Towards Optimizing Search and Indexing in Vector Databases

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Motivation





- Vector searches sit on the critical path in RAG applications; Getting fast responses require searches to be highly performant
- Vector datasets often have billions/trillions of vectors; Getting high-performance at that scale is difficult
- Having an in-depth understanding of the performance characteristics of vector indexing and search algorithms is crucial !

Vector Search



- Finding tokens closely related to a query, requires performing a nearest neighbor search on a set of feature vectors
- Traditionally, KNN algorithms have been used for nearest neighbor searches,
 - > But with billions/trillions of vectors, KNN search durations become unrealistic quickly
 - ANN (Approximate Nearest Neighbor) algorithms allows faster searches by trading some accuracy using a combination of techniques such as space-partitioning, indexing, and quantization



Vector Similarity Metrics



- Popular metrics used for calculating the distance between two vectors in the euclidean space include
 - > Cosine Similarity
 - > Dot Product
 - > Manhattan Distance (L1)
 - > Euclidean Distance (L2)

$$d(\mathbf{a},\mathbf{b}) = \sqrt{(\mathbf{a_1} - \mathbf{b_1})^2 + (\mathbf{a_2} - \mathbf{b_2})^2 + ... + (\mathbf{a_n} - \mathbf{b_n})^2}$$

Vector Indexing Techniques

CRSS

- Given below are some widely-used vector indexing algorithms
 - ≻ Flat
 - > IVF or Inverted File Index (Clustering-based)
 - > HNSW or Hierarchical Navigable Small World (Graph-based)
 - ➤ LSH or Locality Sensitive Hashing (Hashing-based)
 - > Examples of other indexing algorithms include
 - Microsoft DiskANN
 - Google ScaNN
 - Spotify ANNOY

Hierarchical Navigable Small World



- We start from layer 0,
 - > pick a entry node
 - compare its neighbors with the query vector
 - move to the neighbor closest to the query vector
 - Once we find a local minima, we move to that exact node in the next layer and start the search again
 - The local minima that we find in the last layer is the closest one to our query vector



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Vector Data Management Systems

- Some widely-used vector data management systems include
 - Client-Server
 - Milvus, Qdrant, Weavite
 - Embedded
 - LanceDB, Deeplake, Chroma
 - ➤ Extensions
 - PgVector
 - > Libraries
 - FAISS (Meta), hnswlib, usearch





Machine Information



CPU:

- Intel(R) Xeon(R) Silver 4114 @ 2.20GHz
 - 2 Sockets
 - 10 Cores / Socket
 - Hyperthreading enabled
 - L2: 20 MB, L3: 27.5 MB
- Memory:
 - ➢ 192 GB ECC DDR4

Benchmark and Profile Setup



Dataset

- GIST dataset (<u>http://corpus-texmex.irisa.fr/</u>)
- > Learn Set: 1,000,000 x 960 / 3.84 GB
- > **Query Set:** 500,000 x 960 / 1.92 GB
- Indexes
 - ≻ Flat
 - HNSW (M = 32 / efSearch = 16 / efConstruction = 40)
- 🛠 ТорК
 - > 10

FAISS vs hnswlib



Search Duration



hnswlib is faster at vector searches than FAISS

FAISS vs hnswlib





Although index sizes are similar, FAISS is slower in indexing than hnswlib

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Effect of parallelism in hnswlib





Index and Search operations can scale well with increasing parallelism, hence opportunities for using GPUs, FPGAs

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Profiling hnswlib searches: CPU Hotspots



_mm_mul_ps mm mul ps Others 1.4% mm loadu ps mm loadu ps Others 121% 23.0% mm_add_ps mm add ps searchBaseLaver 8.6% 16.9% _mm_sub_ps _mm_sub_ps 53.3% 54 9%

Searching an HNSW Index

Searching a Flat Index

Distance calculation operations (subtractions in this case) dominate the total search duration

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Profiling hnswlib searches: Micro-Architecture





Search operations are highly memory bandwidth bound, more so on an HNSW index than on a Flat index

Profiling hnswlib indexing





Index operations have similar performance characteristics to searches being memory bandwidth bound and dominated by distance calculations

Conclusion and Next Steps



Conclusion

- > Vector search libraries are still not in their most performant state and needs optimizations
- Understanding the performance characteristics of vector indexing/searches is necessary to find opportunities for acceleration using modern hardware
- Vector indexing/search operations are memory bandwidth bound and the query duration is dominated by distance calculations
- Next Steps
 - Study GPU-based indexes, for example NVIDIA Cagra
 - > Perform billion-scale experiments (for example, with the BigANN dataset)
 - Explore using GPUs, specialized accelerators, and CXL memory expanders for billion-scale searches
 - > Look at end-to-end performance characteristics by profiling databases besides libraries

Thank You



Questions?

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