Jack Spalding-Jamieson (Jack S-J)
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Independent

Scalable k-Means Clustering for Large k via Seeded Approximate Nearest-Neighbor Search

Joint work with Eliot Robson and Da Wei Zheng

k-Means/Sum of Squares Clustering: Quick Review

Input

- k: a parameter (e.g., $k = 3$)
- n d-dimensional vectors

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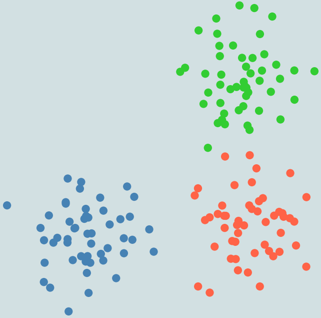

- Clusters $\{C_i\}_{i \in [k]}$ with centroids $\{\mu_i\}_{i \in [k]}$
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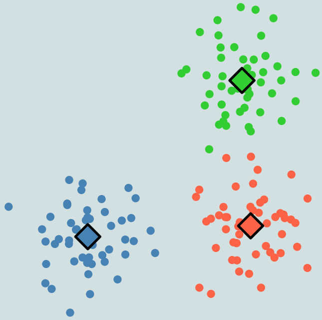

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(Equivalent by Huygens' theorem)

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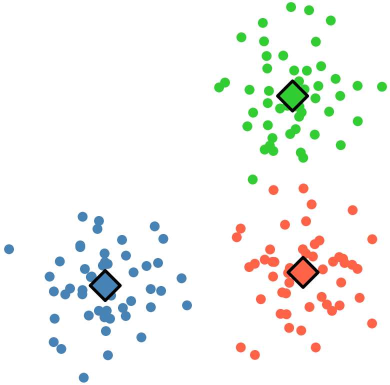

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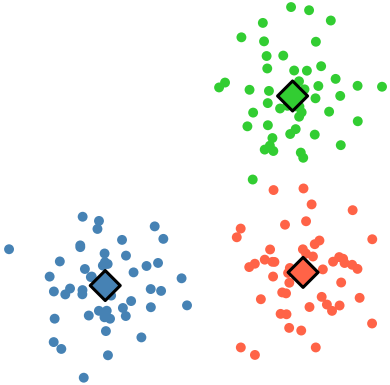

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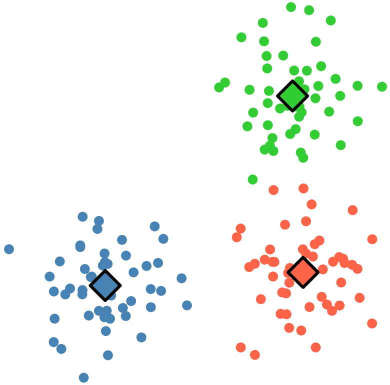

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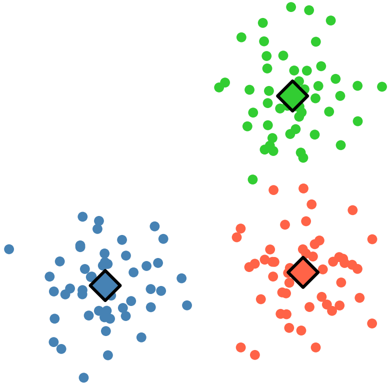

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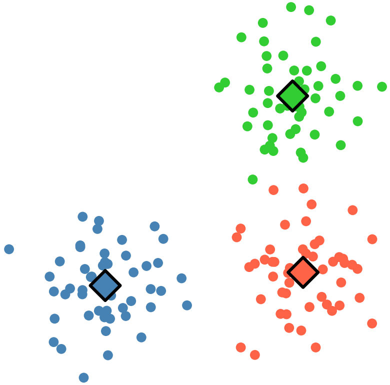

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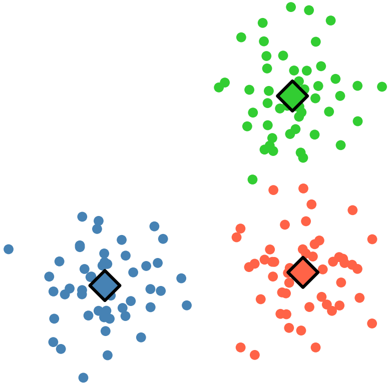

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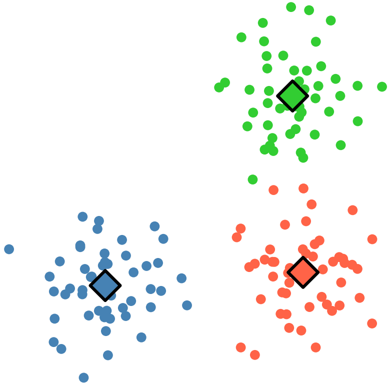
Better approximations known, not used in practice.



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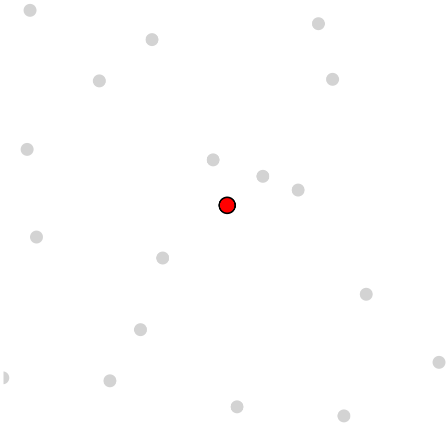

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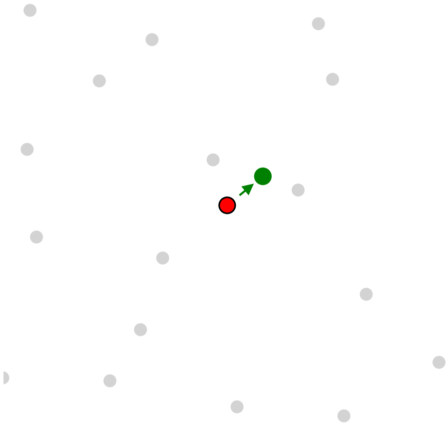

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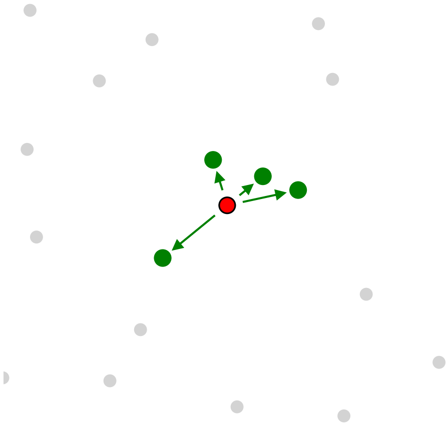

