Representation Learning

Publications
- Yang-TPAMI'18
- Krizhevsky-NIPS'2012

- Deep-Learned Hashing
  - Main Idea:
    - Modify conventional DNN models (eg, AlexNet classification model) by replacing ouput layer with deep hashing modules



AI and Similarity Search

Representation Learning

- Deep-Learned Hashing

Publications

Cai-Arxiv'17

Luo-Arxiv'20

Wang-TPAMI'18

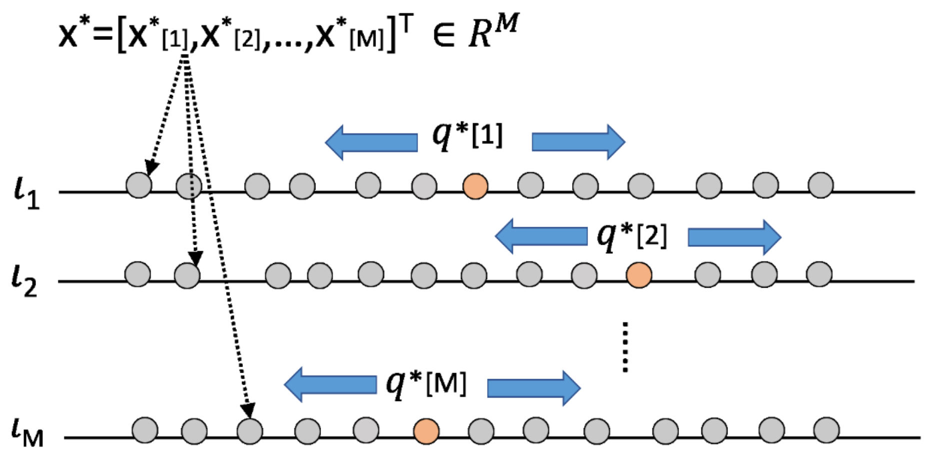
Network	AE, CNN, GAN, Siamese/Triplets, Attention Networks, etc.
Loss Functions	Pair-wise similarity, multi-wise similarity, semantic similarity (label-based), quantization loss, regularization loss, etc.
Optimization	Backpropagation, relaxation, optimizing subproblems, continuation

AI and Similarity Search
Representation Learning

Publications

Li et al. – ICDE'20

- Deep-Learned Hashing
  - OPFA, NeOPFA: approximate NN search for disk-based data
    - learn hashing (i.e., mapping) functions that map vectors to (lower dimensional) embeddings, preserving data locality
    - build indexes (e.g.,. B+-trees) on lists of values of individual dimensions of the embeddings
    - query answering makes bi-directional sequential access to each list, leading to sequential I/O



AI and Similarity Search
Representation Learning

- Deep-Learned Hashing
  - How do they compare?
    - Evaluation Metrics: precision, recall, search time
  - Conflicting results:
    - [Luo-20]: Deep-learned hashing greatly outperforms traditional hashing methods (e.g., SDH and KSH) overall.
    - [Cai17]: Deep-learned hashing is inferior to traditional hashing methods if the later exploit multiple hash tables.
  - [Sablayrolles17]:
    - Need better evaluation criteria: retrieval of unseen classes and transfer learning.

Publications

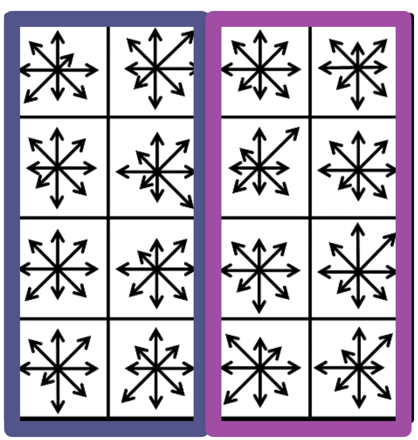
- Cai-Arxiv'17
- Luo-Arxiv'20
- Wang-TPAMI'18
- Sablayrolles-ICASSP'17

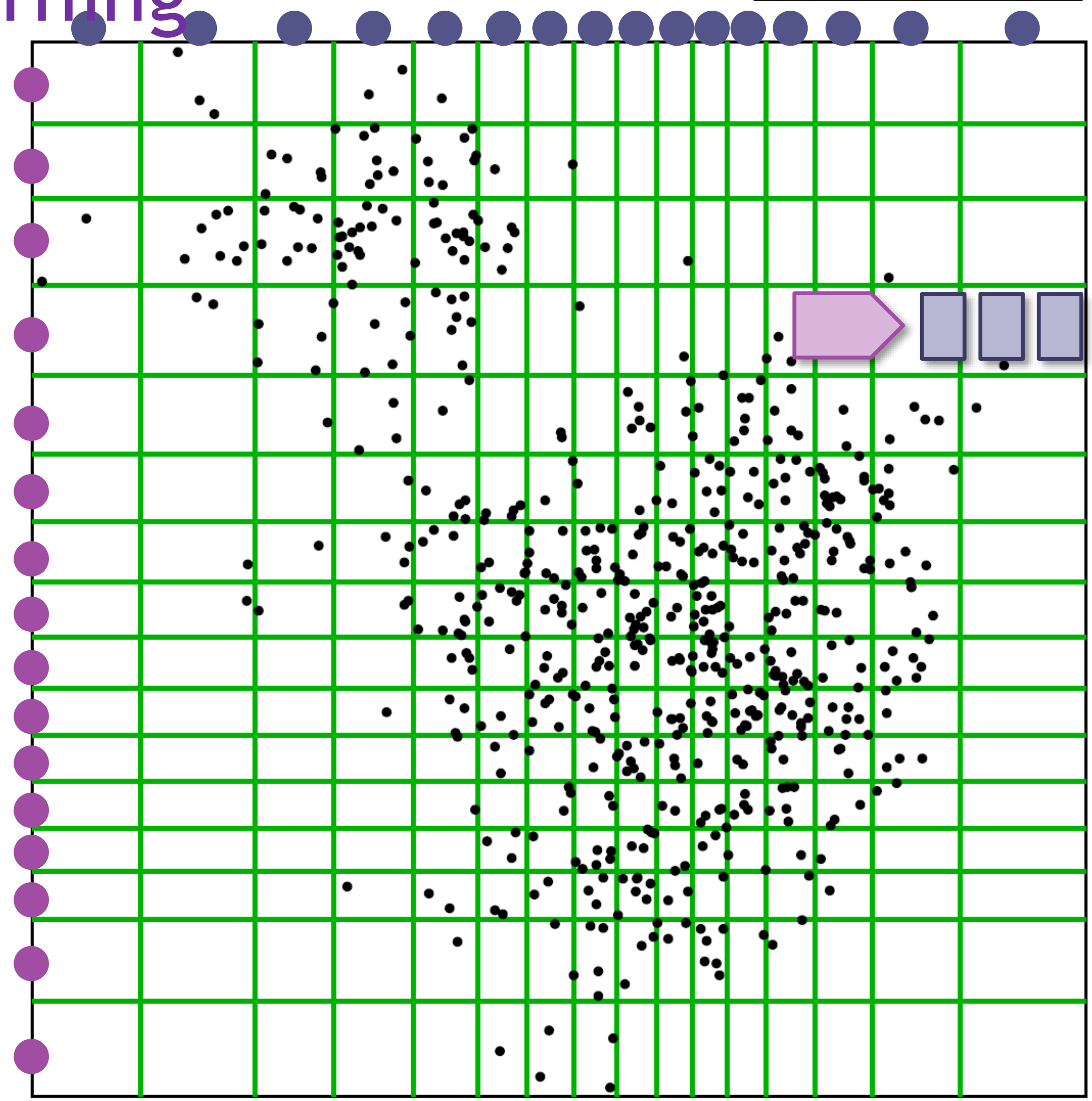
AI and Similarity Search
Representation Learning

