VLDB 2020 Tutorial

Similarity Query Processing for High-Dimensional Data

Jianbin Qin
Shenzhen Institute of Computing Sciences
Shenzhen University

Wei Wang
University of New South Wales

Chuan Xiao
Osaka University and Nagoya University

Ying Zhang
University of Technology Sydney

Subtitles

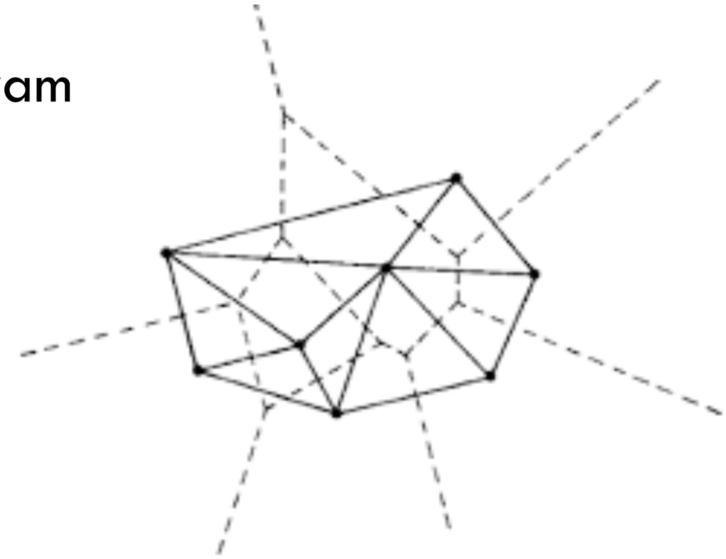
Neighbourhood-based Nearest Neighbour Search

Motivation

Delaunay graph – dual of Voronoi Diagram

For 2 dimension space

- Greedy without backtracking
- Expected log(n) steps



Curse of dimensionality !

Neighbourhood-based Nearest Neighbour Search

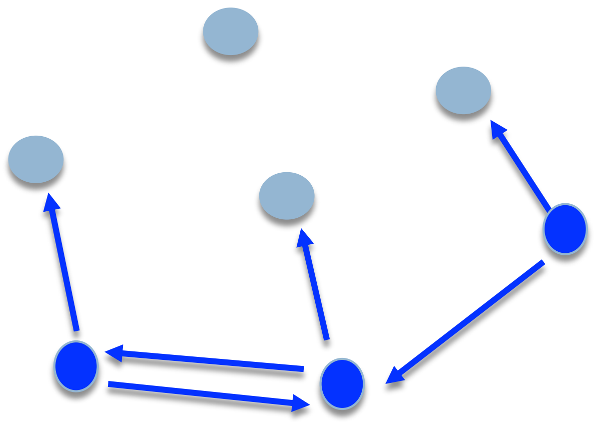
- **KNN graph based methods**
- Small world graph based methods
- Relative neighbourhood graph based methods
- Investigations under some specific settings
- Benchmark

KNN graph based Methods

KNN graph

Each point x in high dimensional space → a **vertex** x in the KNN graph

For it's k nearest neighbours {y} → add a directed **edge** x → y



K = 2

KNN Graph Construction

- **Exact KNN graph construction**
  - Brute-force costs $O(n^2)$
  - Other exact algorithms, e.g., **L2Knng** (CIKM'15)
- **Approximate KNN graph construction**
  - Reducing to individual KNN search

    e.g., based on LSH methods, but still expensive
  - Jointly find KNN for everyone, such as

    L2 distance: data partition (Jie JLMR09) , space filling curve (Connor TVVG10).

    general metric distance: **Kgraph** (WWW'11), etc

    sparse data: **KIFF** (ICDE'16), etc

Important properties for KNN graph construction

- General
- Scalable
- Space efficient
- Fast
- Accurate

Kgraph (www'10) – Motivation

- Neighbors' neighbors are likely to be neighbors

- By exploring each point's neighbors' neighbors, we can
  - Recover missing true K-NN graph edges
  - Find approximations better than current ones

Slides from Dr. Wei Dong (WWW'11)

Kgraph (www'10)

NN-Descent

1. Initialize K-NN graph approximation

   Each point randomly picks K neighbors

2. Loop, each point

   Explores its current neighbors' neighbors

   Updates K-NN list if better ones are found

   Until no improvements can be made

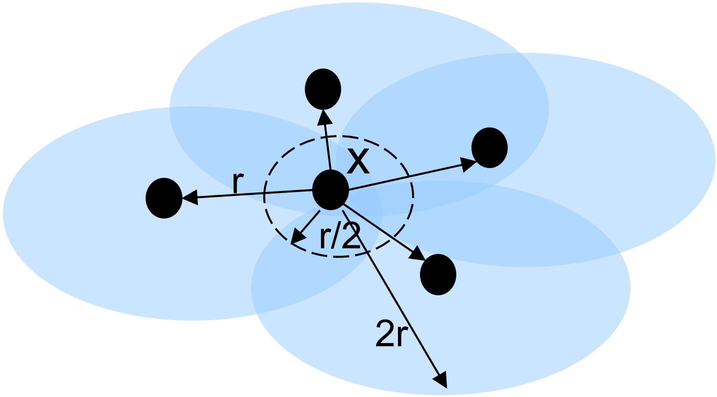
Implementation: https://github.com/aaalgo/kgraph

Slides from Dr. Wei Dong (WWW'11)

