Approximate 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

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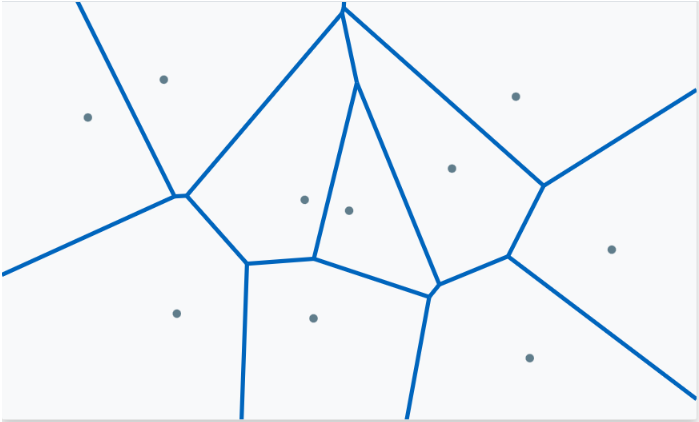
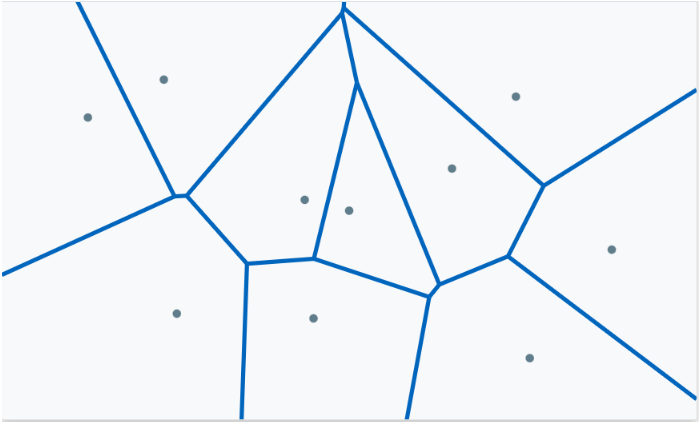


Voronoi diagram to Delaunay graph



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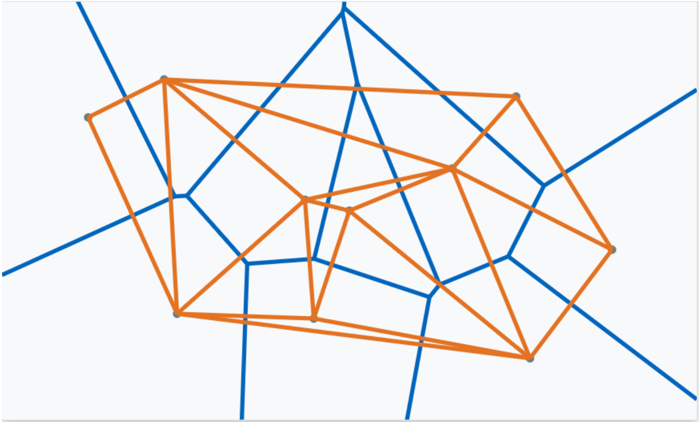
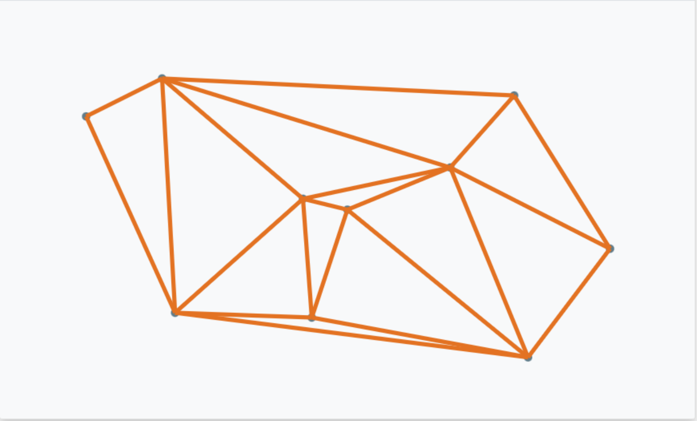
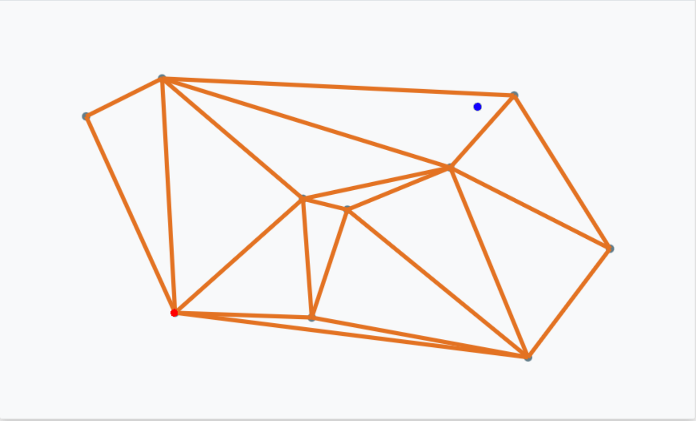


