Accelerating Vector Search with RAPIDS cuVS

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https://github.com/nwstephens/ASU-GPU-Day-2024

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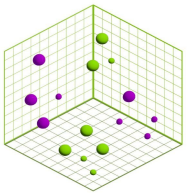
Vector Search



Overview

Embeddings

Vector Search

Applications

Algorithms

IVF-Flat

IVF-PQ

CAGRA

RAPIDS

Notebooks

jupyter

TL/DR

Why GPU accelerated vector search matters

1. **Vector Search is commonly used with AI**
   Examples: Retrieval augmented generation (RAG), recommenders, genomics, finance, chemistry, finance, and cybersecurity.

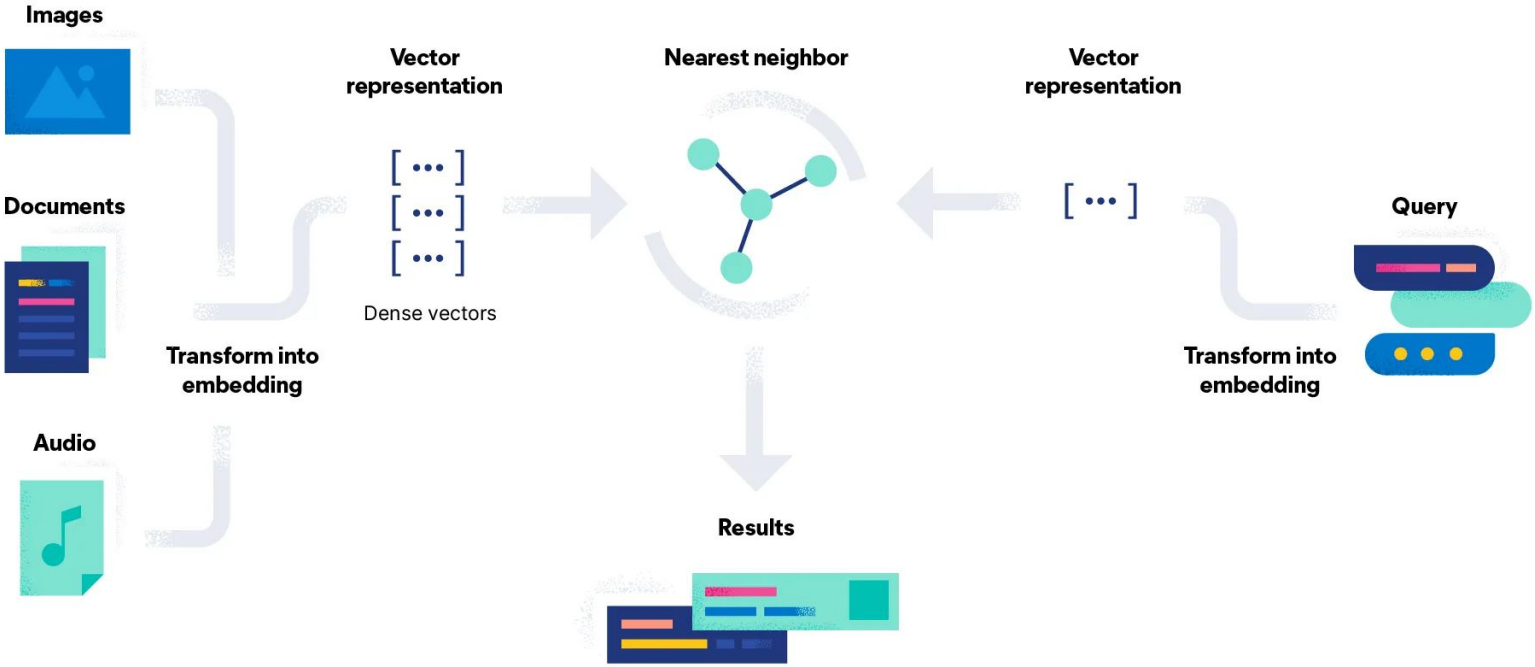
2. **Vector data types are everywhere**
   Nearly all data sources will support them if they don't already.

3. **GPUs increase throughput, lower latency, and decrease build times**
   GPUs can increase performance by +10X and cut index build times from days to minutes.

Vector Search Overview

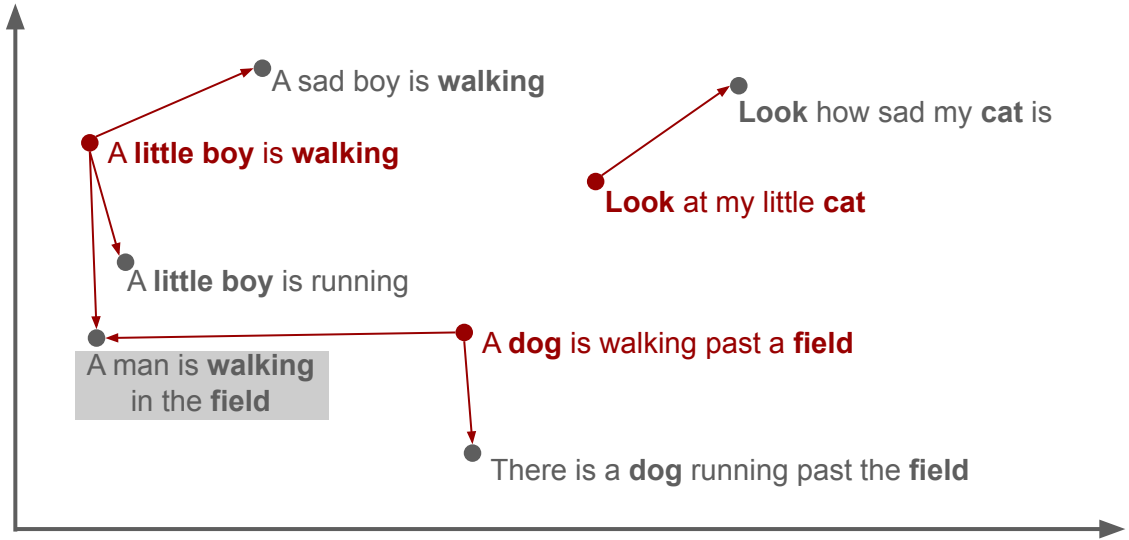
Vector Search Overview

Nearest Neighbor Analysis



Vector Search Overview

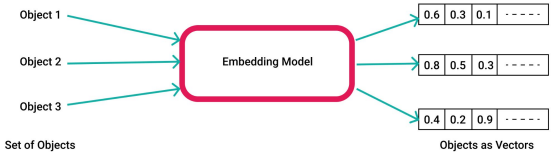
Example of Text Vectors

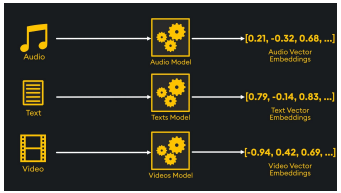


Vector Search Overview

What is an embedding?

