Machine Learning

Clustering and Manifold Learning

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Lecture Overview

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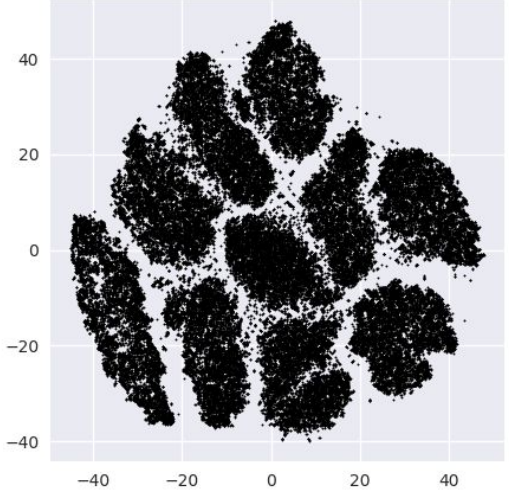
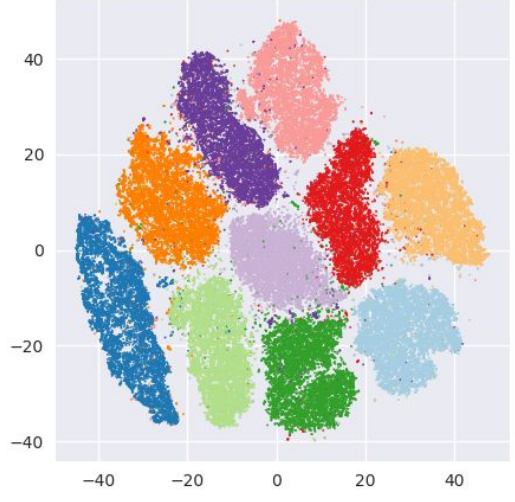
Recap

- Reinforcement Learning, RNNs
- Density Estimation

Today's lecture

- Clustering
  - Theory
  - k-Means
  - DBSCAN
  - ...
- Manifold Learning
  - T-SNE, UMAP
  - AE Embeddings, ...





Relation to Density Estimation

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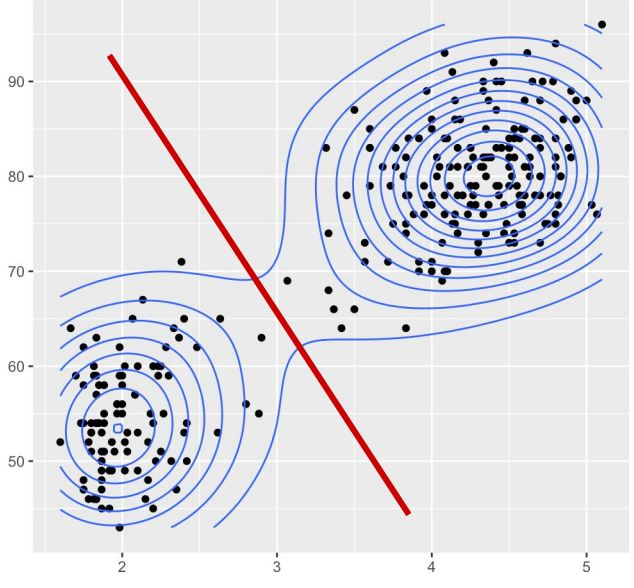
Manifold Learning

- Given some unorganised (high-dimensional) data can we learn some (low-dimensional) structure?

Clustering

- Given some (structured) data, can we learn the decision boundaries?



Manifold Learning & Clustering Applications

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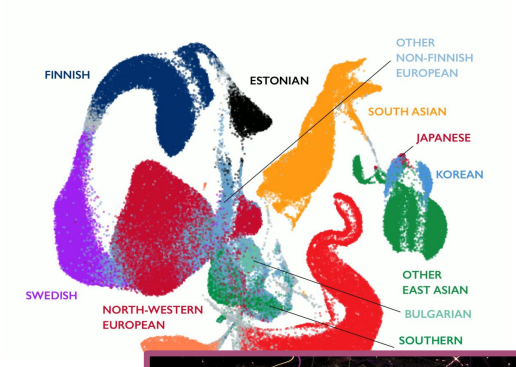
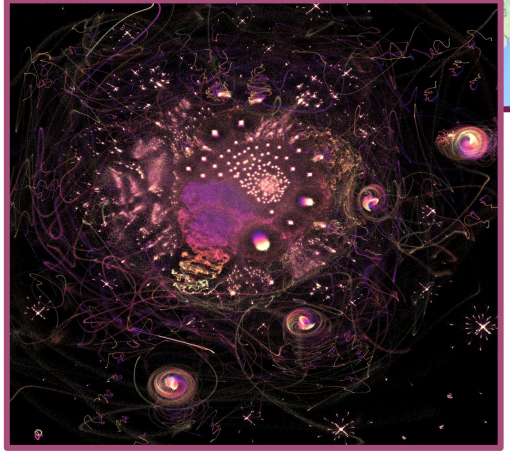
- Plant and animal ecology
- Transcriptomics
- Business and marketing
- Credit risk & insurance
- Medicine
- Crime analysis
- Education
- Politics and demographics
- Chemistry
- Climatology
- *Pointless* but beautiful math
- ...