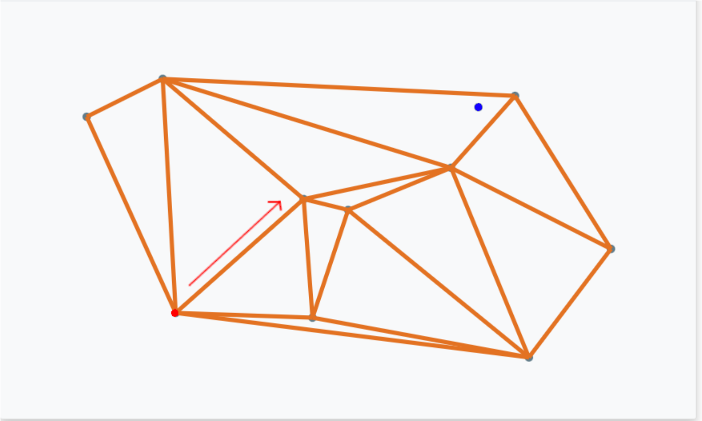
Delaunay graph



Greedy NN search start - Query and entry point



Greedy NN search - iteration



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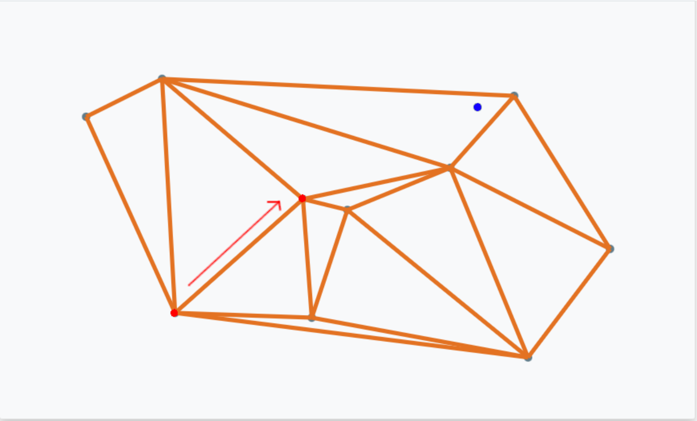

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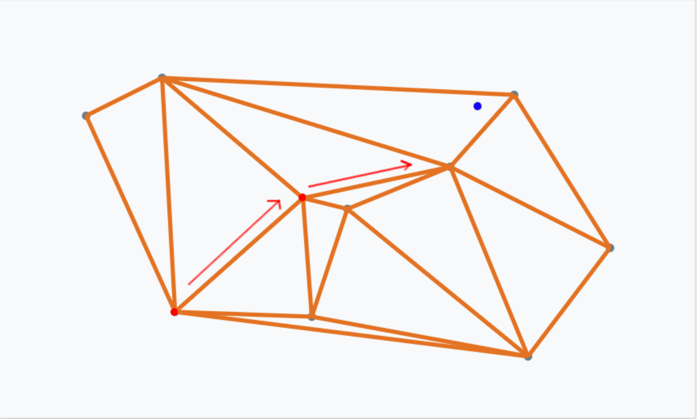