Embedding: Numerical representation of typically non-numerical data objects





Text

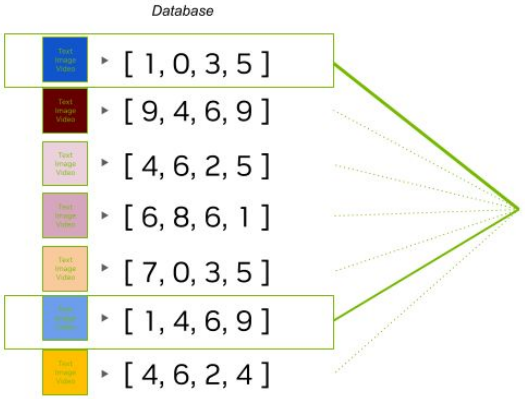
- TF-IDF (Term Frequency — Inverse Document Frequency)
- Word2Vec
- BERT (Bidirectional Encoder Representations from Transformers)

Audio

- Spectrogram-based Representations
- MFCCs (Mel Frequency Cepstral Coefficients)
- Convolutional Recurrent Neural Networks (CRNNs)

Image

- Convolutional Neural Networks
- Transfer Learning with Pre-trained CNNs like ResNet and VGG
- Autoencoders

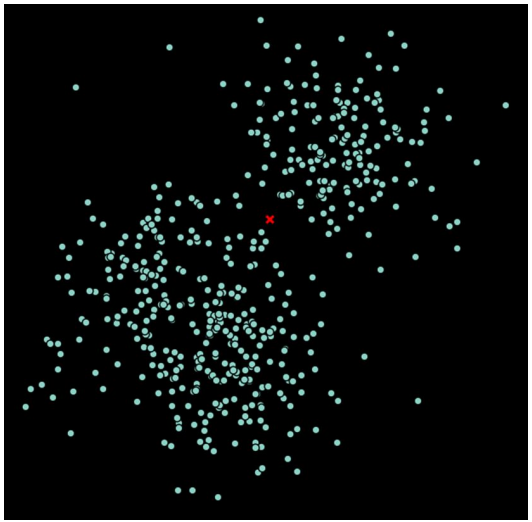


"Find the two most similar images, documents, or videos"

Vector Search Overview

Nearest Neighbor Search

Question: How to find the closest k points to the red marker?



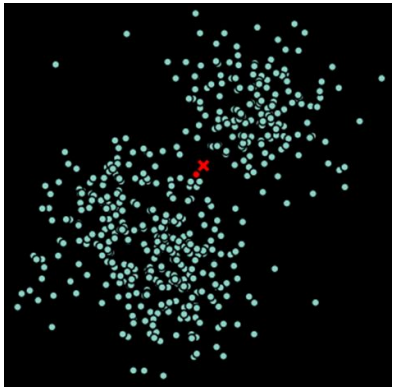
Vector Search Overview

Nearest Neighbor Search

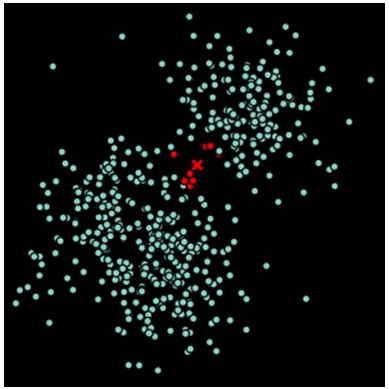
Question: How to find the closest k points to the red marker?

Answer: Measure the distance to all points and choose the shortest!

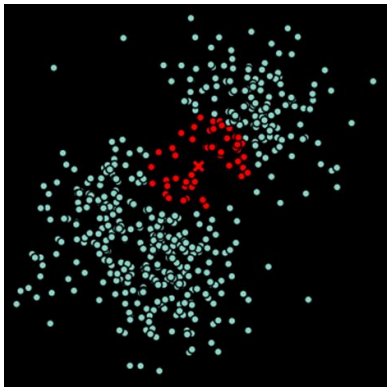
K=1



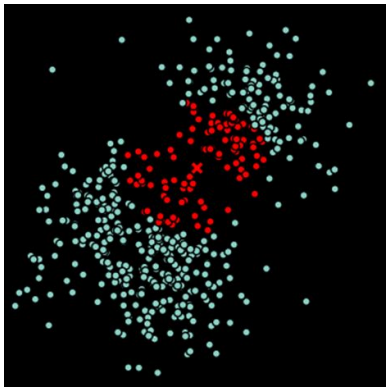
K=10



K=50

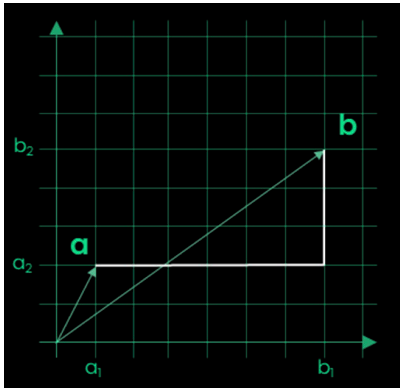


K=100

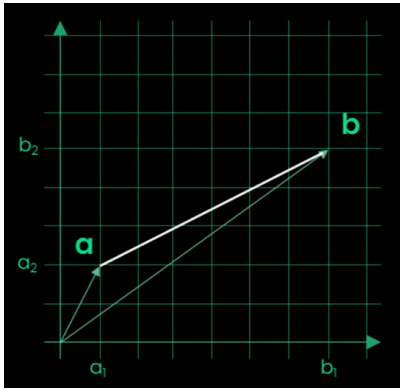


Vector Search Overview

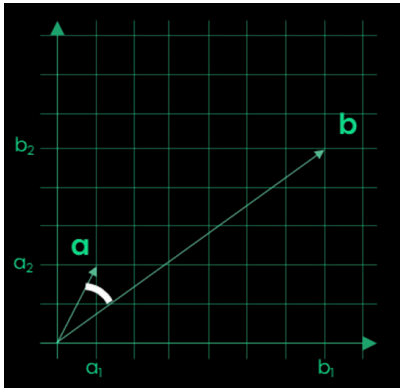
Example Distance Metrics



L1
(Taxi Distance)



L2 or Euclidean
Distance



Cosine
Similarity

Vector Search Overview

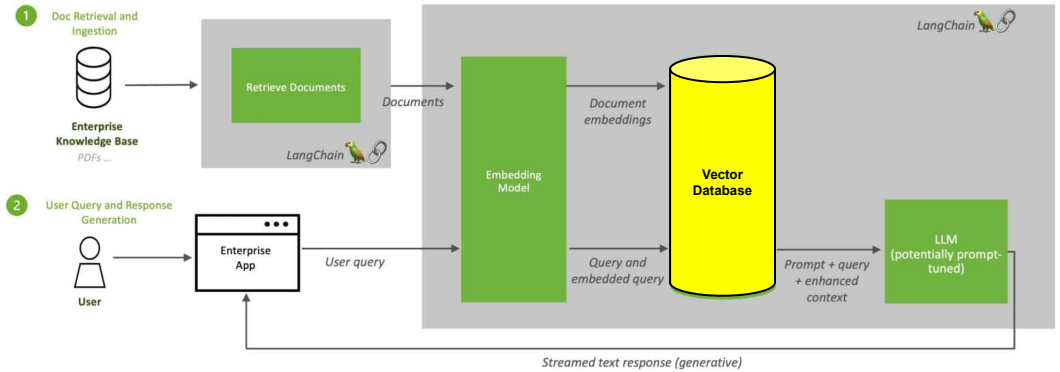
Applications

- **Recommender systems**. Provide personalized suggestions according to what a user has shown interest in or interacted with.
- **Finance.** Fraud detection models vectorize user transactions, making it possible to determine whether those transactions are similar to typical fraudulent activities.
- **Cybersecurity**. Uses embeddings to model and search behaviors of bad actors and anomalous activities.
- **Genomics.** Finds similar genes and cell structures in genomics analysis, such as single-cell RNA analysis.
- **Chemistry.** Models molecular descriptors or fingerprints of chemical structures to compare them or find similar structures in a database.