Kgraph (www'10) - Analysis under assumptions

- Assume *growth restricted* - doubling constant c :

$$|B_{r/2}(x)| \geq \frac{1}{c}|B_r(x)| \geq \frac{1}{c^2}|B_{2r}(x)|$$



- If for every x we have K points in $B_r(x)$

  → explore K^2 points in $B_{2r}(x)$

  → expect to hit $\frac{K^2}{c^2}$ points in

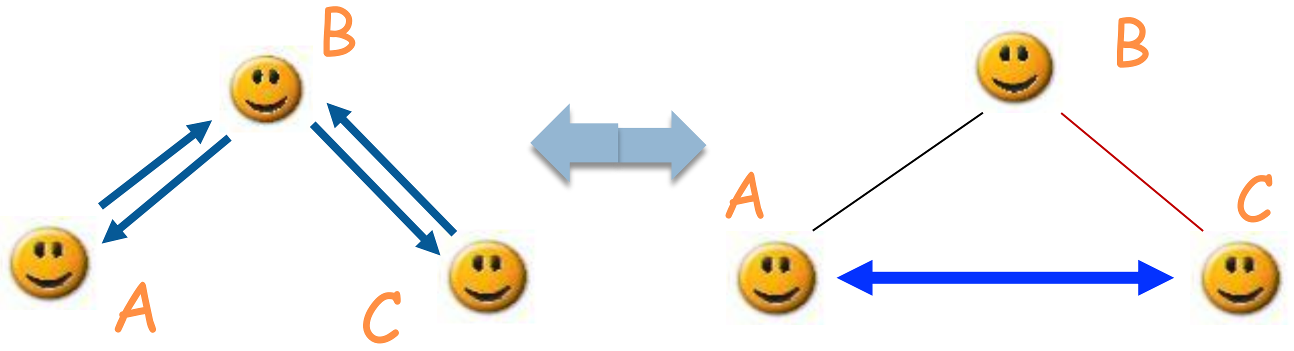
  Set $\frac{K^2}{c^2} \geq K$, or $K \geq c^2$, and we can repeatedly improve!

- It should converge in $\log \Delta$ iterations (Δ: diameter of dataset)

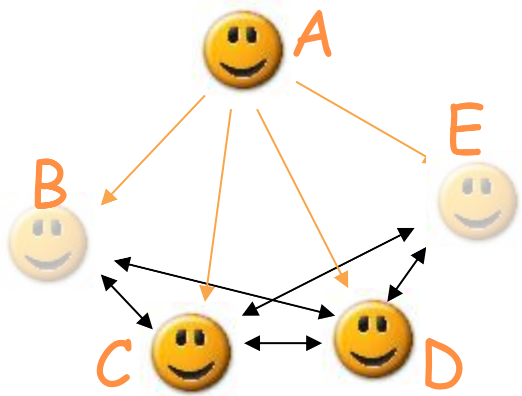
Slides from Dr. Wei Dong (WWW'11)

Kgraph (www'10), Computation Speedup

- Local Join



- Incremental search



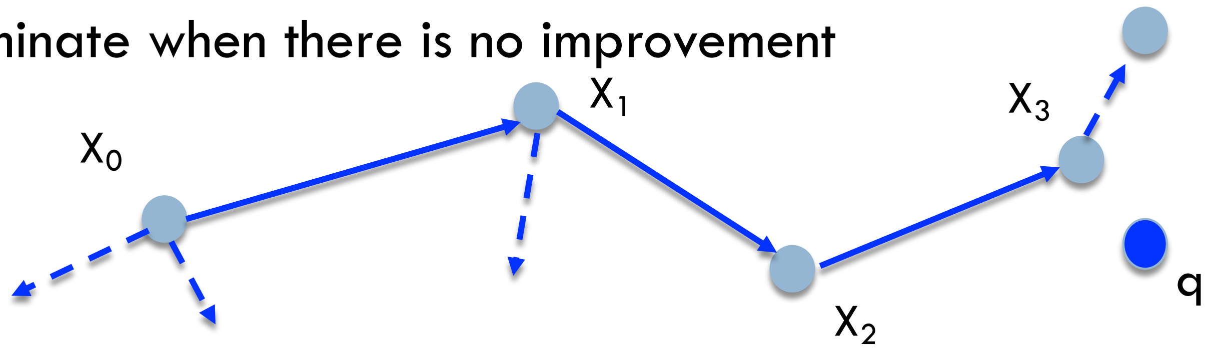
- Sampling
- Early termination

Slides from Dr. Wei Dong (WWW'11)

Search on KNN graph – Greedy heuristic

[e.g., ChávezEric MCPR'10, Hajebi ICJAI'11, k-DR KDD'11]

- One or more random selected starting nodes
- Keep on finding the closest node among unvisited neighbor nodes
- Terminate when there is no improvement



In practice, a candidate node list with limited budget is used to avoid local optimum (beam search):

e.g., implementation of Kgraph [https://github.com/aaalgo/kgraph] from Dr. Wei Dong

Vairants of kNN graph

- Sparsification of KNN graph (**k-DR** KDD'11)
- Diversified KNN graph (**DPG** TKDE'20, CoRR'16)
- Pruned Bi-directed KNN graph (**PANNG**, SISAP'16)

k-DR KDD’11

- **k-DR graph**: Degree reduced undirected kNN graph

How approximate?

