

SIGMOD PODS 2024

Vector Database Management Techniques and Systems

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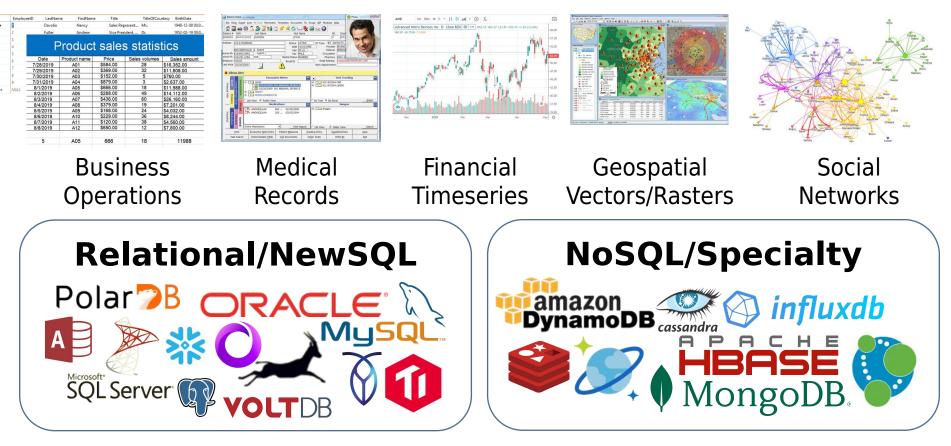






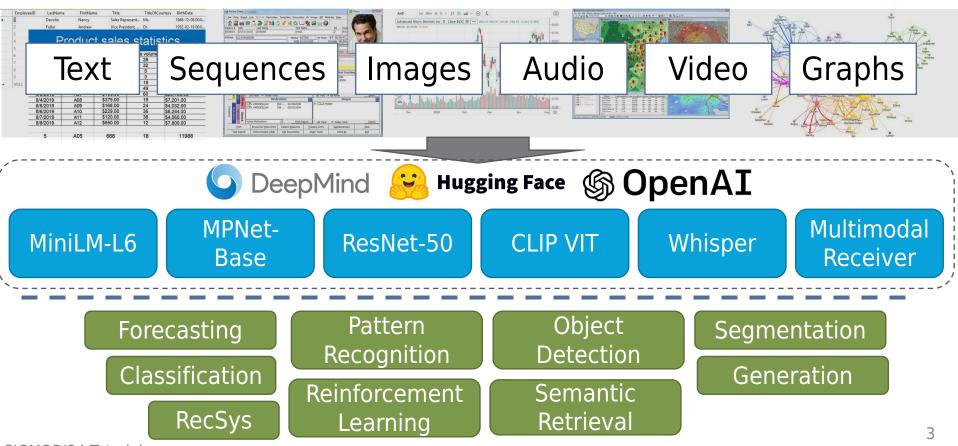
Modern DBMS Landscape

Modern DBMSs are designed for data that humans can understand

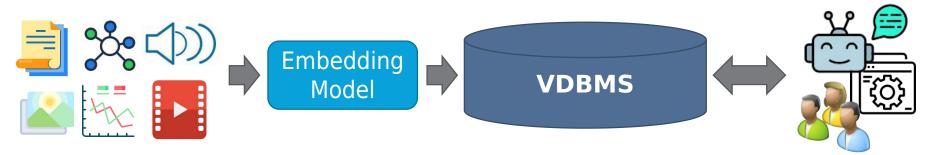


Embeddings: Building Blocks of the Future

More and more applications rely on deep-learning embedding vectors that can only be understood by machines



Goal: Vector DBMS (VDBMS)

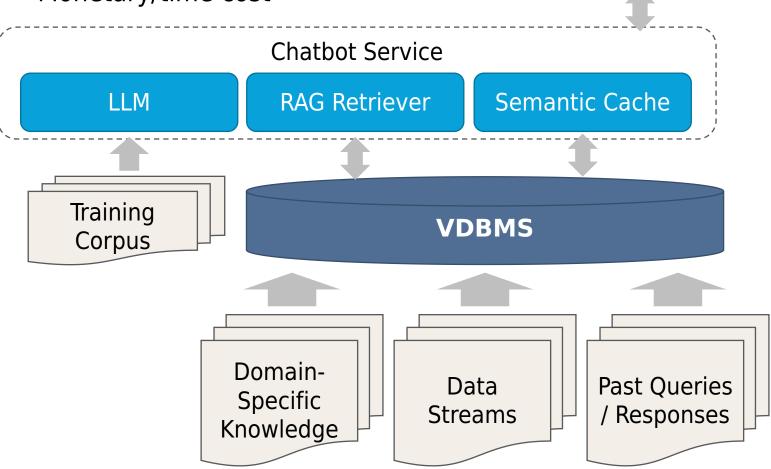


Store embeddings in a database and retrieve desired embeddings for whatever downstream task

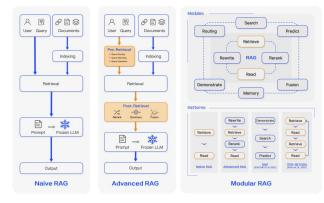
- Capabilities: similarity-based top-k/range retrieval, hybrid attribute-vector retrieval, multi-modal (multivector) retrieval
- Characteristics: read/write latency/throughput, retrieval accuracy, scalability, availability, consistency, fault tolerance, privacy & security, elasticity

Example: LLMs + VDBMS

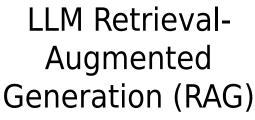
- Lack of domain-specific knowledge
- Data freshness
- Monetary/time cost



Some of Today's Commercial Applications







https://arxiv.org/abs/2312.10997



News Classification

E-Commerce & Recommendation Systems



Writing Assistant





Photo/Video Search & Deduplication Threat Detection

Why is Building a VDBMS Hard? Embeddings are...

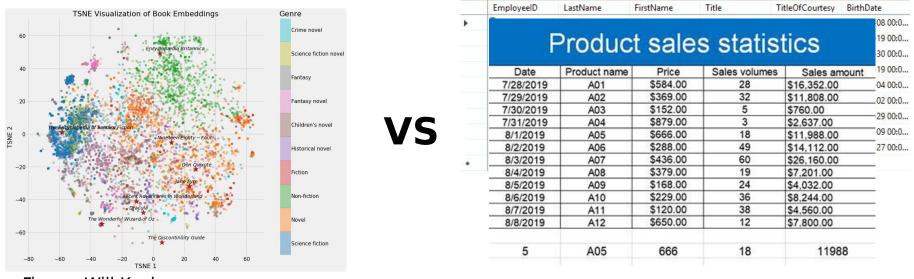


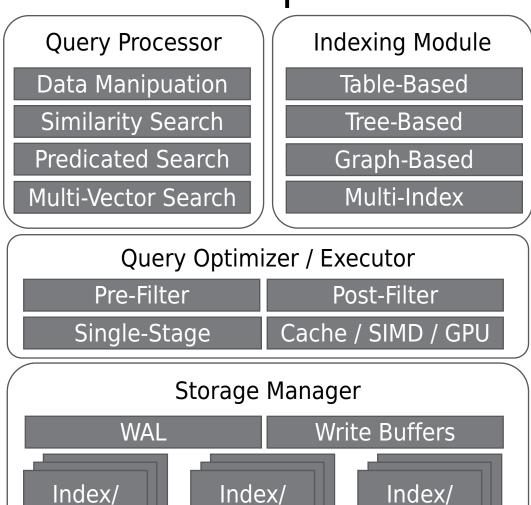
Figure: Will Koehrsen

- Huge (1024 x float64) \rightarrow costly to move, clog storage
- Hard to retrieve without ambiguity
- Hard to index
- Costly to compare
- Hard to index together with attributes



Part 1: VDBMS Techniques

Data



Data

Physical Storage (SSD / S3 / HDFS)

Data

Overview of Query Processing

Query Processor

Data Manipuation

Similarity Search

Predicated Search

Multi-Vector Search

- High dimensionality
- Large data volume
- Low latency
- High accuracy

Query Definition

Similarity Score

- Metrical Scores
- Non-Metrical Scores

Query Type

- Data Manipulation
- Range Search
- (c,k)-Search
- Variants

Query Interface

• API, SQL

Operators & Algorithms

Vector Operators

- In/Up/Del
- Object Embedding
- Vector Math
- Vector Projection

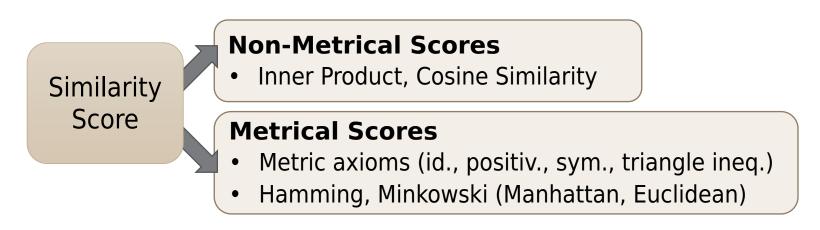
Search Operators

- Table Scan, Top-K
- Index-Based Operators

Search Algorithms

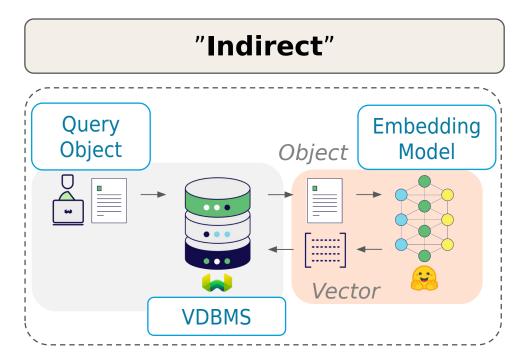
- Brute-Force Search
- Index-Based Search

Query Definition: Similarity Scores

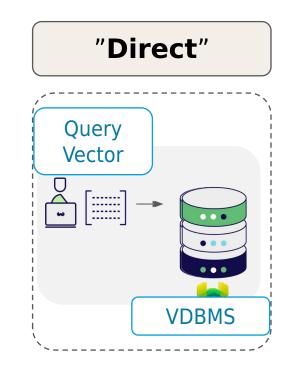


- A function $f: \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}$ indicating degree of similarity
- Similarity calculations are expensive
 - Sq. Euclidean (D=1024 floats) takes 62us on my machine (Intel i5 @ 2.3 GHz), about the same as SSD random seek

