UMAP

What is Dimension reduction?

Dimension reduction, is the transformation of data from a high-dimensional space into a low-dimensional space so that the low-dimensional representation retains some **meaningful properties** of the original data

Dimension reduction algorithms tend to fall into two categories;

•those that seek to preserve the pairwise distance structure amongst all the data samples.

Eg. PCA , MDS, and Sammon mapping.

•those that favor the preservation of local distances over global distance.

Eg. t-SNE, Isomap, LargeVis, Laplacian eigenmaps, UMAP

Why not PCA?

For **visualization**, our humans could only visualize 2 or 3-dimensional plot. Since PCA preserves the global picture of the dataset, if the dataset is complex, it normally remains complex in 2 or 3 PCs space.

Three steps of UMAP:

1.Constructs a high dimensional graph

2.Constructs a low dimensional graph

3.Optimizes the low-dimensional graph to be high dimensional one as similar as possible

Algorithm 1 UMAP algorithm

function UMAP(X, n, d, min-dist, n-epochs)

1 *# Construct the relevant weighted graph*
for all $x \in X$ **do**
fs-set[x] ← LocalFuzzySimplicialSet(X, x, n)

 # Perform optimization of the graph layout
2 Y ← SpectralEmbedding(top-rep, d)
3 Y ← OptimizeEmbedding(top-rep, Y, min-dist, n-epochs)
return Y

1.Constructs a high dimensional graph

What is the desired graph? A particular weighted k-neighbour Graph

With **neighbors** and **distance (weight)**

How to construct this graph?

- Let $X = \{x_1, ..., x_N\}$ be the input dataset with metric d
- Find set of nearest k-neighbours $\{x_{i_1}, ..., x_{i_k}\}$ of x_i under metric d
- Weight function:

$$w((x_i, x_{i_j})) = \exp\left(\frac{-\max(0, \boxed{d(x_i, x_{i_j})} - \boxed{\rho_i})}{\boxed{\sigma_i}}\right)$$

- $d_{\mathbb{R}_N}(x_i, x_{i_j})$ is the Euclidean distance in $\mathbb{R}^N$
- $\rho_i = \min\{d(x_i, x_{i_j}) \mid 1 \le j \le k, d(x_i, x_{i_j}) > 0\}$ ensures that x i connects to at least one other data point with an edge of weight 1
- normalisation factor σ_i such that

$$\sum_{j=1}^{k} \exp\left(\frac{-\max(0, d(x_i, x_{i_j}) - \rho_i)}{\sigma_i}\right) = \log_2(k)$$

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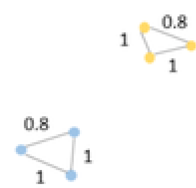
What is the property of the final umap high dimentional graph?

1.Explore final weighted graph

Why ?

- Undirected graph
- The largest weight is always 1
- Sum of weights is no longer $\log_2(k)$
- New sum $\geq \log_2(k)$
- Each point is now connected to at least k-1 other points

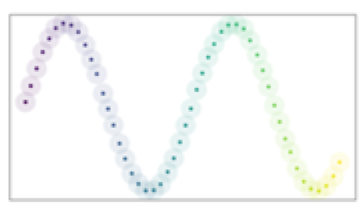


	A	B	C
A	0	1	0.8
B	1	0	1
C	0.8	1	0

why?

Approximating underlying manifold

- Assume D is uniformly distributed on the manifold M $D \in \mathbb{R}^N$
  - Then a ball of fixed volume V on M should contain the same number of points
  - Conversely a ball centred on point x that contains its k-nearest neighbours has fixed volume regardless of the choice of x



	A	B	C
A	0	1	0.8
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C	0.8	1	0

$\mathbb{R}^N$ is the high dimensional space

2. Standard steps of optimization:

Initialize low dimension distribution

Sample high and low dimension pairs

Calculate distances of sampled pairs in both high and low dimensions

Calculate the cost of dis-similarity of distances

Minimize the cost

Two different steps in the UMAP to do optimization.