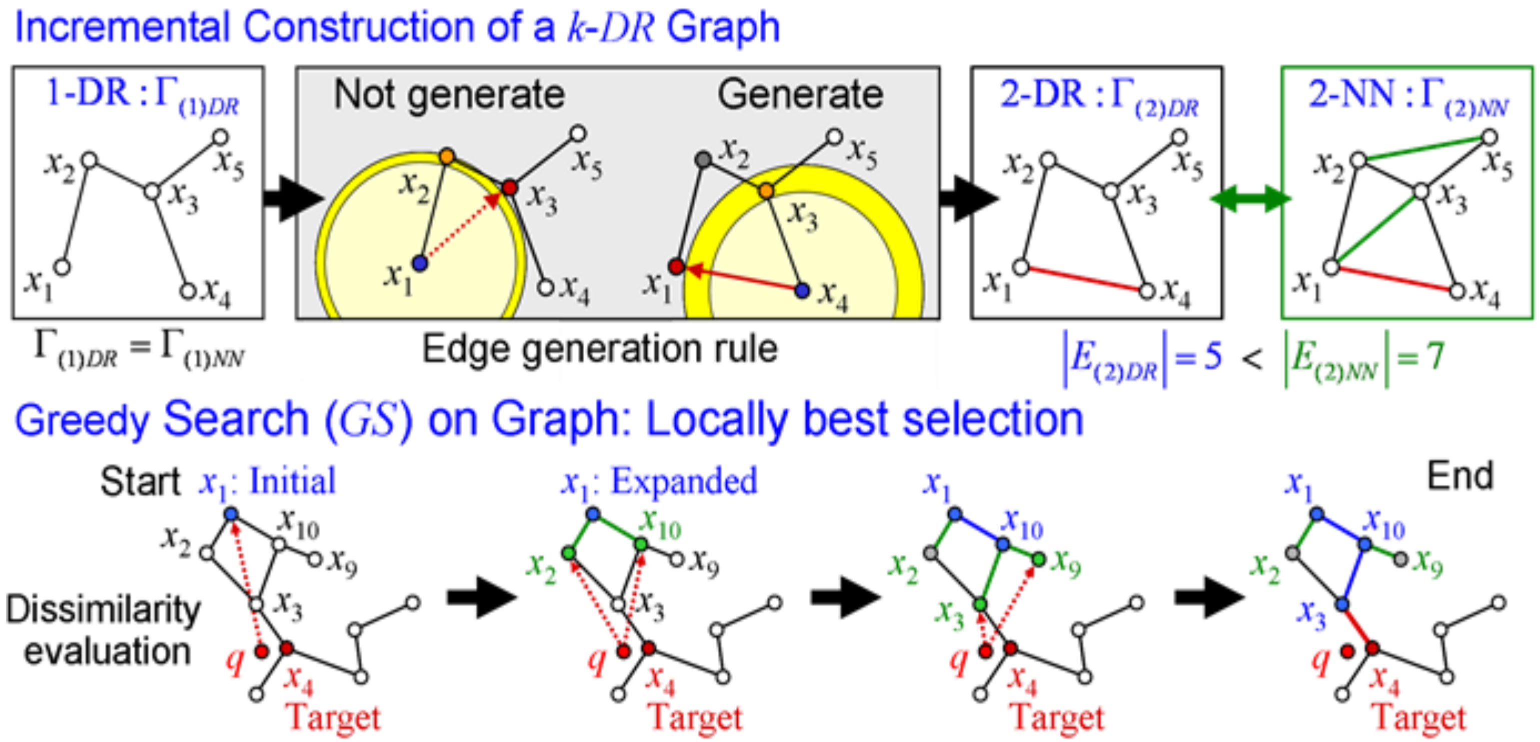
Given: Failure probability δ and # search trials L

Determined: Graph structural parameter k

$$\boxed{\text{Probability that at least one of } L \text{ search trials succeeds} > 1-\delta}$$

Slides from Prof. Sawada *(KDD’11)*

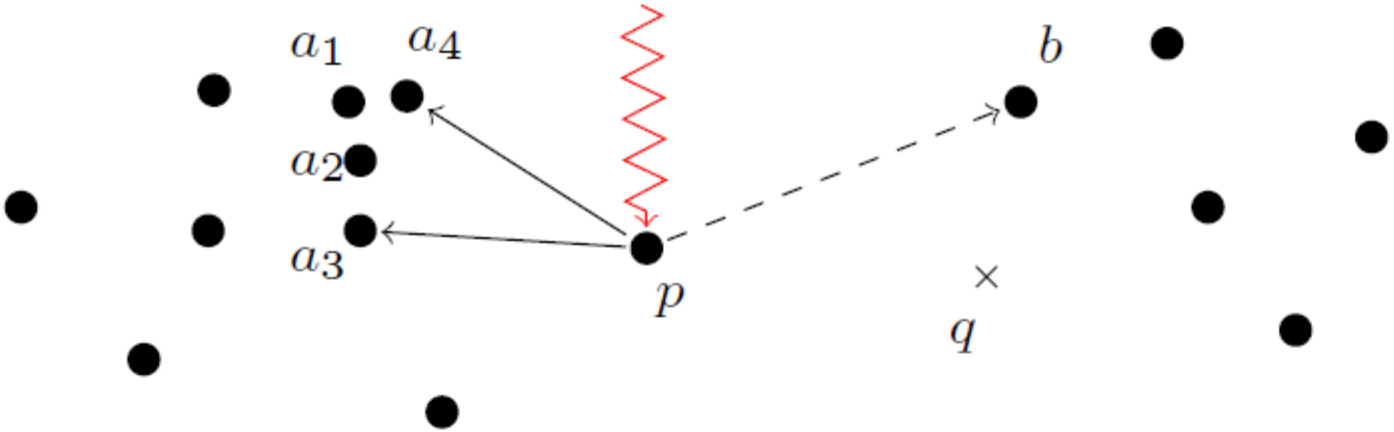
k-DR KDD'11



Slides from Prof. Sawada *(KDD'11)*

DPG TKDE'20, CoRR'16

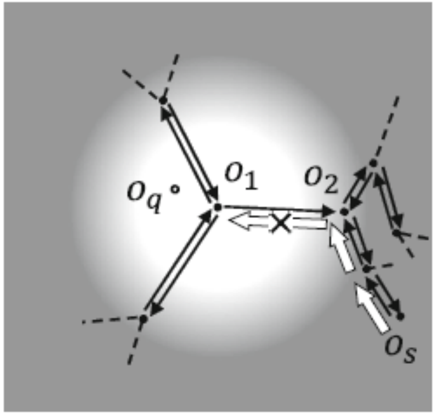
- **DPG**: Diversified Proximity Graph
  (https://github.com/DBWangGroupUNSW/nns_benchmark/tree/master/algorithms/DPG)

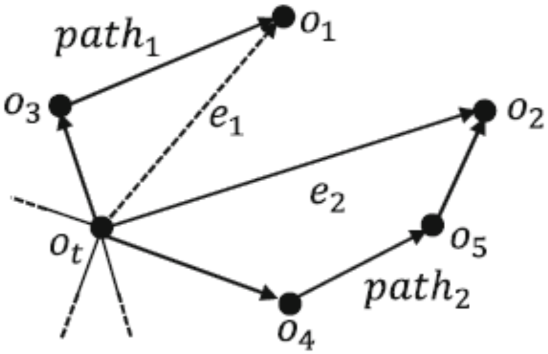


Build KNN graph, then (1) choose K/2 diversified neighbours; (2) add reverse edge when necessary