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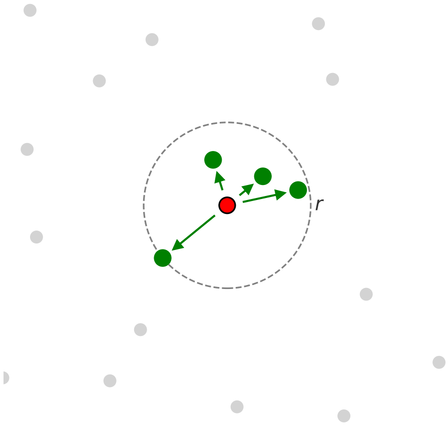

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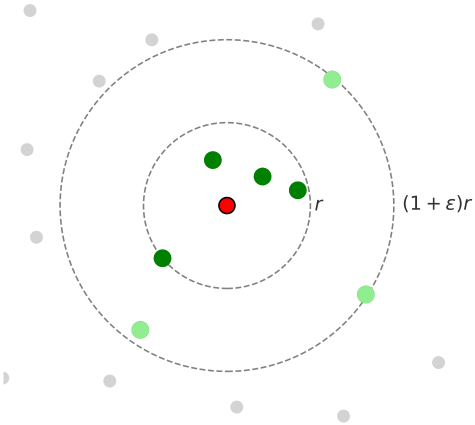

Approximation factor: $(1 + \varepsilon)$

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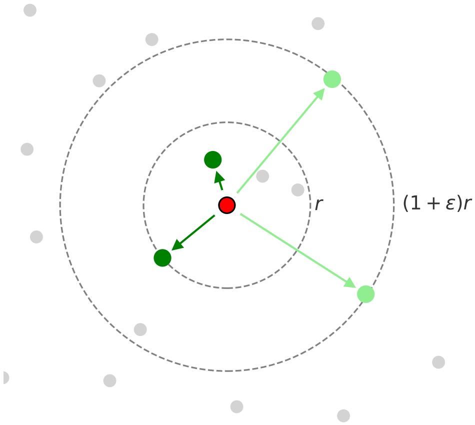

Approximation factor: $(1 + \varepsilon)$
Recall: $\frac{2}{4} = 0.5$

Dataset sizes vs Existing Approaches

ANNS has three broad families of practical approaches:

- Quantization
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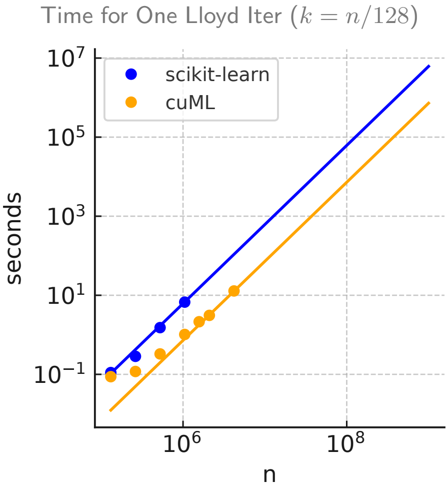
e.g. 200-dimensional f32 dataset with $20,000,000$ points requires 16GB (plus data structure size).

Some Motivation

"Vector Similarity Search" is very popular in machine learning recently, with a lot of active development.



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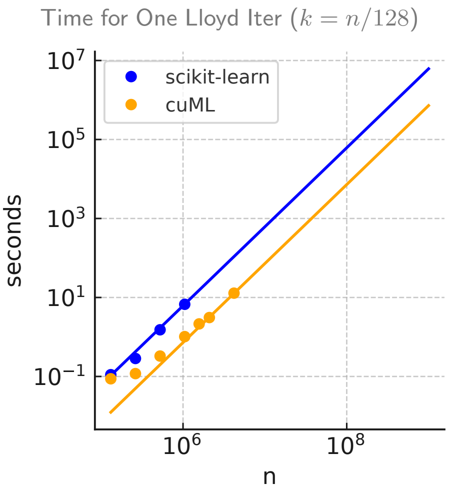

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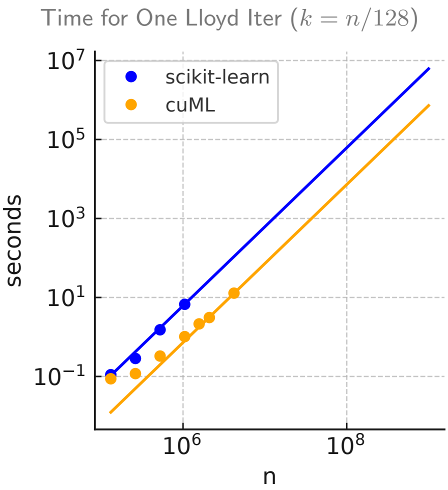

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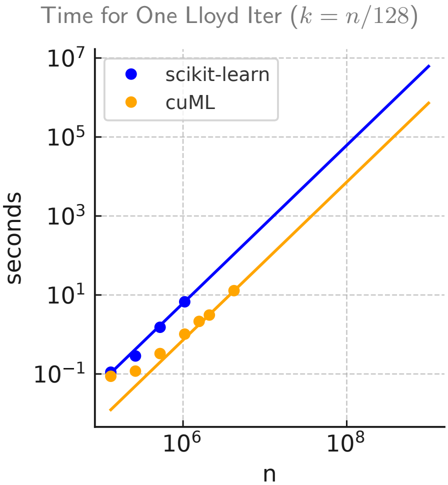

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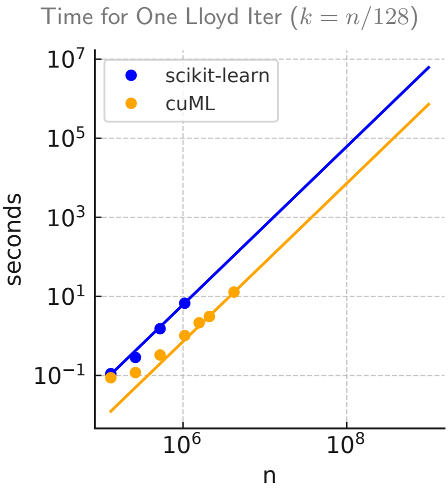

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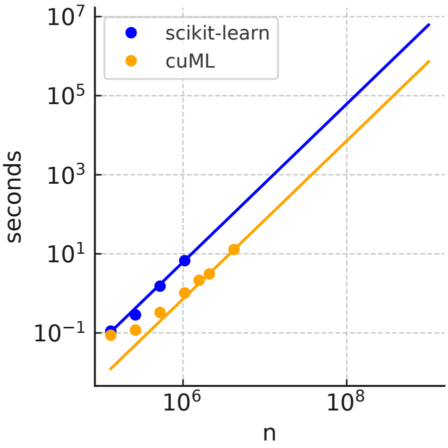

