Manifold Modelling with Minimum Spanning Trees

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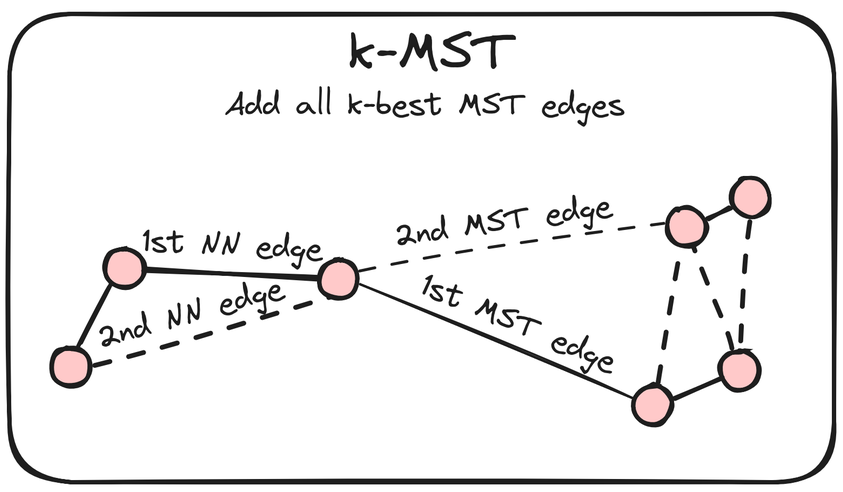
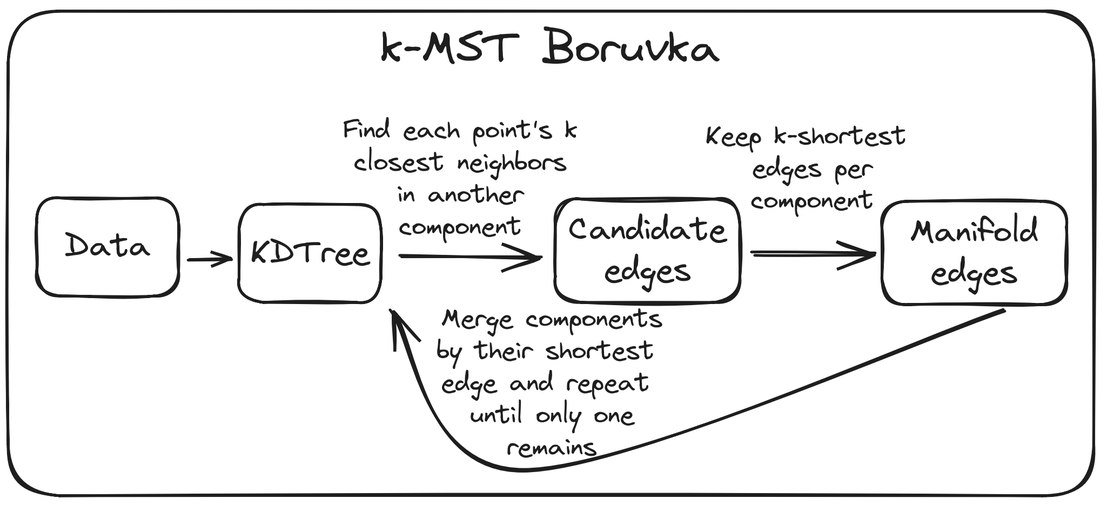
Background

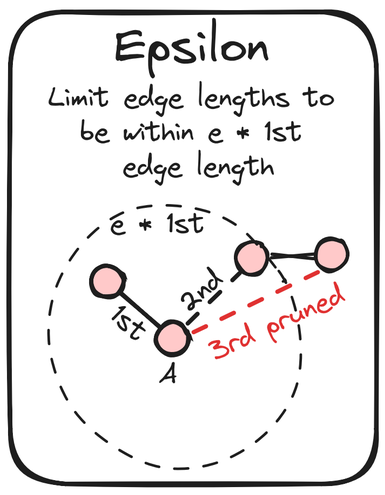
Recent dimensionality reduction algorithms assume data is uniformly sampled from an underlying manifold (e.g., [RS00, Ten00, vdMH08, MHM18]. While some algorithms are fairly robust against this assumption, there are scenarios in which more than the k-nearest neighbours (k-NN) are needed to approximate a manifold. This poster presents a k-nearest Minimum Spanning Tree (k-MST) manifold approximation approach that can deal with non-uniform sampling.