PANNG, SISAP'16

- **PANNG** : Pruned bi-directed KNN graph
  (https://github.com/yahoojapan/NGT)





(1) bi-directed edge; (2) remove edges according to distance & connectivity

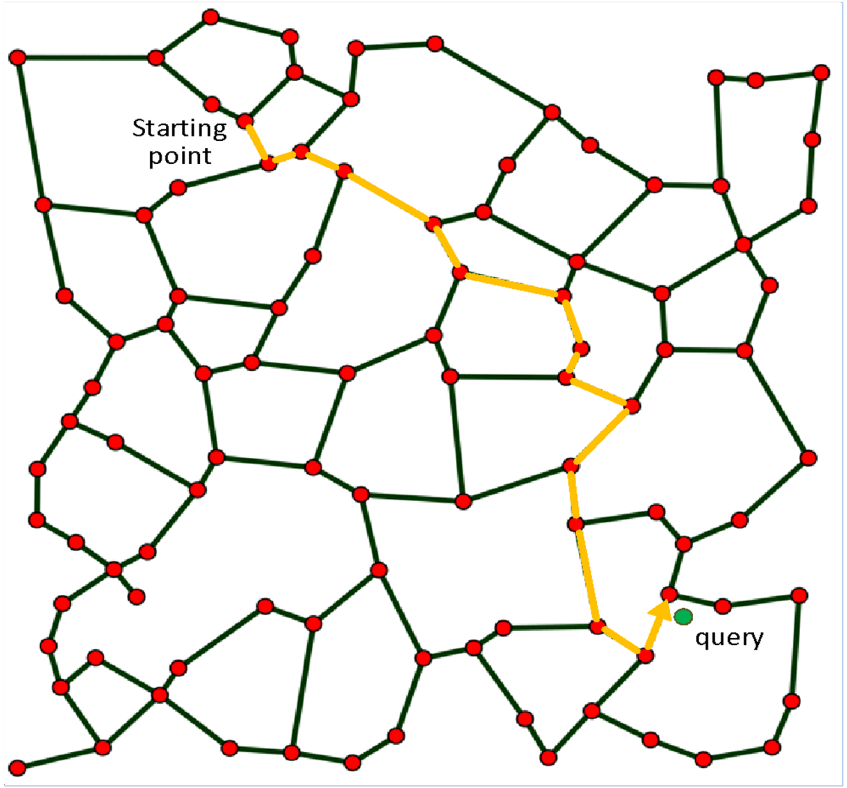
Neighbourhood-based Nearest Neighbour Search

- KNN graph based methods
- Navigable small world graph based methods
- Relative neighbourhood graph based methods
- Investigation under some specific settings
- Benchmark

NSW IS'14

Problem: Long paths in proximity graphs.

Idea: Social networks are searchable e.g. Milgram experiment.



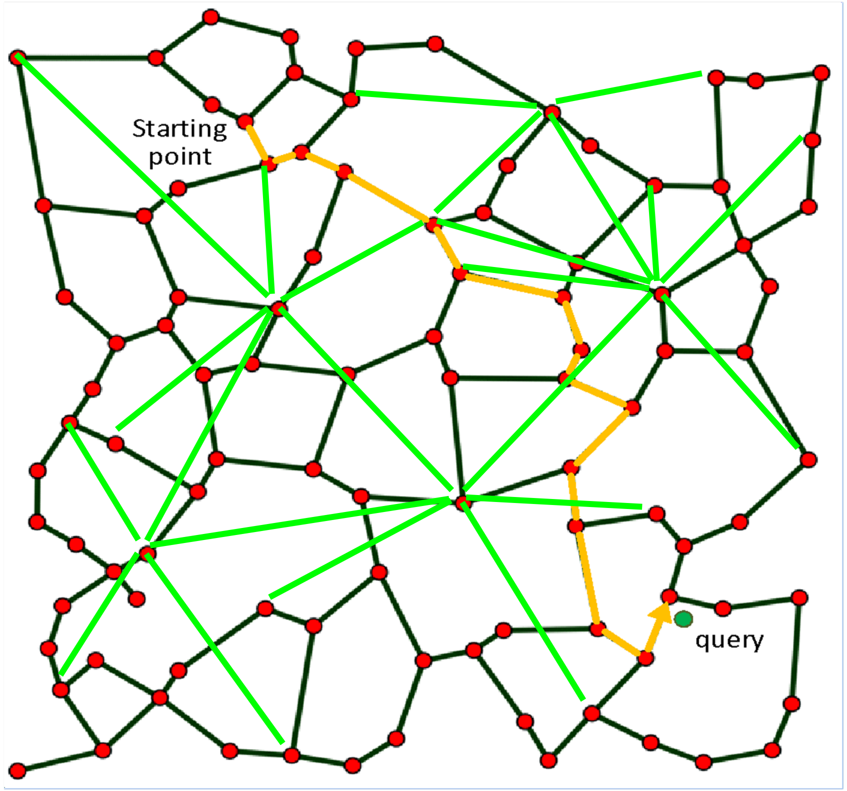
Slides from Dr. Malkov *(IS'14)*

NSW IS'14

Problem: Long paths in proximity graphs.

Idea: Social networks are searchable e.g. Milgram experiment.

Solution: Just add “long” links (e.g. with NSW algorithm) to get log(N) hops.

