

Graph-Based Vector Search Recent Advances & Future Directions

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Talk at the University of Waterloo, Canada

July 28th, 2025

Introduction

Research Main Topics





Main Topics

- Scalable and responsible data science
 - Similarity search
 - Data structures/algorithms
 - Representation learning
 - Data science
 - GenAl pipelines (e.g., RAG)
 - Data valuation
 - Health
- Computer science education
 - Survey on leading universities across the Arab region
 - Study of CS programs in the African/Arab region
 - Booklet on best practices for supporting transitions from PhD to Professorship



Research Collaborators





Research Collaborators

Topic	Collaborators	Affiliation
Vector Search/ Data Mining	Damien Hilloulin, Marco Arnaboldi, Ioannis Alagiannis, Vlad Haprian Themis Palpanas Theophanis Tsandilas Anastasia Bezerianos Panagiota Fatourou	Oracle Labs, Zurich Paris Cite, France Inria, France Paris Saclay, France Univ. Crete, Greece
Data Valuation	Mardavij Roozbehani, Thibault Horel, Munther Dahleh	MIT, USA
Health Analytics	Yousef Yeganeh, Azade Farshad, Nassir Navab Amal Fadaili Anis Hasnaoui Gbenga Peter Oderinde, Stephen Peter Akpulu Kun-Hsing Yu	TUM, Germany Amana Pathology Lab, Morocco Faculty of Medicine, Tunisia Ahmadu Bello Univ., Nigeria Harvard Medical School, USA
Computer Science Education	Sherif G. Aly, Seif Eldawlatly Slim Abdennadher Khaled Shuaib Joe Tekli	AUC, Egypt GUC, Egypt UAE Univ., UAE Lebanese American Univ, Lebanon





Research Team







Name	Hasnae Zerouaoui
Position	Postdoctoral Fellow
Awards/ Employment	Microsoft Research PhD Fellowship NUDIA Ambassador
Project	Representation Learning & Health Analytics









Name	Hasnae Zerouaoui	Ilias Azizi
Position	Postdoctoral Fellow	Alumni PhD Student
Awards/ Employment	Microsoft Research PhD Fellowship NUDIA Ambassador	amazon Research Internship PostDoc 2 VLDB Grants
Project	Representation Learning & Health Analytics	Approximate Graph-Based Vector Search











Name	Hasnae Zerouaoui	llias Azizi	Khaoula Abdenouri	
Position	Postdoctoral Alumni PhD Fellow Student		3 rd year PhD Student	
Awards/ Employment	Microsoft Research PhD Fellowship NUDIA Ambassador	amazon Research Internship PostDoc 2 VLDB Grants		
Project	Representation Learning & Health Analytics	Approximate Graph-Based Vector Search	Exact Tree- Based Vector Search	











Name	Hasnae	llias	Khaoula	Anas
	Zerouaoui	Azizi	Abdenouri	Ait Aomar
Position	Postdoctoral	Alumni PhD	3 rd year PhD	2 nd year PhD
	Fellow	Student	Student	Student
Awards/ Employment	Microsoft Research PhD Fellowship NVIDIA. Ambassador	amazon Research Internship PostDoc 2 VLDB Grants		Research PhD Fellowship WATERLOO SIGMOD Grant
Project	Representation Learning & Health Analytics	Approximate Graph-Based Vector Search	Exact Tree- Based Vector Search	Approximate Graph-Based Hybrid Vector Search















Name	Hasnae	llias	Khaoula	Anas	Firdawse
	Zerouaoui	Azizi	Abdenouri	Ait Aomar	Guerbouzi
Position	Postdoctoral	Alumni PhD	3 rd year PhD	2 nd year PhD	1 st year PhD
	Fellow	Student	Student	Student	Student
Awards/ Employment	Microsoft Research PhD Fellowship NUDIA Ambassador	amazon Research Internship PostDoc 2 VLDB Grants		Research PhD Fellowship WATERLOO SIGMOD Grant	Print Research Associate MICCAI Travel Grant
Project	Representation Learning & Health Analytics	Approximate Graph-Based Vector Search	Exact Tree- Based Vector Search	Approximate Graph-Based Hybrid Vector Search	Representation Learning & Health Analytics



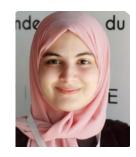














Name	Hasnae	llias	Khaoula	Anas	Firdawse	Mehdi
	Zerouaoui	Azizi	Abdenouri	Ait Aomar	Guerbouzi	Touil
Position	Postdoctoral	Alumni PhD	3 rd year PhD	2 nd year PhD	1 st year PhD	1 st year PhD
	Fellow	Student	Student	Student	Student	Student
Awards/ Employment	Microsoft Research PhD Fellowship NUDIA Ambassador	amazon Research Internship PostDoc 2 VLDB Grants		Research PhD Fellowship WATERLOO SIGMOD Grant	Print Name of the	IlliT
Project	Representation Learning & Health Analytics	Approximate Graph-Based Vector Search	Exact Tree- Based Vector Search	Approximate Graph-Based Hybrid Vector Search	Representation Learning & Health Analytics	Data Valuation





















Name	Hasnae	llias	Khaoula	Anas	Firdawse	Mehdi	Reda	Abdelatif
	Zerouaoui	Azizi	Abdenouri	Ait Aomar	Guerbouzi	Touil	Lefdali	Bouzid
Position	Postdoctoral	Alumni PhD	3 rd year PhD	2 nd year PhD	1 st year PhD	1 st year PhD	Data	Data
	Fellow	Student	Student	Student	Student	Student	Scientist	Engineer
Awards/ Employment	Microsoft Research PhD Fellowship NUIDIA Ambassador	amazon Research Internship PostDoc 2 VLDB Grants		Research PhD Fellowship WATERLOO SIGMOD Grant	Research Associate MICCAI Travel Grant	PliT	⊗ OCP	(E) OCP
Project	Representation Learning & Health Analytics	Approximate Graph-Based Vector Search	Exact Tree- Based Vector Search	Approximate Graph-Based Hybrid Vector Search	Representation Learning & Health Analytics	Data Valuation	Health Analytics/ Data Mining	RAG





Vector Search

Vector Search Overview



High-D Data is Everywhere



Finance



Paleontology



Manufacturing



Aviation



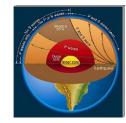
Agriculture



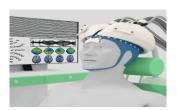
Astronomy



Criminology



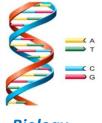
Seismology



Neuroscience



Medicine



Biology







High-D Collections are Massive



 \approx 500 ZB per year



 \approx 130 TB



> 40 PB per day



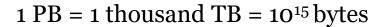
> 5 TB per day



> 500 TB per day



$$1 ZB = 1 billion TB$$



$$1 \text{ ZB} = 1 \text{ billion TB} = =10^{21} \text{ bytes}$$

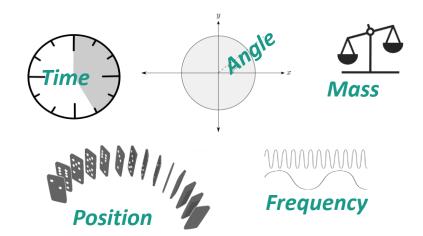






Data Series

A collection of points ordered over a dimension

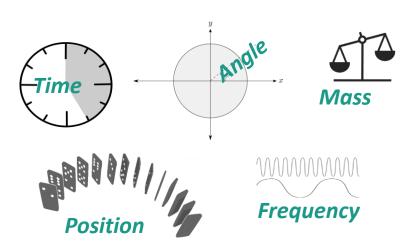






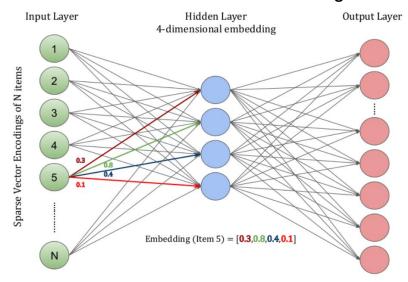
Data Series

A collection of points ordered over a dimension



Deep Embeddings

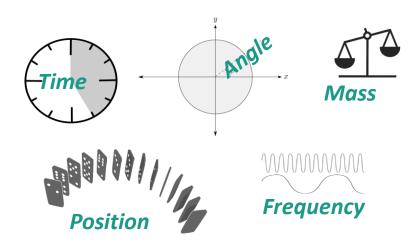
A feature vector learned from data using a DNN





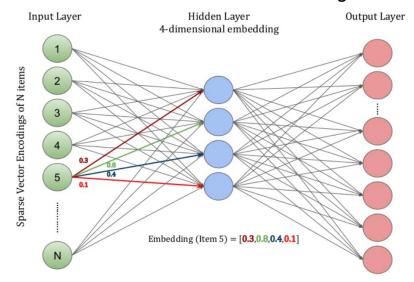
Data Series

A collection of points ordered over a dimension



Deep Embeddings

A feature vector learned from data using a DNN



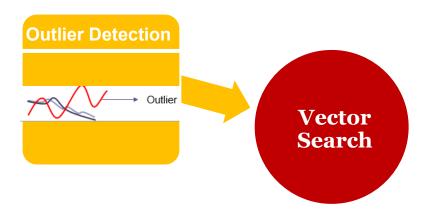
embedded text, images, video, graphs, etc.





