Are You My Neighbor? Bringing Order to Neighbor Computing Problems.

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Part III: Approximate Search

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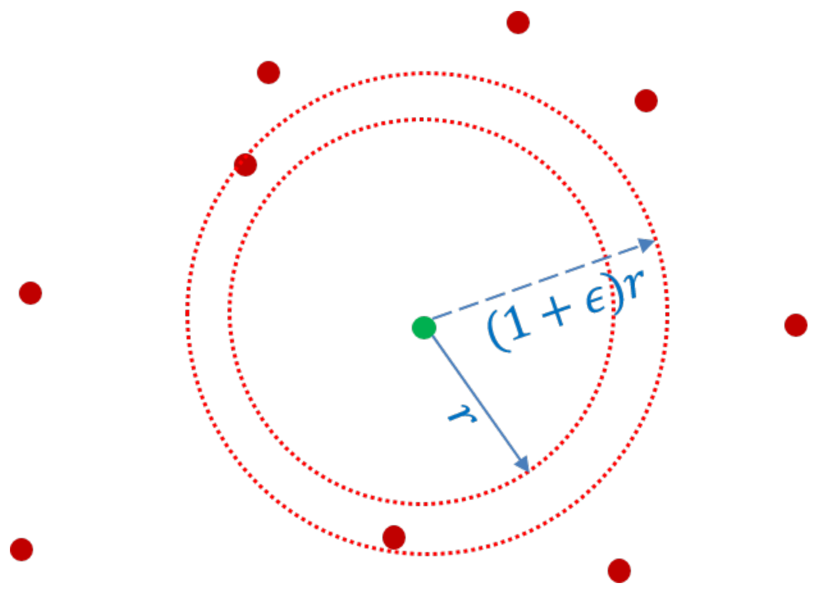
Tutorial Outline

- **Part I: Problems and Data Types**
  - Dense, sparse, and asymmetric data
  - Bounded nearest neighbor search
  - Nearest neighbor graph construction
  - Classical approaches and limitations
- **Part II: Neighbors in Genomics, Proteomics, and Bioinformatics**
  - Mass spectrometry search
  - Microbiome analysis
- **Part III: Approximate Search**
  - Locality sensitive hashing variants
  - Permutation and graph-based search
  - Maximum inner product search
- **Part IV: Neighbors in Advertising and Recommender Systems**
  - Collaborative filtering at scale
  - Learning models based on the neighborhood structure
- **Part V: Filtering-Based Search**
  - Massive search space pruning by partial indexing
  - Effective proximity bounds and when they are most useful
- **Part VI: Neighbors in Learning and Mining Problems in Graph Data**
  - Neighborhood as cluster in a complex network system
  - Neighborhood as influence trigger set

Approximate near(est) neighbor search

- Input: $\mathrm{P}, \mathrm{q}, r, \epsilon$
- Output:
  - If some points exists with $\mathrm{dist}(\mathrm{p}, \mathrm{q}) \leq r$, output any such ANN and return YES
  - If no points exists with $\mathrm{dist}(\mathrm{p}, \mathrm{q}) \leq (1+\epsilon)r$, return NO
  - Otherwise, return any point with $\mathrm{dist}(\mathrm{p}, \mathrm{q}) \leq (1+\epsilon)r$

