

Projections and clusterings

Formation IA biodiversité

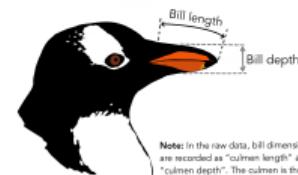
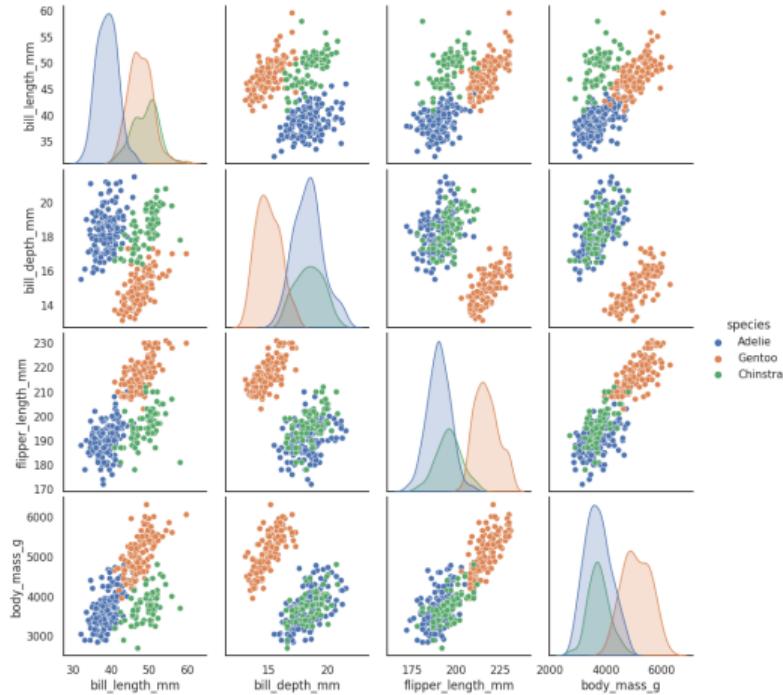
Paul Tresson

May 14, 2025

UMR AMAP

Introduction

Visualize what is happening in higher dimensions



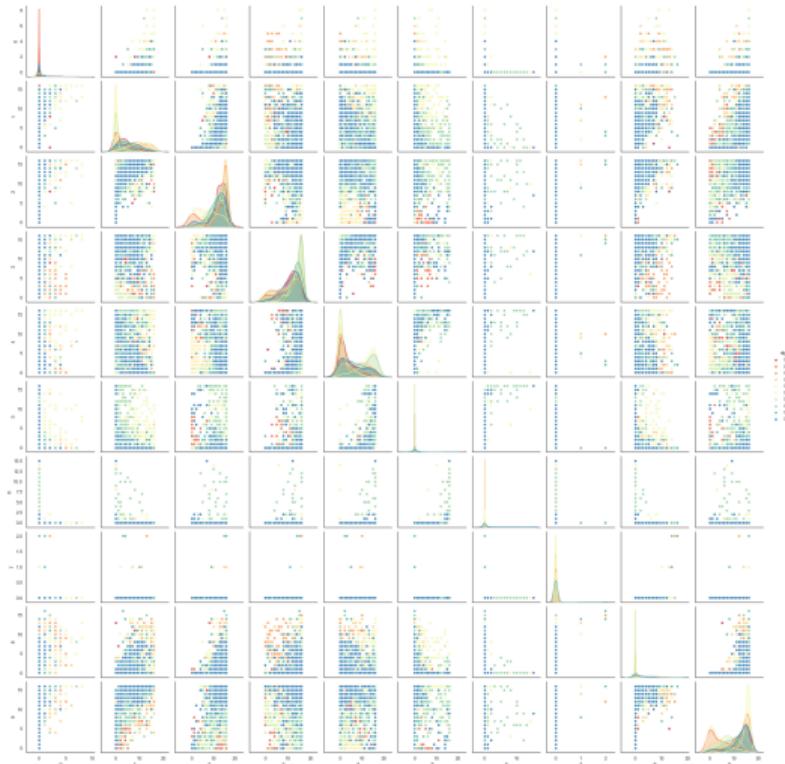
Note: In the raw data, bill dimensions are recorded as "culmen length" and "culmen depth". The culmen is the dorsal ridge atop the bill.

Visualize what is happening in higher dimensions

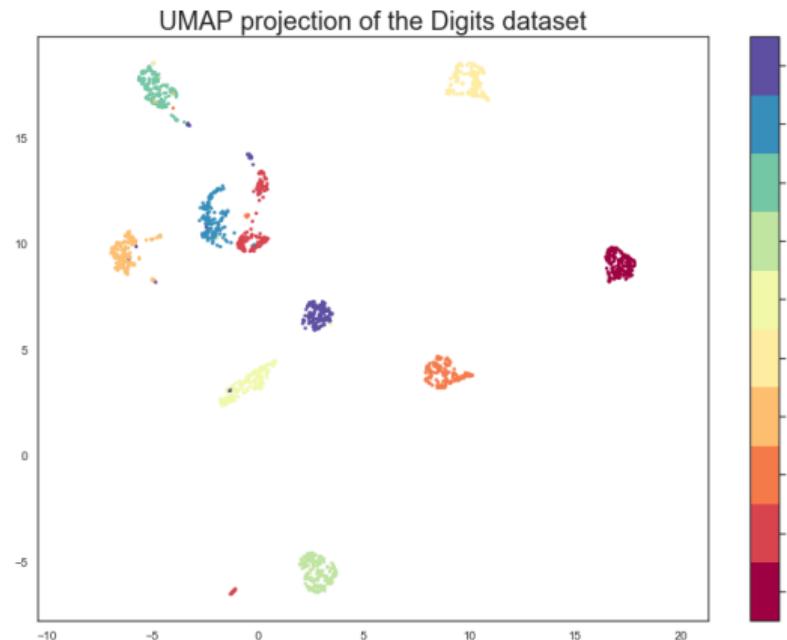
A 4x4 grid of numbers from 0 to 9, representing a 2D projection of a 3D cube. The numbers are arranged in a pattern that shows the relative positions of vertices in a cube, though they are not in a standard 3D coordinate system.

0	0	8	5
1	1	9	6
2	2	0	7
3	3	1	4
4	4	2	5
5	5	3	6
6	6	4	7
7	7	5	8
8	8	6	9
9	9	0	1

Visualize what is happening in higher dimensions



Visualize what is happening in higher dimensions

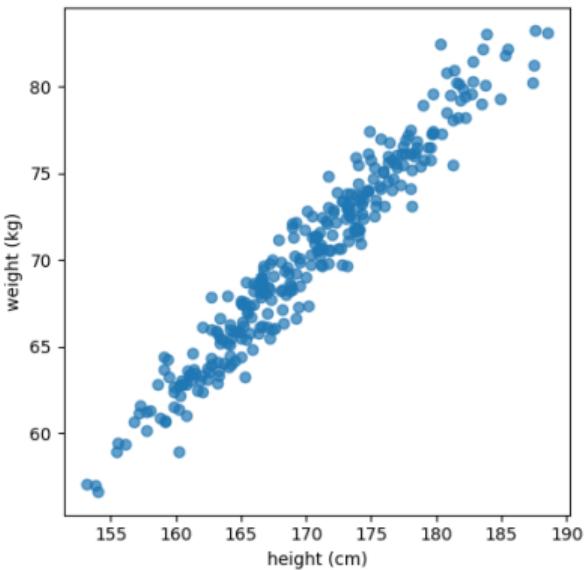


Projections

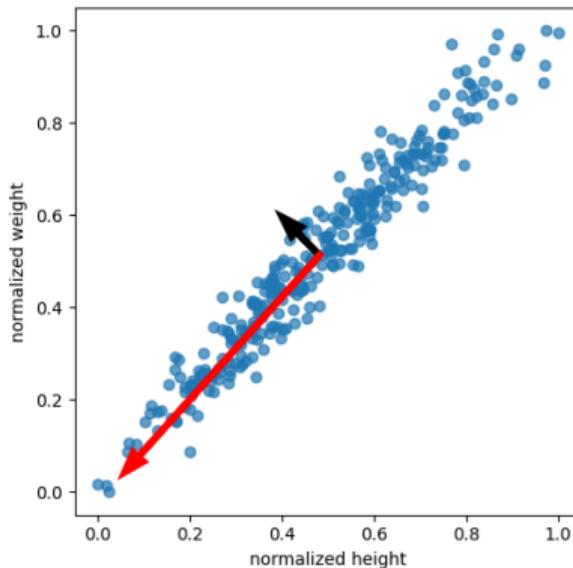
Projections

PCA

PCA



PCA



PCA calculation

$$X = \begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ x_3 & y_3 \\ \dots & \dots \end{bmatrix}$$

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$$C = \begin{bmatrix} \sigma_x^2 & \sigma_{xy} \\ \sigma_{yx} & \sigma_y^2 \end{bmatrix}$$

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$$Cv = \lambda v$$

$$\begin{bmatrix} \sigma_x^2 & \sigma_{xy} \\ \sigma_{yx} & \sigma_y^2 \end{bmatrix} \begin{bmatrix} v_x \\ v_y \end{bmatrix} = \lambda \begin{bmatrix} v_x \\ v_y \end{bmatrix}$$

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$$P = \begin{bmatrix} v_x & v_y \end{bmatrix}$$

PCA calculation

```
# normalize
normalized_data = (points - np.min(points, axis=0)) / (
    np.max(points, axis=0) - np.min(points, axis=0)
)

# get covariance
cov = np.cov(normalized_data, rowvar=False)

# calculate eigenvalues and eigenvectors of the covariance matrix
eigvals, eigvecs = np.linalg.eig(cov)

# scale eigenvectors
scaled_eigvecs = eigvecs * np.sqrt(eigvals)
```

PCA advantages and drawbacks

Advantages

- fast

Drawbacks

PCA advantages and drawbacks

Advantages

- fast
- scales well

Drawbacks

PCA advantages and drawbacks

Advantages

- fast
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- explanatory

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PCA advantages and drawbacks