Publications

Jegou et al. TPAMI' 11

- Learned Quantization Techniques
  - Prior works:
    - Product Quantization
    - Efficient search with lookup tables





Slide by A. Babenko

AI and Similarity Search
Representation Learning

Publications

Wang-CVPR'16

Cao-AAAI'16

- Learned Quantization
  - Main goal: learn encodings that minimize quantization errors
  - Early works:
    - SQ learns features and quantization separately
      - Exploits Semantic (label-based) loss.
    - DQN learns them simulatenaneously
      - First end-to-end model
      - Combines a similarity-preserving loss and a product quantization loss.
      - But DQN's codebook is trained with k-means clustering.
  - No exhaustive survey

  - we will focus on state-of-the-art deep-learning approaches

AI and Similarity Search
Representation Learning

Publications

Klein-CVPR'19

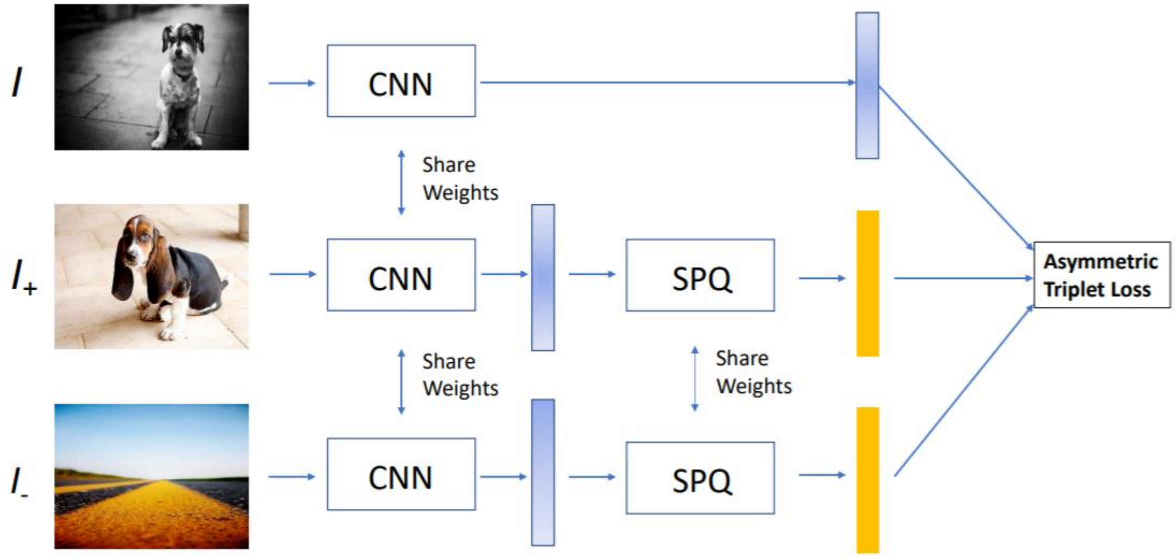
- Supervised Learned Quantization
  - DPQ:
    - Learns centroids and parameters end-to-end
    - Learns a cascade of two fully-connected layers followed by a softmax layer to determine a soft codeword assignment.
    - In contrast to original PQ, codeword assignment is no longer determined by distance between the original feature and codewords.

AI and Similarity Search
Representation Learning

Publications

Yu-ECCV'18

- Supervised Learned Quantization
  - PQN:
    - Codewords are assigned based on similarity between the original features and codewords
    - Less prone to over-fitting compared to DPQ due to the smaller number of parameters.

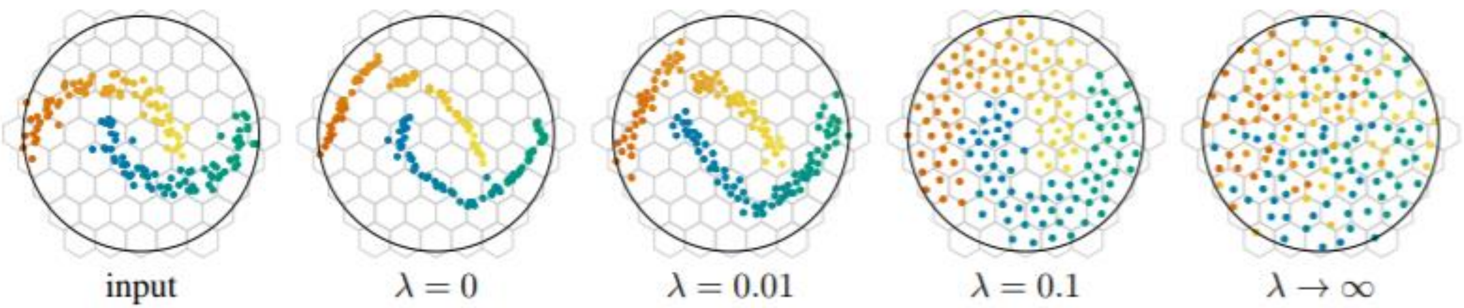


AI and Similarity Search
Representation Learning

Publications

Sablayrolles-ICLR'19

- Unsupervised Learned Quantization
  - Catalyst-Lattice
    - Idea: adapt the data to the quantizer rather than the opposite
      - Train a neural network that maps input features to a uniform output distribution on a unit hypersphere, making high-dimensional indexing more accurate

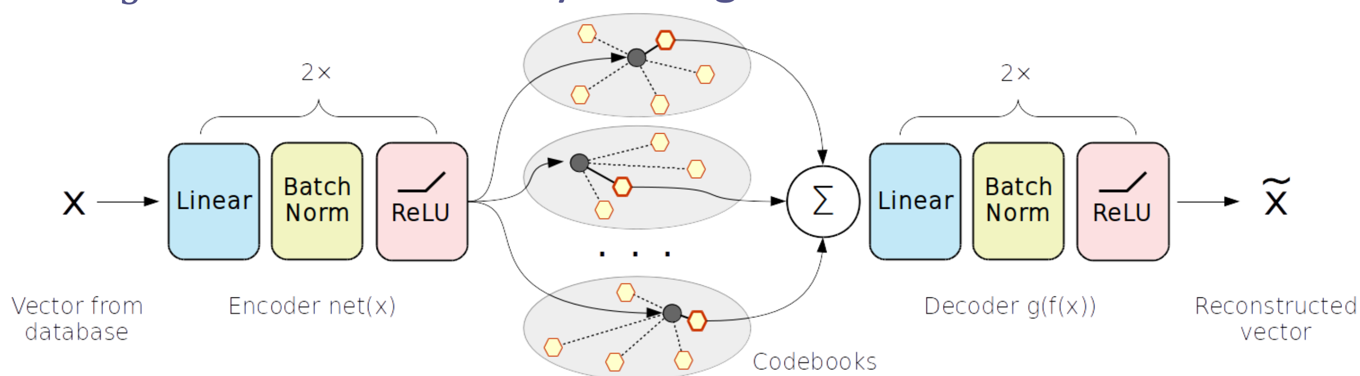


AI and Similarity Search
Representation Learning

Publications

Morozov-ICCV'19

- Unsupervised Learned Quantization
  - Unsupervised Neural Quantization (UNQ)
    - Idea: train multi-layer encoder/decoder in end-to-end fashion in unsupervised setup
  - UNQ Training Loss: $L = L_1 + \alpha L_2 + \beta L_3$
    - L_1 – reconstruction loss
    - L_2 – triplet loss in compressed domain
    - L_3 – enforces diversity among codebooks



AI and Similarity Search
Representation Learning

Publications

Morozov-ICCV'19

Slide by S. Morozov

- Learned Quantization Techniques
  - UNQ vs. Catalyst-Lattice[1] and LSQ[2]

