

Nearest neighbor search using the Hierarchical Navigable Small World (HNSW) algorithm

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Outline

1 Theoretical foundations

- Voronoi diagram
- Delaunay graph
- Greedy NN search using Delaunay graph

2 HNSW algorithm

- Idea behind algorithm
- Construction of search index
- Nearest neighbor search using index

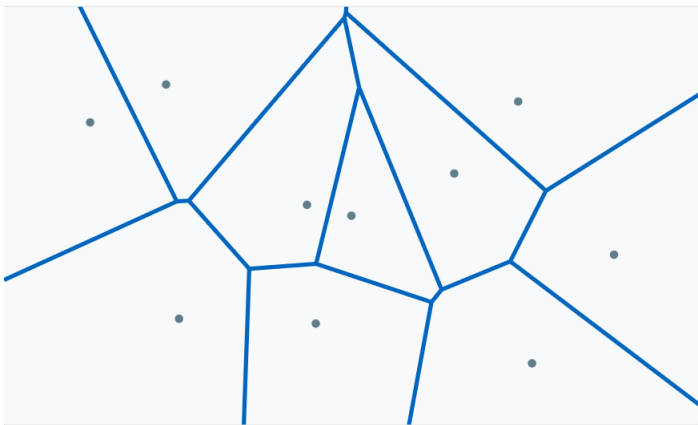
3 Performance

- Search accuracy
- Build time