Advantages

- fast
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Drawbacks

- **not suited for non-linear data**

Non linear data

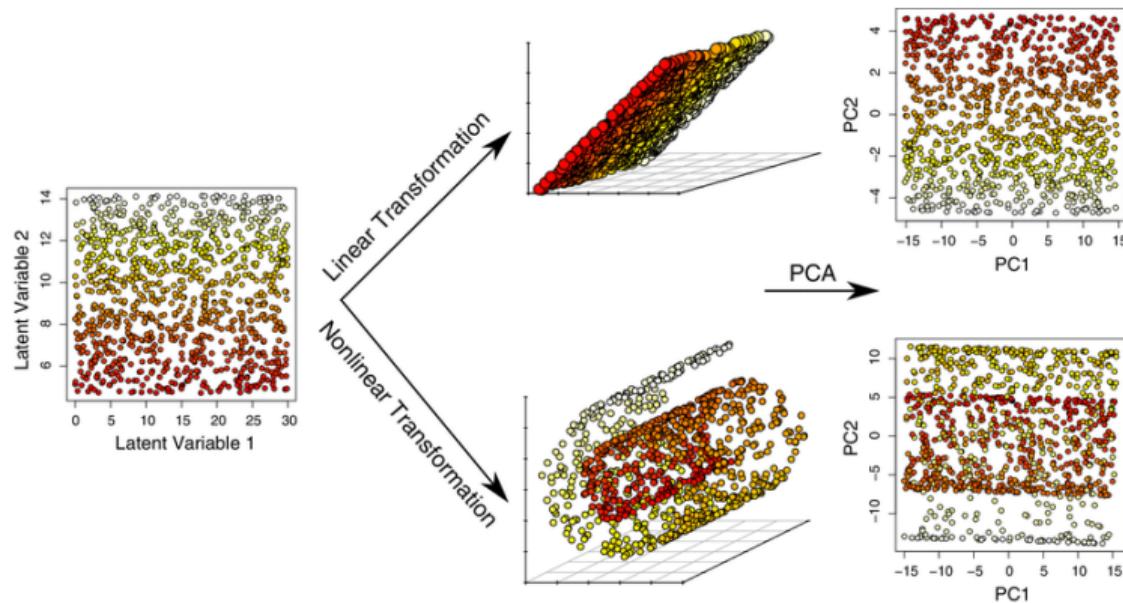


Figure from Du, 2019

Projections

UMAP

How to work with non linear data

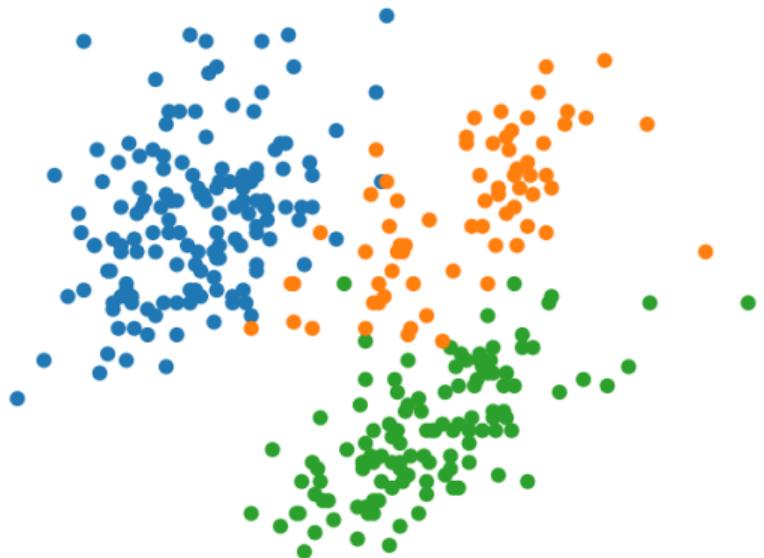
1. Find a good representation of the data in high dimension
2. Fit a good representation of in low dimension

- **SNE** (Stochastic Neighbor Embedding) Hinton and Roweis, 2002

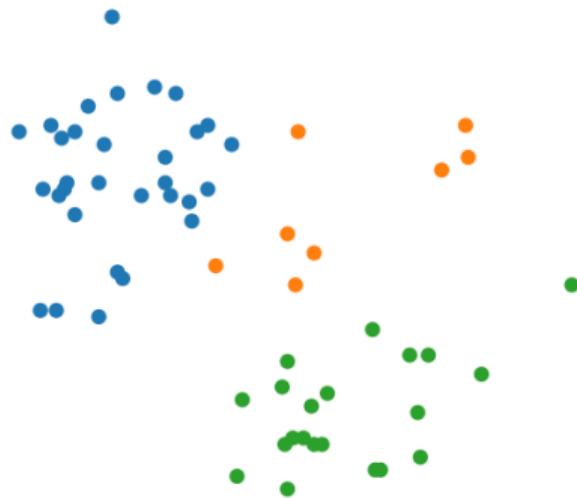
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- **T-SNE** (T-distributed SNE) Van der Maaten and Hinton, 2008

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- **UMAP** (Uniform Manifold Approximation and Projection) McInnes et al., 2018

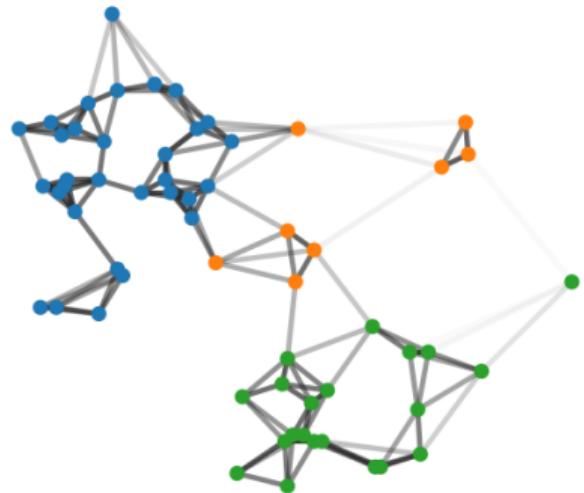
UMAP : Finding high dimension graph



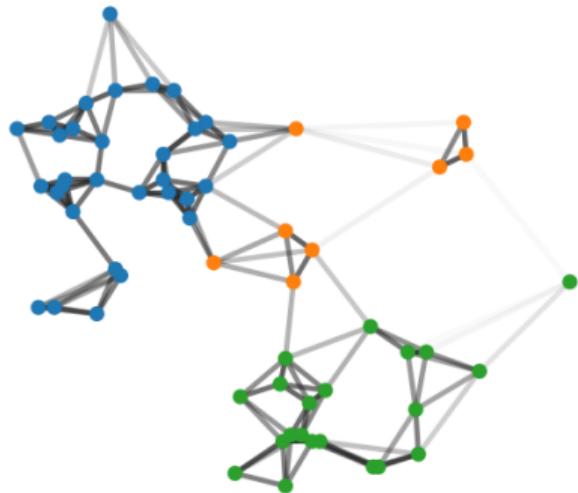
UMAP : Finding high dimension graph



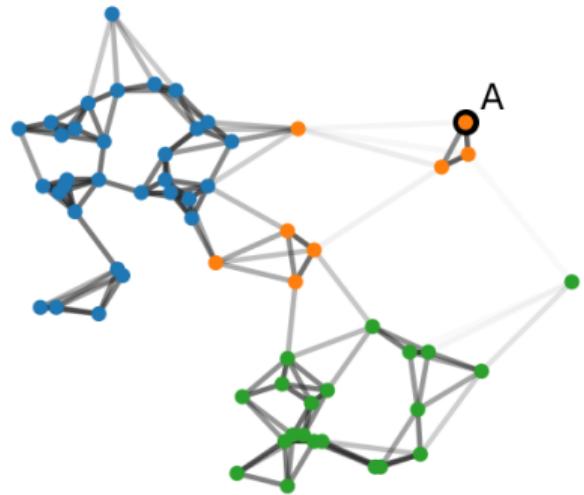
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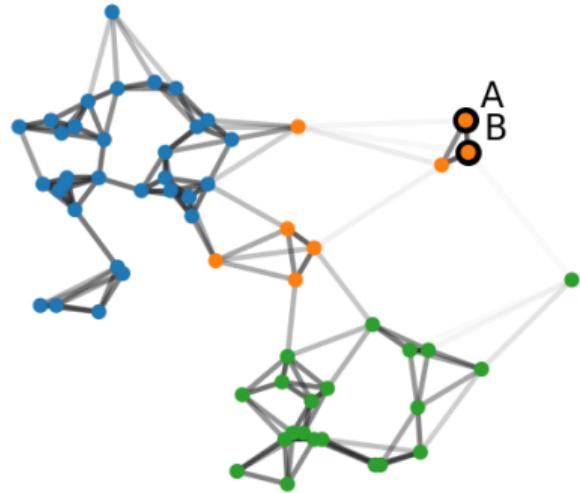
UMAP : Fitting low dimensional representation