https://macarthurlab.org/2018/10/17/gnomad-v2-1/





https://johnhw.github.io/umap_primes/index.md.html

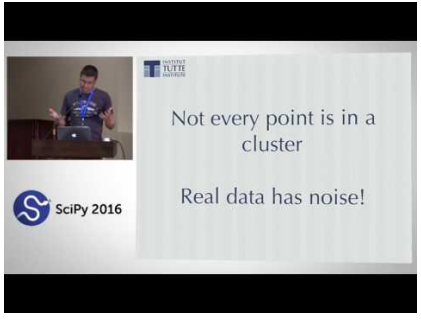
Clustering

The **task**

- Assign observations of a PDF to coherent clusters or label them as noise

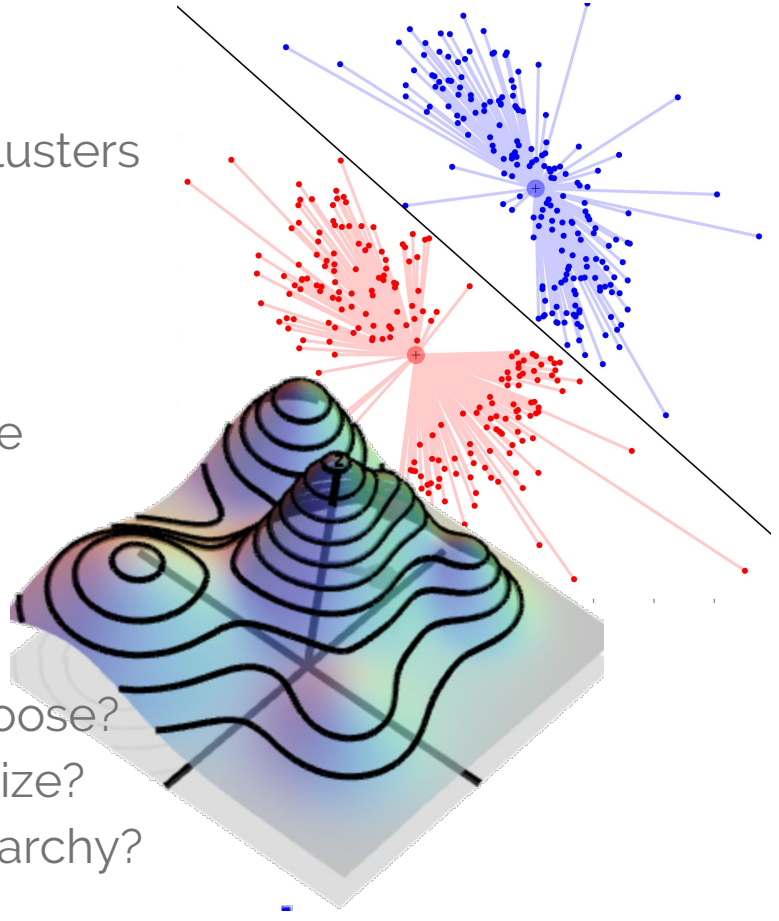
A **cluster** is a...

- **Connected-component** of a **level set** of the **unknown PDF** over our data **observations**



Some of the **challenges**

- What algorithm to choose?
- What metric to minimize?
- What scale, what hierarchy?



Types of Clustering Algorithm

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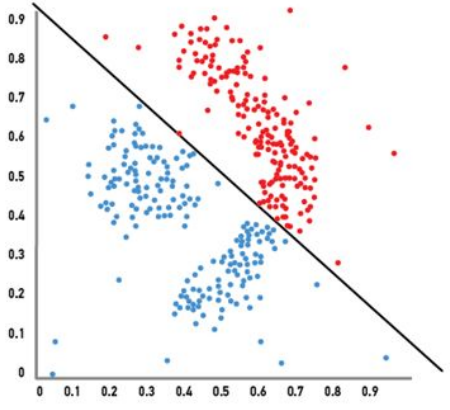
Assignment:

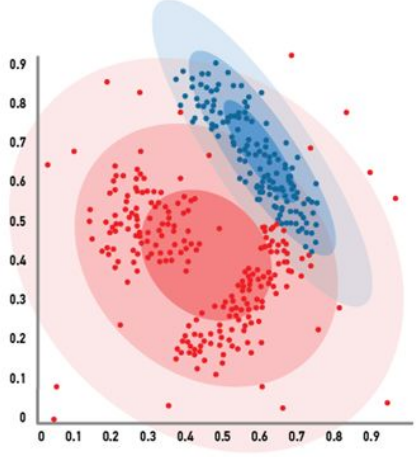
1. **Hard** clustering
2. **Soft** (fuzzy) clustering

Categories

- Centroid-based
- Density-based
- Distribution-based
- Connectivity-based
  - Bottom-up
  - Top-down



Hard clustering



Fuzzy clustering

k-Means Clustering Algorithm

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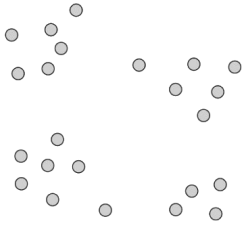
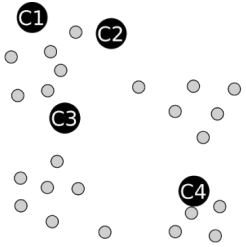
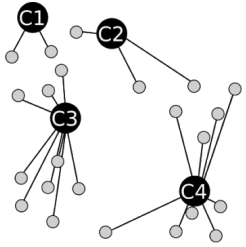


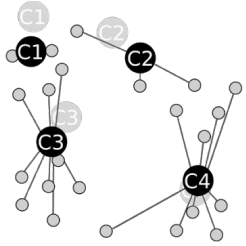
Input data



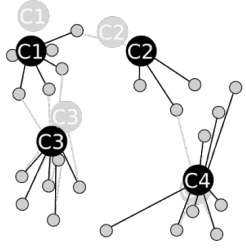
(1) Pick *k* random centroids



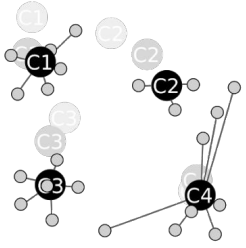
(2) Assign each point to nearest centroid



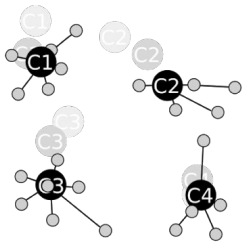
(3) Update centroids to mean of assigned



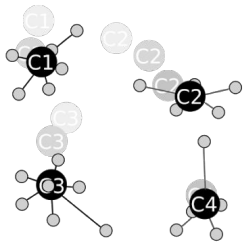
Repeat (2)



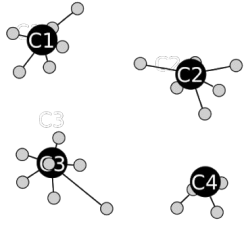
Repeat (3)



Repeat (2)

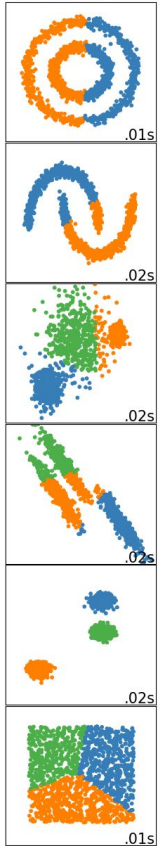


Repeat (3)