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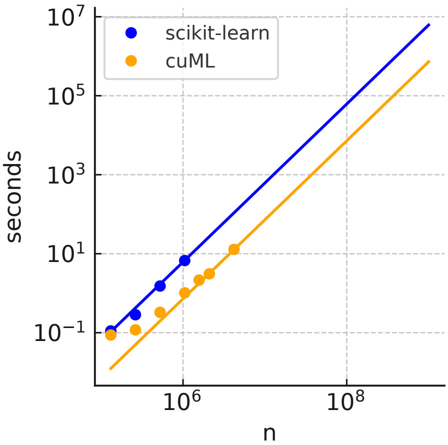

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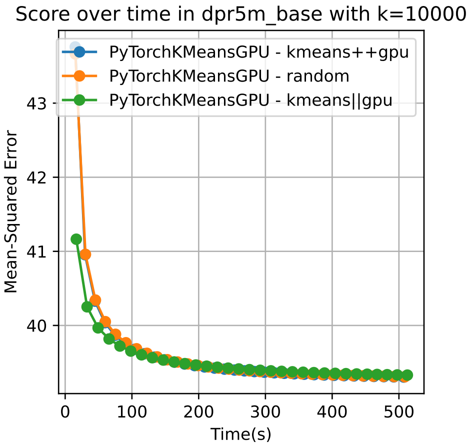
Large n/k: Only Lloyd's algorithm matters (right)
Conclusion: Want to accelerate Lloyd's algorithm



Checkpoint 1

Out-of-Core Similarity Search

(used by your favourite semantic search engine)

Basically out-of-core ANNS with n base points

↓

k-Means Clustering

↓

Exact NNS

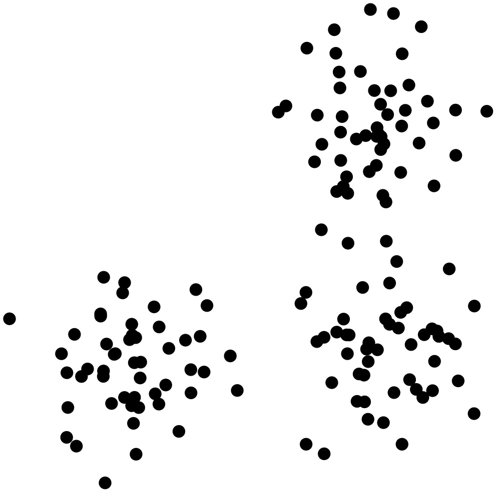
k base points

↓

GPU Acceleration

1. **Initialization:** Sample k centroids uniformly from the dataset.
2. Iterate (local search):
   - **Assignment:** Assign each point to the nearest centroid.
   - **Mean Computation:** Update each centroid to be the average of points assigned to it.

Bottleneck is **Assignment** step.



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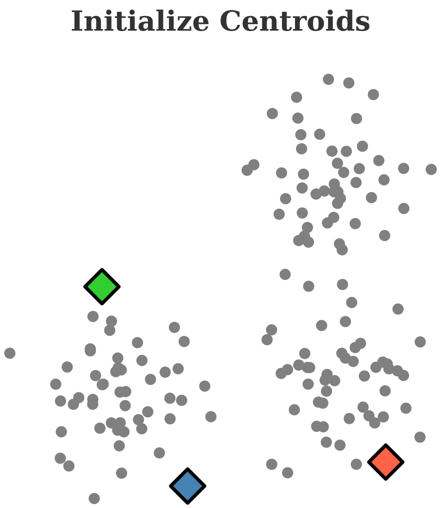

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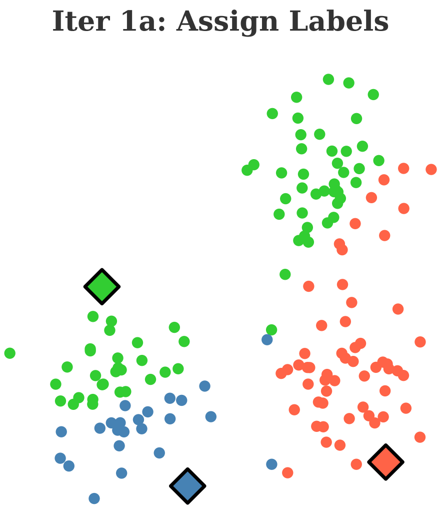

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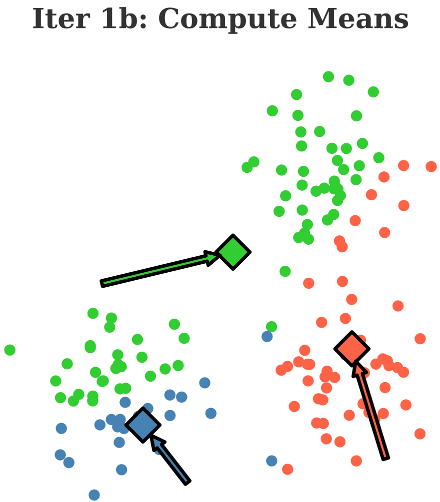

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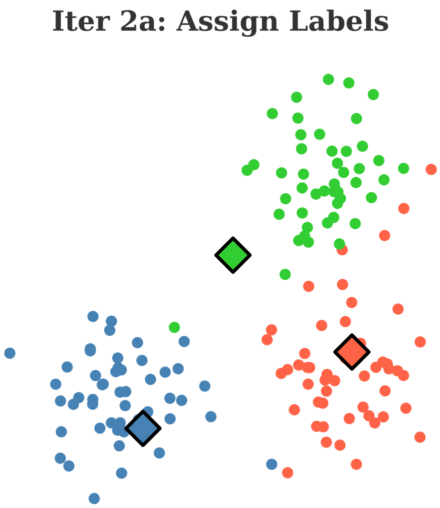

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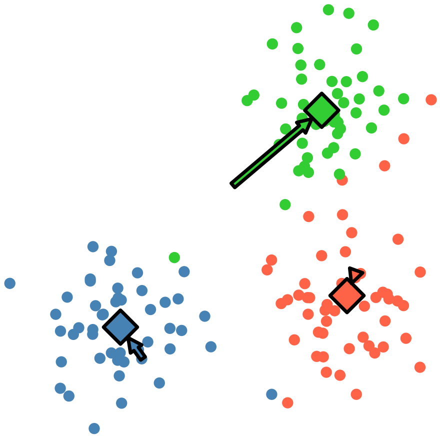
Iter 2b: Compute Means



