

Projections and clusterings

Formation IA biodiversité

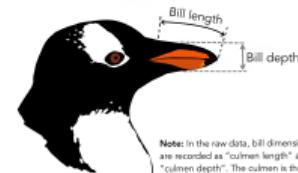
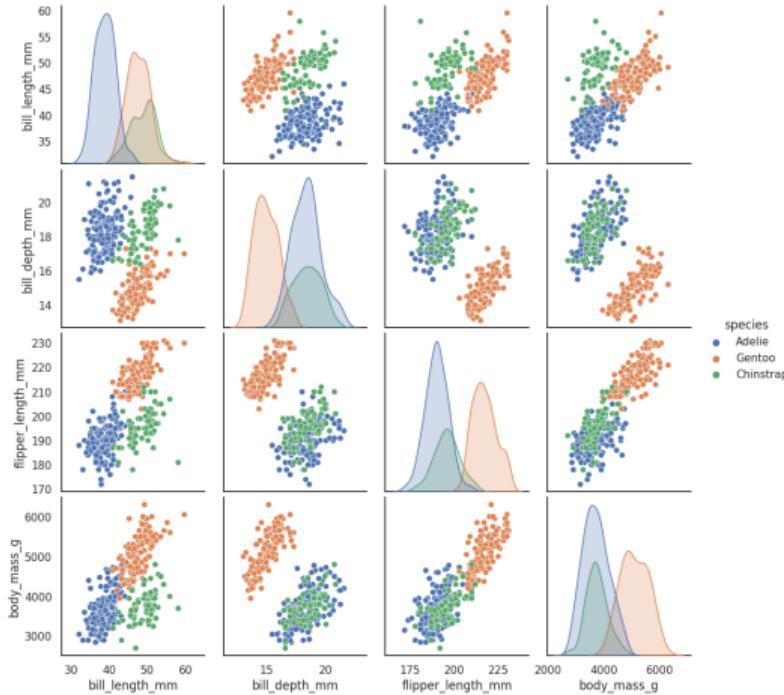
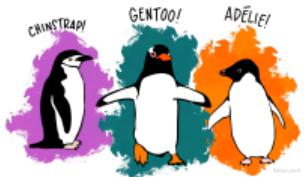
Paul Tresson

May 14, 2025

UMR AMAP

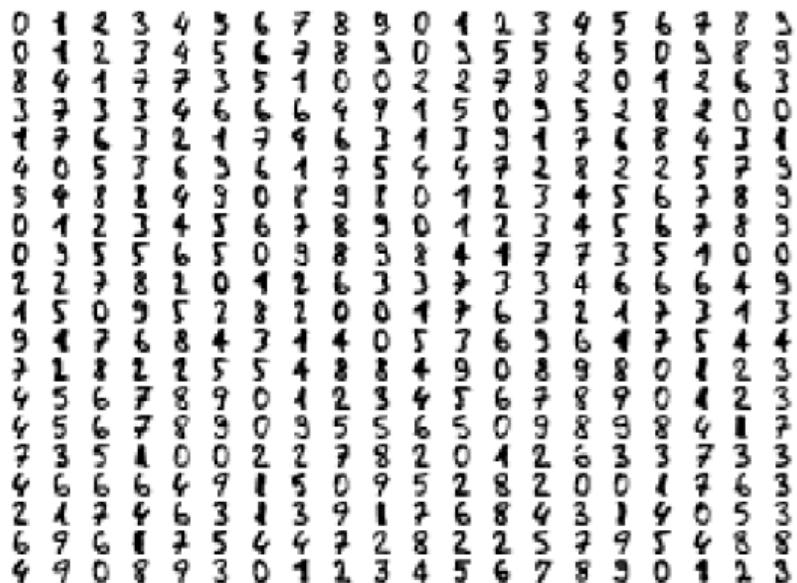
Introduction

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.

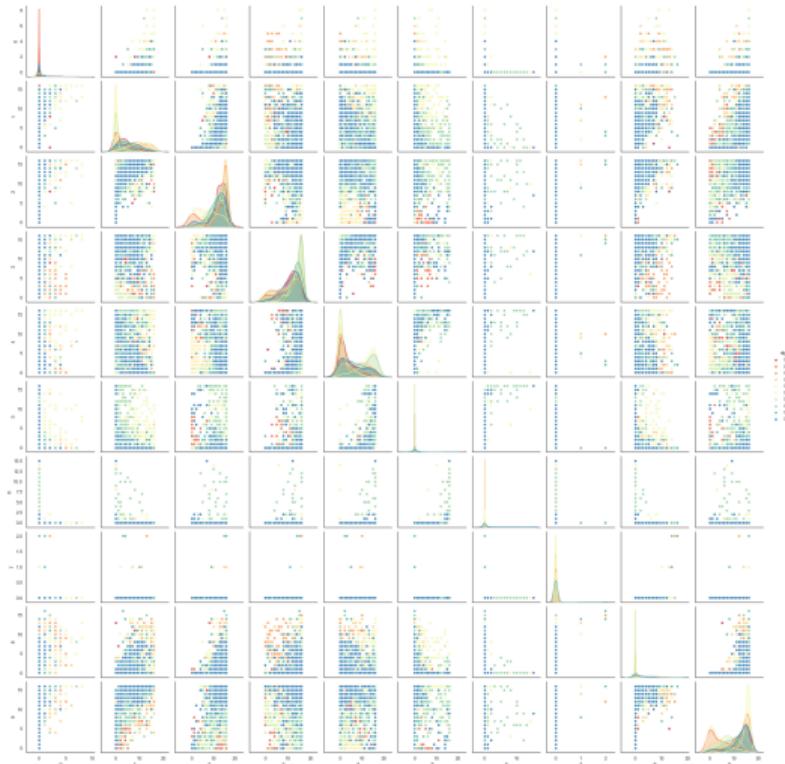
Visualize what is happening in higher dimensions