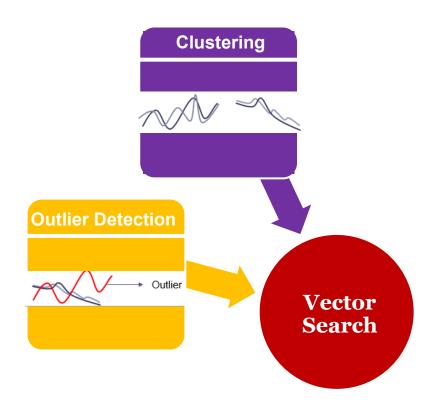






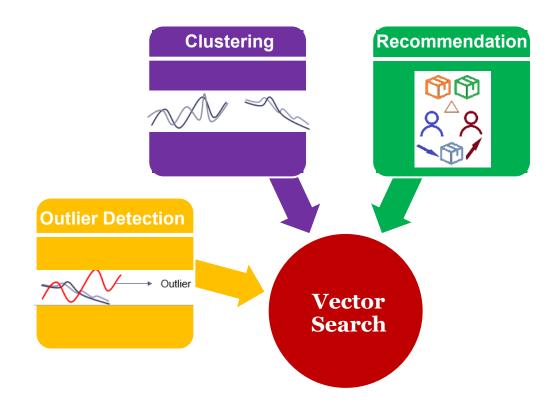






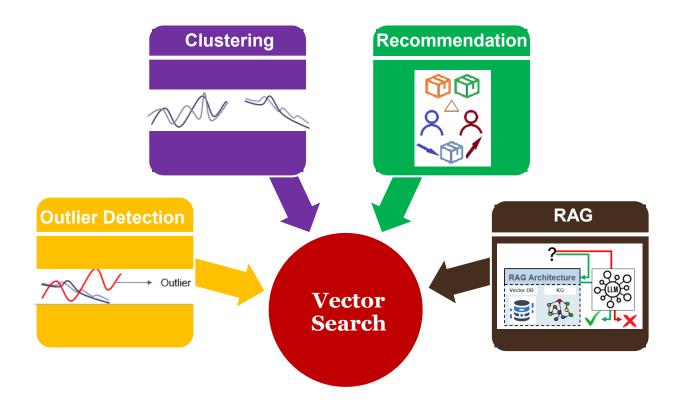






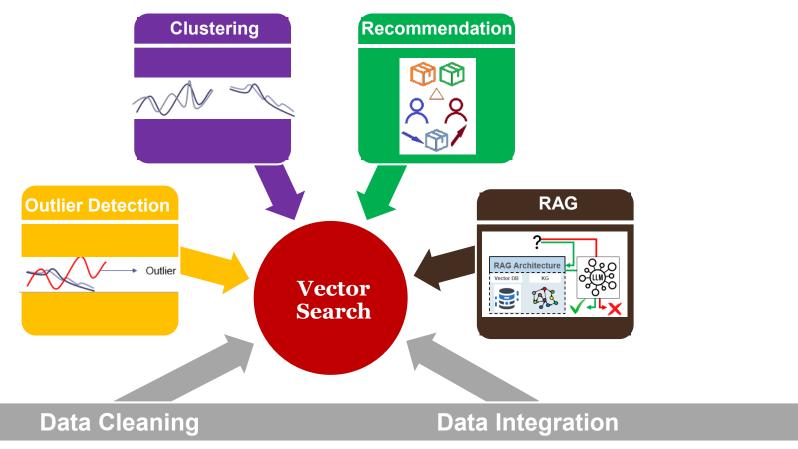






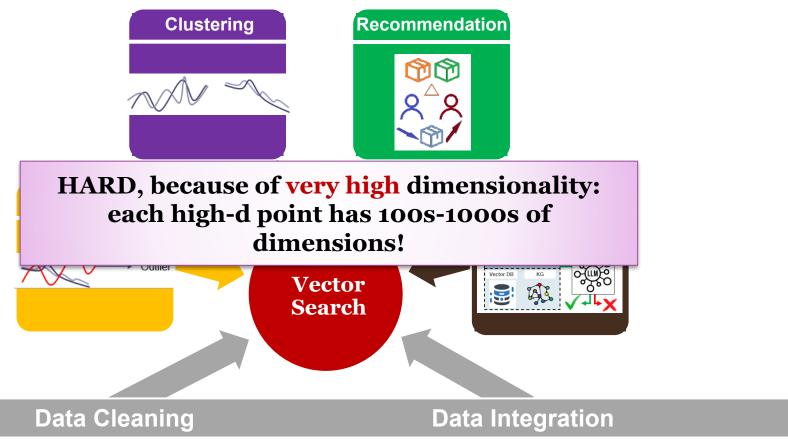






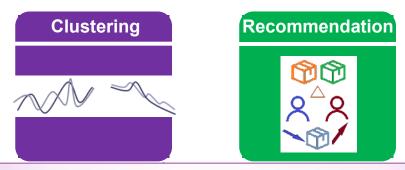












HARD, because of very high dimensionality: each high-d point has 100s-1000s of dimensions!