Vector Search Overview

Retrieval Augmented Generation (RAG)

RAG Workflow



Vector Search Technologies

Milvus

redis kinetica

Weaviate DATASTAX

APACHE LUCENE

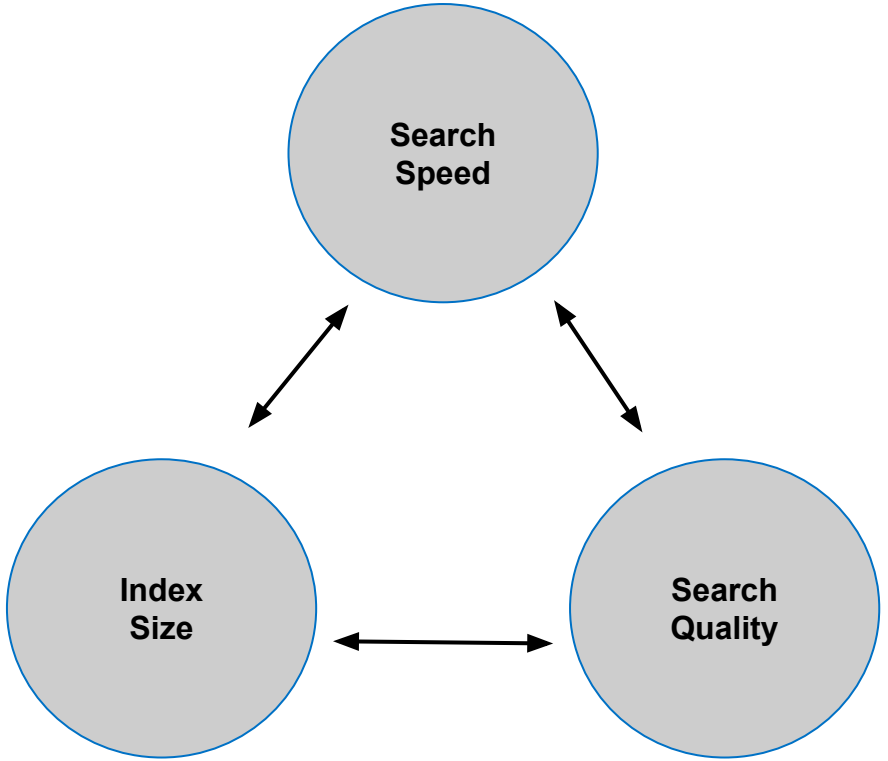
OpenSearch Solr

Vector Search Algorithms

Vector Search Challenges

Competing priorities cause computational challenges and tradeoffs

- Higher throughput requires larger batch sizes but latency requirements may require small batch sizes.
- Indexing is slow and choice of index affects search quality, size, and speed.
- Higher quality search requires larger storage and is more thorough, reducing speed.
- Higher dimensionality embeddings can improve quality at the expense of storage and speed.
- Larger datasets increase computational needs, reducing speeds and increasing storage size.



RAPIDS cuVS Overview

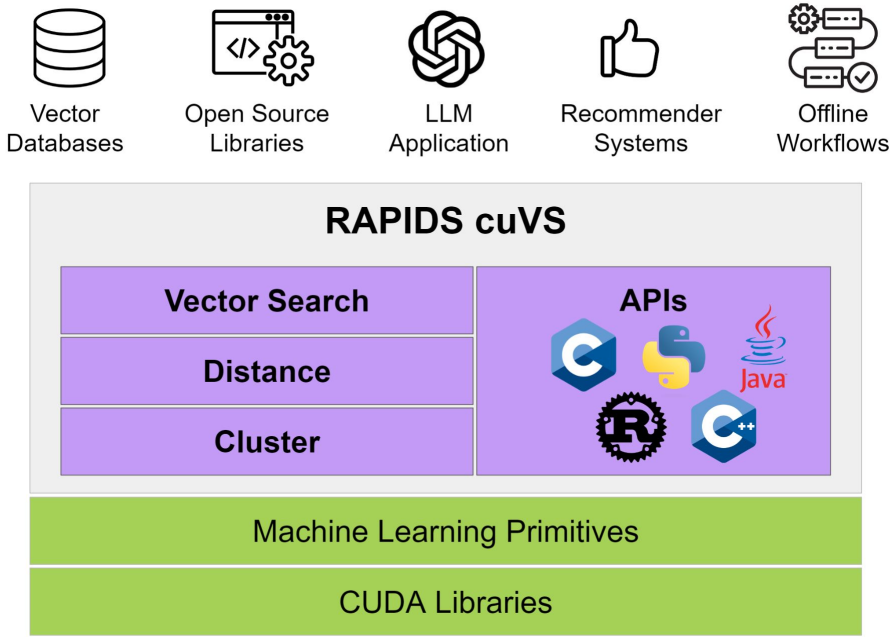
Open-Source GPU Accelerated Vector Search and Clustering

Vector search:

- Underpins many data mining and AI applications
- Requires efficient handling of massive workloads.

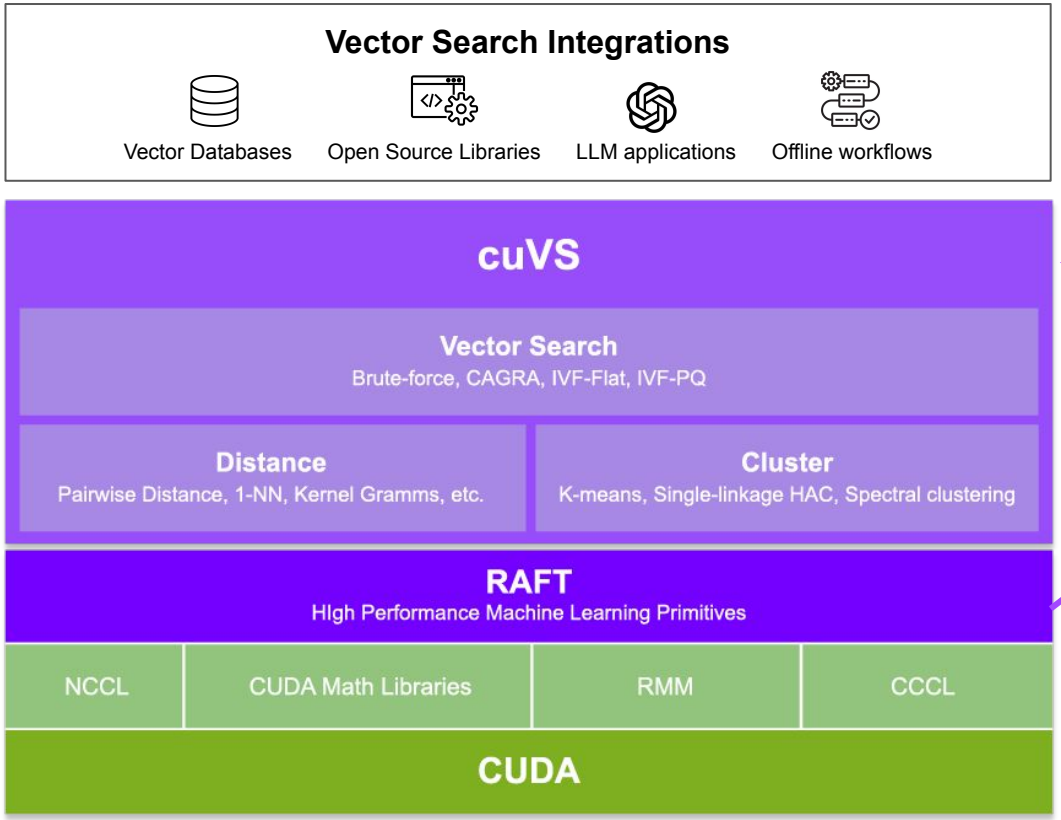
RAPIDS cuVS contains optimized algorithms for:

- Approximate nearest neighbors
- Clustering



RAFT to cuVS Migration

Winter 2024 - Summer of 2024



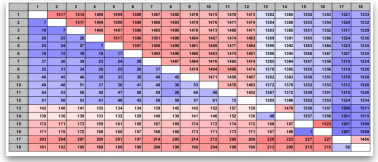
Vector Search extracted from RAFT and into cuVS

Approximate Nearest Neighbors

Building an Index

Brute force is slooooowwww for large data

- **Solution**: Build an index!
- **Examples**: Inverted file index (IVF) or graph based (HNSW)
- Gives **approximate** results (less than 100% recall)