Query Types: Data Manipulation

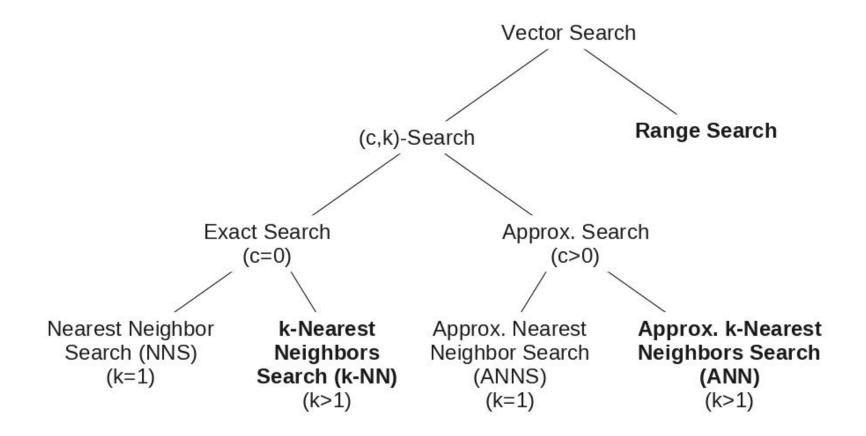


- VDBMS interacts with embedding model via plugin/add-on/extension
- More user friendly



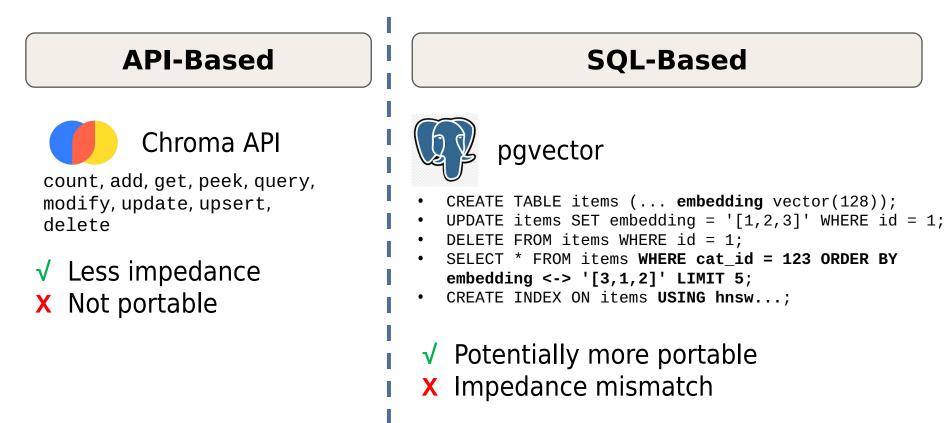
- User is responsible for producing embeddings
- More controllable (e.g. custom embedding model)

Query Types: Vector Search Queries

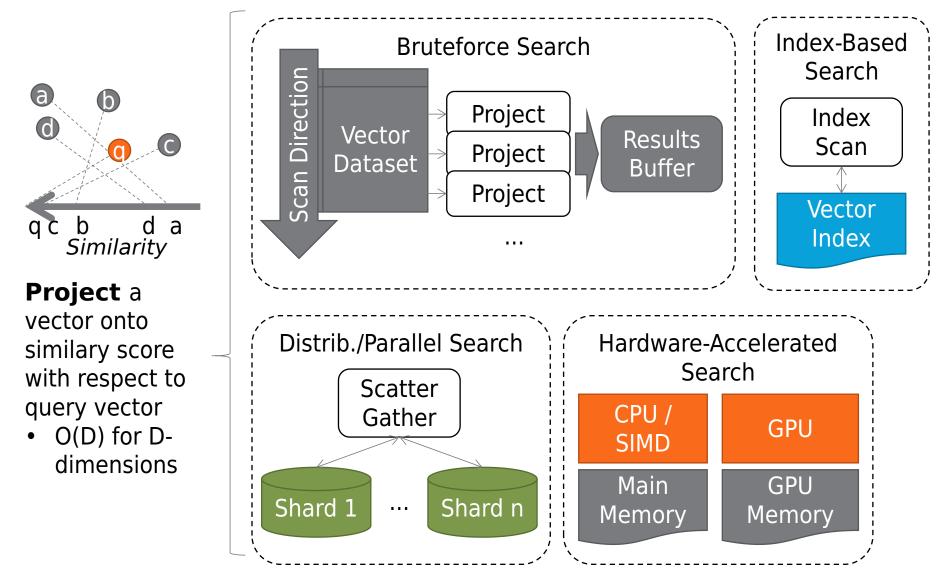


Query Variants: predicated, batched, multi-vector

Query Interfaces



Operators & Algorithms



Characteristics of Search Algorithms

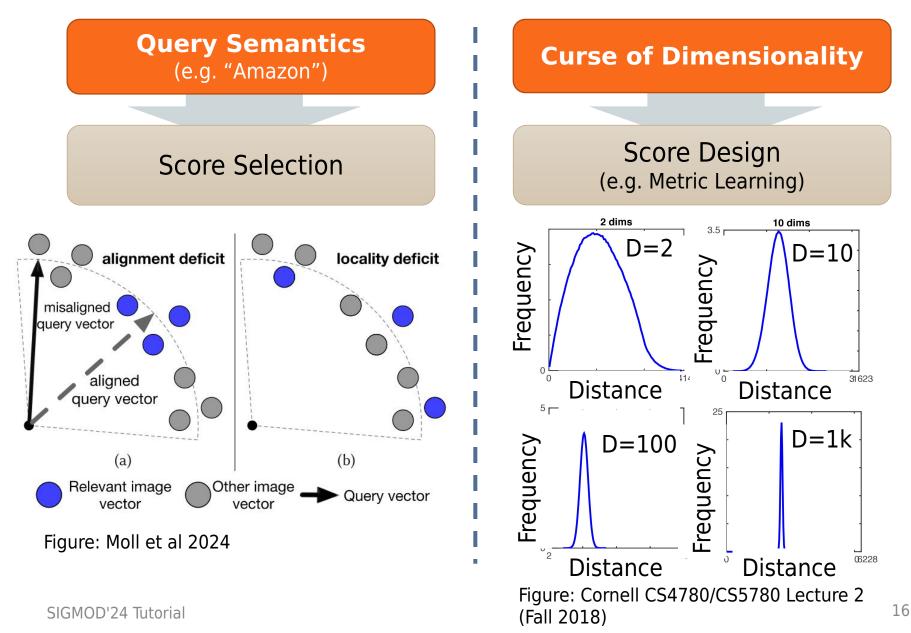
Performance

• Amount of visited vectors, similarity comparisons

Accuracy

- Recall: (true positives) / (true positives + false negatives)
- Recall@K
 - Recall when k=K for k-NN, ANN (Li et al 2020)
 - Proportion of queries where 1-NN is ranked in first k results (Jegou et al 2011)
 - Proportion of true nearest-neighbors within the first K results of a k-NN or ANN query (K \leq k) (RecSys)
- Precision: (true positives) / (true positives + false positives)

Challenges to Query Processing



Overview of Storage & Indexing

Indexing Module

Table-Based

Tree-Based

Graph-Based

Multi-Index

- High dimensionality
- Large data volume
- Low latency
- High accuracy
- Construction cost
- Storage cost
- Maintenance cost

Construction / Search / Maint.