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

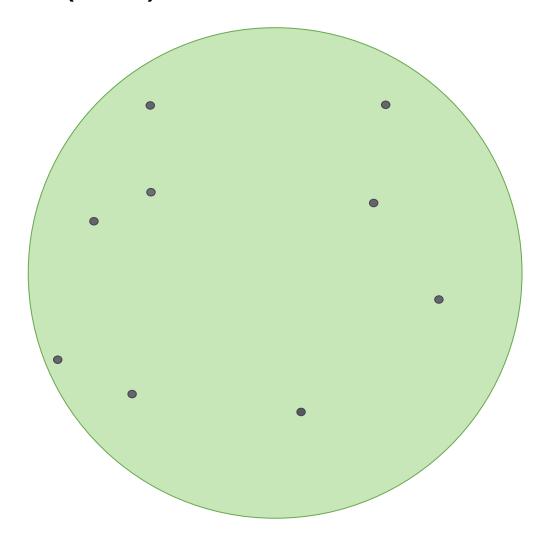
Data Cleaning

Data Integration





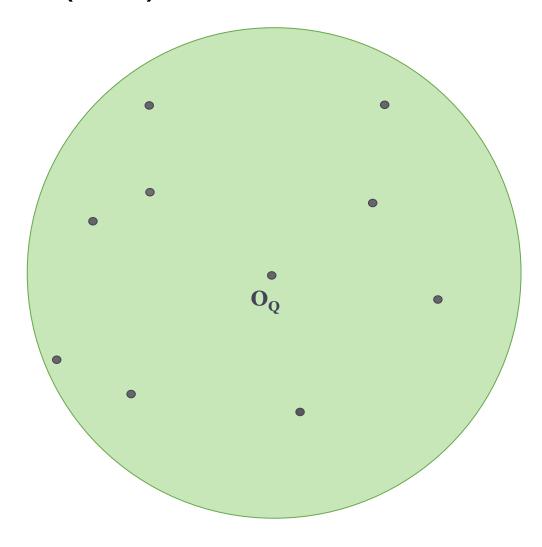








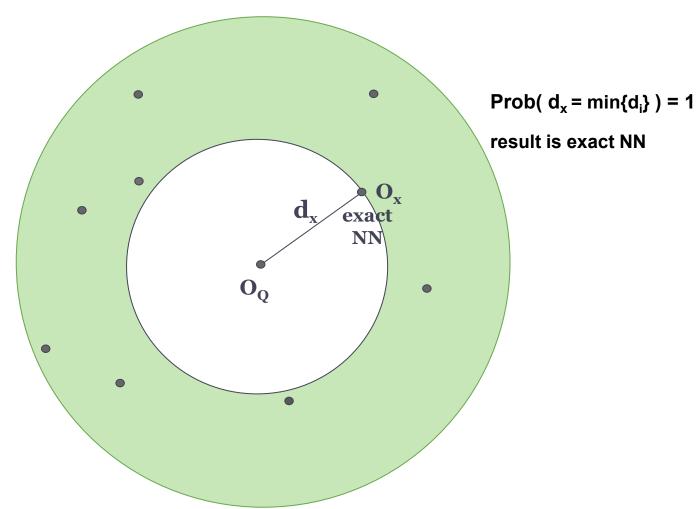








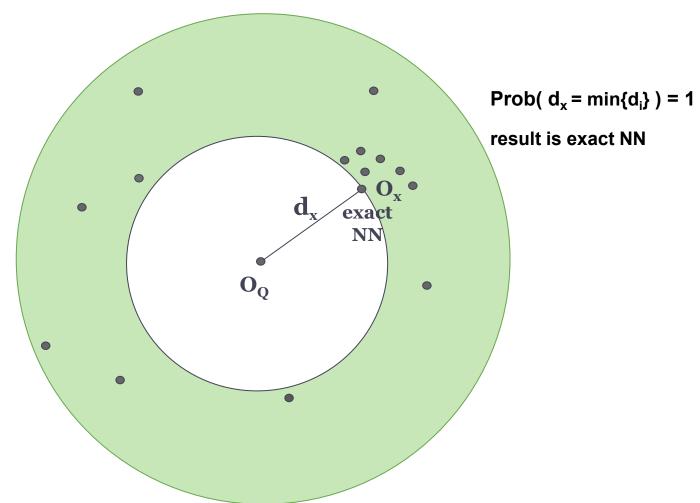








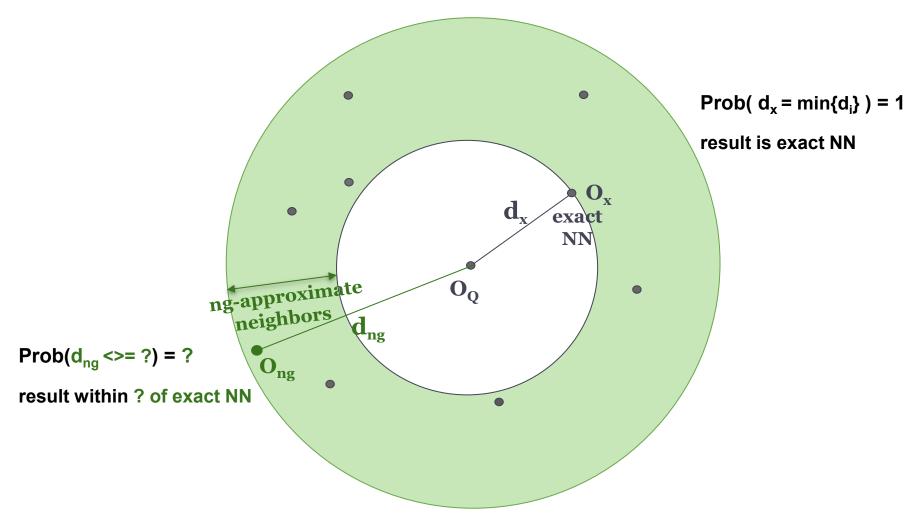








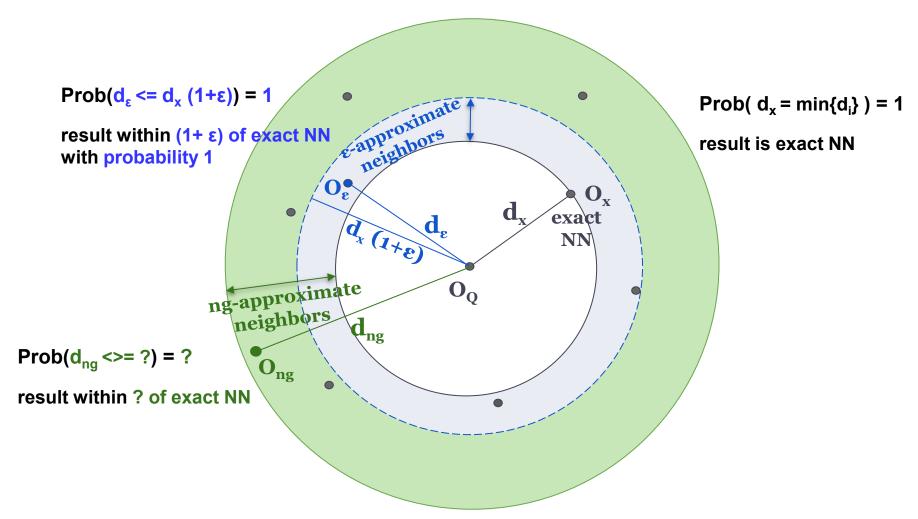










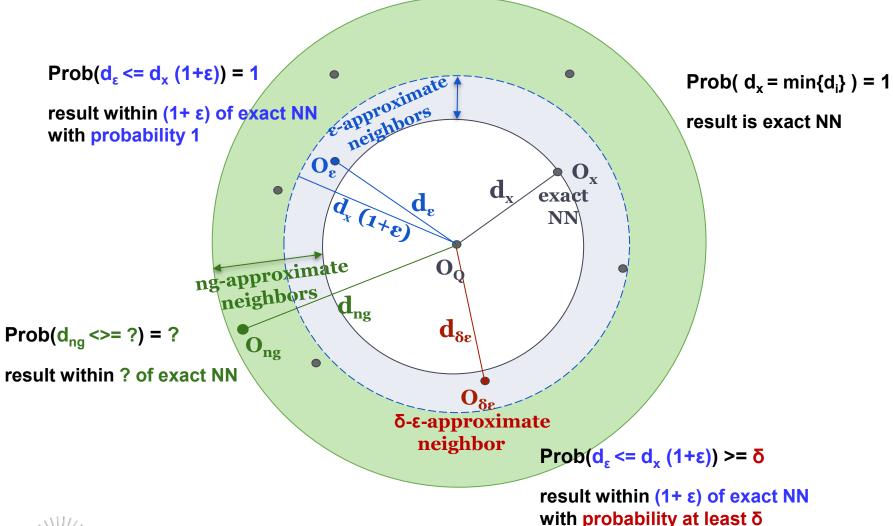






Nearest Neighbor (NN) Queries







Vector Search Main Contributions

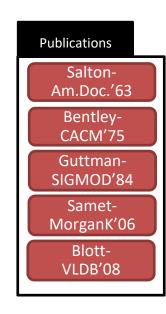


Large body of work (> 50 years)



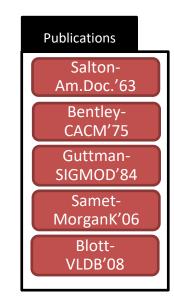


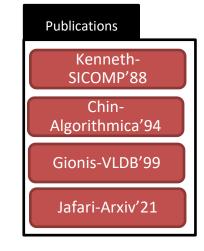
- Large body of work (> 50 years)
- Exact search:
 - Different communities working in isolation
 - Data series vs generic high-d vectors
 - Typically scan (e.g. VA-file) or tree-based (e.g., KD-Tree, RTree)
 - High-d vector techniques scale to a few GBs over 10s of dimensions
 - Data series techniques scale to 100s GBs over 1000s of dimensions





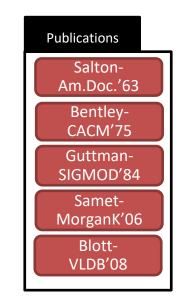
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- Approximate search:
 - with guarantees relatively slow
 - LSH family

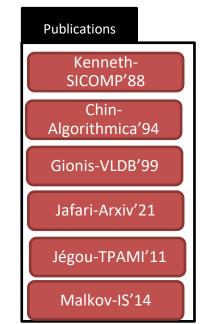






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- Approximate search:
 - with guarantees relatively slow
 - LSH family
 - without guarantees relatively efficient
 - Inverted indexes and graph-based techniques







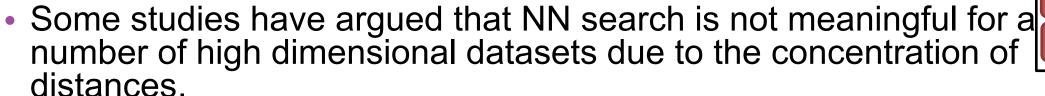
Meaningfulness of NN queries in high-d spaces



- Some studies have argued that NN search is not meaningful for a number of high dimensional datasets due to the concentration of distances.
 - However, these conclusions were based on over-restrictive assumptions



Meaningfulness of NN queries in high-d spaces



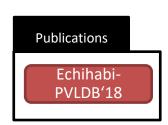
- Beyer et al.
 ICDT'99

 Aggarwal et al.
 ICDT'01

 He et al.
 ICML'12
- However, these conclusions were based on over-restrictive assumptions
- Other studies have shown that high-dimensional NN search is meaningful for:
 - non-i.i.d data
 - data with low intrinsic dimensionality
 - for a variety of real world datasets



Reconciled terminology/taxonomy across different communities

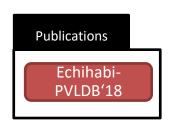




Reconciled terminology/taxonomy across different communities



- Data series techniques work well for generic high-d vectors
 - Evaluated on images, deep network embeddings.
 - Scaled to a few TBs of data over 1000s dimensions.

