High-Dimensional Vector Similarity Search





Université Paris Cité French University Institute





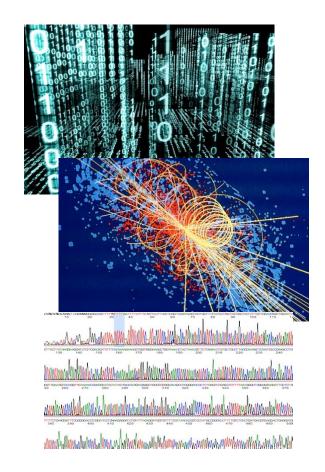
Acknowledgements

- thanks to all my collaborators from:
 - Harvard University
 - Cornell University/Microsoft
 - University of Chicago
 - University of Toronto
 - Ohio State University
 - Inria
 - University of California at Riverside
 - University of Crete/FORTH
 - University of Trento
 - EDF
 - CEA
 - Huawei

diN

Executive Summary

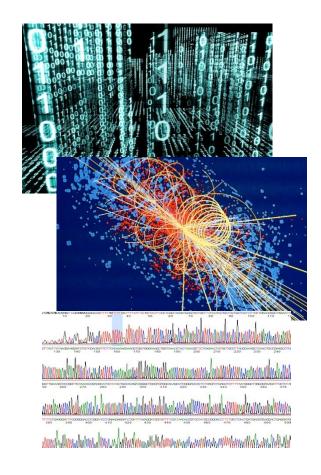
- data collected at unprecedented rates
- they enable data-driven scientific discovery
- lots of these data are high-d vectors
 takes days-weeks to analyze big high-d vector collections



dil

Executive Summary

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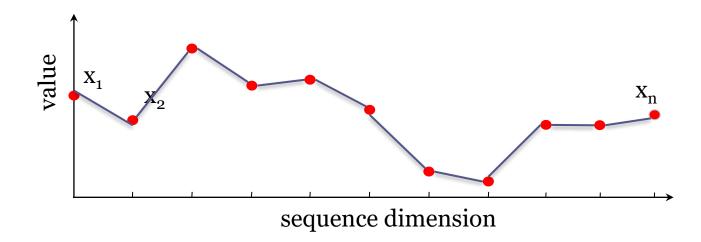


dil

goal: analyze big high-d vectors in seconds

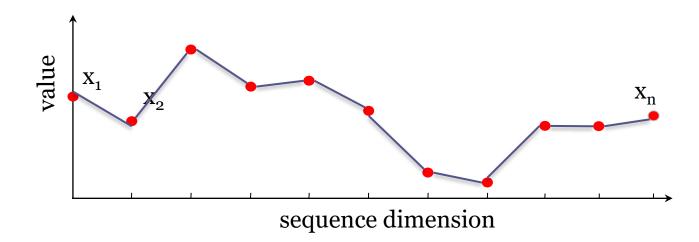
din

• Sequence of points ordered along some dimension



dive

• Sequence of points ordered along some dimension

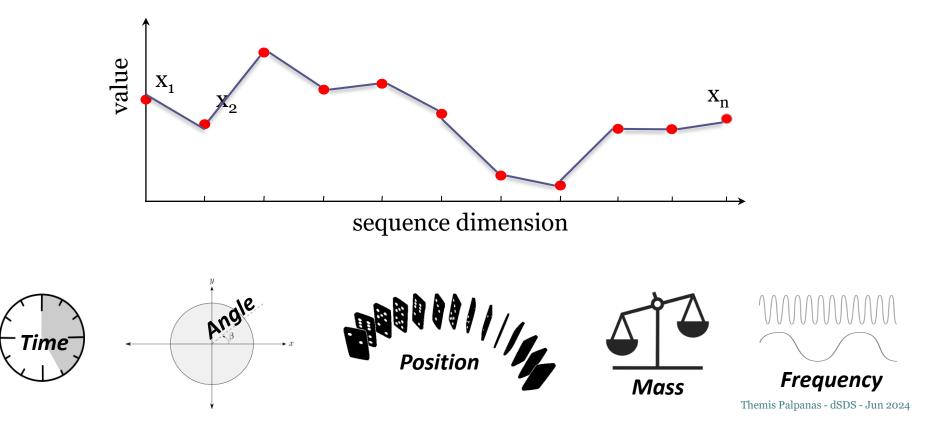




dive

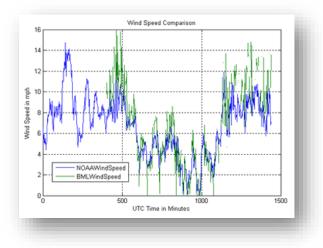
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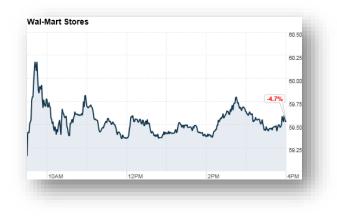
div

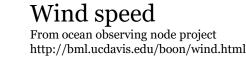


Scientific Monitoring

 meteorology, oceanography, astronomy, finance, sociology, ...







Time

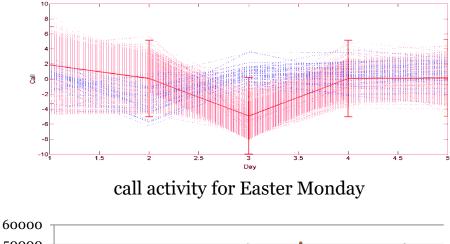
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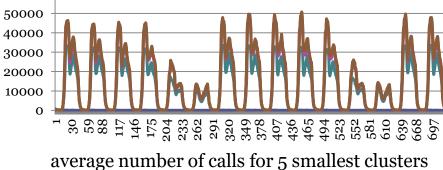
16

din

Telecommunications

- analysis of call activity patterns
 - Telecom Italia







clustermap of incoming calls time series

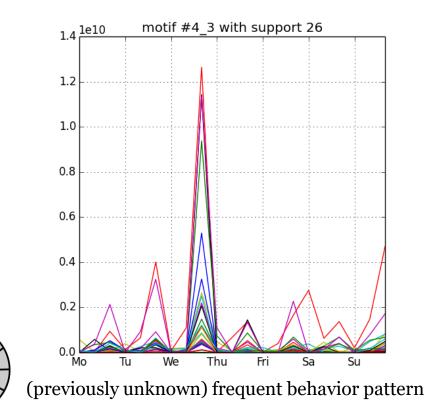


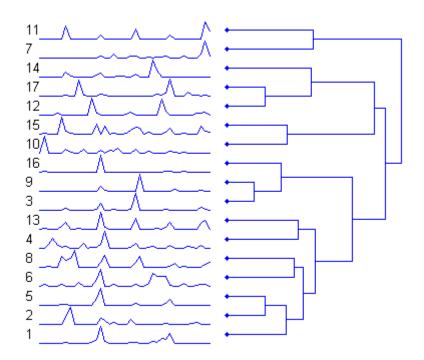
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Home Networks

- temporal usage behavior analysis of home networks
 - Portugal Telecom

Time



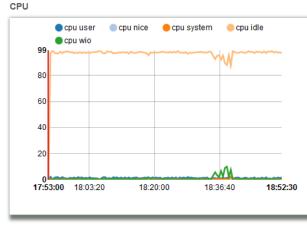


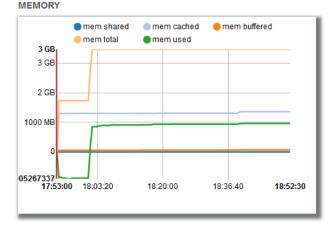
clustering based on user activity patterns

dive

Data Centers

cloud utilization/operation/health monitoring









LOAD



Time

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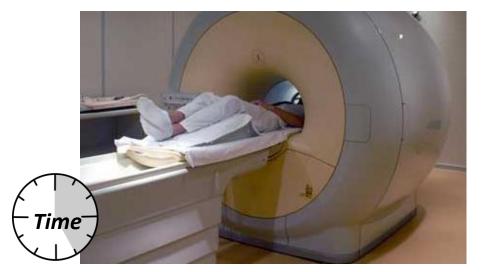
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- functional Magnetic Resonance Imaging (fMRI) data
 - primary experimental tool of neuroscientists
 - reveal how different parts of brain respond to stimuli



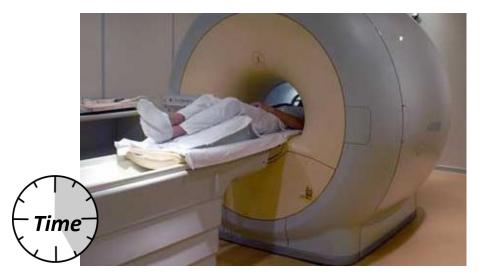
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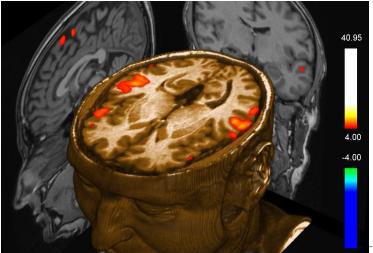
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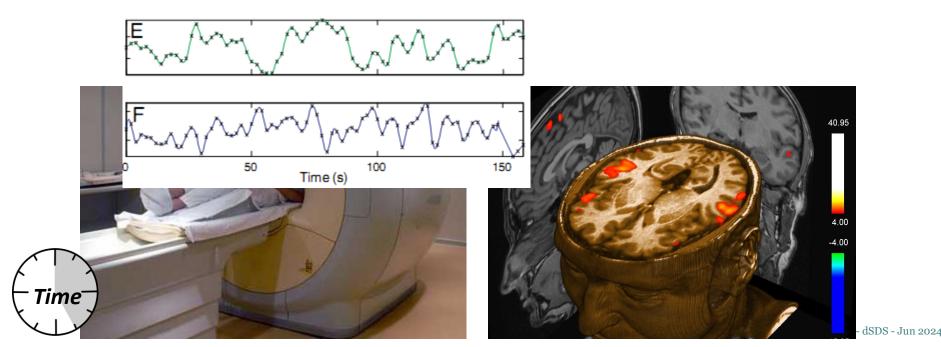


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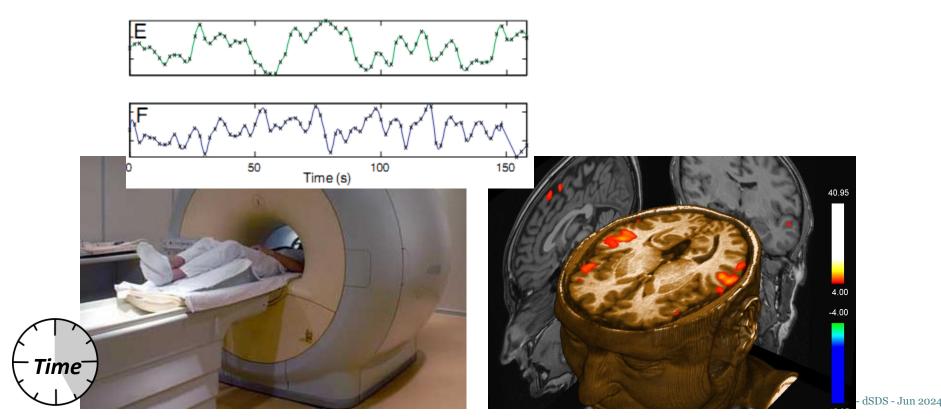
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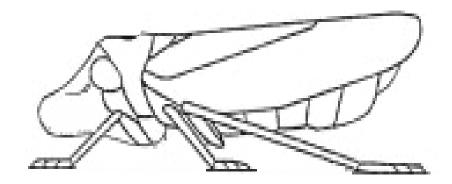
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Entomology

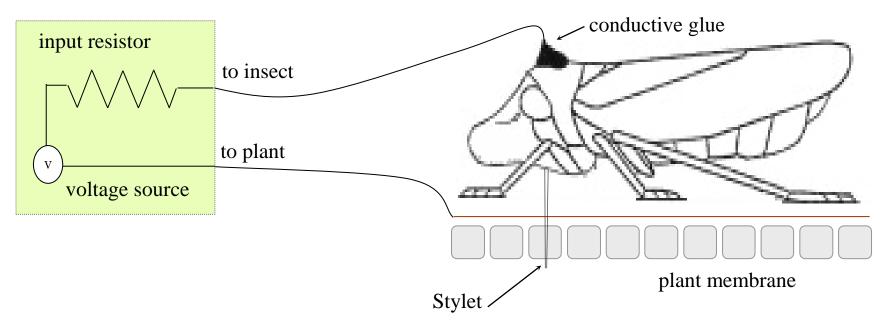




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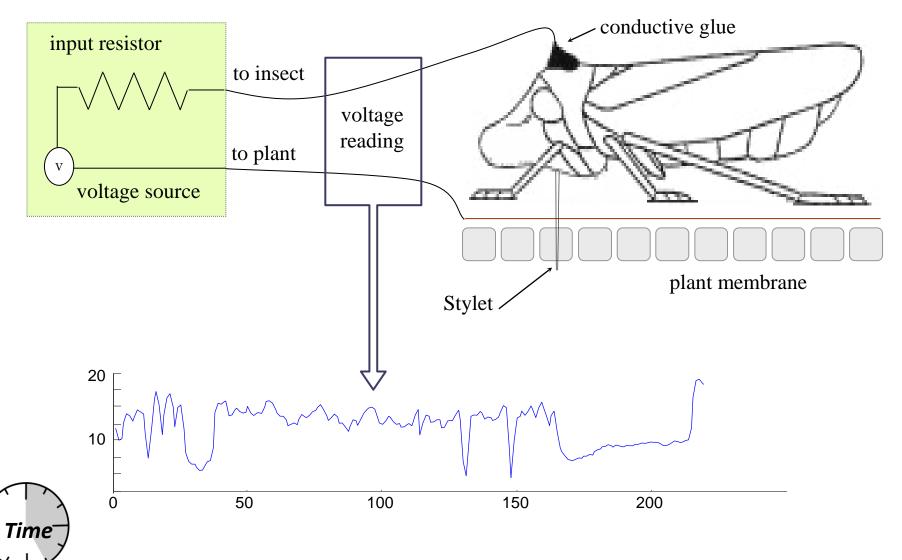
Entomology





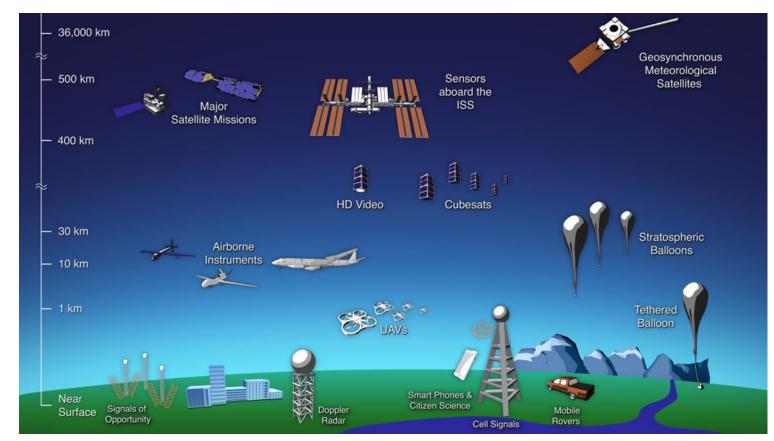
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Entomology



divo

• Earth monitoring



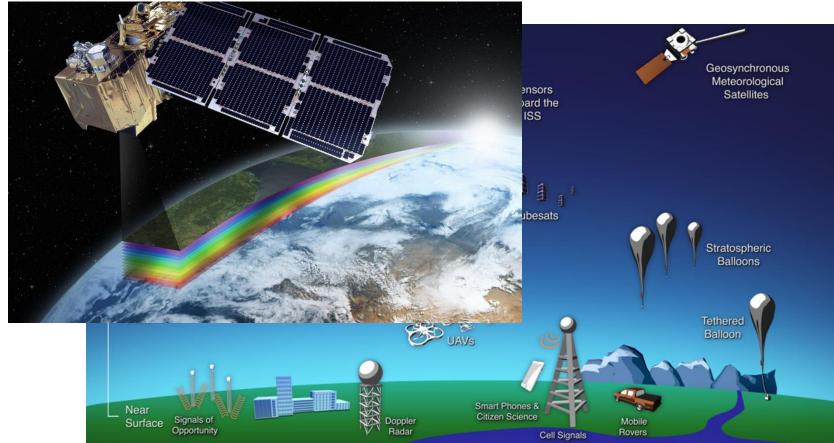


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div

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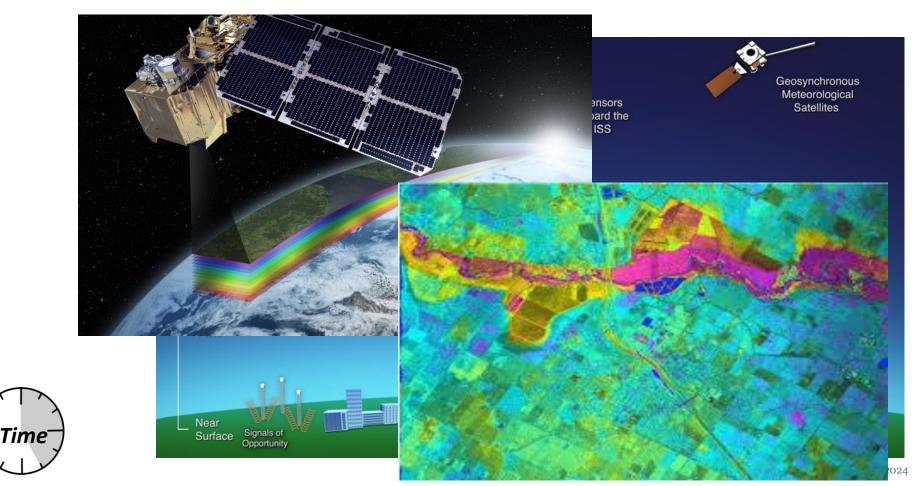
Time



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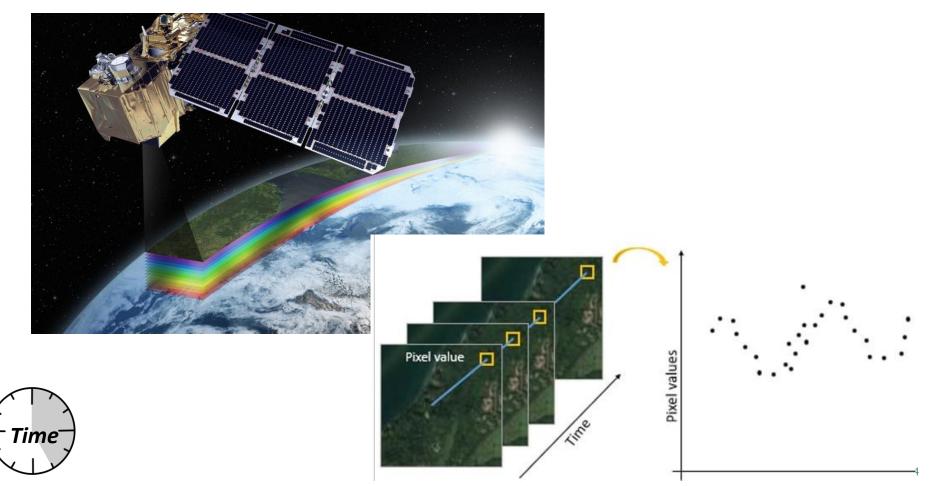
dive

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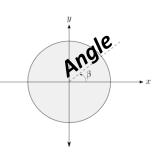
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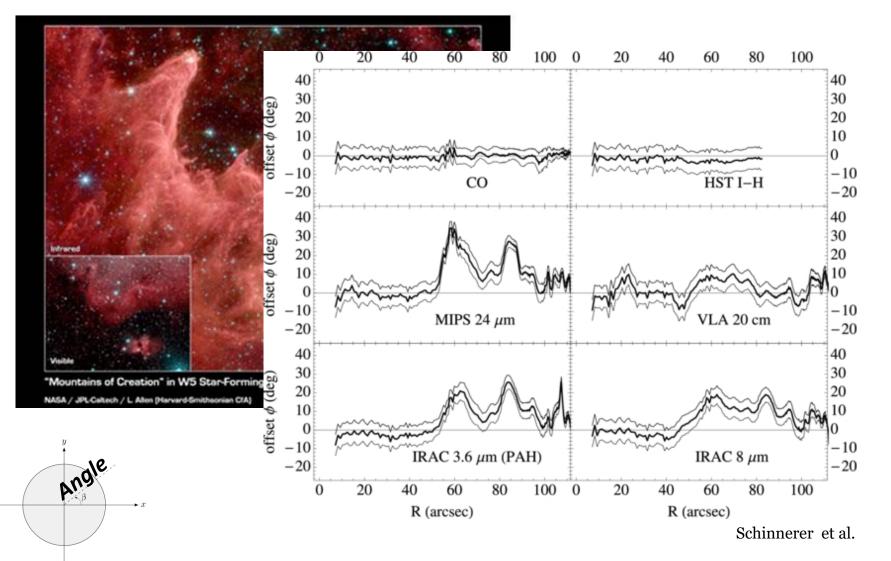
Astrophysics





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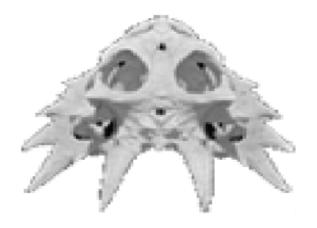
Astrophysics

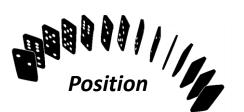


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Paleontology

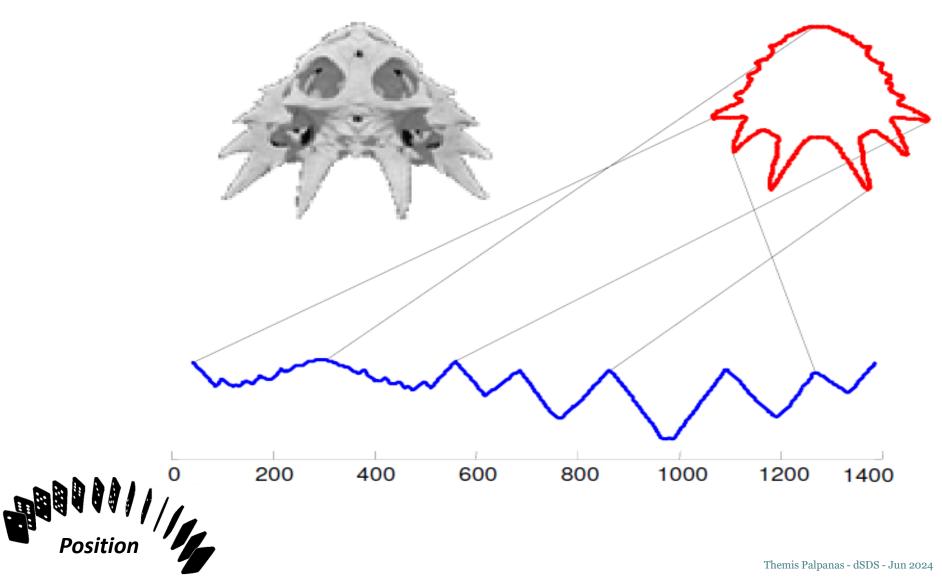




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Paleontology

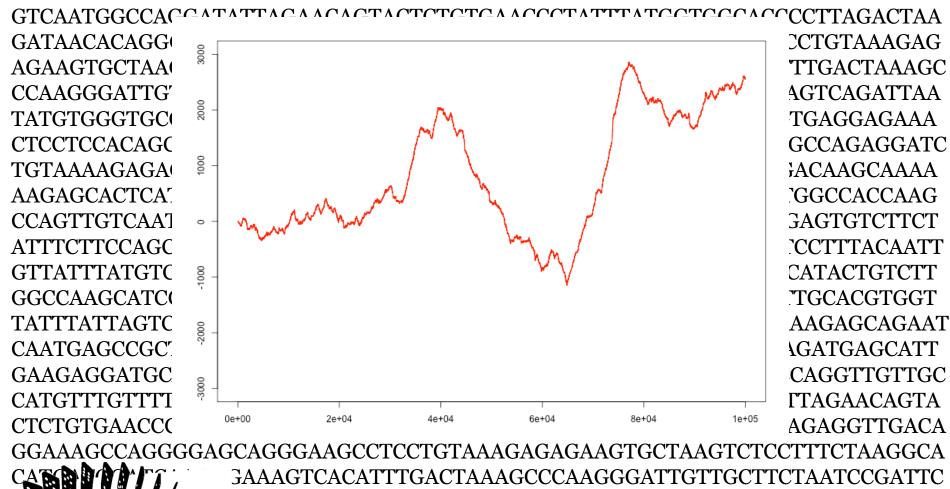


din

Biology

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Biology



Position

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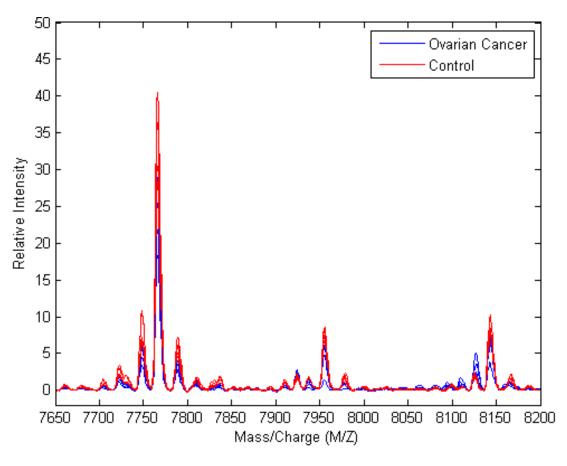
Biology

GATAACACAGG(CCTGTAAAGAG 3000 TTGACTAAAGC AGAAGTGCTAA(**CCAAGGGATTG'** AGTCAGATTAA 2000 TATGTGGGTGC(TGAGGAGAAA CTCCTCCACAGC GCCAGAGGATC 1000 **TGTAAAAGAGA** ACAAGCAAAA AAGAGCACTCA **'GGCCACCAAG CCAGTTGTCAA** GAGTGTCTTCT 0 ATTTCTTCCAGC **'CCTTTACAATT** GTTATTTATGTC -1000 CATACTGTCTT GGCCAAGCATC(TGCACGTGGT TATTTATTAGTC AAGAGCAGAAT -2000 CAATGAGCCGC^r AGATGAGCATT GAAGAGGATGC CAGGTTGTTGC -3000 CATGTTTGTTTT ΓΤΑGΑΑCAGTΑ 0e+00 2e+04 4e+04 6e+04 8e+04 1e+05 CTCTGTGAACC(AGAGGTTGACA **JAAAGTCACATTTGACTAAAGCCCAAGGGATTGTTGCTTCTAATCCGATTC**

