KDD 2021 Tutorial

# High-Dimensional Similarity Query Processing for Data Science


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# Neighbourhood-based Nearest Neighbour Search

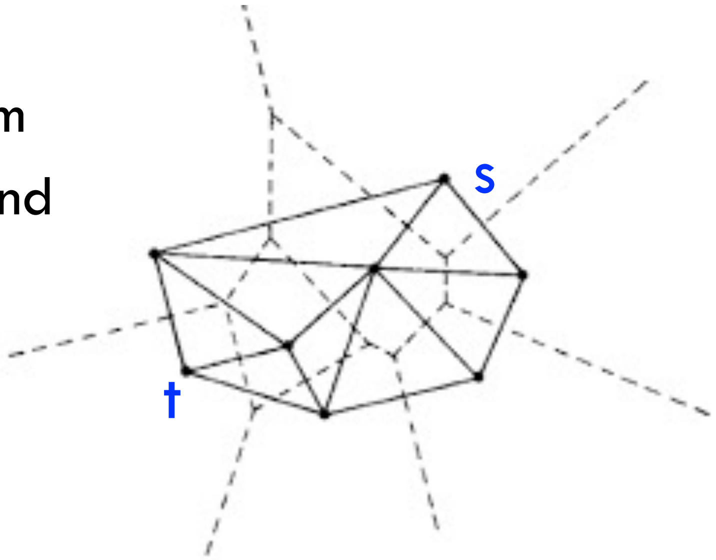


## Motivation

Delaunay graph – dual of Voronoi Diagram

For 2-dimension space, for a source node and a target node, always find a path

- 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

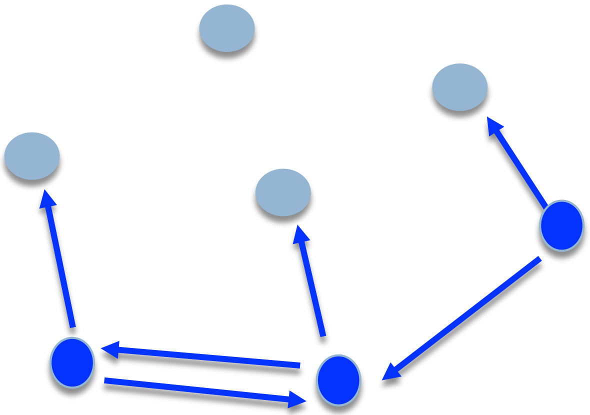
# KNN graph based methods



- **K nearest neighbour (KNN) graph**

Each point x in the space → a **node** x in the KNN graph

For it's k nearest neighbours {y} regarding the given distance metric → add a directed **edge** x → y



K = 2

# KNN Graph Construction



- **Exact KNN graph construction**
  - Brute-force costs $O(dn^2)$
  - Other exact algorithms, e.g., **L2Knng** (CIKM'15)
- **Approximate KNN graph construction**
  - Reducing to individual approximate KNN search
    e.g., based on LSH methods, but still expensive
  - Jointly find KNN for everyone, such as
    **L2 distance:** data partition (Jie JLMR'09) , space filling curve (Connor TVVG'10).
    **sparse data:** **KIFF** (ICDE'16), etc
    **general metric distance:** **NN Descent** (WWW'11), etc

# Important properties for KNN graph construction



- General
- Scalable
- Space and index size
- 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