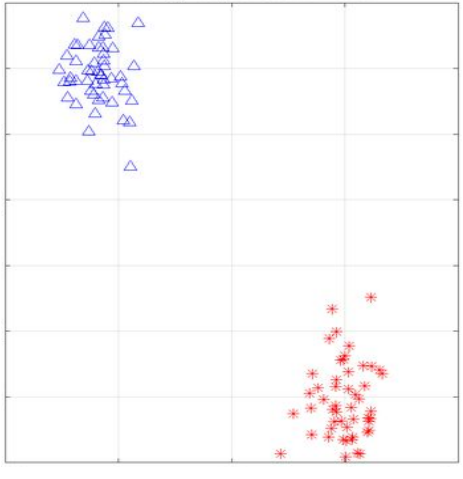


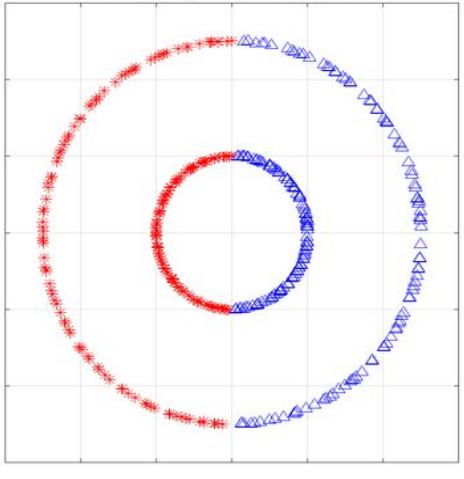
No movement = convergence

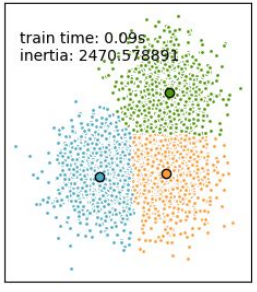
Properties (limitations) of *k*-Means



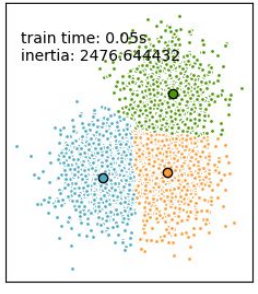
- Requires *k* to be known in advance (a prior)
- Assigns noise to clusters
- Can exhibit slow convergence
  - Mini-batch *k*-means, spatial index data structure
- Requires data to be <u>linearly</u> separable (convex clusters):



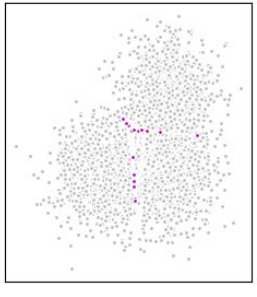




k-Means



Mini-batch k-Means



Difference

Hierarchical Clustering

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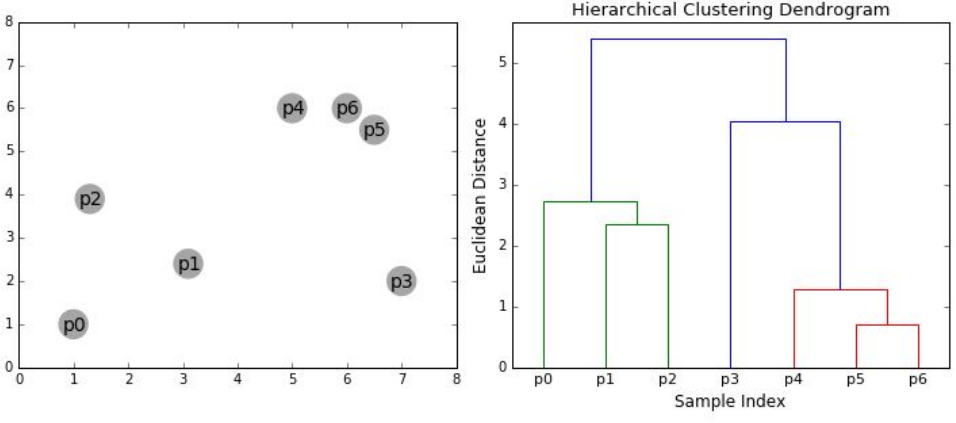
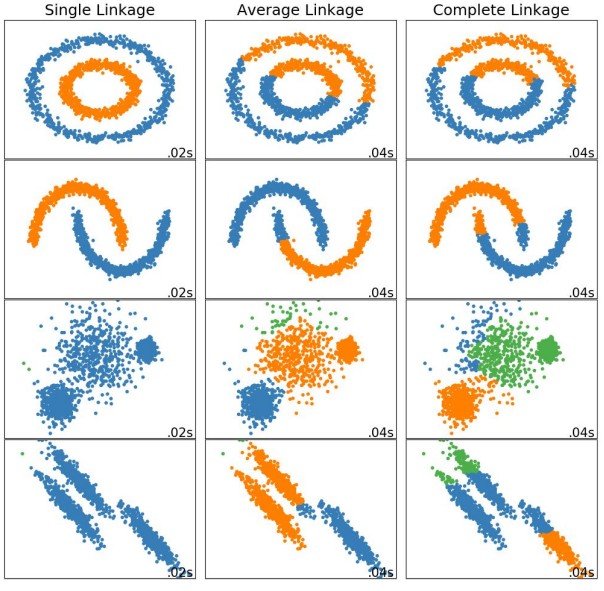
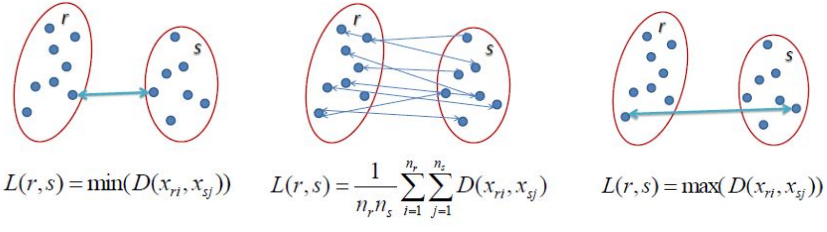
Hierarchical clustering methods are:

1. **Top-down** (divisive)
2. **Bottom-up** (agglomerative)

Various splitting/merging strategies….