Methodology

The k-nearest Minimum Spanning Tree (k-MST) adapts MST unions from Pathfinder networks for distances. Our implementation adapts the Boruvka Algorithm from [MC23] to keep the k shortest edges between connected components. Since data points start as distinct components, all k-NN edges are included in the k-MST. A distance threshold ε provides an upper distance limit for the 2-to-k alternative edges to avoid shortcuts or sparsify the network.

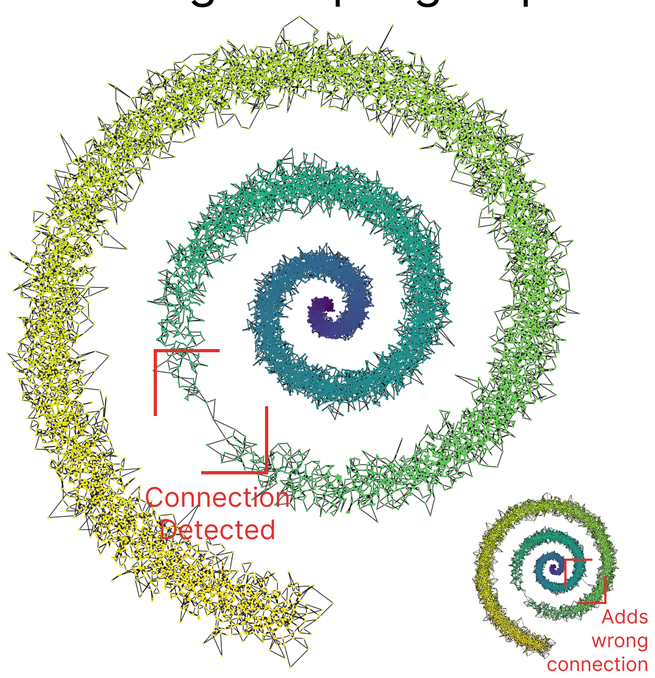






How do k-NNs and k-MSTs compare in modelling non-uniformly sampled manifolds?

Crossing Sampling Gaps

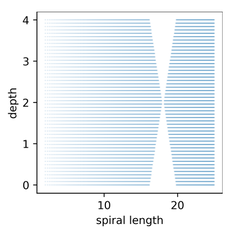


2-MST *time: 105ms*

5-NN *time: 124ms*

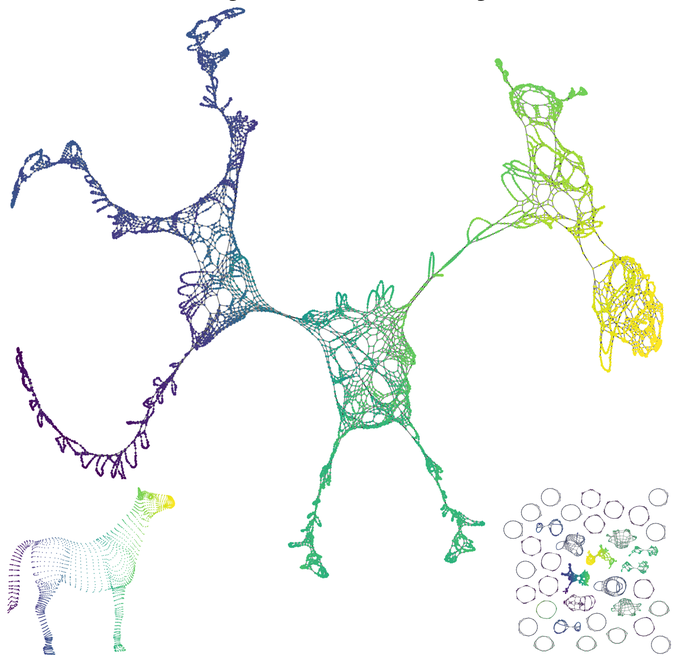
The ability to cross sampling-gaps was evaluated on a non-uniformly sampled Swiss Roll built from lengths `l` and depths `d`:

$$x = sl^2\cos(l) + \mathcal{N}(0, nl)$$
$$y = sl^2\sin(l) + \mathcal{N}(0, nl)$$
$$z = d + \mathcal{N}(0, nl)$$
$$s = 0.03, n = 0.0395$$



Some samples were removed along the manifold, resulting in a dataset with `22.196` samples and `3` features.

Layout Quality



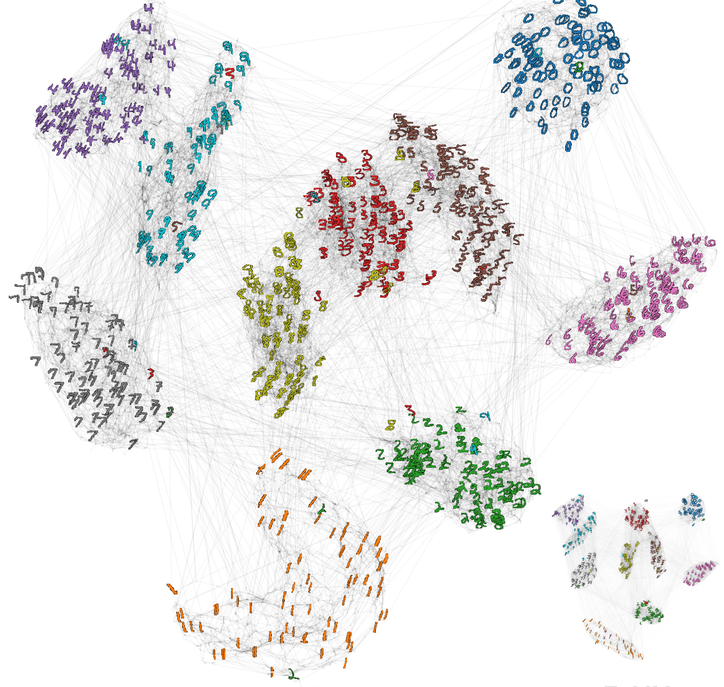
side-view

3-MST *time: 40ms sortedness: 0.90*

5-NN *time: 68ms sortedness: 0.72*

The methods' quality as dimensionality reduction approach was quantified by the Sortedness [PSNCP23] of their force-directed layouts [Hu05] on a horse-shaped dataset [SP04] with `8.431` samples and `3` features. The `3`-MST recovers a small, connected graph. The `5`-NN does not create a fully connected graph. At `10`-NN the Sortedness improves to `0.89`, but the graph remains disconnected.

Clustered Data



2-MST *time: 647ms edges: 201.032*

5-NN *time: 68ms edges: 427.046*

The methods' behavior on data with clusters was compared using MNIST [LBBH98], which has `70.000` samples and `784` features. UMAP layouts show the created networks. The `2`-MST was computed with `ε=1.1` to sparsify the graph. It balances local and global structures in a small model that is relatively cheap to lay out. The `5`-NN creates a larger network with more in-cluster connectivity.

Conclusions

k-MST discovers connectivity at all distance scales, balancing local and global structure and creating small models. A limitation of our implementation is the compute cost associated with KDTrees on some data sets. A NNdescent-based approximation for MSTs could make our techniques computationally competitive for larger datasets.

References

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