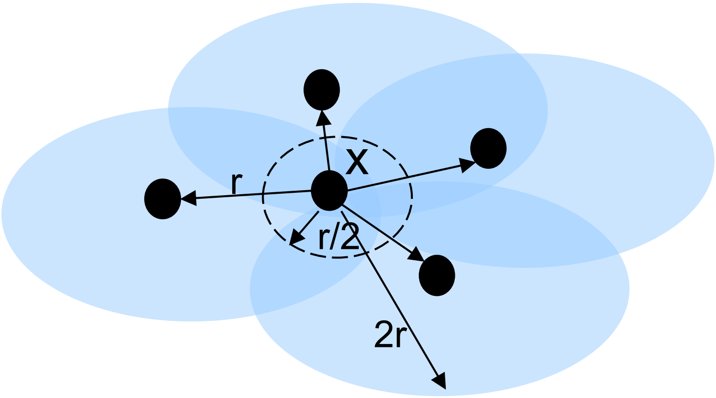
*Slides from Dr. Wei Dong (WWW'11)*

# 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 $B_{r/2}(x)$

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

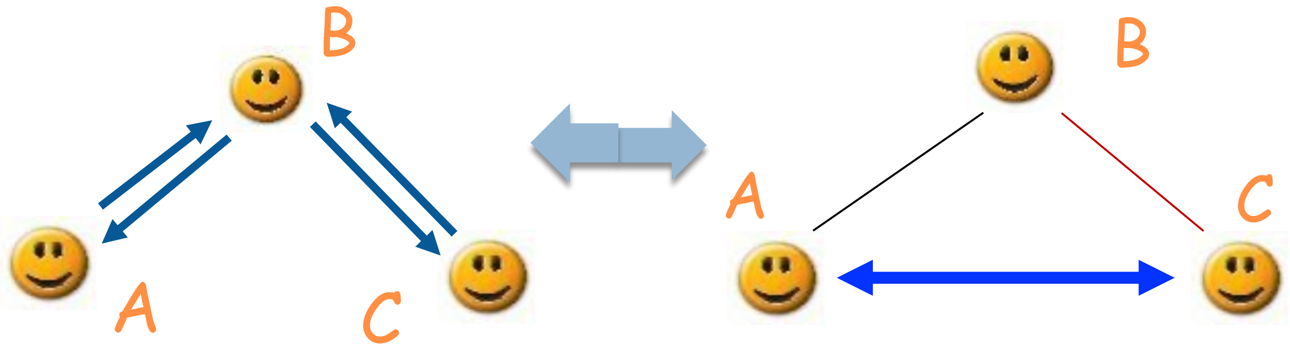
- It should converge in $\log \Delta$ iterations ( $\Delta$: diameter of dataset)