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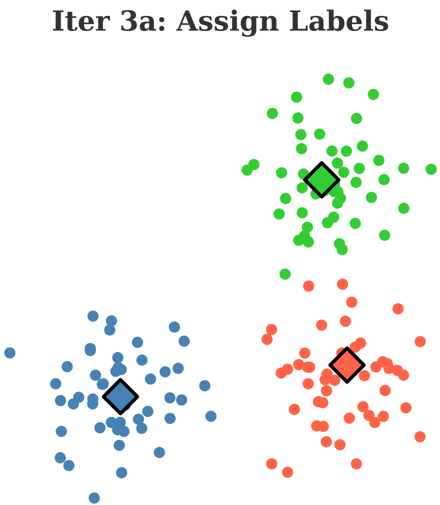

Lloyd's k-Means Method

1. **Initialization:** Sample k centroids uniformly from the dataset.
2. Iterate (local search):
   - **Assignment:** Assign each point to the nearest centroid.
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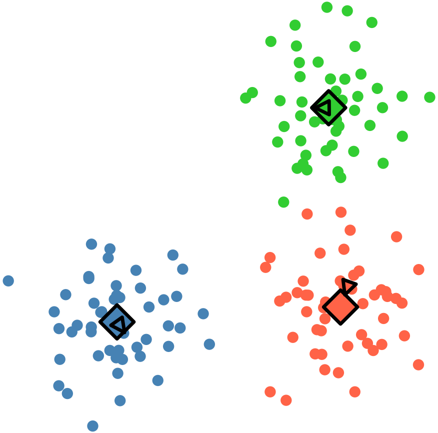
Iter 3b: Compute Means



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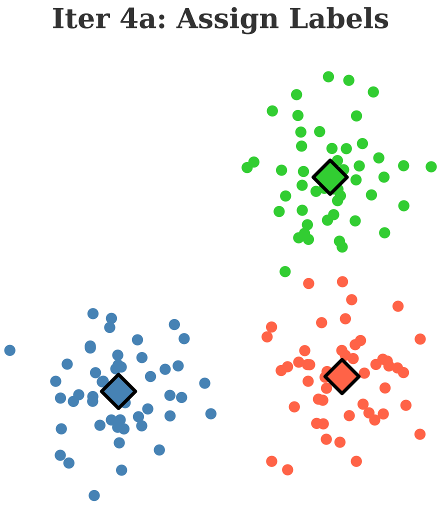

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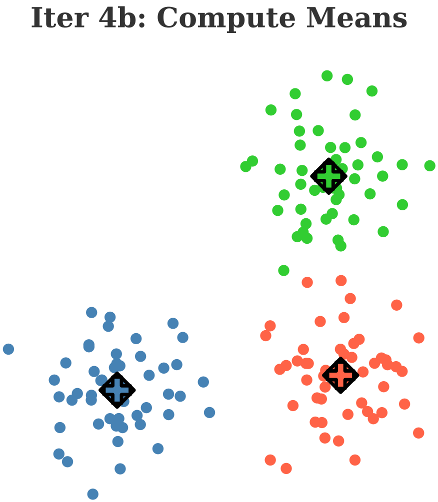

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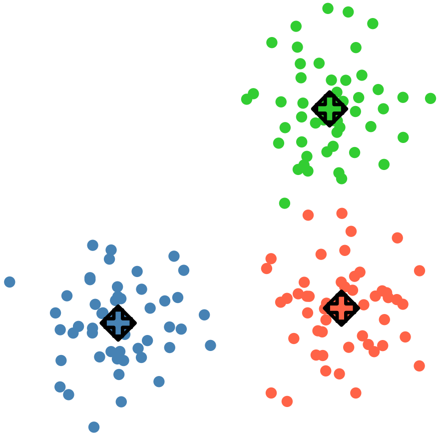
Lloyd's algorithm is very limited in theory.
But it's very good in practice.

Iter 4b: Compute Means



Lloyd Iterations with a Black-box ANNS Data Structure

Alternative iteration approach:

- **Build**: Construct an **approximate nearest neighbor search (ANNS) data structure** on the centroids.
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Why ANNS? Exact-NN has a linear lower bound in high-dimensions[1].
ANNS has strong lower bounds too[2], but good widely-used heuristics exist.

---

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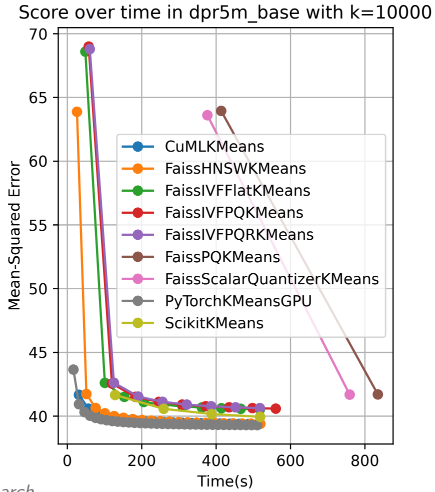

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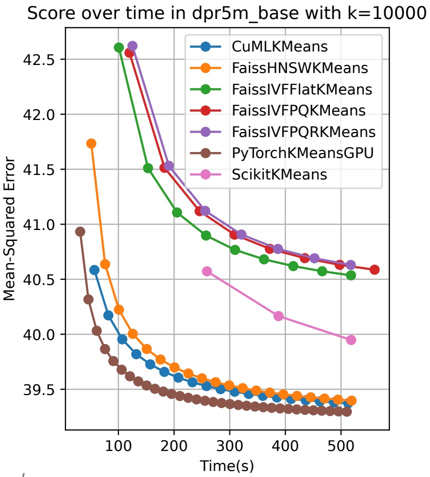

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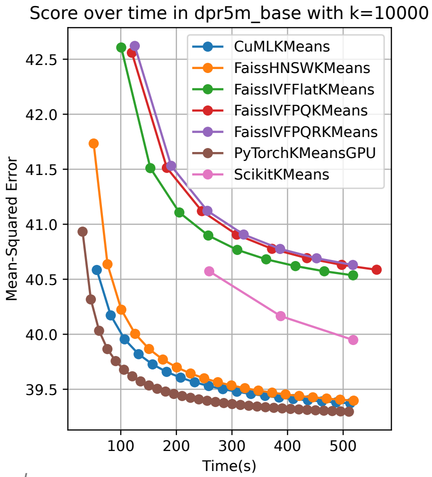