Method	BigANN1B			Deep1B		
	R@1	R@10	R@100	R@1	R@10	R@100
	8 bytes per vector					
Catalyst+Lattice[1]	10.4	37.6	76.6	**16.8**	**38.7**	68.2
LSQ[2]	9.6	35.9	73.3	13.2	32.3	59.9
LSQ+rerank	9.9	36.1	73.8	12.3	31.6	59.7
UNQ	**13.0**	**44.5**	**82.4**	14.5	37.8	**68.5**
	16 bytes per vector					
Catalyst+Lattice	31.1	77.8	98.3	35.3	72.8	95.6
LSQ	38.0	85.6	99.3	30.5	65.0	91.1
LSQ+rerank	37.6	86.0	99.3	30.1	65.8	91.4
UNQ	**38.3**	**86.8**	**99.4**	**35.5**	**74.2**	**96.1**

[1] Alexandre Sablayrolles, Matthijs Douze, Cordelia Schmid and Hervé Jégou. Spreading vectors for similarity search. ICLR'19
[2] Julieta Martinez, Shobhit Zakhmi, Holger H. Hoos, and James J. Little. LSQ++: lower running time and higher recall in multi-codebook quantization, ECCV'2018

Slide by S. Morozov

AI and Similarity Search
Representation Learning for Data Series

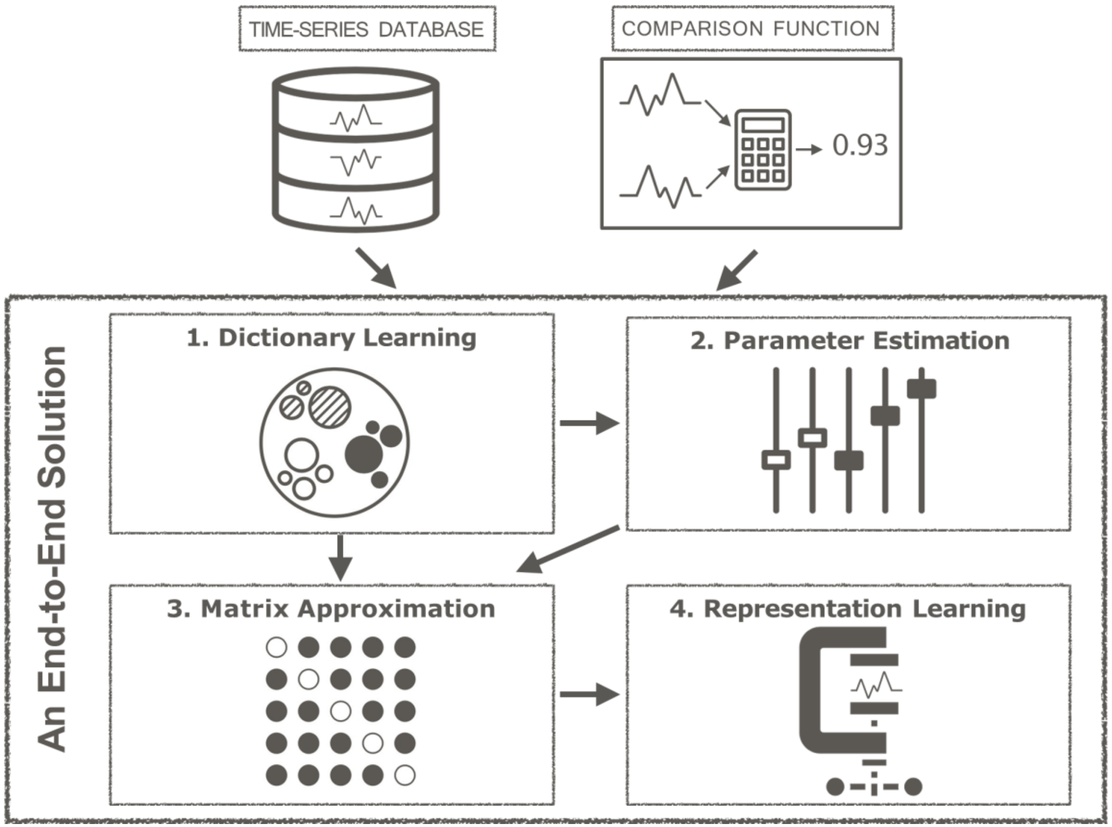
- learn compact similarity-preserving representations
- use those for
  - similarity search
  - classification
  - clustering
  - …

AI and Similarity Search
Representation Learning for Data Series

Publications

Paparrizos - PVLDB'19

- GRAIL
  - learns representations that preserve a user-defined comparison function
  - for a given comparison function:
    - extracts landmark series using clustering
    - optimizes parameters
    - exploits approximations for kernel methods to construct representations by expressing each series as a combination of the landmark series



AI and Similarity Search

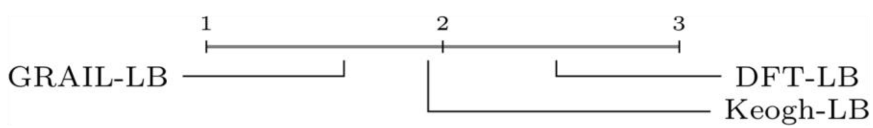
Representation Learning for Data Series

Publications

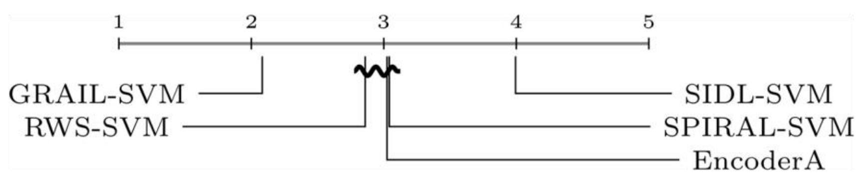
Paparrizos - PVLDB'19

- GRAIL
  - uses the learned representations for querying, classification, clustering, …

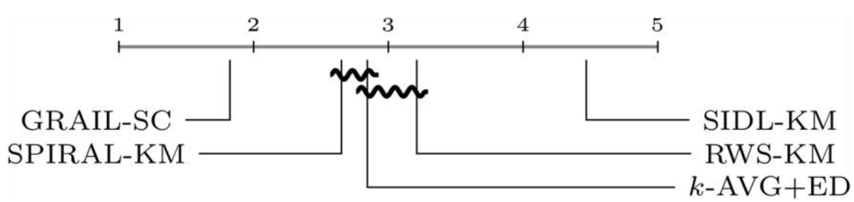
QUERYING: GRAIL Lower Bound vs. Lower Bounds for DFT & DTW



CLASSIFICATION: GRAIL with SVM vs. other Learned Representations



CLUSTERING: GRAIL with Spectral Clustering vs. other Learned Representations



AI and Similarity Search

Representation Learning for Data Series

Publications

Wang - KDD'21

- Series Approximation Network (SEAnet)
  - novel autoencoder architecture
  - learns deep embedding approximations
  - uses those for similarity search