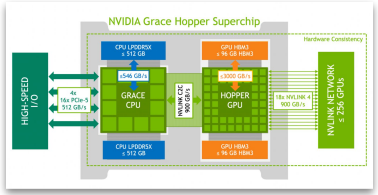


Building an index

- Used for **efficiently querying** several vectors at a time.
- **Speed up** the search by approximating the closest vectors
- Index vectors in an **efficient** way
- Sometimes use compression **compression**

Great for GPUs

- Indexes can take hours or even **days to build on the CPU**
- **These indexes can often be built much faster on the GPU**



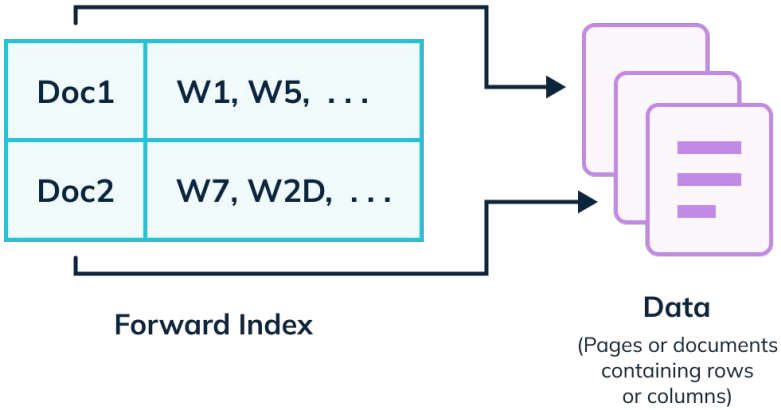
IVF-Flat

Inverted File Index

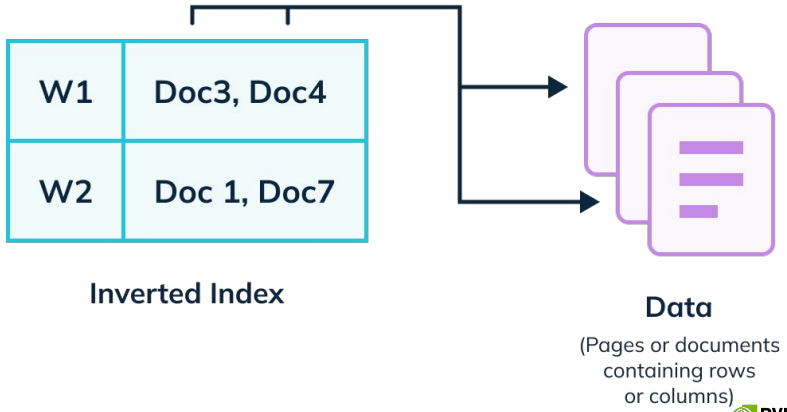
IVF-Flat

- Flat == unmodified vectors (i.e. no compression)
- Simple knobs to reduce the overall search space
- Trade-off accuracy for speed.

Forward Index (~ table of contents)



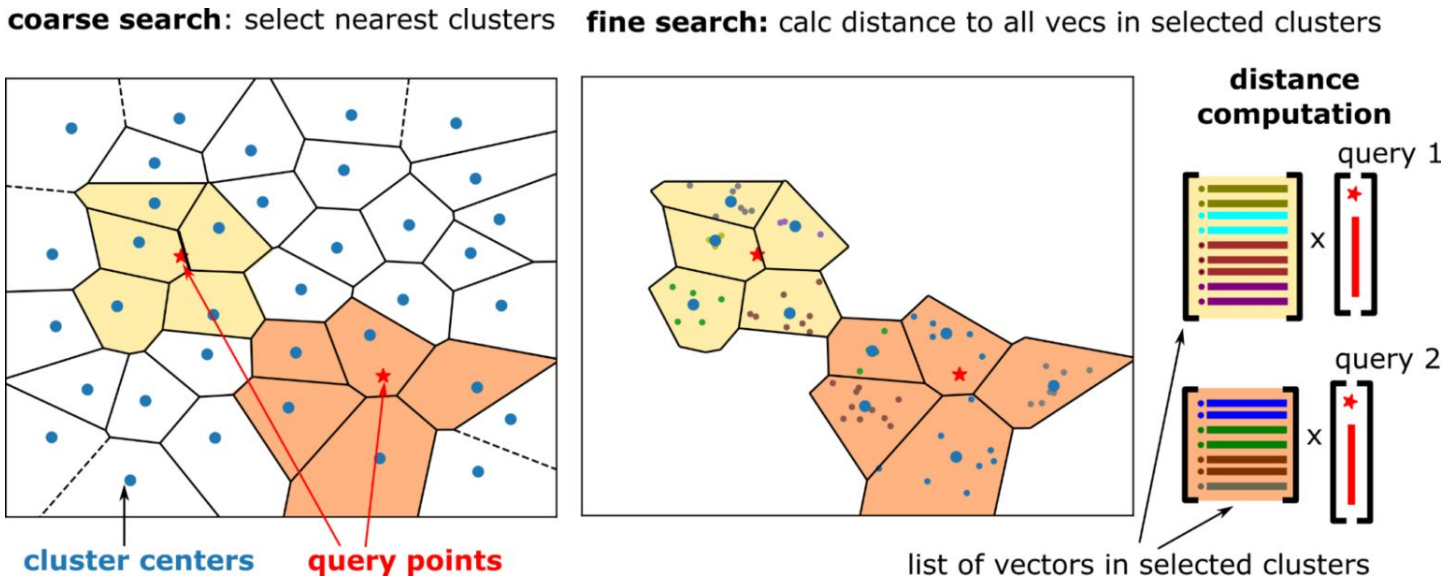
Inverted Index (~ back of the boo index)



IVF-Flat

Coarse Search and Fine Search

The top-k neighbors from each probed cluster are selected, which results in **n_probes * k_neighbor** candidates for each query. This is reduced to the k-nearest neighbors.



IVF-Flat

Tuning parameters for index building

Tuning n_lists parameter

- **n_lists** parameter determines the number of clusters to partition the training dataset.
- **n_probes** determines the number of closest clusters to search through to compute the nearest neighbors for a set of query points.
- n_lists == sqrt(n_samples) is a good starting point (where n_samples is the number of vectors in the dataset).
- n_lists == n_probes is like an exact (brute force) search

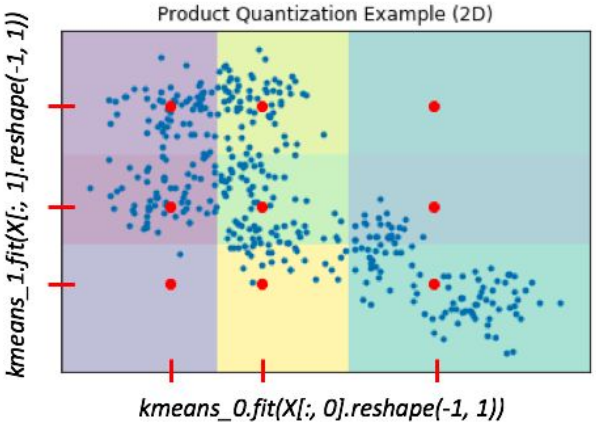
Optimizations

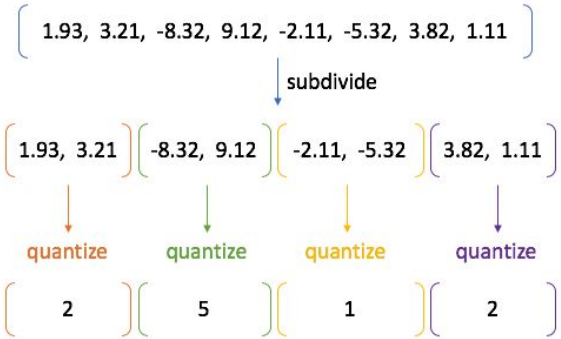
- **High throughput**. cuVS uses Tensor Cores to accelerate the k-means clustering during index building.
- **Improved algorithm**. cuVS uses a balanced hierarchical k-means clustering, which clusters the dataset efficiently even as the number of vectors reaches hundreds of millions.
- **Optimized top-k candidates**. cuVS has highly optimized methods to select the top-k candidates.