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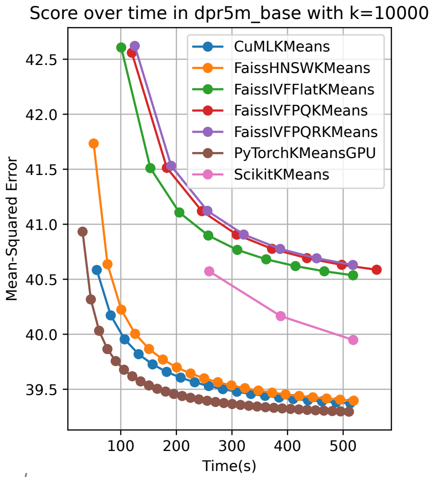

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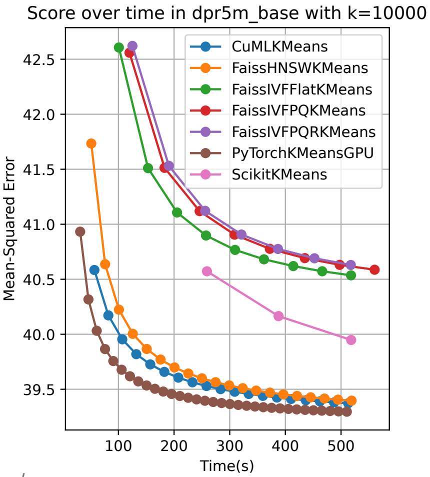
  - **Almost as good as Nvidia's own GPU imlementation.[4]**



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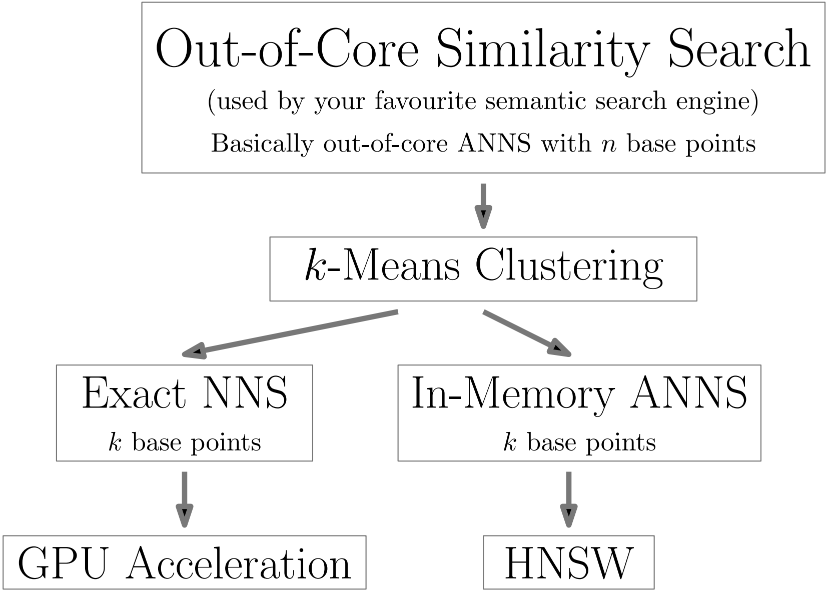
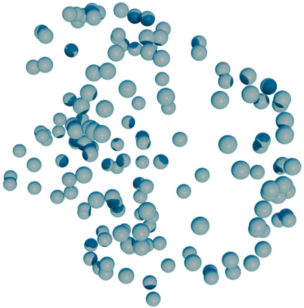
Checkpoint 2



HNSW Review



Structure

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- Prune edges with a heuristic
- Randomly subsample points to get higher layers (similar to skip list)
- Build/insertions also similar to skip list

Search

- Start at arbitrary point on top level
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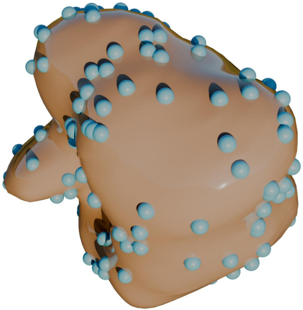

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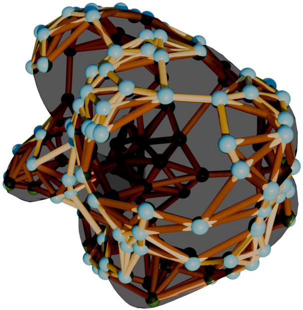

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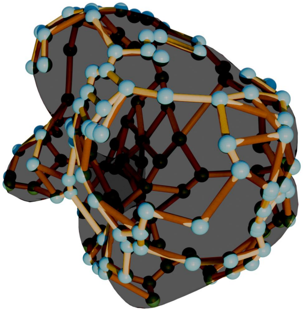

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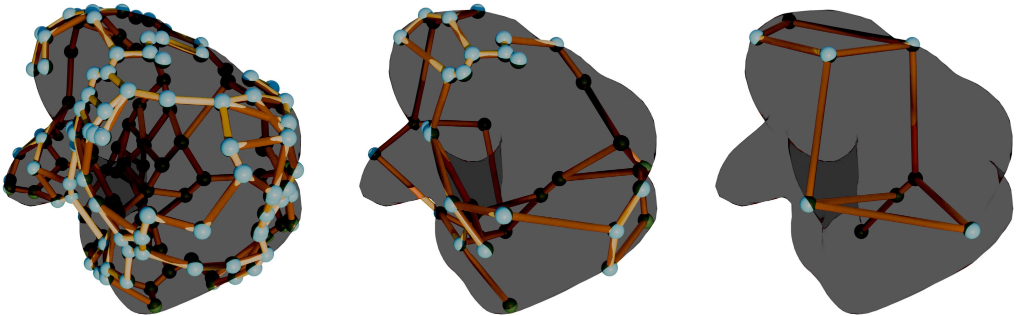

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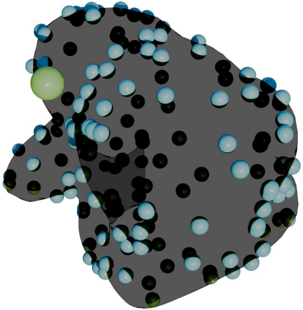

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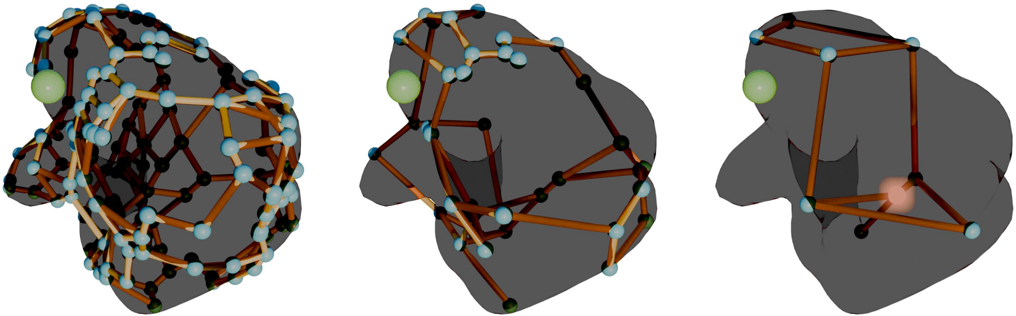