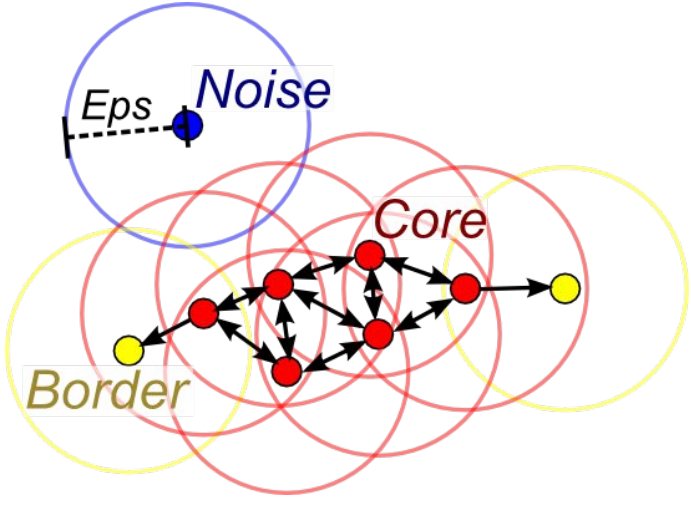
Density-based (DB)
Clustering

A Density-Based Algorithm for Discovering Clusters in Large Spatia
https://www.aaai.org/Papers/KDD/1996/KDD96-037.pdf
by M Ester - Cited by 13952 - Related articles
In this **paper**, we present the new clustering algorithm **DBSCAN** relying on density-based notion of clusters which is designed to dis- cover clusters of

DBSCAN: Density-Based Spatial Clustering of Applications with Noise

Two parameters:

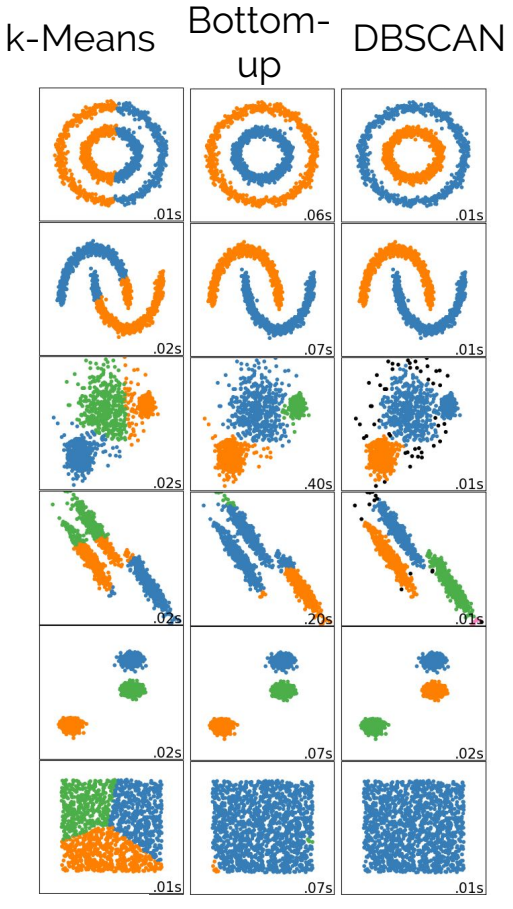
- Maximum radius $\varepsilon = 0.4$
- Minimum points $\delta = 5$



Algorithm:

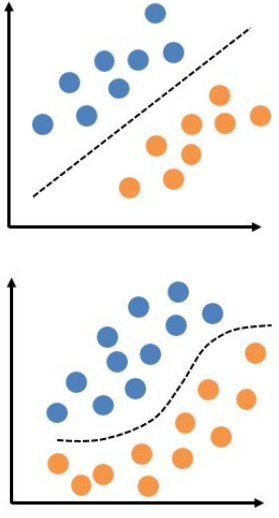
1. For all points, identify core points
2. Find core points connected components, these are the clusters
3. Assign density-reachable borders also to clusters, otherwise its noise

Properties of DBSCAN



Main **strengths**

- Creates arbitrarily shaped clusters
- Classifies noise
- Average runtime $n \log n$ with spatial indexing structure



Main **limitations**

- Quite difficult to tune ε and δ
- Non-deterministic
  - Although modification exists
- Relies on euclidean distance measure

HDBSCAN (Hierarchical DBSCAN)

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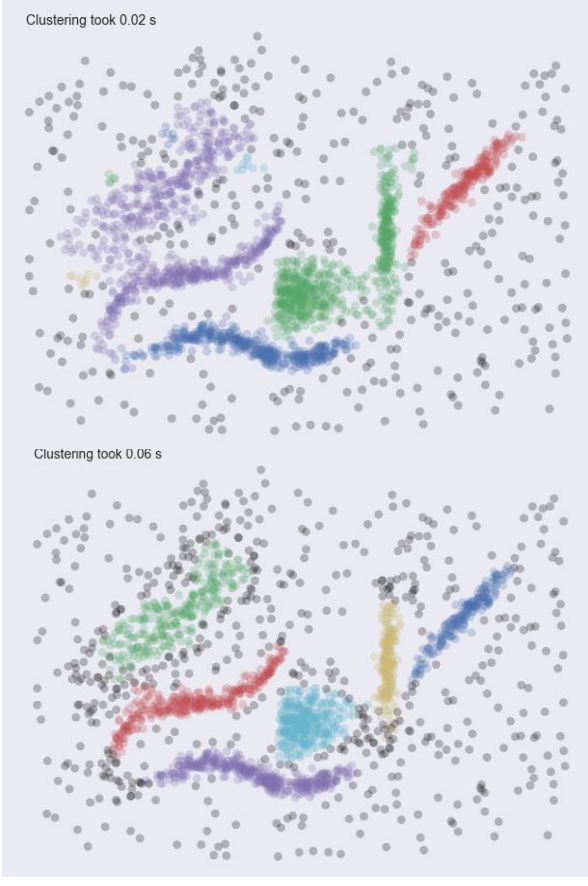
- More recent algorithm by some of same authors of DBSCAN
- Combines Hierarchical clustering with DBSCAN
- Just one intuitive parameter:
  - **minClusterSize**
- (Also has a *minSamples* parameter but is insensitive to it and can be set with sane defaults)
- Supports clusters of varying density
- Can be implemented reasonably efficiently