*Slides from Dr. Wei Dong (WWW'11)*

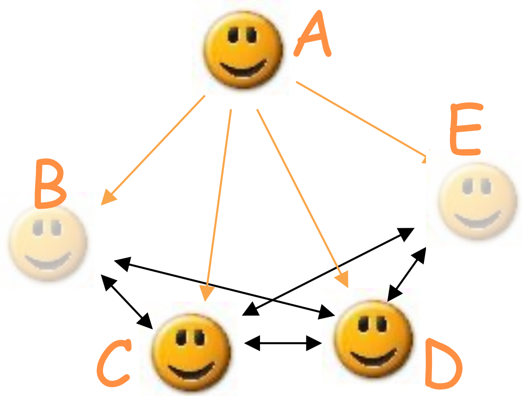
# Kgraph (www'10), Computation Speedup



- Local Join




- Incremental search




- Sampling
- Early termination

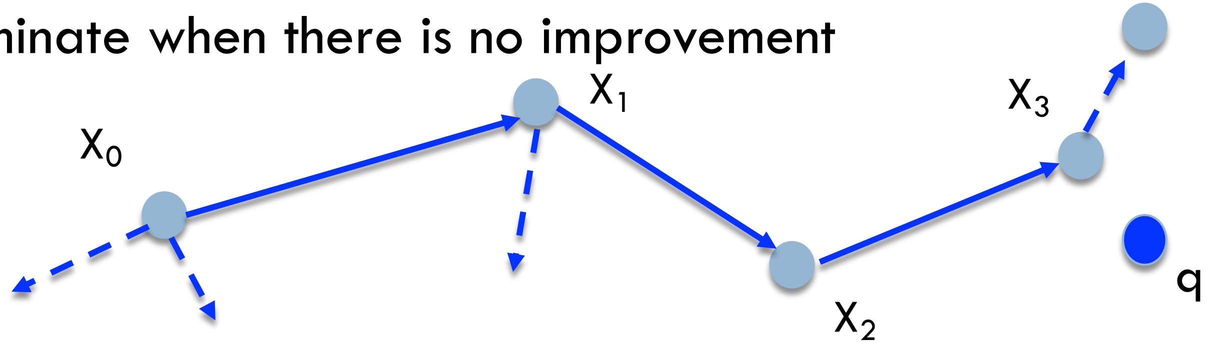
*Slides from Dr. Wei Dong (WWW'11)*

# Search on KNN graph – Greedy heuristic



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

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




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

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

# Variants 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 $\delta$ and # search trials $L$

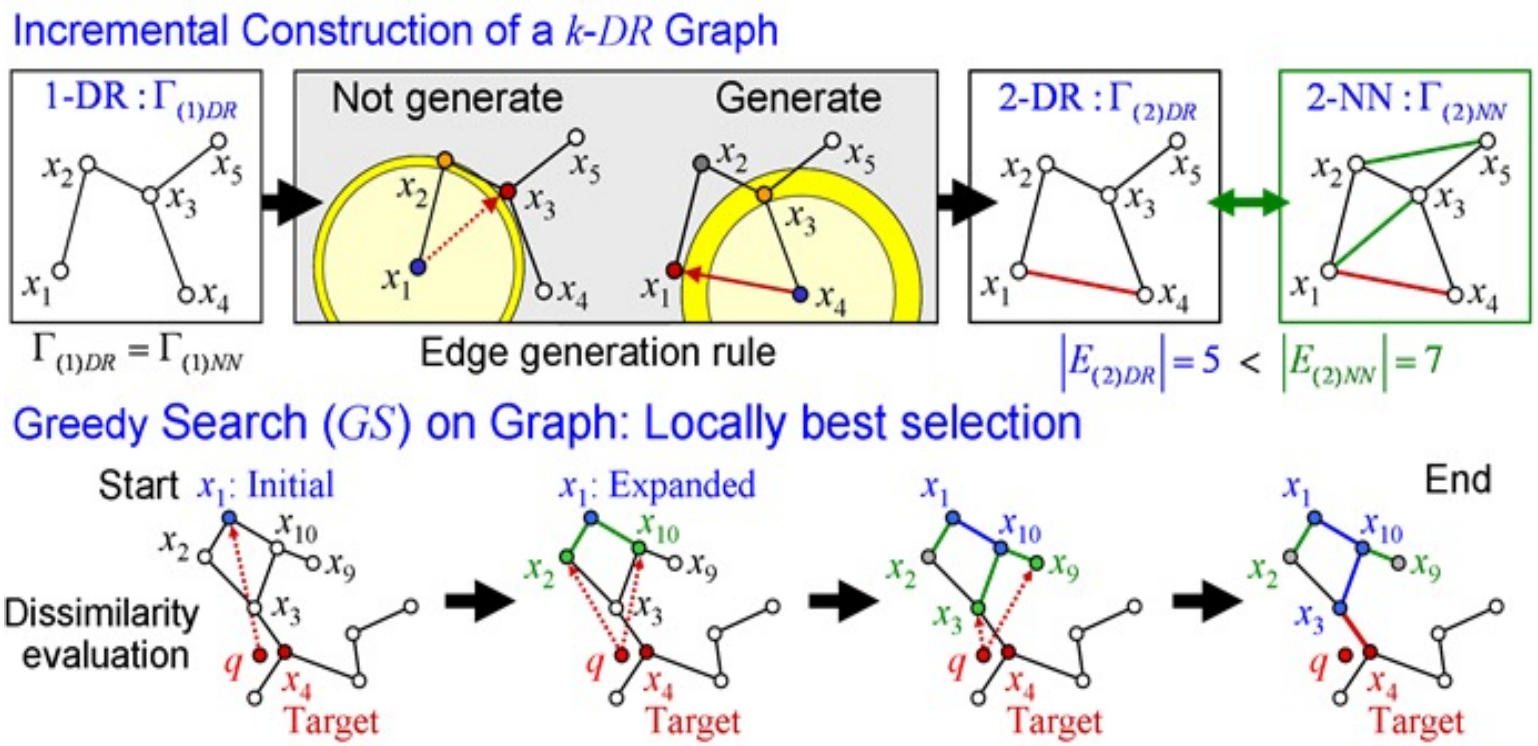
Determined: Graph structural parameter $k$

| | |
|---|---|
| Probability that at least one of $L$ search trials succeeds | $> 1-\delta$ |