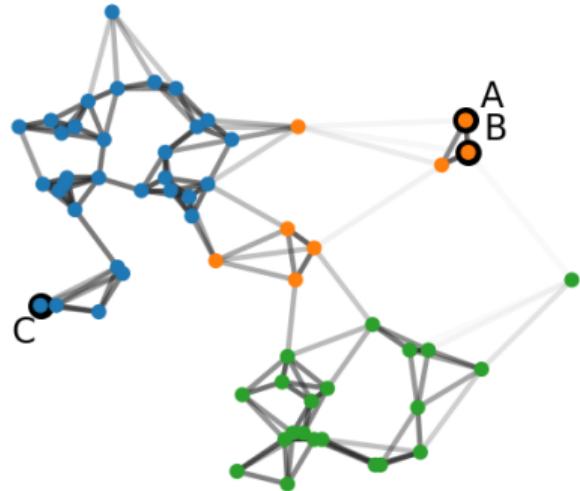
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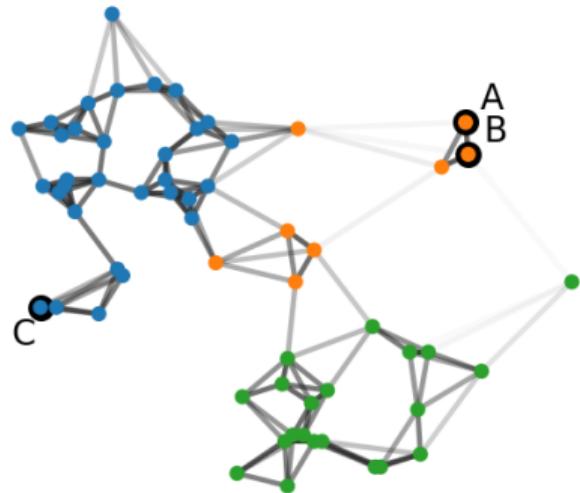
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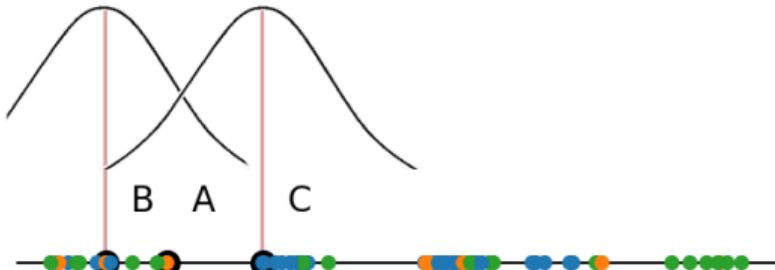
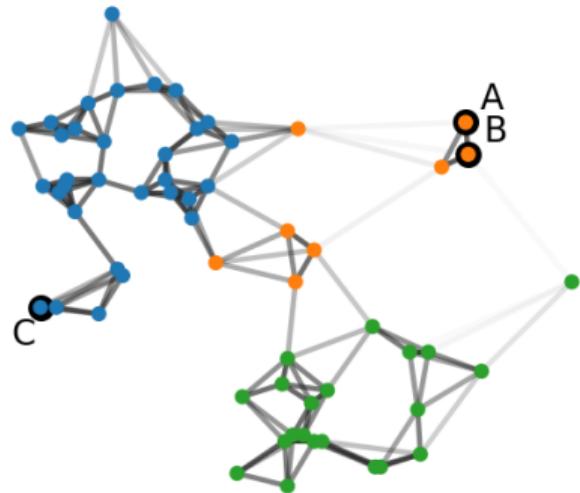
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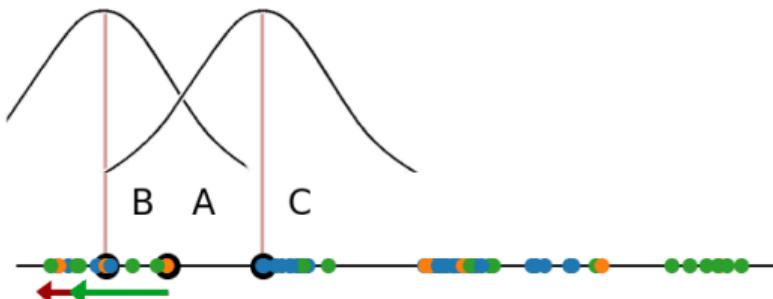
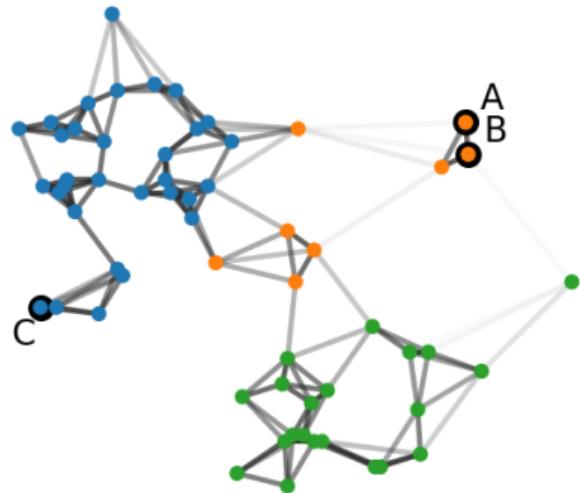
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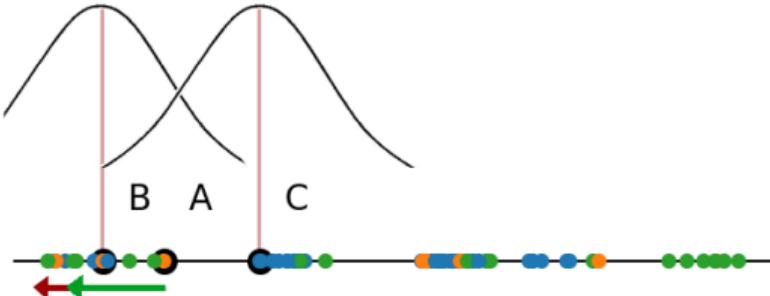
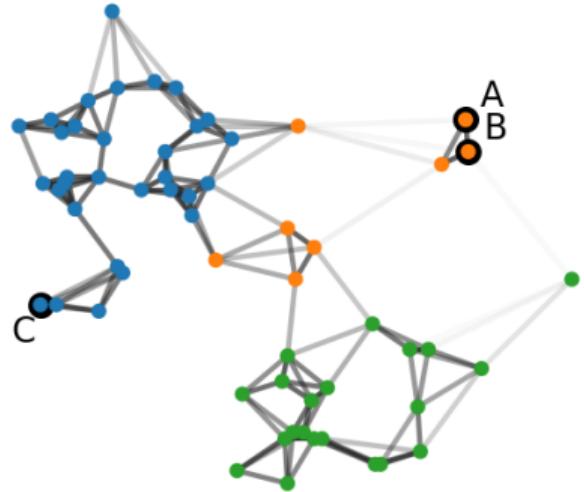
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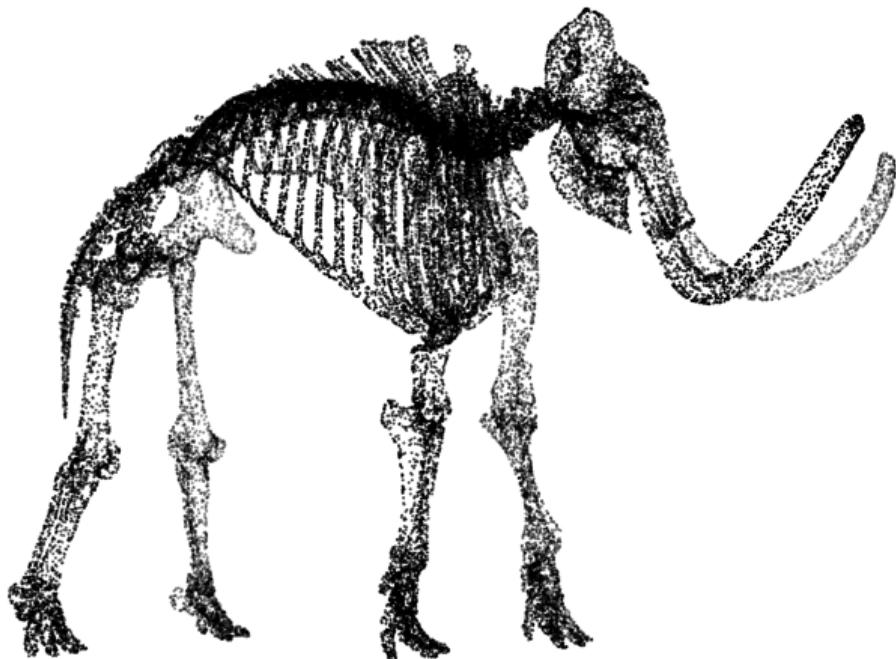


