

SingleStore: Do you need a specialized vector database? CMU 15-445/645 (Fall 2023)

Cheng Chen Dec 2023

CONFIDENTIAL

Specialized Database Systems

- Transaction processing
- Data warehousing
- Time series analysis
- Fulltext search
- ...
- Vector search



Outline

- SingleStore Overview
- Vector Search Overview
- Vector Index at SingleStore
- Vector Search at SingleStore



SingleStore Overview



What is SingleStore?

- SingleStore is a distributed general-purpose SQL database
- HTAP
 - Operational and analytical workloads
 - Can run TPC-H and TPC-DS competitively with data warehouses
 - Can run TPC-C competitively with operational databases
- Cloud-native
- Scale out to efficiently utilize 100s of hosts, 1000s of cores and 10s of TBs of RAM

Benchmarks

Product	vCPU	Size (warehouses)	Throughput (tpmC)	Throughput (% of max)
CDB	32	1000	12,582	97.8%
S2DB	32	1000	12,556	97.7%
S2DB	256	10000	121,432	94.4%

Table 1: TPC-C results (higher is better, up to the limit of 12.86 tpmC/warehouse)

Product	Cluster price per hour	TPC-H geomean (sec)	TPC-H geomean (cents)	TPC-H throughput (QPS)
S2DB	\$16.50	8.57 s	3.92 ¢	0.078
CDW1	\$16.00	10.31 s	4.58 ¢	0.069
CDW2	\$16.30	10.06 s	4.55 ¢	0.082
CDB	\$13.92	Did not finish within 24 hours		

Table 2: Summary of TPC-H (1TB) results



Product Overview





Cluster Architecture

- SingleStore is a horizontally-partitioned, shared-nothing DBMS with an optional shared storage for cold data
- Aggregators
 - Clients connect to aggregators
 - Handle query optimization and planning
 - Coordinate distributed query
- Leaves
 - Perform most computation





Distributed Query Processing

- Tables are hash partitioned by shard key
- Distributed Join
 - Shard key matching, push down execution to individual partitions
 - Otherwise, redistribute data via broadcast or reshuffle
- Optimizer needs to take into account data movement cost
- Certain queries need to be transformed in order to be efficiently executed



Distributed Query Processing



10 CONFIDENTIAL



Hybrid Workloads

- Analytical workloads
 - \circ $\,$ Scan 100s of millions to trillions of rows in a second $\,$
- Transactional workloads
 - Write or update millions of rows per second
- Real-time analytical workloads
 - Running analytics concurrently with high-concurrency point reads and writes



Unified Table Storage For Hybrid Workload

- Efficient for analytical workloads
- Efficient for transactional workloads
 - Operational-Optimized Columnstore



Operational-Optimized Columnstore

- On-disk columnstore LSM + in-memory rowstore segment
- Rows are first written into in-memory rowstore segment
- Flusher flushes a new segment when in-memory rowstore segment is full
- Merger merges segments
- Columnstore segments are immutable
 - DELETE/UPDATE mark rows as deleted in the segment



Optimized For Tiered Storage

- Immutable blobs
- No blob writes are on commit (no files either, only WAL)
- Out-of-order replication



Optimized for Analytical Workloads

- Vectorized execution
- Encoded execution
- Late materialization



Optimized for Operational Workloads

- Seekable encoding
- Segment Elimination
 - In-memory metadata (MIN/MAX/deleted bits/...)
 - Sort key
- Secondary index
- Row-level locking



Full-Query Code Generation

- Queries are parametrized
 - SELECT a + 1 AS x FROM t WHERE b = "abc"
 - SELECT a + @ AS x FROM t WHERE b = ^
- Parameterized queries are compiled to MBC bytecodes
- Interpret MBC while compiling MBC to machine code in the background
- Switch to machine code when compilation completes





Secondary Indexes

- Common indexing approaches for LSM tree
 - External index: extra LSM tree lookup per matched row
 - Per-segment index: O(logn) write amplification
- Index generally have sub-linear search complexity
 - Searching a larger index is cheaper than several small ones
- Index LSM tree
 - Per-segment index + index merger
 - Index merger builds cross-segment indexes on multiple segments



Secondary Hash Index

- Two-level indexes
- Per-segment index
 - Posting lists: value -> [row offset]
- Cross-segment index
 - hash(value) -> [(segment id, posting list offset)]





Figure 3: Two-level secondary index structure. A segment and a global hash table from the corresponding LSM trees are shown here