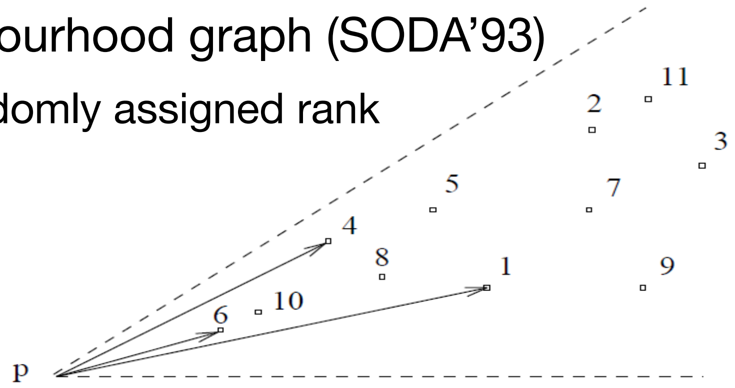


Slides from Dr. Malkov *(IS’14)*

Construction of SW graph

- Randomized neighbourhood graph (SODA'93)

Based on **distance** & randomly assigned rank



- Navigable small world (**NSW**) graph (IS'14)

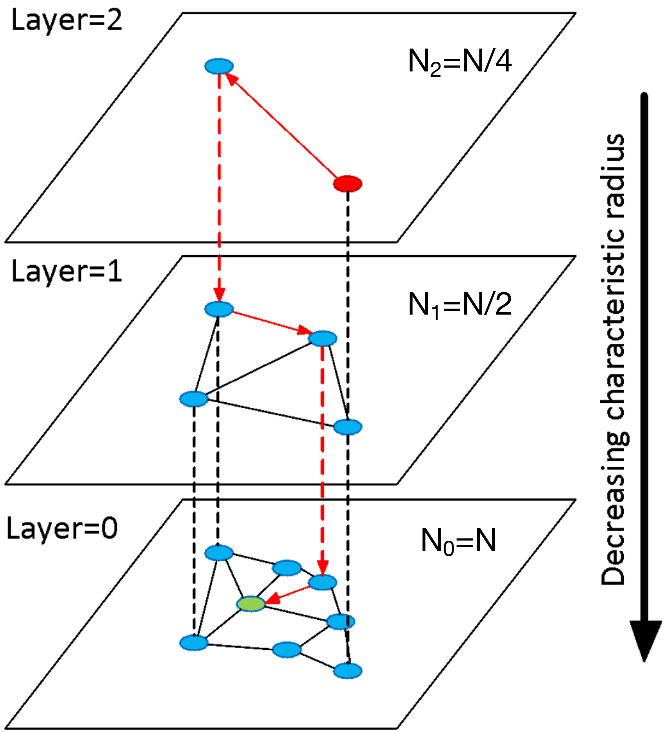
Incremental construction of NSW graph:

(1) k-NNS for each new node;

(2) updates it's neighbours after other nodes are inserted (keep old edges)

HNSW TPAMI'20, CoRR'16

- In HNSW we split the graph into layers (fewer elements at higher levels)
- Search starts for the top layer. Greedy routing at each level and descend to the next layer.
- Maximum degree is capped while paths ~ log(N) → log(N) complexity scaling.
- Incremental construction



Slides from Dr. Malkov *(TPAMI'20)*

HNSW implementation

- Carefully implemented in C/C++:

https://github.com/nmslib/nmslib (**2.1k stars**)
https://github.com/nmslib/hnswlib (**1k stars**)

- Third-party open-source implementations in Java, C#, Rust, Go, Python, Julia, including the ones by **Facebook** (Faiss) and **Microsoft** (HNSW.Net)

- Used in production in **Amazon, Snapchat, Yandex, Twitter, Pinterest** and other s.

Slides from Dr. Malkov *(TPAMI'20)*

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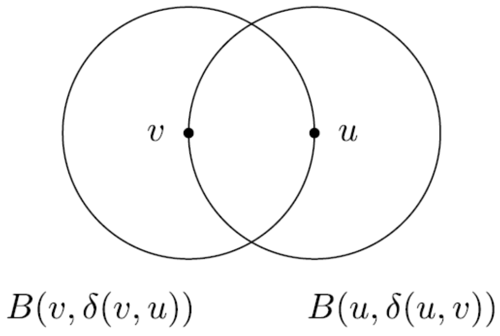
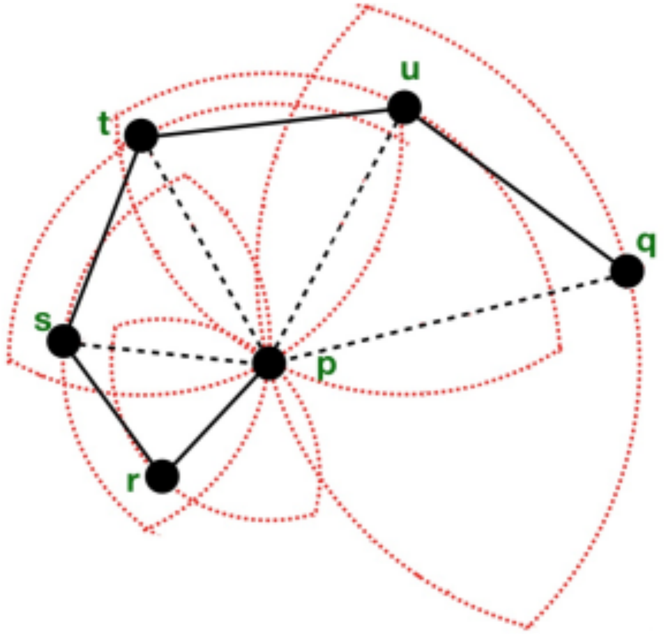
Relative Neighbourhood graph

- **Relative Neighbourhood Graph (RNG)**





Vertices u and v are connected if there is no vertex in the intersection of the two balls.

Brute-force costs $O(n^3)$

FANNG CVPR'16

Occlusion definition

edge(p_1, p_2) occludes edge(p_1, p_3) if

$$d(p_1, p_2) < d(p_1, p_3) \text{ and } d(p_2, p_3) < d(p_1, p_3)$$

Diagram form

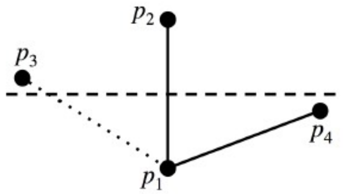


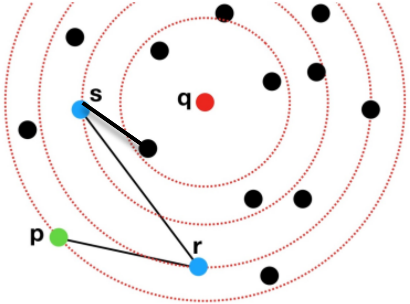
Figure 1. An edge from p_1 to p_2 occludes an edge from p_1 to p_3 because p_3 is closer to p_2 than p_1. The edge to p_4 is not occluded.