AI and Similarity Search
Representation Learning for Data Series

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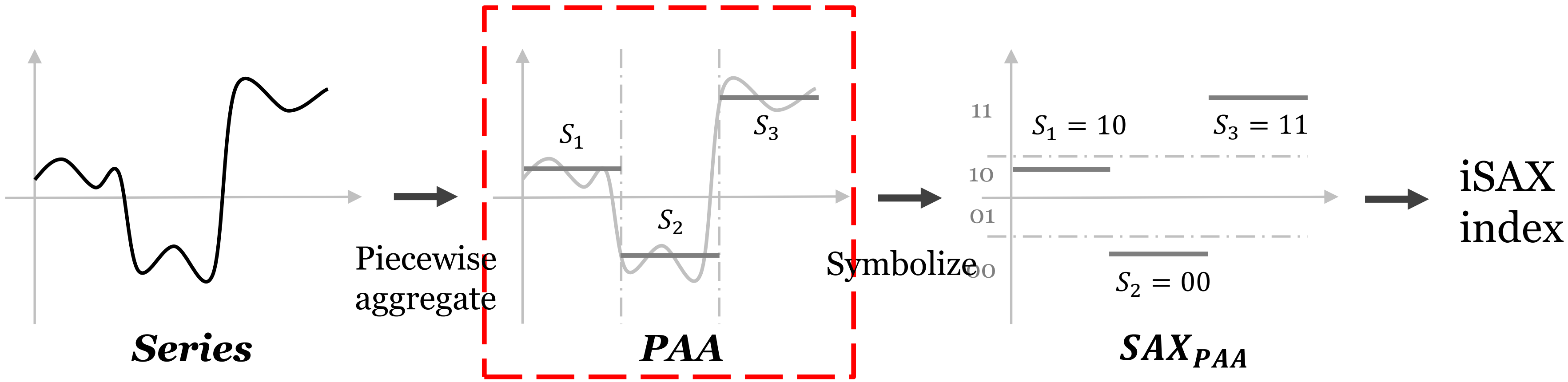

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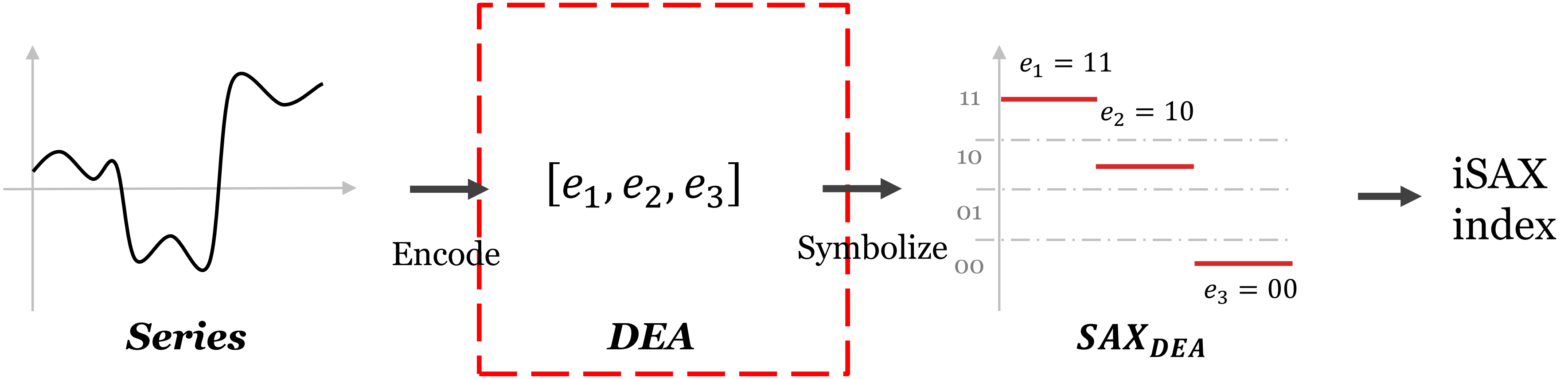

AI and Similarity Search

Representation Learning for Data Series

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- Series Approximation Network (SEAnet)
  - is an exponentially dilated ResNet architecture + Sum of Squares regularization
  - minimizes
    - reconstruction error
    - difference between distance of two vectors in embedded space and distance in original space

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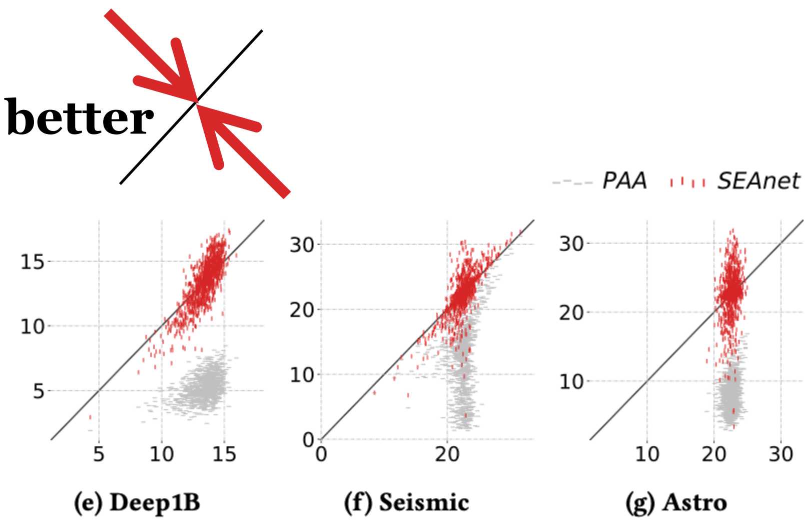
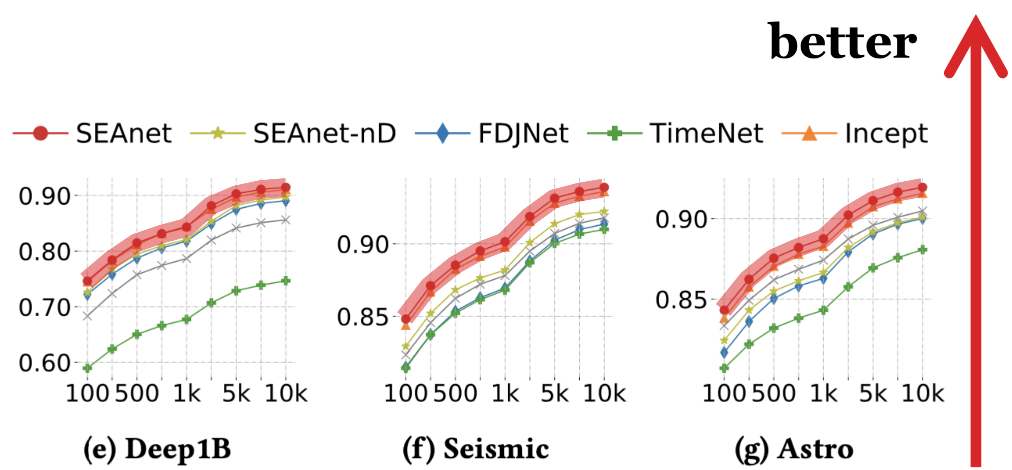




AI and Similarity Search
Search and Indexing

- Search and Indexing
  - Problem:
    - High-d vector similarity search is hard
    - Massive datasets and high dimensionality in 100s-1000s
    - Sophisticated indexing structures and search algorithms
  - Solutions:
    - Learned Indexes
    - Improve search efficiency using deep learning
    - Indexing for learned embeddings