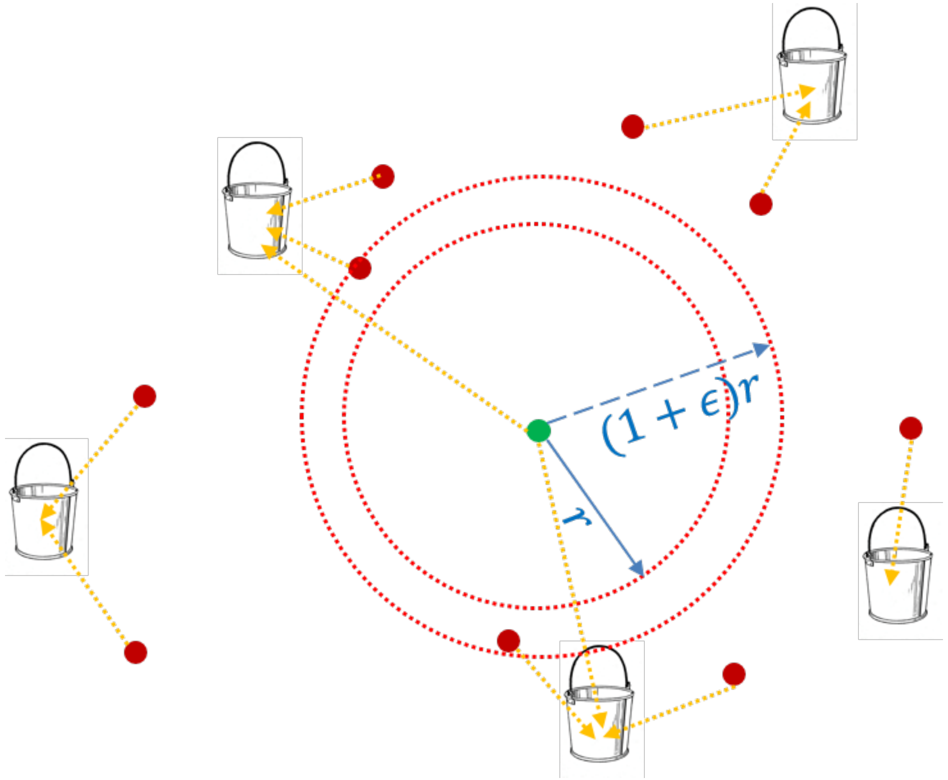


Directions of approximate methods

- Plethora of methods, especially in recent years
- Deep learning and abundance of data lead to a push towards
  - Faster and faster methods
  - Methods that can search 1 Billion+ objects
  - While accuracy is sought after, scaling and efficiency seem to be of primary concern
- Methods fall into one or more of the following categories:
  - Locality-sensitive hashing
  - Graph traversal
  - Quantization
  - GPU-focused
  - Other

Locality sensitive hashing

- A set of functions is *locality-sensitive*, if, for a **random** hash function h in the set, for any pair of points p, q:
  - $Pr[h(p) = h(q)]$ is "high" if p is "close" to q
  - $Pr[h(p) = h(q)]$ is "low" if p is "far" from q



Locality sensitive hashing

- *Preprocessing* :
  - Hash the data-point using several LSH functions so that probability of collision is higher for closer objects (increases recall, but hurts precision)
    - E.g., partition with random Gaussian noise vectors for Euclidean distance search
- *Querying* :
  - Hash query point and retrieve elements in the buckets containing the query point
- Give-and-pull between # hashes and # tables
  - Increase precision by repeating the search multiple times (use several hash functions) and keeping only common points (set intersection)
  - Increase recall by repeating the search multiple times (use several hash functions) and keeping all found points (set union)

Recent directions in LSH

- C2LSH
  - Identifies candidates by collision counting
  - Good candidates express a large number of collisions with the query when tested against dynamically-generated compound hash functions derived from a set of m initial functions.
- QALSH
  - A query-aware data-dependent LSH scheme
  - Boundaries of the buckets are query-dependent, decided once query is received
    - Leads to improved effectiveness

Quantization methods

- Main idea is to reduce the size of the vectors so more can fit in memory/cache
  - A quantizer is a function mapping real-valued vectors into a vector of integers from a finite set

- PQ
  - Decomposes the space into a Cartesian product of low dimensional subspaces, which are separately quantized.
  - A vector is represented by a short code composed of its subspace quantization indices.
- OPQ
  - Improves quantization accuracy by a linear transformation applied to the input vectors