Position

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Medicine

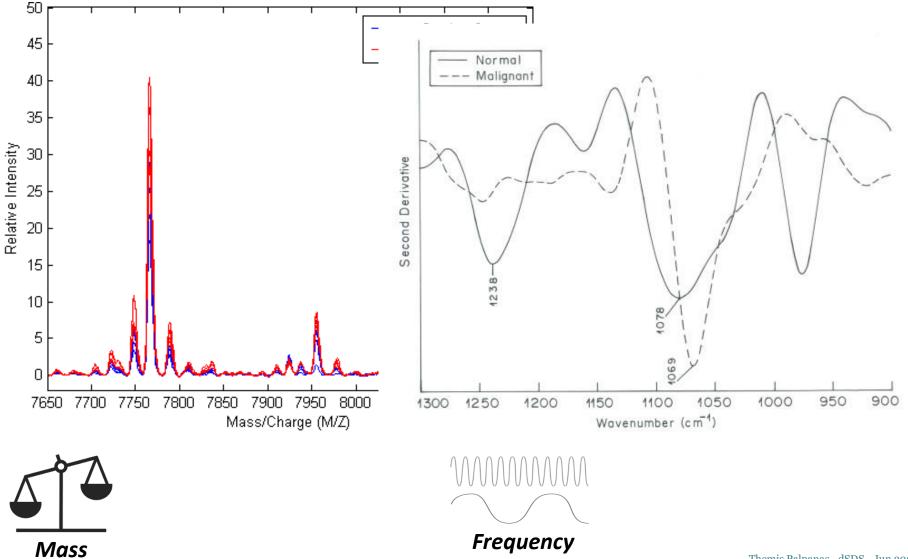




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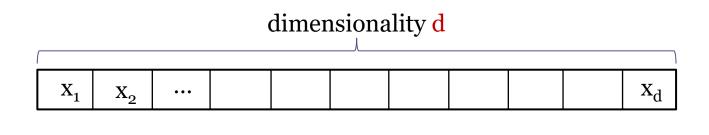
Medicine

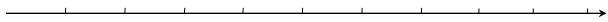


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• represented as *d*-dimensional vector



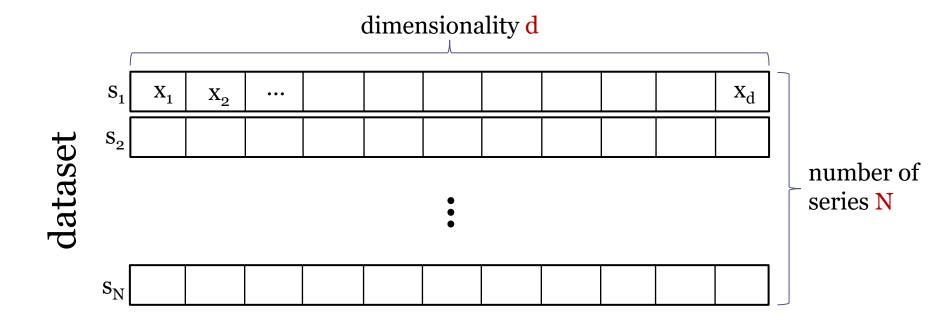


sequence dimension

diN

Data Series Collections

• represented as *N d*-dimensional vectors



div

What do we want to do with them? - simple query answering

select values in time interval select values in some range

select some data series combinations of those

divo

What do we want to do with them? - simple query answering

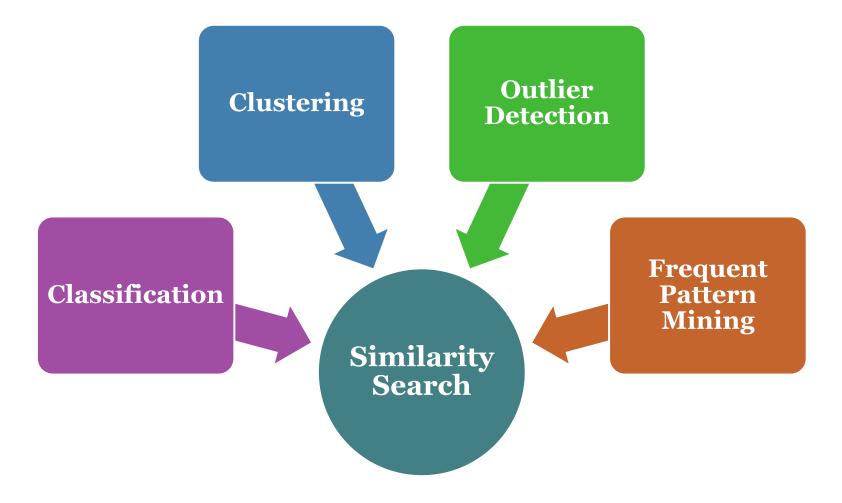
- a solved(?) problem
 - vour favorite DBMS
 - •••
 - InfluxData
 - kx
 - Riak TS
 - OpenTSDB
 - Gorilla/Beringei
 - TimescaleDB
 - KairosDB
 - Druid

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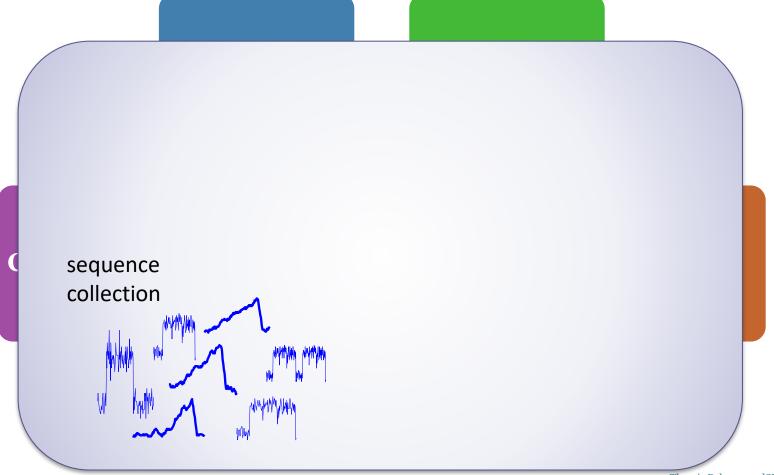
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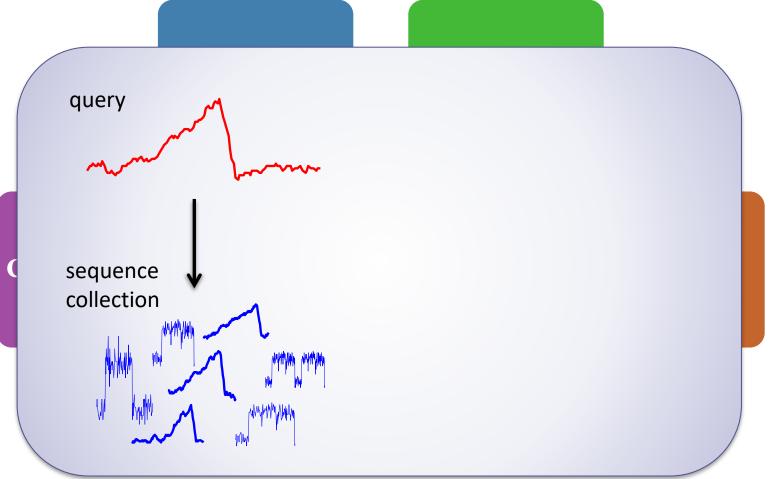


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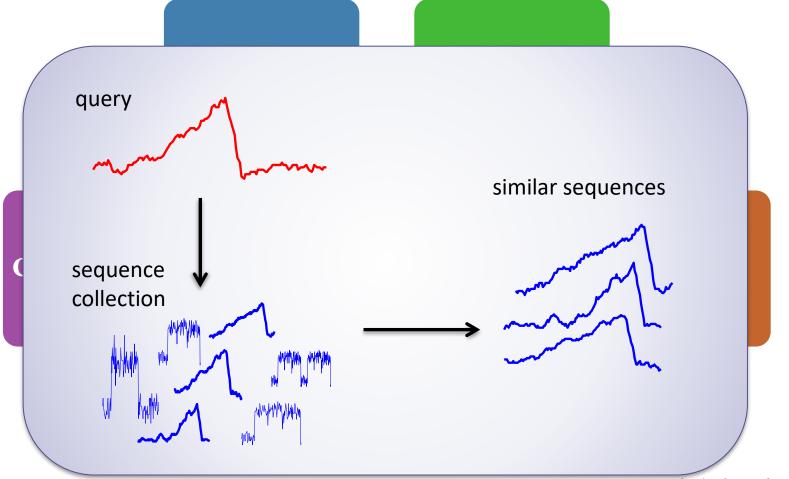
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diN



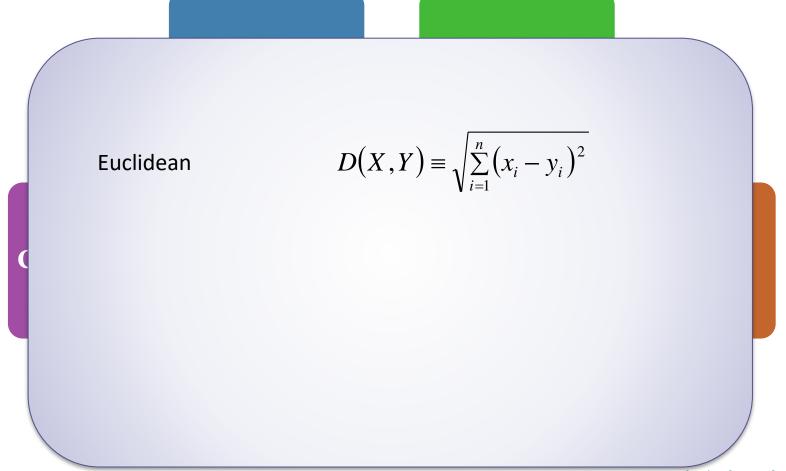
Themis Palpanas - dSDS - Jun 2024

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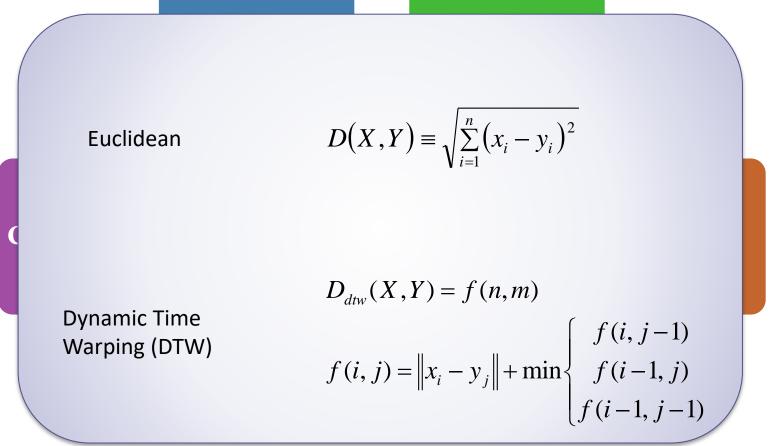


Themis Palpanas - dSDS - Jun 2024

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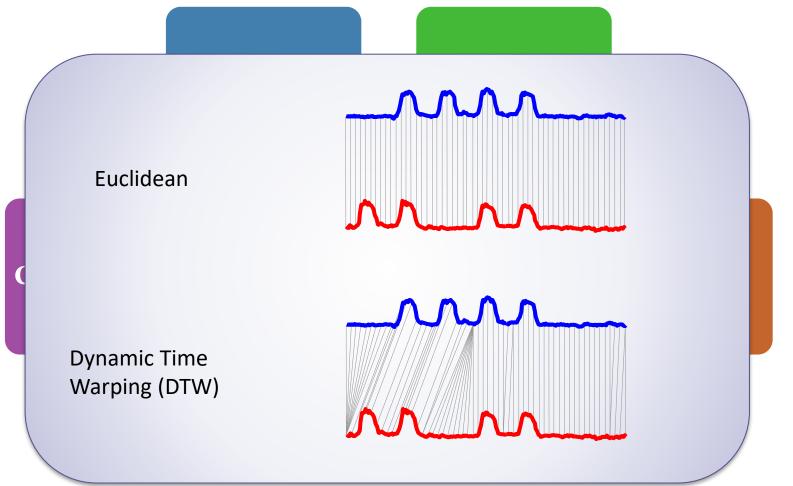


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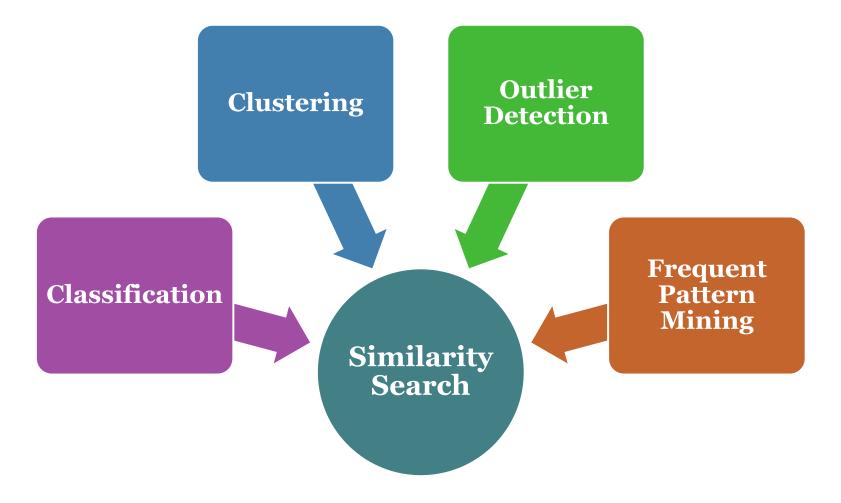
Themis Palpanas - dSDS - Jun 2024

diN

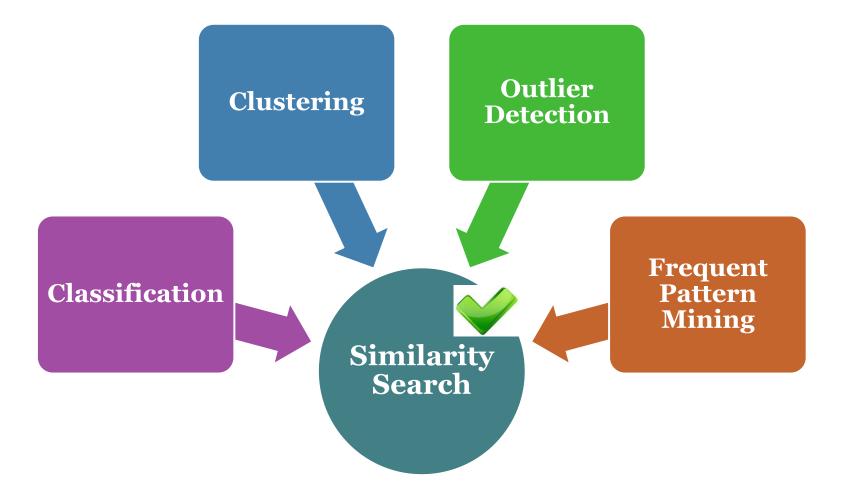


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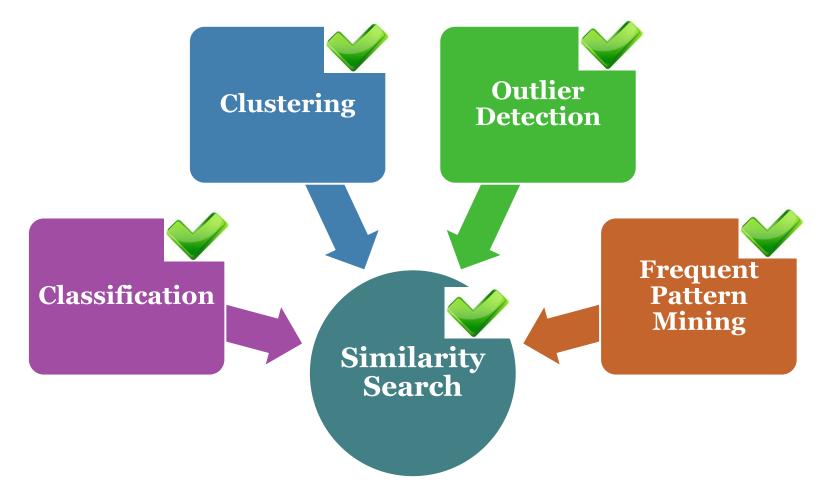
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diNo



diNo



diNo



HARD, because of very high dimensionality: each data series has 100s-1000s of points!



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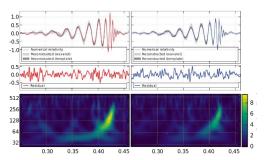
HARD, because of very high dimensionality: each data series has 100s-1000s of points!

even HARDER, because of very large size: millions to billions of data series (multi-TBs)!

diNc

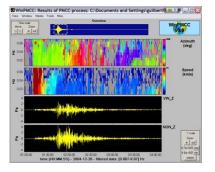
Real Use-Cases

astrophysics: gravitational waves, **TB/hour** partner: European Gravitational Observatory (EGO) *Pisa, Italy*



diNc

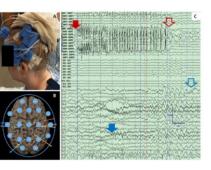
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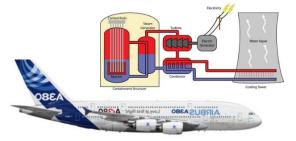


seismology: seismic sequences, 100s of TB partner: Atomic Energy Commission (CEA) *Paris, France*

neuroscience: intracranial EEG sequences, **TB/patient** partner: **Paris Brain Institute (ICM)**

Paris, France



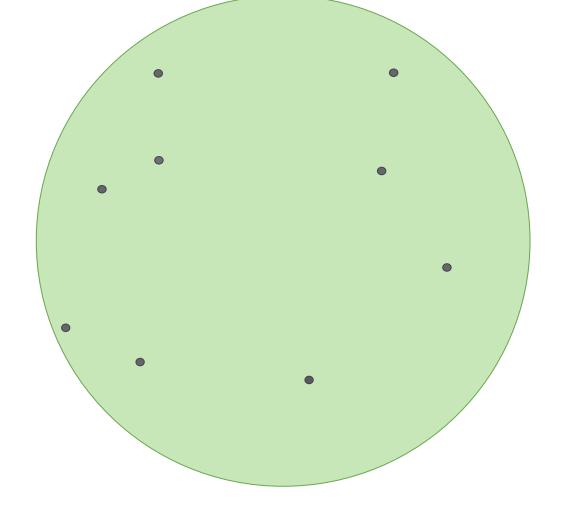


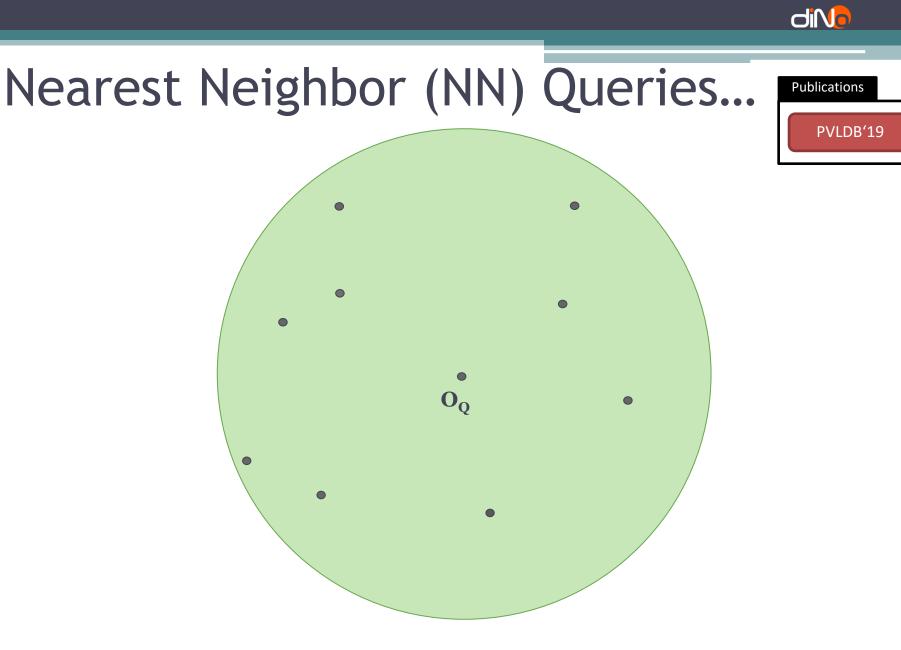
engineering: operation monitoring, **TB-PB** partners: **Airbus / Électricité de France (EDF)** *Toulouse / Paris, France*

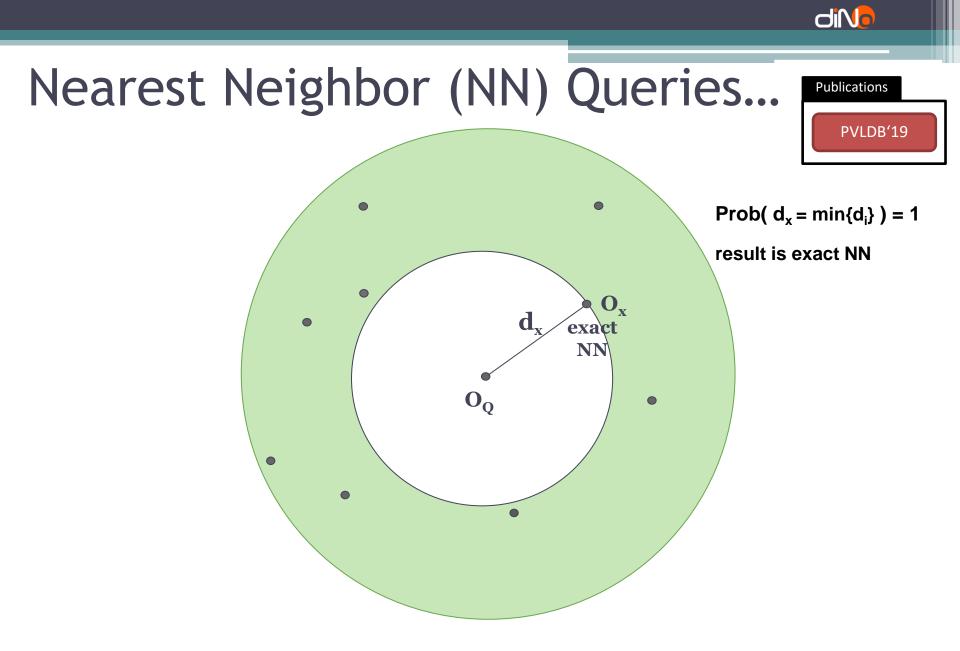
Nearest Neighbor (NN) Queries...