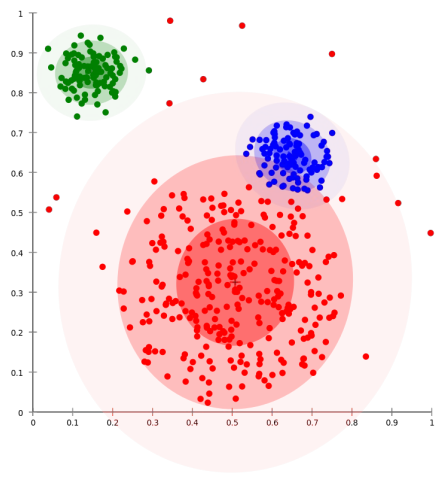


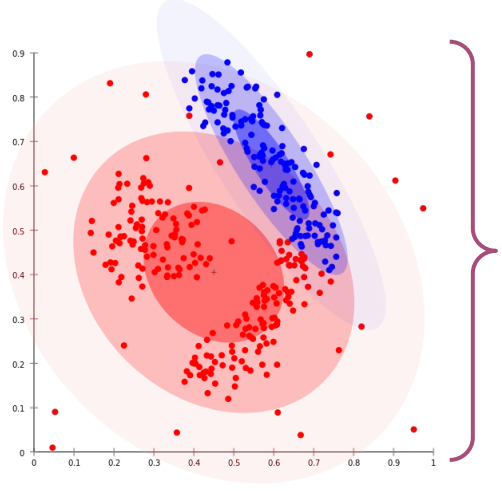
Distribution-based Clustering

Supposing our data points are generated from a mixture of a finite number of Gaussian distributions with unknown parameters, we can...

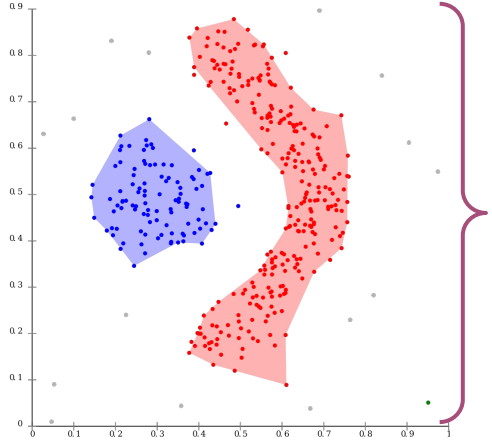
- Assign to distribution in a k-Means like fashion
- Optimise the parameters of the prior distributions such as to maximize the likelihood of the data given those assignments. Then repeat.

GMMa (good case)





GMM (bad case)



DBSCAN

Clustering Algorithms...

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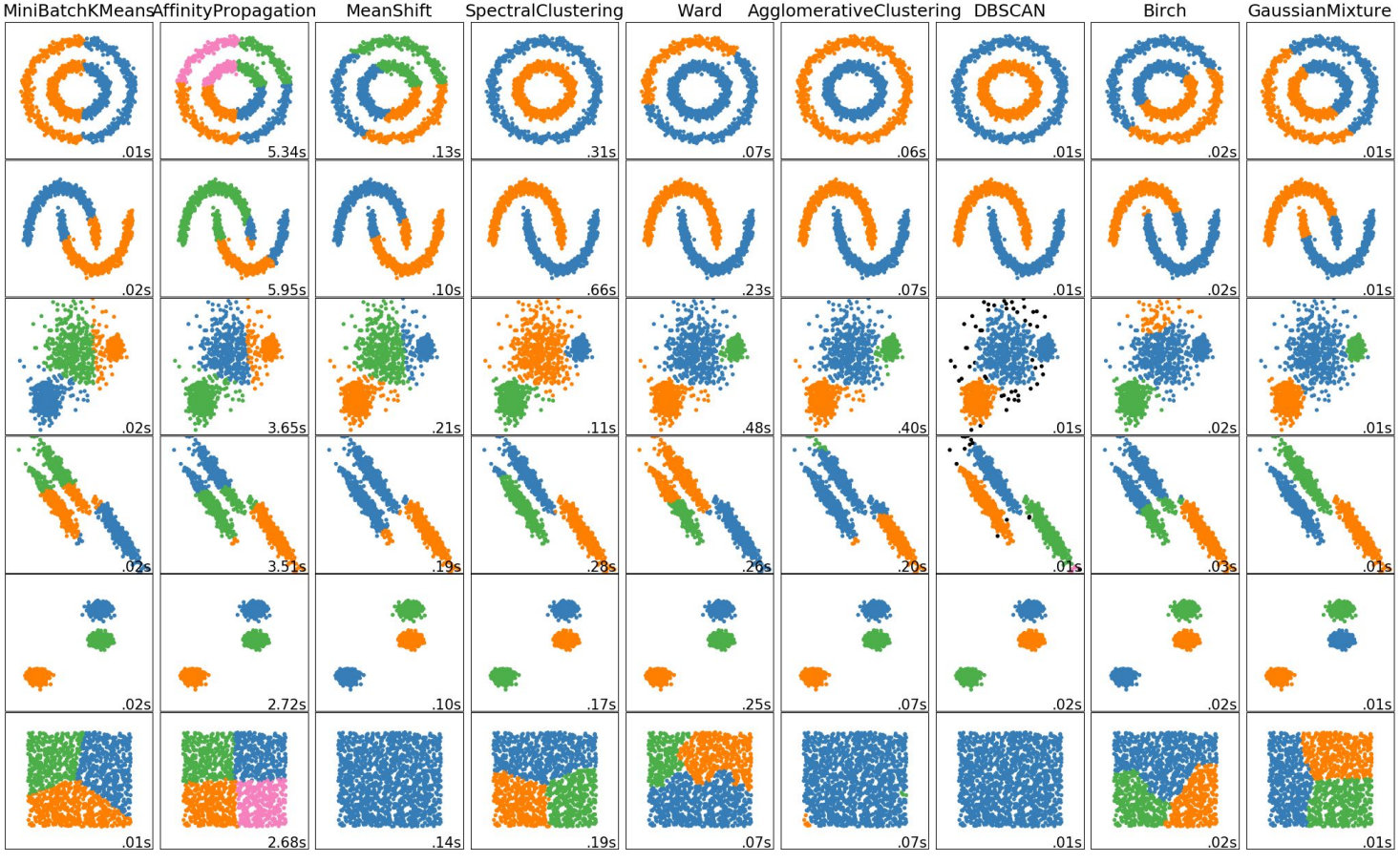

Python implementations in **scikit-learn**

https://scikit-learn.org/stable/modules/clustering.html

HDBSCAN separate: https://hdbscan.readthedocs.io/

Manifold Learning (or NLDR)

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The **task**

- Given some unorganised (high-dimensional) data can we learn some organised (low-dimensional) manifold that captures the data distribution?