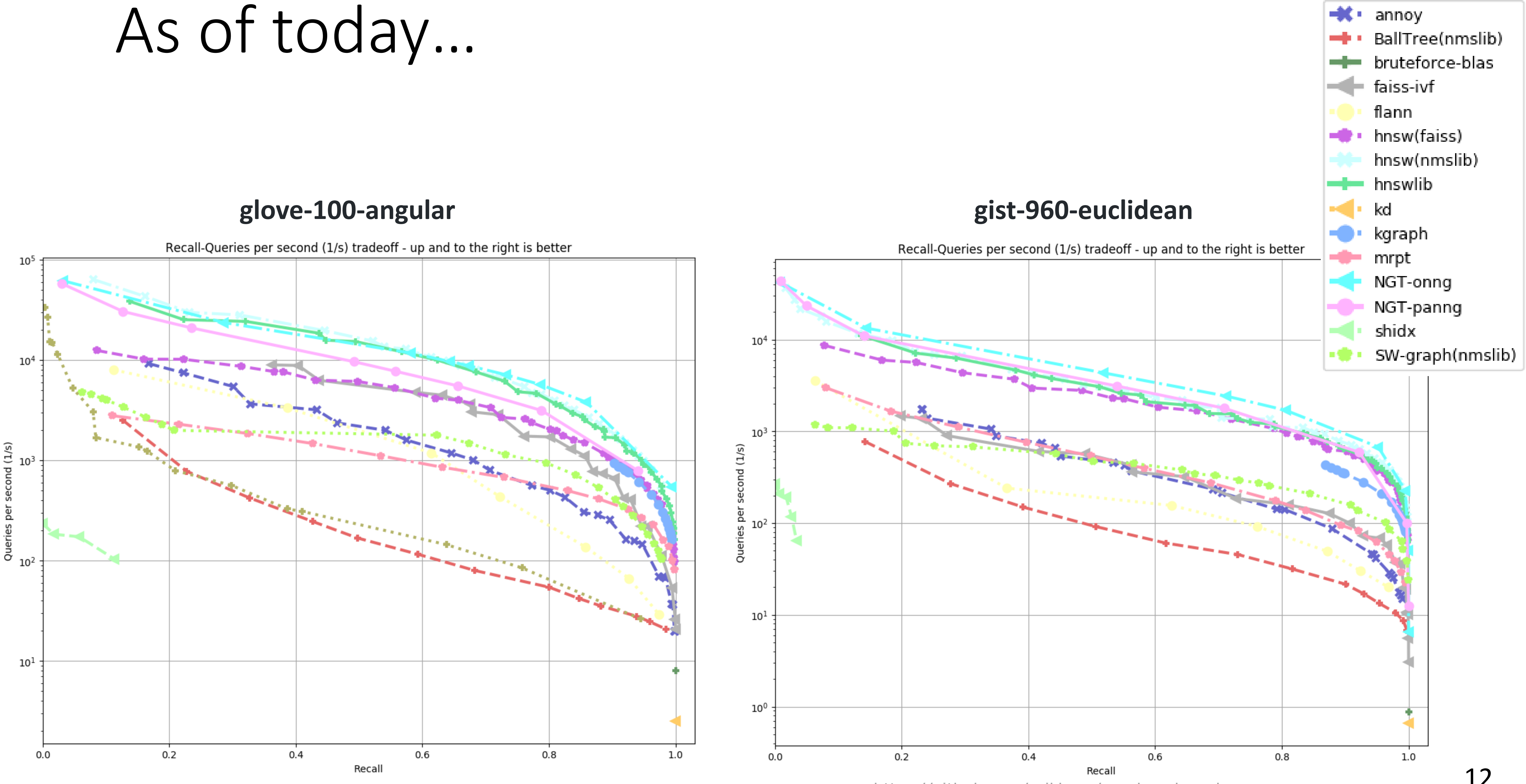
Graph traversal method

- Main idea is to pre-process the objects and build a k-NNG including all database objects
- At search time, the k-NNG is traversed in search of better and better neighbors for the query
- The methods largely differ in:
  - Starting point in traversing the graph
    - NGT, e.g., uses a secondary tree structure to identify better/optimum starting points
  - Traversal strategy
    - kGraph, e.g., looks only among the neighbors of the query's current neighbors for possible better neighbors
  - Local or global graph construction
    - HNSW creates a tree of k-NNGs at different granularities
      - During the search, it also expands the search space with less-similar candidates, as a way to prevent getting stuck in a local structure (think simulated annealing, or restarts in PageRank).

So, what's the best search method?

- It depends on your data (primarily dimensionality and number of objects)
- Erik Bernhardsson put together a benchmarking framework for approximate nearest neighbor codes
- It provides
  - Realistic data sets
  - Standard evaluation metrics
  - A platform to showcase algorithm comparisons
- It requires
  - Python bindings for the tested methods
- https://github.com/erikbern/ann-benchmarks

As of today…



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