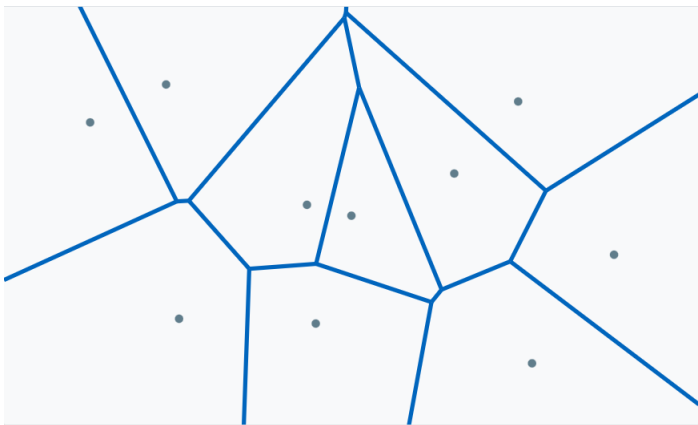
Voronoi diagram for a set of points



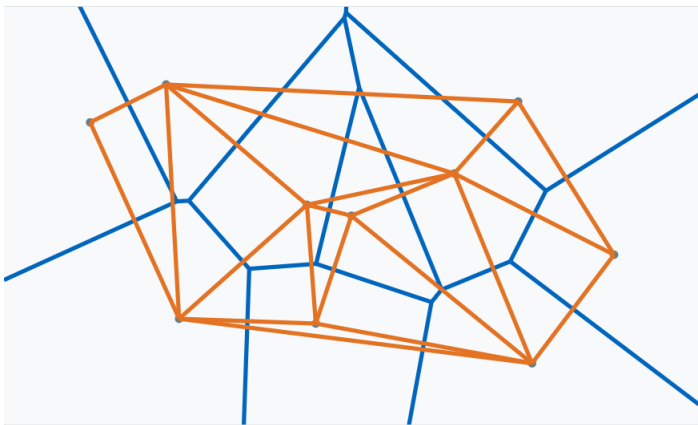
Voronoi diagram for a set of points



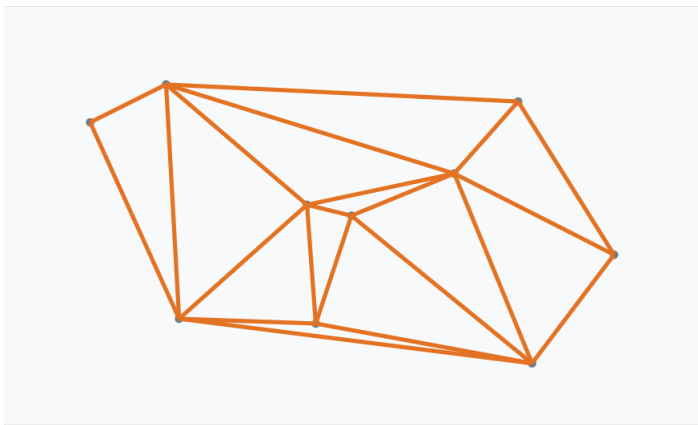
Voronoi diagram to Delaunay graph



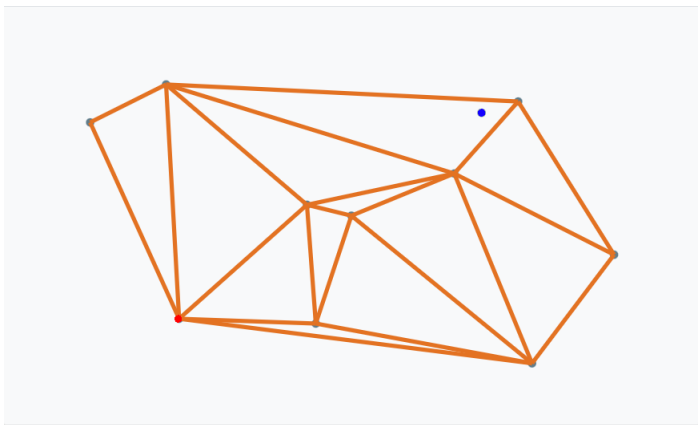
Voronoi diagram to Delaunay graph



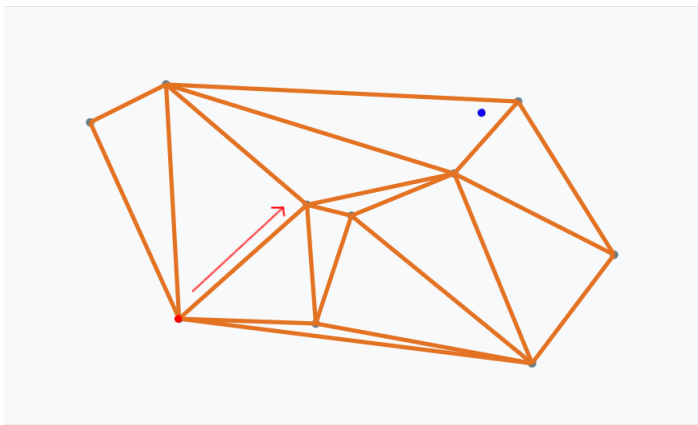
Delaunay graph



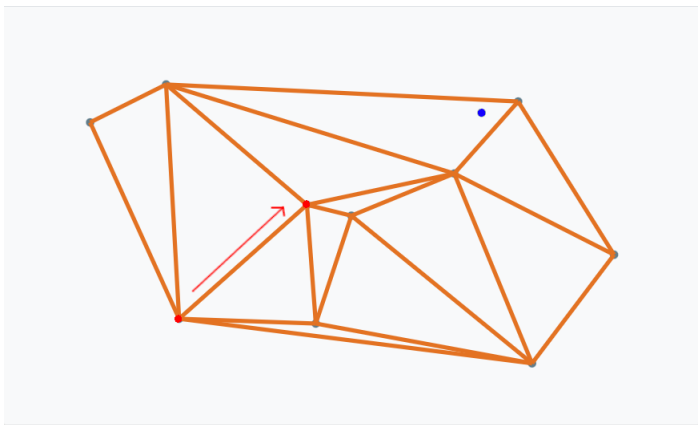
Greedy NN search start - Query and entry point