The **challenges**

- What should the manifold look like, and why?
- Curse of dimensionality
  - Distances in high-dimensional spaces are all similar
- What neighborhood to define?
- What metric to minimize?

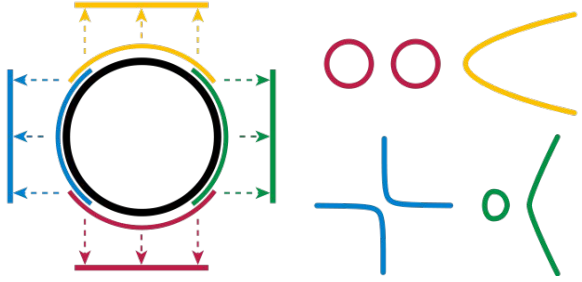
The **application:**

- Save space, understand data patterns, ...

Terminology

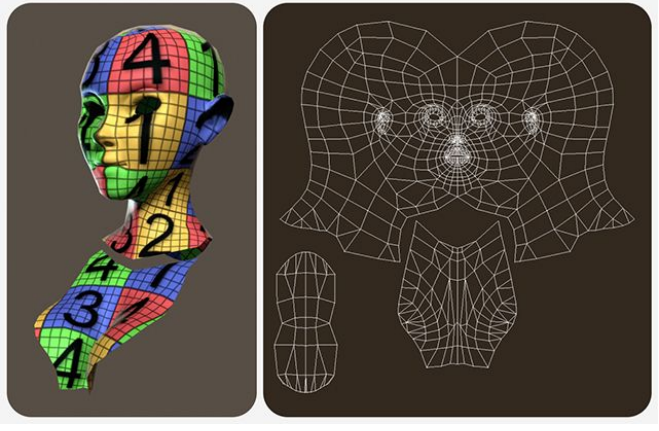
Manifold

- A space that locally resembles Euclidean space.
- Hierarchy of types of manifold:
  - Topological
  - Differentiable
  - Riemannian



Embedding

- An injective map $\phi : \mathcal{M} \to \mathcal{N}$ that preserves the underlying structure.



"Recovering the riemannian metric"

Autoencoders

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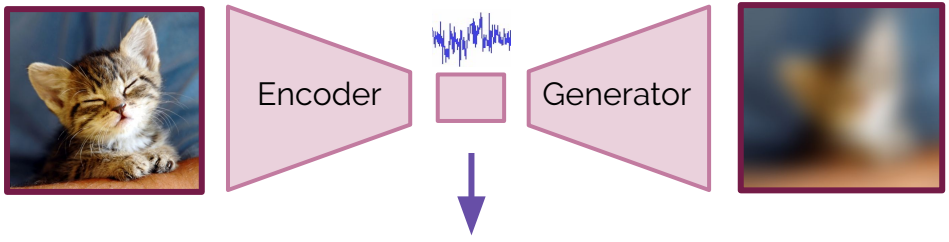
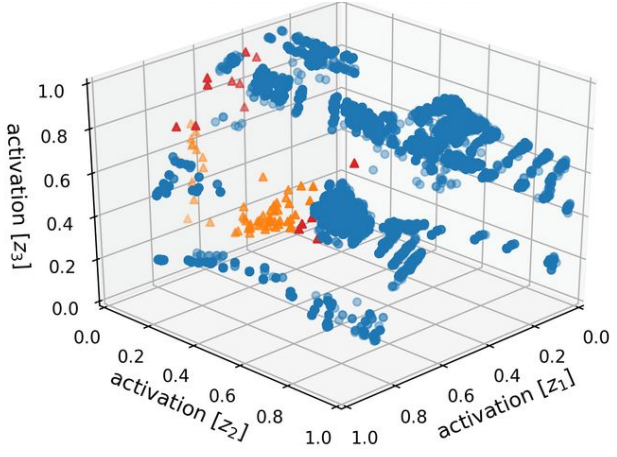
Learn a non-linear mapping from high-dimensional to an embedded space



- Local variations with $L2$
- **Can fracture** a manifold into many different domains (giving different regions for nearby data points)
- If we have **prior knowledge** about data, we can split the manifold into lovely categories easily
  - Global coherency

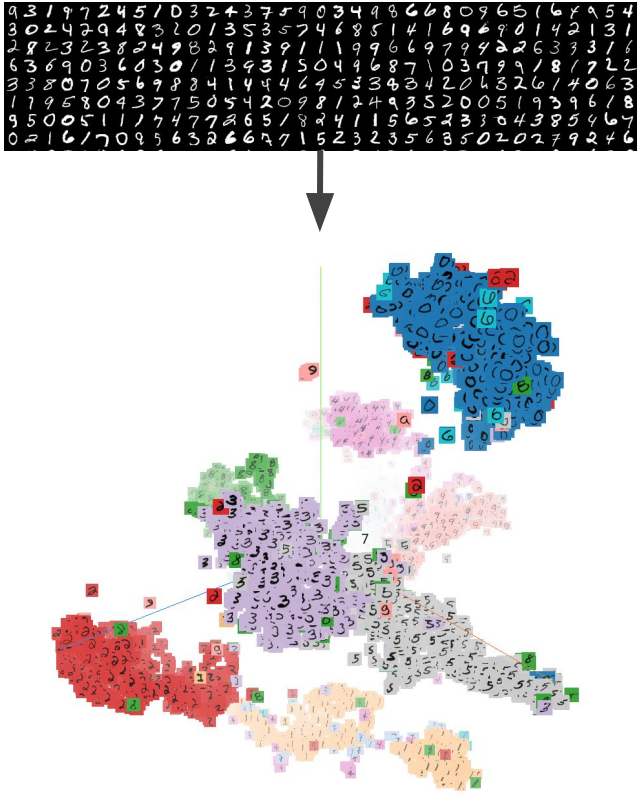


T-**D**istributed **S**tochastic **N**eighbor **E**mbedding

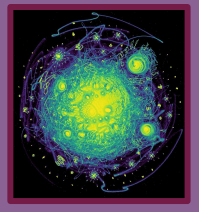
Visualizing Data using t-SNE - Journal of Machine Learning Research
www.jmlr.org/papers/volume9/vandermaaten08a/vandermaaten08a.pdf ▾
by L Maaten - 2008 - Cited by 7224 - Related articles
We present a new technique called "**t-SNE**" that visualizes high-dimensional da
.... present in the **paper** are sufficient to demonstrate the superiority of **t-SNE**.