UMAP : Fitting low dimensional representation

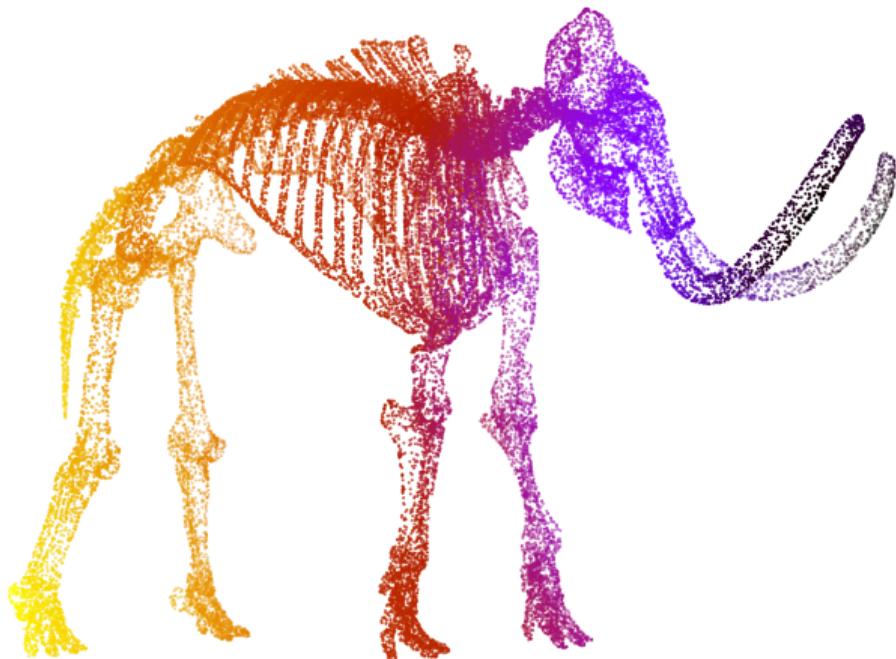


→ Update with cost function so that
neighbours in HD are neighbours in LD

Mammoth example



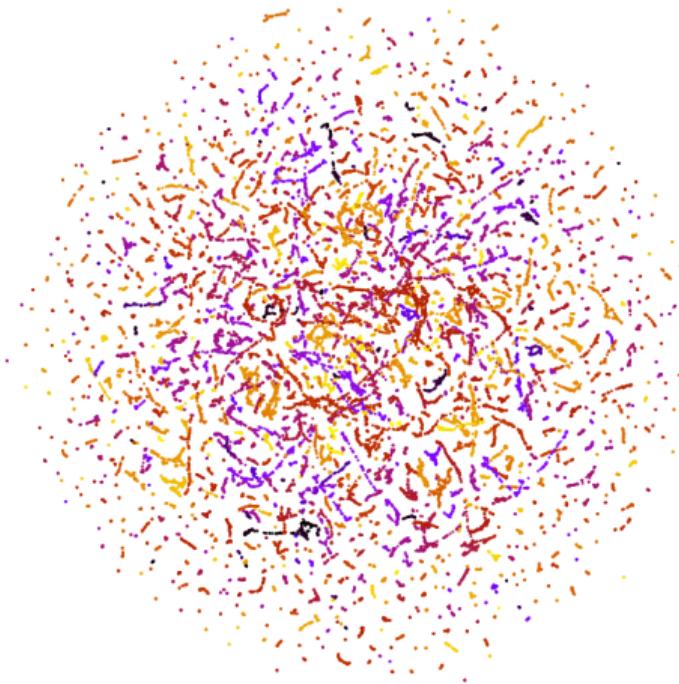
Mammoth example



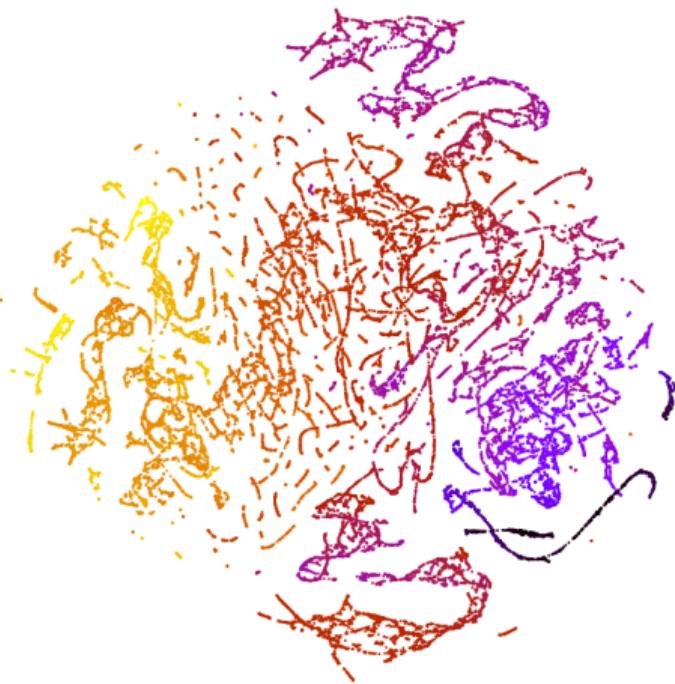
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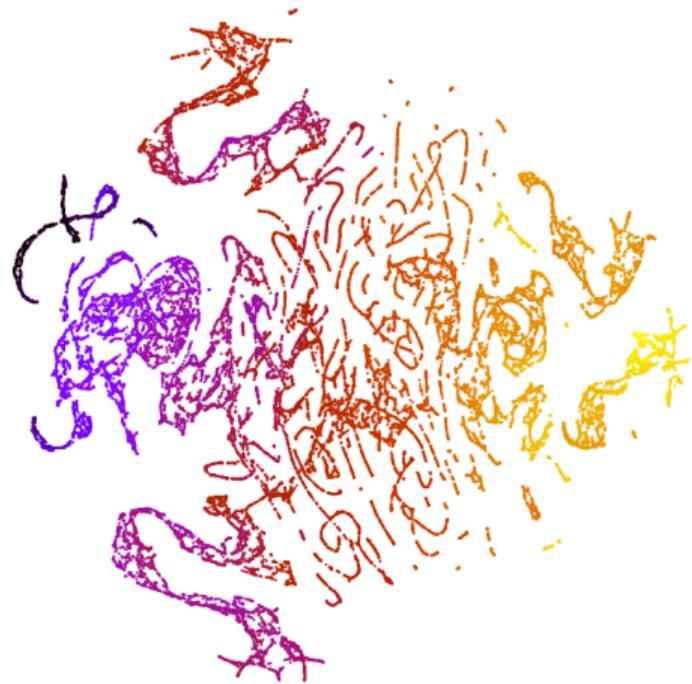
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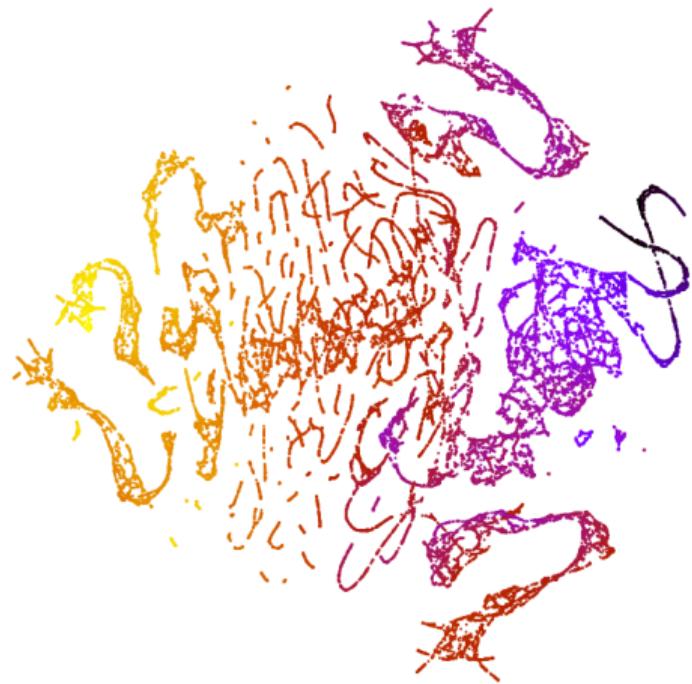
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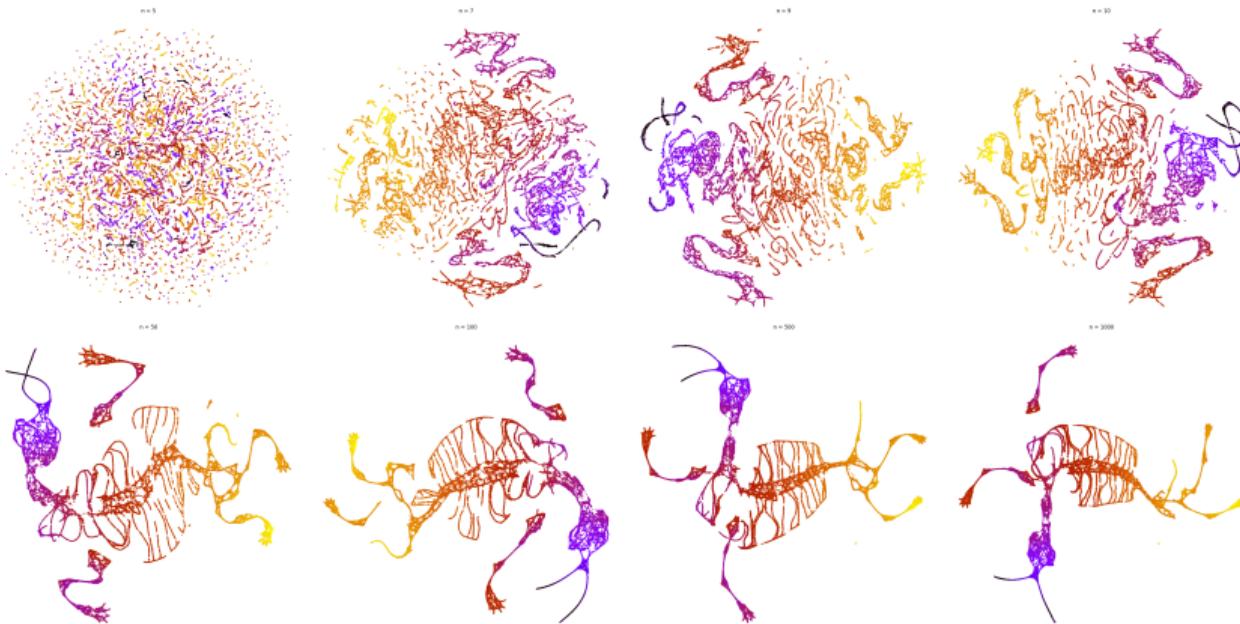
Mammoth example



Mammoth example



Mammoth example



UMAP vs. T-SNE

UMAP

- graph theory, fuzzy logic

T-SNE

- probabilities

UMAP vs. T-SNE

UMAP

- graph theory, fuzzy logic
- deterministic initialization

T-SNE

- probabilities
- random initialization

UMAP vs. T-SNE

UMAP

- graph theory, fuzzy logic
- determinist initialization
- \log_2 similarity scores

T-SNE

- probabilities
- random initialization
- gaussian distribution similarity

UMAP vs. T-SNE

UMAP

- graph theory, fuzzy logic
 - determinist initialization
 - \log_2 similarity scores
 - update by pairs
- scales well for large datasets

T-SNE

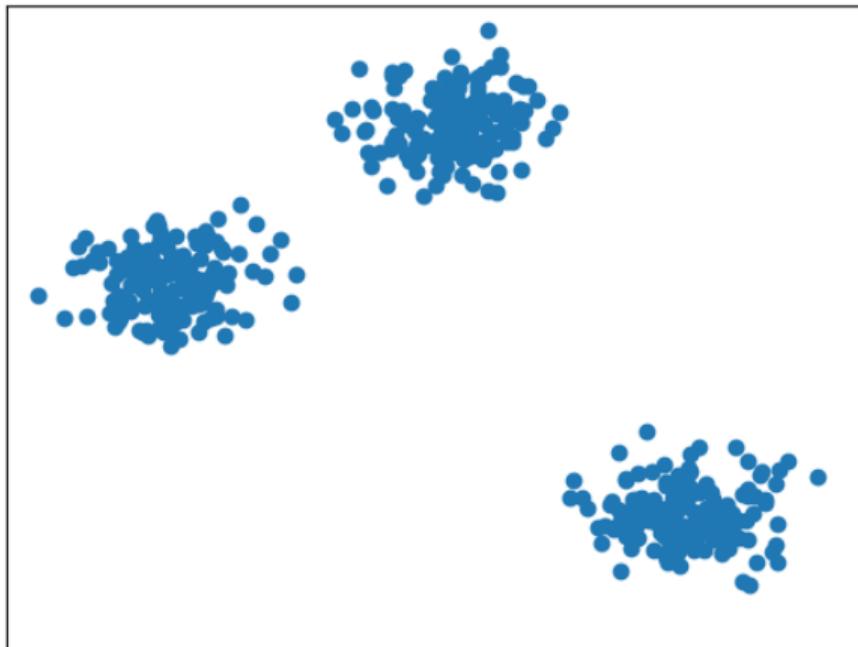
- probabilities
 - random initialization
 - gaussian distribution similarity
 - update all points
- scales less