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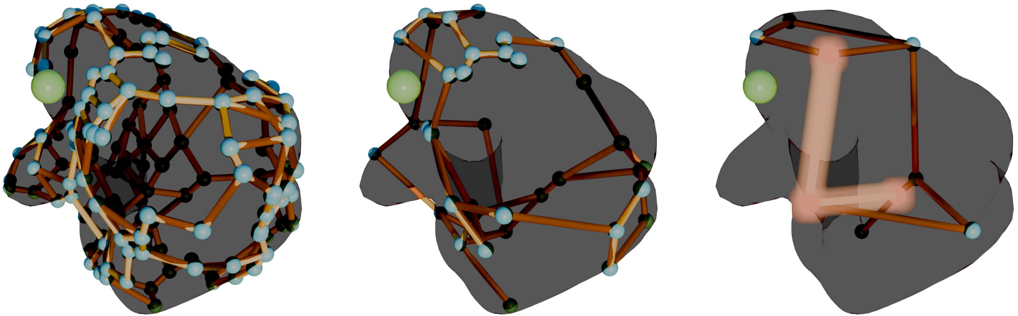

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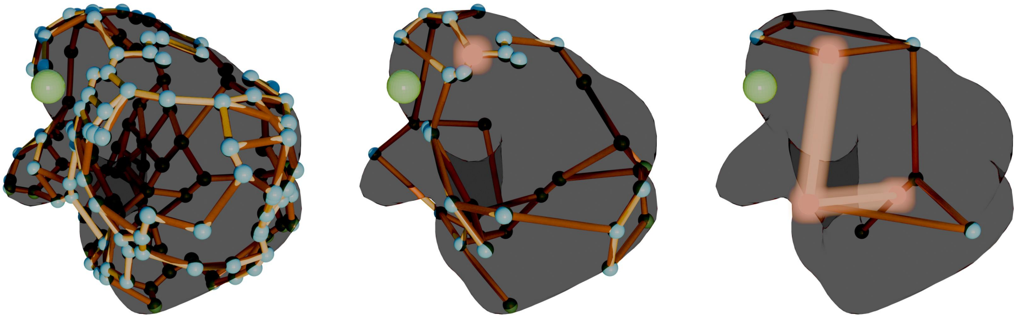

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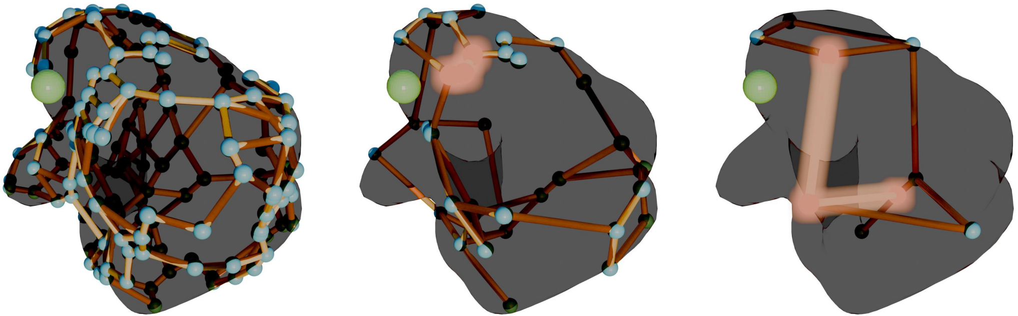

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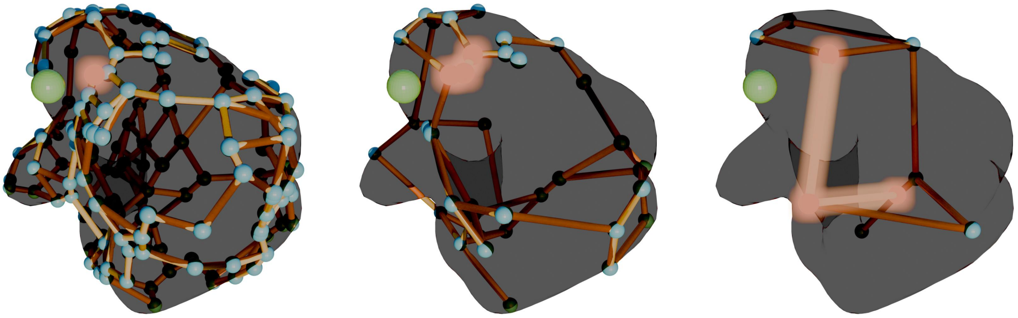

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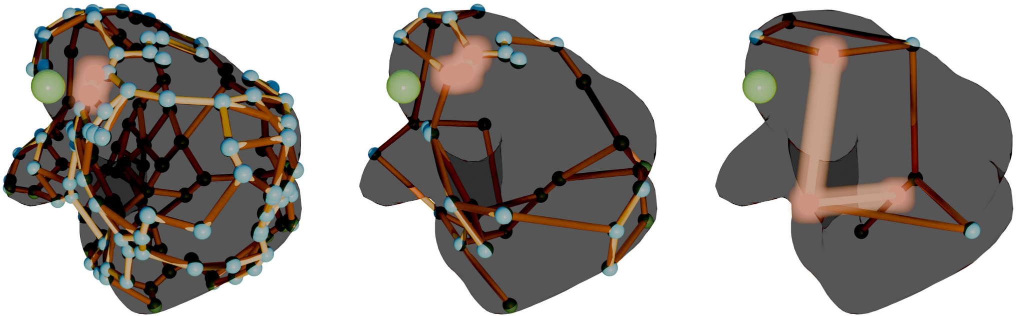

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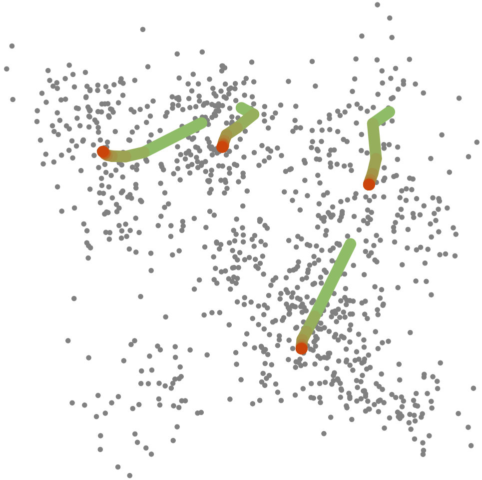
In HNSW: Add seed points right at start of search on last level. Similar for other search-graph methods (result: **seeded search-graphs**).