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

# **k-DR** KDD’11



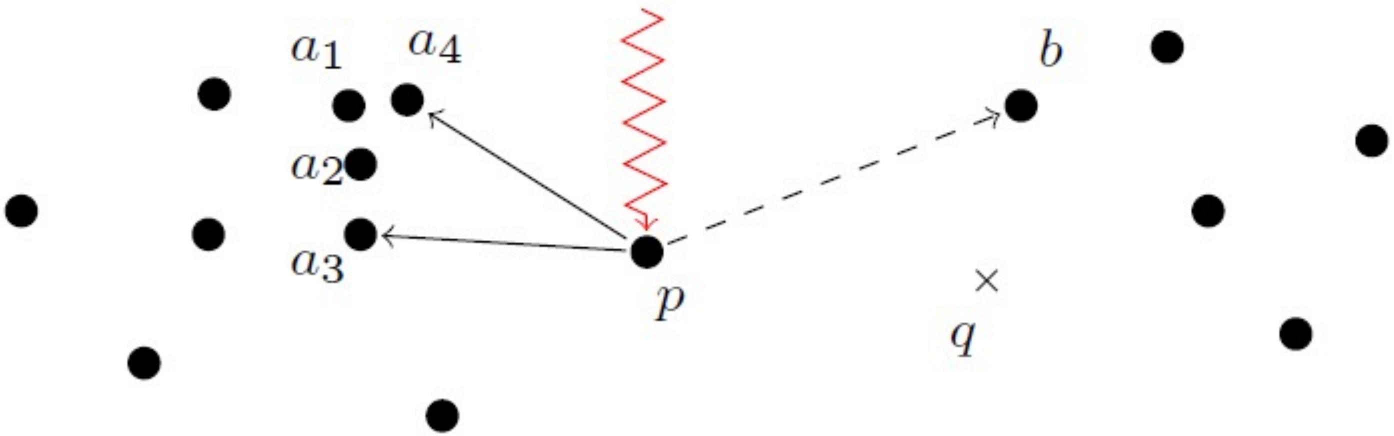



*Slides from* Prof. Sawada *(KDD’11)*

# **DPG** TKDE’20, CoRR’16



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

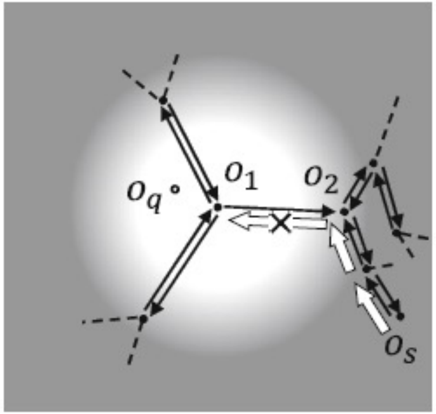


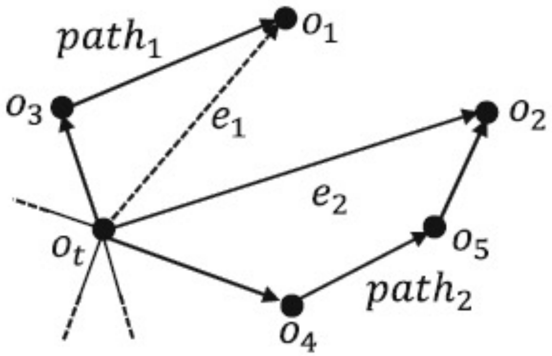

Build KNN graph, then (1) choose K/2 diversified neighbours; (2) add reverse edge when necessary

# **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



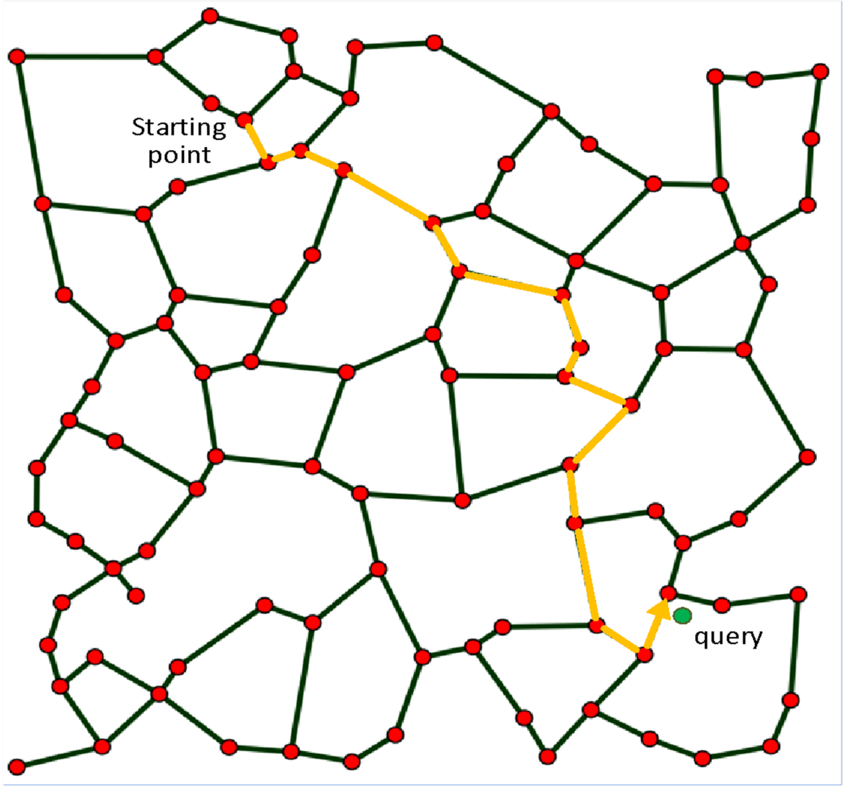
- KNN graph based methods
- Navigable small world graph based methods
- Relative neighbourhood graph based methods
- Investigation under some specific settings
- Benchmark

# NSW IS'14



Problem: Long paths in proximity graphs.