AI and Similarity Search
Search and Indexing

Publications

Kraska-SIGMOD'18

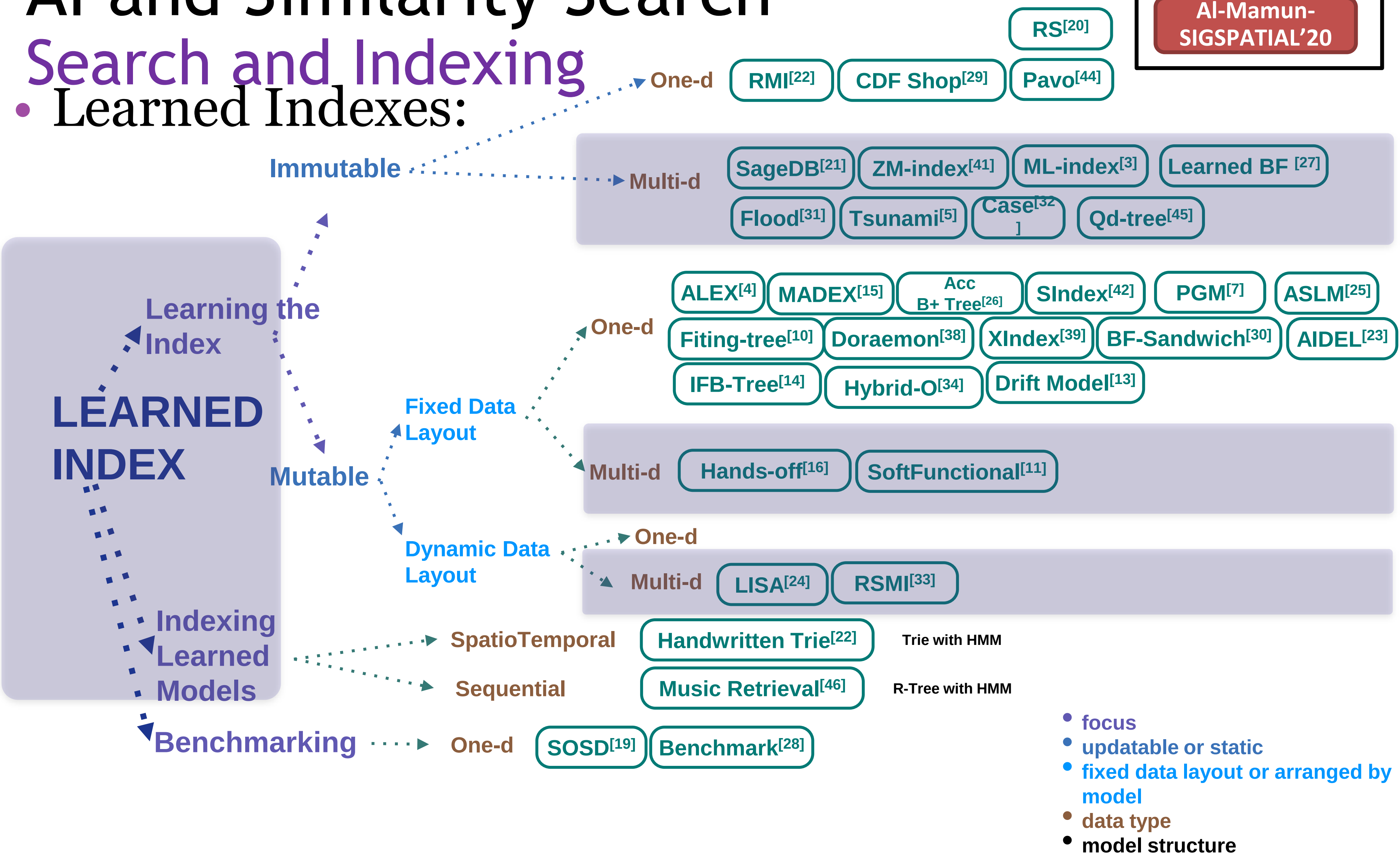
Al-Mamun-SIGSPATIAL'20

- Learned Indexes:
  - Main idea: replace an index with a learned model
    - One-dimensional learned indexes
      - Seminal work: The Case for Learned Indexes
    - Multi-dimensional indexes
      - Exhaustive tutorial on this topic at SIGSPATIAL'20: https://www.cs.purdue.edu/homes/aref/learned-indexes-tutorial.html
    - Some initial attempts for similarity search
  - Main challenges for multi-dimensional indexes:
    - How to sort the data?
    - How to correct prediction errors?
    - Which ML model to choose?
    - How to store the data?

AI and Similarity Search

Search and Indexing

- Learned Indexes:



Slide from W. Aref

AI and Similarity Search
Search and Indexing

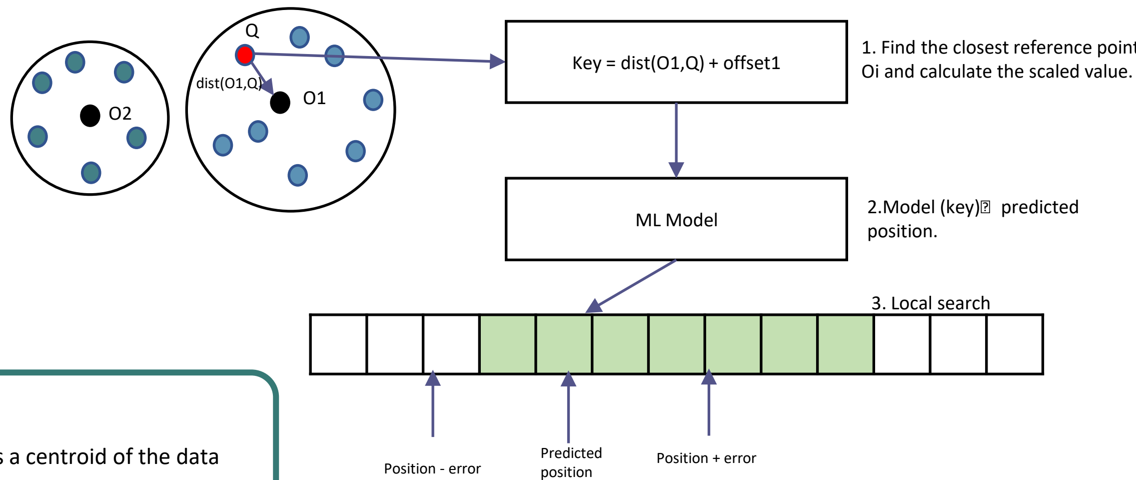
Publications: Davitkova-EDBT'20

- Learned Indexes for similarity search:
  - The ML-Index: A multidimensional, learned index for point, range and NN queries

Core Idea

ML-Index:

- Z/Morton order cannot be easily learned by ML models.
- Multi-dimensional data should be sorted in an order that can be easily learned.
- Partition and transform the data into one-dimensional values based on distribution-aware reference points.
- Combines the scaled ordering with ML models



Query Processing (Point)

Efficient Scaling

Offset Method:

- *m* reference points *Oi* are chosen each can be thought as a centroid of the data partition *Pi*.
- The closest reference points of *Oi* are used to build the partition *Pi*.
- The minimal distance of a point to the reference points is *dl*
- Scaled value = $offset_i + dist(O_i, dl)$
- For reference points *O1, O2,…Om* and their partitions *P1,P2,…Pm*,
- r: The maximal distance from *Oj* to the points in partition *Pj*

Slide from W. Aref

Publications

Davitkova-EDBT'20

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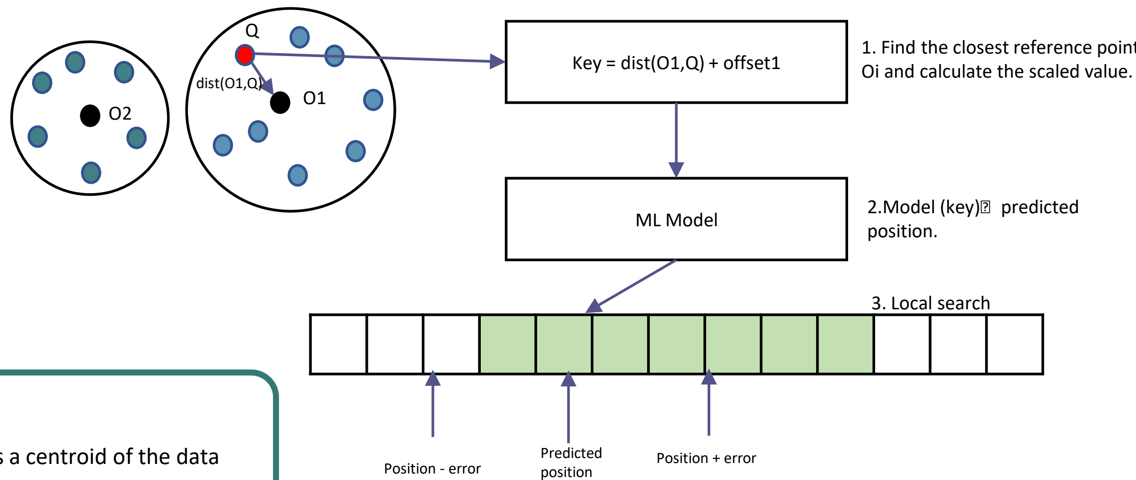