Clustering

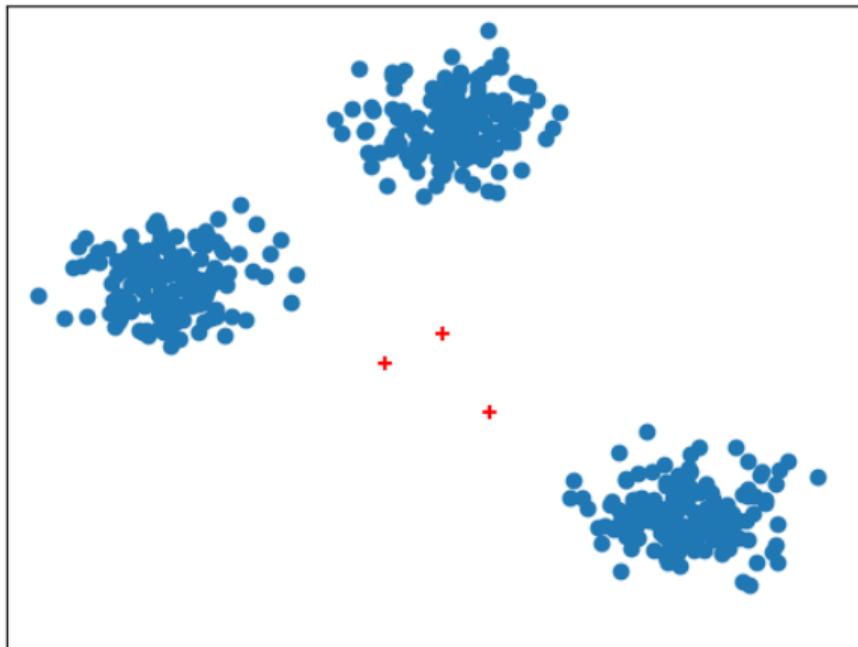
Clustering

K-means

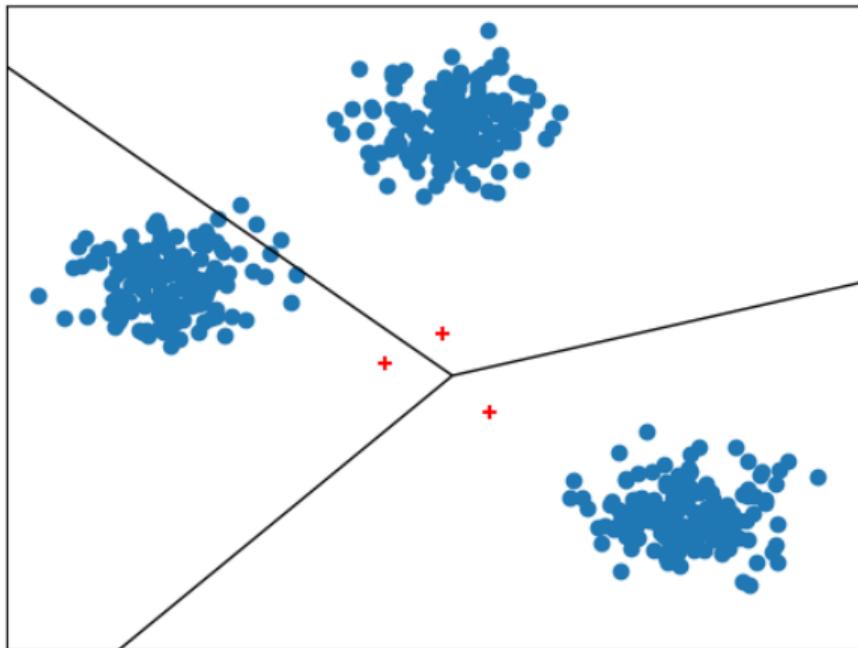
K-means



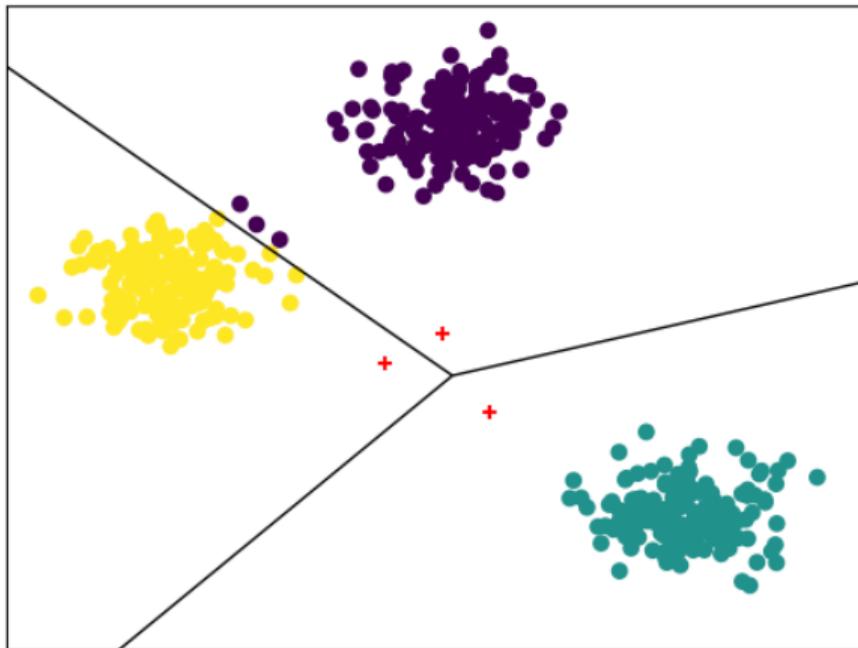
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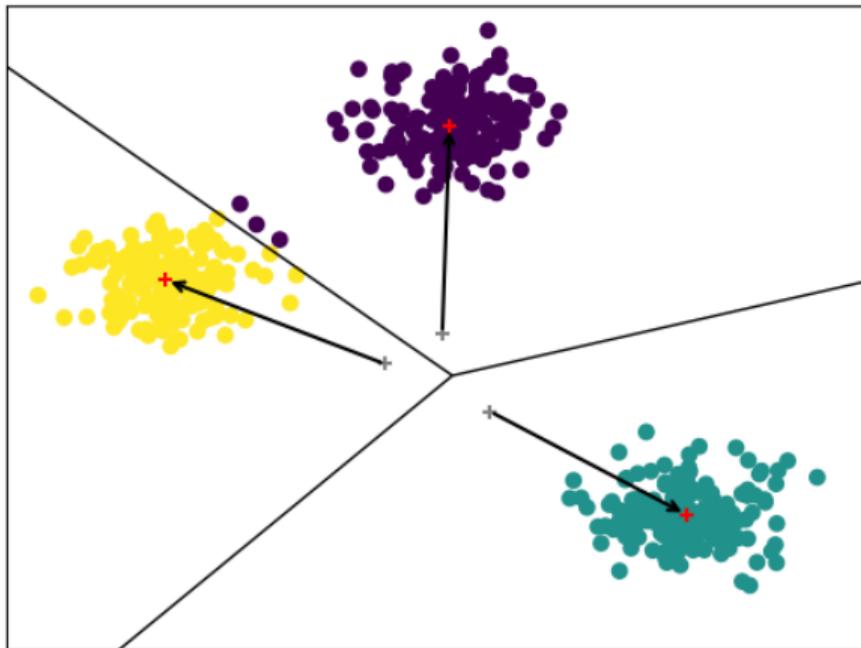
K-means



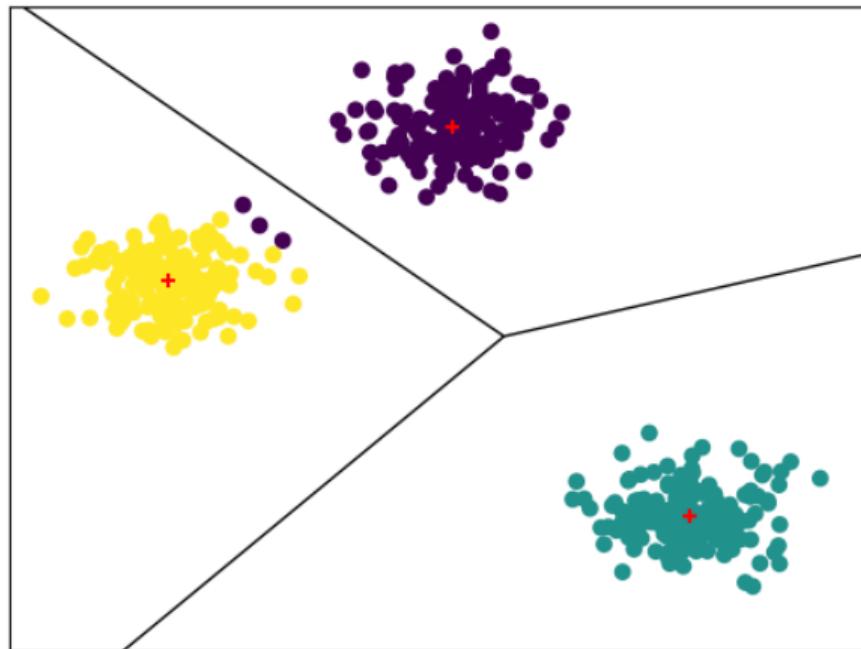
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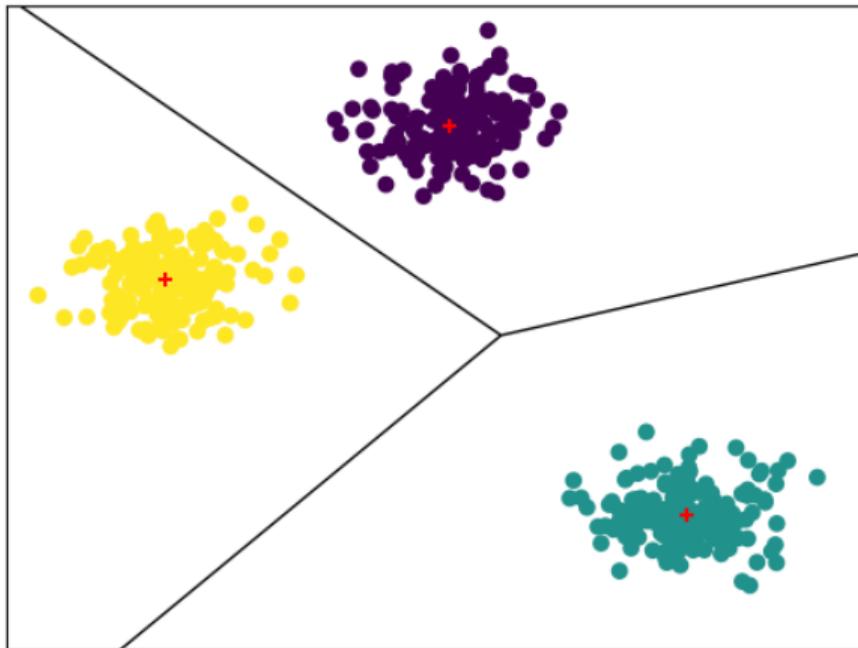
K-means



K-means



K-means



Determine the good K ? Elbow method

K-means advantages and drawbacks

Advantages

- fast

Drawbacks

K-means advantages and drawbacks

Advantages

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- scales well

Drawbacks

K-means advantages and drawbacks

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- scales well
- converges well

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K-means advantages and drawbacks

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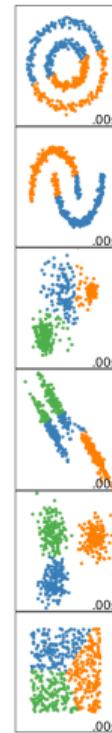
K-means advantages and drawbacks