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




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

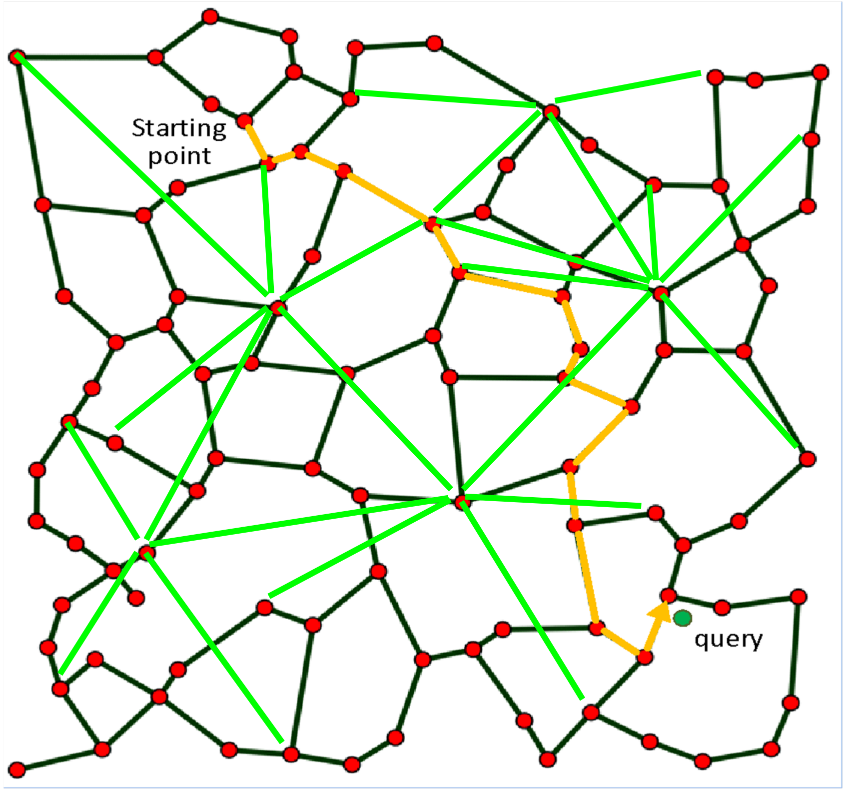
# NSW IS'14



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.



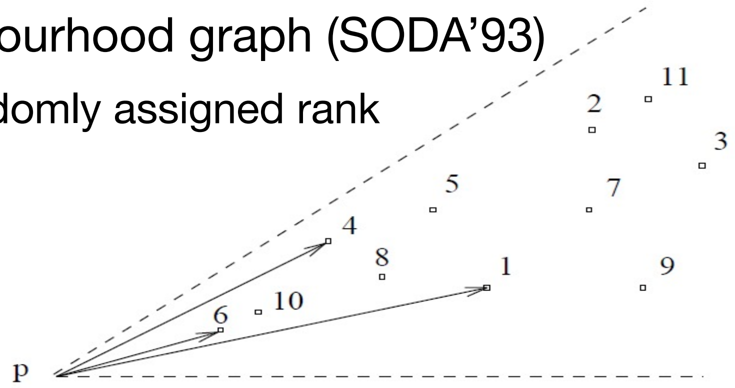

*Slides from* Dr. Malkov *(IS'14)*

# 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:

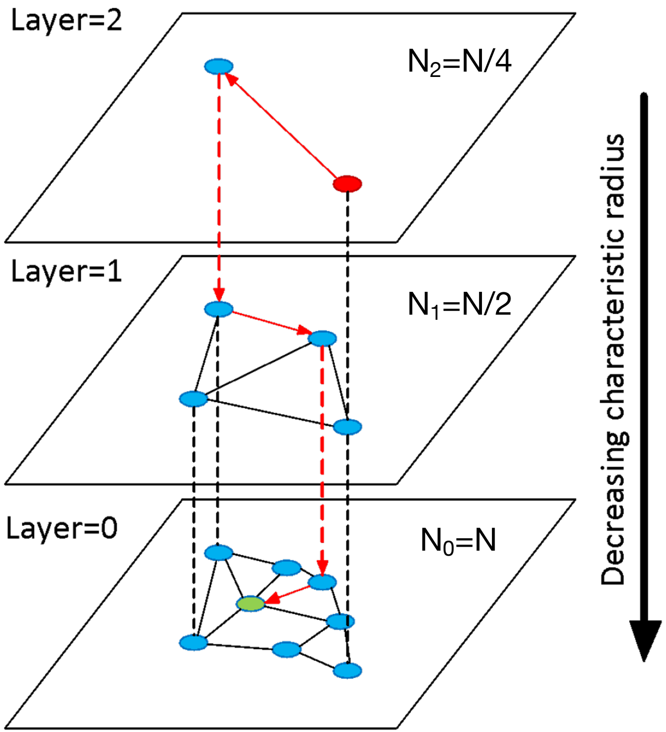
(1) k-NNS for each new node;