IVF-PQ

Product Quantization

- Lower PQ bits (4-8) provide ***better compression*** and more ***efficient use of shared memory***
- Configurable lookup table and distance precision provide ***faster computation*** and ***efficient use of shared memory***
- Support for ***reduced precision*** (uint8 and int8)
- Supports custom predicate ***pre-filter***
- ***pq_dim*** sets the target dimensionality of the compressed vector.
- ***pq_bits*** sets the number of bits for each vector element after compression.

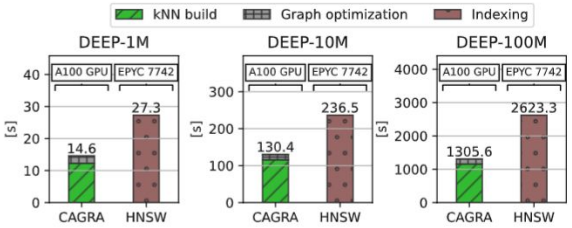


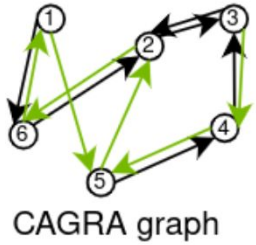


CAGRA

GPU-Accelerated State-of-the-Art Graph-Based ANN

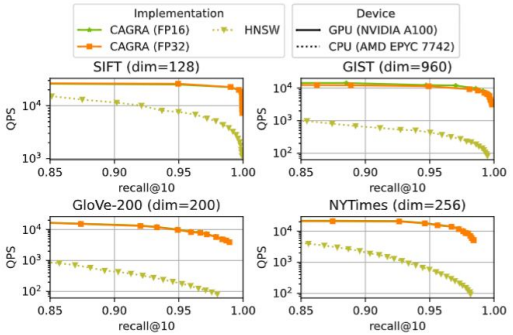
- ***Individual queries*** parallelized during search
- Setting records for both ***single query*** and ***large batch*** performance
- ***Higher throughput*** than existing GPU Graph ANNs and ***lower latency*** than SOTA CPU Graph ANNs



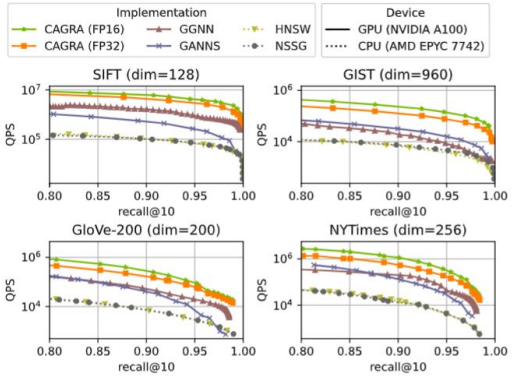


CAGRA graph

Single query at a time



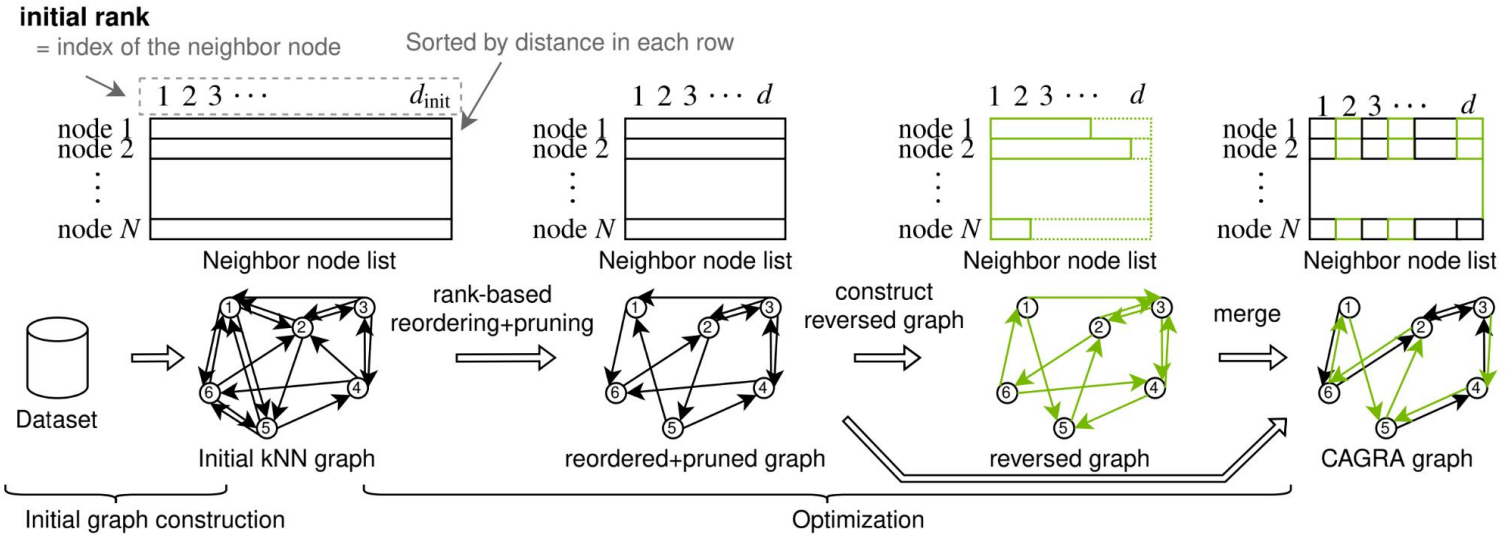
Batches of 10k queries



"CAGRA: Highly Parallel Graph Construction and Approximate Nearest Neighbor Search on the GPU", Ootomo et al., 2023

CAGRA

GPU-Accelerated State-of-the-Art Graph-Based ANN



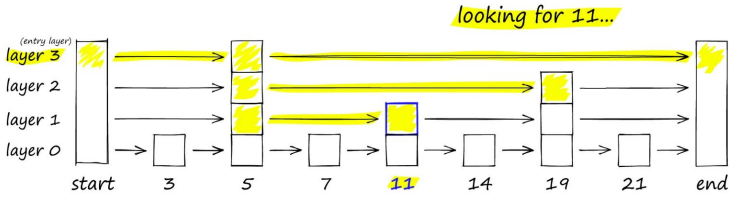
"CAGRA: Highly Parallel Graph Construction and Approximate Nearest Neighbor Search on the GPU", Ootomo et al., 2023