Advantages

- fast
- scales well
- converges well
- robust

Drawbacks

- **not suited for non-linear data**



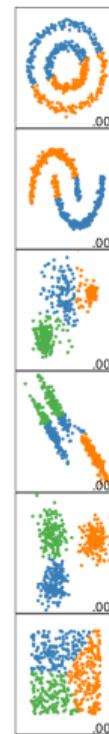
K-means advantages and drawbacks

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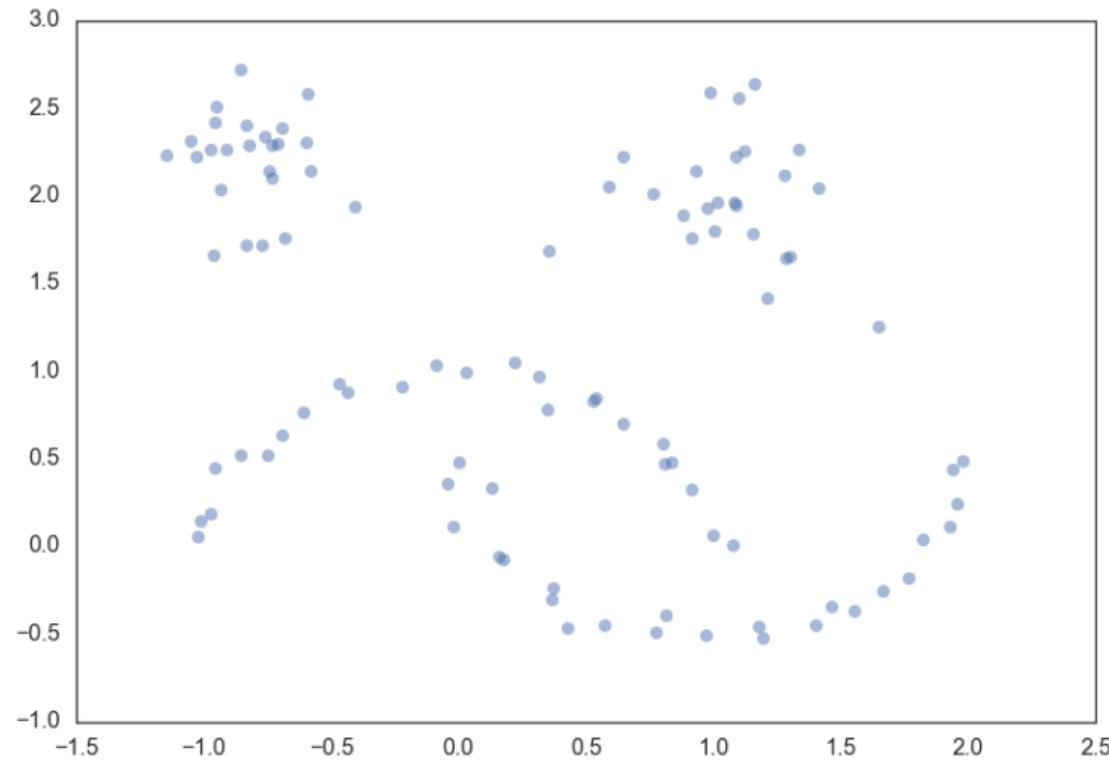
- **not suited for non-linear data**
→ Density based clustering



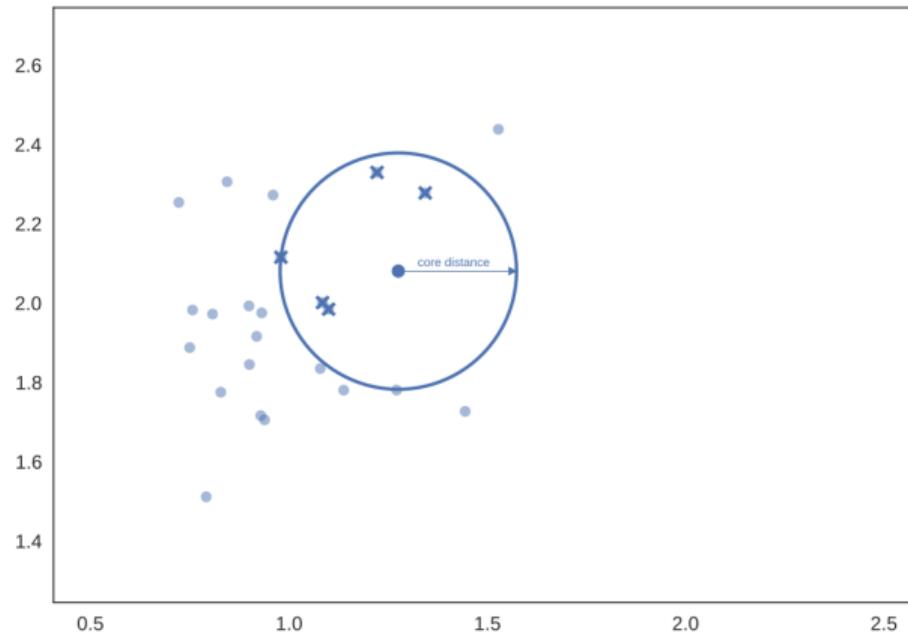
Clustering

HDBSCAN

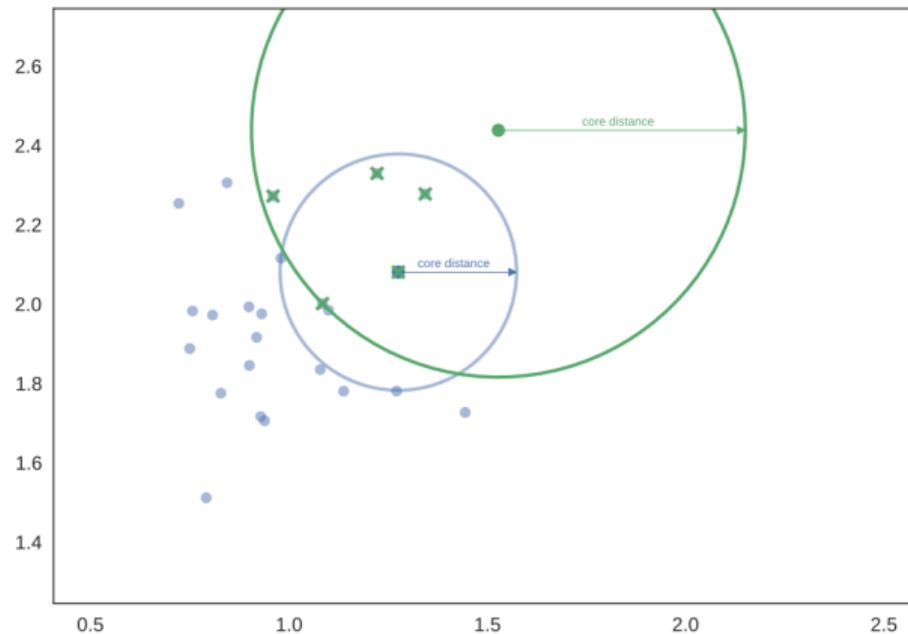
HDBSCAN



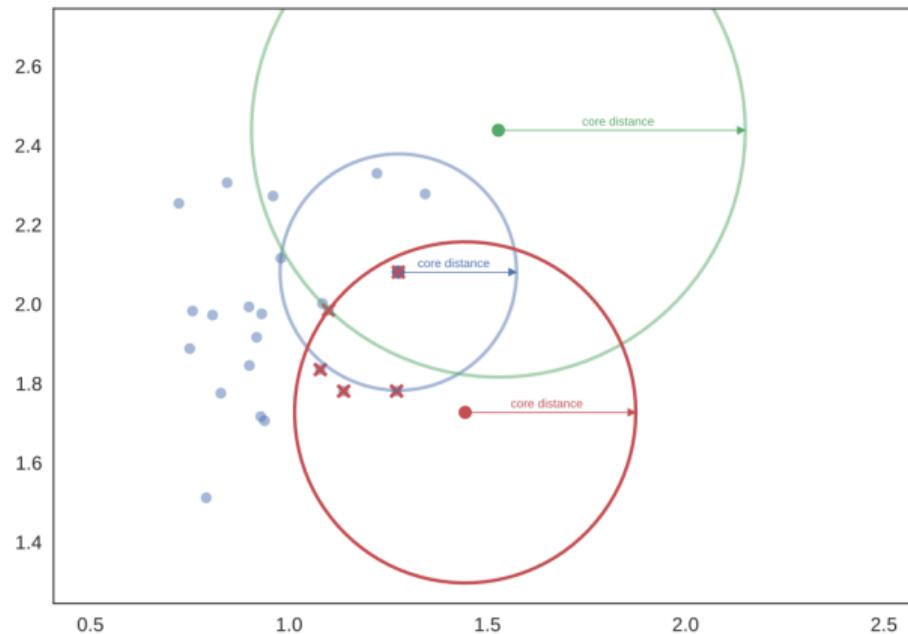
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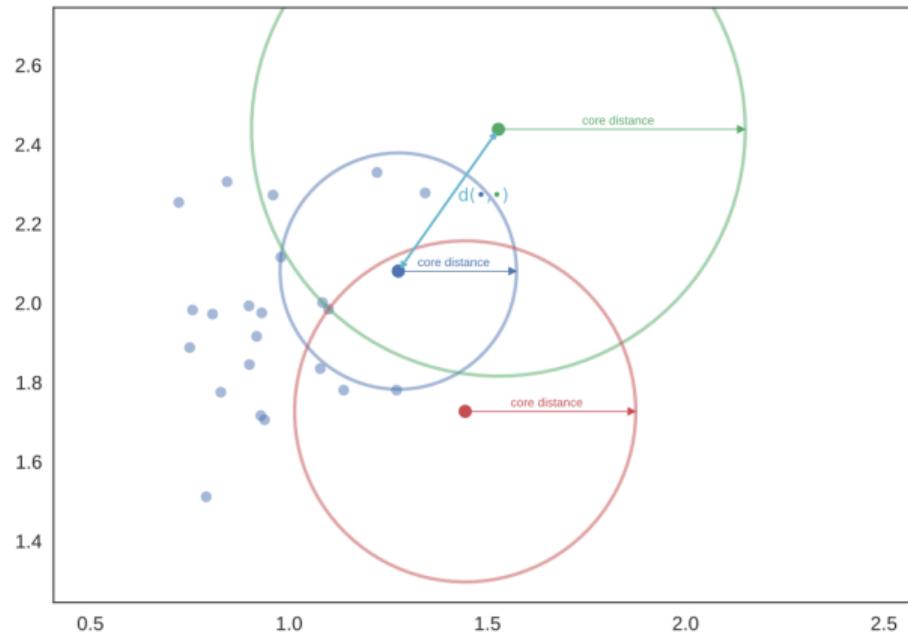
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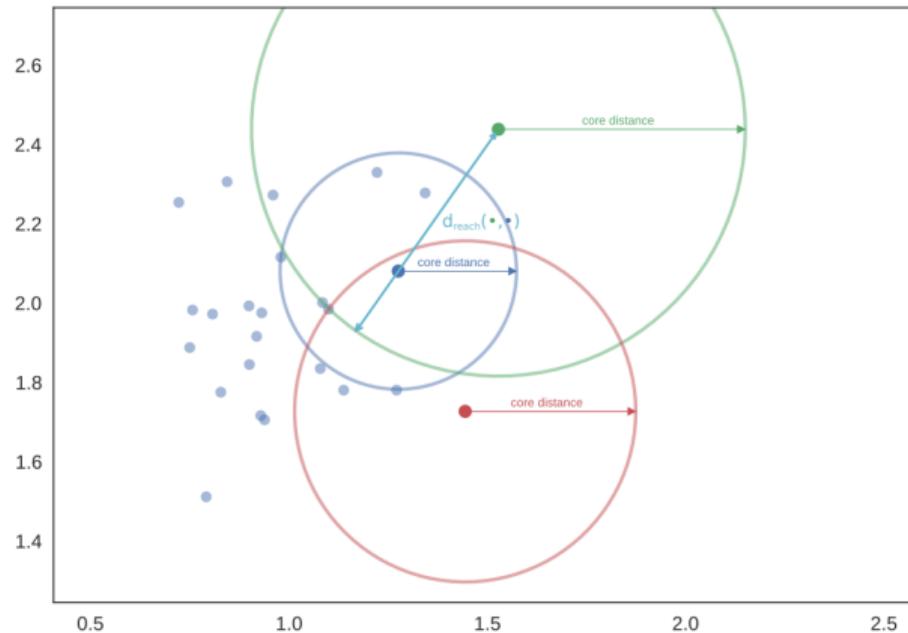
HDBSCAN



