Fast Inner Product Search on Graph

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Outline

- General setting.
- Search on graph.
- Voronoi Cell and Delaunay graph.
- Search on Delaunay graph.
- ℓ^2-Delaunay graph and IP-Delaunay graph.
- Möbius transformation and graph isomorphism.
- Proposed algorithm.
- Experimental results.

General Setting

- $X, Y \subset \mathbb{R}^d$.
- Dataset $S = \{x_1, \ldots, x_n\} \subset X$.
- Real valued function $f : X \times Y \to \mathbb{R}$.
- Aim to solve the optimization problem:

$$\arg\max_{x_i \in S} f(x_i, q) \quad \text{for} \quad q \in Y.$$

- Allow prepossessing on dataset S.
- Most interesting examples:

$$f(x, y) = -\|x - y\| \quad \text{and} \quad f(x, y) = x^\top y.$$

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Search on Graph for Nearest Neighbor Search

- Let $f(x, y) = -\|x - y\|$.
- $\arg\max_{x_i \in S} f(x_i, q)$ aims to find the nearest point of q in S.
- Search on graph strategy
  1. Build a proximity graph G on S by connecting certain points, e.g., k-NN graph.
  2. Randomly select a vertex x from the graph.
  3. Evaluate the ℓ^2-distance $\|x - q\|$ and $\|y - q\|$, where y's are neighbors of x on the graph G.
  4. If x' is closer to q than x, then replace x by y and repeat step 3.
  5. Stop if x is closer to q than x's neighbors on graph.
- This procedure finds the exact solution if and only if G contains *Delaunay graph* as a subgraph.

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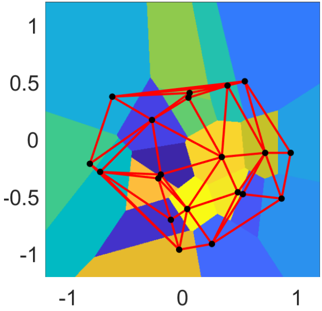
Voronoi Cells and Delaunay Graph

- Goal: to find $\arg\max_{x_i \in S} f(x_i, q)$.
- Voronoi cells: solution area of the problem.
- Delaunay graph: the dual graph of Voronoi diagram.



ℓ^2-Delaunay graph

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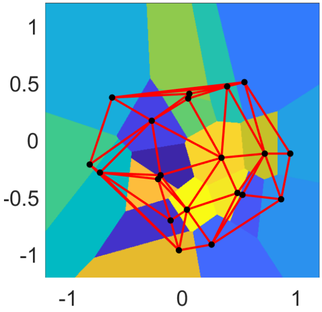

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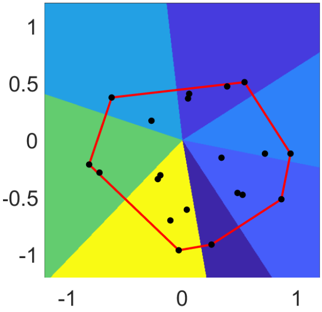

IP-Delaunay graph

- Every ℓ^2-Voronoi cell is nonempty, but IP-Voronoi cell can be empty.

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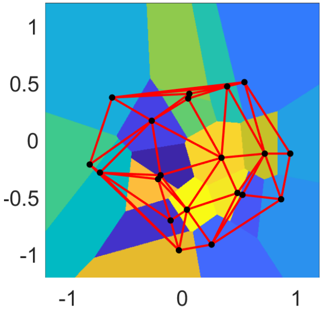

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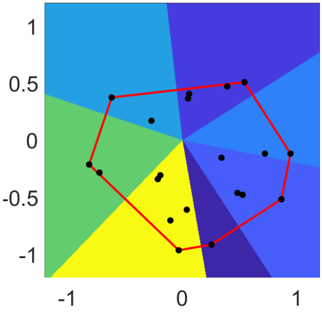

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Sufficiency and Necessity Delaunay Graph

Theorem

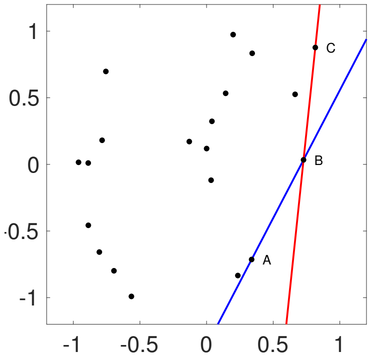
For given f, suppose its Voronoi cells w.r.t. any dataset are connected, then

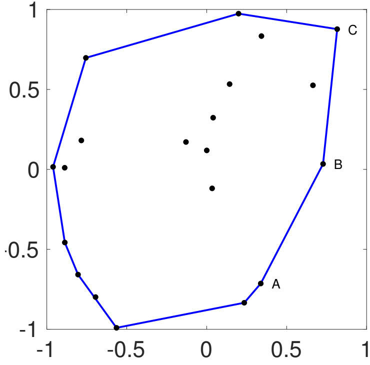
- *for $q \in Y$, performing greedy search on Delaunay graph returns the solution of $\arg\max_{x_i \in S} f(x_i, q)$;*
- *conversely, for any G' does not contain Delaunay graph as a subgraph, there exists a query $q \in Y$ such that greedy search on G' does not always retrieve the exact solution.*

- Any ℓ^p-norm and inner product satisfy the assumption on f.
- Delaunay graph is the smallest graph such that greedy search always return exact solution.