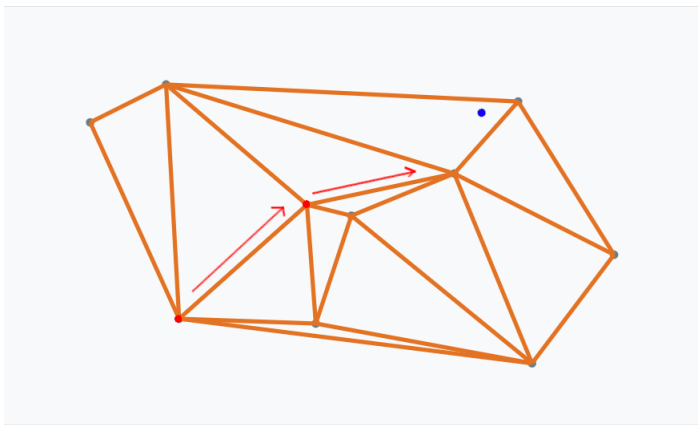
Greedy NN search - iteration



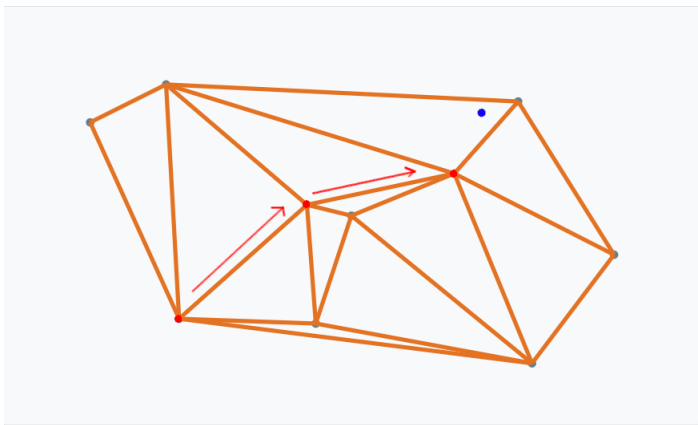
Greedy NN search - iteration



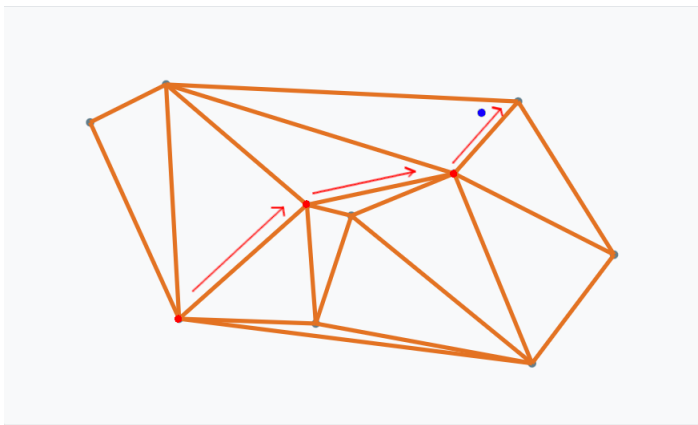
Greedy NN search - iteration



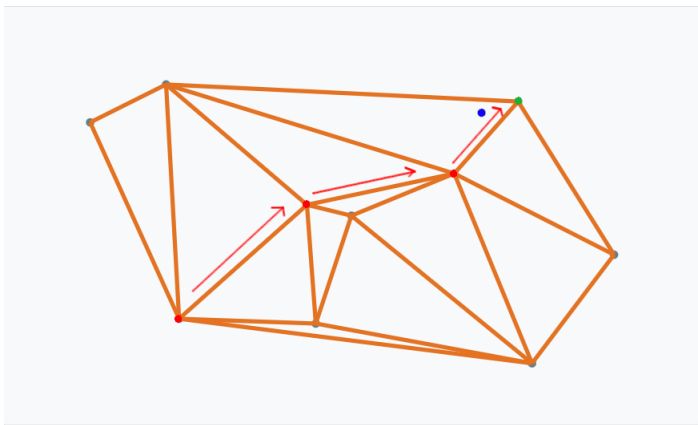
Greedy NN search - iteration



Greedy NN search - iteration



Greedy NN search done!



Drawbacks

- Delaunay graph intractable to construct for large, high-dimensional data sets
- Greedy search might be slow if graph is large

Navigable small world graph

Why?

- Can help us the direction of the prior art
- User might be interested also in finding infringing patents
- Currently we can't model this asymmetry

How?

- We can learn a distribution for a document instead of just a single vector
- Model prior art relation as KL divergence of distributions

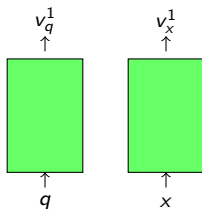
Distance functions for metadata

Why?

- We can do soft filtering (by country, patent class etc.)
- Can be useful if match is not found by strict filters

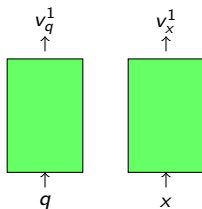
Learning multiple distance functions - naive way