CPU Only

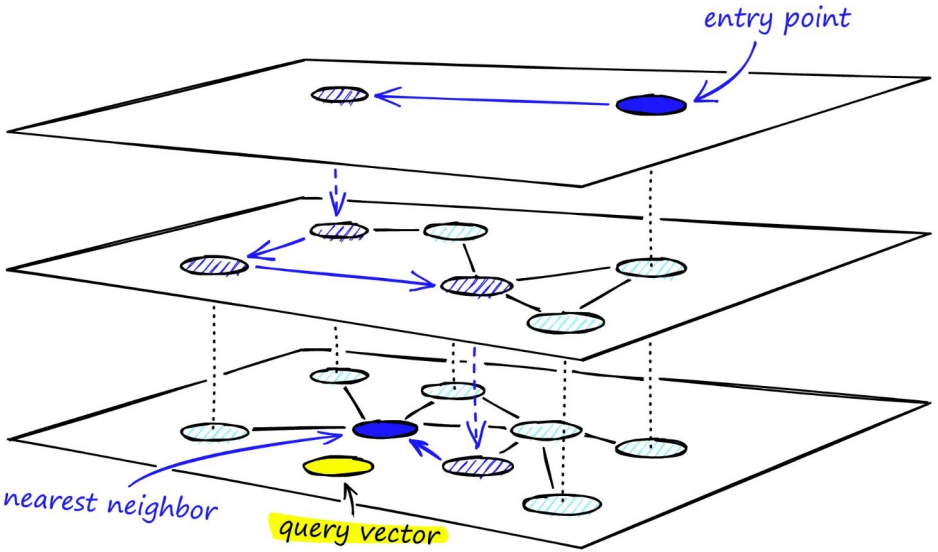
HNSW Overview

Hierarchical Navigable Small World (HNSW) algorithm

Skip List



HNSW Graph

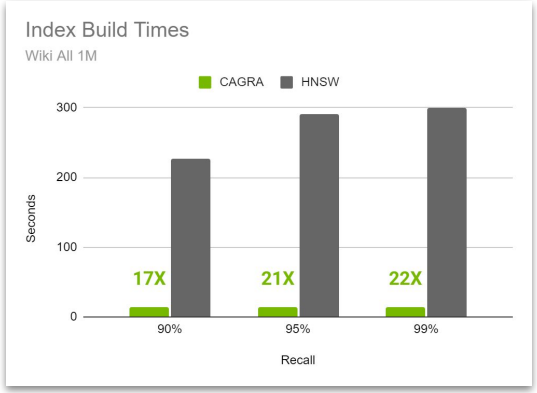


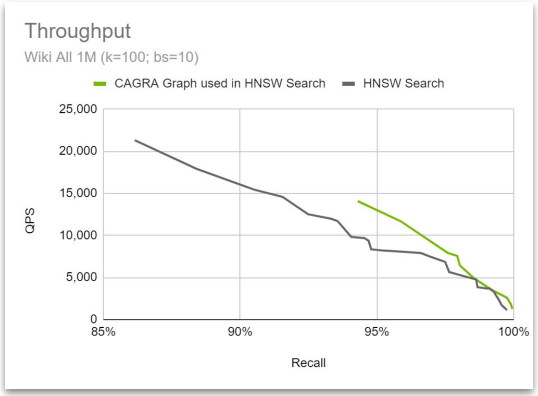
CAGRA+HNSW

Building index on GPU and searching on CPU

Organizations that prefer to use CPU infrastructure for search can still benefit from GPU accelerated build times, because CAGRA indexes built on GPUs are compatible with HNSW.

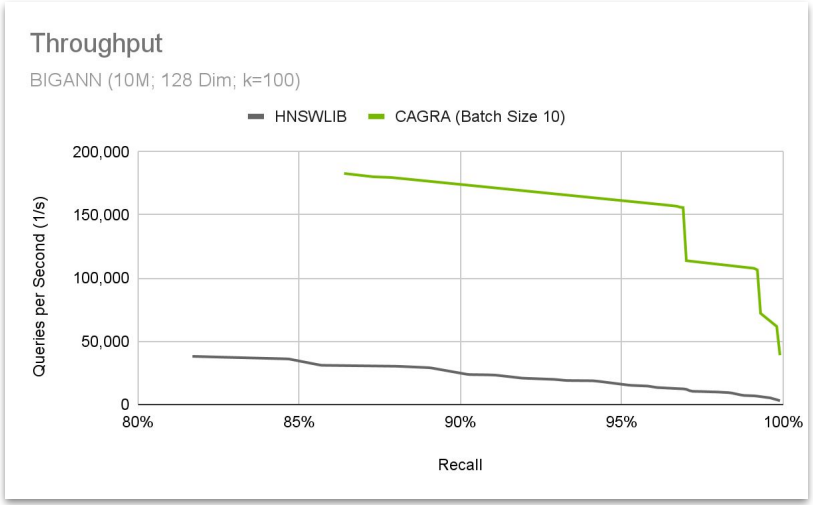
- HNSW can be slightly modified to accept CAGRA graphs
- CAGRA graphs are then deployed to HNSW on the CPU
- The result is the CAGRA graph often outperforms HNSW on CPU search – especially for larger dimensional data

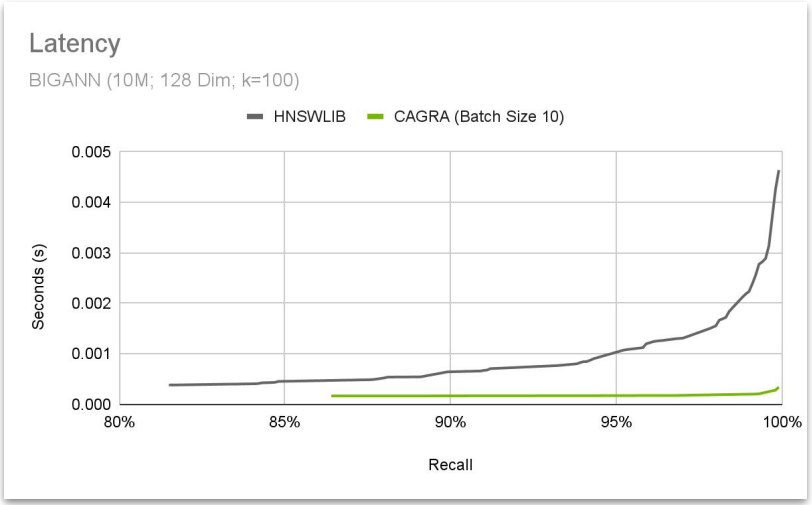




CAGRA (GPU) vs. HNSW (CPU)

Small batches (bs=10): Low latencies drive higher throughput



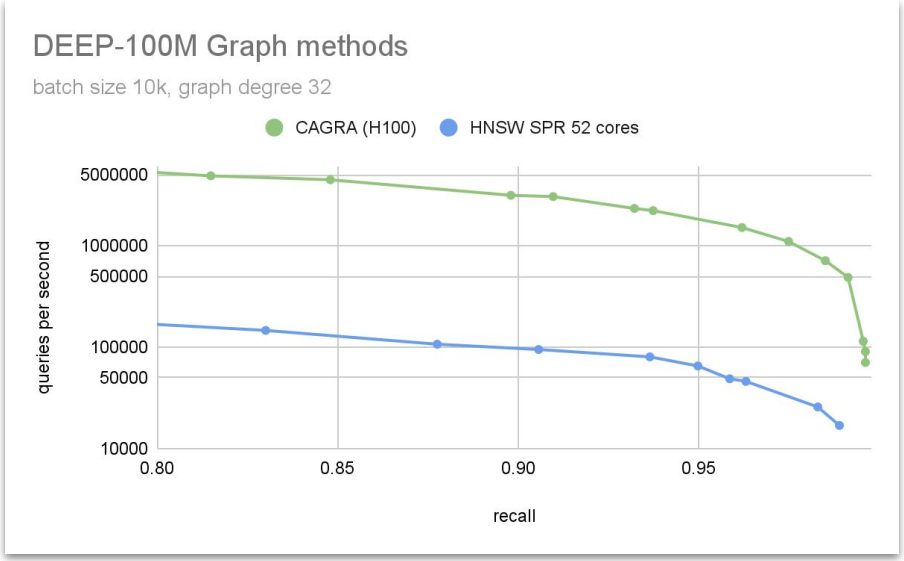


Recall	CAGRA	HNSW	Speedup
90%	174,153	24,816	**7.0X**
95%	161,356	16,008	**10.1X**
99%	108,029	6,940	**15.6X**

Recall	CAGRA	HNSW	Speedup
90%	0.000171	0.000647	**3.8X**
95%	0.000176	0.001035	**5.9X**
99%	0.000204	0.002236	**11.0X**