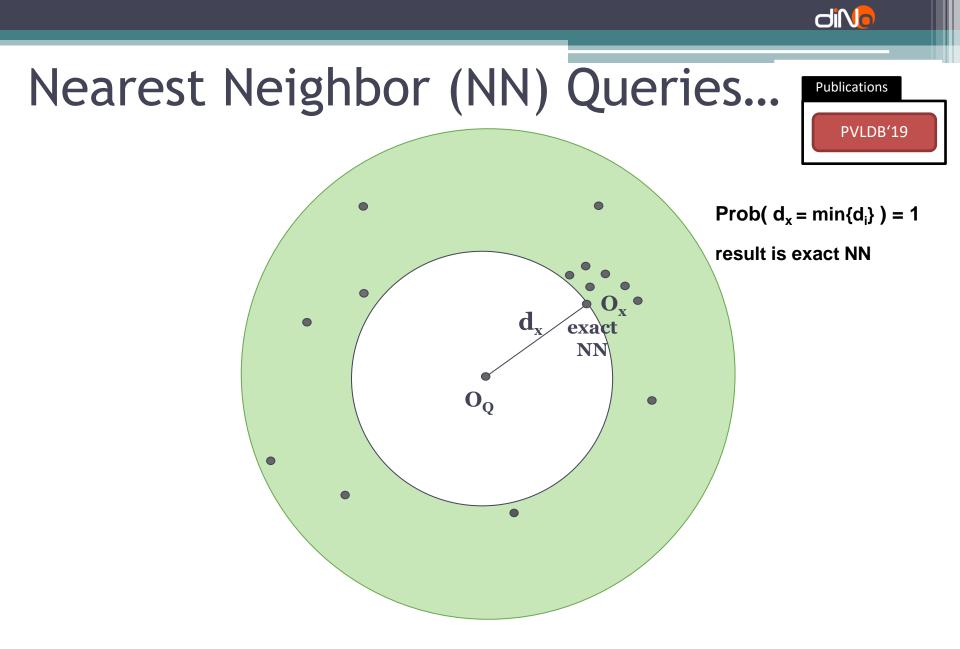


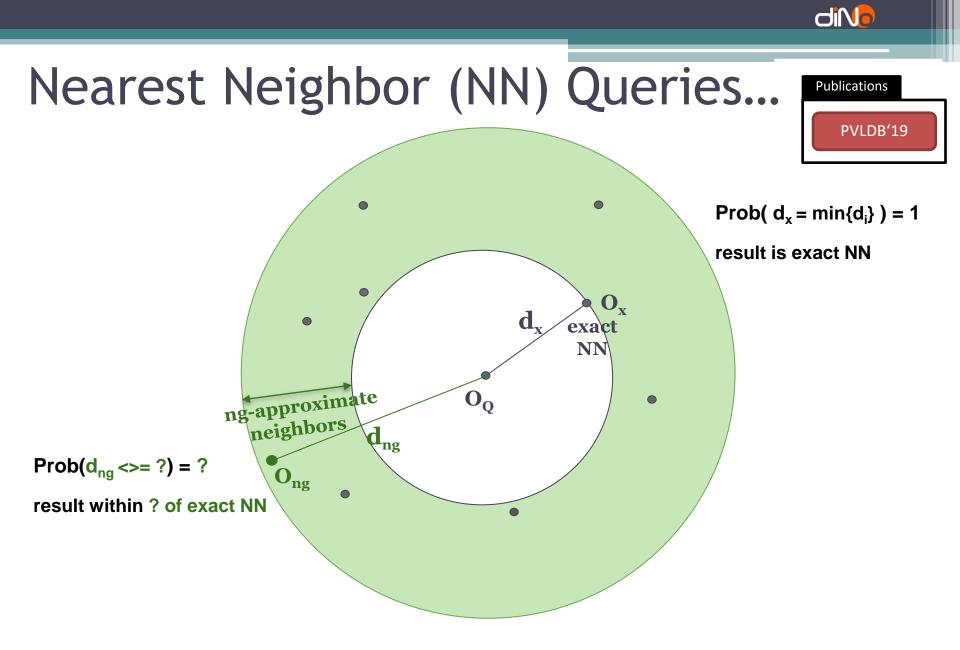
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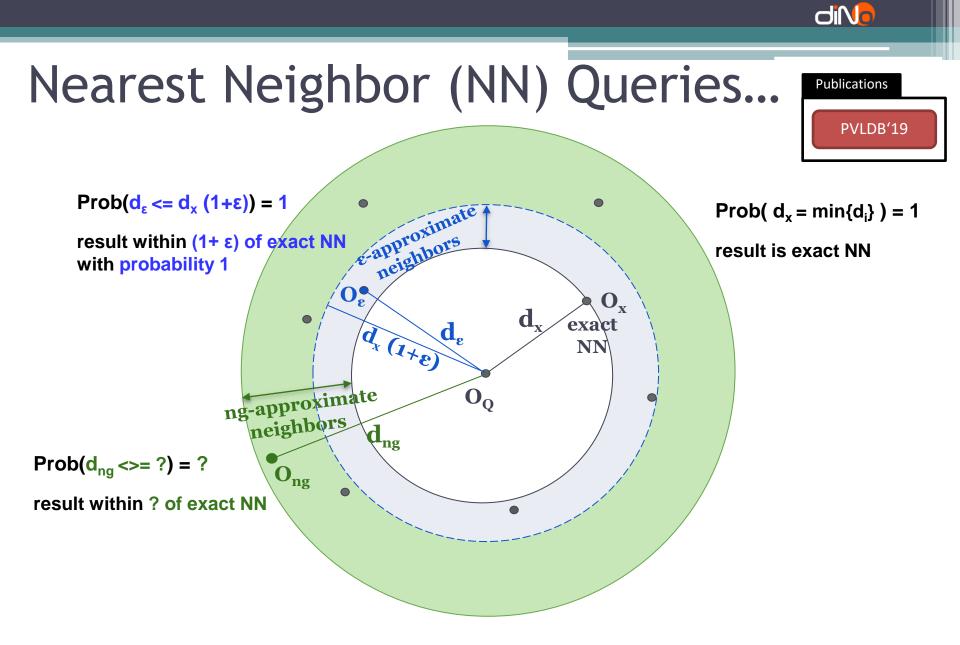


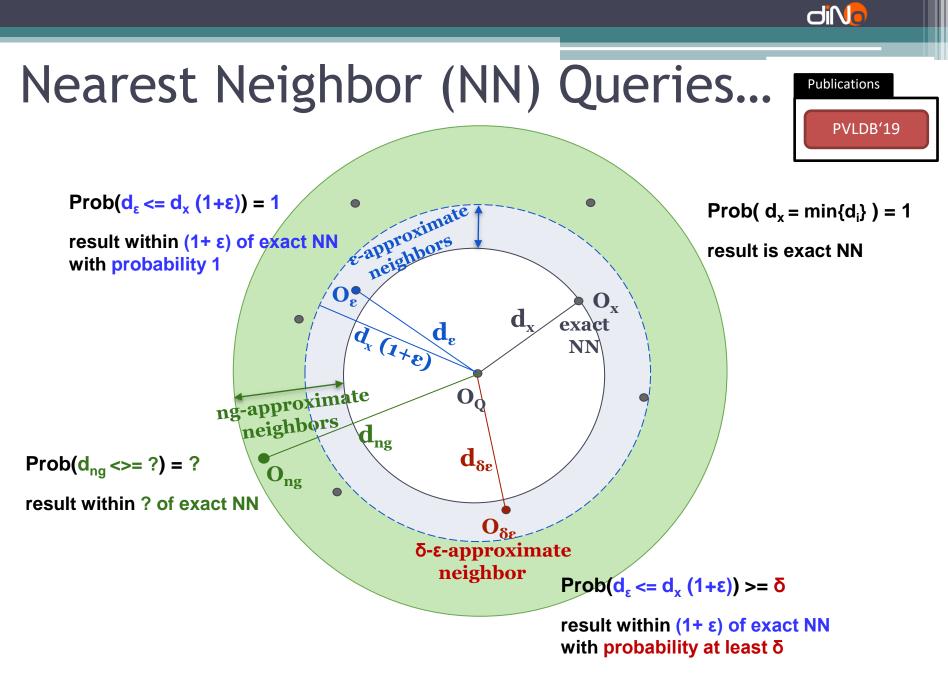


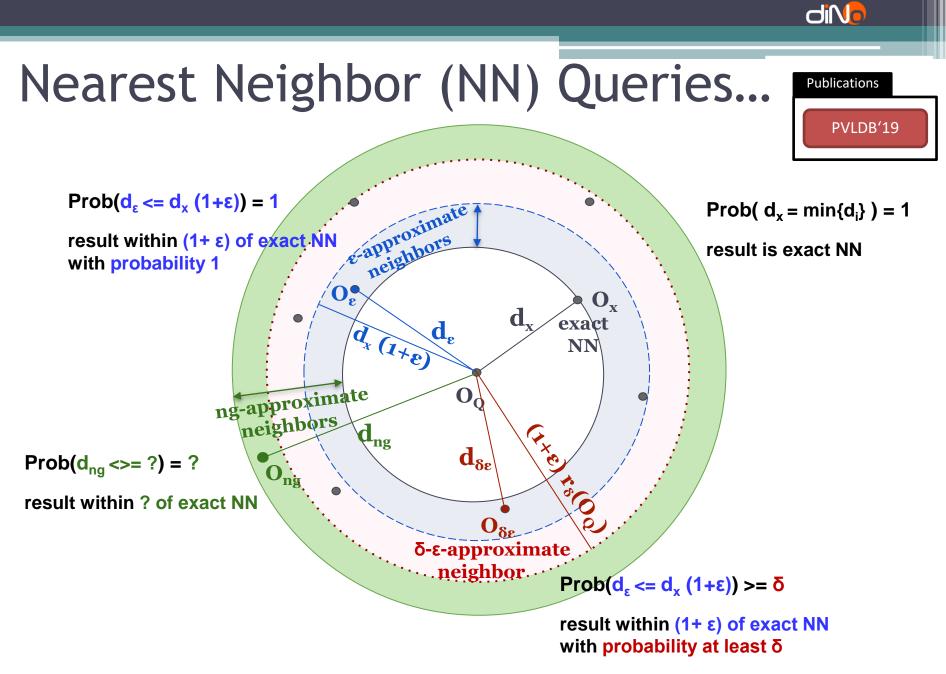












Problem Variations

High-d Vectors Distance Measures

- similarity search is based on measuring distance between vectors
- A variety of distance measures have been proposed
 - L_p distances (0<p≤2, ∞), (Euclidean for p = 2)
 - Cosine distance
 - Correlation
 - Hamming distance

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Problem Variations

High-d Vectors Distance Measures

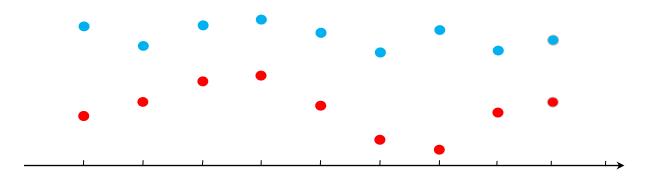
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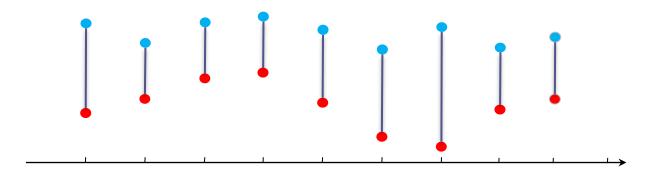
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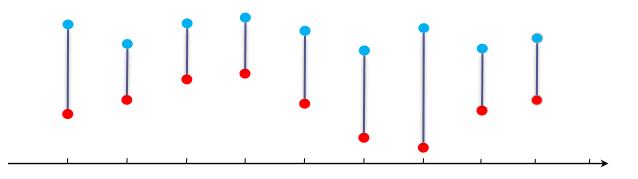
Euclidean Distance



Euclidean Distance



Euclidean Distance



• Euclidean distance pair-wise point distance ED(X,Y)

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

- similarity matching requires many distance computations
 - can significantly slow down processing
 - because of large number of data series in the collection
 - because of high dimensionality of each data series

din

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- in case of Euclidean Distance, we can speedup processing by
 - smart implementation of distance function
 - early abandoning

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- in case of Euclidean Distance, we can speedup processing by
 - smart implementation of distance function
 - early abandoning
- result in **considerable** performance improvement

smart implementation of distance function

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

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Publications

Keogh-DMKD'03





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Similarity Matching Fast Euclidean Distance

smart implementation of distance function

• do not compute the square root (of the Euclidean Distance) $n = \frac{n}{2}$

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



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Similarity Matching Fast Euclidean Distance

smart implementation of distance function

• do not compute the square root (of the Euclidean Distance) $\sum_{n=1}^{n} \sum_{n=1}^{n} (n - n)^2$

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

- does not alter the results
- saves precious CPU cycles

Publications

Keogh-

DMKD'03

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div

Similarity Matching Fast Euclidean Distance

early abandoning

stop the distance computation as soon as it exceeds the value of bsf

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

Publications Keogh-

DMKD'03

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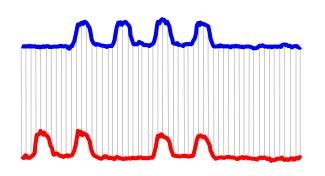
Similarity Matching Fast Euclidean Distance

- early abandoning
 - **stop** the distance computation as soon as it exceeds the value of bsf $ED(X,Y) = \sum_{i=1}^{m} (x_i - y_i)^2, \quad m \le n$

- does not alter the results
- avoids useless computations

Distance Measures: Euclidean, DTW, LCSS

- Euclidean
 - rigid



diNo

Distance Measures: Euclidean, DTW, LCSS

- Euclidean
 - rigid

- Dynamic Time Warping (DTW)
 - allows local scaling

div

Distance Measures: Euclidean, DTW, LCSS Euclidean • rigid • Dynamic Time Warping (DTW) allows local scaling Longest Common SubSequence (LCSS) allows local scaling ignores outliers

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Pearson's Correlation Coefficient

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

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

div

Pearson's Correlation Coefficient

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- 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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Pearson's Correlation Coefficient

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- 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

diNc

PC and ED

• Euclidean distance:
$$ED = \sqrt{\sum_{i=1}^{n} (x_i - y_i)^2},$$

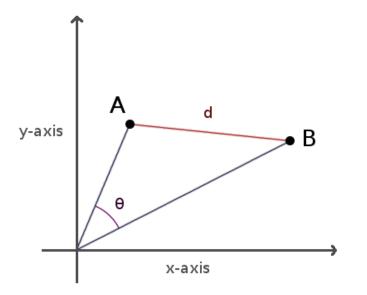
• In case of Z-normalized data series (mean = 0, stddev = 1):

$$PC = \frac{1}{n-1} \sum_{i=1}^{n} x_i \cdot y_i$$
 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: Cosine Distance



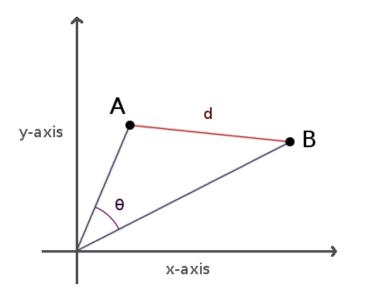
$$ext{similarity} = \cos(heta) = rac{\mathbf{A} \cdot \mathbf{B}}{\|\mathbf{A}\| \|\mathbf{B}\|} = rac{\sum\limits_{i=1}^n A_i B_i}{\sqrt{\sum\limits_{i=1}^n A_i^2} \sqrt{\sum\limits_{i=1}^n B_i^2}},$$

• Cosine distance = 1 - cosine similarity

87

diNo

Distance Measures: Cosine Distance



$$ext{similarity} = \cos(heta) = rac{\mathbf{A} \cdot \mathbf{B}}{\|\mathbf{A}\| \|\mathbf{B}\|} = rac{\sum\limits_{i=1}^n A_i B_i}{\sqrt{\sum\limits_{i=1}^n A_i^2} \sqrt{\sum\limits_{i=1}^n B_i^2}},$$

• Cosine distance = 1 - cosine similarity

- ED vs. Cosine similarity
 - If A and B are normalized to unit length in L₂, the square of ED is proportional to the cosine distance:
 - $||A||_2 = ||B||_2 = 1 \rightarrow ||A B||_2 = 2 2\cos(A, B)$

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diNc

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 $Q \in R^d$, $C = \operatorname{argmax}_{X \in S} Q^T X$

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 $Q \in R^d$, $C = argmax_{X \in S} Q^T X$
- 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).

Data Series Similarity Search Pre-processing Tasks

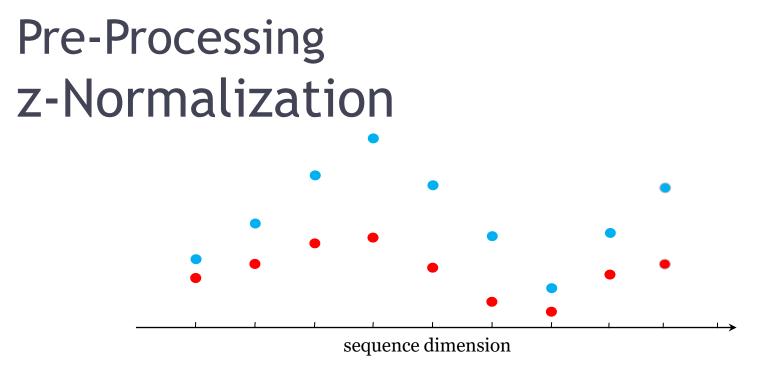
diNo

- data series encode trends
- usually interested in identifying similar trends

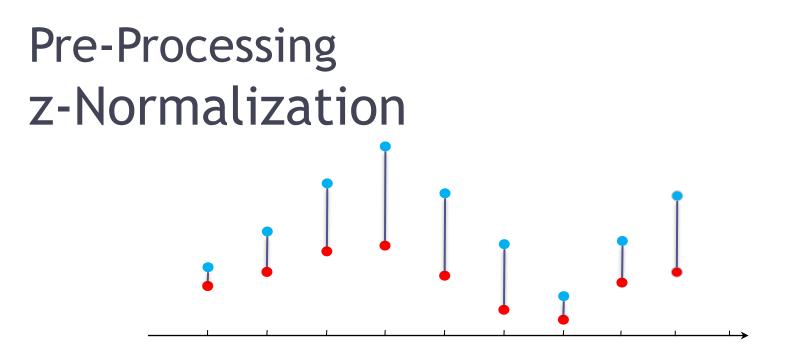
div

- data series encode trends
- usually interested in identifying similar trends
- but absolute values may mask this similarity

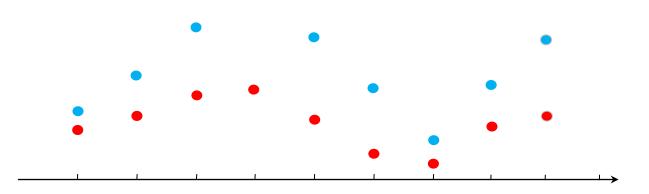
diN



• two data series with similar trends

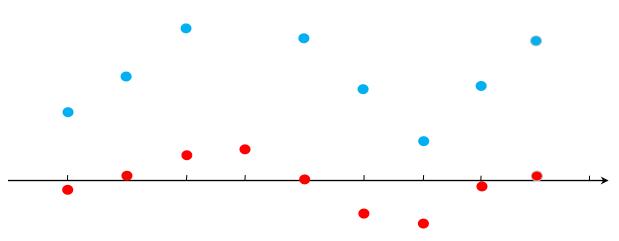


- two data series with similar trends
- but large distance...



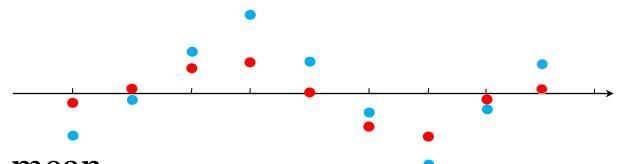
zero mean

- o compute the mean of the sequence
- subtract the mean from every value of the sequence



zero mean

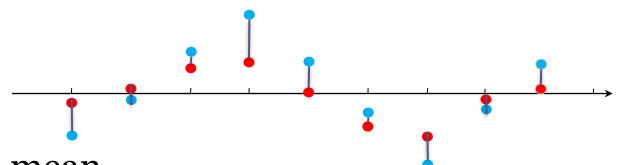
- o compute the mean of the sequence
- subtract the mean from every value of the sequence



zero mean

o compute the mean of the sequence

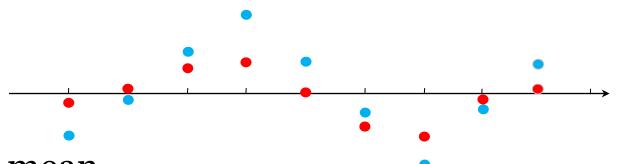
• subtract the mean from every value of the sequence



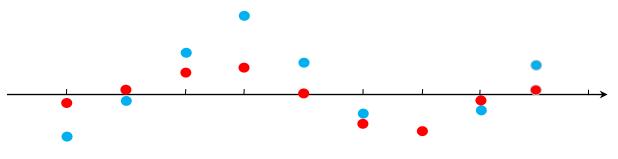
zero mean

o compute the mean of the sequence

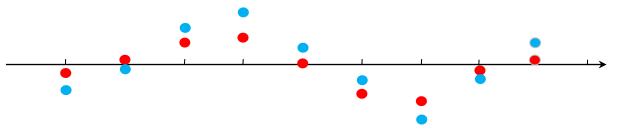
• subtract the mean from every value of the sequence



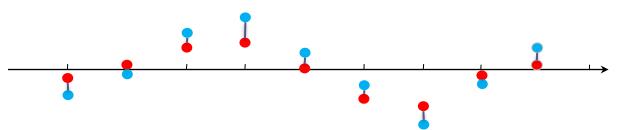
- zero mean
- standard deviation one
 - o compute the standard deviation of the sequence
 - divide every value of the sequence by the stddev



- zero mean
- standard deviation one
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- zero mean
- standard deviation one
 - o compute the standard deviation of the sequence
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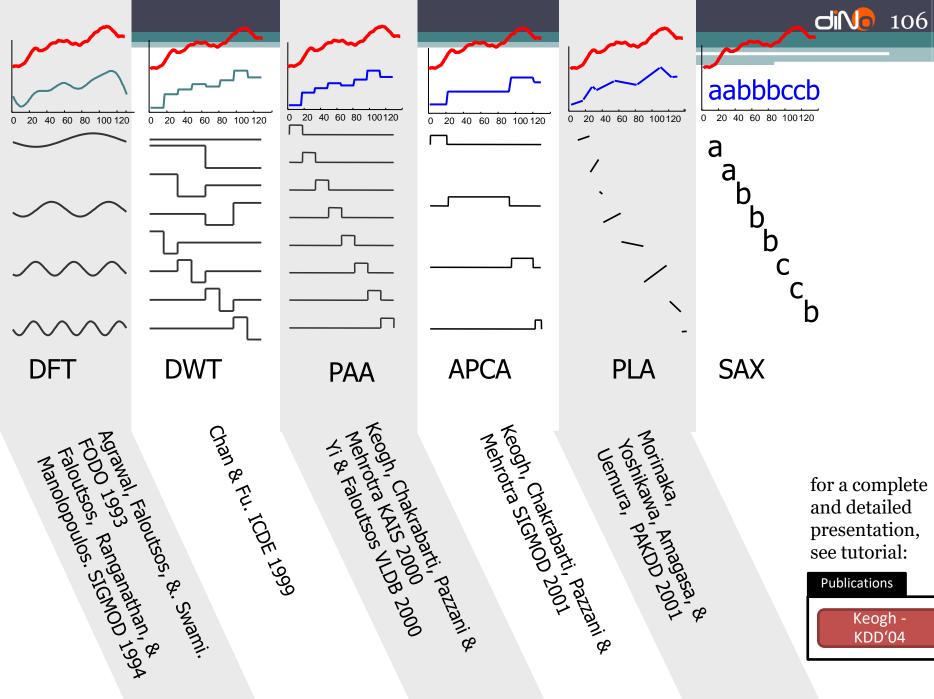
- zero mean
- standard deviation one

- when to z-normalize
 - interested in trends

dino 104

- when to z-normalize
 - interested in trends
- when not to z-normalize
 - interested in absolute values

diNo 105



Comparison of Representations

• which representation is the best?

divlo 107

Comparison of Representations

- which representation is the best?
- depends on data characteristics
 periodic, smooth, spiky, ...

diNo 108

diNo 109

Publications

Palpanas et al. ICDE'04

Palpanas et al.

TKDE'08 Shieh et al. KDD'08

Comparison of Representations

- which representation is the best?
- depends on data characteristics
 periodic, smooth, spiky, ...
- overall (averaged over many diverse datasets, using same memory budget), when measuring reconstruction error (RMSE)
 - no big differences among methods
 - DFT, PAA, DWT (Haar), iSAX slightly better
- should also take into account other factors
 - visualization, indexable, ...

Data Series Similarity Search Common Framework

GEMINI Framework

Publications Faloutsos-SIGMOD'94

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diNo

- Raw data: original full-dimensional space
- Summarization: reduced dimensionality space
- Searching in original space *costly*
- Searching in reduced space *faster*:
 - Less data, indexing techniques available, lower bounding
- Lower bounding enables us to
 - prune search space: throw away data series based on reduced dimensionality representation
 - guarantee correctness of answer
 - no false negatives
 - false positives filtered out based on raw data

GEMINI Framework



GEMINI Solution: Quick filter-and-refine:

- extract *m* features (numbers, e.g., average)
- map to point in *m*-dimensional feature space
- organize points
- retrieve the answer using a NN query
- discard false positives



GEMINI: contractiveness

• GEMINI works when:

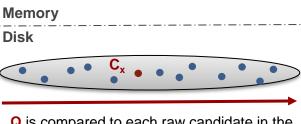
 $D_{feature}(F(x), F(y)) \leq D(x, y)$

• Note that, the closer the feature distance to the actual one, the better

Data Series Similarity Search Classes of Methods

diNo 114

Similarity Matching Serial Scan



Q

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

(a) Serial scan

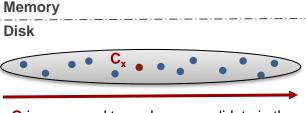
Answering a similarity search query using different access paths

divo



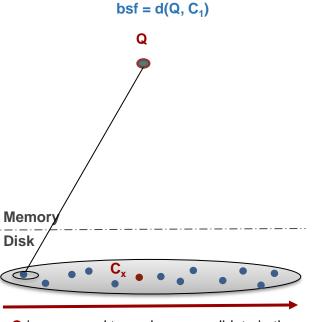






Q is compared to each raw candidate in the dataset before returning the answer C_x

(a) Serial scan



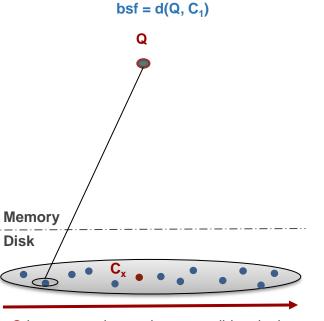
Q is compared to each raw candidate in the dataset before returning the answer C_x

(a) Serial scan

Answering a similarity search query using different access paths

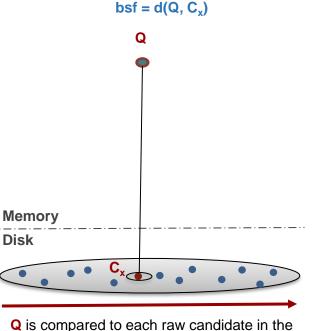
divo





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

(a) Serial scan



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

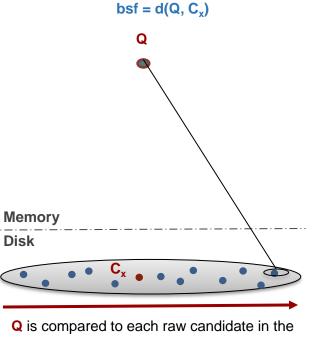
(a) Serial scan

Answering a similarity search query using different access paths

divo

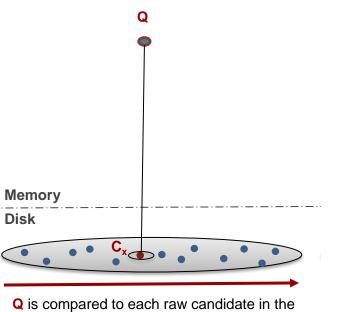
diNo 120

Similarity Matching Serial Scan



dataset before returning the answer C_x

(a) Serial scan

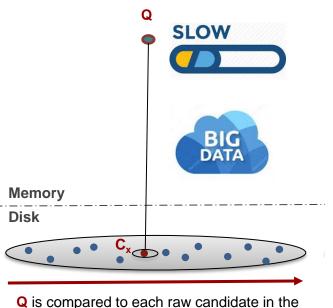


dataset before returning the answer C_x

(a) Serial scan

Answering a similarity search query using different access paths

divo

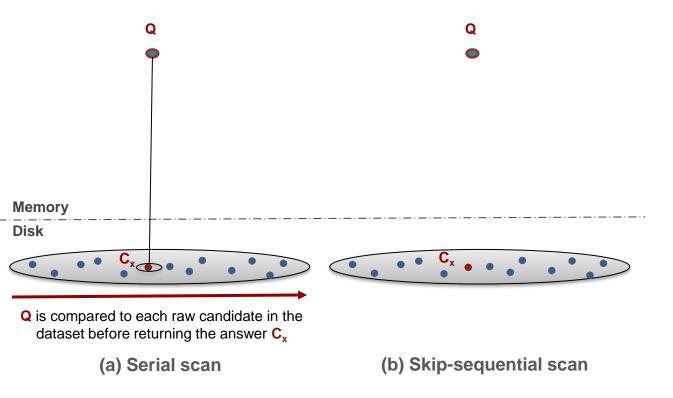


Q is compared to each raw candidate in the dataset before returning the answer C_x