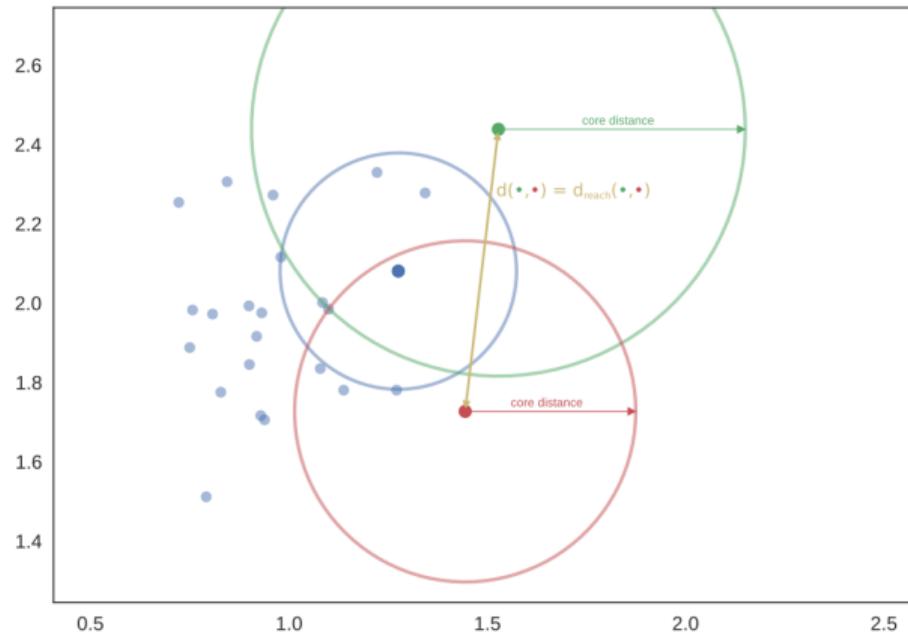
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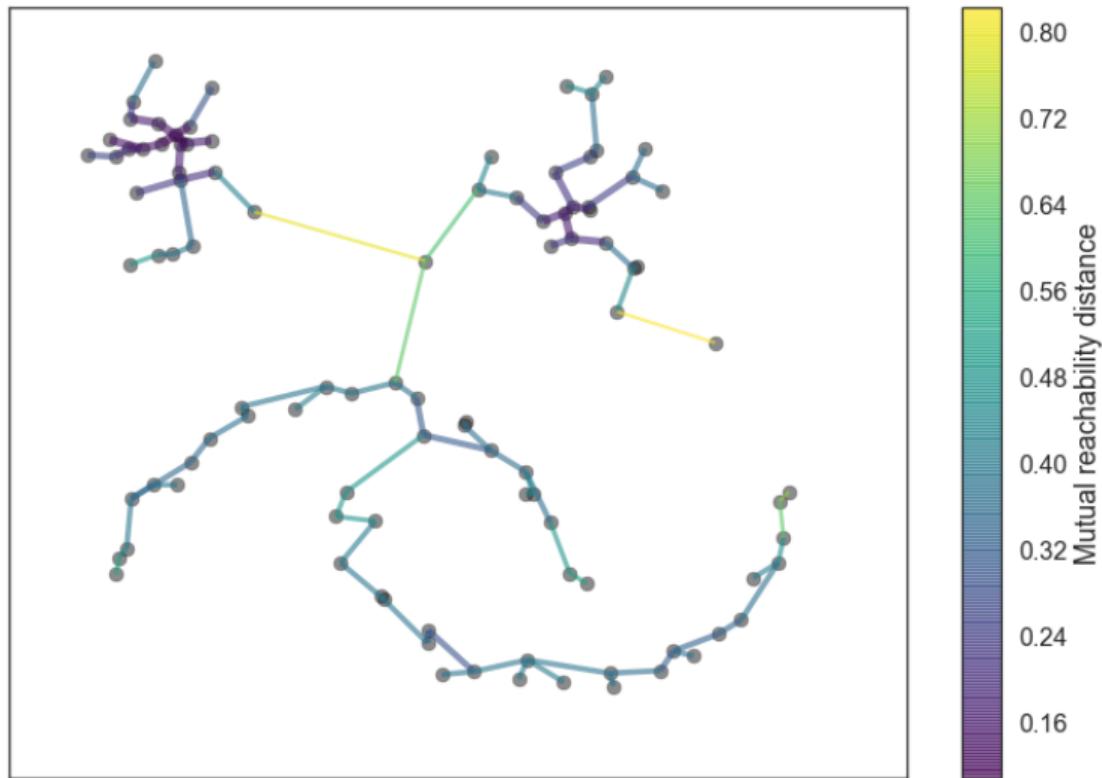
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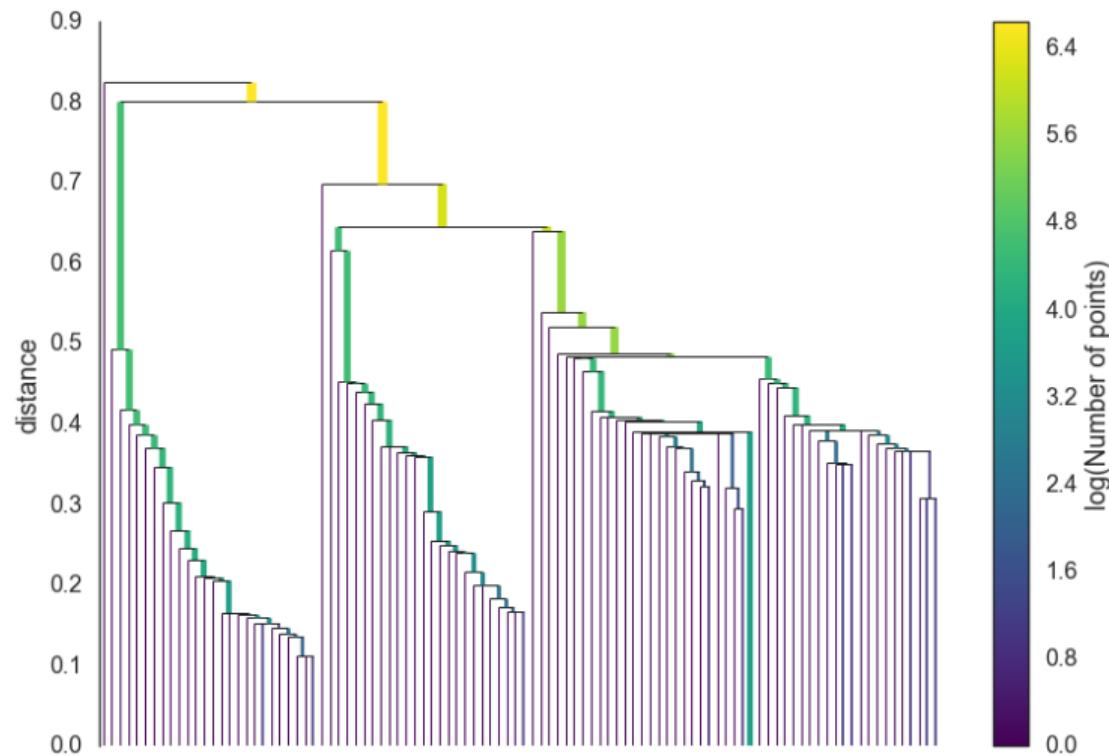
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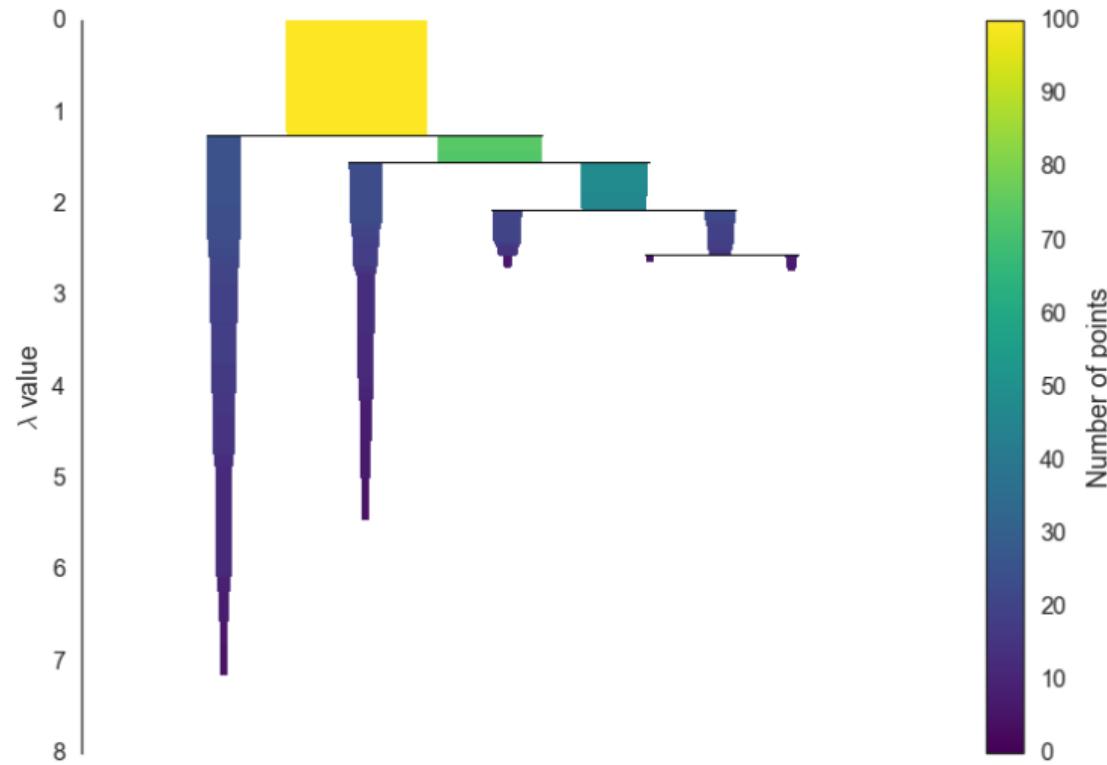
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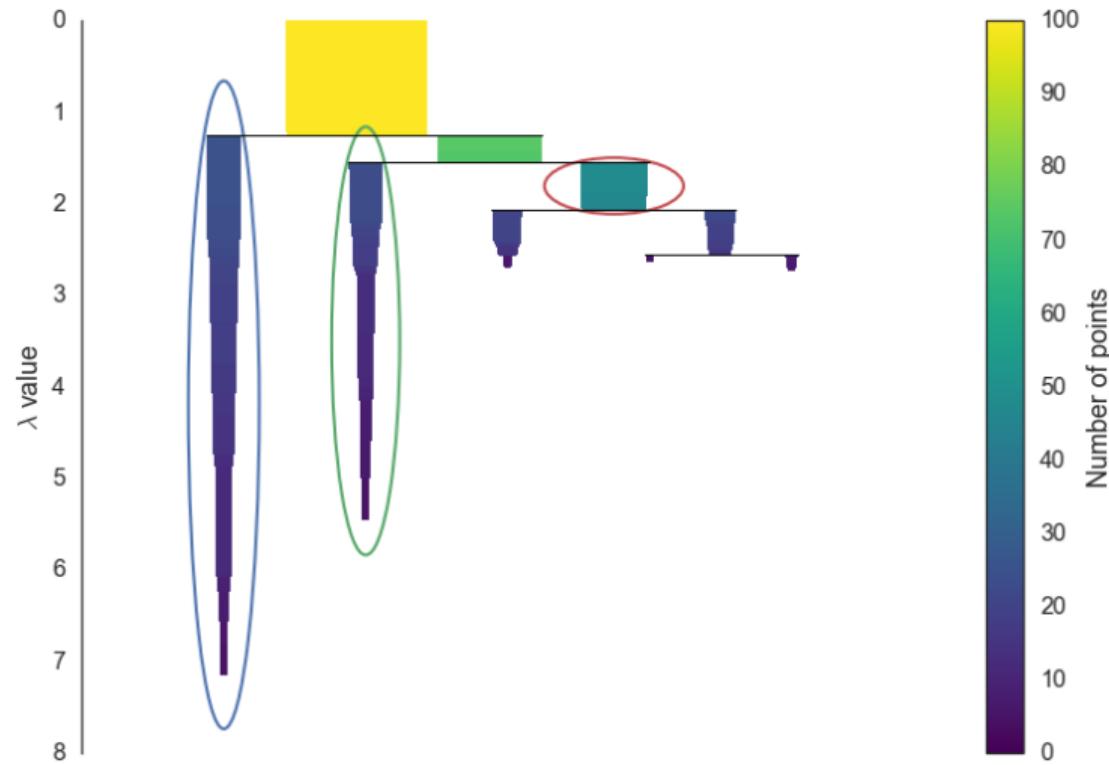
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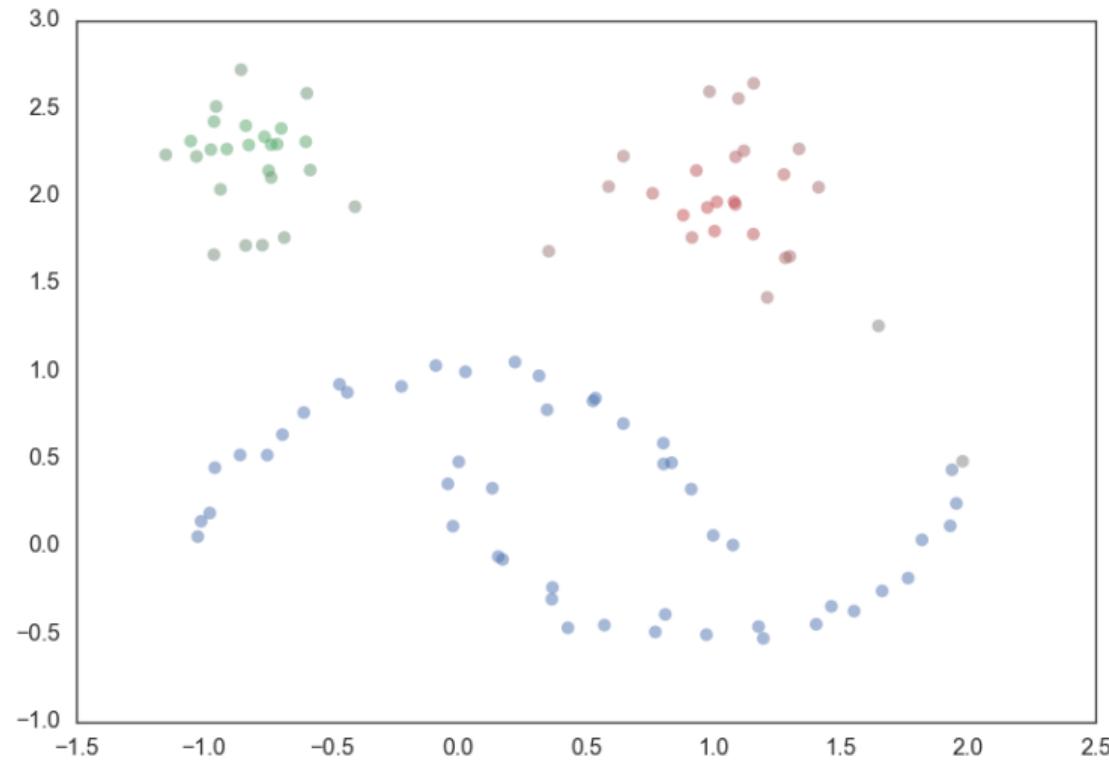