Construction

- Randomization
- Learned Partitions
- Navigable Partitions

Search

- Bucket Scan
- Defeatist Search
- Best-First Search

Maintenance

• Rebalancing

Logical / Physical Storage

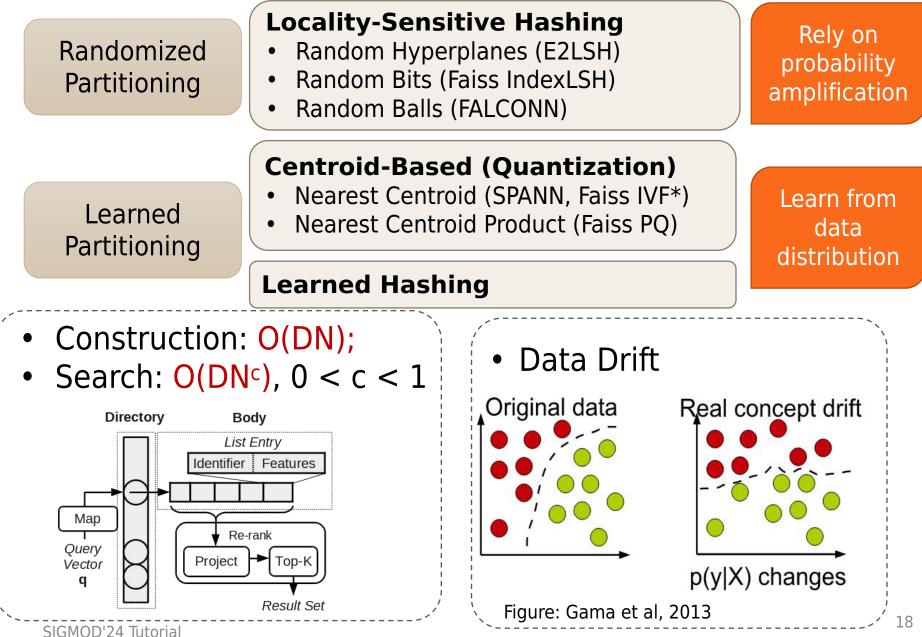
Logical Structure

- Tables
- Trees
- Graphs

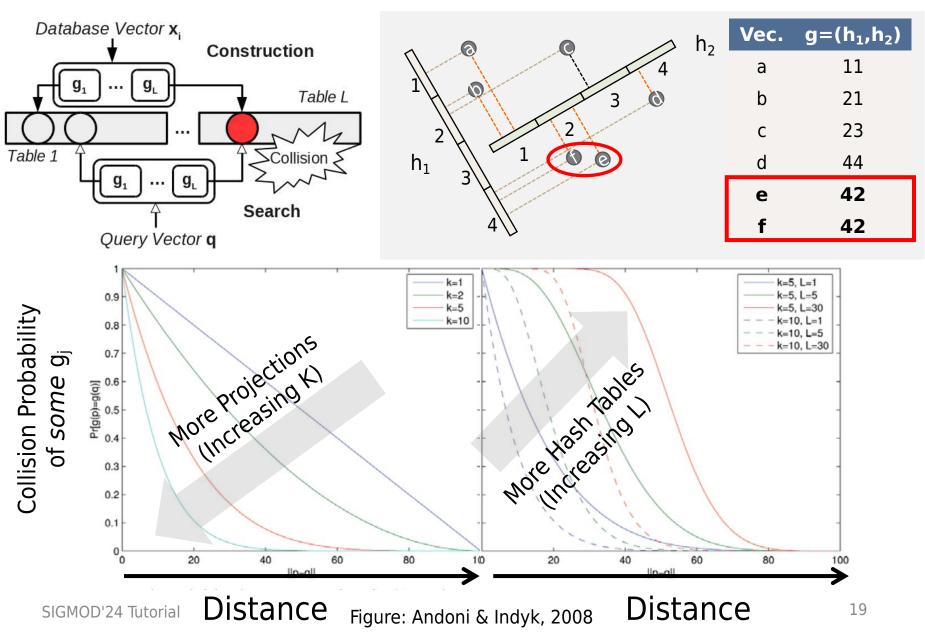
Physical Structure

- Quantization
- Disk-Resident Indexes

Table-Based Indexes

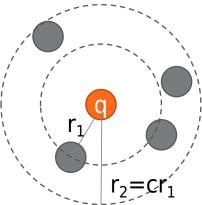


Locality-Sensitive Hashing (LSH) e.g. E2LSH L=2, K=4

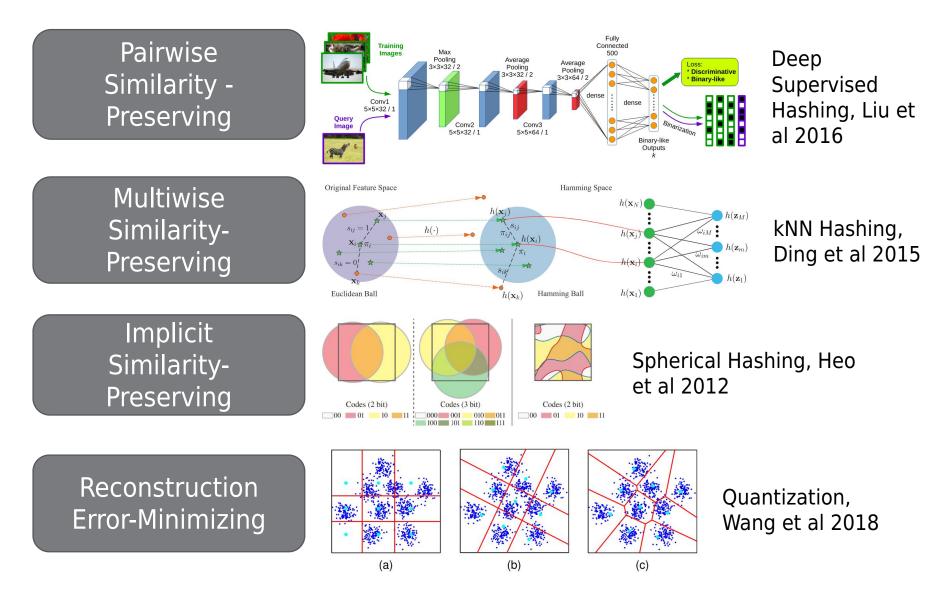


LSH Families

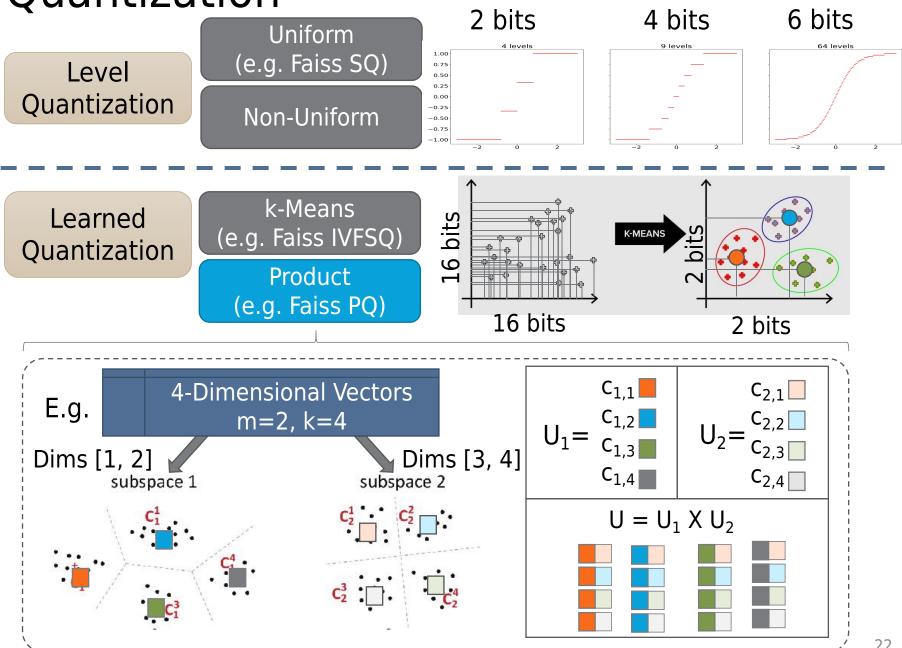
- "Hash Family": For any r_1 , r_2 , $x \in S$, and q:
 - if $d(x, q) \le r_1$, then collision prob. $\ge p_1$ Large is Better
 - if $d(x, q) \ge r_2$, then collision prob. $\le p_2$ Small is Better
- Typically storage ~ $O(DN^{1+\rho})$, search ~ $O(DN^{\rho})$ where $\rho = \frac{log(1/p_1)}{log(1/p_2)}$
- Interesting families:
 - Hamming (Faiss IndexLSH) $\rho = 1/c$
 - Random hyperplans (E2LSH) $\rho = 1/c$
 - Spherical LSH (FALCONN) $\rho = 1/(2c^2-1)$



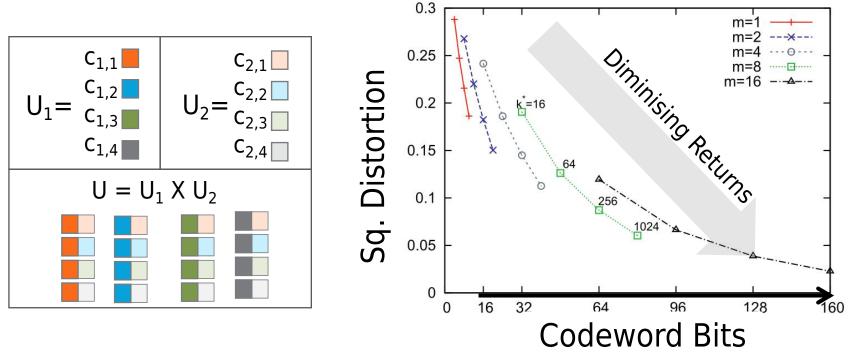
Learning to Hash (L2H)



Quantization

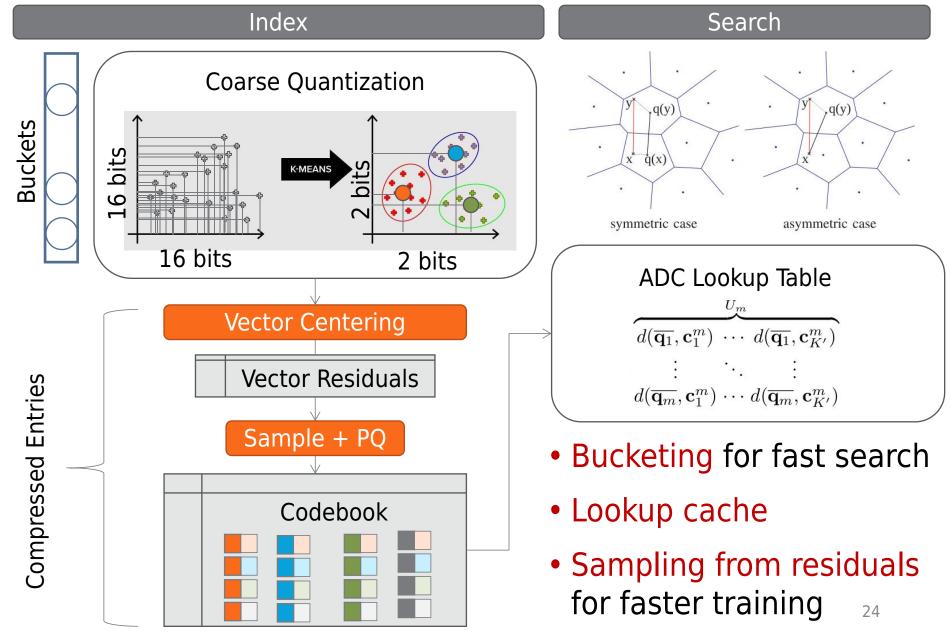


Product Quantization

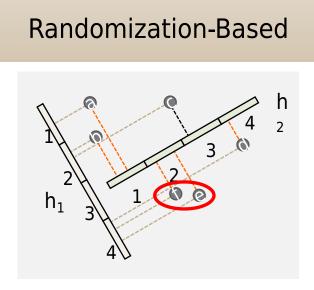


- Preserves dimensions, e.g. $R^4 = R^2 X R^2$
- Faster training
 - 4 centroids per subspace = 16 total codes
 - k-means O(DN*k): 2(2N*4) = 16N vs 4N*16 = 64N

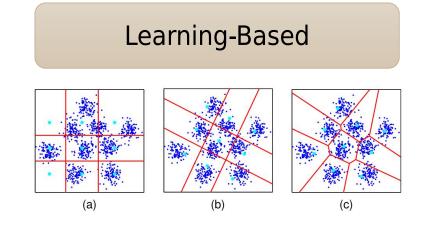
"IVFADC" Asymmetric Distance Comp.



Summary of Table-Based Indexes



- E.g. Faiss IndexLSH, E2LSH, FALCONN
- ✓ Theoretical guarantees✓ No rebalancing
- X High storage costs



E.g. L2H, SQ, PQ, IVFADC

- ✓ Low storage costs
- ✓ Low latency
- **X** Susceptible to data drift

Table-Based Indexes: Discussion

Advantages

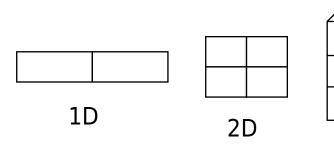
- ✓ Disk-friendly, E.g. LSH, SPANN
- ✓ Readily supports in-distribution insert/update/delete
- ✓ Easier to derive error bounds

Disadvantages

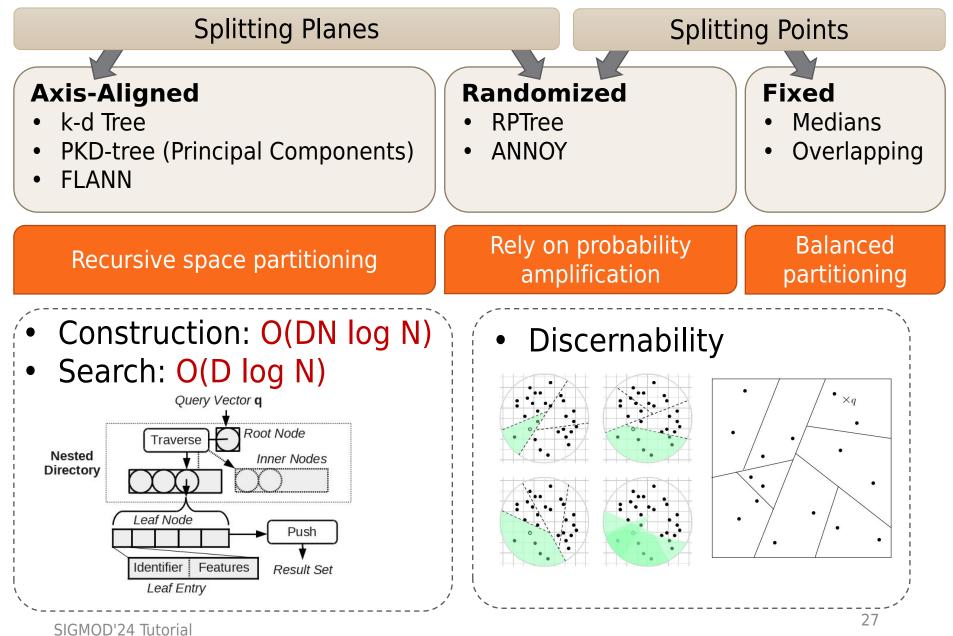
X Hard to deal with queries near borders/corners

• How many buckets are adjacent to a corner in a D-dimensional space?