- ❑ In practice, the trade-off between recall and computational cost is managed by placing a hard limit on the number of distances that will be computed.

NSG VLDB'19

- **Monotonic Path**

distance to the end point monotonically decrease



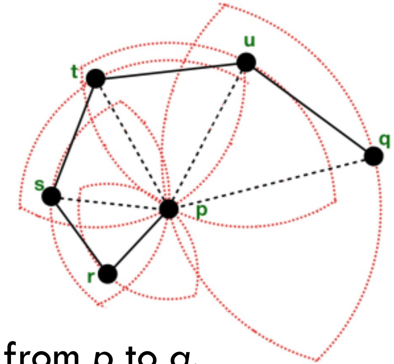
- **Monotonic Search Network (MSN)**

Any pair of nodes x, y, there is at least one monotonic path

property: if q is a node of network, start from any node, we can find exact NN with greedy search (no backtracking !)

- **Relative Neighbourhood Graph (RNG)**

is not a MSN [Dearholt SSC'88]



When the search goes from *p* to *q*, the path is non-monotonic (*e.g.*, *rq* < *pq*)

NSG VLDB'19

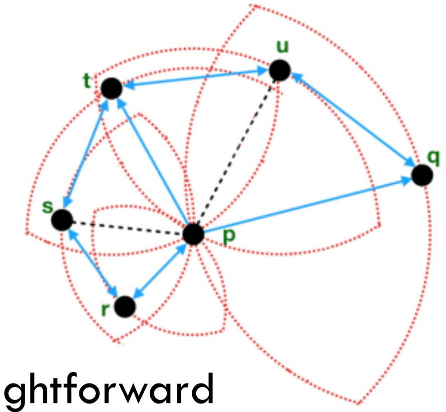
- **Monotonic Relative Neighbourhood Graph (MRNG)**

For any edge $\overrightarrow{pq}$, $\overrightarrow{pq} \in MRNG$ *if and only if* $\boxed{lune_{pq} \cap S = \emptyset}$ *or*

$\boxed{\forall r \in (lune_{pq} \cap S), \overrightarrow{pr} \notin MRNG.}$

RNG

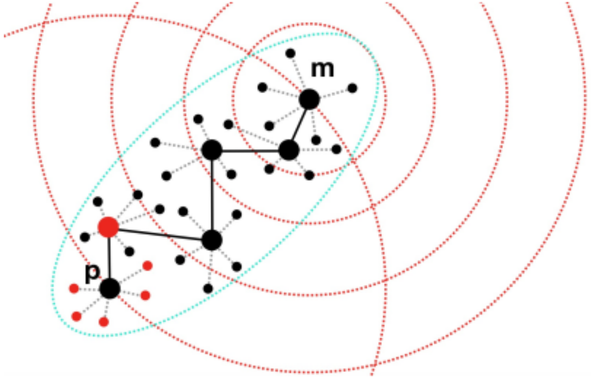
Add edges -> ensure the existence of monotonic path



The search from p to q is straightforward

NSG VLDB'19

- **Navigating Spreading-out Graph (NSG)： approximate MRNG**
  - Build an approximate *k*NN graph.
  - Find the *Navigating Node*. (All search will start with this fixed node – center of the graph).
  - For each node p, find a relatively small candidate neighbour set. (*sparse*)
  - Select the edges for p according to the definition of MRNG. (*low complexity*)
  - leverage Depth-First-Search tree (*connectivity*)



Neighbourhood-based Nearest Neighbour Search

- KNN graph based methods
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How ML can help?

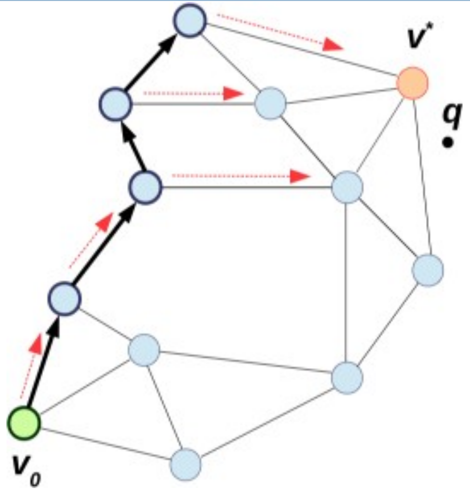
Learning to Route in Similarity Graphs (ICML'19)

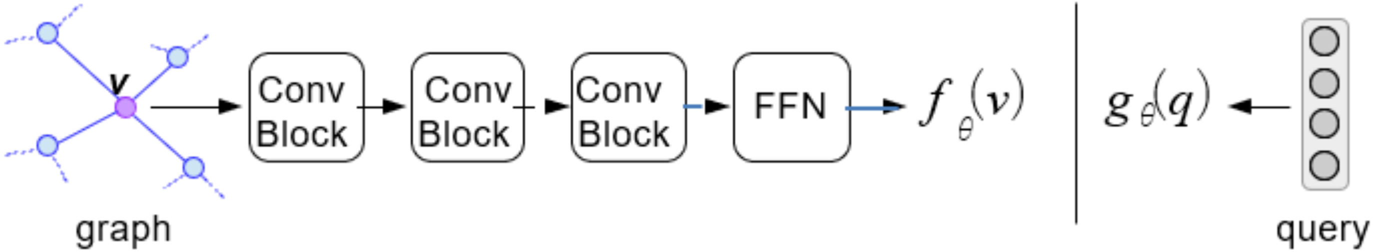
- **Greedy routing:** Pick the best neighbor of the current vertex
- **Beam search:** Expand the most promising vertex in the candidate pool
- **New method:** Learn a routing algorithm directly from data

Slides from ICML'19

How ML can help?