(a) Serial scan

Answering a similarity search query using different access paths

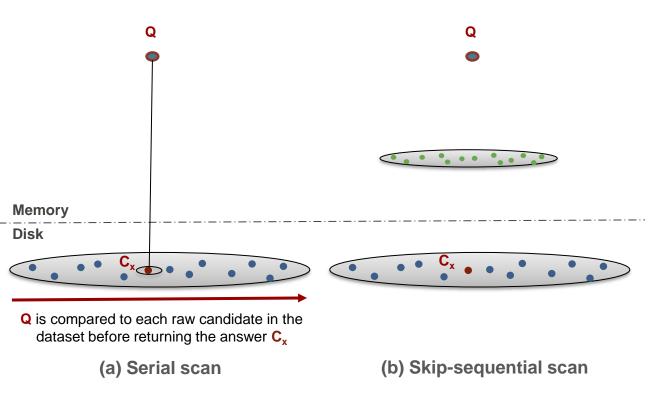
Indexes vs. Scans



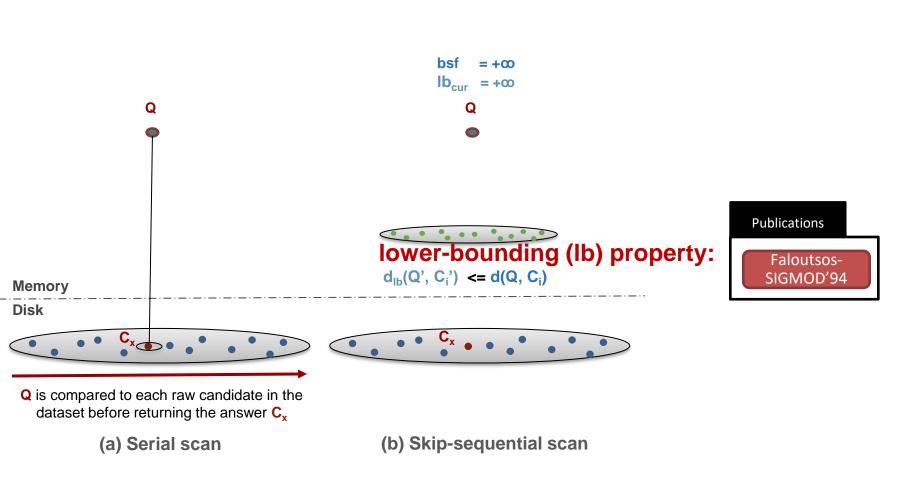
Answering a similarity search query using different access paths

diNb 123

Indexes vs. Scans



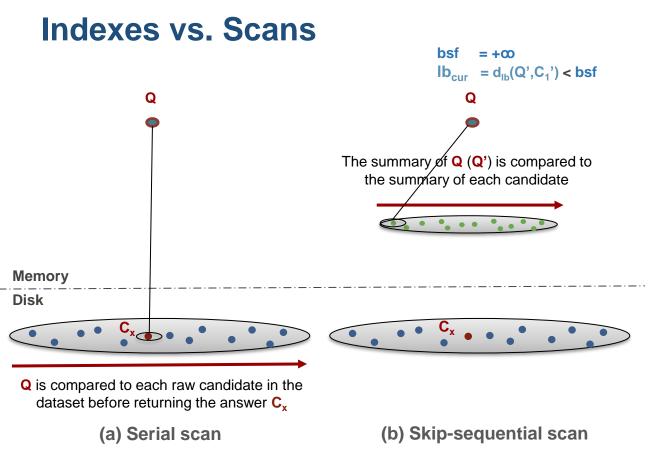
Answering a similarity search query using different access paths



diNo

Indexes vs. Scans $bsf = +\infty$ $Ib_{cur} = d_{Ib}(Q',C_1')$ Q Q The summary of Q (Q') is compared to the summary of each candidate Memory Disk C_x C, Q is compared to each raw candidate in the dataset before returning the answer C_x (a) Serial scan (b) Skip-sequential scan

Answering a similarity search query using different access paths

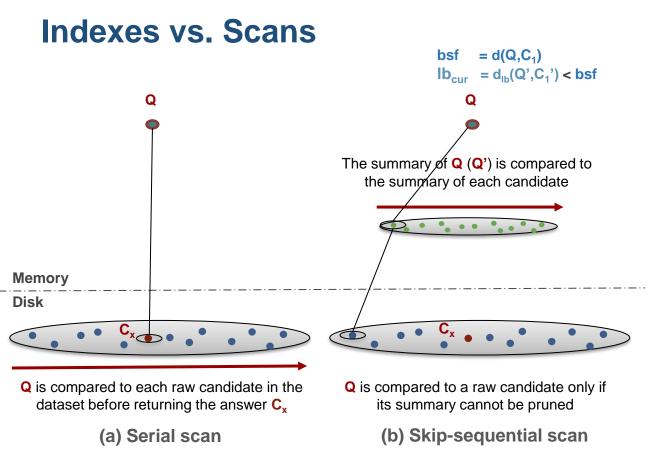


divo

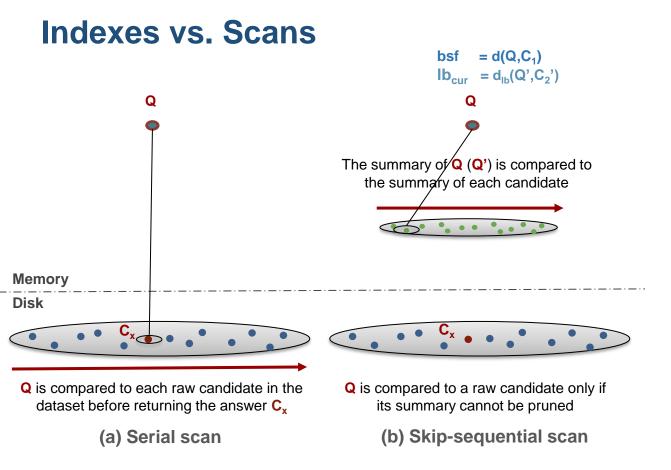
Indexes vs. Scans bsf = +00 $lb_{cur} = d_{lb}(Q', C_1') < bsf$ Q Q The summary $\oint \mathbf{Q} (\mathbf{Q}')$ is compared to the summary of each candidate • • • • • • Memory Disk C_x **Q** is compared to each raw candidate in the Q is compared to a raw candidate only if dataset before returning the answer C_x its summary cannot be pruned (a) Serial scan (b) Skip-sequential scan

Answering a similarity search query using different access paths

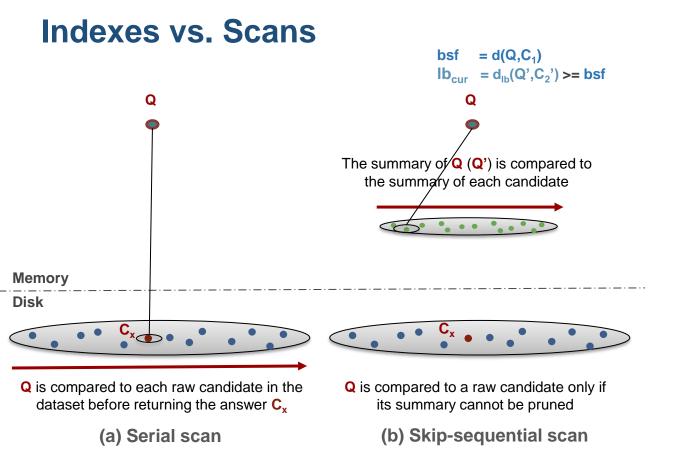
divo 128



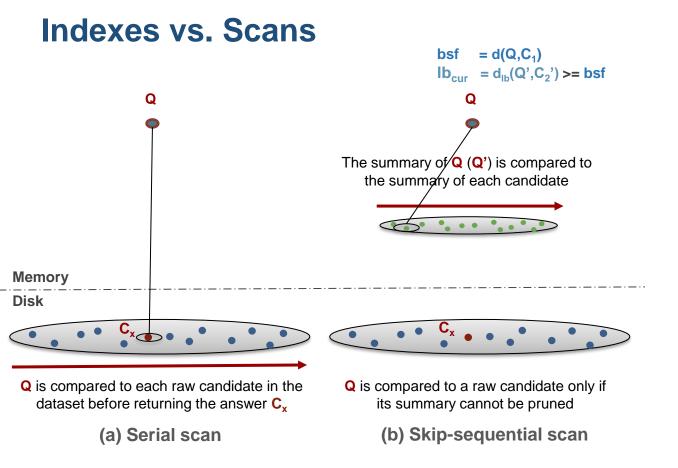
diNo



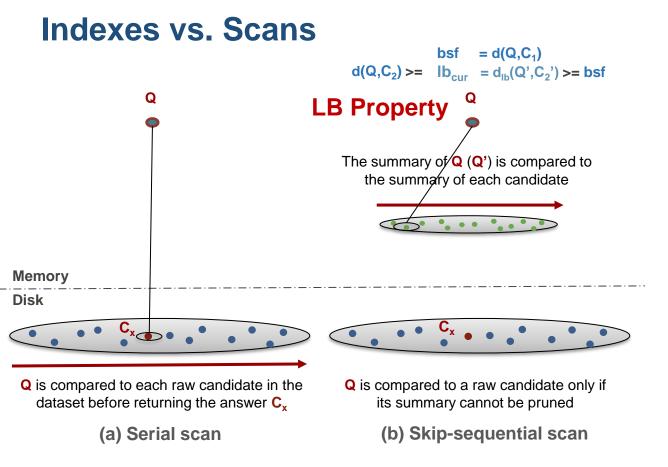
dino 130



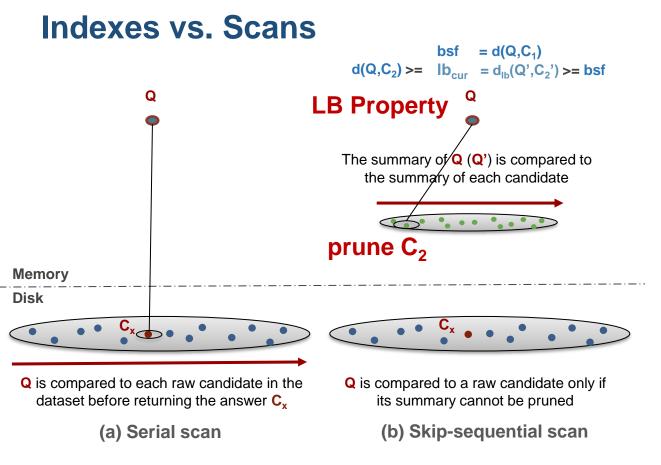
diN



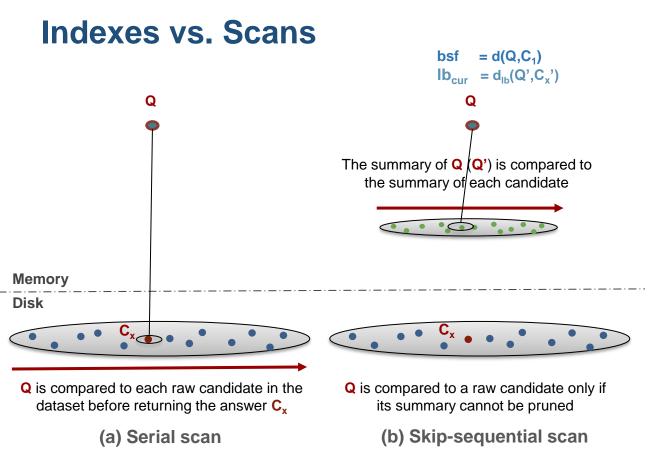
divo



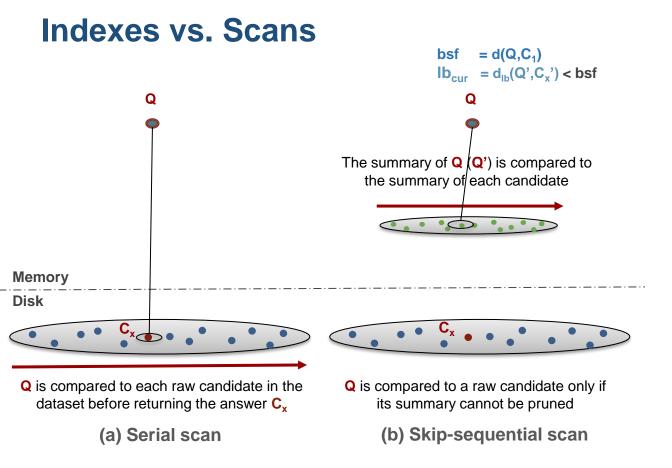
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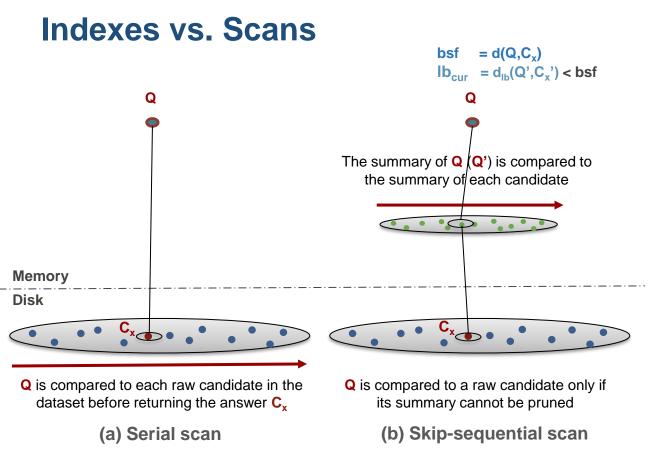


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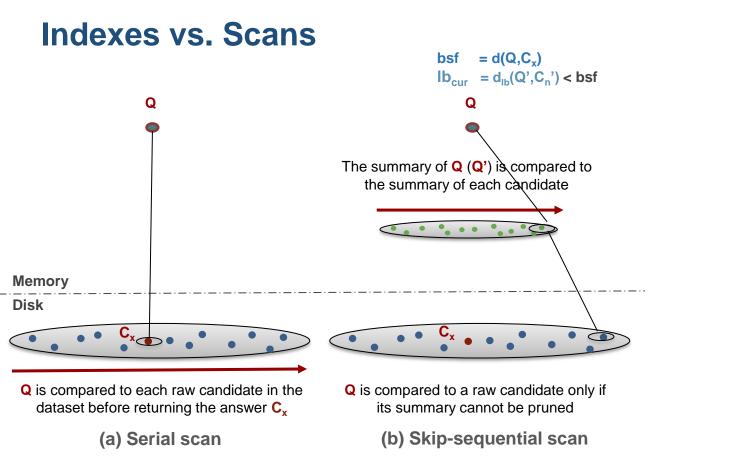


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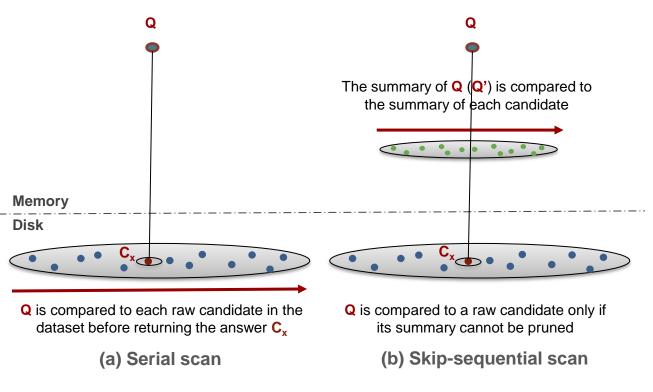


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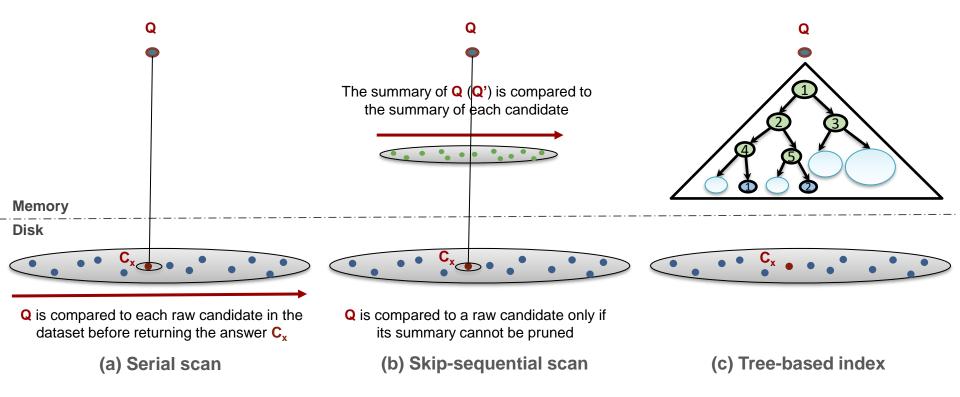


dino 138





Indexes vs. Scans



Answering a similarity search query using different access paths

Indexes vs. Scans bsf $=+\infty$ Q Q Q The summary of Q (Q') is compared to the summary of each candidate Memory Disk Cx C_x **Q** is compared to each raw candidate in the Q is compared to a raw candidate only if dataset before returning the answer C_x 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

diNo

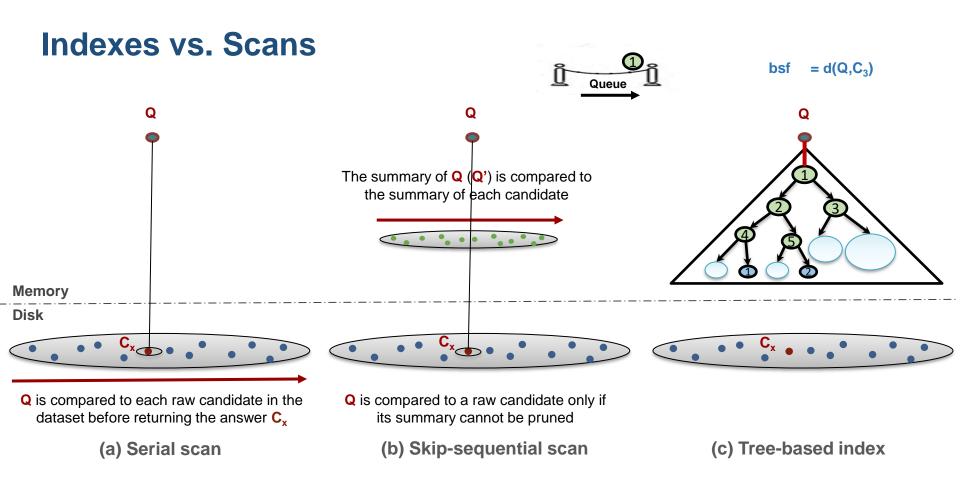
Indexes vs. Scans bsf $=+\infty$ Q Q Q The summary of Q (Q') is compared to the summary of each candidate Memory Disk C_x C_x C_x **Q** is compared to each raw candidate in the Q is compared to a raw candidate only if dataset before returning the answer C_x its summary cannot be pruned (a) Serial scan (b) Skip-sequential scan (c) Tree-based index

Answering a similarity search query using different access paths

Indexes vs. Scans bsf = $d(Q,C_3)$ Q Q Q The summary of Q (Q') is compared to the summary of each candidate Memory Disk C_x C_x **Q** is compared to each raw candidate in the Q is compared to a raw candidate only if dataset before returning the answer C_x 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

diNo 144

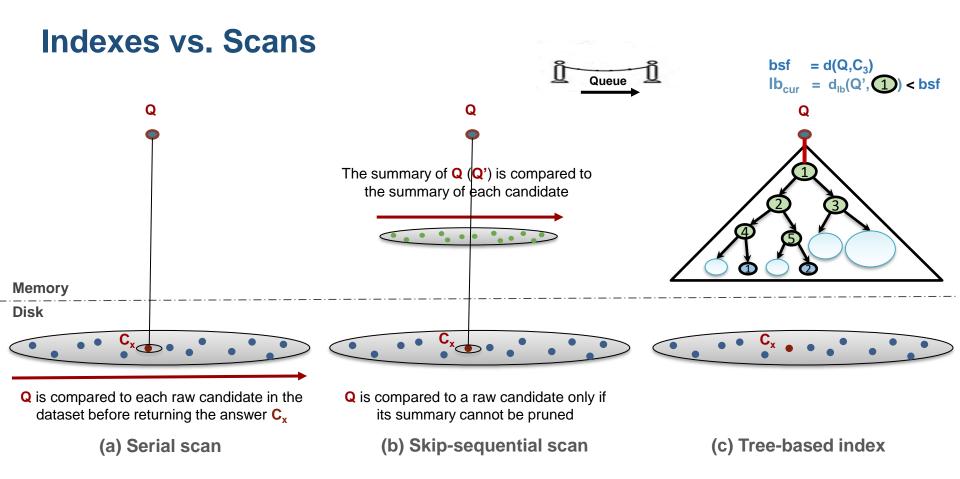


Indexes vs. Scans bsf $= d(Q,C_3)$ $lb_{cur} = d_{lb}(Q', 1)$ Queue Q Q Q The summary of Q (Q') is compared to the summary of each candidate Memory Disk Cx C_x **Q** is compared to each raw candidate in the Q is compared to a raw candidate only if dataset before returning the answer C_x its summary cannot be pruned (a) Serial scan (b) Skip-sequential scan (c) Tree-based index

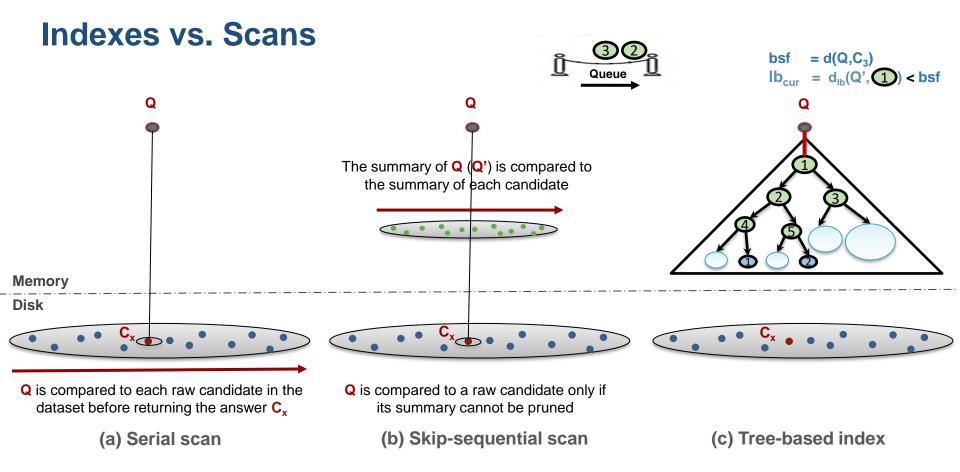
Answering a similarity search query using different access paths

dino 145

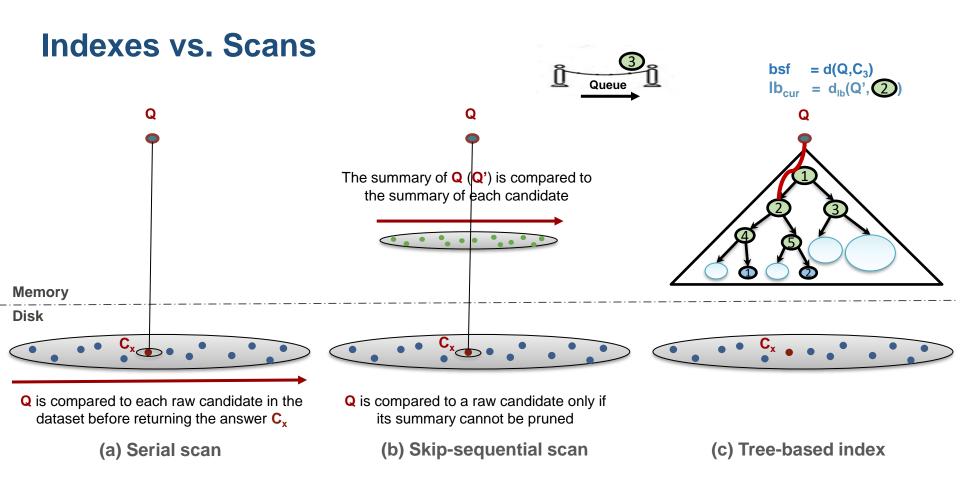
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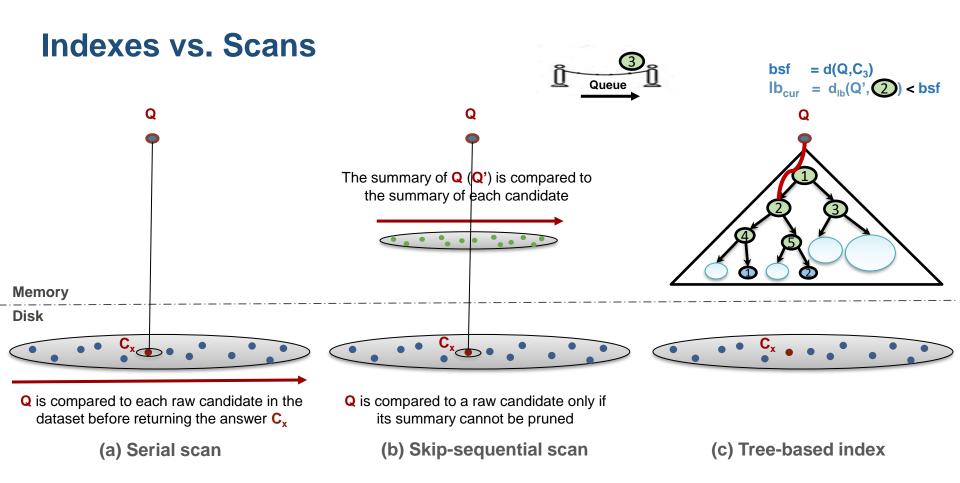
diNo 147



diNo 148



diN0 149

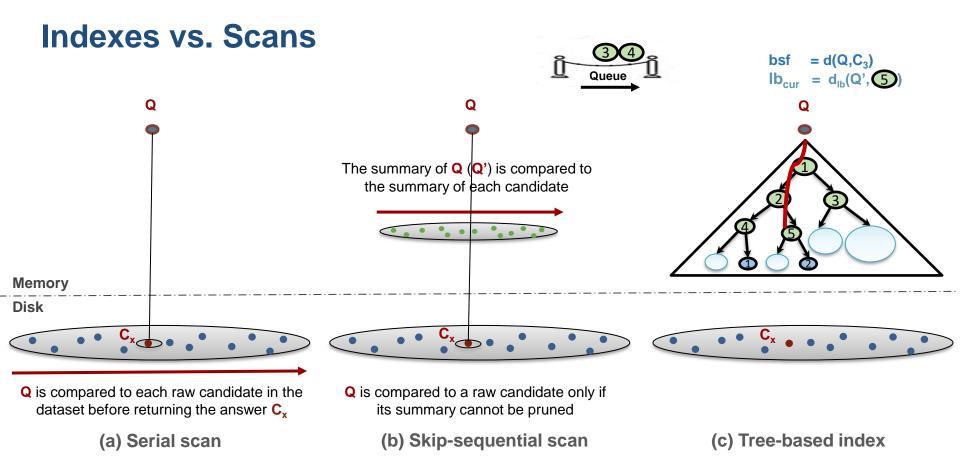


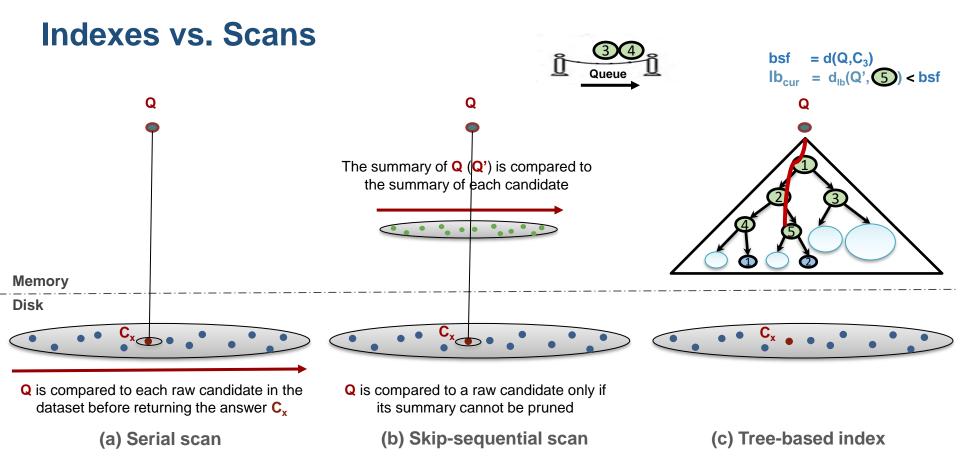
Indexes vs. Scans bsf $= d(Q,C_3)$ $Ib_{cur} = d_{Ib}(Q', 2) < bsf$ Q Q Q The summary of Q (Q') is compared to the summary of each candidate Memory Disk Cx C_x **Q** is compared to each raw candidate in the Q is compared to a raw candidate only if dataset before returning the answer C_x its summary cannot be pruned (a) Serial scan (b) Skip-sequential scan (c) Tree-based index