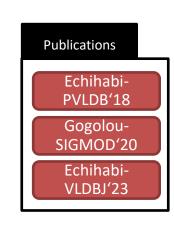




Reconciled terminology/taxonomy across different communities



- Data series techniques work well for generic high-d vectors
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- Progressive search
 - Proposed progressive search algorithms for interactive search.

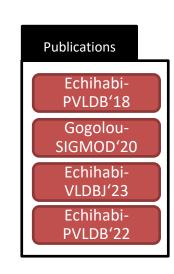




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Exact search:

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 - Proposed progressive search algorithms for interactive search.
- No technique was an overall winner
 - Proposed Hercules with state-of-the-art performance across all popular query workloads.

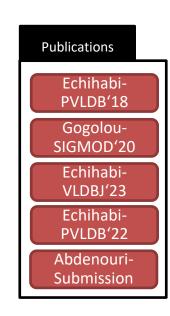




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Exact search:

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- Progressive search
 - Proposed progressive search algorithms for interactive search.
- No technique was an overall winner
 - Proposed Hercules with state-of-the-art performance across all popular query workloads.
- An exact technique better suited for embeddings
 - Proposed a new state-of-the-art technique with logarithmic averagecase/worst-case query time complexity.





Publications

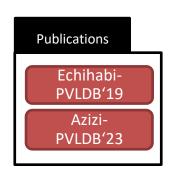
EchihabiPVLDB'19

- Approximate search:
 - Provided techniques that answer all flavors of search and are alternatives to:
 - the LSH family for approximate search with guarantees based on trees.
 - graph-based and quantization-based methods for search without guarantees on disk.



Approximate search:

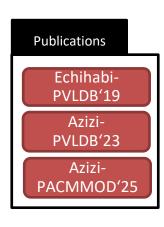
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- Proposed Elpis to address the indexing scalability of graph-based techniques
 - builds the index 3x-8x faster than competitors, using 40% less memory.
 - achieves a high recall of 0.99, up to 2x faster than the state-of-the-art methods.





Approximate search:

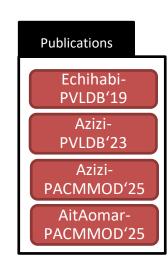
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- Conducted an experimental evaluation of in-memory graph-based vector indexes
 - Incremental insertion and neighborhood diversification lead to better query performance.
 - Efficient seed selection can improve both indexing and search performance.





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- Conducted an experimental evaluation of in-memory graph-based vector indexes
 - Incremental insertion and neighborhood diversification lead to better query performance.
 - Efficient seed selection can improve both indexing and search performance.
- Proposed RWalks, an index-agnostic graph-based filtered vector search method
 - Efficiently supports both filtered and unfiltered vector search.
 - Can perform filtered search up to 2x faster than the second-best competitor (ACORN), while building the index 76x faster and answering unfiltered search 13x faster.

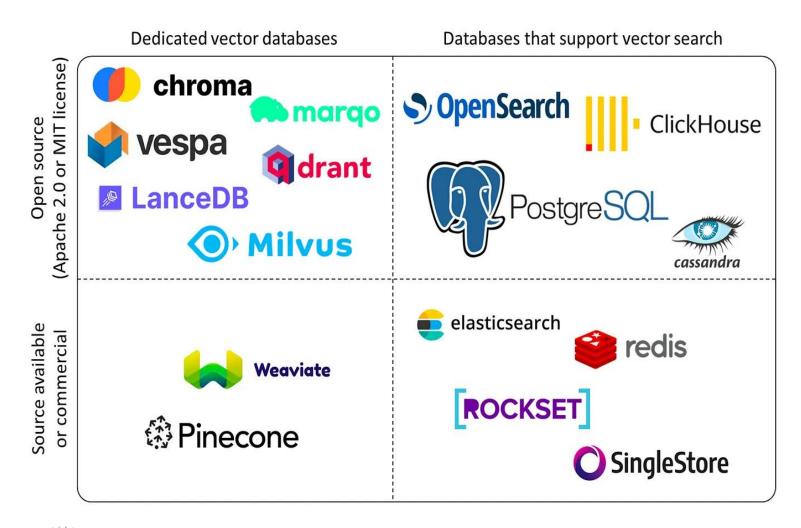






Vector Search Experimental Evaluation of Graph-Based Methods



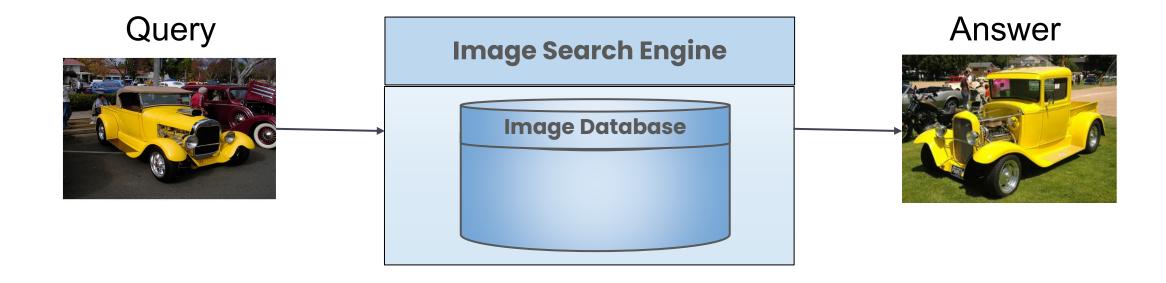






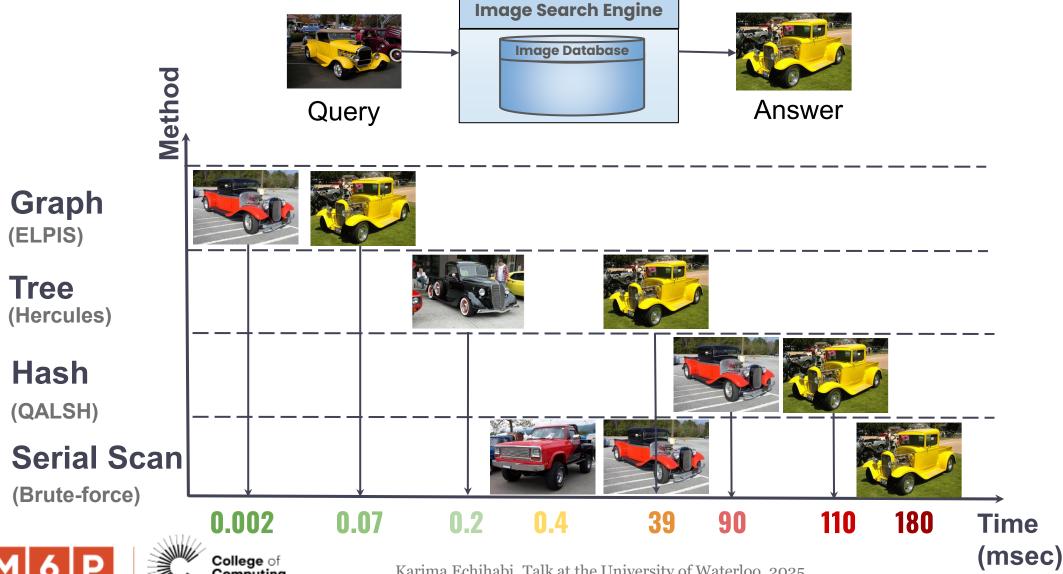
Proprietary composite index
milvus/*zilliz Flat, Annoy, IVF, HNSW/RHNSW (Flat/PQ), DiskANN
Weaviate Customized HNSW, HNSW (PQ), DiskANN (in progress)
qdrant Customized HNSW
throma ······ HNSW
LanceDB IVF (PQ), DiskANN (in progress)
vespa ····· HNSW + BM25 hybrid
Vald ····································
elasticsearch Flat (brute force), HNSW
redis Flat (brute force), HNSW
pgvector













Limitations of Existing Studies

- Lack of comprehensive taxonomy
- Limited insights into graph construction's impact on search performance.
- Limited scalability study (up to 1M vectors)



Contributions

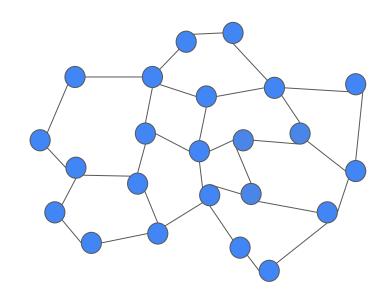
- New taxonomy of five design paradigms
- New insights on the impact of key design choices on performance
- Exhaustive experimental evaluation
- Recommendations
- Promising research directions



Primer - Proximity Graphs

Proximity graphs are geometric graphs G(V,E) in which two vertices p, q are connected by an edge (p, q) if and only if a certain exclusion region for p, q contains no points from the vertex set.