CAGRA (GPU) vs. HNSW (CPU)

Large batches (bs=10k): Increased parallelism drives larger speedups



Recall	CAGRA	HNSW	Speedup
90%	3,133,965	97,451	**32X**
95%	1,861,029	64,988	**29X**
99%	574,209	16,939	**34X**

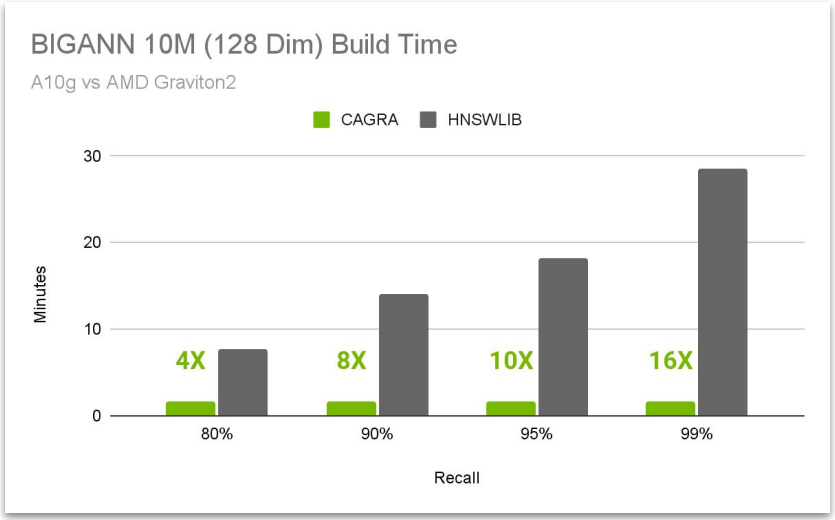
CAGRA Index Build Times

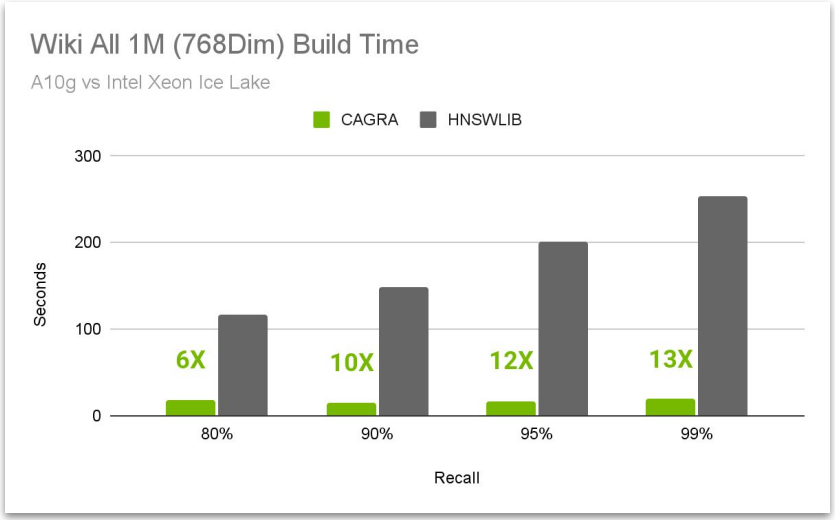
Compared to HNSW

GPUs are especially good at offline processes where large batch sizes can be used

Index build time increases as:

- Recall increases
- Dimensions increases
- Embeddings increase

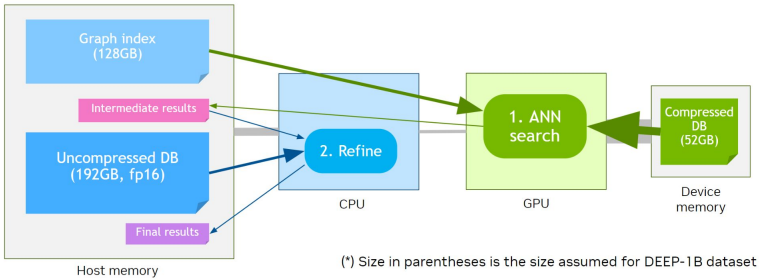




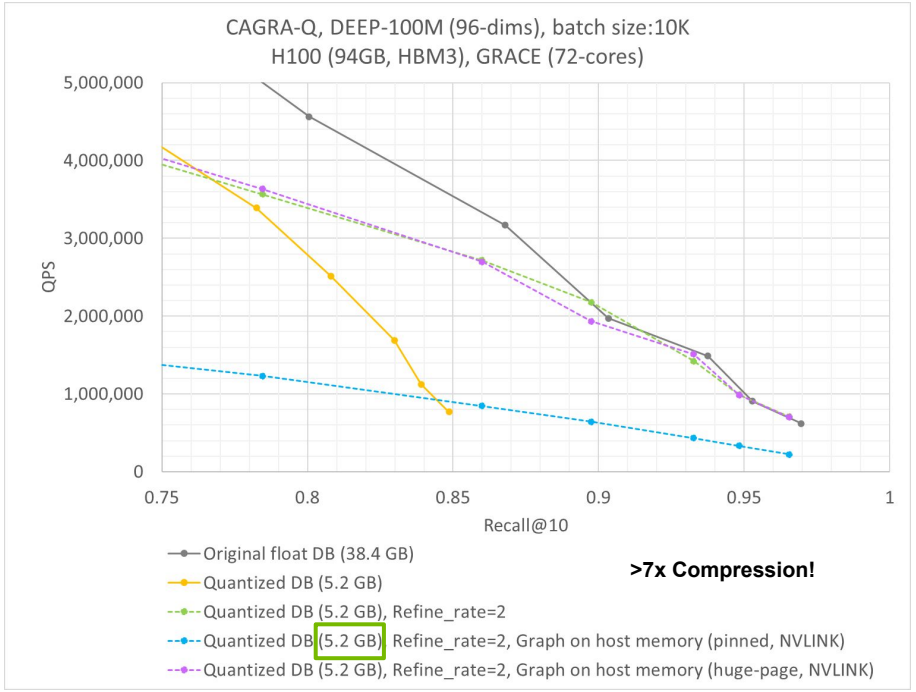
CAGRA-Q

CAGRA + Quantization for improved scale

- CAGRA requires ***original training vectors*** to compute distances
- Can keep original dataset in ***host memory*** (this can be slow)
- CAGRA-Q ***compresses original dataset*** so it can be stored on device for faster search
- Original dataset kept in host memory and used ***only for reranking*** to improve recall



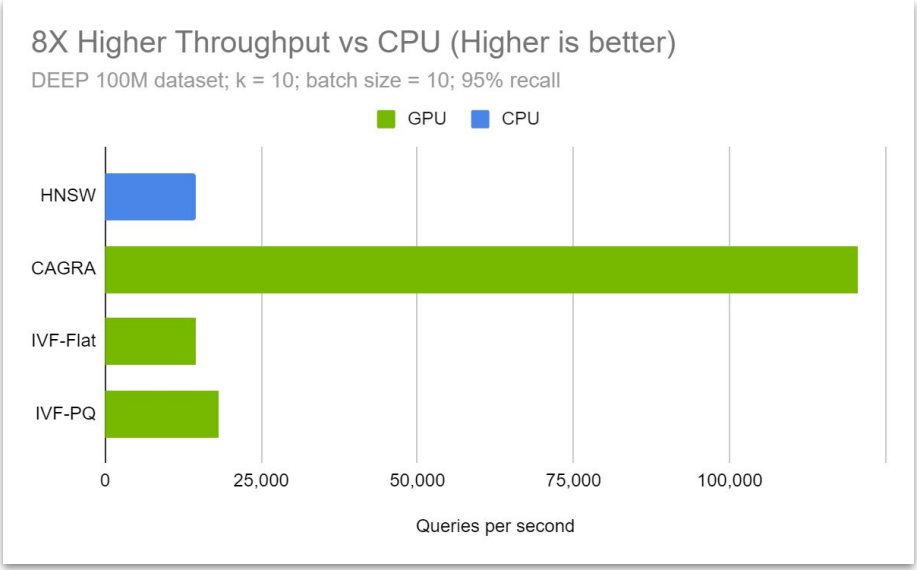
(*) Size in parentheses is the size assumed for DEEP-1B dataset