The t-SNE algorithm:

- Uses local relationships between points to create a low-dimensional mapping.
  - Definies this relation by assuming an **adaptive Gaussian prior** based on a "perplexity" hyperparameter
- Defines a distribution over points in low-dimensional space, and minimizes KL-divergence between the two distributions
  - Ensures dissimilar points are far apart



UMAP



UMAP: Uniform Manifold Approximation and Projection for Dimension ...
https://arxiv.org › stat
by L McInnes - 2018 - Cited by 78 - Related articles
9 Feb 2018 - The **UMAP** algorithm is competitive with t-SNE for visualization quality, and ... Furthermore, **UMAP** has no computational restrictions on

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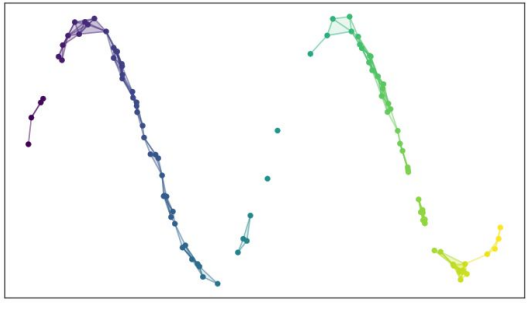
The UMAP algorithm:

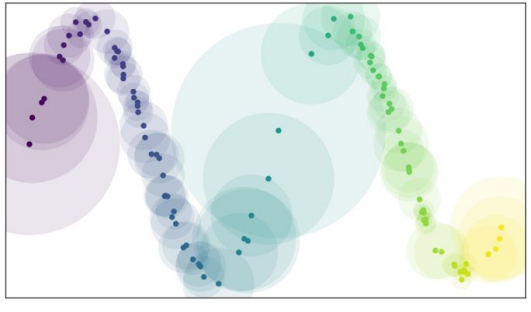
- Finds k-nearest neighbors in dataset
  - Creates edge weights based on diameter of neighborhood graph and distance to nearest neighbor
- Minimize:

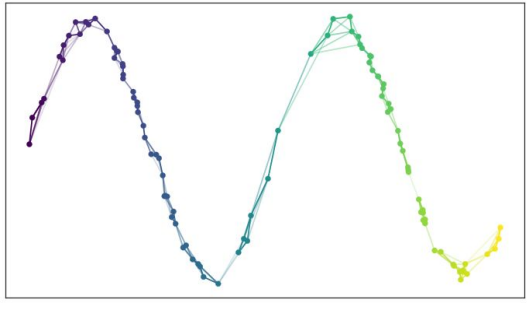
$$\sum_{e \in E} w_h(e) \log\left(\frac{w_h(e)}{w_l(e)}\right) + (1 - w_h(e)) \log\left(\frac{1 - w_h(e)}{1 - w_l(e)}\right)$$