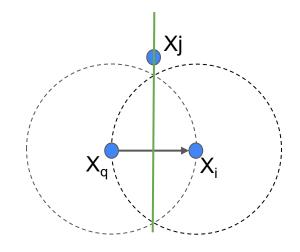




Primer – Example Proximity Graphs



Relative Neighborhood Graph (RNG) Lune (Xq,Xi) is empty



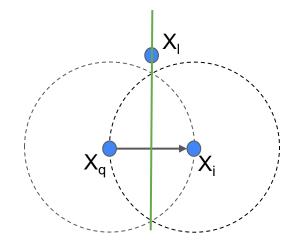




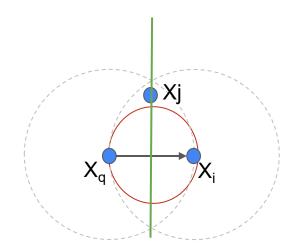
Primer – Example Proximity Graphs



Relative Neighborhood Graph (RNG) Lune (Xq,Xi) is empty



Gabriel Graph (GG) that is not RNG DiameterSphere (Xq,Xi) is empty

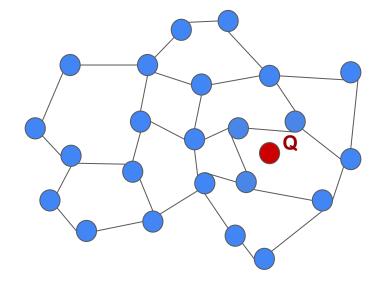




Primer - Beam Search

Beam search is a heuristic search algorithm that explores a graph by expanding the most optimistic node in a limited set of size L

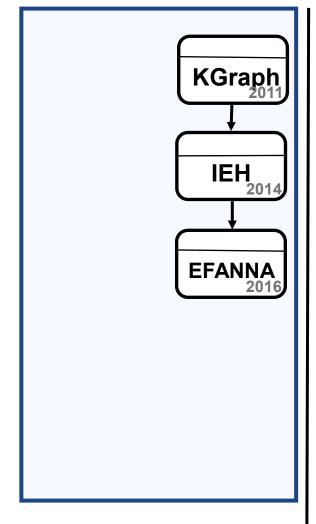
BeamSearch (G, Q, entry_node, K, L)





Proposed Taxonomy

Neighborhood Propagation

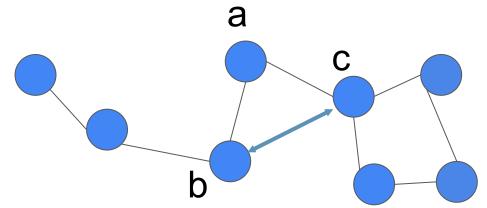






Neighborhood Propagation

Neighborhood propagation through NNDescent



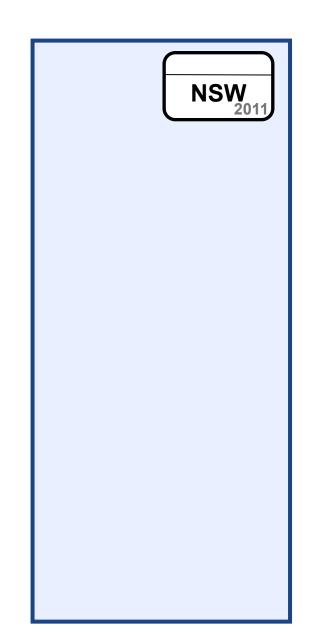
"Hi a, your neighbors can become my neighbors too"

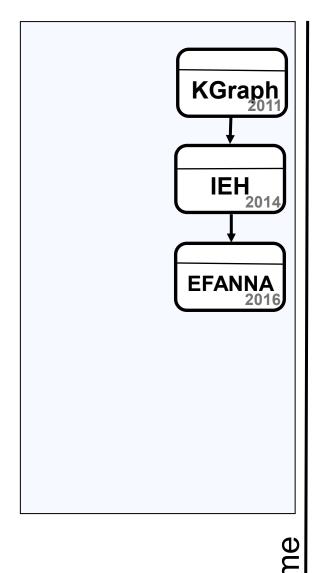


Proposed Taxonomy

Neighborhood Propagation

Incremental Insertion



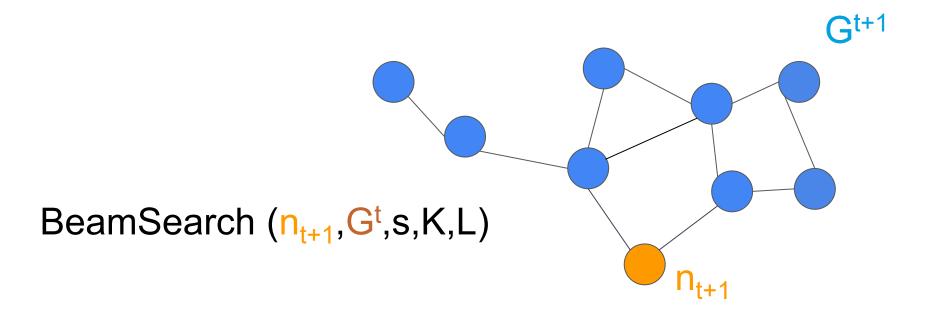






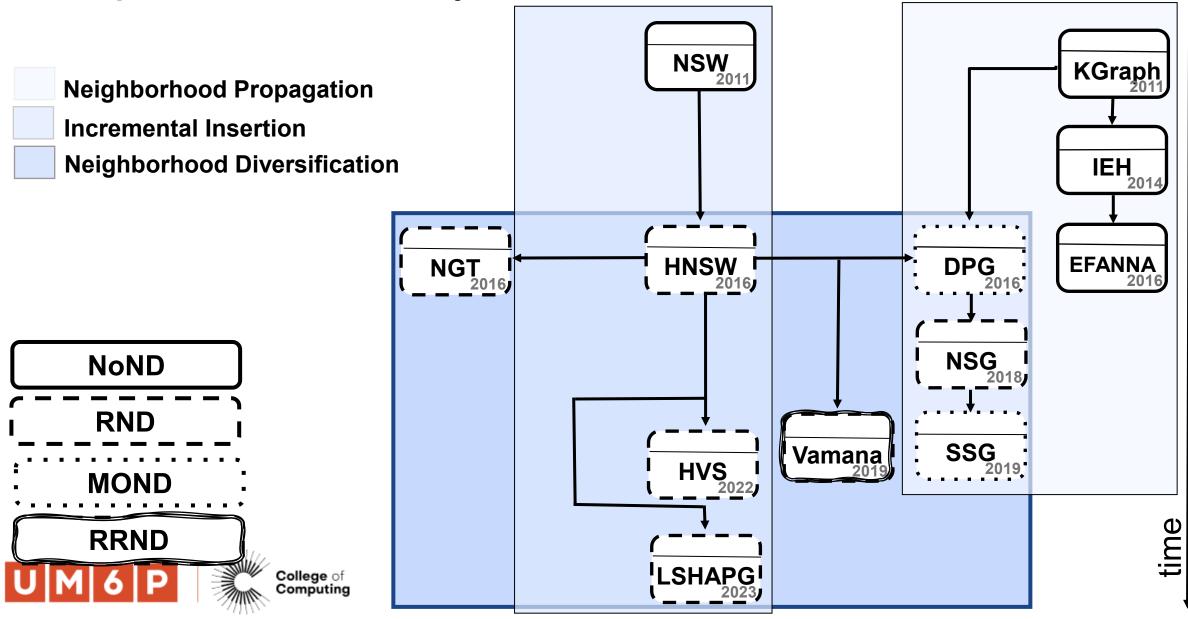
Incremental Insertion

Insert node incrementally into the graph





Proposed Taxonomy



Relative Neighborhood Diversification

For a node X_q and a list of candidate neighbors C_q , the node X_j , which belongs to C_q , is selected into the set of X_q 's neighbors R_q if and only if the following condition holds:

$$\forall X_i \in R_q$$
, $dist(X_q, X_j) < dist(X_i, X_j)$ (eq1)