Answering a similarity search query using different access paths

dino 150

 diN_{0} 151





Answering a similarity search query using different access paths

Indexes vs. Scans bsf $= d(Q,C_3)$ $lb_{cur} = d_{lb}(Q', 5) < bsf$ Q Q Q The summary of Q (Q') is compared to the summary of each candidate Memory Disk Cx C_x **Q** is compared to each raw candidate in the Q is compared to a raw candidate only if dataset before returning the answer C_x 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

diNo

Indexes vs. Scans bsf $= d(Q,C_3)$ $Ib_{cur} = d_{Ib}(Q', Q)$ Q Q Q The summary of Q (Q') is compared to the summary of each candidate Memory Disk C_x C_x **Q** is compared to each raw candidate in the Q is compared to a raw candidate only if dataset before returning the answer C_x its summary cannot be pruned (a) Serial scan (b) Skip-sequential scan (c) Tree-based index

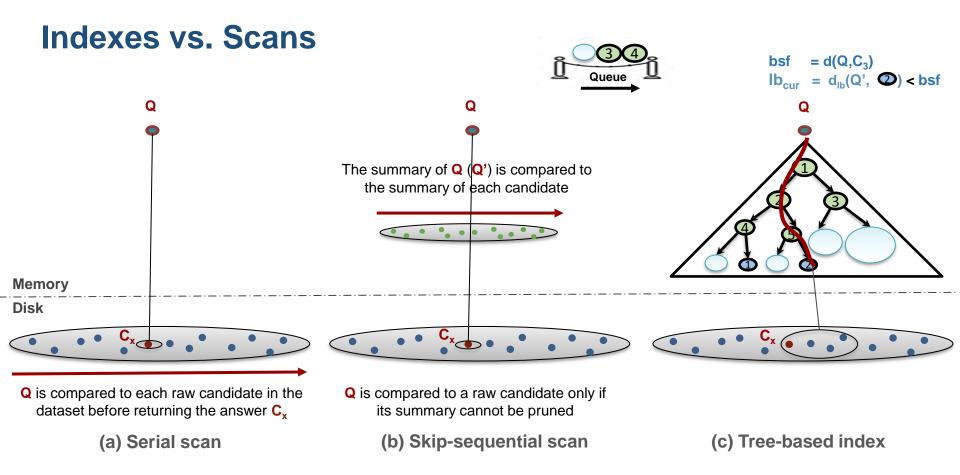
Answering a similarity search query using different access paths

diNo

Indexes vs. Scans bsf $= d(Q,C_3)$ $Ib_{cur} = d_{Ib}(Q', \mathbf{O}) < bsf$ Q Q Q The summary of Q (Q') is compared to the summary of each candidate Memory Disk C_x C_x **Q** is compared to each raw candidate in the Q is compared to a raw candidate only if dataset before returning the answer C_x 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

diNo

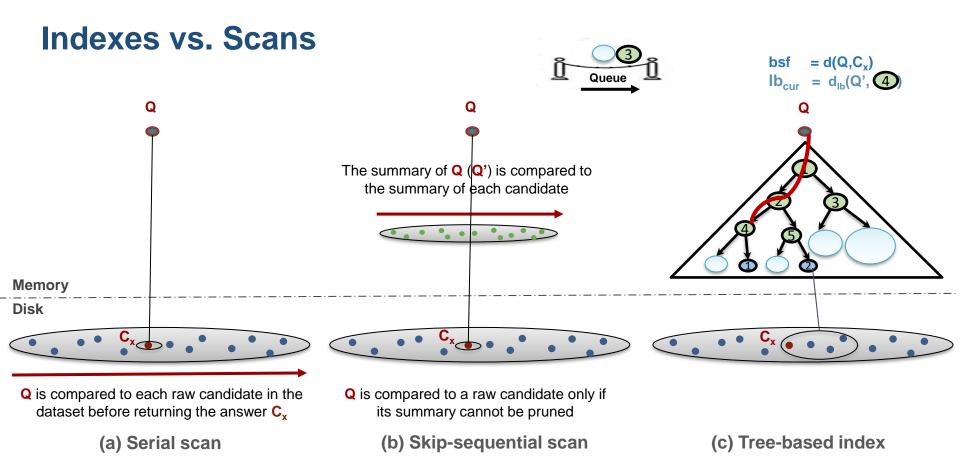


Answering a similarity search query using different access paths

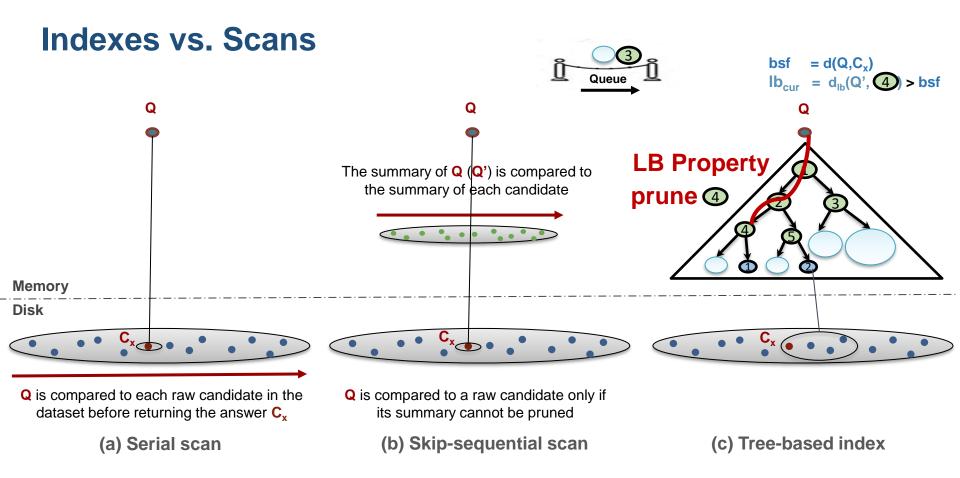
Indexes vs. Scans bsf $= d(Q, C_x)$ $Ib_{cur} = d_{Ib}(Q', \mathbf{O}) < bsf$ Q Q Q The summary of Q (Q') is compared to the summary of each candidate Memory Disk C_x C_x **Q** is compared to each raw candidate in the Q is compared to a raw candidate only if dataset before returning the answer C_x its summary cannot be pruned (a) Serial scan (b) Skip-sequential scan (c) Tree-based index

Answering a similarity search query using different access paths

divo

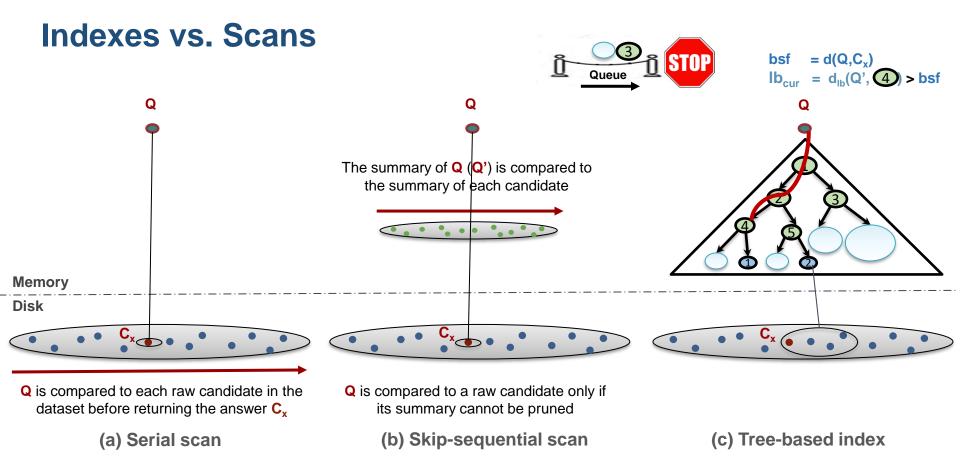


Answering a similarity search query using different access paths



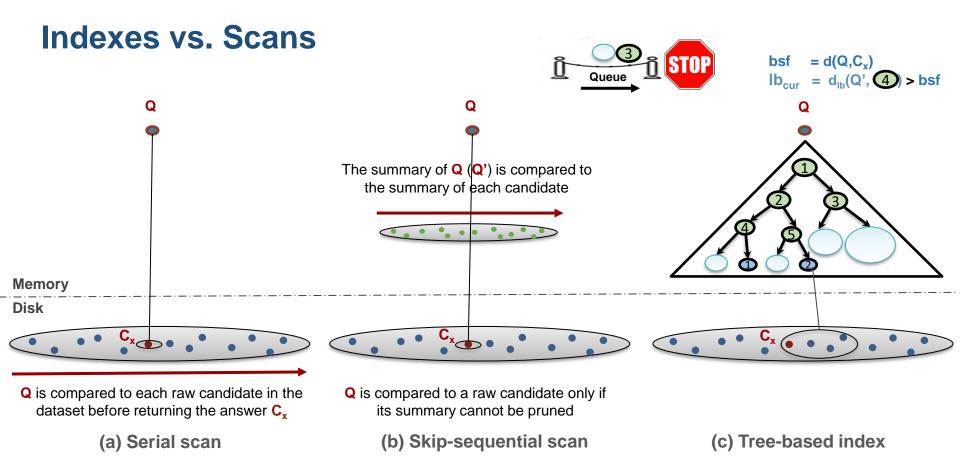
Answering a similarity search query using different access paths

divip 160



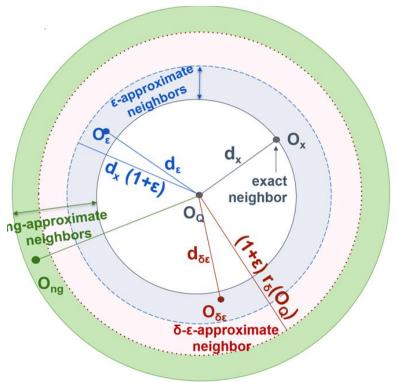
Answering a similarity search query using different access paths

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Answering a similarity search query using different access paths

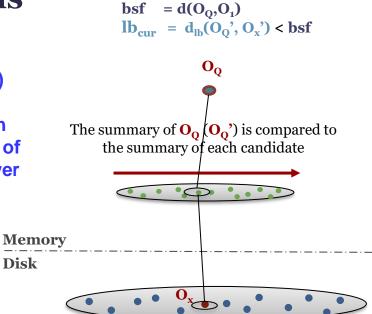
Similarity Search Data Series Extensions



Extensions: Skip-Sequential Scans

 $d_{\epsilon} \ll d_{\chi} (1+\epsilon)$

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



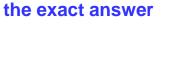
dino 163

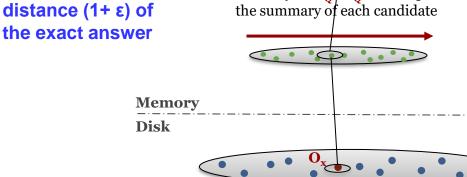
Extensions: Skip-Sequential Scans $bsf = d(O_Q, O_1)$ $\frac{lb_{cur}}{lb_{cur}} = \frac{d_{lb}(O_Q, O_x) < bsf}{d_{lb}(O_Q, O_x) < (1+\epsilon) bsf}$ $d_{\epsilon} \ll d_{x}(1+\epsilon)$ E-approximate neighbors **Result is within** The summary of O_0 (O_0 ') is compared to distance (1+ ε) of the summary of each candidate O, **O**_x the exact answer d_x $d_x(1+\varepsilon)$ d exact neighbor ng-approximate Od Memory neighbors Disk $d_{\delta\epsilon}$ O_x Ong Οδε

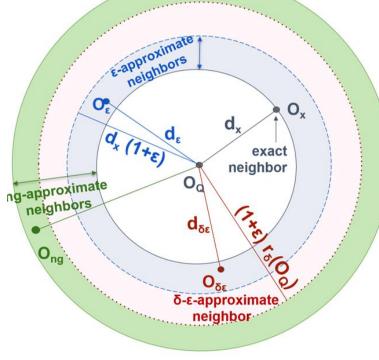
δ-ε-approximate neighbor **dino** 164

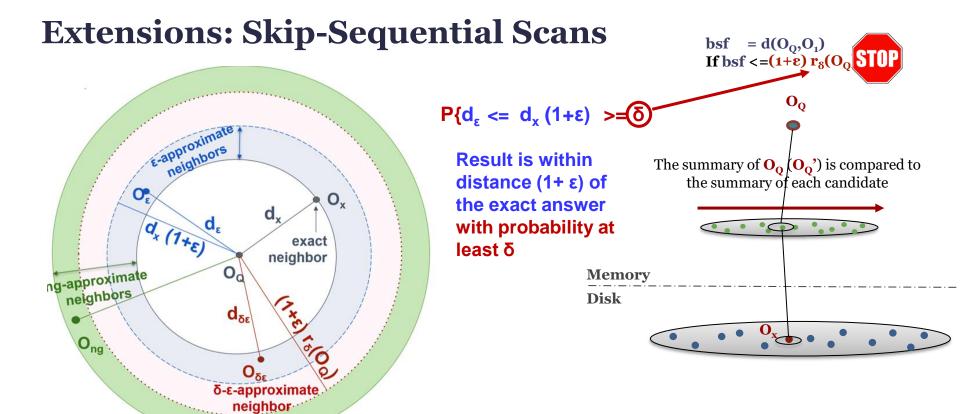
Extensions: Skip-Sequential Scans $bsf = d(O_0, O_1)$ 00 $d_{\epsilon} \ll d_{x} (1+\epsilon)$ **Result is within** The summary of O_0 (O_0 ') is compared to

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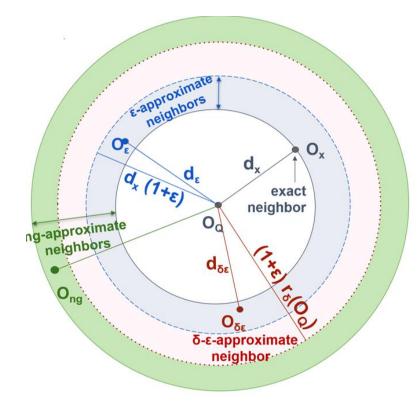






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Extensions: Indexes

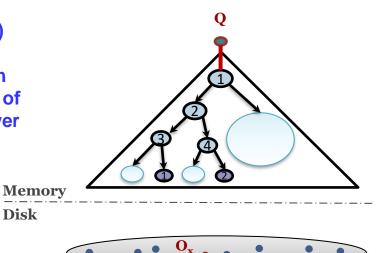


 $d_{\epsilon} \ll d_{x} (1+\epsilon)$

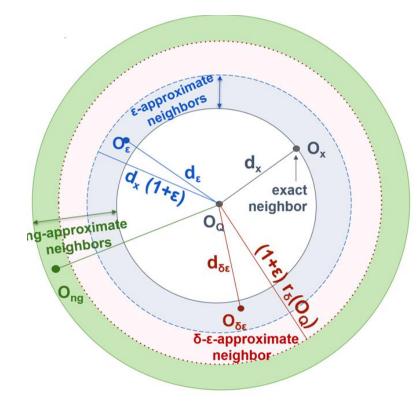
Result is within distance $(1 + \varepsilon)$ of the exact answer

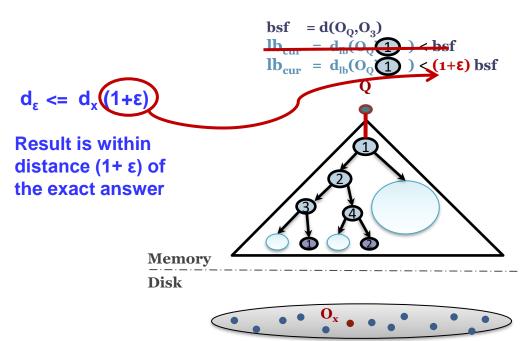
Disk

 $bsf = d(O_Q, O_3)$ $lb_{cur} = d_{lb}(O_Q)$) < bsf

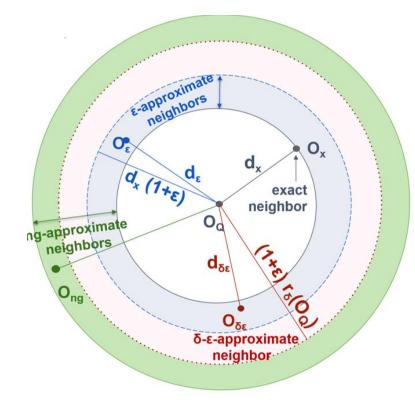


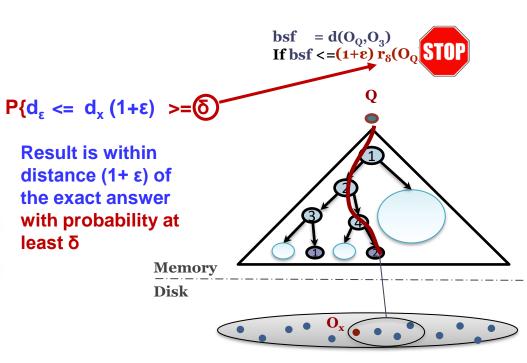
Extensions: Indexes

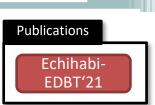




Extensions: Indexes



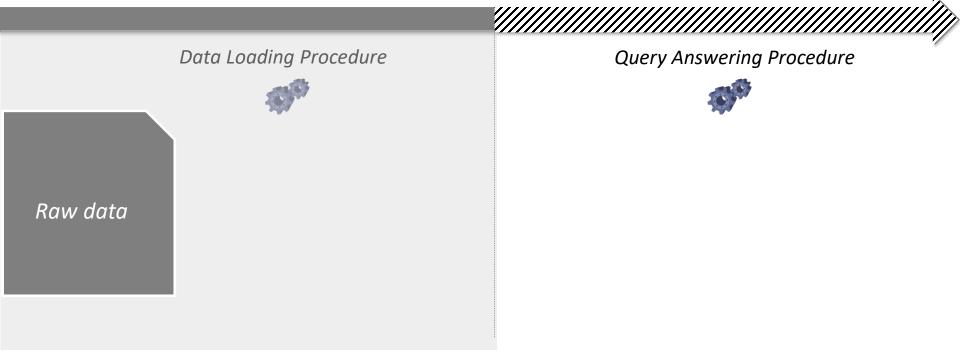


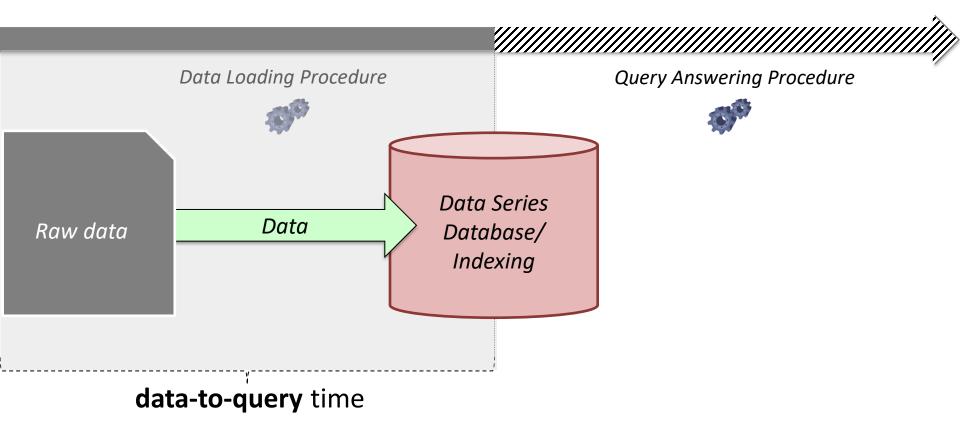


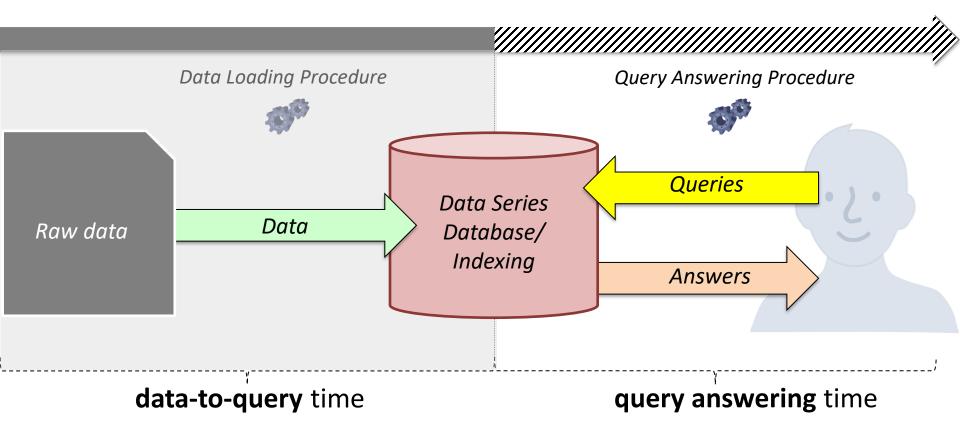
Data Series Similarity Search State-of-the-Art Methods

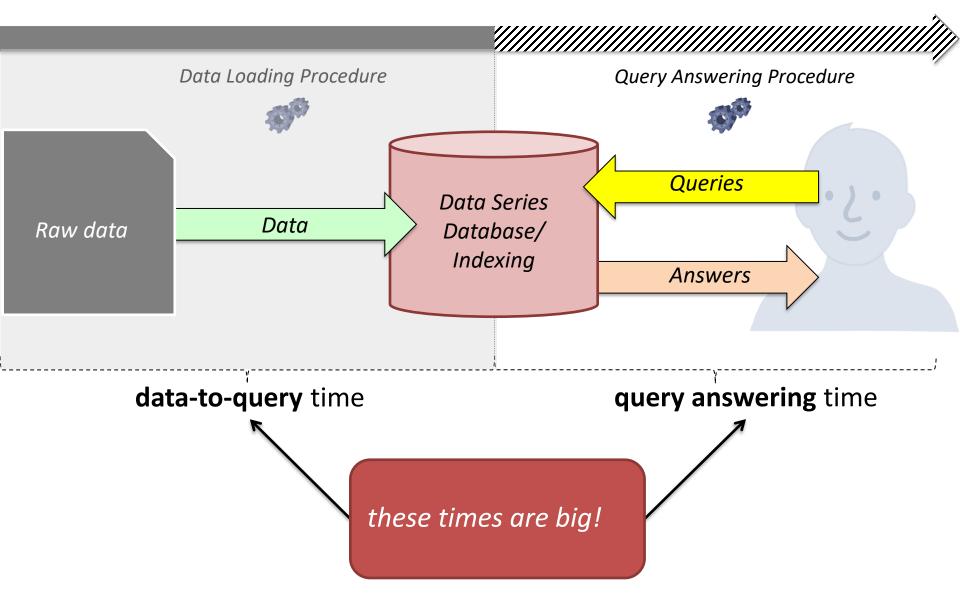
for a more complete and detailed presentation, see tutorial:

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

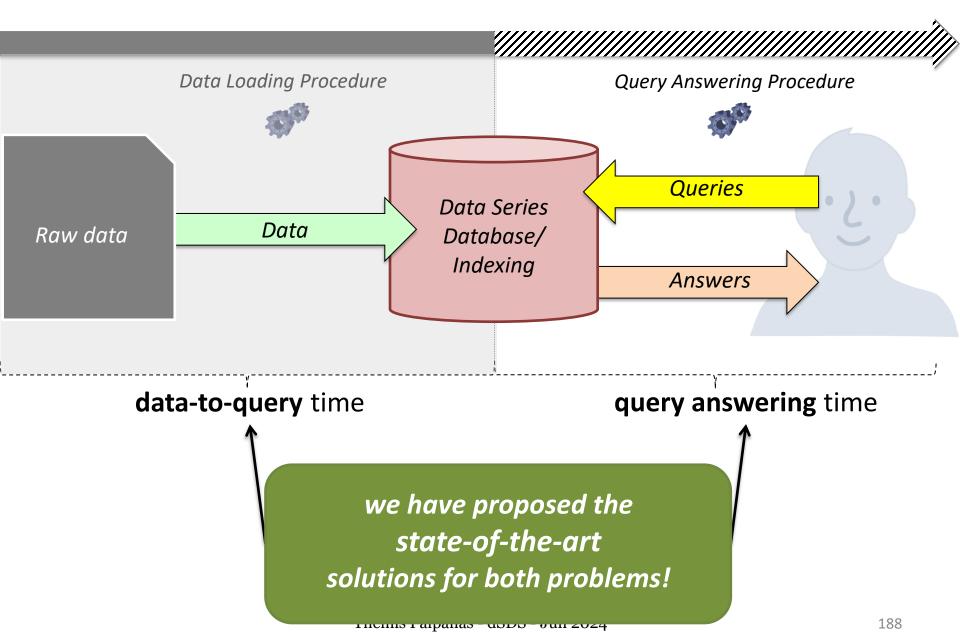




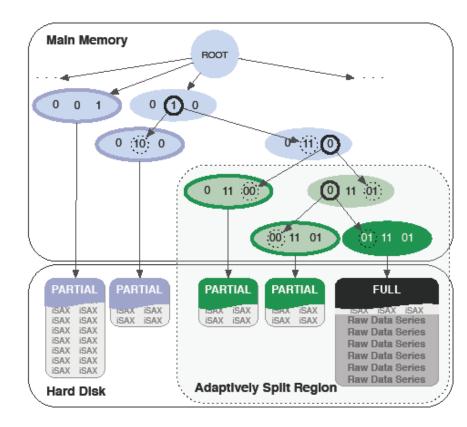


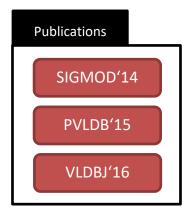


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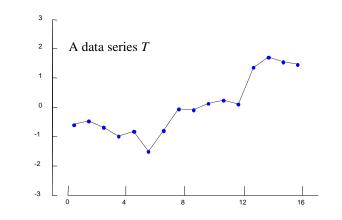
The ADS+ Solution