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Slide from W. Aref

AI and Similarity Search

Search and Indexing

- Learned Indexes for similarity search:
  - Effectively Learning Spatial Indices

Publications

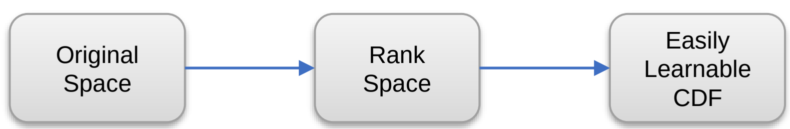
Qi-PVLDB'20

Motivation

- Selecting grid resolution for Z-order for learned multi-dimensional index (e.g. ZM-Index[41]) is difficult:
  - Large cells
    - More false positives due to many points per cell
  - Small cells
    - Hard to learn due to uneven gaps in Cumulative Distribution Function (CDF)

Core Idea

- Spatial index based on ordering the data points by a rank space-based transformation*
  - Simplify the indexing functions to be learned
  - M(search keys) ⟹ disk block Ids (location)



- For scaling to large datasets, proposes:
  - Introduce a Recursive Spatial Model Index (RSMI) (in lieu of RMI)
- Support point, window, and kNN queries
- Support updates

Slide from W. Aref

AI and Similarity Search

Search and Indexing

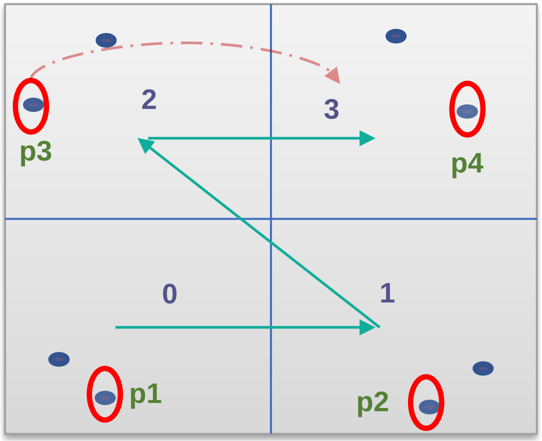
Publications

Qi-PVLDB'20

- Learned Indexes for similarity search:
  - Effectively Learning Spatial Indices

RSMI

- Recursive Spatial Model Index (RSMI):
  - Recursively partitions a dataset
  - Partitioning is learned over the distribution of data
- Steps:
  - Initially distribute the data into equal sized partitions
  - Use a Space Filling Curve (SFC) to assign Ids to partitions
  - Learn the partition Ids using a model $M_{0,0}$
  - Rearrange the data based on the prediction of $M_{0,0}$
  - Recursively repartition
    - Until each partition can be learned with a simple model



Point	p1	p2	p3	p4
Initial partition Id	0	1	2	3
Model predicted Id	0	1	3	3
Learned partition Id	0	1	3	3

Discussion

- Window and kNN query results are highly accurate but not exact.
  - i.e., over 87% across a variety of settings
  - Separate mechanism has been proposed for exact answer.
- Does not support query for spatial objects with non-zero extent

Slide from W. Aref

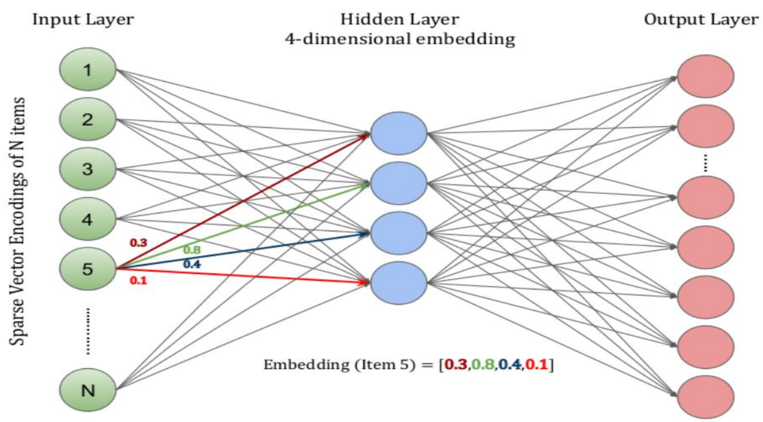
AI and Similarity Search
Search and Indexing

Publications

Echihabi-PVLDB'19

- Indexing Deep Network Embeddings (DNE)

sequences
text
images
video
graphs
…



deep embeddings
high-d vectors learned using a DNN

AI and Similarity Search
Search and Indexing

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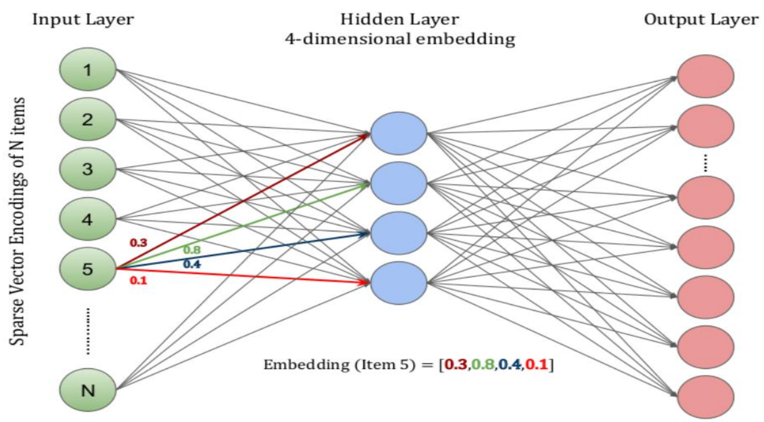


deep embeddings
high-d vectors learned using a DNN

  - Data series techniques provide effective/scalable similarity search over DNE
  - They outperform hashing-based, quantization-based inverted indexes and kNN graphs on many scenarios

High-d Similarity Search: Challenges and Open Problems

Challenges and Open Problems

- we are still far from having solved the problem
- several challenges remain in terms of
  - usability, ease of use
  - scalability, distribution
  - benchmarking
- these challenges derive from modern data science applications

Challenges and Open Problems
Outline

- benchmarking
- interactive analytics
- parallelization and distribution
- deep learning

Massive High-d Data Collections

Publications

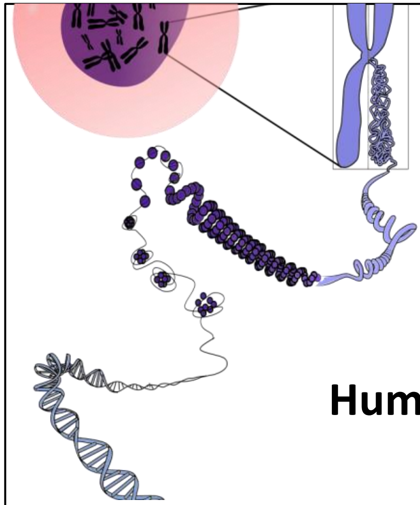
Palpanas-SIGREC'19

NASA's Solar Observatory

1.5 TB per day

Large Synoptic Survey Telescope (2019)