(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)*

## Neighbourhood-based Nearest Neighbour Search



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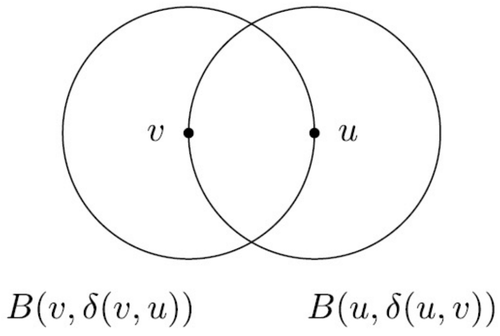
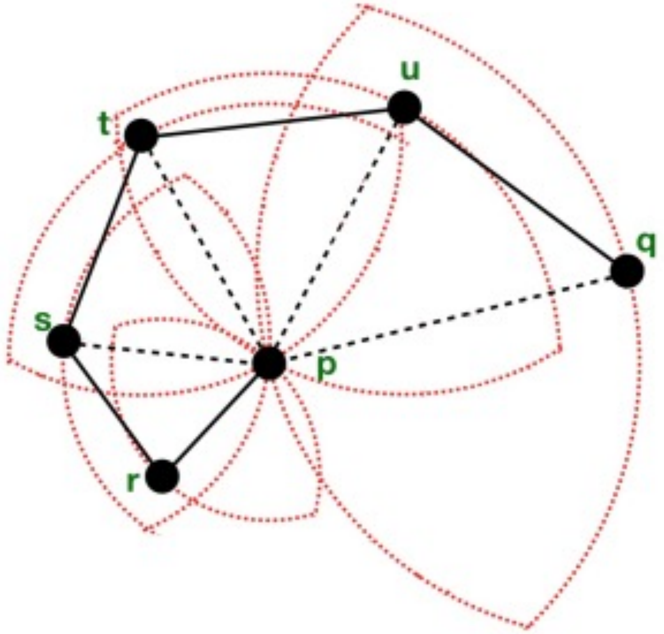
# Relative Neighbourhood graph



- **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

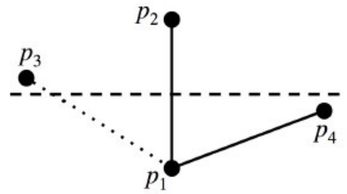



Figure 1. An edge from $p_1$ to $p_2$ occludes an edge from $p_1$ to $p_3$ because $p_3$ is closer to $p_2$ than $p_1$. The edge to $p_4$ is not occluded.

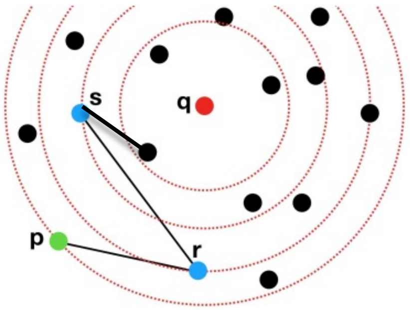
- In practice, the trade-off between recall and computational cost is managed by placing a hard limit on the number of distances that will be computed.

*Slides from authors*

# NSG VLDB'19

- **Monotonic Path**

distance to the end point monotonically decrease




- **Monotonic Search Network (MSN)**

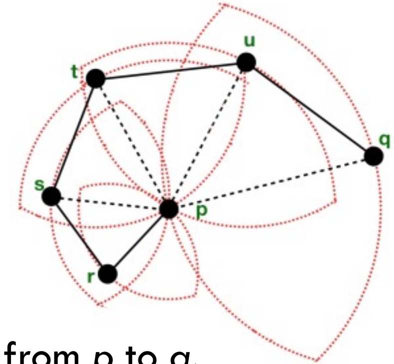
Any pair of nodes x, y, there is at least one monotonic path

**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



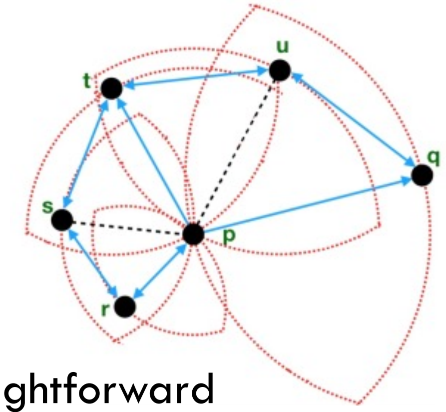
- **Monotonic Relative Neighbourhood Graph (MRNG)**