SAX Representation

- Symbolic Aggregate approXimation (SAX)
 - (1) Represent data series *T* of length *n* with *w* segments using Piecewise Aggregate Approximation (PAA)



divo

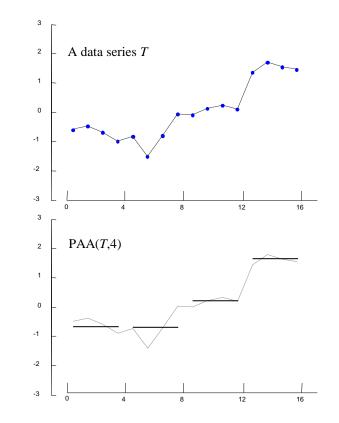
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• PAA(
$$T, w$$
) = $\overline{T} = \overline{t}_1, \dots, \overline{t}_w$
where $\overline{t}_i = \frac{w}{T} \sum_{i=1}^{\frac{n}{w}} T_i$

There
$$t_i = \frac{w}{n} \sum_{j=\frac{n}{w}(i-1)+1} I_j$$



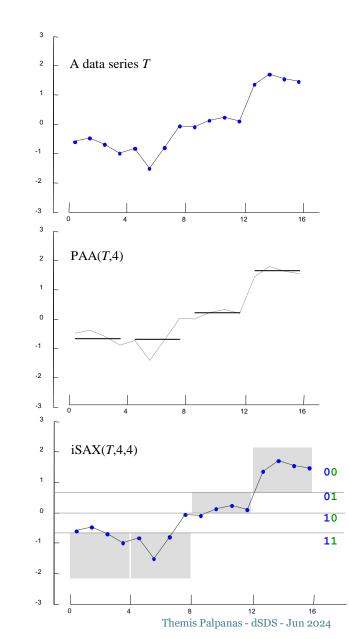
diN0 192

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- (2) Discretize into a vector of symbols
 - Breakpoints map to small alphabet *a* of symbols

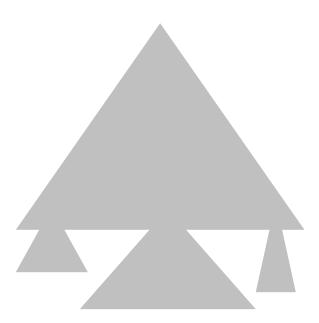


iSAX Representation

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

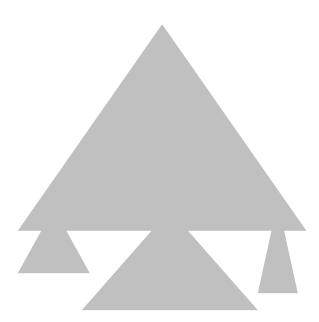
$$= \{ 6, 6, 3, 0 \} = \{ 110, 110, 0111, 000 \}$$
$$= \{ 3, 3, 1, 0 \} = \{ 11, 11, 011, 00 \}$$
$$= \{ 1, 1, 0, 0 \} = \{ 1, 1, 0, 0 \}$$

- 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 $\leq th$



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e.g., th=4, w=4, b=1
$$\begin{bmatrix}
1 & 1 & 1 & 0 \\
1 & 1 & 1 & 0 \\
1 & 1 & 1 & 0 \\
1 & 1 & 1 & 0
\end{bmatrix}$$



dino 196

- non-balanced tree-based index with non-overlapping regions, and controlled fan-out rate
 - base cardinality **b** (optional), segments **w**, threshold **th**
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Insert:
$$\longrightarrow \begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$

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

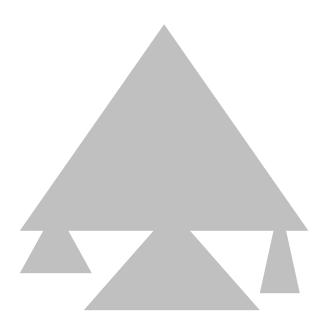
 $d \sim 197$

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$$1 \ 1 \ 1 \ 0$$

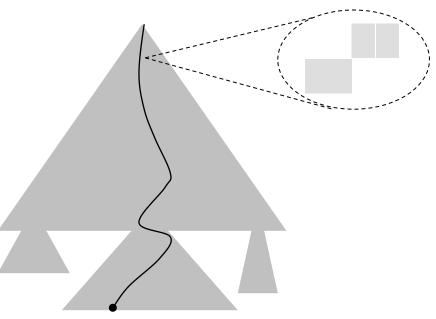
 $1 \ 1 \ 1 \ 0$
 $1 \ 1 \ 1 \ 0$
 $1 \ 1 \ 1 \ 0$
 $1 \ 1 \ 1 \ 0$
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 $1 \ 1 \ 1 \ 0$



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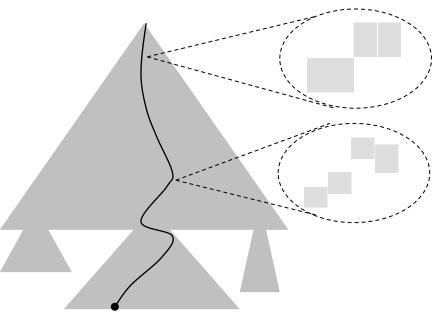
divo 198

- non-balanced tree-based index with non-overlapping regions, and controlled fan-out rate
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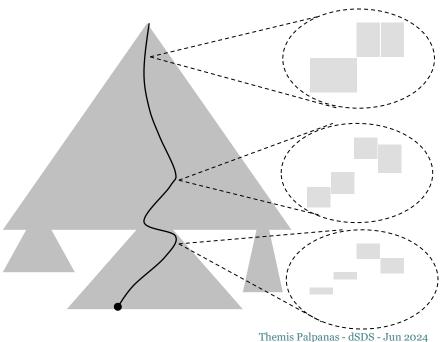


diNb 199

- non-balanced tree-based index with non-overlapping regions, and controlled fan-out rate
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iSAX Index

 non-balanced tree-based index with non-overlapping regions, and controlled fan-out rate

dino 202

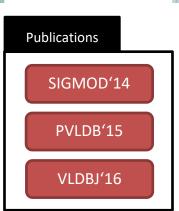
Themis Palpanas - dSDS - Jun 2024

- 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

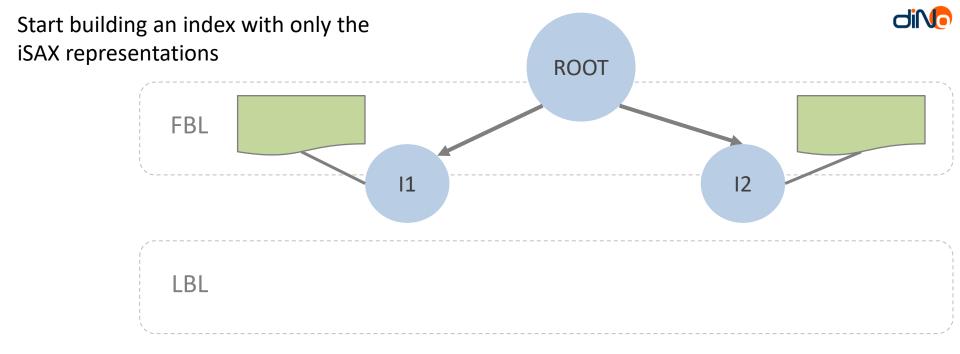
Adaptive Data Series Index: ADS+

- novel paradigm for building a data series index
 - do not build entire index and then answer queries
 - start answering queries by building the part of the index needed by those queries
- still guarantee correct answers

Adaptive Data Series Index: ADS+

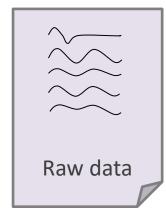


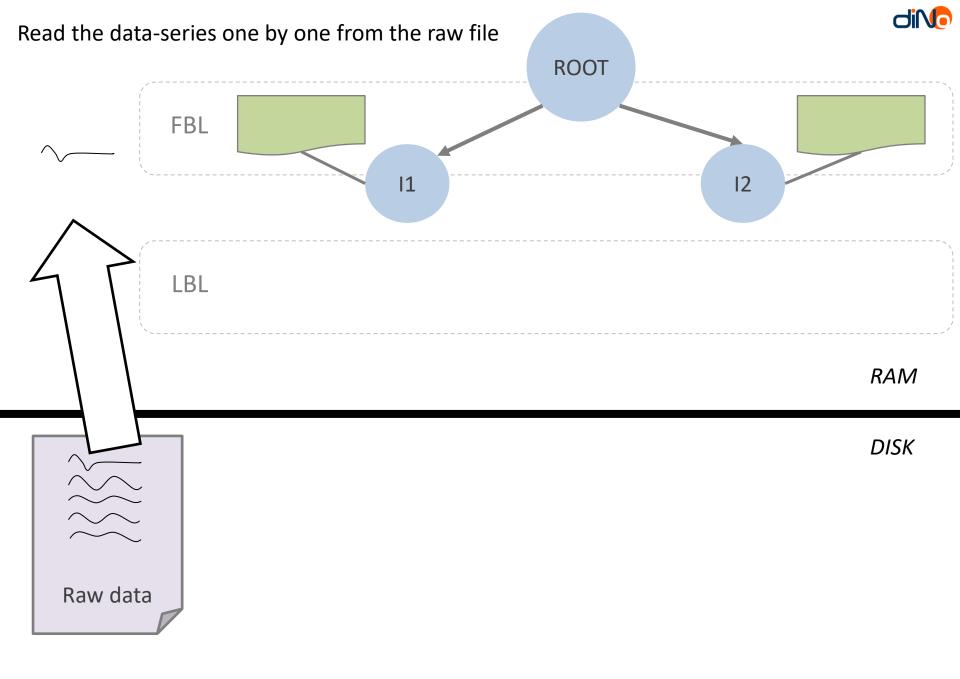
- intuition for proposed solution
 - build the iSAX index using the iSAX representations
 just like iSAX2+
 - but start with a large leaf size
 - minimize initial cost
 - postpone leaf materialization to query time
 - only materialize (at query time) leaves needed by queries
 - parts that are queried more are refined more
 - use smaller leaf sizes (reduced leaf materialization and query answering costs)