$$d_1(q, x) = v_q^1 \cdot v_x^1$$

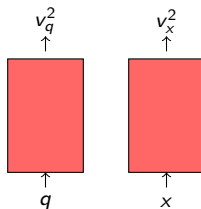


Learning multiple distance functions - naive way

$$d_1(q, x) = v_q^1 \cdot v_x^1$$

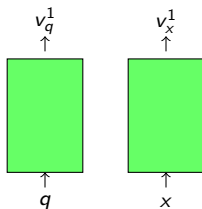


$$d_2(q, x) = v_q^2 \cdot v_x^2$$

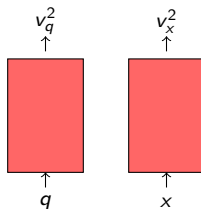


Learning multiple distance functions - naive way

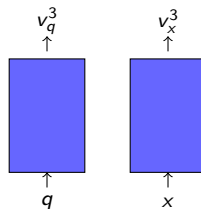
$$d_1(q, x) = v_q^1 \cdot v_x^1$$



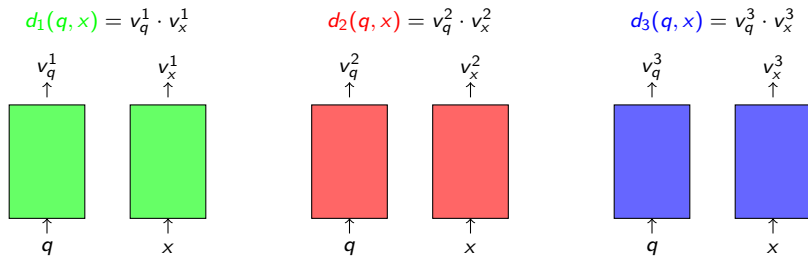
$$d_2(q, x) = v_q^2 \cdot v_x^2$$



$$d_3(q, x) = v_q^3 \cdot v_x^3$$



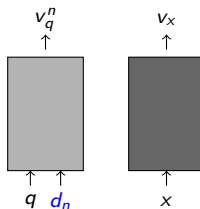
Learning multiple distance functions - naive way



Drawback: multiple embeddings of same document must be indexed!

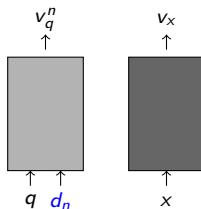
Learning multiple distance functions - efficient way

$$d_n(q, x) = v_q^n \cdot v_x$$



Learning multiple distance functions - efficient way

$$d_n(q, x) = v_q^n \cdot v_x$$



Only one meta-embedding per document is indexed!

Forward thinking



Forward thinking

Why?

- We can train deeper models but keep batch size the same
- Training of deep models can take less wall clock time

Forward thinking - paper

- Forward Thinking: Building and Training Neural Networks One Layer at a Time (Hettinger et al.)
<https://arxiv.org/abs/1706.02480>

Current method - using gradients

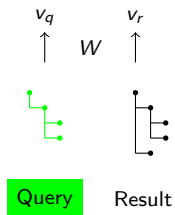


Query

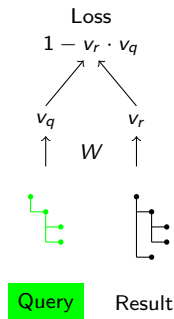


Result

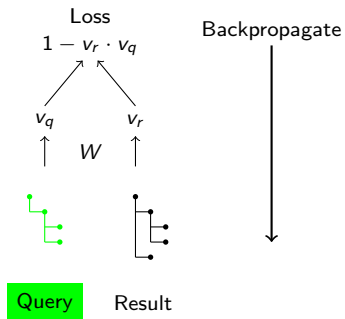
Current method - using gradients



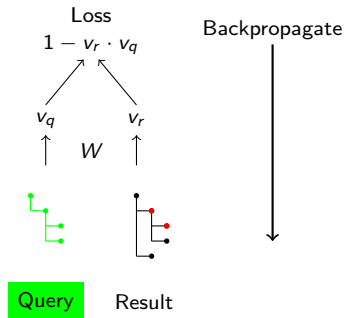
Current method - using gradients



Current method - using gradients



Current method - using gradients



Nodes with highest gradient are considered most important

Drawbacks with using gradients

- Compute-intensive, since we need to do backwards pass
- Quality of explanations is not the best
 - Evaluating Recurrent Neural Network Explanations (Arras et al.) <https://arxiv.org/abs/1904.11829>

Comparing node embeddings

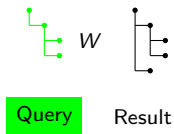


Query



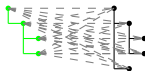
Result

Comparing node embeddings



1 Embed graphs using model

Comparing node embeddings

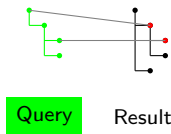


Query

Result

- 1 Embed graphs using model
- 2 Compare each pair of node embeddings

Comparing node embeddings



- 1 Embed graphs using model
- 2 Compare each pair of node embeddings
- 3 Highlight most similar nodes

Comparing node embeddings

Why?

- Faster than using gradients (no backprop step needed)
- Might give more relevant explanations
- Can be useful for finding missing features

References

- *Efficient and robust approximate nearest neighbor search using Hierarchical Navigable Small World graphs (Malkov et al.*
<https://arxiv.org/abs/1603.09320>
- *Approximate nearest neighbor algorithm based on navigable small world graphs (Malkov et al*
<https://doi.org/10.1016/j.is.2013.10.006>
- *Voronoi diagrams—a survey of a fundamental geometric data structure (Aurenhammer)*
<https://dl.acm.org/doi/10.1145/116873.116880>
- *Hierarchical Navigable Small Worlds (HNSW) (Pinecone blog)*
<https://www.pinecone.io/learn/hnsw/>