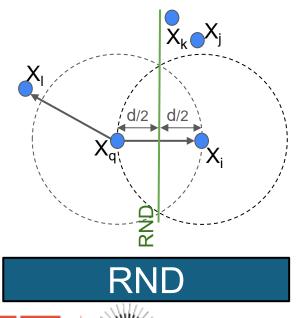
Where:

- \circ X_q is the query node.
- \circ X_j is a candidate neighbor being considered for inclusion in R_q and is part of C_q .
- X_i are nodes already in the set R_q.
- o dist (X_a, X_b) represents the Euclidean distance between nodes X_a and X_b in the d-dimensional space.



Neighborhood Diversification Today

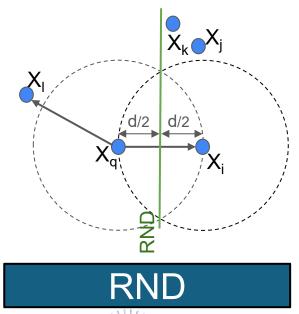
1. Relative ND (RND) → approximate RNG as |Cq| << |V|

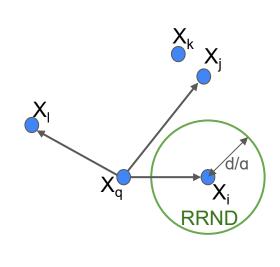




Neighborhood Diversification Today

- 1. Relative ND (RND)
- 2. Relaxed RND (RRND): $(eq_1) \Rightarrow \forall X_j \in R_q$, $dist(X_q, X_j) < \alpha.dist(X_i, X_j)$ for $\alpha > 1$





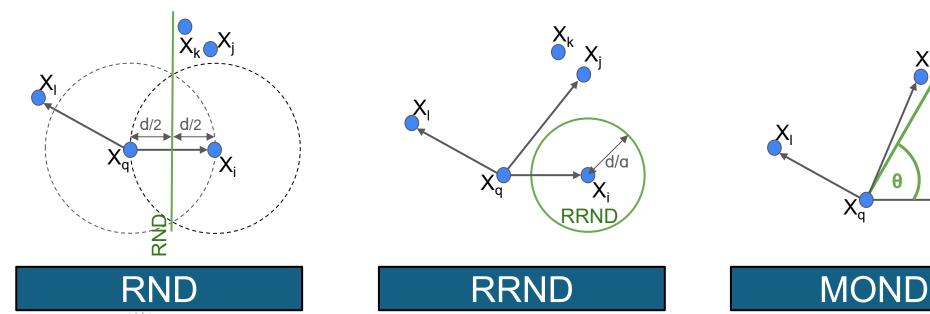
RRND





Neighborhood Diversification Today

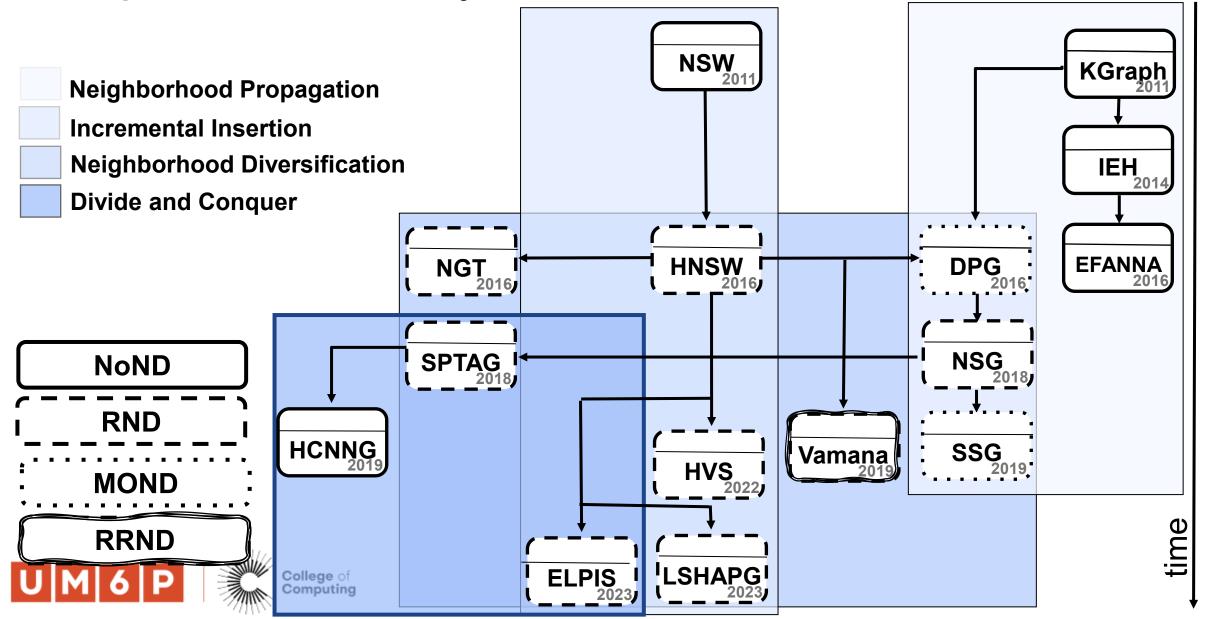
- 1. Relative ND (RND)
- 2. Relaxed RND (RRND): $(eq_1) \Rightarrow \forall X_j \in R_q$, $dist(X_q, X_j) < \alpha.dist(X_i, X_j)$ for $\alpha > 1$
- 3. Maximum-Oriented ND (MOND): $(eq_1) \Rightarrow \forall X_j \in R_q$, $cos(\angle X_i X_q X_j) < cos(\theta)$