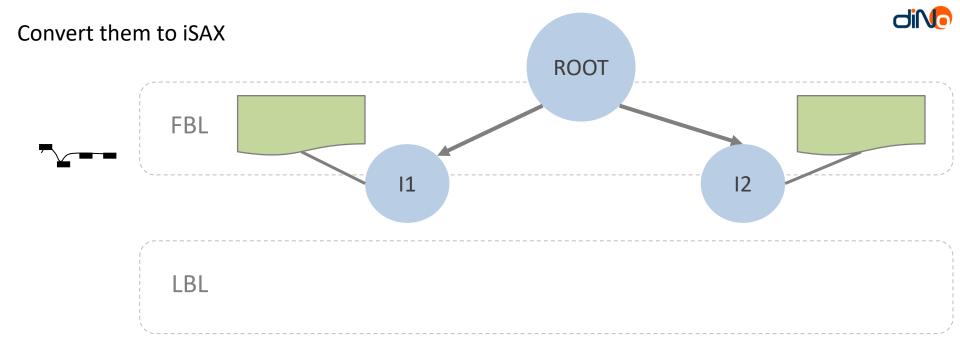


RAM

DISK

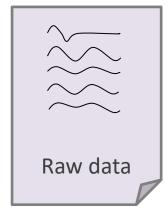


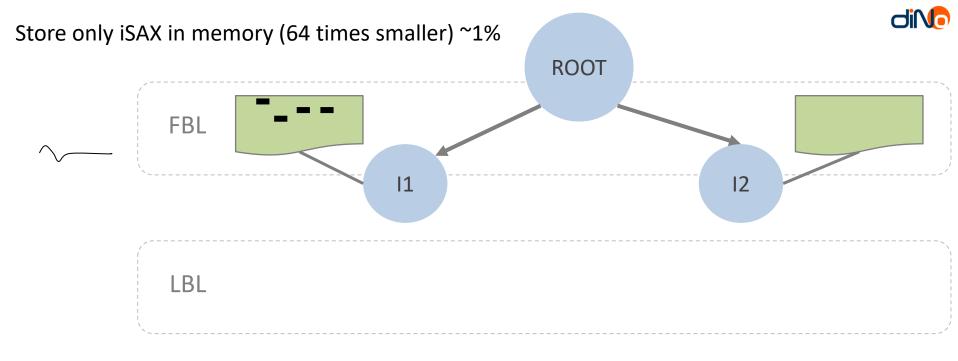




RAM

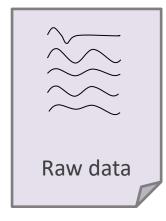
DISK

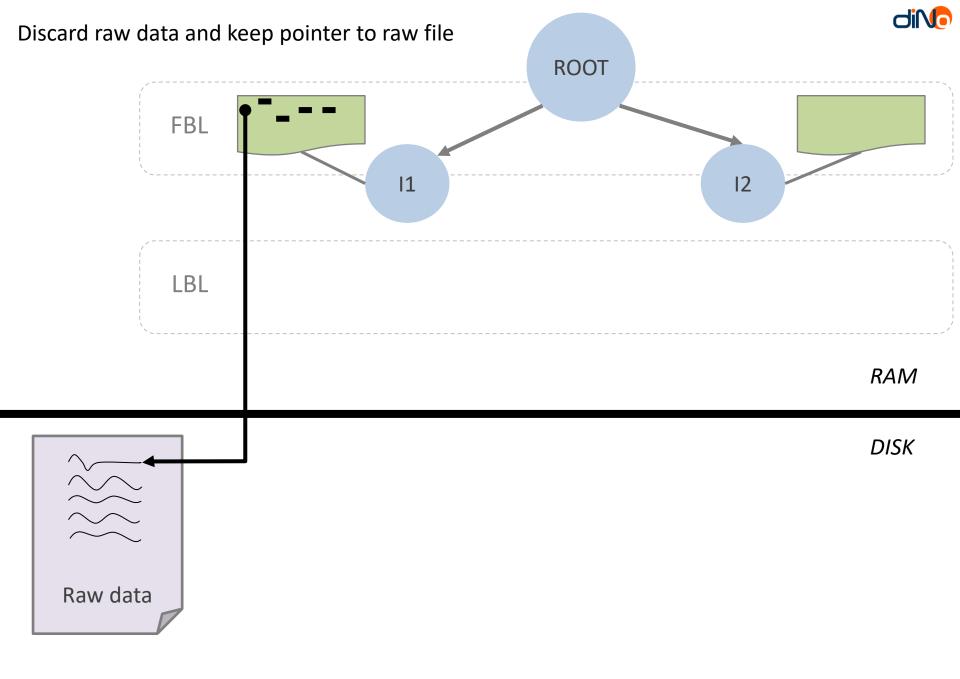


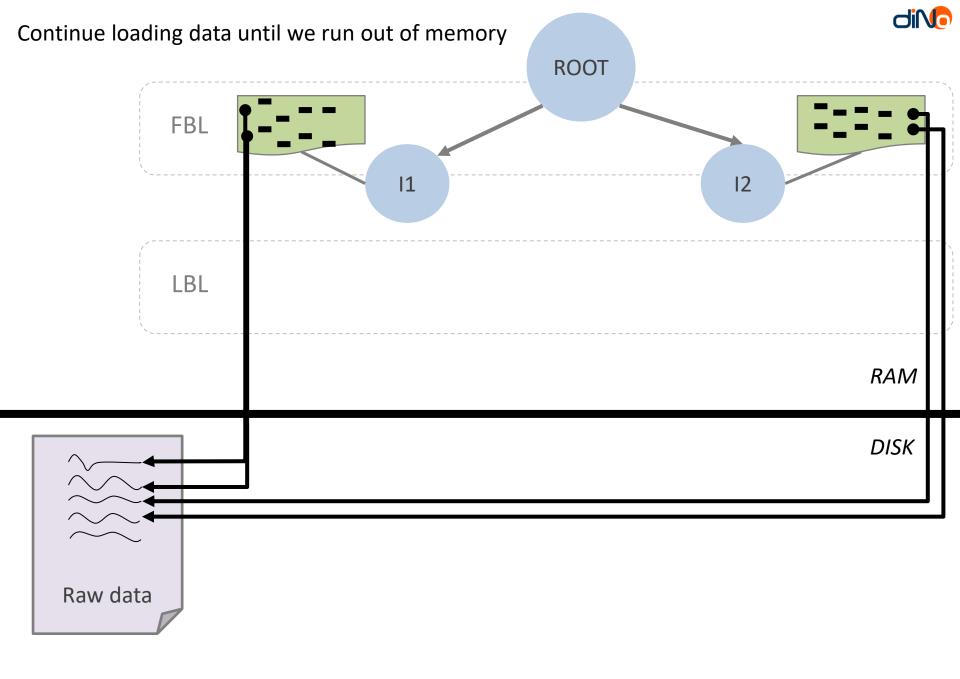


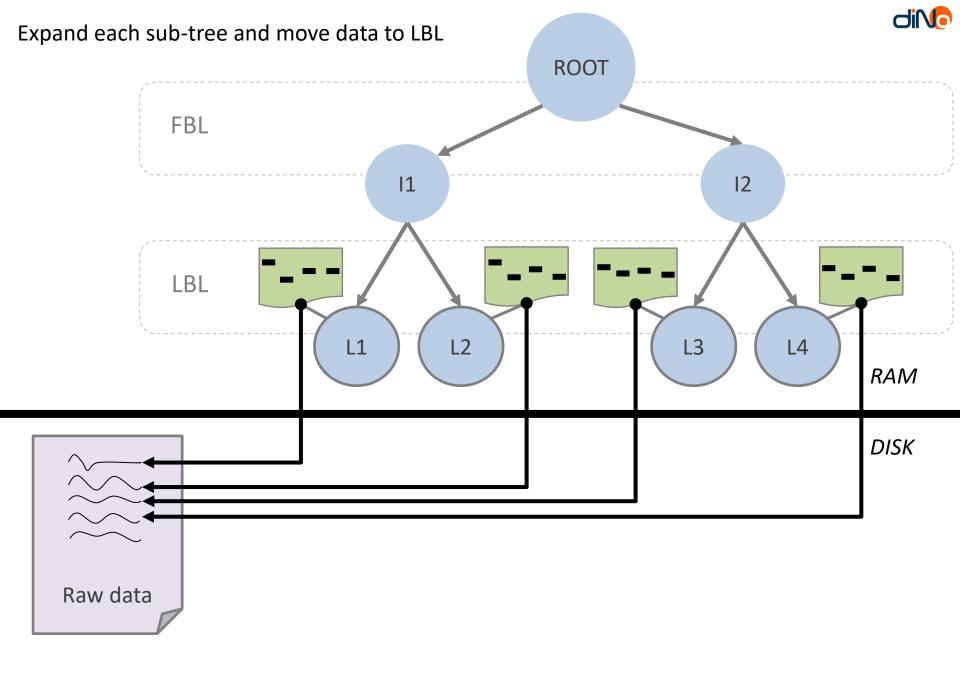
RAM

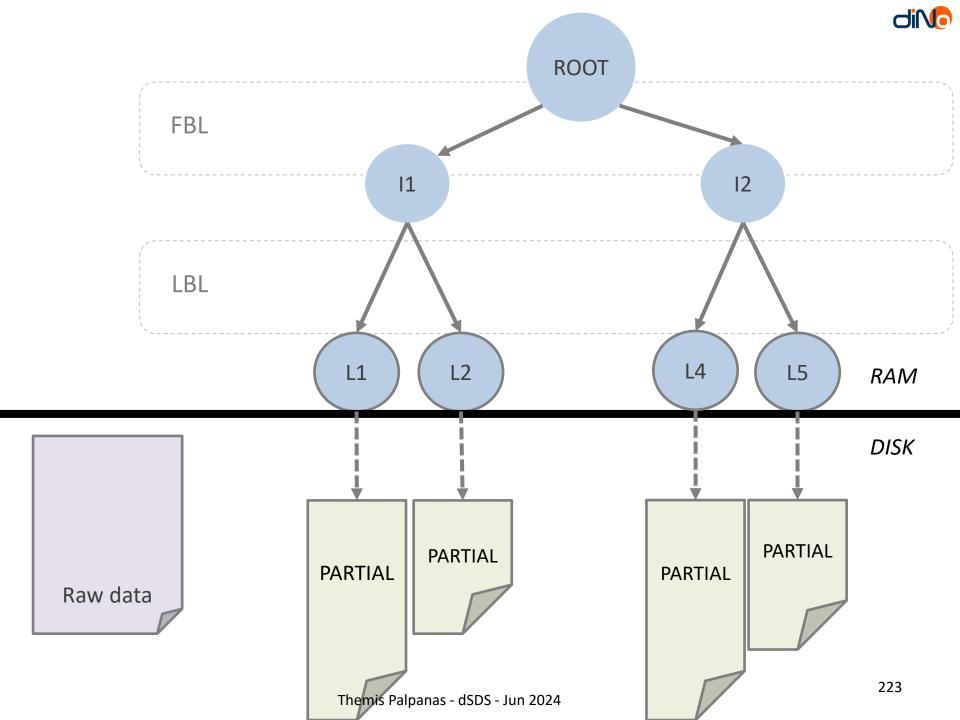
DISK

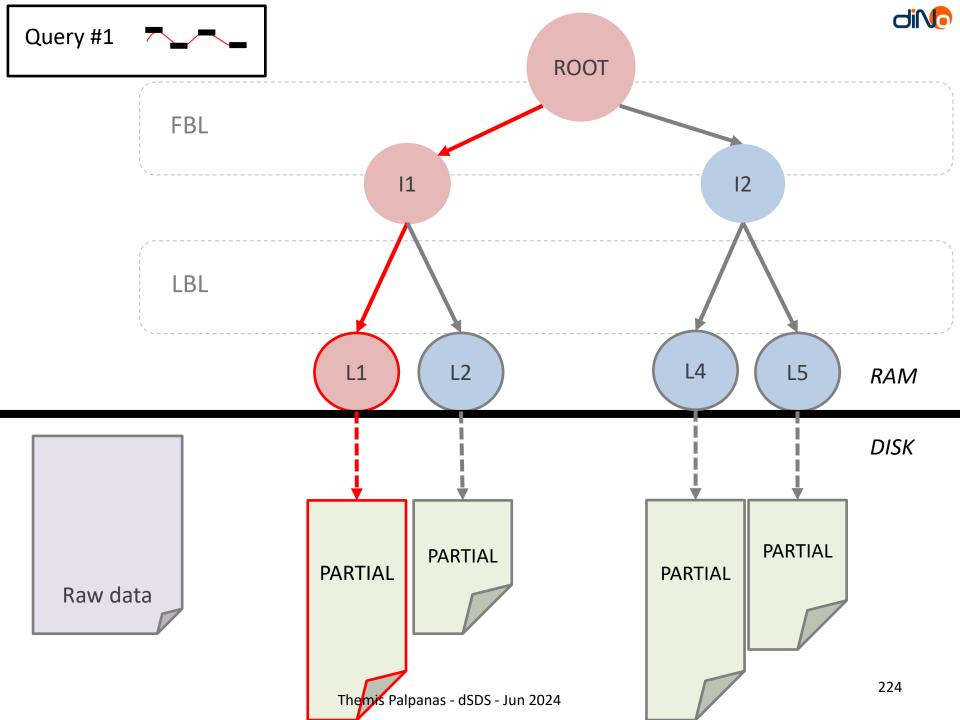


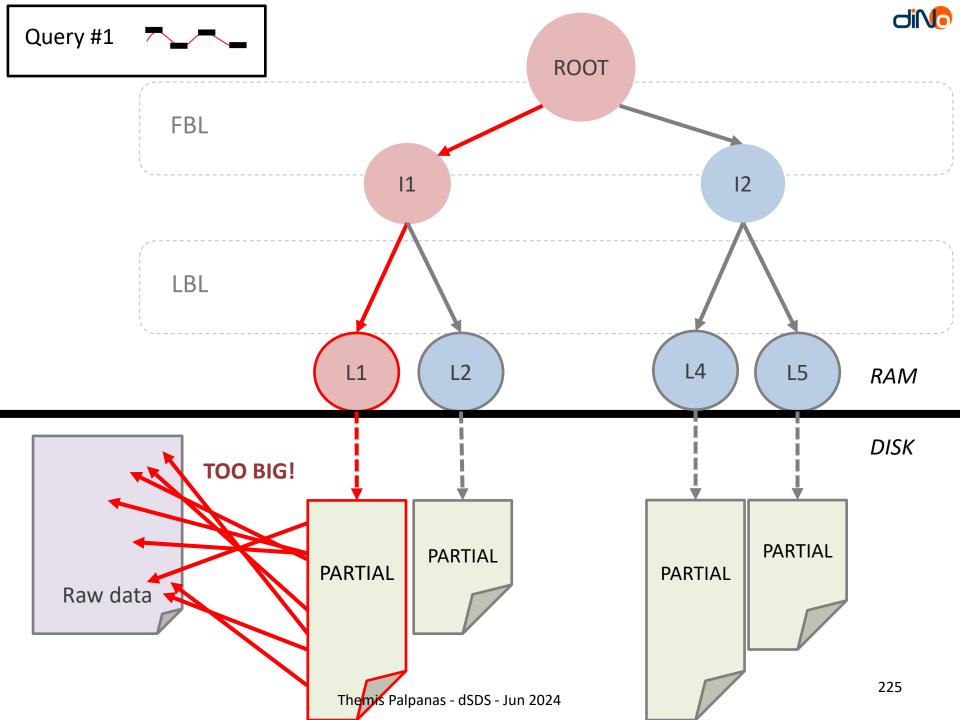


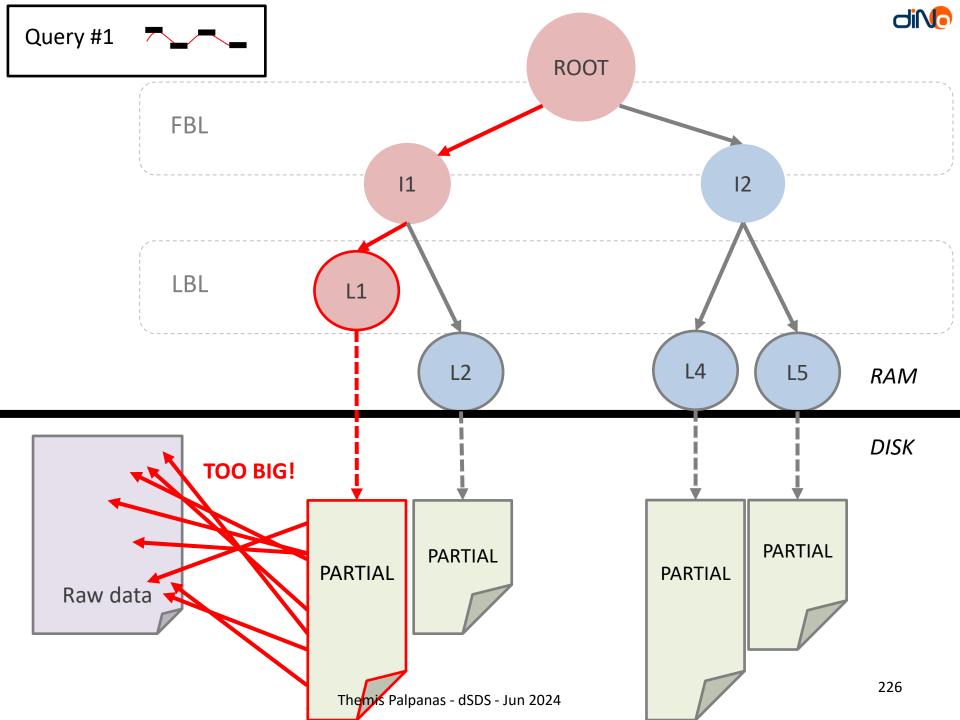


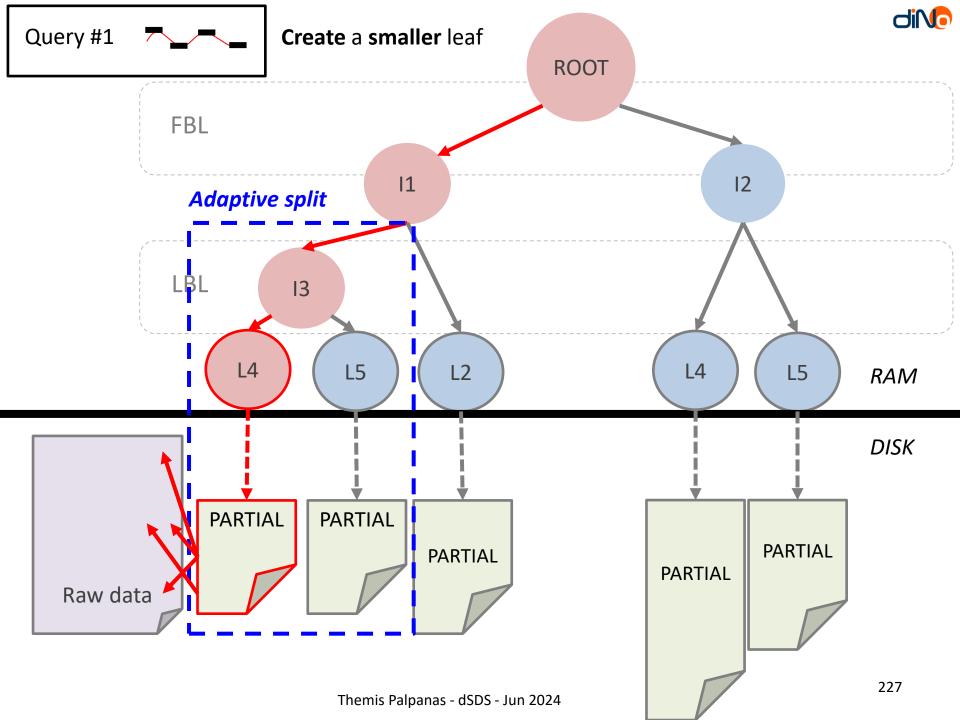


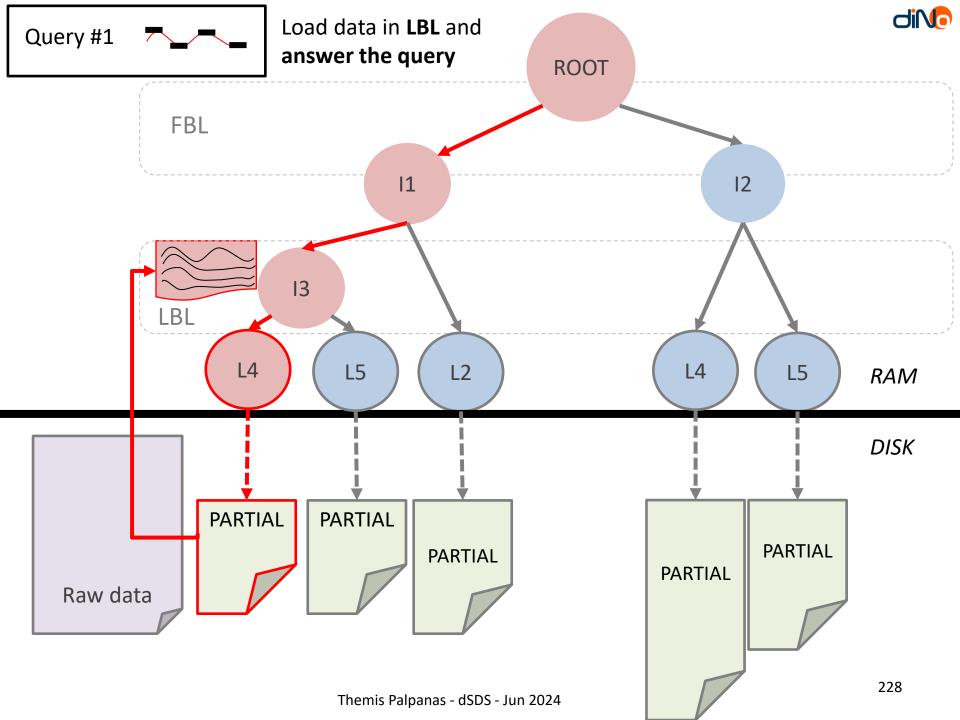


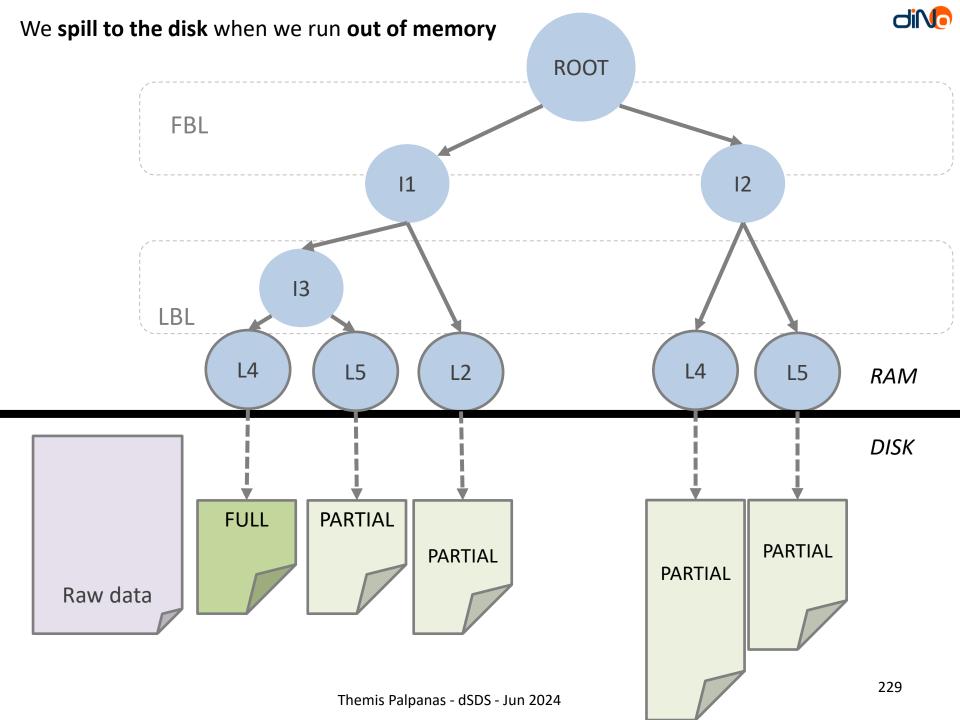












Parallelization/Distribution?

Parallelization/Distribution?

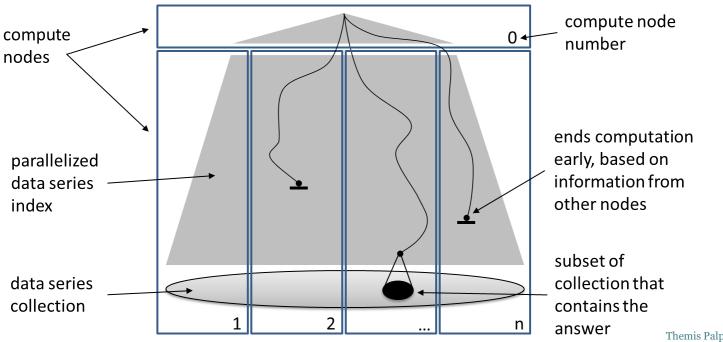
- discussion so far assumed serial execution in a single core
 - focus on efficient resource utilization
 - squeeze the most out of a single core
 - produce scalable solutions at lowest possible cost
 - also suitable for analysts with no access to/expertise for clusters

- take advantage of modern hardware!
 - Single Instruction Multiple Data (SIMD)
 - natural for data series operations
 - multi-tier CPU caches
 - design data structures aligned to cache lines
 - multi-core and multi-socket architectures
 - use parallelism inside each computation server
 - Graphics Processing Units (GPUs)
 - propose massively parallel techniques for GPUs
 - new storage solutions: SSDs, NVRAM
 - develop algorithms that take these new characteristics/tradeoffs into account
 - compute clusters
 - distribute operation over many machines

Publications

HPCS'17

- further scale-up and scale-out possible!
 - techniques inherently parallelizable
 - across cores, across machines



diNo 246

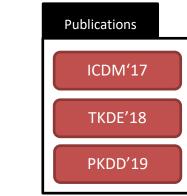
HPCS'17

Publications

• DPiSAX: current solution for distributed processing (Spark)

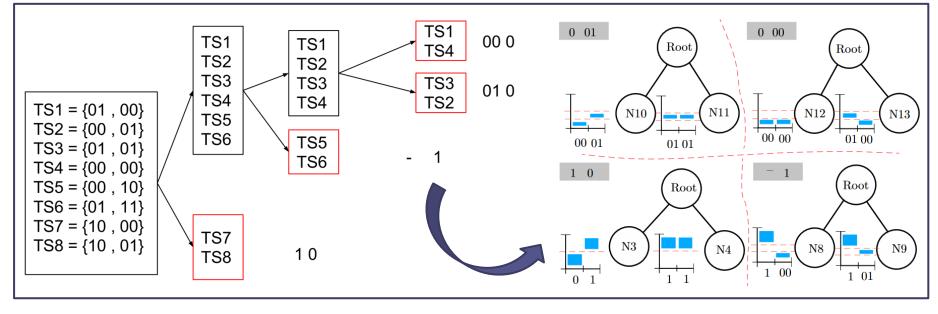
balances work of different worker nodes





• DPiSAX: current solution for distributed processing (Spark)

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Publications ICDM'17 TKDE'18 PKDD'19

PKDD'19

- DPiSAX: current solution for distributed processing (Spark)
 belances work of different worker nodes
 - balances work of different worker nodes
 - performs 2 orders of magnitude faster than centralized solution

diN0 250

Publications

ICDM'17

TKDE'18

DPiSAX: current solution for distributed processing (Sparl

- balances work of different worker nodes
- performs 2 orders of magnitude faster than centralized solution
- ParIS: current single-node parallel solution
 - masks out the CPU cost

diNo 251

ICDM'17

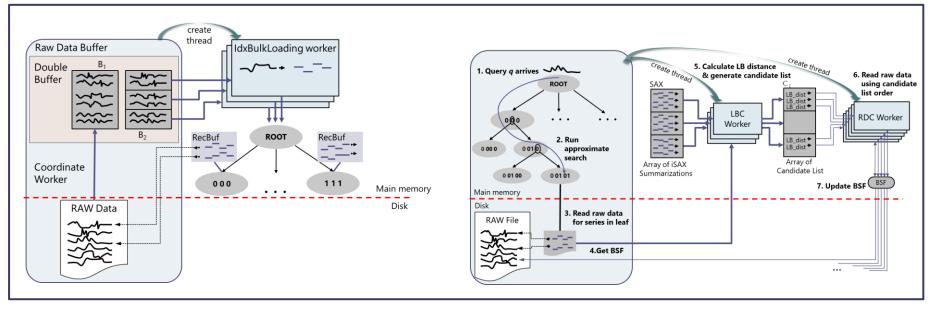
BigData'18

Publications

TKDE'18 PKDD'19

• **DPiSAX**: current solution for distributed processing (Sparl

balances work of different worker nodes



diNo 253

Publications

ICDM'17

TKDE'18

PKDD'19

BigData'18

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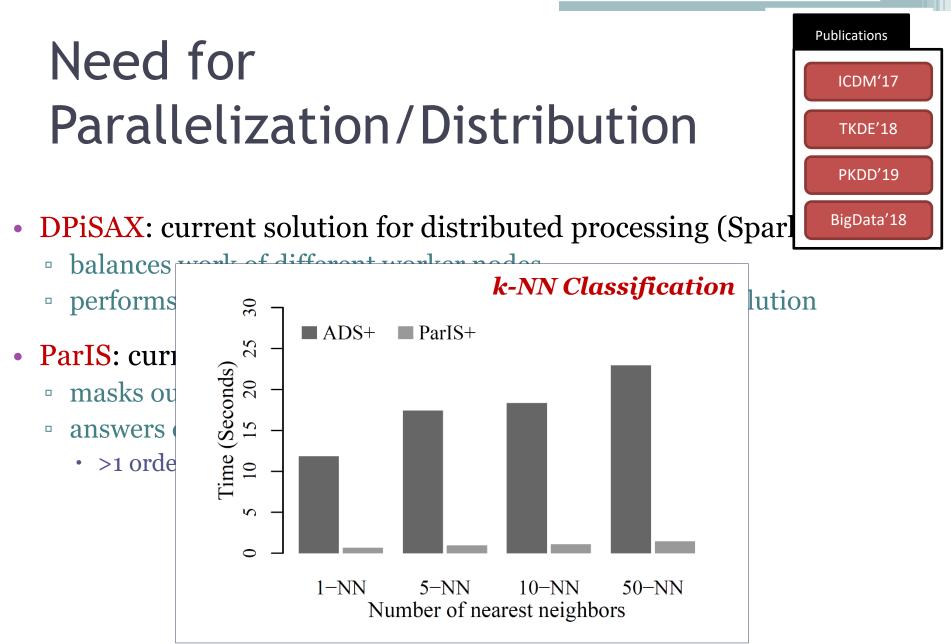
diNo 254

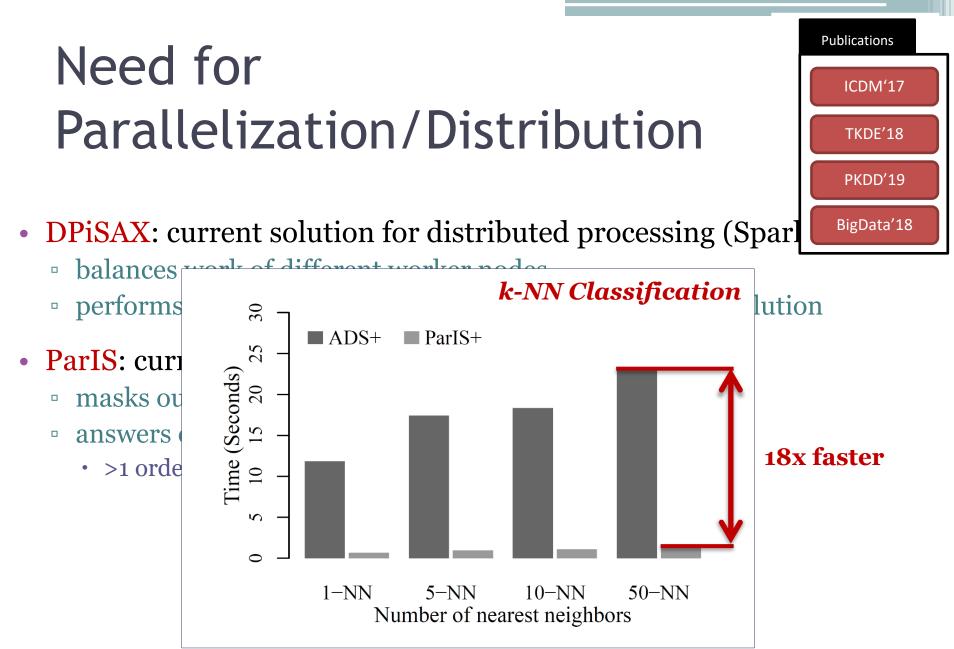
Publications

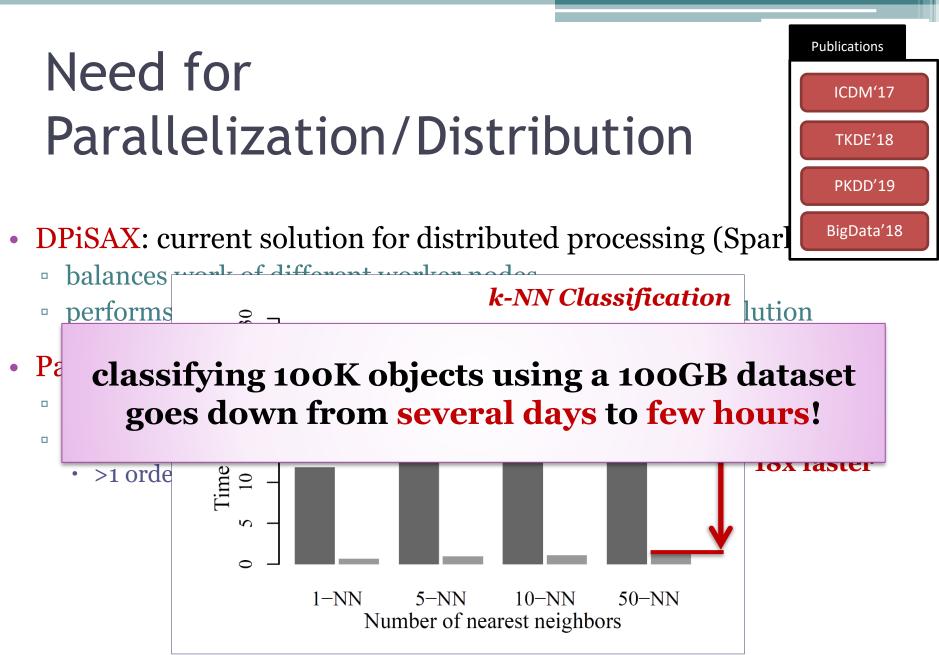
TKDE'18 PKDD'19

ICDM'17

BigData'18







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 - answers exact queries in the order of a few secs
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- MESSI: current single-node parallel solution + in-memory data
 answers exact queries at interactive speeds: ~50msec on 100GB
- **SING**: current single-node parallel solution + GPU + in-memory data
 - answers exact queries at interactive speeds: ~32msec on 100GB

diNo 258

Publications

ICDM'17

TKDE'18

PKDD'19

BigData'18

ICDE'20

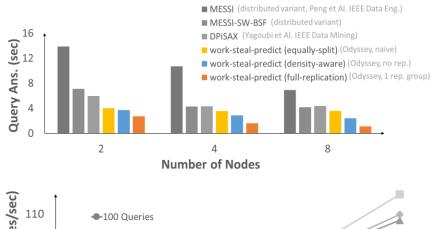
Odyssey Distributed, Parallel, In-Memory Indexing

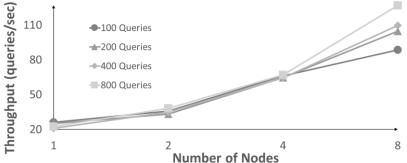
- Distributed, in-memory solution for SIMD, multi-core, multi-socket architectures
 - allows in-memory processing (across machines) of very large datasets
- Odyssey addresses the following challenges
 - **Query Scheduling**: Which queries to which nodes?
 - Query Execution Time estimations
 - Flexible Replication Schemes
 - Dynamic Scheduling
 - Load Balancing: Enable nodes to perform useful and equal work
 - Density-aware Data Distribution
 - Efficient work-stealing

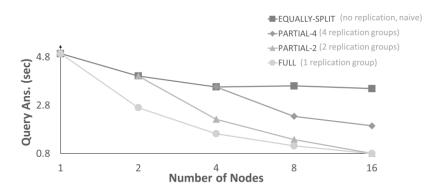
din 260

Odyssey

• achieves all goals







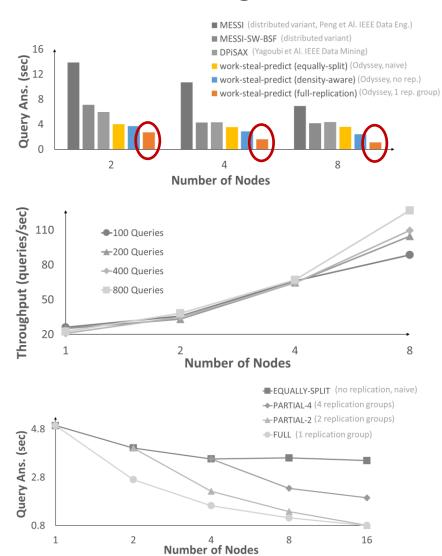
Publications



diND 261

Odyssey

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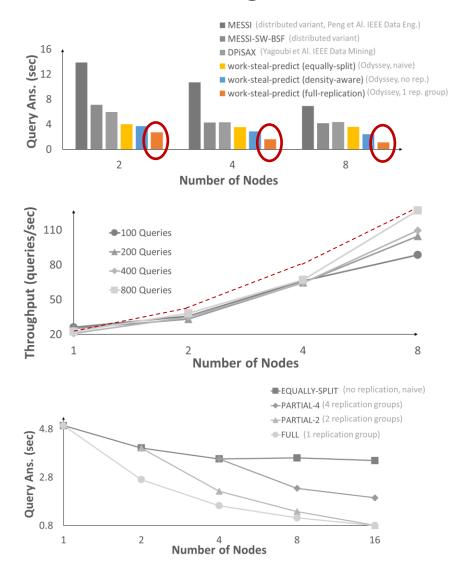


Publications Chatzakis-PVLDB'23

up to 3x faster than best competitor

Odyssey

• achieves all goals



Publications Chatzakis-PVLDB'23

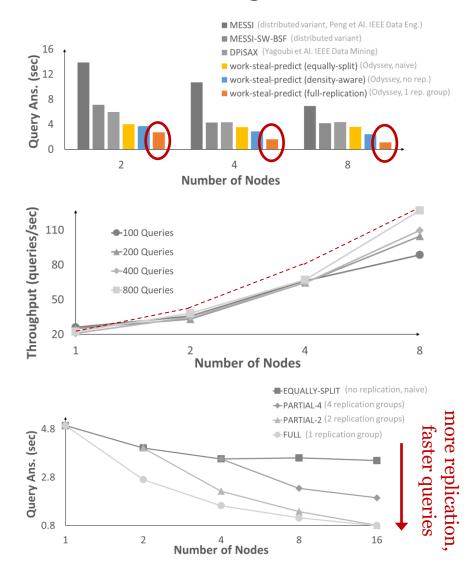
up to 3x faster than best competitor

scalable query answering (almost linear)