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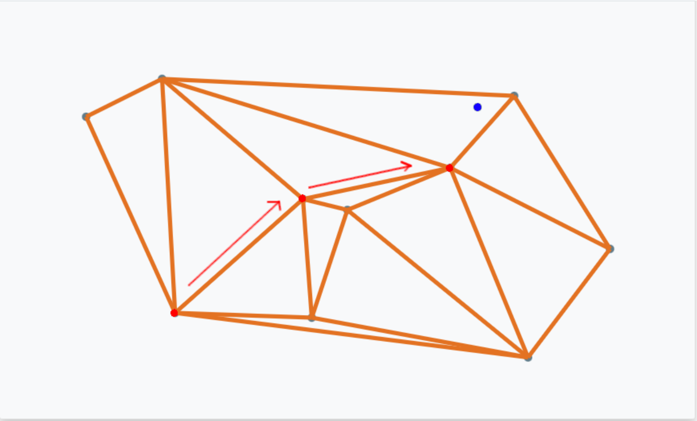

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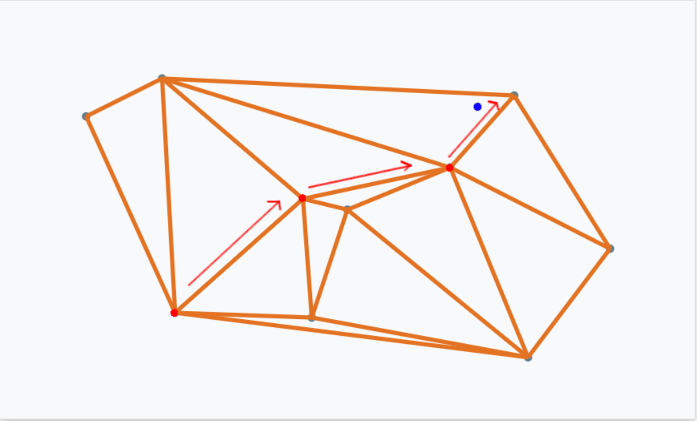
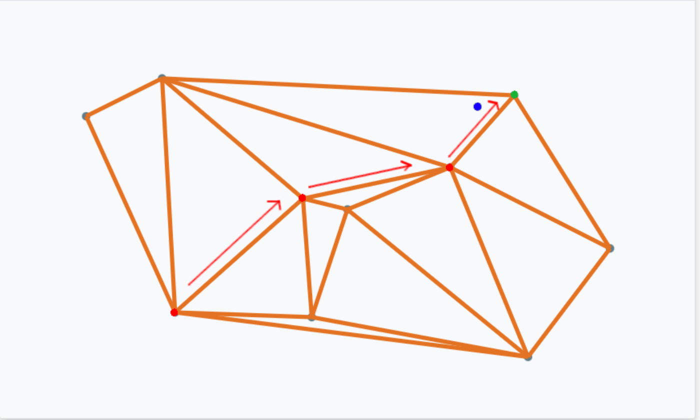


Greedy NN search done!



Drawbacks

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

Navigable small world (NSW) graph

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- Navigability
  - Greedy search algorithm has logarithmic scalability

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- Navigability ensures that the greedy algorithm finds the logaritmic path
- High clustering coefficient lets us zoom in on the actual correct node when we're in the right area

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- Ok since we're doing approximate nearest neighbor search!

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How?

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

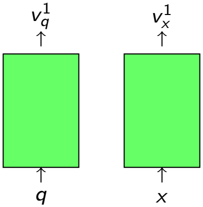
Distance functions for metadata

Why?