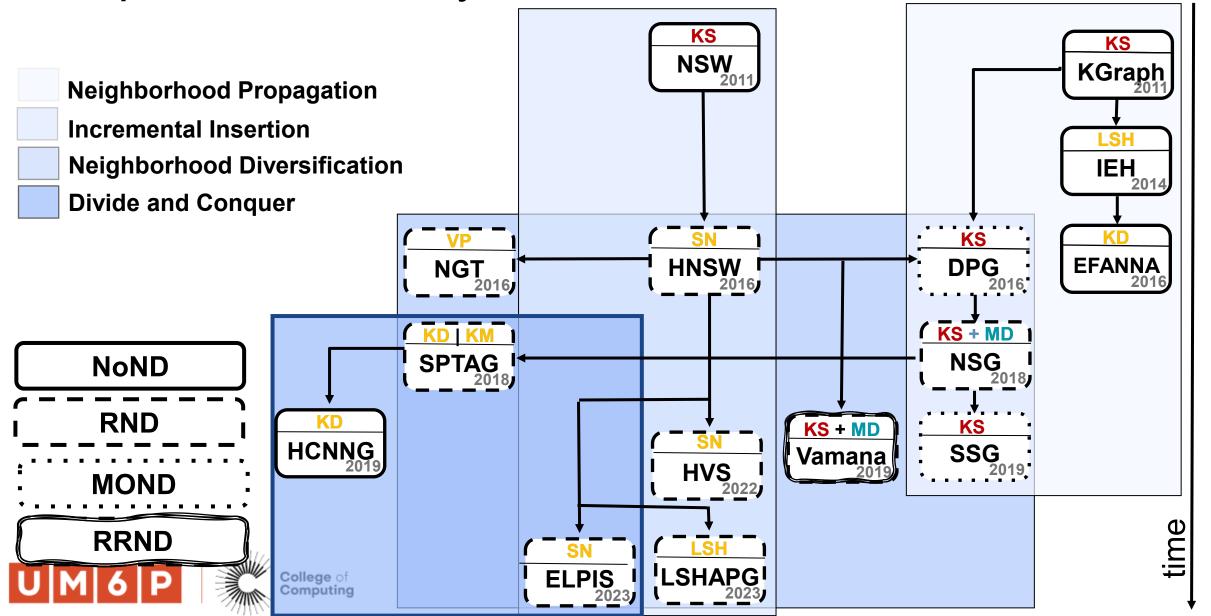


Proposed Taxonomy



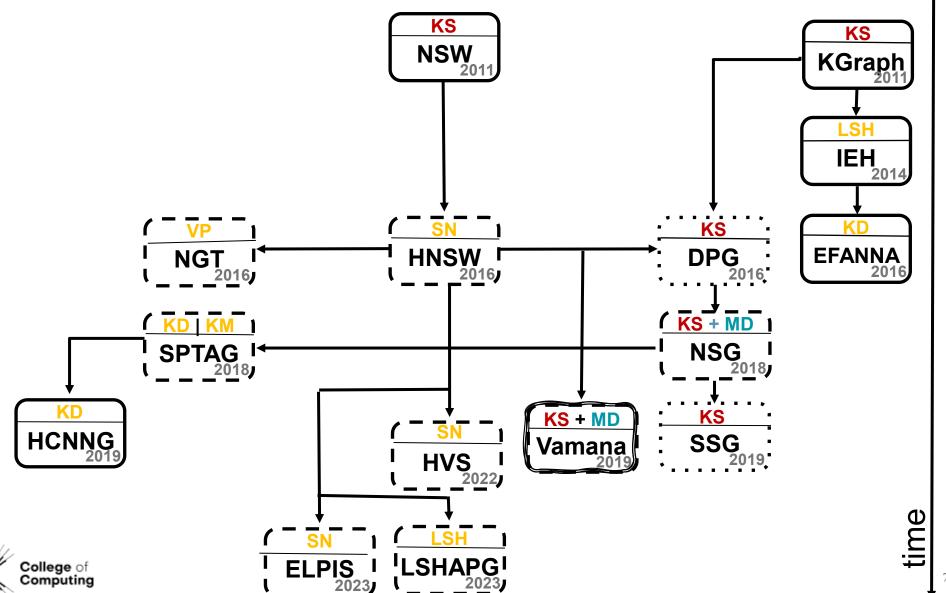
Proposed Taxonomy

Randomized Seed Selection Index-based Seed Selection Predefined Seed Selection



Seed Selection

Randomized Seed Selection Index-based Seed Selection Predefined Seed Selection





Experimental Evaluation – Datasets

- **Sift1B**: 1 billion vectors of 128 dimensions representing the Sift image feature descriptors.
- Deep1B: 1 billion vectors of 96 dimensions extracted from the last layers of a convolutional neural network.
- Sald: 200 million neuroscience MRI data series of size 128.
- **Seismic**: 100 million data series of size 256 representing earthquake recordings at seismic stations worldwide.
- **Gist**: 1 million vectors of 960 dimensions representing image descriptors that capture spatial structure and color layout.
- **ImageNet**: 1 million vectors of 256 dimensions generated from ImageNet using a ResNet50 model, followed by PCA for dimensionality reduction.
- **Text-to-Image**: 1 billion 200-dimensional image embeddings (from Se-ResNext-101) paired with 50 million text queries (from DSSM) for cross-modal retrieval tasks.
- **RandPow***i*: contains vectors of 256 dimensions generated randomly following power law distribution using power law exponent *i*.



Experimental Evaluation – Query Workloads

- Query sets include 100 vectors processed sequentially, not in batches, mimicking a real-world scenario where queries are unpredictable.
- Results with 1 million queries are extrapolated from 100 query sets.
- For Deep, Sift, GIST, and Text-to-Image, queries are randomly sampled from available query workloads.
- For SALD, ImageNet, and Seismic, For SALD, ImageNet, and Seismic, 100 queries are randomly selected from the datasets and excluded from the index-building phase.
- For hardness experiments, we use Deep query vectors of varying complexity, denoted as a percentage ranging from 1% to 10% (percentage indicating the gaussian noise added).



Experimental Evaluation – Hard Query Workloads

Local Intrinsic Dimensionality (LID):

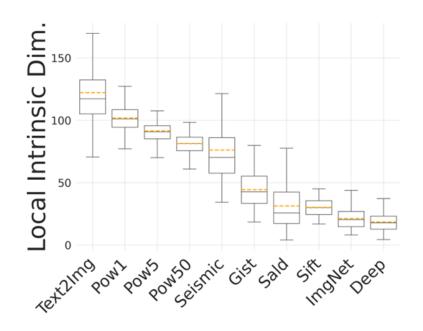
$$\mathrm{LID}(x) = -\left(\frac{1}{k}\sum_{i=1}^k\log\frac{\mathrm{dist}_i(x)}{\mathrm{dist}_k(x)}\right)^{-1}$$

Local Relative Contract:

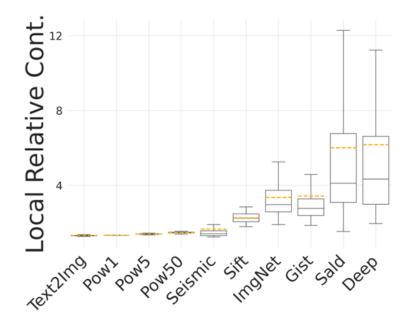
$$LRC(x) = \frac{\operatorname{dist}_{\operatorname{mean}}(x)}{\operatorname{dist}_k(x)}$$



Experimental Evaluation – Query Workloads



(a) Local Intrinsic Dimensionality (LID): low values indicate easy search



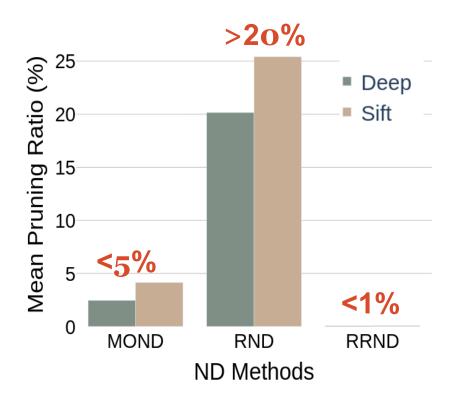
(b) Local Relative Contrast (LRC): high values indicate easy search

Fig. 4. Dataset Complexity

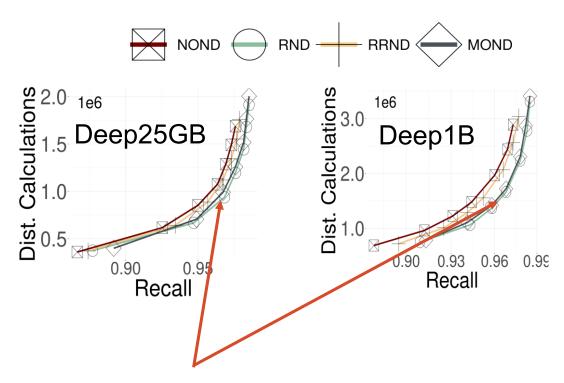




Experimental Evaluation - ND



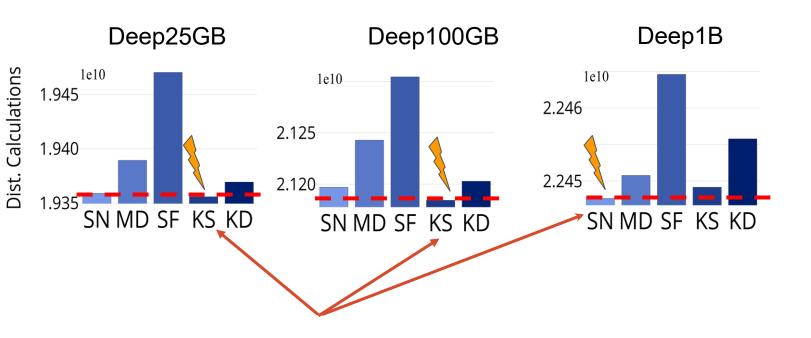
RND prunes at least 5x and 20x more than MOND and RRND, leading to a smaller index size and search memory footprint.



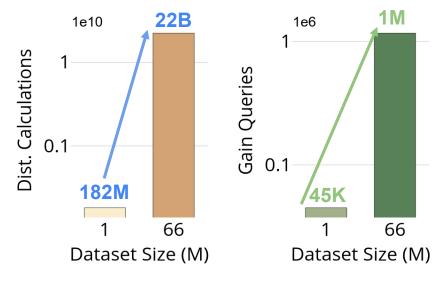
RND leads to the best search efficiency across datasets and dataset sizes.