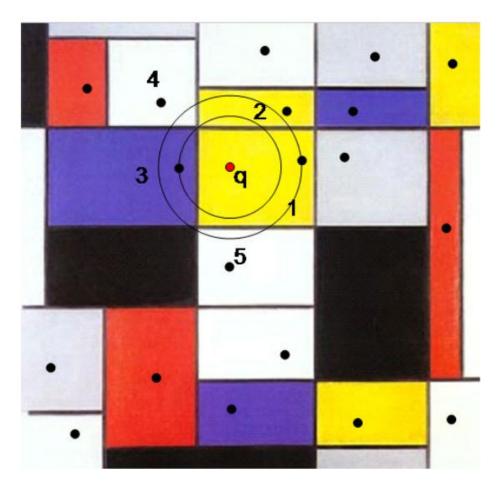
3D



Tree-Based Indexes

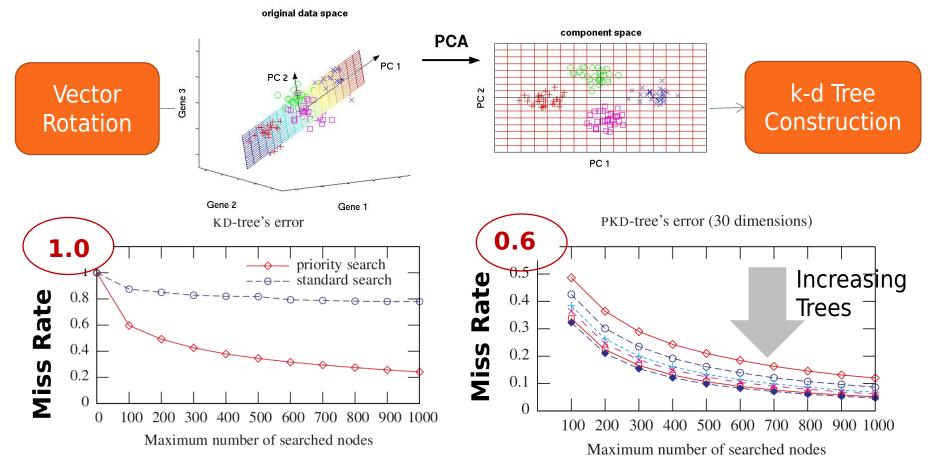


k-d Tree



- O(DN^{1-1/D}) search, O(DN log N) construction
- Tends toward O(DN) as D grows

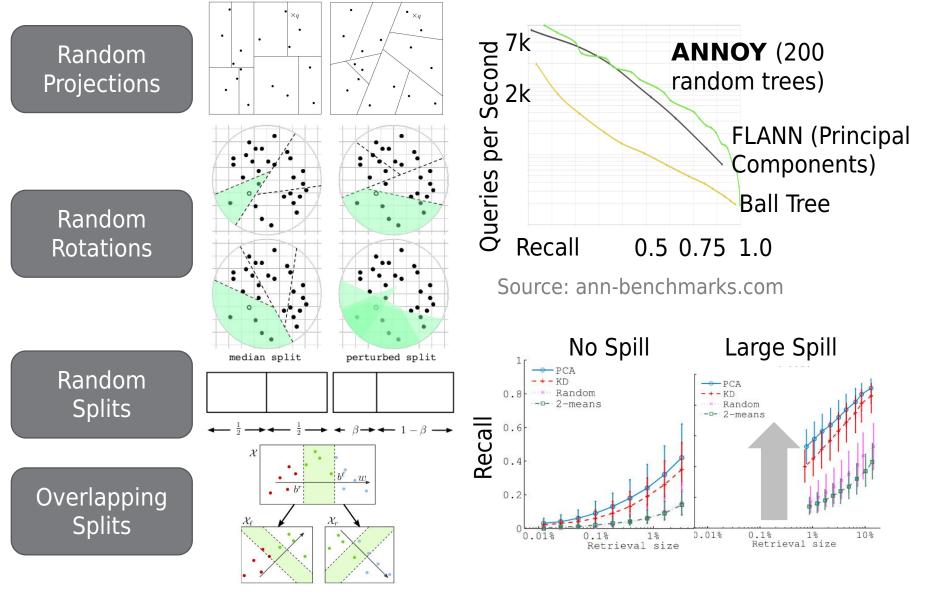
Principal Component Trees



- More discernability by aligning to principal components
- No huge gains from multiple trees

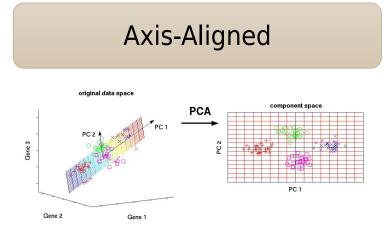
SIGMOD'24 Tutorial

Random Projection Trees



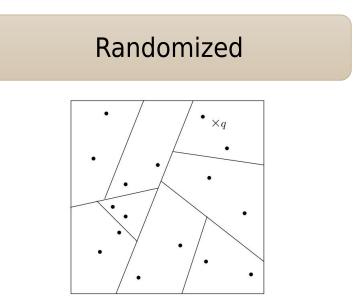
Figures: Dasgupta & Sinha 2013, Dasgupta & Freund 2008, Ram & Sinha 2019, McFee & Lanckriet 2011

Summary of Tree-Based Indexes



E.g. k-d Tree, PKD-Tree, FLANN

✓ High recall for low dims.X Inflexible





✓ High recall for high dims.X High storage (forests)

Tree-Based Indexes: Discussion

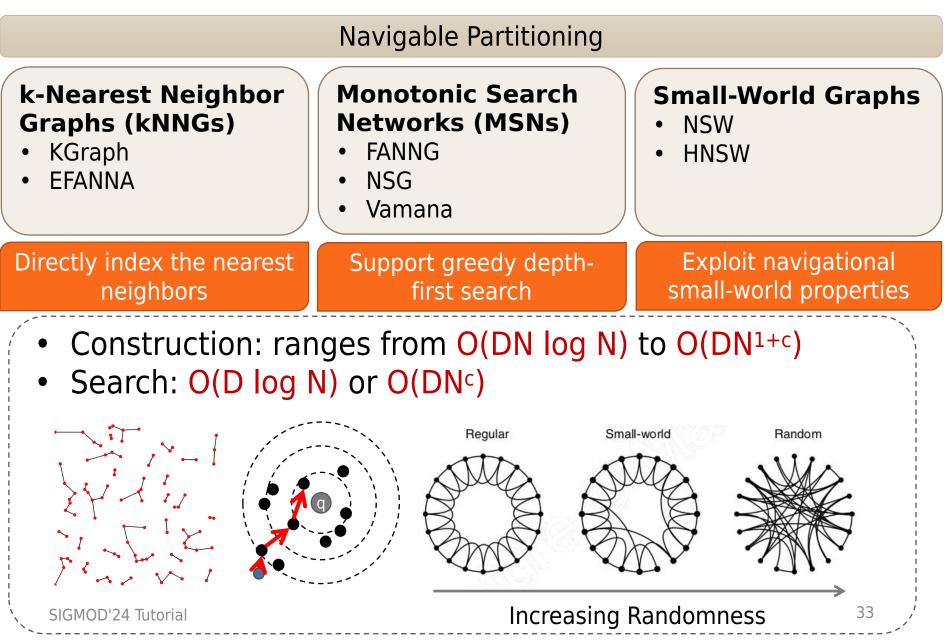
Advantages

- ✓ Disk-friendly in principle (store together by leaf)
- ✓ O(D log N) defeatist search
- ✓ Supports in-distribution insert/update/delete

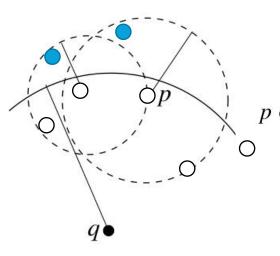
Disadvantages

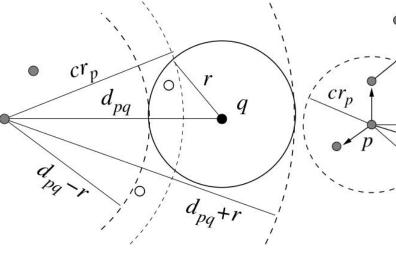
- **X** Hard to keep balanced following data drift
- X Low recall for queries near leaf borders / corners

Graph-Based Indexes



k-Nearest Neighbor Graphs (kNNGs)





A. Sampled point inside query ball \rightarrow check its neighbors

B. Point ball intersects query ball \rightarrow check neighbors in the overlap

C. Point ball outside query ball \rightarrow prune near neighbors of p

 d_{pq}

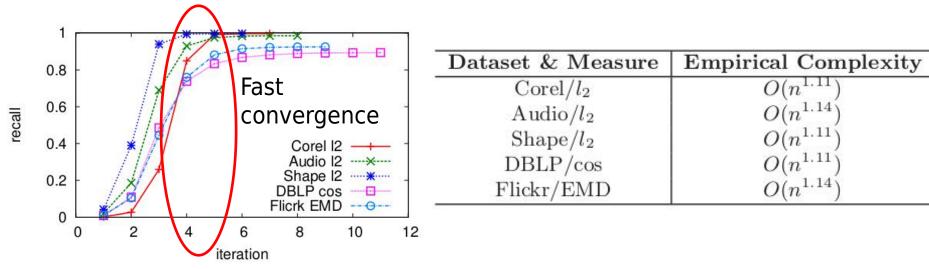
 O(1) search for queries in dataset, else O(DN^{1+c}) via sample and prune (see above)

Construction

• Exact: O(DN²)

KGraph (NNDescent)

"A neighbor of a neighbor is likely to also be a neighbor"



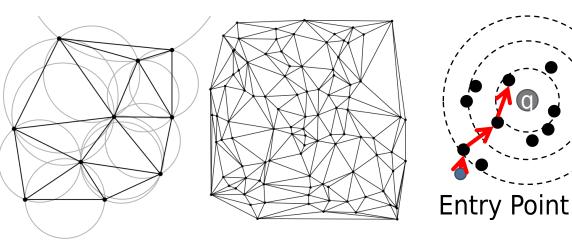
Construction

- Initialize random kNNG
- For each node, change any 2-hop neighbor into a 1-hop neighbor if it is a new k-nearest neigbor
- Repeat until convergence

Monotonic Search Networks (MSNs)

"Greedy search is all you need"

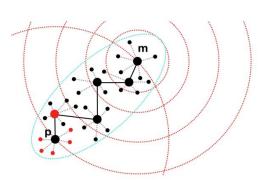
Figures: Delaunay triangulation (Wikipedia)





 Probe the graph by conducting searches from a random entry point to a random query point in the dataset, e.g. FANNG