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Odyssey

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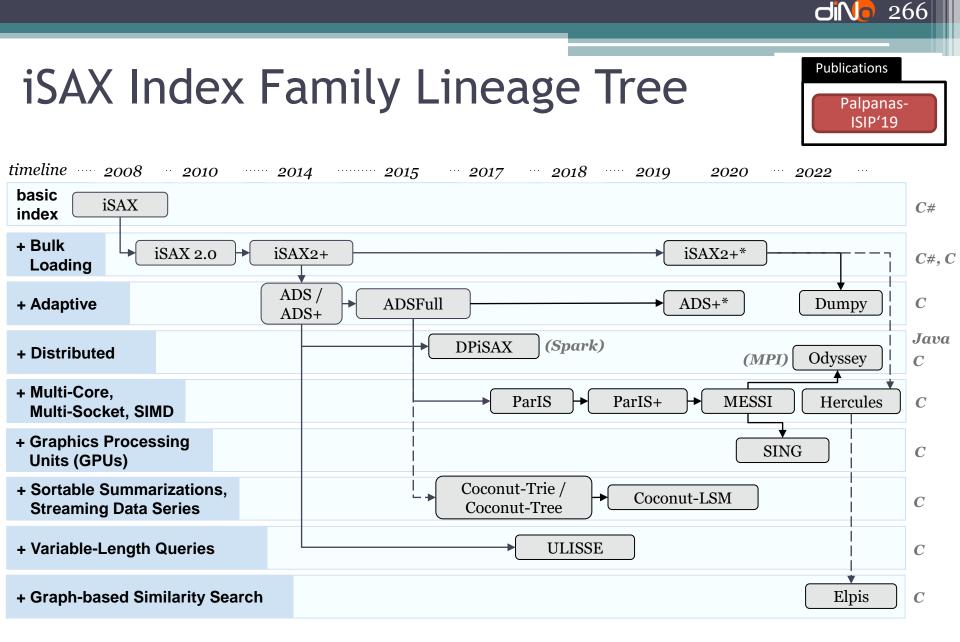
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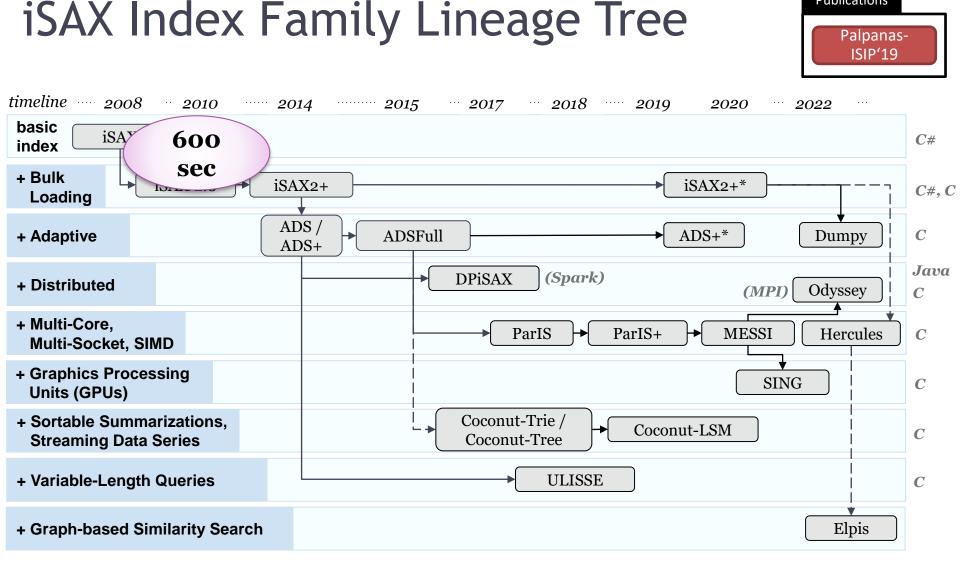
scalable query answering (almost linear)

more replication leads to faster query answering

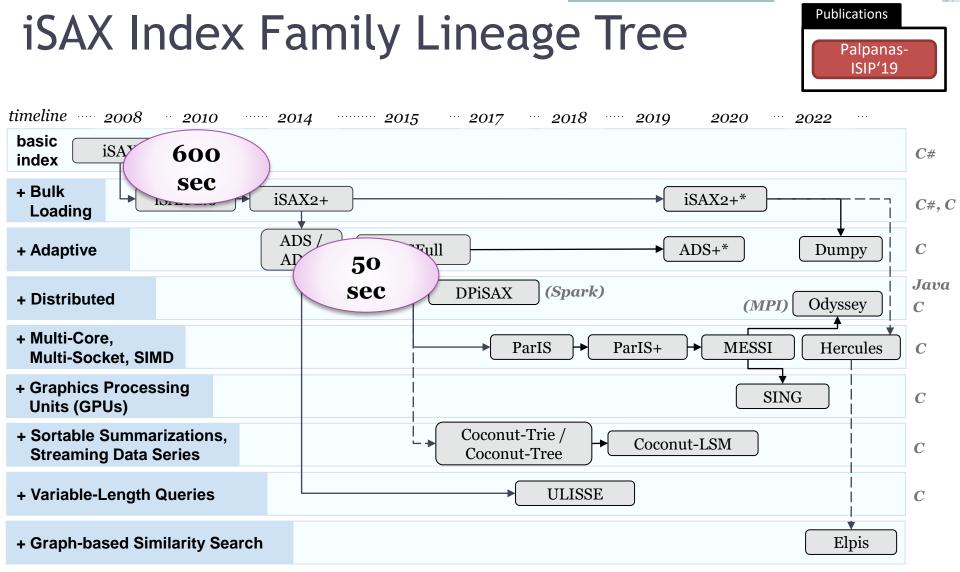
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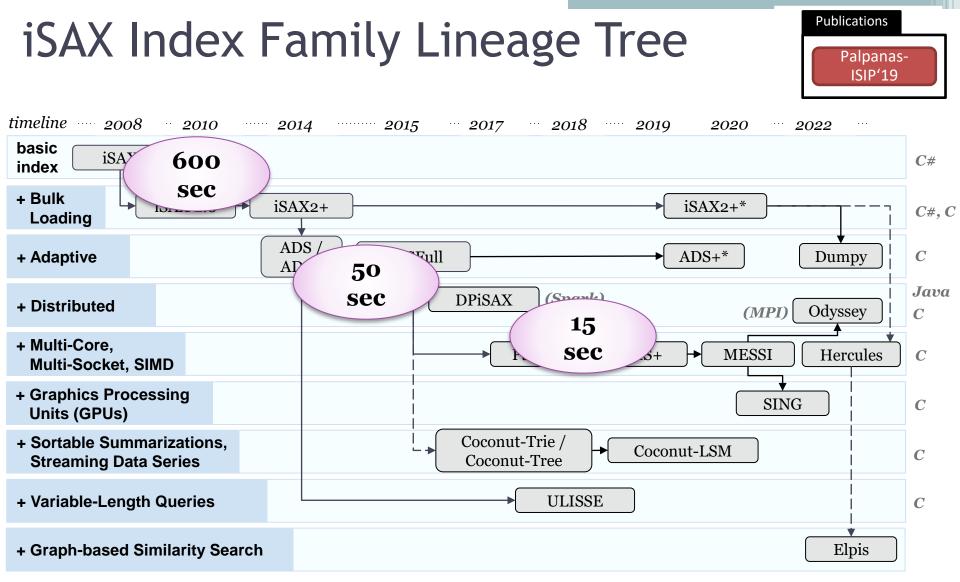
Publications



execution time for 1 similarity search query on a 100GB dataset on disk

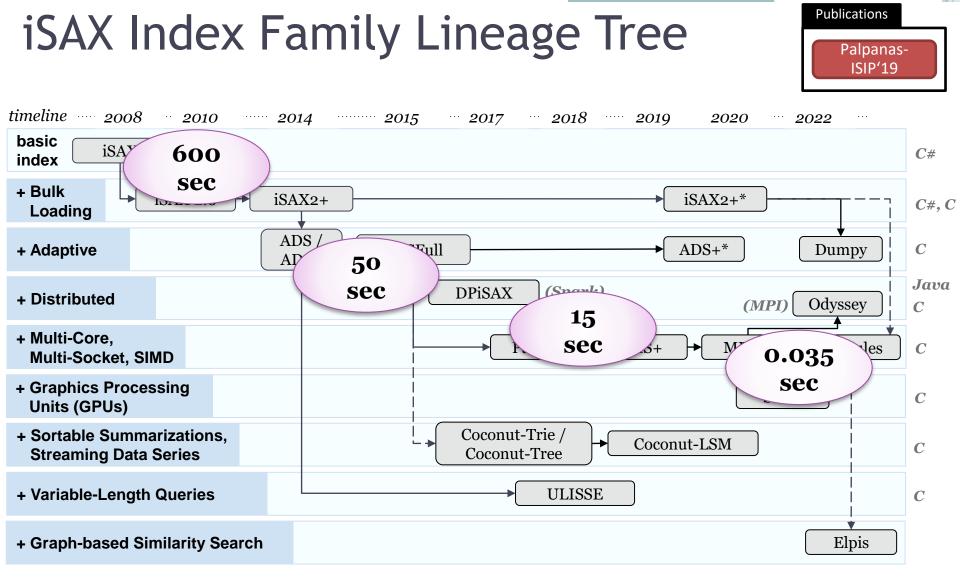


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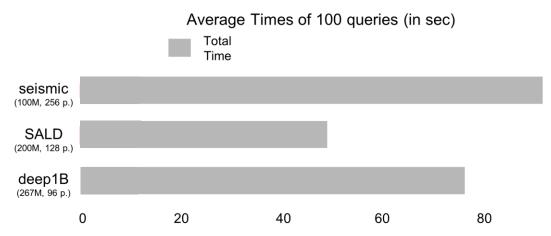
divo 270



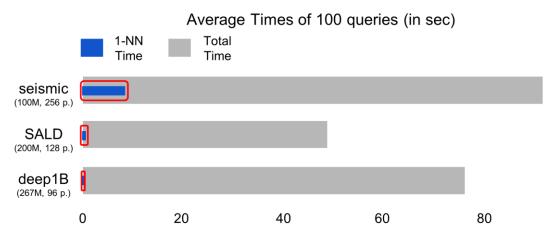
execution time for 1 similarity search query on a 100GB dataset in memory

diNo

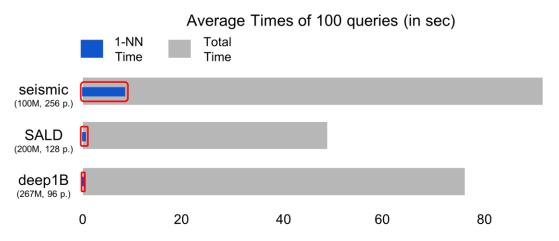
271



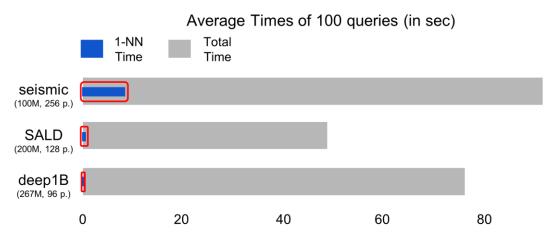
diNp 276



• how do we further reduce the wasted (gray) effort?



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 - progressive query answering
 - produce intermediate answers with (probabilistic) quality guarantees



- how do we further reduce the wasted (gray) effort?
 - progressive query answering
 - produce intermediate answers with (probabilistic) quality guarantees
 - learned summarizations + index structures
 - adapt to data characteristics
 - build more efficient indexes
 - perform more effective pruning

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- two sides of the same(?) coin
 - data series as multidimensional points
 - for a specific ordering of the dimensions



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- everything we discussed applicable to high-d vectors, too!







- two sides of the same(?) coin
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- several techniques for similarity search in high-d vectors
 - using LSH (SRS), space quantization (IMI), k-NN graphs (HNSW)

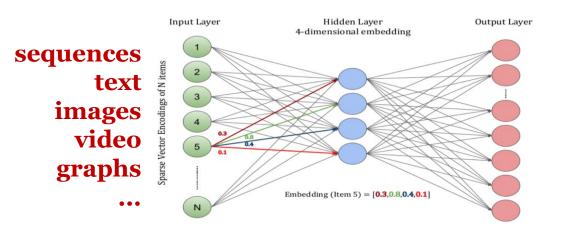


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sequences text images video graphs

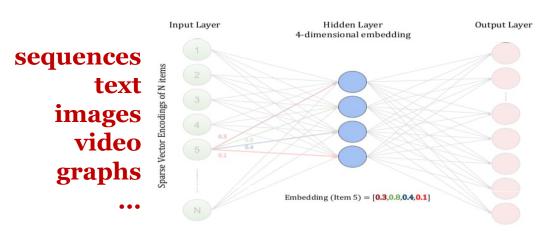


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 - using LSH (SRS), space quantization (IMI), k-NN graphs (HNSW)



deep embeddings

high-d vectors learned using a DNN

High-d Vector Similarity Search Applications

• ocean life monitoring

Introduction

Challenges

- · Animals at different depth levels from the sea surface
- Sun glitters and wave crests
- Various background w.r.t. weather, season, geography location, etc.



Allain and Pham, MACLEAN'22

Themis Palpanas - dSDS - Jun 2024

diNo 306

() IRISA

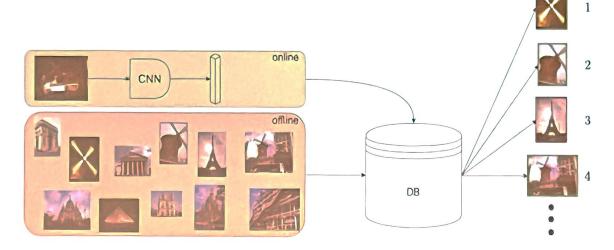
diNo 307

High-d Vector Similarity Search Applications

- ocean life monitoring
- image retrieval

Image Retrieval: the task

Given a query image, rank images of a database from most to least similar.



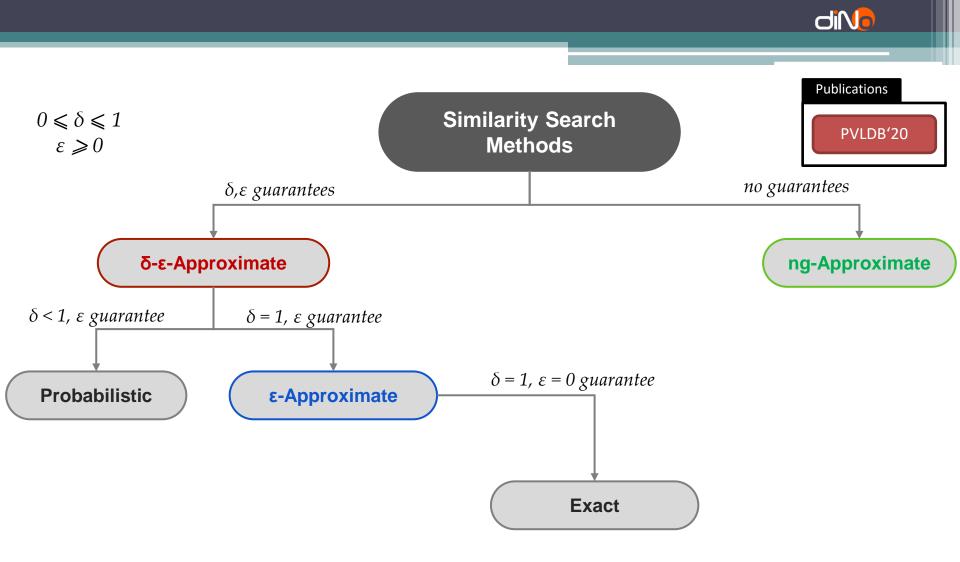
Ramzi et al., Cap&RFIAP'22

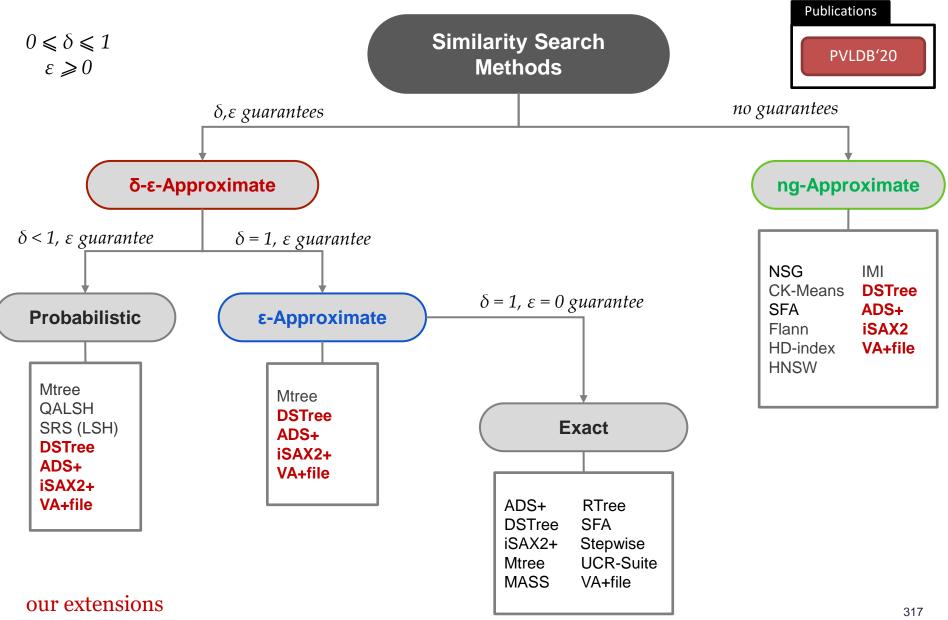
High-d Vector Similarity Search Applications

- ocean life monitoring
- image retrieval
- recommendations
- entity matching
- fraud detection
- • •

- two sides of the same(?) coin
 - data series as multidimensional points
 - for a specific ordering of the dimensions
- everything we discussed applicable to high-d vectors, too!
- several techniques for similarity search in high-d vectors
 - using LSH (SRS), space quantization (IMI), k-NN graphs (HNSW)
- how do these high-d vector techniques compare to data series techniques?
 - have conducted extensive experimental comparison







 data series techniques are the overall winners, even on general high-d vector data

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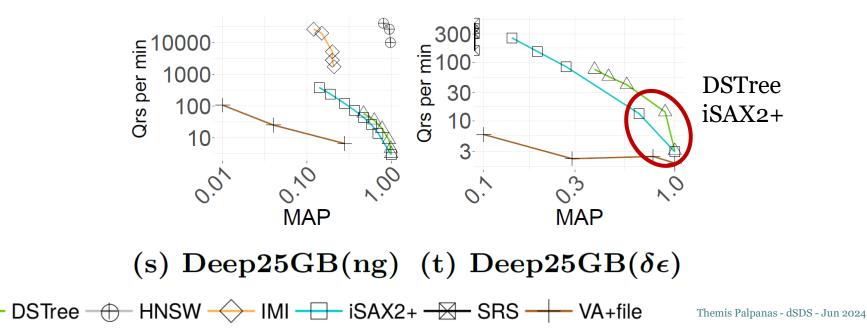
PVLDB²⁰

Publications



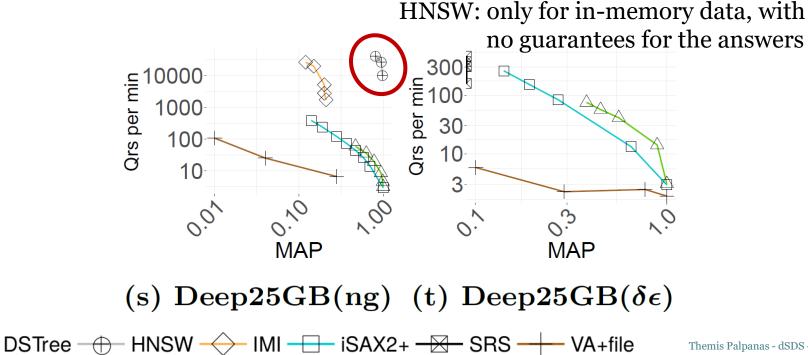
diN 320

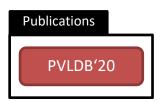
- data series techniques are the overall winners, even on general high-d vector data
 - perform the best for approximate queries with probabilistic guarantees
 (δ-ε-approximate search), in-memory and on-disk



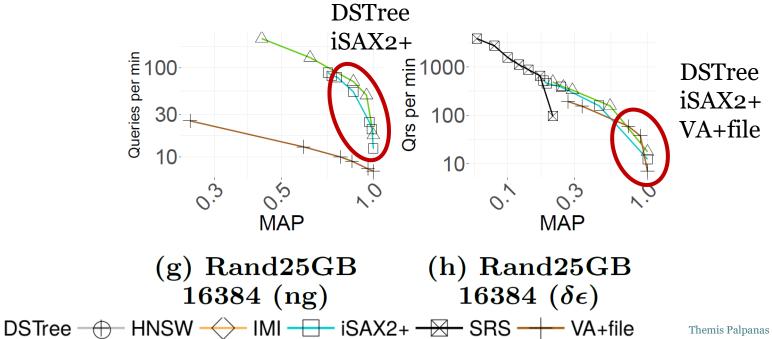


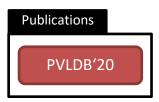
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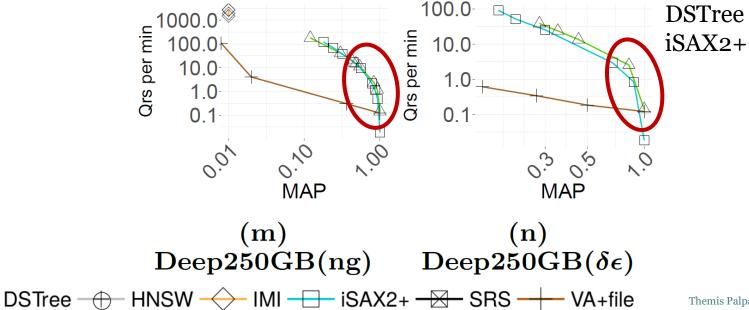


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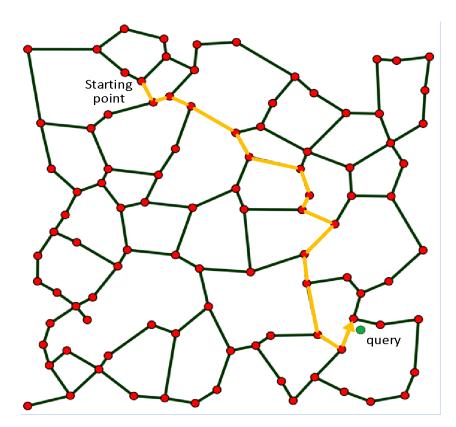


- data series techniques are the overall winners, even on general high-d vector data
 - perform the best for approximate queries with probabilistic guarantees (δ-ε-approximate search), in-memory and on-disk
 - perform the best for long vectors, in-memory and on-disk
 - perform the best for disk-resident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



NSW Graphs

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

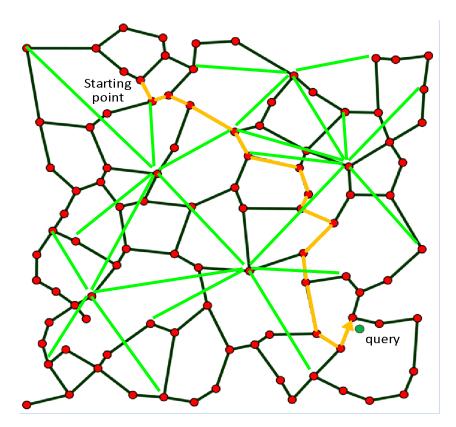




diN 326

NSW Graphs

- Augment approximate kNN graphs with long range links:
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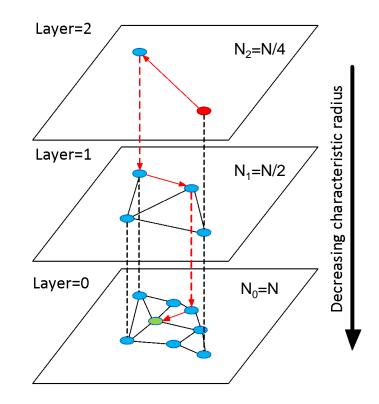






HNSW

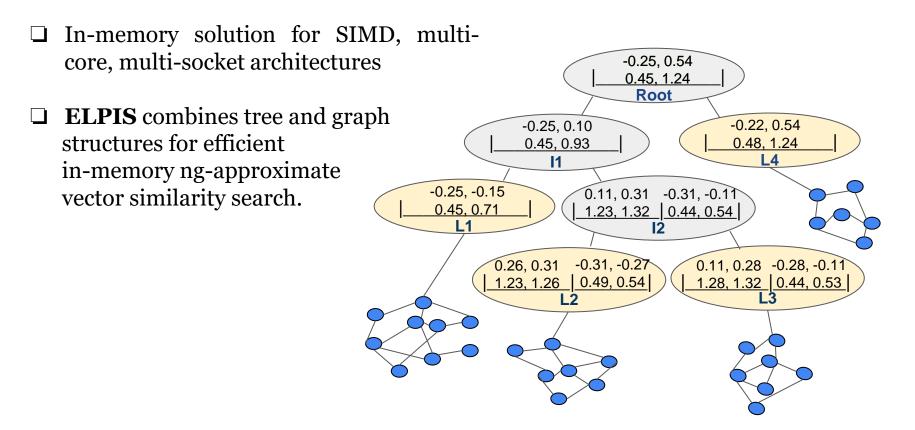
- In HNSW we split the graph into layers (fewer elements at higher levels)
- Search starts for the top layer. Greedy routing at each level and descend to the next layer.
- Maximum degree is capped while paths ~ log(N) → log(N) complexity scaling.
- Incremental construction
- ng-approximate search



Slides by Malkov

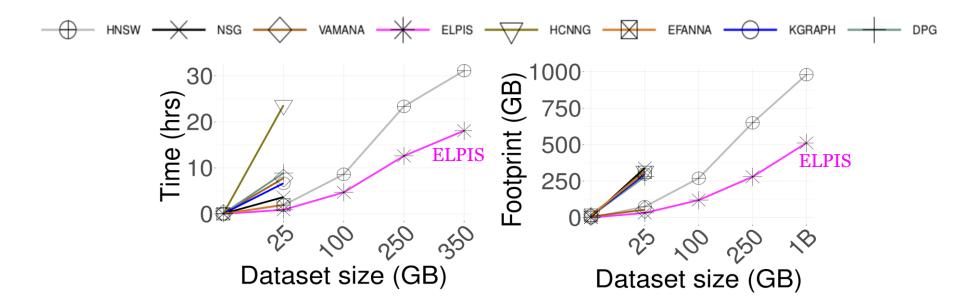
diNp 329

ELPIS Parallel, In-Memory Indexing of Sequences



ELPIS Parallel, In-Memory Indexing of Sequences

• Scalability of indexing time and memory footprint with dataset size (Deep)



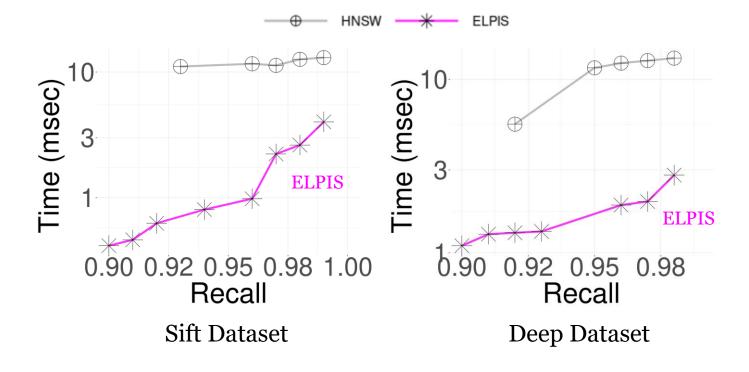
ELPIS builds the index up to **8x faster**, using **40% less memory**

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diN 330

ELPIS Parallel, In-Memory Indexing of Sequences

• Query Performance on 1B vectors datasets (Sift, Deep)



ELPIS answers 10-NN queries in ~3 msec for a dataset of 1 billion vectors with recall 0.99

Available Solutions

libraries

- ELPIS
- HNSW
- FAISS (META/Facebook)
- vector databases
 - Pinecone
 - milvus
- general databases
 - Postgres with HNSW and IVF algorithms (open source)
 - AlloyDB with SCaNN algorithm (Google)
 - Oracle

- high-d vectors is a very common data type
 - across several different domains and applications

diNp 352

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 - across several different domains and applications
- complex high-d vector analytics are challenging
 - have very high complexity

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- data series management/indexing techniques provide much needed scalability
 - work for data series and general high-d vectors (and embeddings)
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 - work for data series and general high-d vectors (and embeddings)
 - lead to fast complex analytics and machine learning
- several exciting research opportunities

thank you!

google: Themis Palpanas
visit: http://nestordb.com

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