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

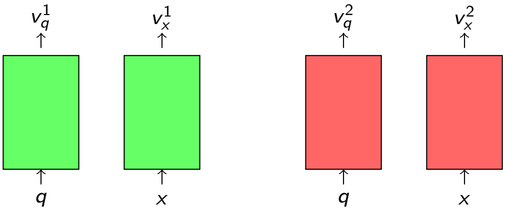
Learning multiple distance functions - naive way

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



Learning multiple distance functions - naive way

$d_1(q,x) = v_q^1 \cdot v_x^1$ $d_2(q,x) = v_q^2 \cdot v_x^2$



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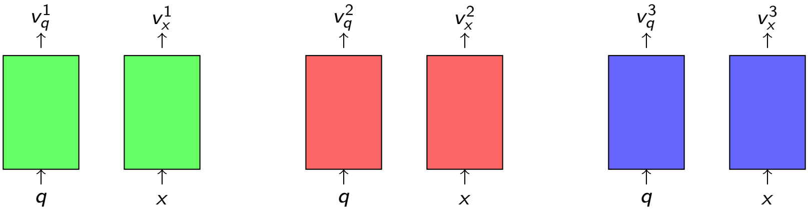

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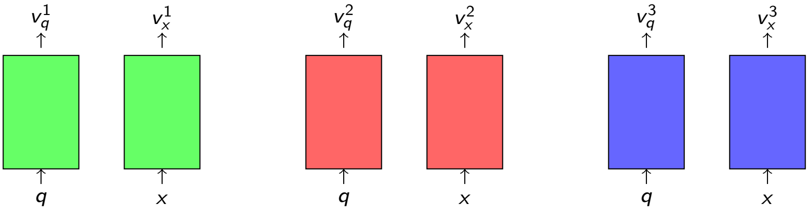
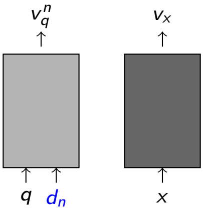


Drawback: multiple embeddings of same document must be indexed!

Learning multiple distance functions - efficient way

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



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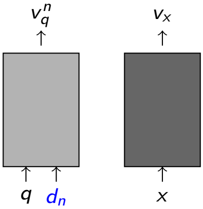


Only one meta-embedding per document is indexed!

Forward thinking

Forward thinking

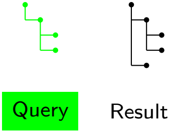
Why?

- 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`

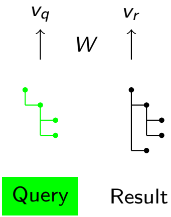
Current method - using gradients



Query

Result

Current method - using gradients



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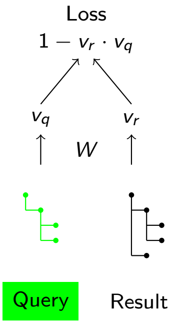

Loss

$1 - v_r \cdot v_q$

v_q

v_r

W

Query

Result

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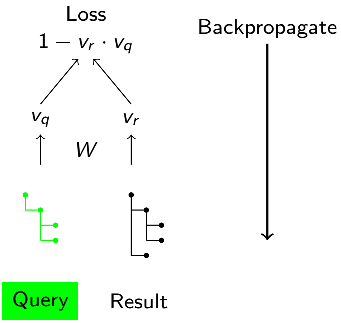

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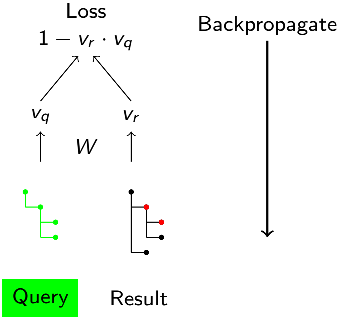
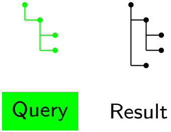


Nodes with highest gradient are considered most important

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



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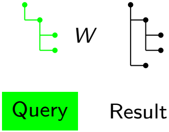
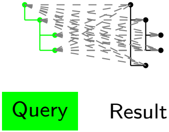


1. Embed graphs using model

Comparing node embeddings



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

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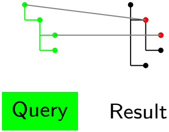

1. Embed graphs using model
2. Compare each pair of node embeddings
3. Highlight most similar nodes

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/`