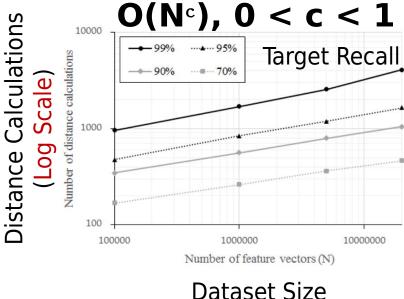




 Designate a point as the sole entry point for all search trials, e.g. NSG, Vamana

Fast ANN Graph (FANNG)





(Log Scale)

Construction

- O(N) trials, each trial O(N^c) to yield O(N^{1+c})
- Occlusion rule prunes redundant edges to limit out-degrees

Navigating Spreading-Out Graph (NSG)

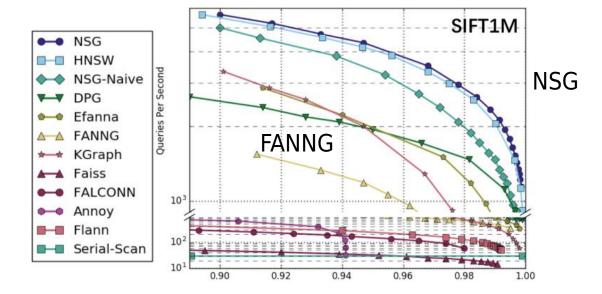
- Single source makes it easier to establish monotonic search paths from this node to all other nodes
- Spanning tree ensures connectivity

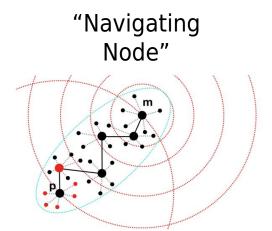
Construction

• O(N1+c log Nc)

Search

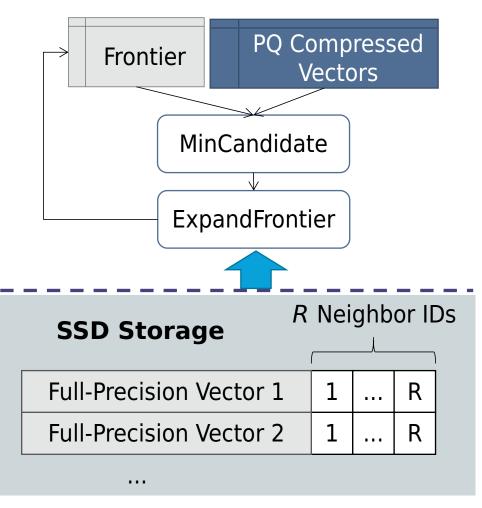
 ~O(log n) due to higher quality neighborhoods



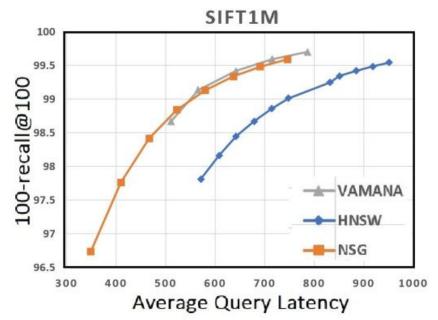


Vamana/DiskANN

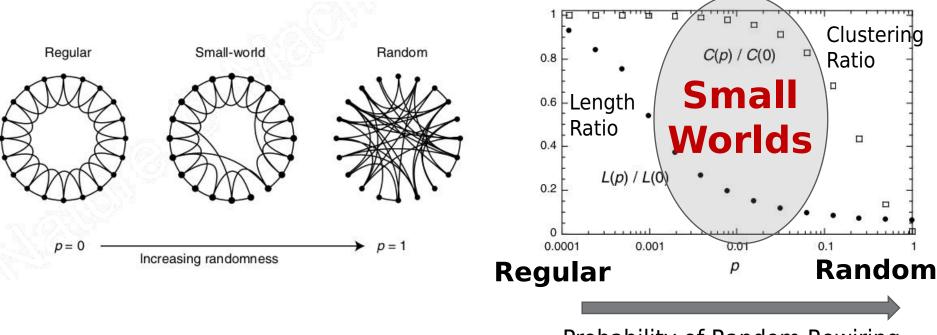
VamanaIndexScan



- Similar to NSG
- On-disk neighborhoods
- Edge traversal performed in memory using compressed vectors



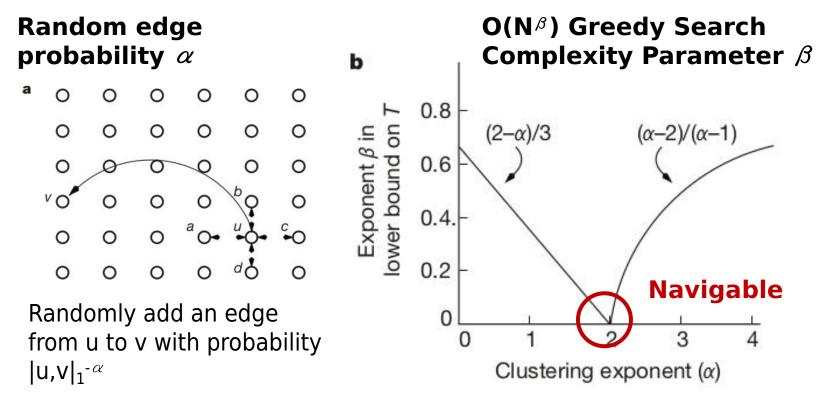
Small-World Graphs



Probability of Random Rewiring

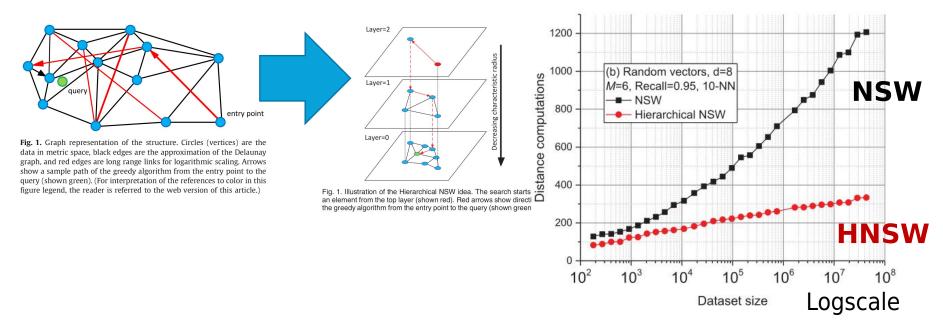
- Small characteristic path lengths (short shortest-paths)
- High clustering (friend of a friend is also my friend)

Navigable Small-World Graphs



- Not all small-world graphs permit O(log N) greedy search
- (In Kleinberg's graph, only $\alpha = 2$ yields a navigable graph)

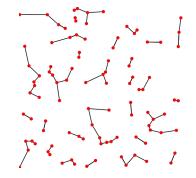
Hierarchical Navigable Small-World Graphs (HNSW)



- Simply **inserting vectors one at a time**, connecting it to its k nearest neighbors already in the graph found via search trial, is navigable and small-world
- Hierarchical levels mitigates high out-degrees

Summary of Graph-Based Indexes

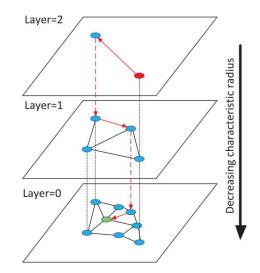
Nearest-Neighbor Graphs



E.g. KGraph (NNDescent)

✓ O(1) offline search
✓ Fast approx. construction
X Slow for online queries

Monotonic Search Networks / Small Worlds



E.g. FANNG, NSG, Vamana, HNSW

✓ ~O(log N) online searchX Slow construction

Graph-Based Indexes: Discussion

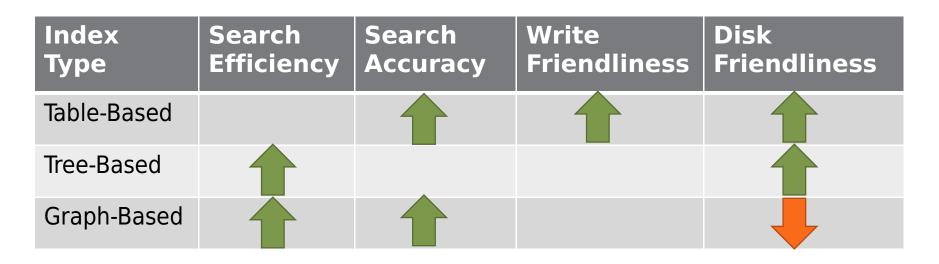
Advantages

Empirically state-of-art throughput/recall

Disadvantages

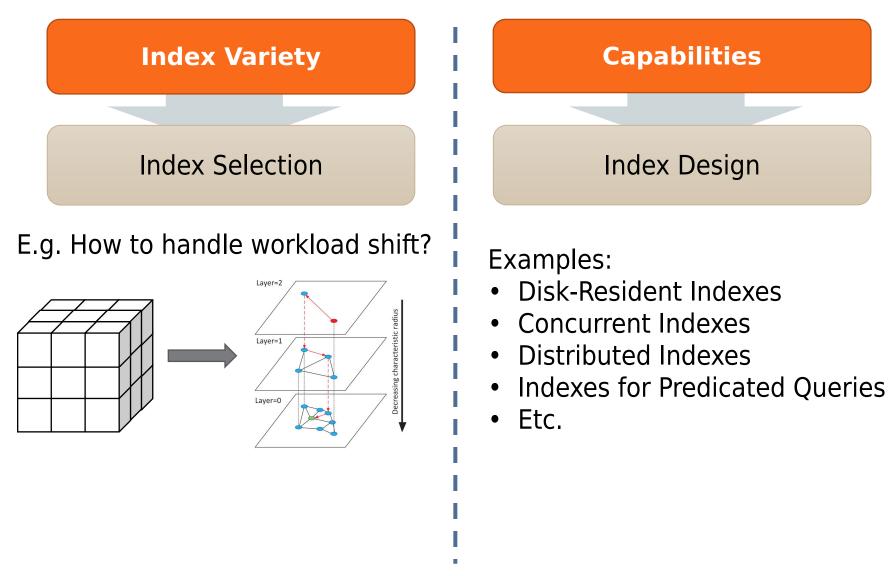
- X Hard to adapt to disk
- **X** Hard to support updates for many graphs
 - For HNSW: accuracy degradation issue
- X Long construction times for graphs based on search trials (incl. HNSW)

Summary of Indexes



Index Type	Construction Efficiency	Storage Efficiency	Ease of Maintenance
Table-Based			
Tree-Based			
Graph-Based			

Challenges to Storage & Indexing



Overview of Query Optimization

Predicated Vector Search Query e.g. select * from items where price < \$10 order by simTo(query) limit k