Main Improvements: Beating Black-Box HNSW

Centroids "slow down" over time:

- Rebuilds (HNSW as a kind of kinetic data structure, omitting details)
- Extra "seed points" from prev assignment: Seeded ANNS



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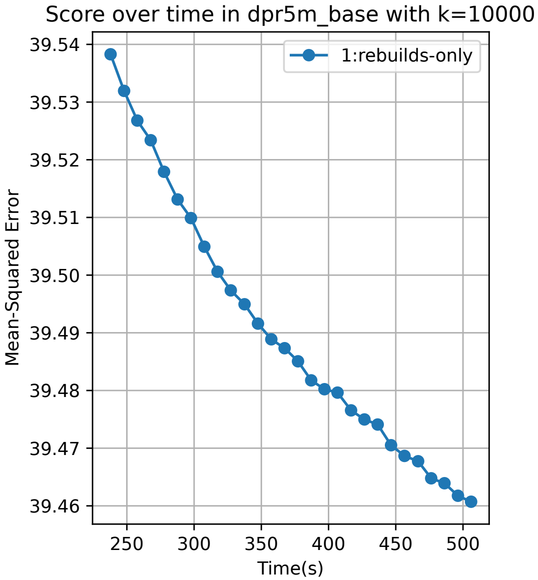

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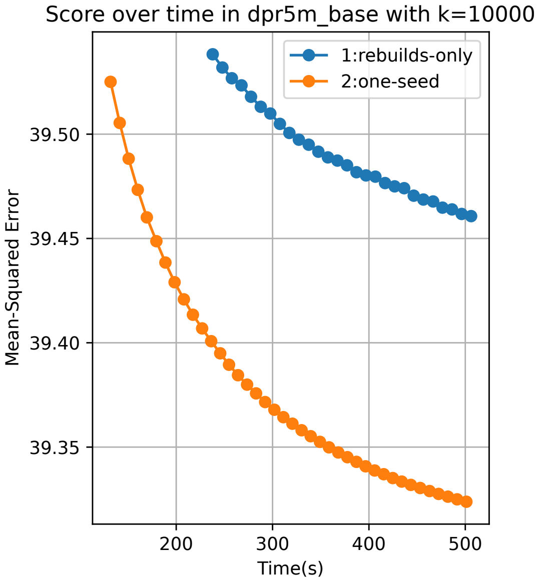

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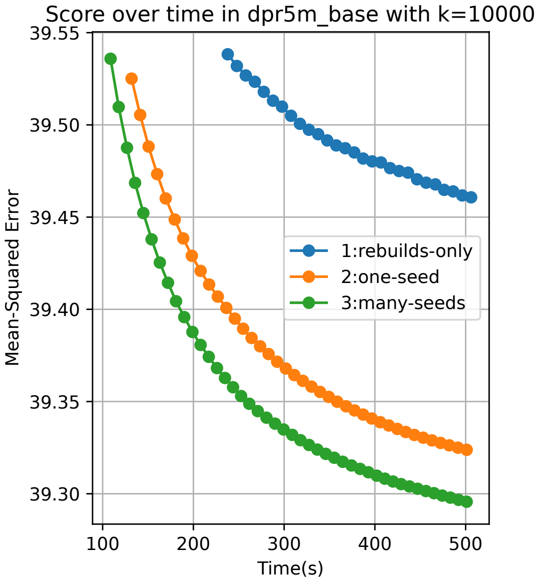

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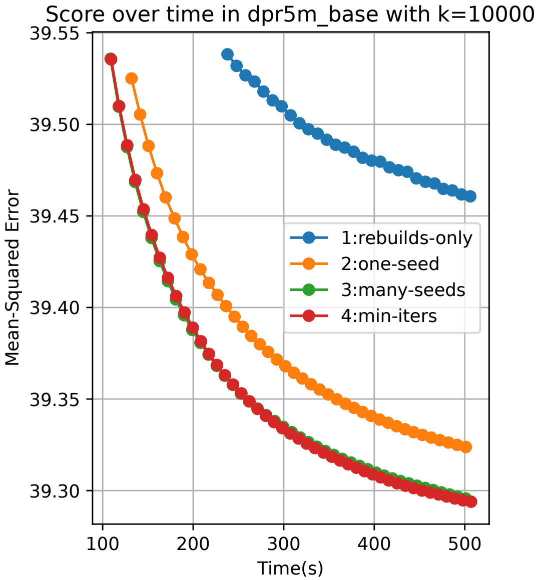

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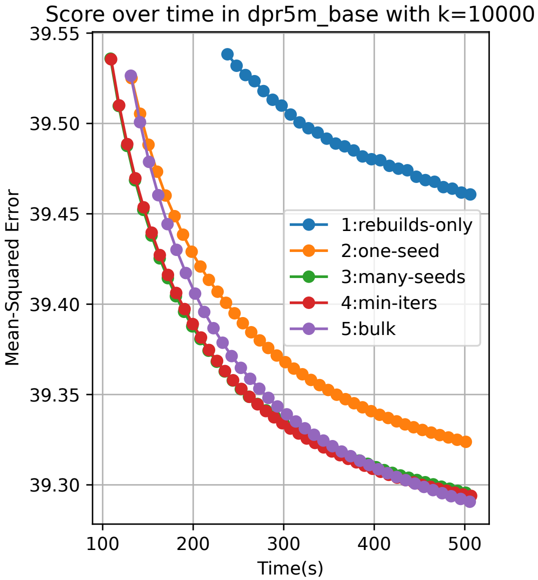