Experimental Evaluation - SS



Optimizing data structures for seed selection enhances search efficiency on large datasets



Deep1M and Deep25GB (SN-KS)

The choice of seed selection impacts index efficiency as well





Experimental Evaluation - Baselines

- HNSW [12]
- NSG [10]
- VAMANA [13]
- SPTAG [14]

- NGT [15]
- SSG [9]
- LSH-APG [17]
- HCNNG [18]

- DPG [11]
- EFANNA [8]
- KGRAPH [7]
- ELPIS [X]

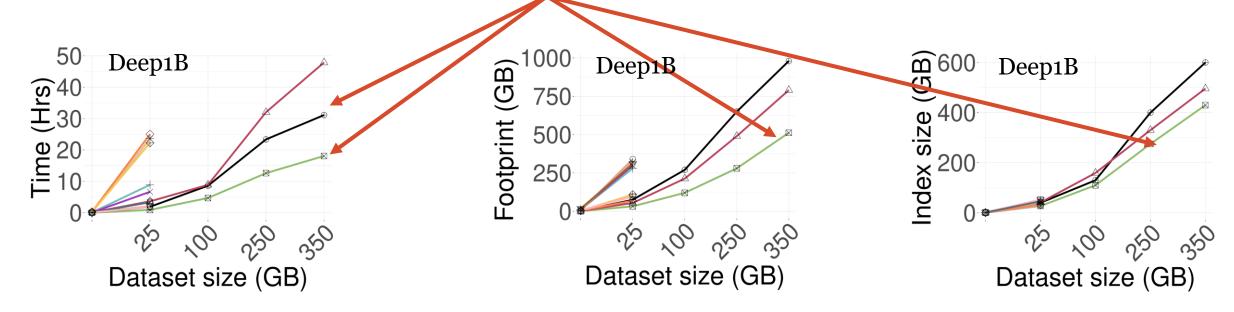




Experimental Evaluation – Indexing Performance



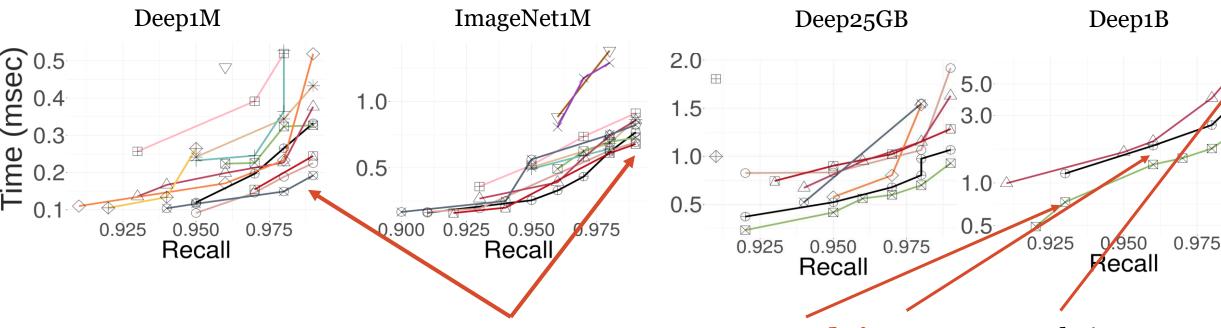
Graph methods based on incremental insertion are the most scalable





Experimental Evaluation – Search Performance





graph-based methods based on ND lead

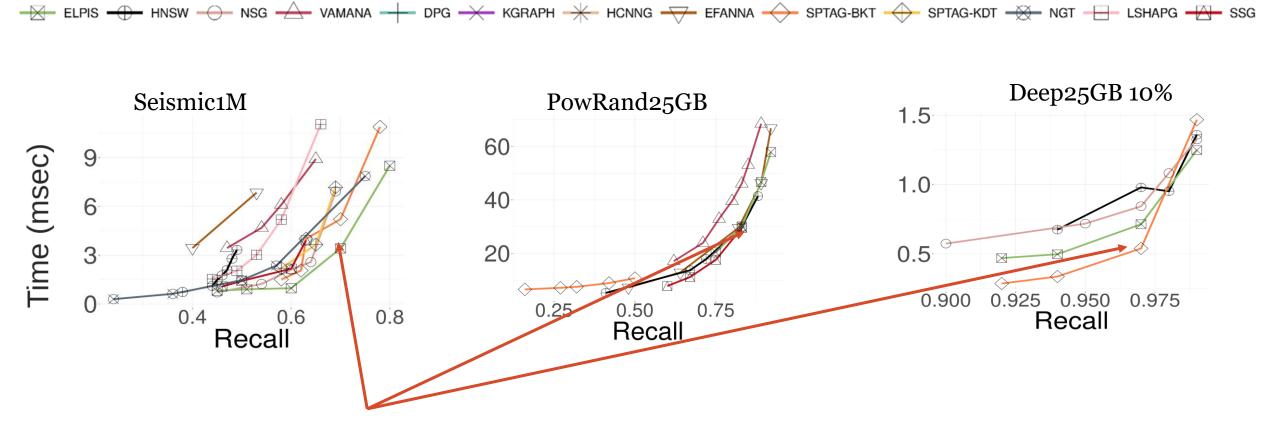
to the best **search performance**

Elpis, **HNSW** scale in billion-scale datasets





Experimental Evaluation – Search Performance

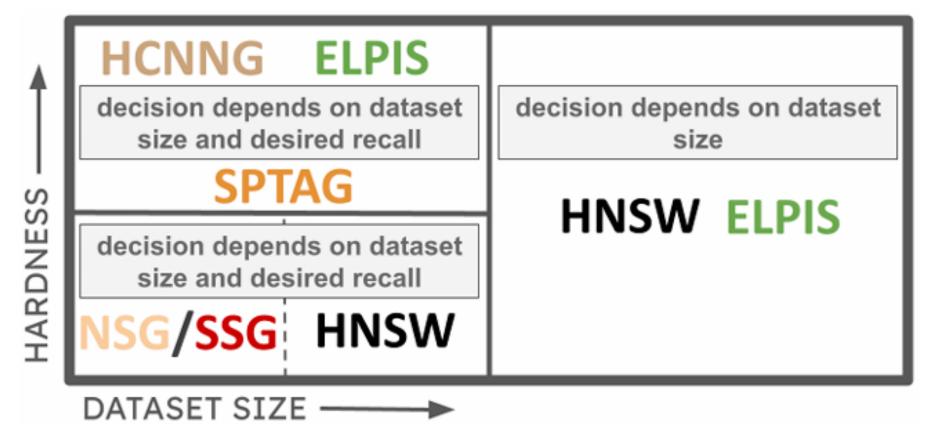


Divide and Conquer graph-based methods lead the best search

performance on hard datasets and workloads



Recommendations



Indexing + 10K queries (0.99 recall)





Unexpected Results

- Simple SS approaches like K-random sampling outperform Stacked NSW on small and medium sized datasets.
- Some methods (SPTAG, NGT, NSG, and SSG) cannot build an index on large datasets (>=100GB) within hours, despite excellent performance on smaller datasets (1M and 25GB).
- DC-based approaches (Elpis, SPTAG) outperform the others on challenging datasets/workloads.



Key Takeaways

- No method wins across the board.
 - II-based methods scale best overall at indexing and query answering
 - ND-based methods have superior query answering
 - DC-based methods scale best at indexing and challenging datasets/query workloads
- Adopting ND to sparsify the graph always leads to better search performance, particularly on large datasets.
- Effective SS plays a crucial role in enhancing both search and indexing performance.



Promising Research Directions

Graph-based search:

- Theoretical studies to better understand the trade-offs between proximity and sparsity.
- Lightweight SS strategies to further improve search and indexing performance, particularly for out-of-distribution queries.
- Hybrid methods that combines the strengths of II, ND and DC.
- Adaptive methods that cater to dataset characteristics such as dataset size, dimensionality, RC and LID.
- Novel base graphs, clustering and summarization techniques tailored for DC-based methods can further improve their performance.
- Filtered search:
 - Range search
 - Updates
 - Non-ED distances
 - Disk-based



Promising Research Directions

- Tree-based search:
 - Improve summarization techniques for exact search
 - Higher tightness of the lower-bound
 - Cheaper to compute
 - Support probabilistic/deterministic approximate search
 - More effective stopping criteria
 - Guarantees on recall not only distance error
 - Exploit modern hardware



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vector search, data mining, data valuation, applications to RAG/GenAI pipelines and health



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