Plan Types

- Naive
- Pre-Filtering
- Post-Filtering
- Single-Stage Filtering



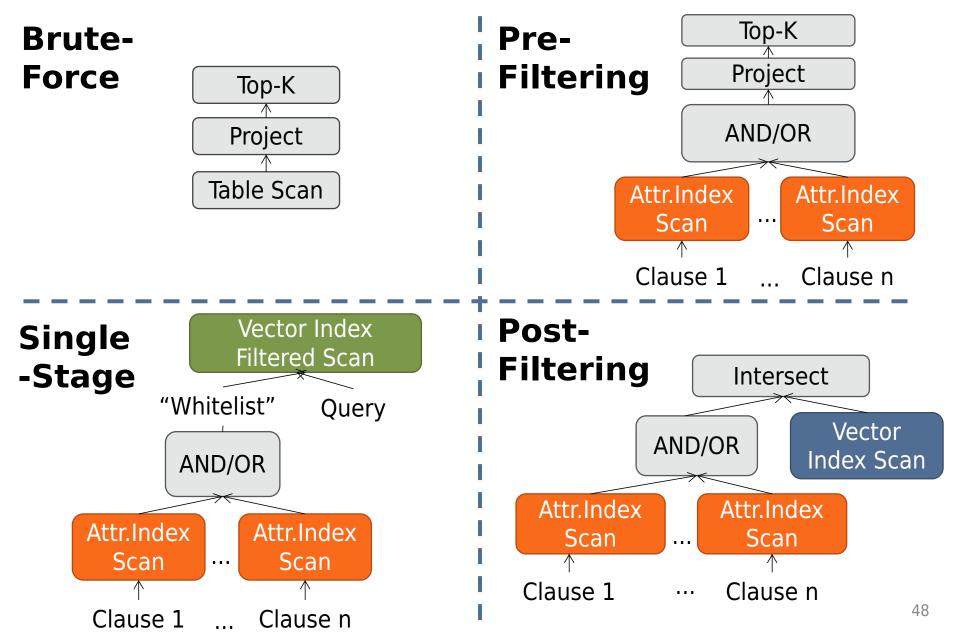
Cost-Based

- Cost Model
- Operator Costs

Rule-Based

• Rule Design

Plan Types for Predicated Queries



Summary of Plan Types

Plan Type	Advantages	Disadvantages	
Brute-Force	✓ Exact (100% Recall)	X High latency for weak filters	
Pre-Filtering	✓ Exact (100% Recall), efficient for strong filters	X High latency for weak filters	
Post-Filtering	✓ Efficient (Native vector search speed & native attribute filter speed)	X Low accuracy risk (e.g. empty intersection). Mitigation: collect (α k) similar vectors, not just k. E.g. ADBV	
Single-Stage Filtering ✓ No loss of recall, often more efficient than pre-filtering		X Possibly high latency for strong filters. Mitigation for graph-based indexes: Encourage visiting satisfying vectors, e.g. FilteredDiskANN, HQANN, NHQ; Increase reachability, e.g. ACORN; Decrease failures via partitioning, e.g. Milvus	

Plan Enumeration

Predefined, e.g. Weaviate, Milvus, ADBV

- Use a single predefined plan for all predicated queries, e.g. Weaviate, Pinecone
- Predefine multiple plans and select which plan to use at query time, e.g. ADBV, Milvus

Automatic, e.g. PASE, pgvector (PostgreSQL)

Let the optimizer automatically enumerate plans

Post-filter low-accuracy risk is real!



pashkinelfe commented on Sep 21, 2023 • edited 👻

Contributor) •••

I suppose the case when post-filtering depletes all (or most) of ann-found tuples is completely legit. Though considering how often are the related complaints I'd suggest it to be mentioned in readme/manual explicitly. Maybe both filtering by other attribute or "filtering" due to dead heap tuples could be mentioned both.

Plan Selection

Rule-Based, e.g. Qdrant, Vespa

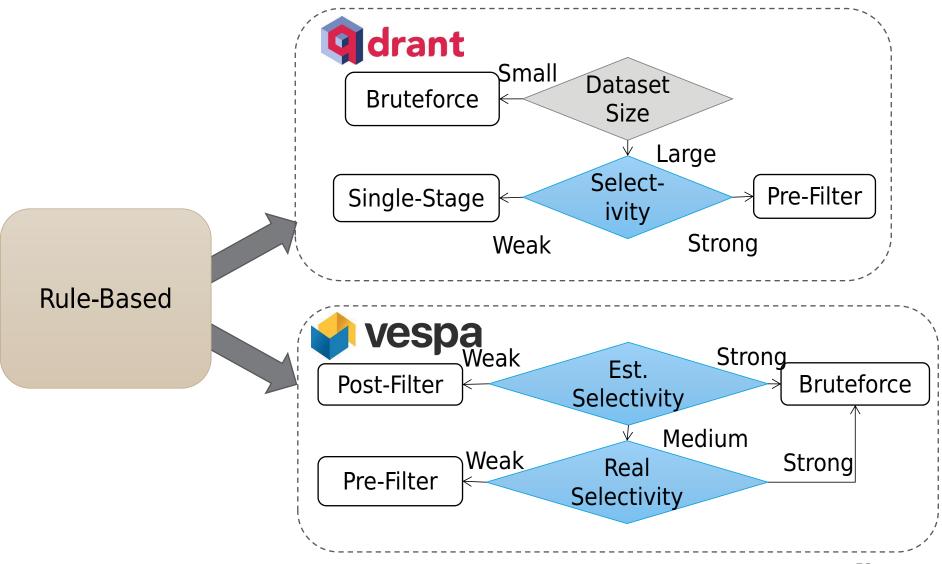
- Simple to implement
- Depends on accurate selectivity estimates

Cost-Based, e.g. ADBV, Milvus

- Select based on a cost model
- Generally more flexible
- Depends on accurate operator cost estimates

Rule-Based Plan Selection

Example: Qdrant and Vespa



Cost-Based Plan Selection in ADBV

Table 1: Notations used by hybrid query optimization

Notation	Meaning		
n	the total number of tuples in database		
α	the ratio between n and the number of records satisfying structured predicate		
β	the visited subcells ratio during VGPQ index search- ing process in VGPQ Knn Bitmap Scan		
γ	the visited subcells ratio during VGPQ index search- ing process in VGPQ Knn Scan		
$\sigma_{\{B,C,D\}}$	amplification factors of ANNS Scan operators in $Plan\{B, C, D\}$		
c_1	the total time cost to fetch a vector and compute pairwise distance		
c_2	the total time cost to fetch a $\tt PQ$ code and run $\tt ADC$		

- Pre-Filter k-NN Scan $cost_A = T_0 + \alpha \times n \times c_1$
- Single-Stage PQ Filtered Scan

 $cost_B = T_0 + \alpha \times n \times c_2 + \sigma_B \times k \times c_1$

• Single-Stage VGPQ Filtered Scan $cost_C = T_0 + \beta \times n \times \alpha \times c_2 + \sigma_C \times k \times c_1$

• Post-Filter VGPQ Scan

$$cost_D = \gamma \times n \times c_2 + \sigma_D \times k \times c_1$$

Challenges to Query Optimization

Cost Estimation



pashkinelfe Pavel Borisov

Single-Stage

 May be difficult to estimate cost of Vector Index Filtered Scan (i.e. backtracking)

Post-Filtering

 Hard to take into account low-accuracy risk I suppose the case when postfiltering depletes all (or most) of ann-found tuples is completely legit. Though considering how often are the related complaints I'd suggest it to be mentioned in readme/manual explicitly.

Source: pgvector Issue #263

Overview of Query Execution

Hardware Acceleration

Data Transfers

CPU Cache

HW Parallelism

• SIMD/GPU

Data Manipulation

Execution Mode

- Immediate
- Deferred

Distributed Query Processing

Partitioning

- Random/Uniform
- Attribute-Based
- Learned

Consistency

- Strong
- Eventual

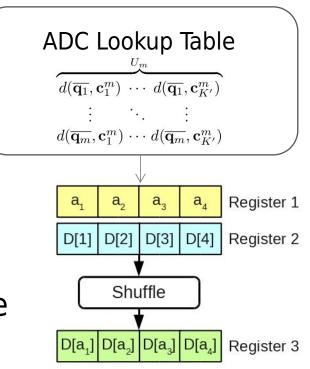
Hardware Acceleration

Data Transfers

 CPU Cache: "Query blocks" keep query vectors cache-resident while assigning threads to data vectors keeps data vectors cache-resident, e.g. Milvus

Data/Task Parallelism

- SIMD/GPU for IVFADC, e.g. Faiss
 - Parallelize lookups by keeping the lookup table inside the SIMD register and simulate lookups via SIMD shuffle (also avoids memory retrieval)
 - Parallelize summations over registers



Data Manipulation

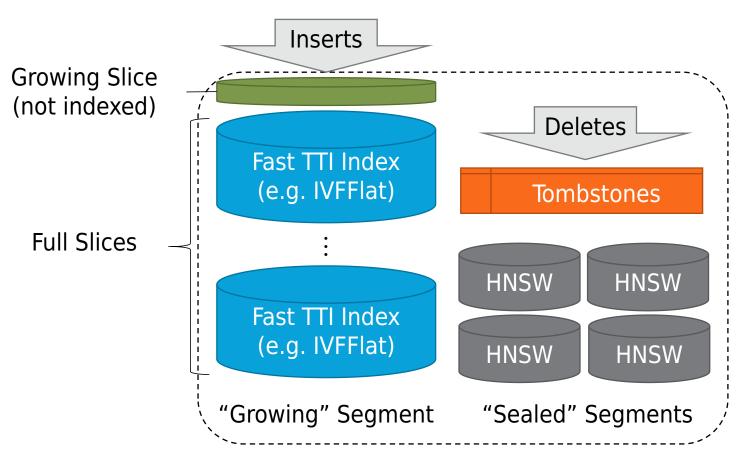
Streaming Updates

- Some indexes support in/up/del, e.g. HNSW
- Vearch: use tombstone deletes to avoid disconnecting the graph + periodic garbage collection

Batched Updates

- Perform in/up/del inside a fast-writeable slowreadable structure which also participates in search
- Reconcile into the slow-writeable fast-readable structure at a convenient time

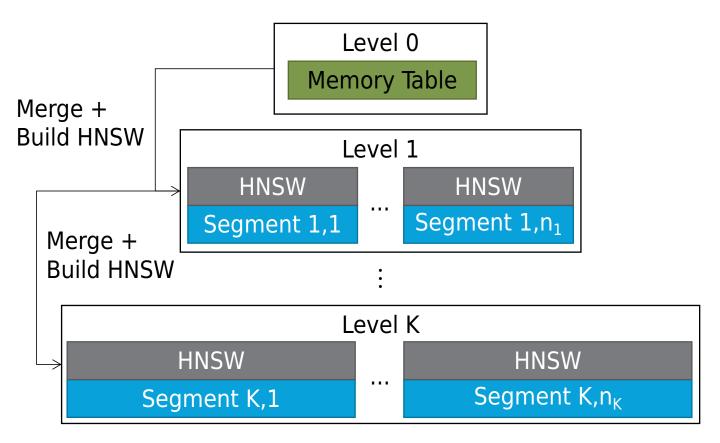
Fast Slices with Slow Segments Manu Vector Database



• HNSW is built over the growing segment once full, and then the temporary slices are discarded