Get the clumps right

Get the gaps right

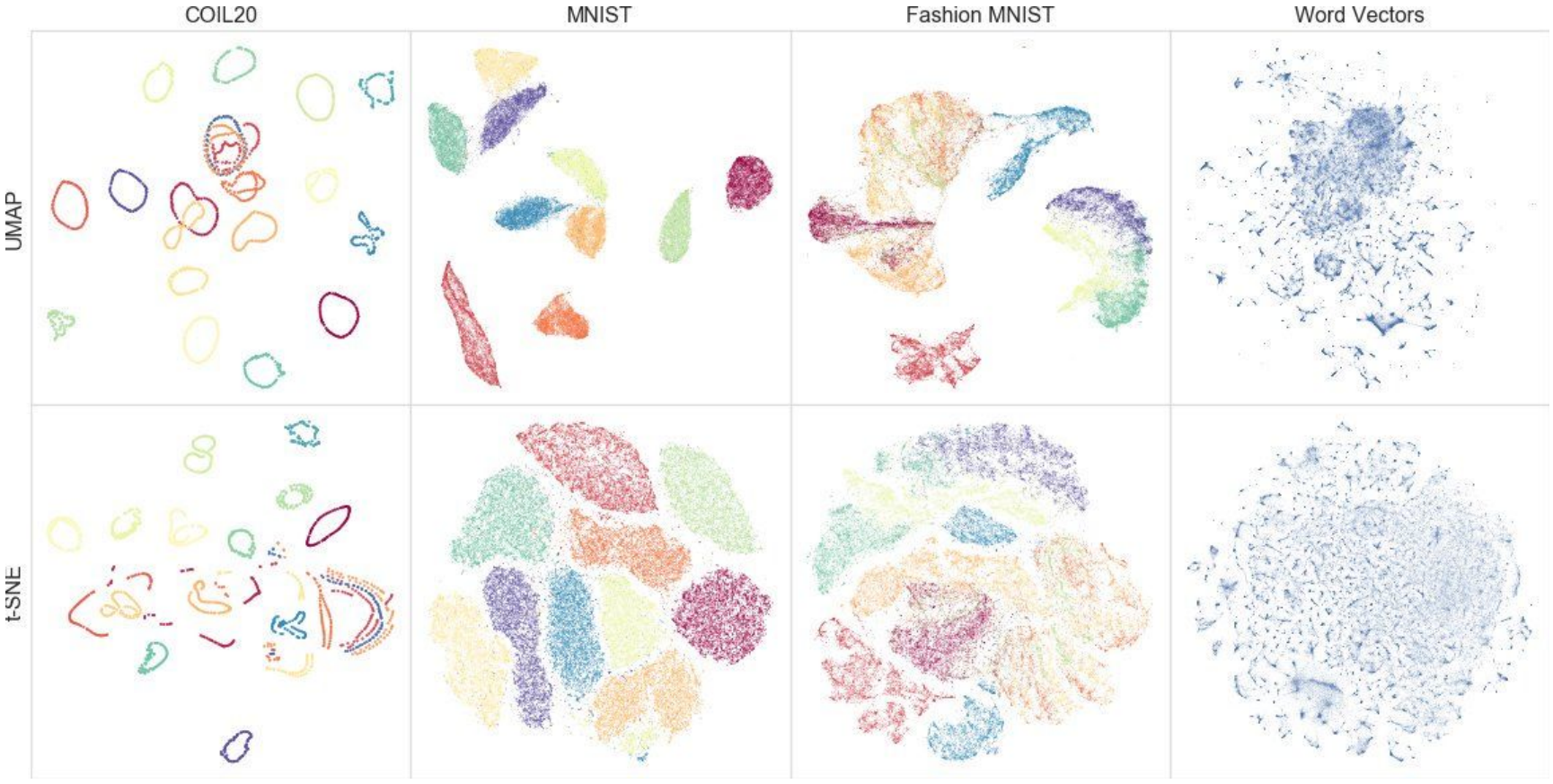






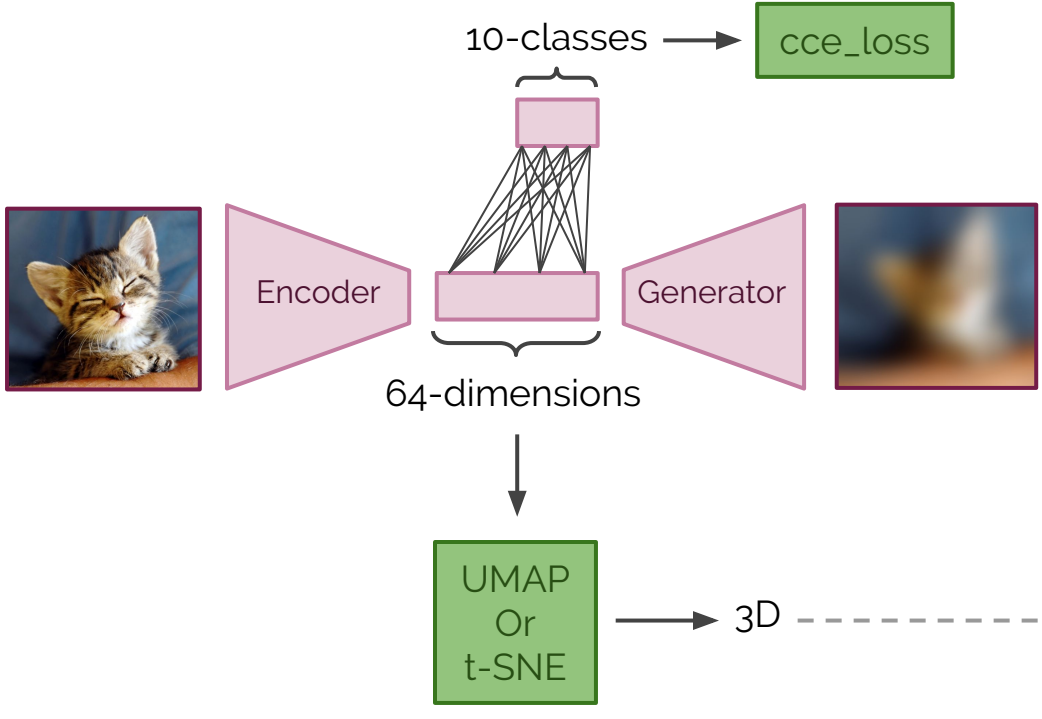
UMAP and t-SNE Examples

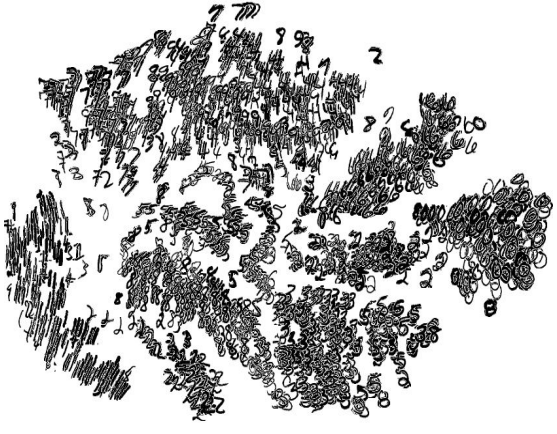
Durham University



Learning Tailored Manifolds

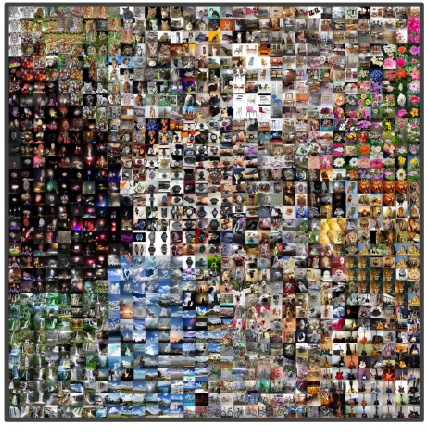
Durham University

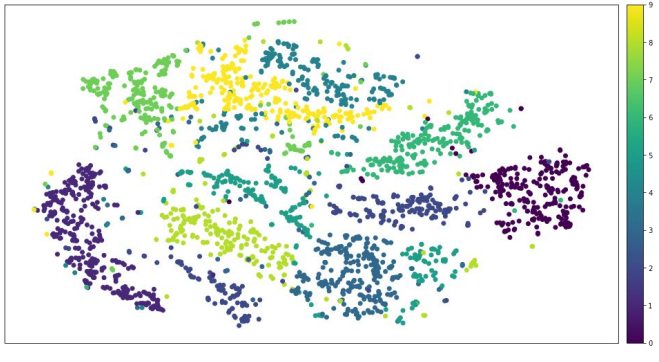


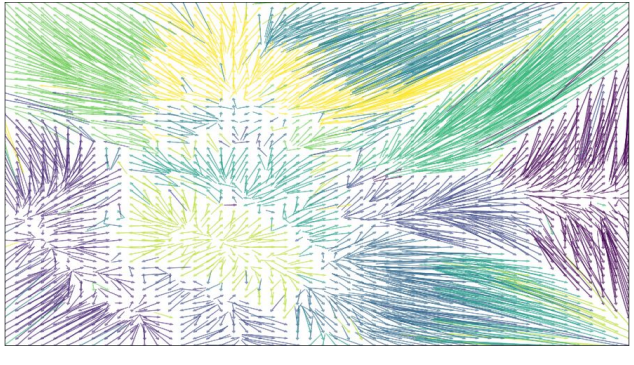


Take Away Points

- There is no one clustering algorithm that outperforms all…
  - But density-based stuff is generally pretty good in low-dimensions
- There's an infinite number of great manifolds out there
  - **UMAP** is currently a pretty good NLDR algorithm
- Good density estimators underpin a lot of this field
  - Especially defining local neighborhoods is important
- In practice, UMAP works pretty well with **HDBSCAN**.
  - See: https://umap-learn.readthedocs.io/en/latest/clustering.html







Jonker-Volgenant algorithm