~30 TB per night



Human Genome project

130 TB

passenger aircrafts

20 TB per hour

data center and services monitoring

2B data series

4M points/sec

facebook

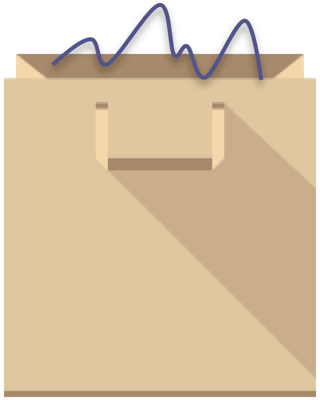
Challenges and Open Problems Outline

- benchmarking
- interactive analytics
- parallelization and distribution
- deep learning

Previous Studies

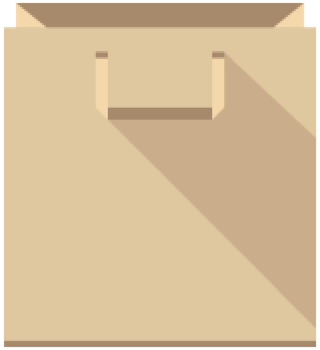
evaluate **performance** of **indexing methods** using **random queries**

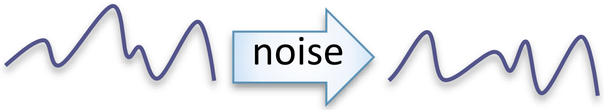
- chosen from the data (with/without noise)



Previous Studies

With or without noise





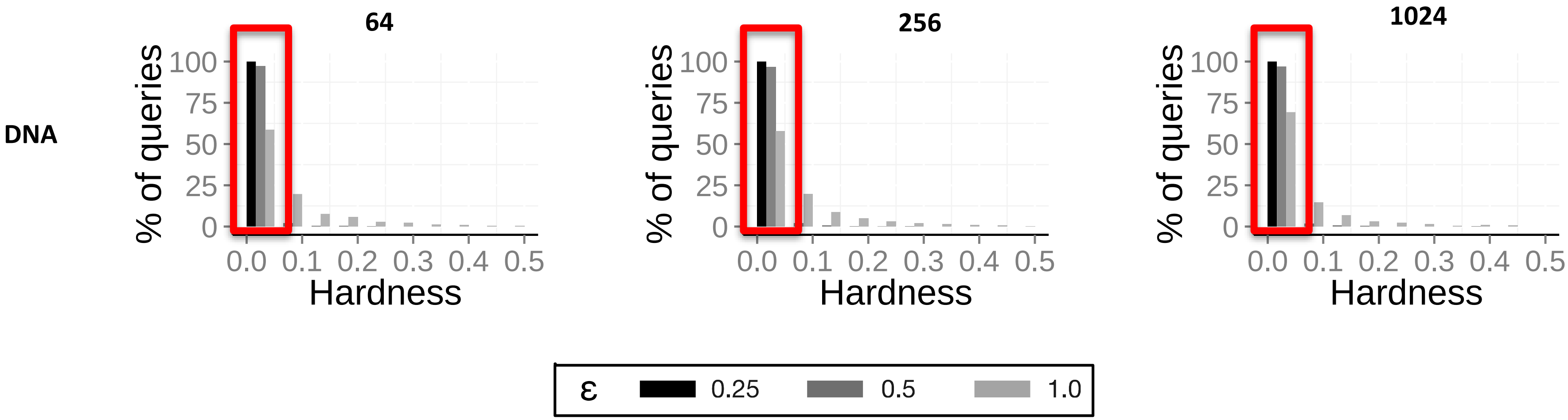
Publications

Zoumbatianos KDD'15

Zoumbatianos TKDE'18

Previous Workloads

Most previous workloads are ***skewed*** to ***easy*** queries



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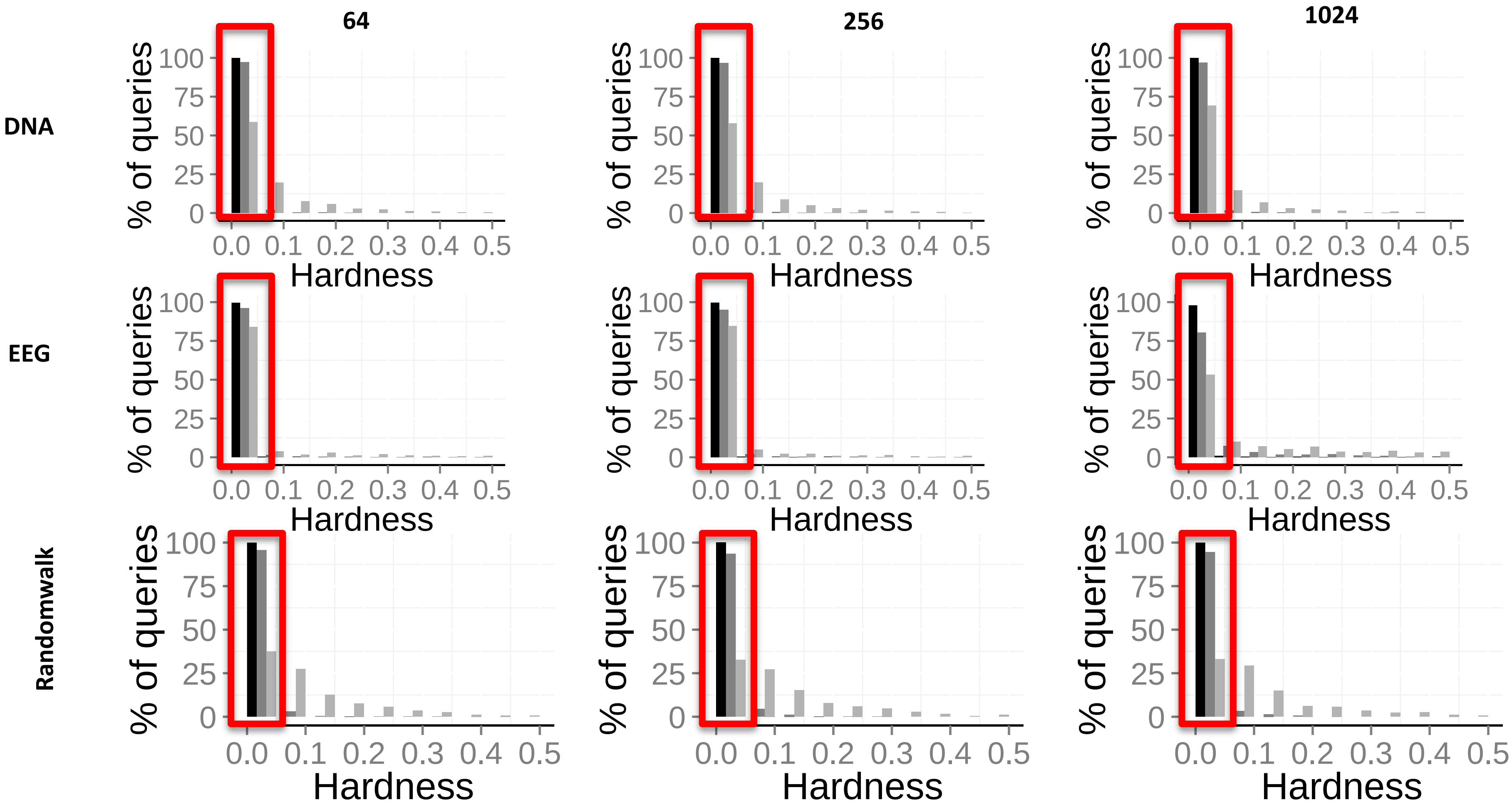