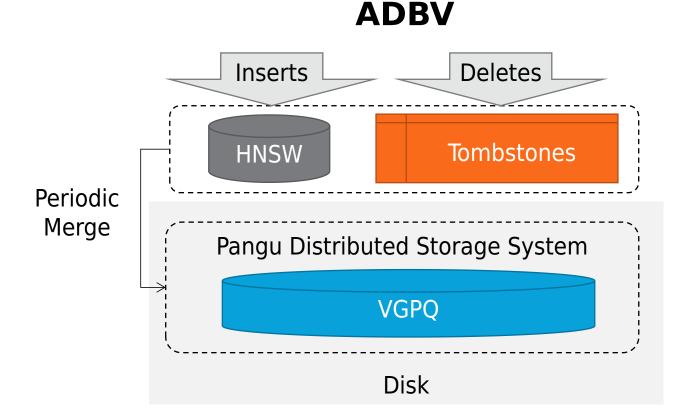
Log-Structured Merge (LSM) Tree

Milvus Vector Database



- HNSW built during segment compaction
- Tombstones are reconciled during compaction

In-Memory HNSW with Disk-Resident Index



- Designed for massive TB+ datasets
- HNSW serves as the fast-writeable structure while disk-resident VGPQ is the slow-writeable structure

Distributed Query Processing

Partitioning

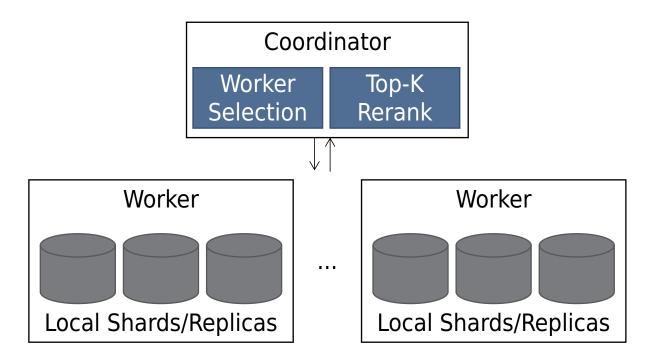
- By attribute if available, e.g. ADBV
- By k-means cluster, e.g. ADBV
- By memory availability, e.g. Vald
- By uniform hashing

Consistency

- Eventual consistency
 - By quorum, e.g. Weaviate
 - By timestamp delta, e.g. Manu
- Strong consistency

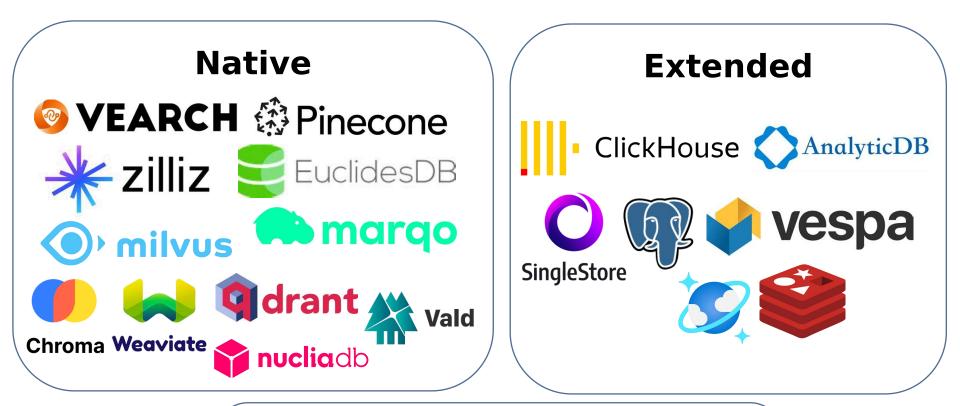
• Concurrent HNSW via internal locks, e.g. Vearch

Scatter-Gather Search



- Hard to know beforehand which workers to select
- k-means partitioning can reduce searched partitions but needs rebalancing

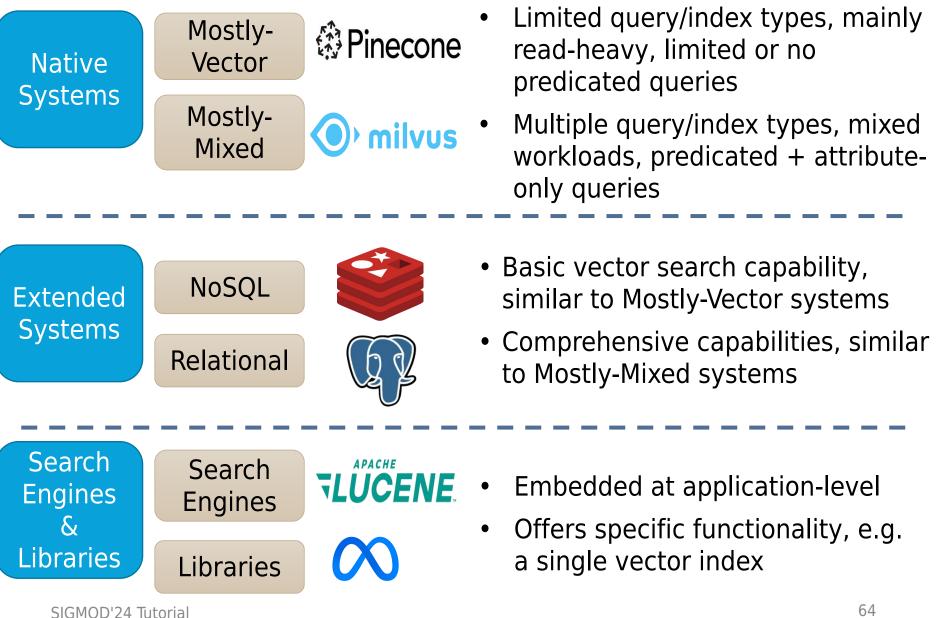
Part 2: Commercial VDBMSs



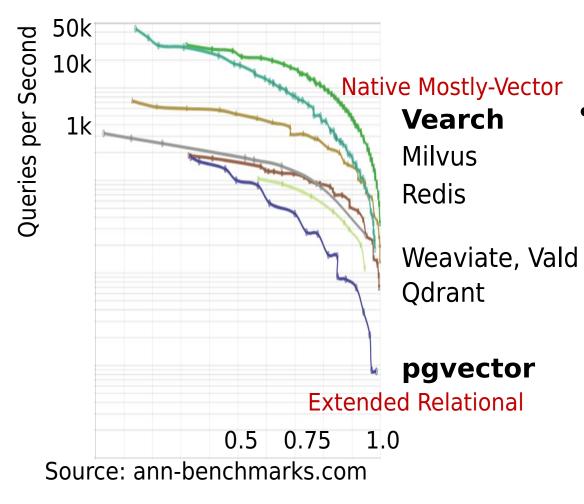
Search Engines / Libraries



VDBMS Types and Capabilities



VDBMS Performance



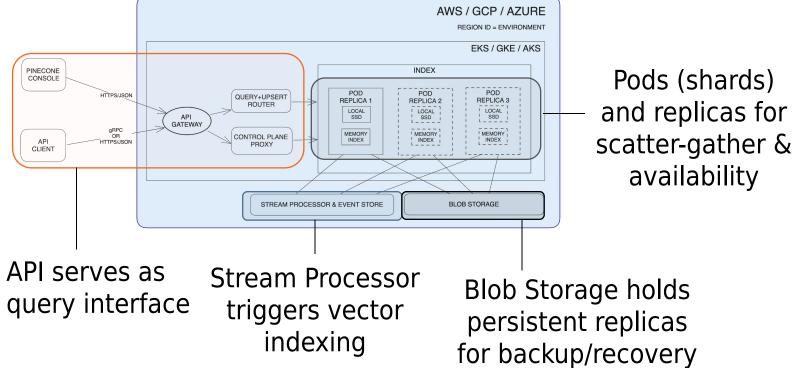
- Native systems "tend to" outperform extended systems
- This view is already being challenged. Zhang et al ICDE'24: "...there is **no** fundamental limitation in using a relational database (e.g., PostgreSQL) to support efficient vector data management"

Design Considerations

Database Management (Distributed QP, Failure Recovery, Storage Management, Query Optimizer) Vector Search Capability (Operators, Indexes, Plans, Interface)

System Type	Examples	Features	Implementation
Native Mostly- Vector	Pinecone, Vearch	Distributed QP, Failure Recovery	Shards/reps, shared- storage persistence
Native Mostly- Mixed	Milvus, Weaviate	Distributed QP, Failure Recovery, Storage Management	Shards/reps, WAL, LSM-Tree
Extended NoSQL	Redis, Vespa	Single Query/Index Types	Bolt on HNSW
Extended Relational	PASE, ADBV	Multi. Query/Index Types, Operators	Tight Integration

Native Mostly Vector **Example:** Pinecone



Advantages

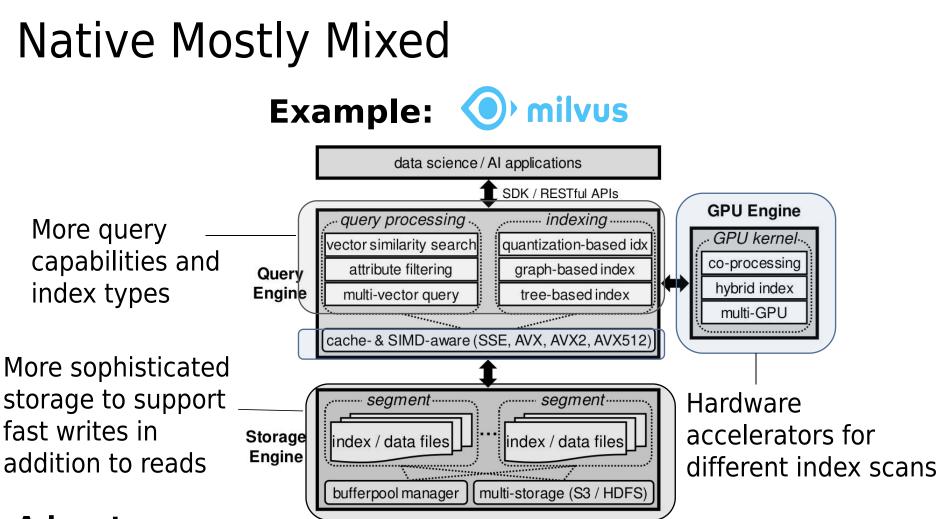
 \checkmark Low-latency searches, high search throughput

Limitations

- X Systems with graph-based index may struggle with writes
- X Systems with table-based index may struggle with latency/accuracy

Other Mostly Vector Systems

- Vald: Architecturally similar to Pinecone, except uses NGT graph index
- Vearch
 - Li et al Middleware 2018: Architecturally similar, except uses table-based index and supports predicated search via post-filtering
 - Latest version: Adds support for attribute-only indexes/queries, pre-filtering, multiple index types (HNSW, IVFPQ)
- EuclidesDB/Chroma: On-premise centralized



Advantages

✓ Many supported query types, can be configured for both read-heavy and write-heavy workloads

Limitations

X Can be resource-intensive due to more sophisticated storage/recovery

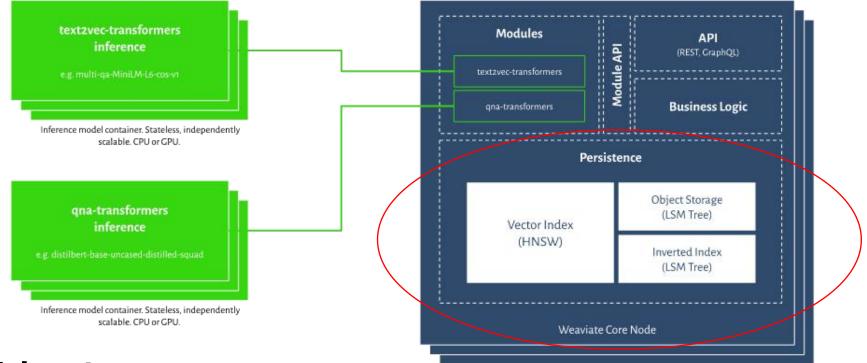
SIGMOD'24 Tutorial Figure: Wang et al "Milvus: A purpose-built vector data management system". SIGMOD 2021

69

Native Mostly Mixed



Example:



Advantages

Weaviate Core, stateful (database), horizontally scalable. CPU only.