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

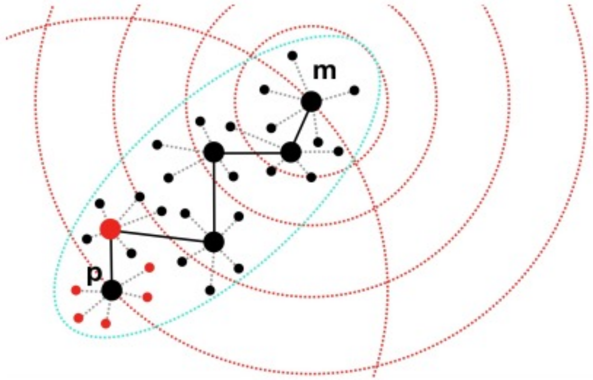



The search from p to q is straightforward

# **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)

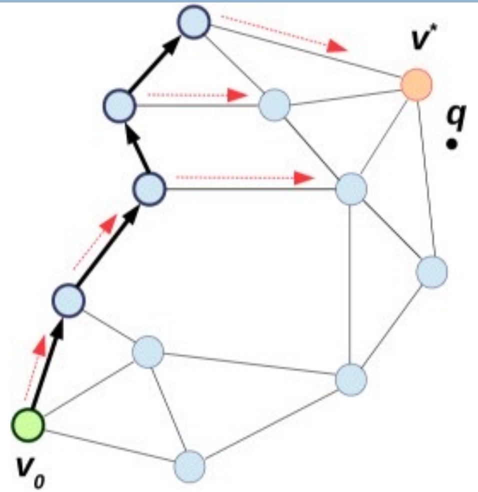
- **Greedy routing:** Pick the best neighbor of the current vertex
- **Beam search**: Expand the most promising vertex in the candidate pool
- **New method**: Learn a routing algorithm directly from data

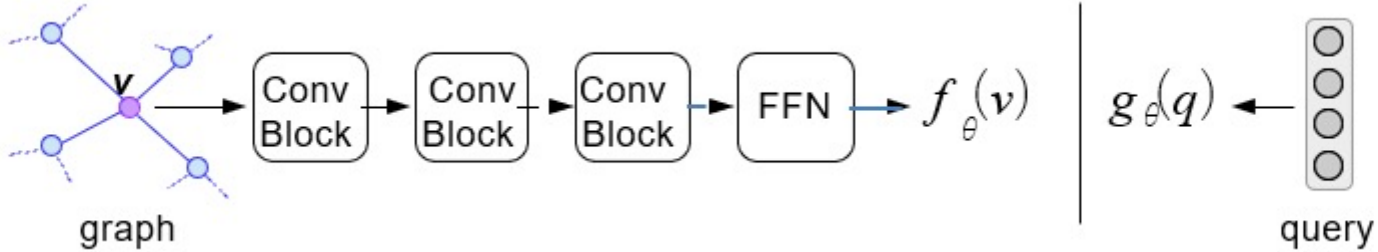

*Slides from ICML'19*

# 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<br>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<br>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

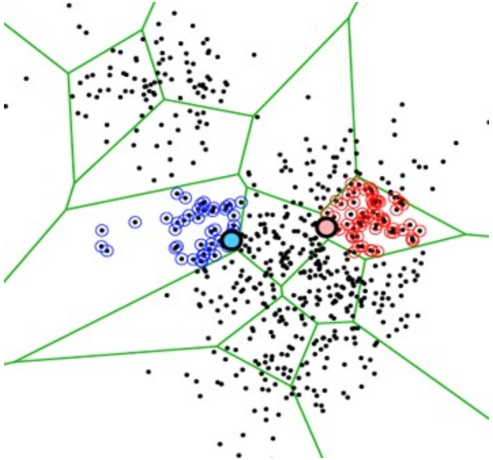


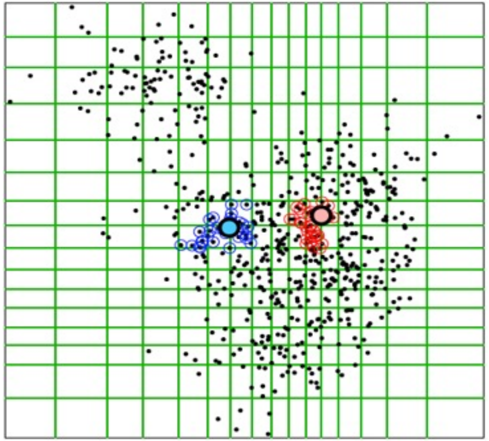
- **Dealing with billion-scale data in a single machine**

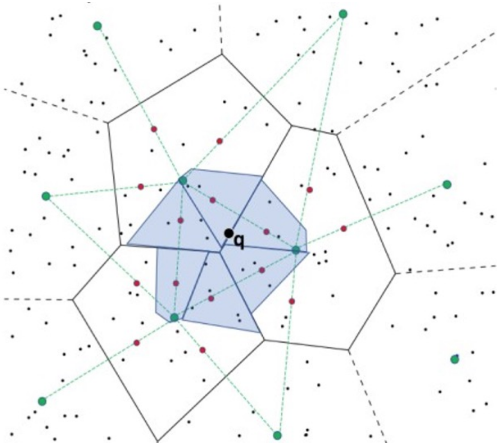
**HNSW** + **Vector quantization** (e.g., ECCV'18, CVPR'18, GRIP CIKM'19, SIGMOD'20)