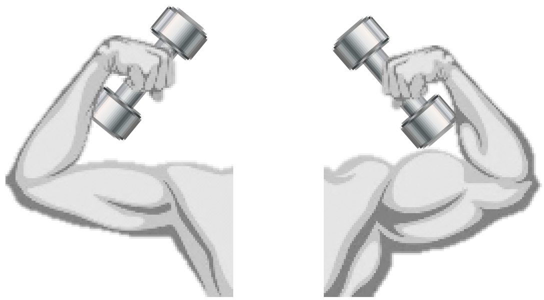
Publications

Zoumbatianos KDD’15

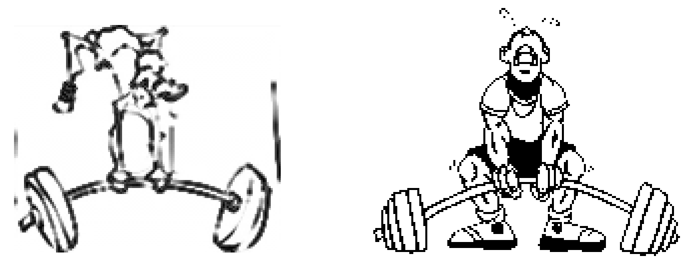
Zoumbatianos TKDE’18

Benchmark Workloads

If all queries are **easy**
all indexes look **good**



If all queries are **hard**
all indexes look **bad**



need **methods** for **generating** queries of **varying hardness**

Publications

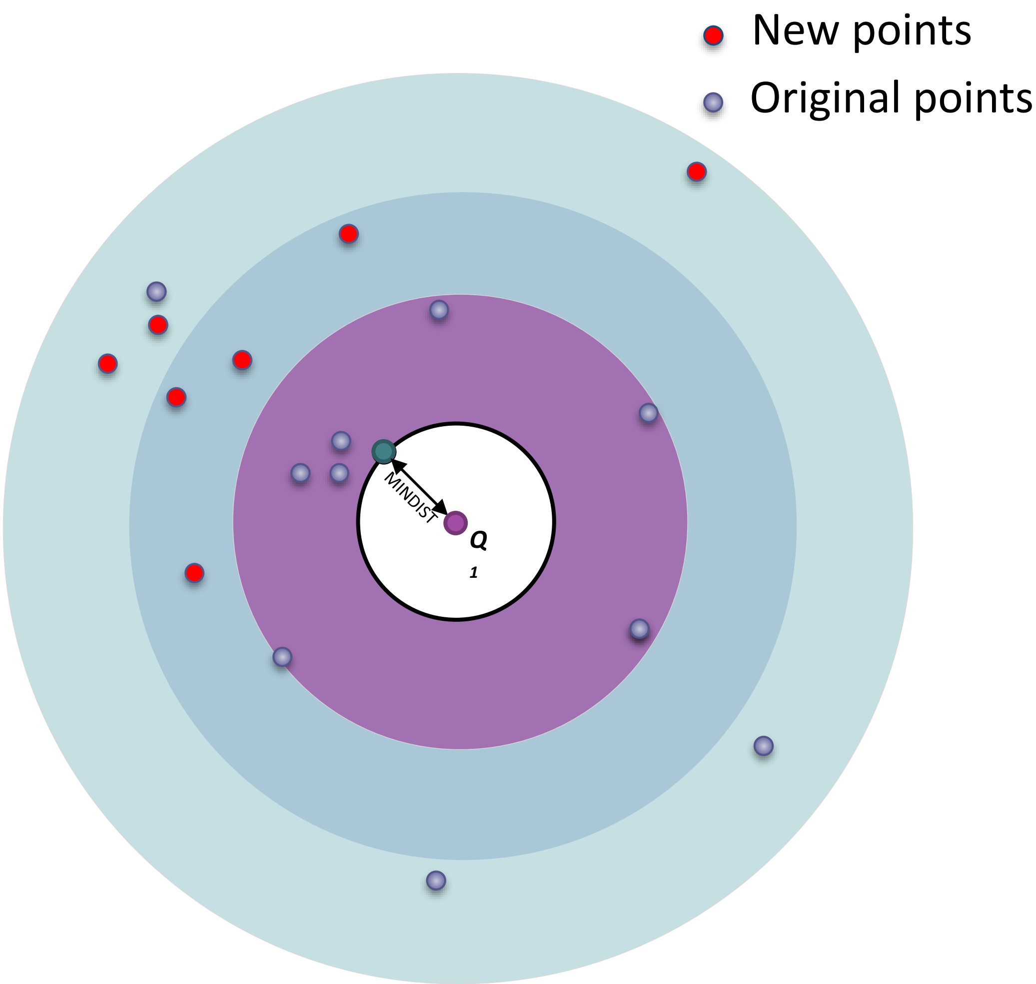
Zoumbatianos KDD’15

Zoumbatianos TKDE’18

Densification Method:
Equi-densification

Distribute points such that:
The **worse** a summarization
the more data it checks

Equal number of points in every “zone”



Publications

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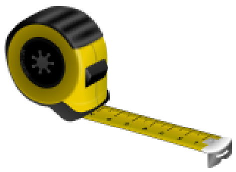
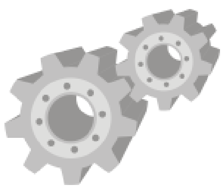
Zoumbatianos TKDE'18

Summary

Pros:



Theoretical background
Methodology for characterizing
NN queries for data series indexes



Nearest neighbor query workload generator
Designed to stress-test data series indexes
at varying levels of difficulty

Cons:

Time complexity
Need new approach to scale to very large datasets

Challenges and Open Problems
Outline

- benchmarking
- interactive analytics
- parallelization and distribution
- deep learning

Need for Interactive Analytics

- interaction with users offers new opportunities
  - progressive answers
    - produce intermediate results
      - iteratively converge to final, correct solution
    - provide bounds on the errors (of the intermediate results) along the way

- several exciting research problems in intersection of visualization and data management
  - *frontend*: HCI/visualizations for querying/results display
  - *backend*: efficiently supporting these operations

Challenges and Open Problems
Outline

- benchmarking
- interactive analytics
- parallelization and distribution
- deep learning

Need for Parallelization/Distribution

Publications

Palpanas-HPCS'17

- further scale-up and scale-out possible!
  - techniques inherently parallelizable
    - across cores, across machines
- need to
  - propose methods for concurrent query answering
  - combine multi-core and distributed methods
  - examine FPGA and NVM technologies
- more involved solutions required when optimizing for energy
  - reducing execution time is relatively easy
  - minimizing total work (energy) is more challenging

Challenges and Open Problems
Outline

- benchmarking
- interactive analytics
- parallelization and distribution
- deep learning

Connections to Deep Learning

- data series indexing for deep embeddings
  - deep embeddings are high-d vectors
  - data series techniques provide effective/scalable similarity search

- deep learning for summarizing high-d vectors
  - different representations for different high-d data types
  - eg, autoencoders can learn efficient data series summaries

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- deep learning for query optimization
  - search space is vast
  - learn optimization function

Connections to Deep Learning

- learning data distributions
  - answer approximate aggregate queries
- learning cardinality estimation
  - estimate query answering cost

Publications

- Thirumuruganathan-ICDE'20
- Sun et al. – SIGMOD'21

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- deep learning for query optimization
  - search space is vast
  - learn optimization function
- dimensionality of high-d vectors and overall dataset size are major challenges!
  - transfer learning to play an important role

Overall Conclusions

- High-d data is a very common data type
  - across several different domains and applications
- Complex analytics on high-d data are challenging
  - have very high complexity

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  - exact similarity search
  - approximate similarity search with quality guarantees
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Overall Conclusions

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  - disk-based datasets

- Several exciting research opportunities
  - parallel, progressive, and deep learning techniques can lead to further performance improvements

thank you!

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