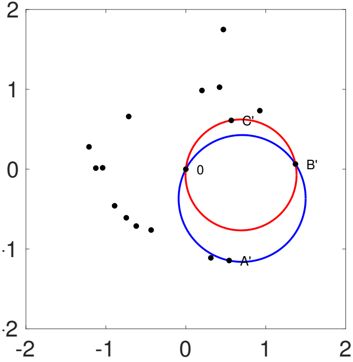
Empty Half Space Criterion

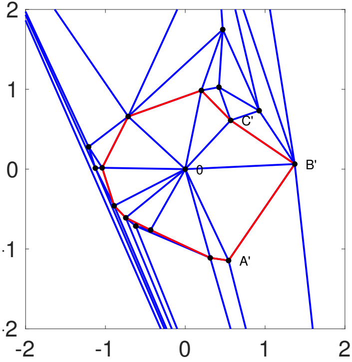
- The line AB in divides the plane into two open half-spaces. One of the half-space does not contain any data points, so A and B are connected in IP-Delaunay graph.





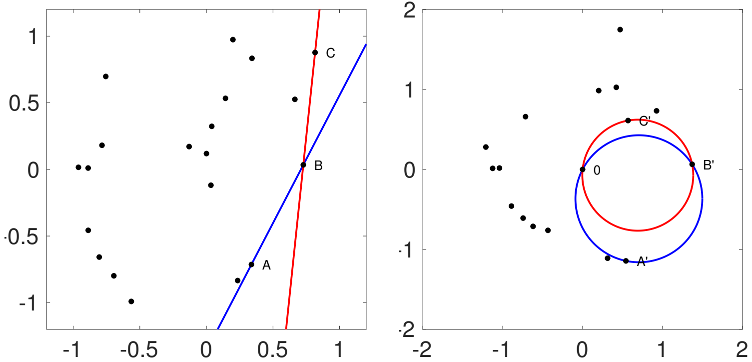
- The circumcircle of 0, A and B does not contain any data points inside, so there is a simplex with vertices 0, A' and B' in the ℓ^2-Delaunay graph.





Möbius Transformation

- Möbius transformation $y = \frac{x}{\|x\|^2}$.
- Maps hyperplanes to spheres.
- Maps lines to circles in $\mathbb{R}^2$.
- Let $y_i = x_i/\|x_i\|^2$.



$S = \{x_1, \ldots, x_n\}$ $S' = \{0, y_1, \ldots, y_n\}$

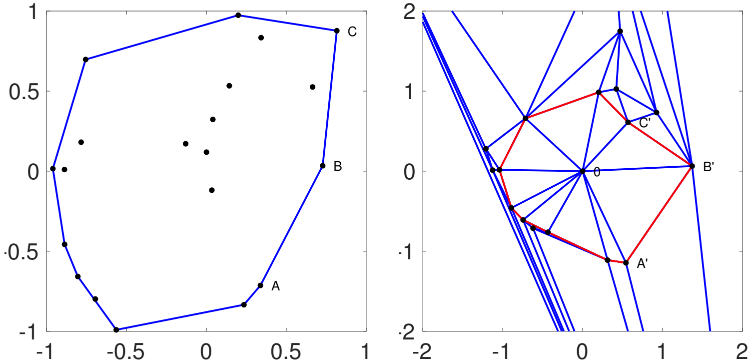
Graph Isomorphism

Theorem

The following two graphs are isomorphic:

(a) *IP-Delaunay graph before transformation (blue graph on the left);*

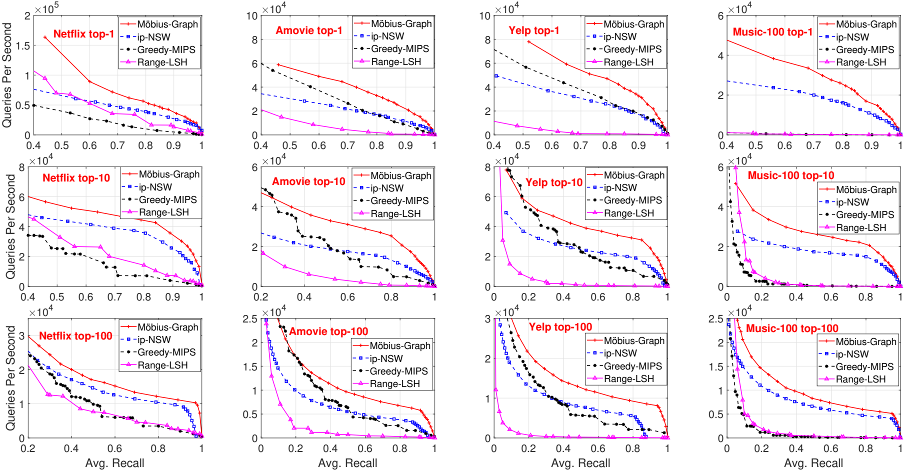
(b) *The neighborhood of 0 (in the graph sense) of ℓ^2-Delaunay graph after transformation (red graph on the right).*



Proposed algorithm

1. Let $\tilde{S} := \{y_i = x_i/\|x_i\|^2 \mid x_i \in S\} \cup \{0\}$ be the transformed dataset.
2. Construct approximate ℓ^2-Delaunay graph, e.g., HNSW, w.r.t. $\tilde{S}$.
3. Replace the vertices y_i by original data vectors x_i.
4. Start from 0, perform greedy inner product search on the graph.

Experiments



Experimental results for Recall vs. Queries Per Second on different datasets. We focus on top-1, top-10, and top-100 ground-truth labels. Here the best results are in the upper right corners.