Unified Way To Identify A Row Efficiently

- Everything identifies a row by (segment id, row offset)
 - Columnar storage
 - Deleted bits
 - Secondary indexes
 - Hash index
 - Fulltext index
 - Row index
 - Vector index

21 CONF Gan correlate between them efficiently



Adaptive Table Scan

- Hybrid workloads needs to combine different access methods and apply them in the optimal order
- Static decision made by optimizer doesn't always work
 - Cost depends highly on query parameters and encodings used



Adaptive Table Scan

- Per-partition segment selection
 - segment elimination with index or MIN/MAX
- Per-segment row selection
 - filter reordering in next slide
- Per-block row projection
 - Seek or scan?
 - Use column group?
 - Selective column decoding or send encoded values upstream to AGGREGATE or JOIN



Filter Tree





Filtering

- Different ways to evaluate filters each with different tradeoffs
 - Regular filter
 - Encoded filter
 - Group filter
 - Index filter
- Adaptive filter reordering for each block
 - Each segment estimates the cost of each strategy by timing it on a small number of rows

 Each block reorders the filters based on the cost estimate and ^{25 CONFIDENTIAL} selectivity from previous block



Vector Search Overview

26 CONFIDENTIAL



Vector Search

- Given n vectors and another query vector
- Find k nearest neighbors to the query vector
- Dense vectors in d-dimensional space
- Distance metrics
- Approximate nearest neighbors (ANN)





Representation Learning

- Learn to represent objects with vector embeddings
- Semantic similar objects are closer to each other





Retrieval Augmented Generation (RAG)

- LLMs are inefficient and costly to train/fine-tune
- RAG as a cost-efficient approach to GenAI
 - Up-to-date knowledge
 - Domain-specific knowledge
 - Source citation



Vector Search vs Fulltext Search

- Fulltext search relies on keyword matching and can't capture semantics
 - I like apple
 - I don't like apple
 - I don't dislike the fruit company
- Vector search can be multimodal: text, image, audio, video etc
- Vector search is more computationally costly



Vector Index Algorithms

- Tree-Based: KD-Tree
- Hash-Based
- Quantization-Based: IVF, SPANN
- Graph-Based: HNSW, DiskANN, CAGRA



Inverted File (IVF)

- Partition vectors into clusters
- Use the centroids to represent each cluster





Inverted File (IVF)

• Build an inverted index from clusters to vectors





Inverted File (IVF): Search

- Find nearby centroids to the query vector
- Only search within nearby clusters



Hierarchical Navigable Small World (HNSW)

- Skiplist over proximity graph
- Each node is only connected to a small number of neighbors
- Greedy search starts from coarsest layer and refine with finer layers



C) SingleStore



Credit: Pinecone

IVF vs HNSW

- HNSW has higher recall
- HNSW is faster to search
 - O(logn) vs O(sqrt(n))
- IVF is faster to build
- IVF has much smaller index size



Product Quantization (PQ)

- Vector compression technique that applies to various algorithms
 - IVF_PQ
 - HNSW_PQ
- Not only saves space, but also speeds up distance computation
- Even faster with PQ Fast Scan
- Compression is lossy so need to refine the results for better recall



Index Composition

- In IVF, searching nearest centroids is yet another ANN
- Can build another vector index on centroids: IVF + HNSW
 - Centroids are much smaller
 - Searching nearest centroids requires very high recall



Vector Search Offerings (08/19/2023)



Credit: https://thedataquarry.com/posts/vector-db-4/





Vector Index at SingleStore

40 CONFIDENTIAL



Overview

- On-disk columnstore LSM + in-memory rowstore segment
- In-memory rowstore segment is small
 - No vector index, just full scan
- Build vector index for on-disk columnstore LSM
 - Per-segment vector index + vector index merger



Per-Segment Vector Index

- Background flusher/merger create a new vector index for each new segment created
- ALTER TABLE creates a new vector index for each segment
- If too many rows are deleted in a segment, its vector index gets rebuild



C) SingleStore

42 CONFIDENTIAL

Vector Index Merger

- Vector indexes have sub-linear search complexity
 - Searching a larger index is cheaper than several small indexes
- Vector index LSM tree
 - Build cross-segment vector indexes on multiple segments
- Vector index is expensive to build so O(logn) write amplification due to merge can be significant
 - Merge only cold data

Pluggable Vector Index Algorithms

- We are using vector index algorithm as a black box
- This allows us to plug in any vector index algorithm
- In 8.5, we support many popular in-memory vector index algorithms:
 - IVF_FLAT, IVF_PQ, IVF_PQFS
 - HNSW_FLAT, HNSW_PQ
- Post 8.5, we are planning to support on-disk vector index algorithms
- Vector index can be built in an external service
 - Build vector index on GPU