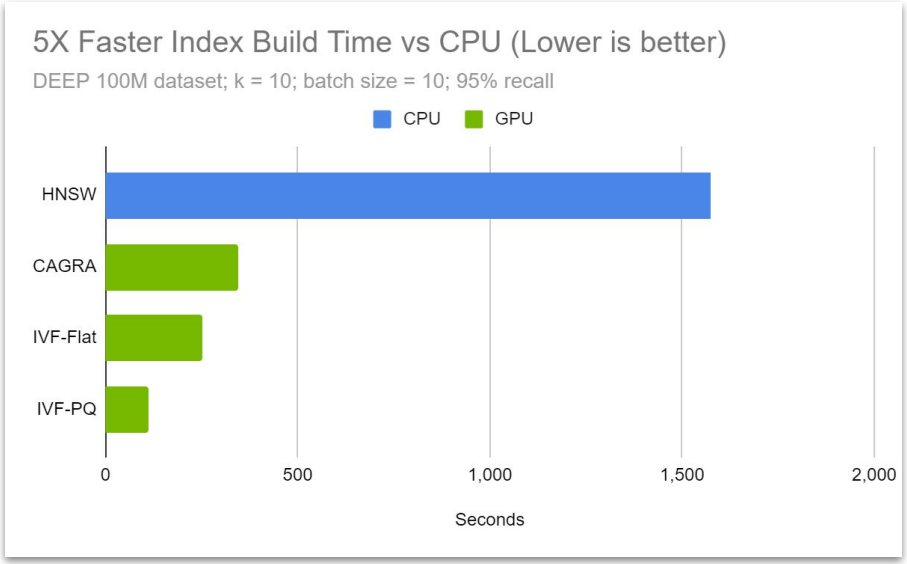


- CAGRA-Q makes a great companion for ***Grace Hopper*** and improved chip-to-chip (C2C) bandwidth.
- **TLDR;** Compressed dataset on device and graph stored in huge page pinned memory has ***equivalent performance*** to original dataset and graph stored on device at high recall levels.

Scaling up cuVS

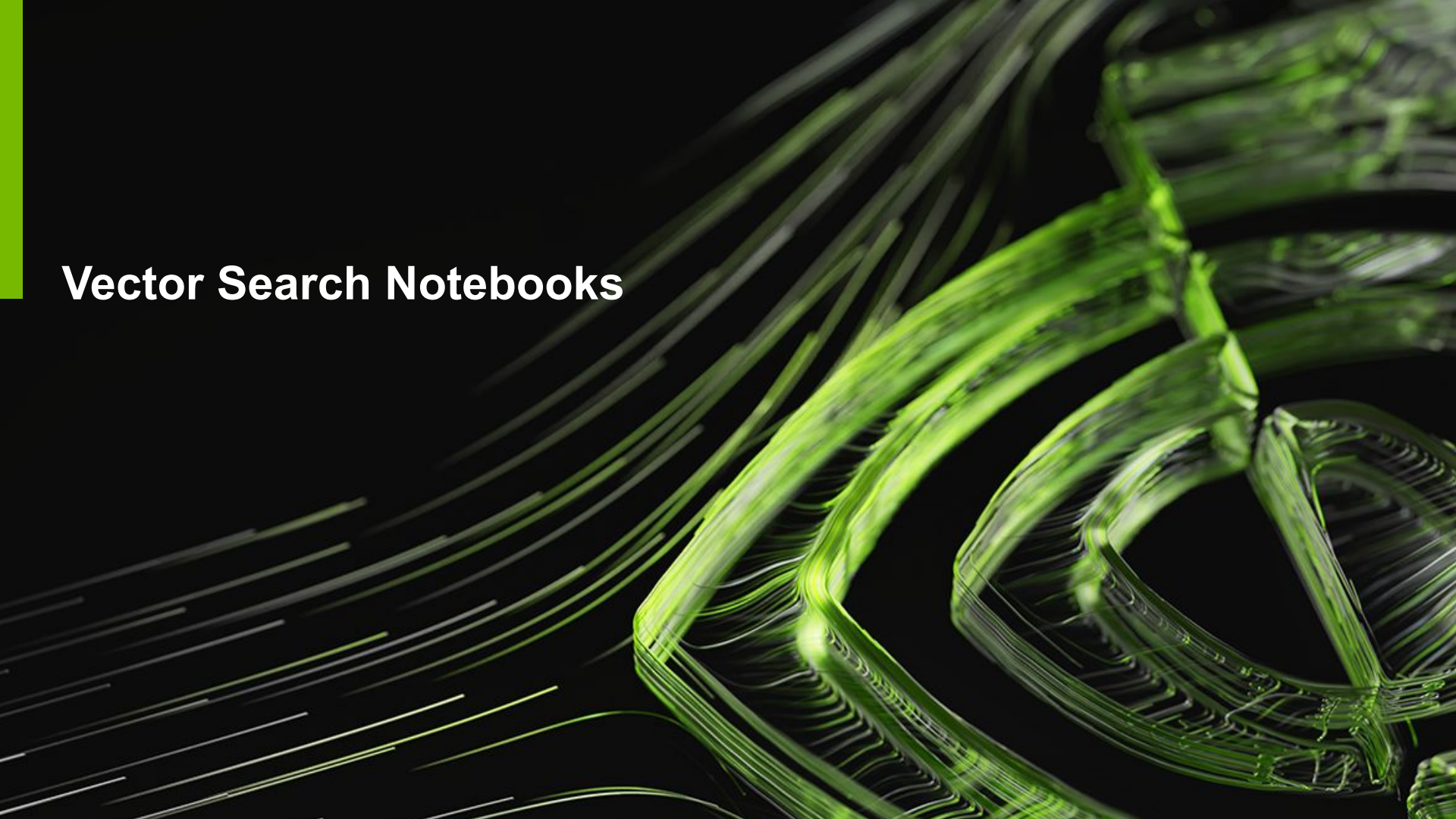
Deep 100M; 96 Dimensions; Single GPU; 38GB





NVIDIA DGX H100 SXM GPU vs Intel Sapphire Rapids 8480CL CPU (224 threads)

Vector Search Notebooks



Scaling cuVS - Multiple GPUs (1TB)

Massive-scale indexing on a DGX H100

GPU
Benchmark

Raw Text
1TB

GPU Ingest
11.5 hours

635M x 1024 Vectors
Tumbling window chunking (size 300)

Vectors
2.5TB

GPU Index Build
56 Minutes

CPU
Estimate

GPU Index Build Time	56 Min
Number of GPUs	× 8
GPU / CPU Performance	× 20
Minutes per day	÷ 1440 Min/Day
CPU Estimated Index Build	**6.22 Days**

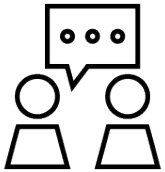
Assumes weak scaling

Resources

A Variety of Ways to Get Up & Running

More about RAPIDS cuVS

- RAPIDS GTC Talk
- cuVS IVF-PQ GTC Talk
- cuVS CAGRA arXiv
- NVIDIA Tech Blog



Discussion & Support

- Check the RAPIDS cuVS GitHub
- C++ API documentation
- Python API documentation
- Talk to NVIDIA Services

@RAPIDSai

https://github.com/rapidsai/cuvs

https://rapids.ai/slack-invite/

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https://rapids.ai


NVIDIA