CAGRA: Highly Parallel Graph Construction and Approximate Nearest Neighbor Search for GPUs

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The paper tackles a fundamental challenge in the field of Approximate Nearest Neighbor Search (ANNS) by introducing a GPU-optimized approach to handle increasingly large datasets in applications spanning NLP, computer vision, and recommender systems. While existing CPU-centric methods like HNSW face performance bottlenecks on GPUs due to their variable out-degree nodes and hierarchical designs, CAGRA introduces a **fixed-out-degree**, **flat graph structure that better aligns with GPU architecture capabilities**. This makes CAGRA particularly valuable for fundamental machine-learning tasks like **clustering and manifold learning**.

The **key innovation** of CAGRA lies in its **GPU-optimized proximity graph architecture**. The system employs a two-phase construction methodology: first building a k-NN graph, then enhancing it through a combination of rank-based reordering and reverse edge addition techniques. This rank-based approach delivers substantial memory efficiency gains, achieving **1.9**x faster graph construction while preserving high recall rates. Such optimization enables CAGRA to handle large-scale datasets like DEEP-100M, where traditional distance-based methods often fail due to memory constraints. The fixed out-degree design proves especially beneficial for GPU processing by eliminating the load-balancing issues common in hierarchical structures.

CAGRA implements several GPU-specific optimizations, most notably the warp splitting technique, and forgettable hash table system. Through warp splitting, CAGRA divides 32-thread warps into smaller units, optimizing resource usage for different data dimensionalities. Empirical testing reveals optimal configurations: **4-8 thread teams for lower-dimensional data** (e.g., DEEP-1M with 96 dimensions) and **full 32-thread warps for higher-dimensional cases** (e.g., GIST with 960 dimensions). The forgettable hash table innovation periodically clears cached computations, effectively managing memory usage without compromising search accuracy. These features, combined with CAGRA's dual-mode architecture (single-CTA for batch processing and multi-CTA for individual queries), deliver remarkable performance gains: **33-77x higher throughput** versus HNSW and **3.8-8.8x improvement over existing GPU solutions at 90-95% recall rates**.

Performance evaluations across various dataset scales demonstrate CAGRA's effectiveness. When tested on datasets from DEEP-1M through DEEP-100M, the system achieves a **53x speedup compared to HNSW for individual queries** while maintaining 95% recall accuracy. Construction time improvements are equally impressive: **2.2-27x faster than HNSW** and **31x faster than GGNN**, primarily due to the memory-efficient rank-based optimization strategy. By eliminating the need for extensive distance calculations and lookup tables, CAGRA achieves superior scalability for large-scale data processing.

One notable **strength** of CAGRA is its potential **algorithmic generality**. Although the paper focuses on Approximate Nearest Neighbor Search (ANNS), CAGRA's **rank-based reordering technique** may be beneficial for other graph-based algorithms where distance computations are computationally intensive. This broader applicability to parallel graph algorithms could extend CAGRA's impact beyond ANNS. Moreover, CAGRA's **design demonstrates a deep, GPU-specific adaptation**, especially in optimizing for GPU memory bandwidth constraints and Cooperative Thread Array (CTA) efficiency. The dual-mode implementation, featuring distinct single-CTA and multi-CTA designs, allows for flexibility across batch sizes and optimally

leverages GPU hardware—an uncommon level of adaptation that enhances CAGRA's practical deployment in settings with varying batch sizes.

One **limitation** of CAGRA's design is that like many ANNS algorithms, **CAGRA assumes a static dataset for graph construction**, which may hinder its performance in real-world applications with dynamic data, such as social networks or recommendation systems. Without a mechanism for updating or retraining the graph in real-time, CAGRA might not be as effective in applications that require ongoing adjustments to reflect new data. Another consideration, which the paper does not address, is the **thermal and power consumption implications of intensive GPU use**, particularly in large-batch processing scenarios. In production environments that may be power-constrained, it would be valuable to understand CAGRA's energy efficiency relative to other CPU-based ANNS methods.

To address these limitations, future enhancements could focus on **enabling real-time graph updates for dynamic, streaming data.** Techniques for incremental graph construction could allow efficient updates to nodes and edges, making CAGRA more suitable for dynamic datasets. Furthermore, **expanding CAGRA's compatibility to support a broader range of GPUs (e.g., AMD, Intel) and hybrid CPU-GPU implementations** could widen its applicability across diverse environments. Research into generalizable frameworks, such as Vulkan or OpenCL, could make CAGRA more versatile, particularly in contexts where exclusive reliance on NVIDIA GPUs is less feasible.