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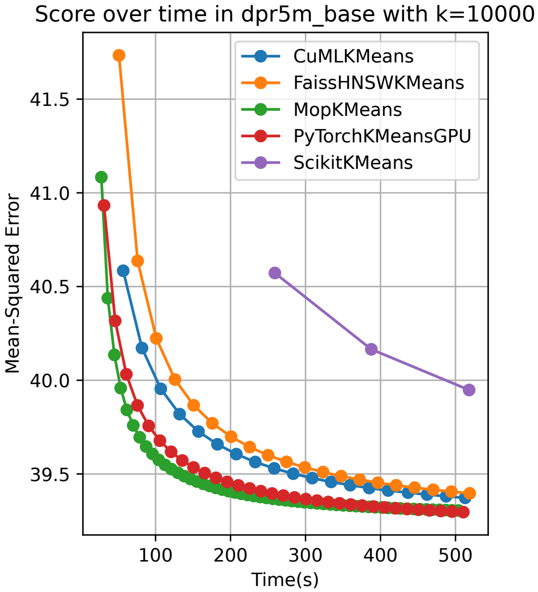
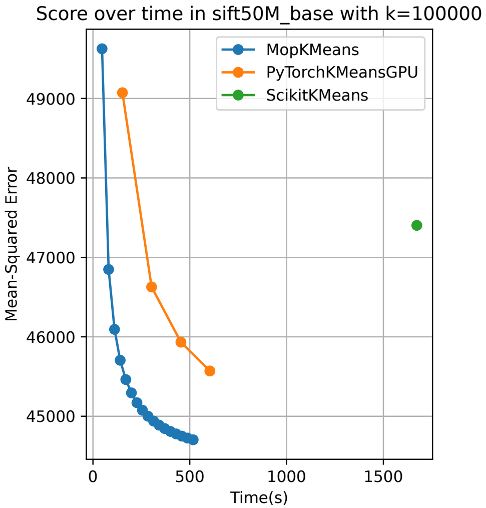
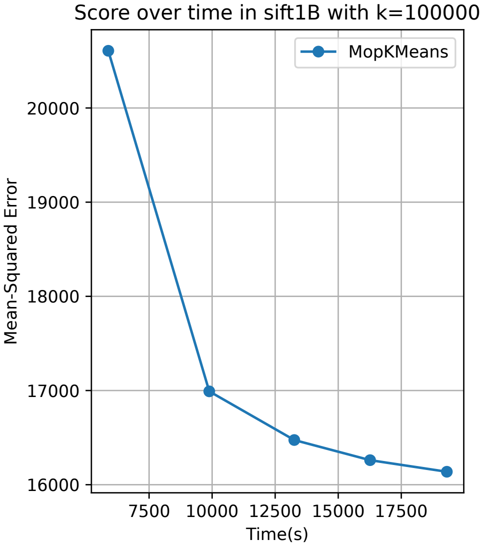
- Bulk queries for more seed points

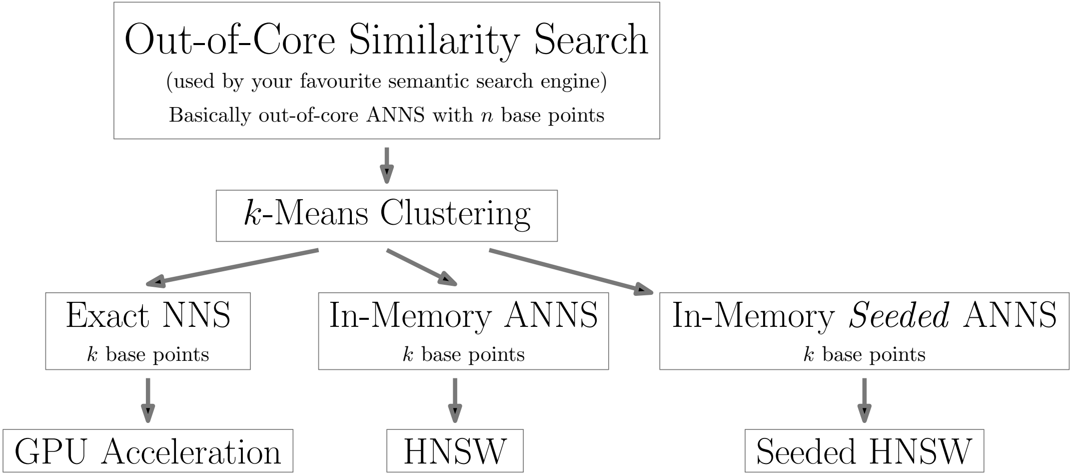
Now (mostly) **beating GPU implementations with CPU**.



More Results



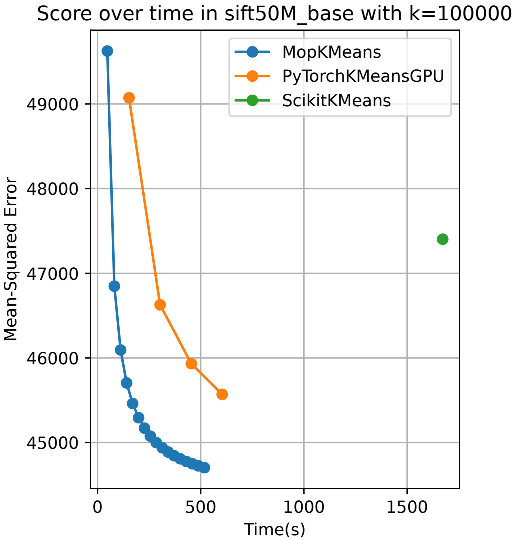



Out-of-Core Similarity Search
(used by your favourite semantic search engine)
Basically out-of-core ANNS with n base points
k-Means Clustering
Exact NNS
k base points
In-Memory ANNS
k base points
In-Memory *Seeded* ANNS
k base points
GPU Acceleration
HNSW
Seeded HNSW

Open Problems

- GPU-acceleration of SANNS? No current methods for ANNS on GPU extend well.
- Perfect consistency guarantees for SANNS in fixed doubling dimension? Search-graph methods don't seem to work.
- General open ANNS problem: Better theoretical understanding of why search-graphs work well? Best known is (tunable) additive approximation known for one specific graph algorithm, with fixed doubling-dimension[1].

arxiv.org/abs/2502.06163



[1] Indyk & Xu, *Worst-case performance of popular approximate nearest neighbor search implementations [...]*

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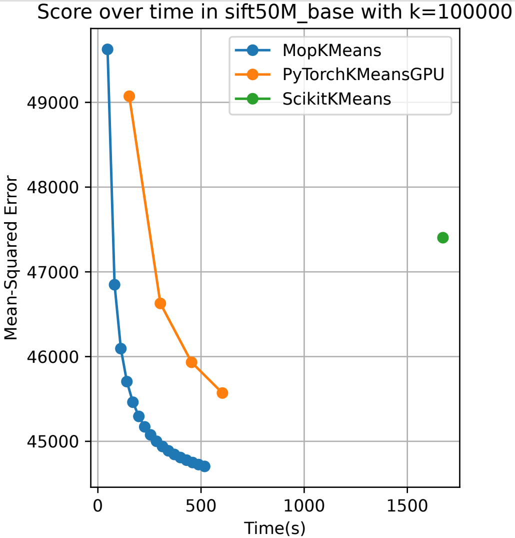

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Fin.

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