- **Learning to Route in Similarity Graphs** (NIPS'19)
  1. **Imitation Learning:** Train the agent to imitate expert decisions
  2. **Agent** is a beam search based on learned vertex representations
  3. **Expert** encourages the agent to follow a shortest path to the actual nearest neighbor $v*$





Slides from ICML'19

How ML can help? (2)

□ Learned adaptive early termination (SIGMOD'20)

- Consider the IVF index and HNSW index
- Get features
- Apply the decision tree models (Gradient boosting decision trees)
- Integrated into the existing search algorithm

Feature	Description
F0: query	The query vector Each dimension is a single feature
F1: c_xth_to_c_1st (10 features)	Dist(q, xth nearest cluster centroid) / Dist(q, 1st nearest cluster centroid) where x ∈ {10, 20, 30, …, 90, 100}
F2: d_1st	Dist(q, 1st neighbor after a certain fixed amount of search)
F3: d_10th	Dist(q, 10th neighbor after a certain fixed amount of search)
F4: d_1st_to_d_10th	F2: d_1st / F3: d_10th
F5: d_1st_to_c_1st	F2: d_1st / Dist(q, 1st nearest cluster centroid)

Table 2: IVF index input features.

Feature	Description
F0: query	The query vector Each dimension is a single feature
F1: d_start	Dist(q, base layer start node)
F2: d_1st	Dist(q, 1st neighbor after a certain fixed amount of search)
F3: d_10th	Dist(q, 10th neighbor after a certain fixed amount of search)
F4: 1st_to_start	F2: d_1st / F1: d_start
F5: 10th_to_start	F3: d_10th / F1: d_start

Table 5: HNSW index input features.

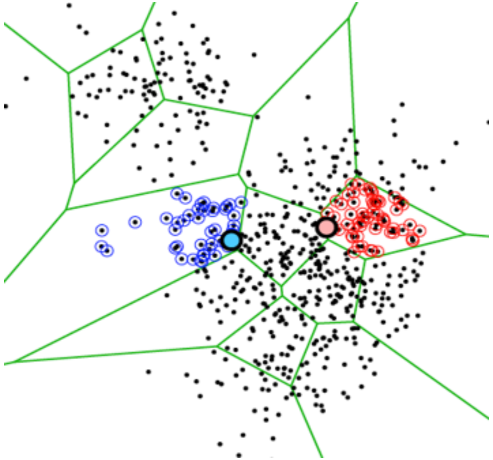
Neighbourhood-based graph under other settings

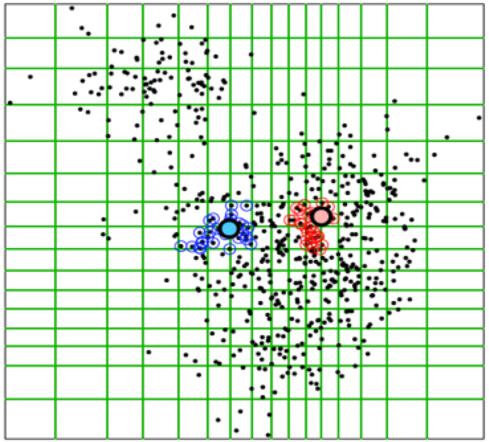
- **Dealing with billion-scale data in a single machine**

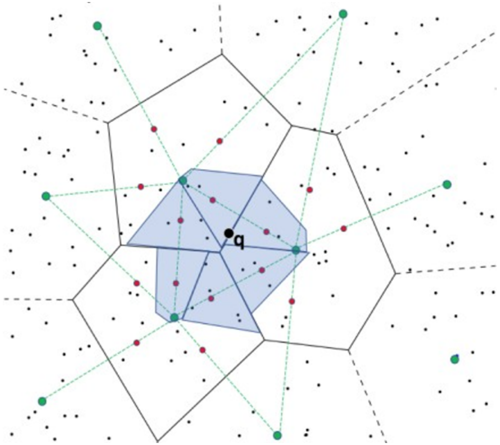
HNSW + **Vector quantization** (e.g., ECCV'18, CVPR'18, GRIP CIKM'19, SIGMOD'20)

- Increase the number of regions in the inverted (multi-) index (larger codebook)

- Use HNSW for fast search of promising regions





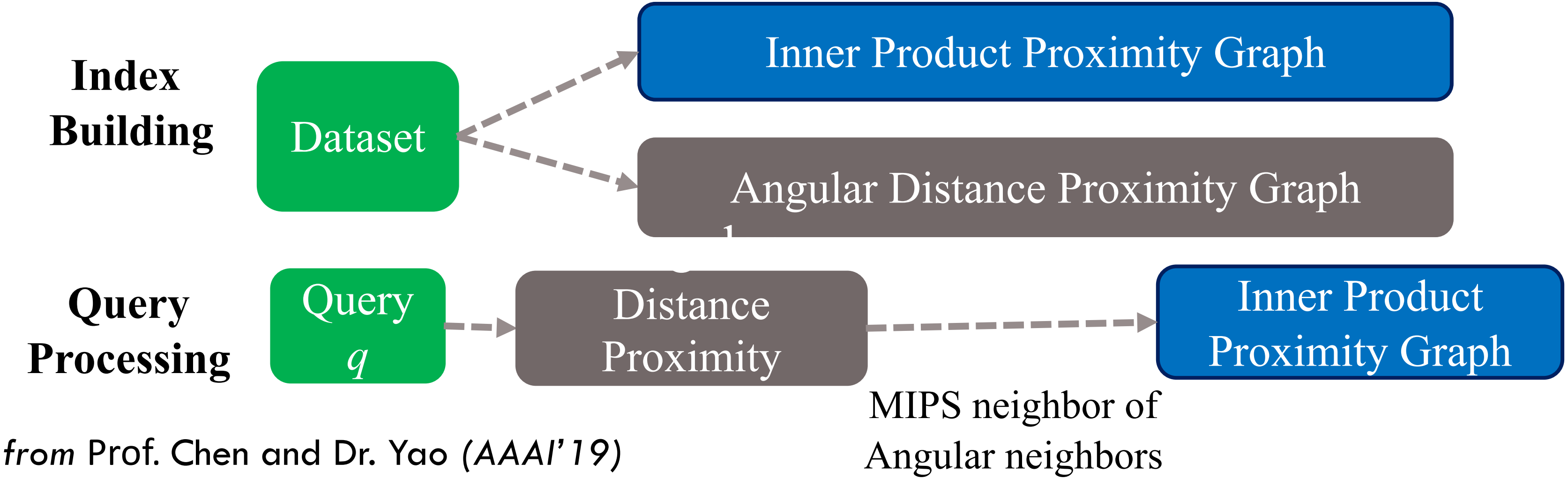


Slides from Dr. Baranchuk *(ECCV'18)*

Neighbourhood-based graph under other settings

Non-metric distance

- SISAP'19,
- Maximum Inner Product (MIP) distance: ip-NSW (NeurIPS'18), IPDG (EMNLP'19), **ip-NSW+** (AAAI'19)