70

 Many supported query types, can be configured for both read-heavy and write-heavy workloads

Limitations

X Can be resource-intensive due to more sophisticated storage/recovery

SIGMOD'24 Tutorial Figure: Wang et al "Milvus: A purpose-built vector data management system". SIGMOD 2021

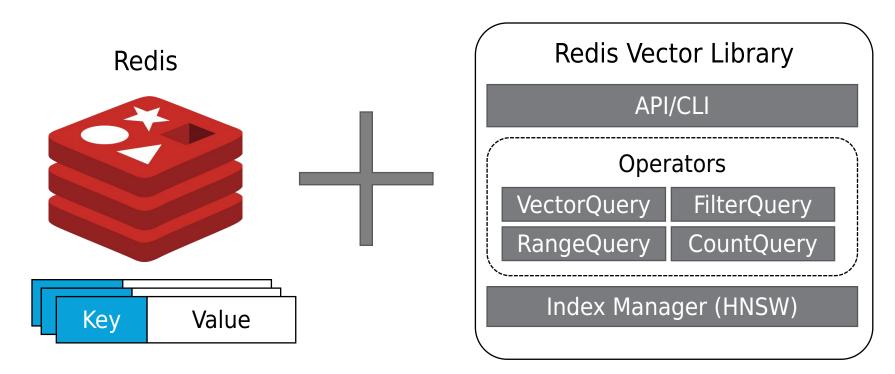
Other Mostly Mixed Systems

• Weaviate

- Targeted at documents over a graph model; supports both vector search and traditional graph queries via GraphQL
- HNSW + LSM-Tree, used for raw records + inverted index over keywords and attributes
- Pre-filtering for predicated search queries
- **Qdrant:** rule-based optimizer for predicated queries
- NucliaDB/Marqo

Extended NoSQL

Example: RedisVL



Advantages

✓ High-performance vector search, similar to Native Mostly-Vector

Combined vector search + non-vector capabilities

Limitations

X As with Mostly-Vector, performance is tied to specific workload 72

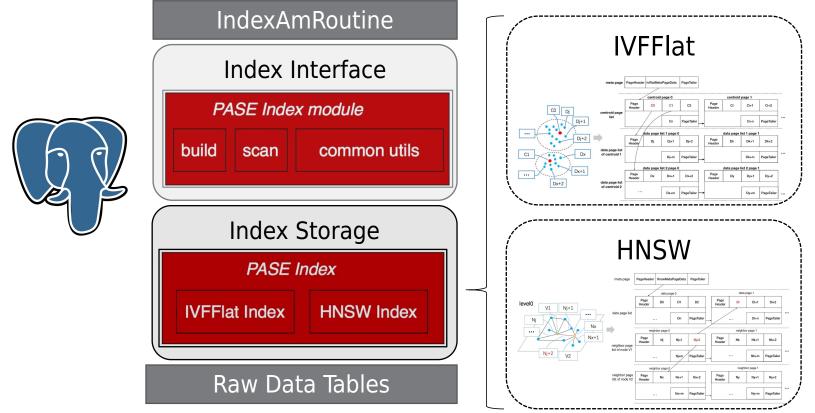
Other NoSQL Systems

• Vespa

- Document model
- SQL-like query language for complex big data analytics
- Rule-based optimizer for predicated queries
- Cosmos DB: proprietary vector index
- MongoDB: HNSW bolt-on
- Neo4j: HNSW bolt-on
- Cassandra: HNSW bolt-on

Extended Relational

Example: PASE



Advantages

Adaptable to different types of workloads

 \checkmark As with Ext NoSQL systems, offers diverse capabilities

Limitations

X May suffer performance overhead (e.g. page indirection)

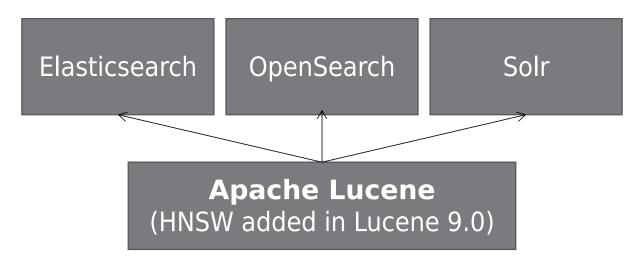
Figure from Yang et al "PASE...". SIGMOD 2020

Other Relational Systems

- **pgvector:** similar to PASE
- AnalyticDB+V
 - Relational OLAP DBMS over disaggregated compute-storage
 - Adds indexing and fast-slow write structures for supporting real-time read/writes over slowupdateable vector indexes, plus accuracy-aware cost estimation model for ANN
- **SingleStoreDB:** Adds sim. scores to enable bruteforce vector search
- ClickHouse, MyScale

Search Engines and Libraries Lin et al "Vector Search with OpenAl Embeddings: Lucene Is All You Need" (2023) arXiv:2308.14963

Search Engines



Libraries: Meta Faiss, hnswlib, ANNOY, Microsoft SPTAG, KGraph, E2LSH, FALCONN, etc.

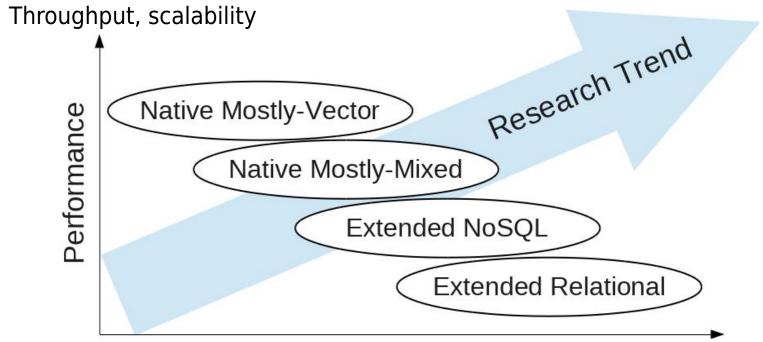
Benchmarks

- Surprisingly few benchmarks
- ann-benchmarks.com
 - Real implementations, highly implementationdependent
- Li et al TKDE 2020
 - Idealized implementations

Li et al "Approximate nearest neighbor search on high dimensional data — Experiments, analyses, and improvement." IEEE Trans. Knowl. Data Eng. 32(8), 1475–1488 (2020)

Summary of Vector Database Systems

• Latency



Capabilities

- Retrieval methods
- Storage methods
- Recovery methods
- Elasticity, availability, consistency, security

Part 3: Challenges and Open Problems

Score Design/Selection

A particular score may not return maximally relevant results, even under high recall:

"The total prod [negative user feedback] rate are 7.3%, 32.6%, and 43.1% at top 1, 3, and 5... roughly 70% are generated by the EBR node during the retrieval stage"

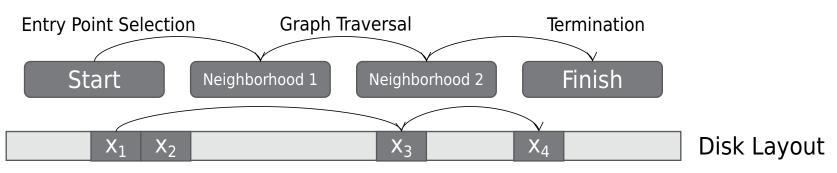
Failure reasons	Percentage	Category
irrelevant result (fuzzy text match)	53%	junkiness
Location mismatch	18%	junkiness
Language mismatch	4%	junkiness
Misinformation	10%	integrity
Untrustworthy results	10%	integrity
Offensive results	5%	integrity

Table 1: Distribution of EBR failures

Wang et al "Integrity and junkiness failure handling for embedding-based retrieval: A case study in social network search". SIGIR 2023

Disk-Friendly/Distributed Indexes

Graphs are slow for disk-resident datasets



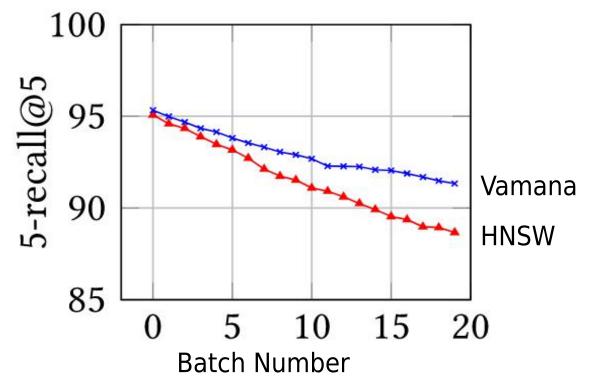
Meanwhile, **trees/tables** are disk-friendly but have worse QPS/recall



Update-Friendly Graphs

Accuracy degradation following series of updates

Effect of Repeated Delete-Reinsert Cycles



Singh et al "FreshDiskANN: A Fast and Accurate Graph-Based ANN Index for Streaming Similarity Search" 2021. arXiv 2105.09613

Easy-to-Build Graphs

- O(DN log N) still too high for huge N (billions)
- ANN_SIFT1B (128 dimensions):
 - Vamana single: 2 days @ 1100 GB peak memory
 - Vamana merged: 5 days @ 64 GB peak memory
- 200M subset of ANN_SIFT1B:
 - HNSW, ef=500: 5.6 hours @ 64 GB peak memory

Sources:

- Malkov & Yashunin "Efficient and robust approximate nearest neighbor search using hierarchical navigable small world graphs" IEEE Trans. Pattern Anal. and Mach. Intell. 2020
- Subramanya et al "DiskANN: Fast accurate billion-point nearest neighbor search on a single node". NeurIPS 2019

New Capabilities

- Multi-Vector Search
 - NRA only works with bounded scores (e.g. cosine)
- Incremental k-NN
- Secure k-NN
- VDBMS Benchmark

Thanks!

Q and A

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