Auto Vector Index

- It's hard for average users to pick which vector index algorithm to use and to tune various parameters for the given algorithm
- Note that our vector index is always build on immutable data
- We can make smart decision for the users
- The user just need to tell us what the requirements are
 - High-recall
 - Cost-effective

Vector Search at SingleStore

Example 1: ANN

SELECT

```
t.v <-> vector AS d
```

FROM t

ORDER BY d

LIMIT k;

ORDER BY ... LIMIT Pushdown

- Agg already pushes down ORDER BY ... LIMIT to leaves
 - Currently Merge TopSort, but we can prob do better
- Leaf pushes down ORDER BY ... LIMIT to table scan as a Top filter

Example 1: ANN

Project [t.v <-> vector AS d]

TopSort limit:k [t.v <-> vector]

ColumnStoreFilter [Top(t.v <-> vector, k) index]

ColumnStoreScan t

Example 1: ANN

- Per-partition segment selection
 - Scan all vector indexes within the partition and select top-k for the entire partition
 - Select segments that contain these top-k rows
- Per-segment row selection
 - Top filter evaluates to true iff the row is selected above
- Per-block row projection

Example 2: Pre-Filtered ANN

SELECT

- t.v <-> vector AS d
- FROM t
- WHERE <filters>
- ORDER BY d
- LIMIT k;

Pre-Filters

- If <filters> are executed after vector index scan
 - There will be less rows after filters
 - We can let vector index scan to output more rows at the beginning, but in practice it's very hard to predict
- <filters> need to be executed before vector index scan
 - Make vector index filter aware of its pre-filters

Example 2: Pre-Filtered ANN

Project [t.v <-> vector AS d]

TopSort limit:k [t.v <-> vector]

ColumnStoreFilter [Top(t.v <-> vector, <filters>, k) index]

ColumnStoreScan t

Example 2: Pre-Filtered ANN

- Per-partition segment selection
 - a. Segment elimination with pre-filters

- **b.** Scan all vector indexes within the filtered segments and select top-I for the entire partition
- c. Run pre-filters on these top-I rows
 - If there are at least k output rows, select top-k.
 - If there are less than k output rows
 - Either retry b with a larger l
 - Or fall back to not using vector index scan

Top Filter

- Top(expr, <filters>, k) is true iff expr of this row ranks within the top-k among all the rows that pass <filters>
- Top filter is just a regular leaf node in the filter tree
- Can have many Top filters in the filter tree with different pre-filters
- Filters outside of Top filter are post-filters
- Filter reordering can happen within pre-filter tree and post-filter tree
- Retry happens within Top filter

Example 3: Join

SELECT

t.v <-> vector AS d

FROM t JOIN s

ON t.id = s.id

WHERE <s.filters>

ORDER BY d

LIMIT k;

Example 3: Join

Project [t.v <-> vector AS d]

TopSort limit:k [t.v <-> vector]

HashJoin

|---HashTableProbe [t.id = s.id]

HashTableBuild alias s

ColumnStoreFilter [<s.filter>]

ColumnStoreScan s

ColumnStoreFilter [Top(t.v <-> vector, t.id = s.id, k) join index] ColumnStoreScan t

- Each query contains multiple subqueries
- Each subquery has its own type: fulltext or knn
- For a given row
 - Each subquery produces a score
 - The final score is a weighted sum of all individual scores
- The query selects rows with the highest final score

- Execute each subquery individually as a filter to select rows that have a positive score for that subquery
- Union all rows selected by each subquery
- Compute the final score for all rows in Step 2 and output the highest ones

SELECT

```
MATCH(t.s) AGAINST ('pattern') AS score1,
t.v <-> vector AS score2
```

FROM t

```
WHERE <filters>
```

```
ORDER BY weight1 * score1 + weight2 * score2
```

LIMIT k;

Project [

MATCH(t.s) AGAINST ('pattern') AS score1,

```
t.v <-> vector AS score2]
```

```
TopSort limit:k [weight1 * score1 + weight2 * score2]
```

ColumnStoreFilter [

(<filters> AND MATCH(t.a) AGAINST ('pattern') index) OR Top(t.v <-> vector, <filters>, k) index] ColumnStoreScan t

More Examples

- Vector index join
- Cross apply
 - Batched workload, good for GPU

Other Vector Index Filters

- Vector range search
 - o t.v <-> vector > threshold
- Maximal Marginal Relevance (MMR)
 - Representatives of nearest neighbors
 - New neighbor can't be too close to previously selected neighbors