Slides from Prof. Chen and Dr. Yao *(AAAI'19)*

Neighbourhood-based graph under other settings

- **GPU** (**SONG** ICDE'20, CoRR'13)
- **External memory** (Zoom CoRR'18)
- **Distributed computing** (JPDC'07)

Neighbourhood-based Nearest Neighbour Search

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Benchmarks for ANNS on high dimensional data

- https://github.com/erikbern/ann-benchmarks (NNS Benchmark IS'19)

- https://github.com/DBWangGroupUNSW/nns_benchmark (DPG TKDE'20, DPG CoRR'16)
- Many implementations/Libraries are public available, e.g.,:

- Non-Metric Space Library (NMSLIB) https://github.com/nmslib/nmslib available for Amazon Elasticsearch Service
- NGT (https://github.com/yahoojapan/NGT/wiki)
- FLANN http://www.cs.ubc.ca/~mariusm/flann
- ANN http://www.cs.umd.edu/~mount/ANN

Benchmark (DPG TKDE'20, CoRR'16)

Why do we need ANNS benchmark

- Coverage of competitor Algorithms and Datasets from different areas

- 16 representative algorithms   - 20 real-life datasets and two synthetic dataset

- Overlooked Evaluation Measures/Settings

- 7 measurements (e.g., search time, quality, scalability, index time/size, robustness, updatability, tuning of parameters

- Discrepancies in existing results
- Comparison fairness. Scope:

- L2 distance
- Dense vector
- No hardware specific optimizations (e.g., multi-threads, SIMD instructions, hardware pre-fetching, or GPU)
- Exact kNN as the ground truth

Benchmark (DPG TKDE'20, CoRR'16)

Category	Search Performance	Index		Index Scalabiliity		Search Scalabiliity		Theoretical Guarantee	Tuning Difficulty
		Size	Time	Datasize	Dim	Datasize	Dim		
DPG	**1st**	4th	7th	=4th	**=1st**	**=1st**	5th	No	Medium
HNSW	**1st**	3rd	5th	=4th	4th	**=1st**	4th	No	Medium
KGraph	3rd	5th	6th	=4th	**=1st**	**=1st**	7th	No	Medium
Annoy	4th	7th	2nd	7th	3rd	6th	=2nd	No	**Easy**
FLANN	5th	6th	4th	=2nd	7th	**=1st**	6th	No	Hard
OPQ	6th	2nd	3rd	**1st**	=5th	5th	=2nd	No	Medium
SRS	7th	**1st**	**1st**	=2nd	=5th	7th	**1st**	**Yes**	**Easy**

Table 6: Ranking of the Algorithms Under Different Criteria

Benchmark (DPG TKDE'20, CoRR'16)

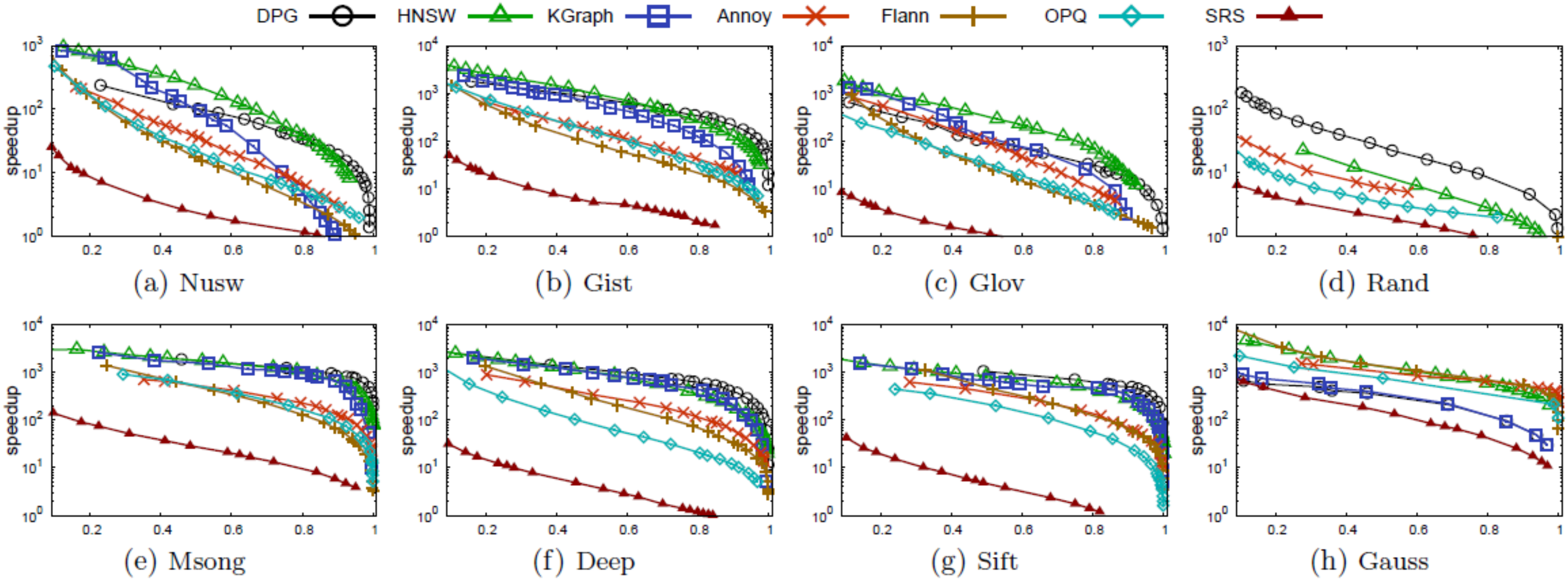

Figure 8: Speedup vs Recall on Different Datasets

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