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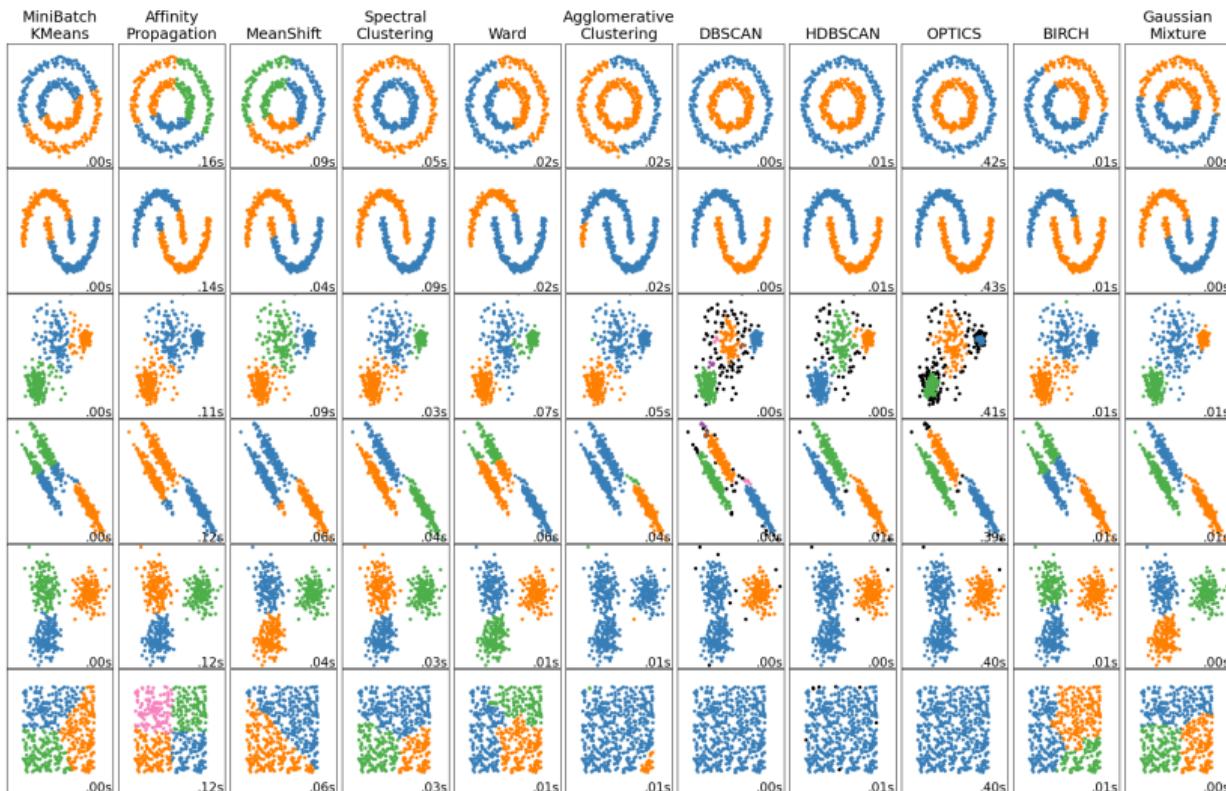
HDBSCAN



HDBSCAN



A lot of options !



Usefull ressources

- scikit-learn docs !
- deepia
- StatQuest

Thanks for you attention !

Let's practice !

References i

- Du, Trina Y (2019). “**Dimensionality reduction techniques for visualizing morphometric data: Comparing principal component analysis to nonlinear methods**”. In: *Evolutionary Biology* 46.1, pp. 106–121.
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