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

- Use HNSW for fast search of promising regions







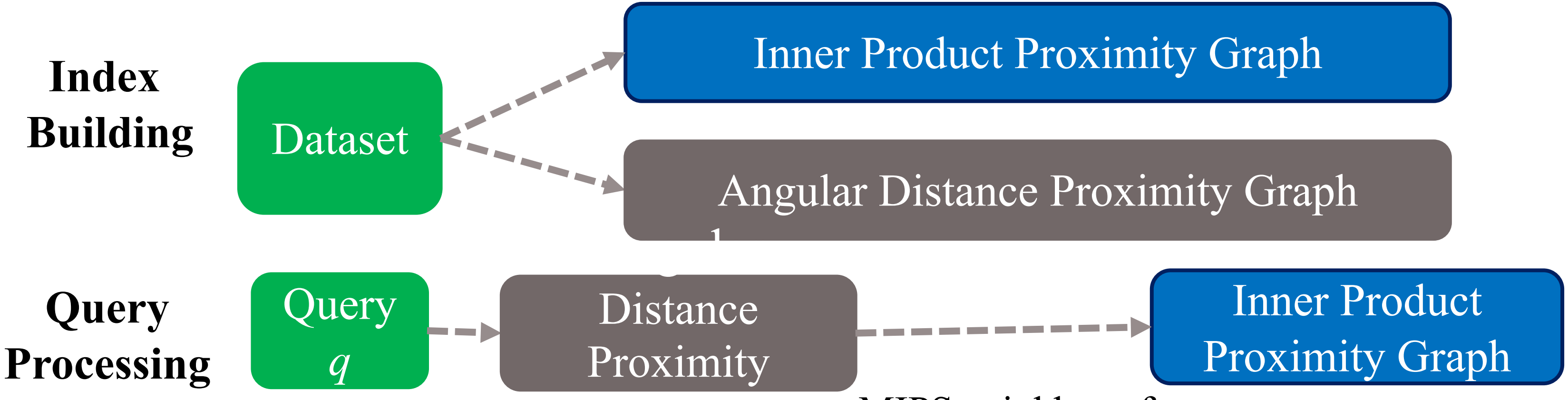

*Slides from* Dr. Baranchuk *(ECCV'18)*

# 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)
- Benchmark for similarity search on series data (Benchmark VLDB'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)



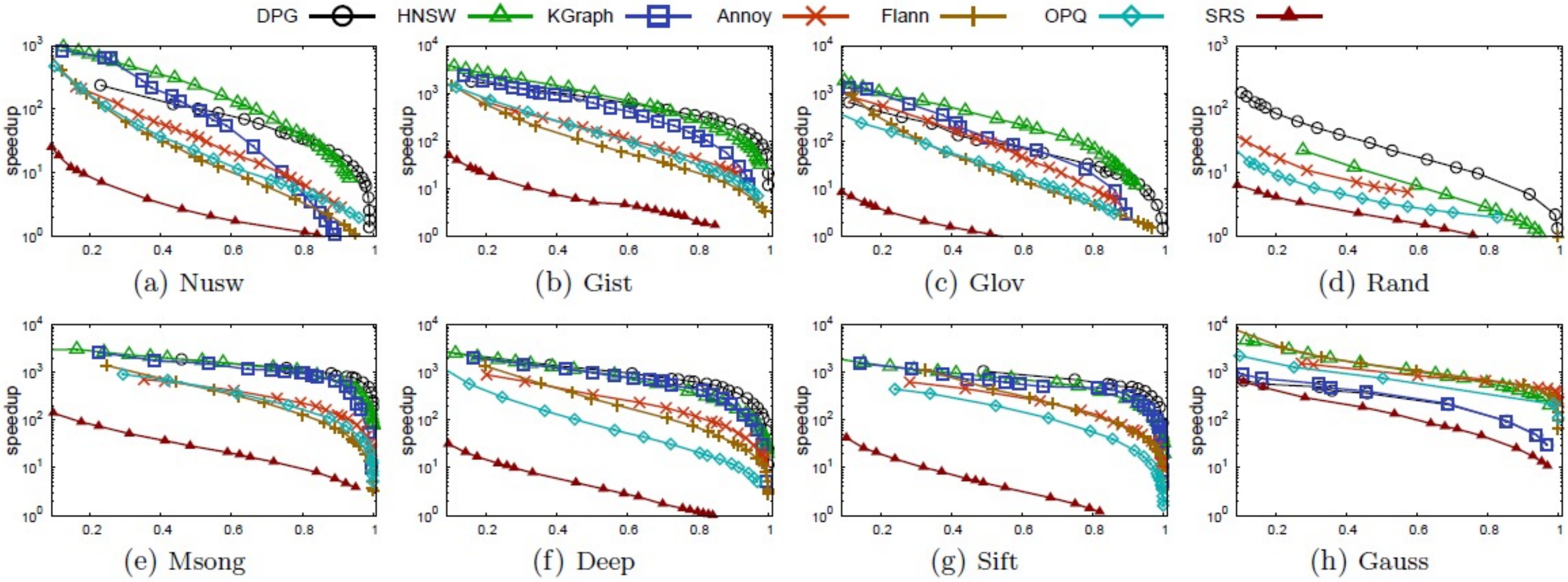


**Figure 8: Speedup vs Recall on Different Datasets**

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