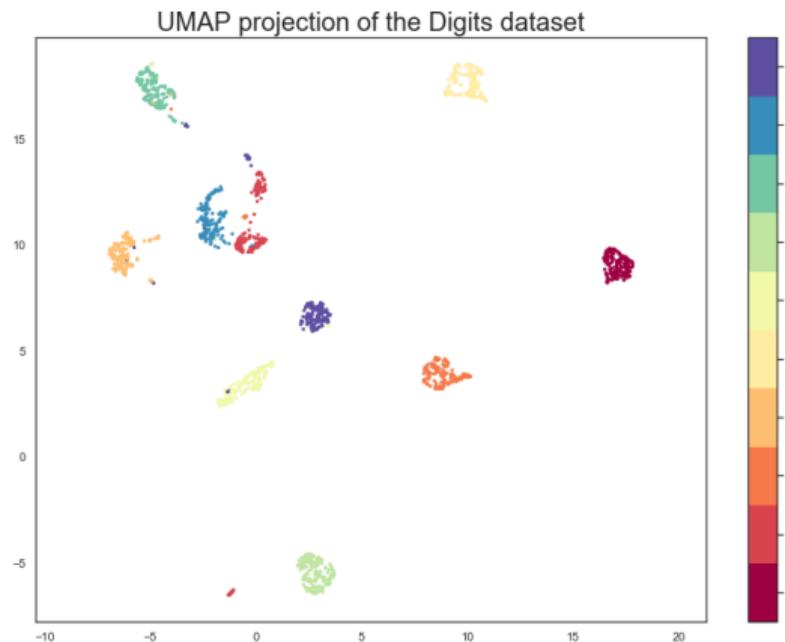
A 10x10 grid of numbers from 0 to 9, arranged in a pattern that suggests a 2D visualization of a 10-dimensional dataset. The numbers are distributed in a non-uniform, somewhat diagonal pattern across the grid.

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

Visualize what is happening in higher dimensions



Visualize what is happening in higher dimensions

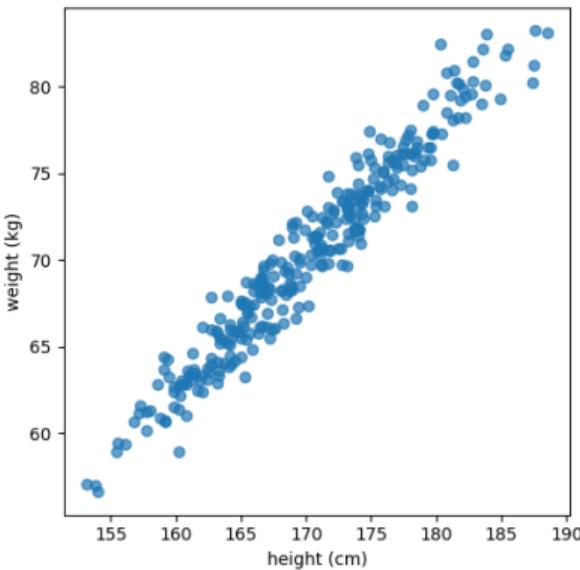


Projections

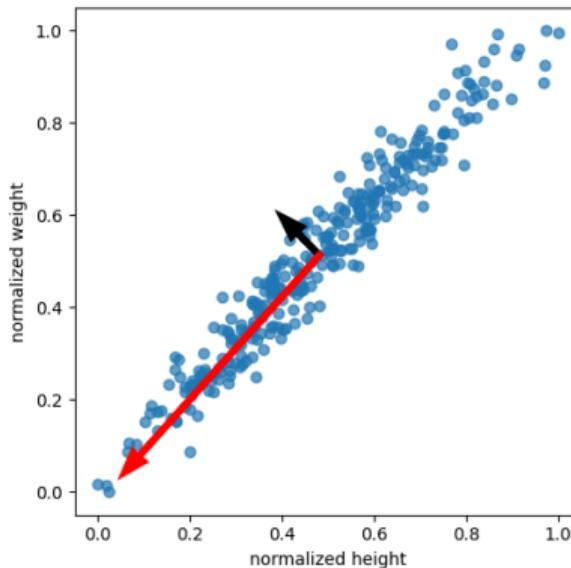
Projections

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

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- scales well

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PCA advantages and drawbacks

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PCA advantages and drawbacks

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Drawbacks

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

Non linear data

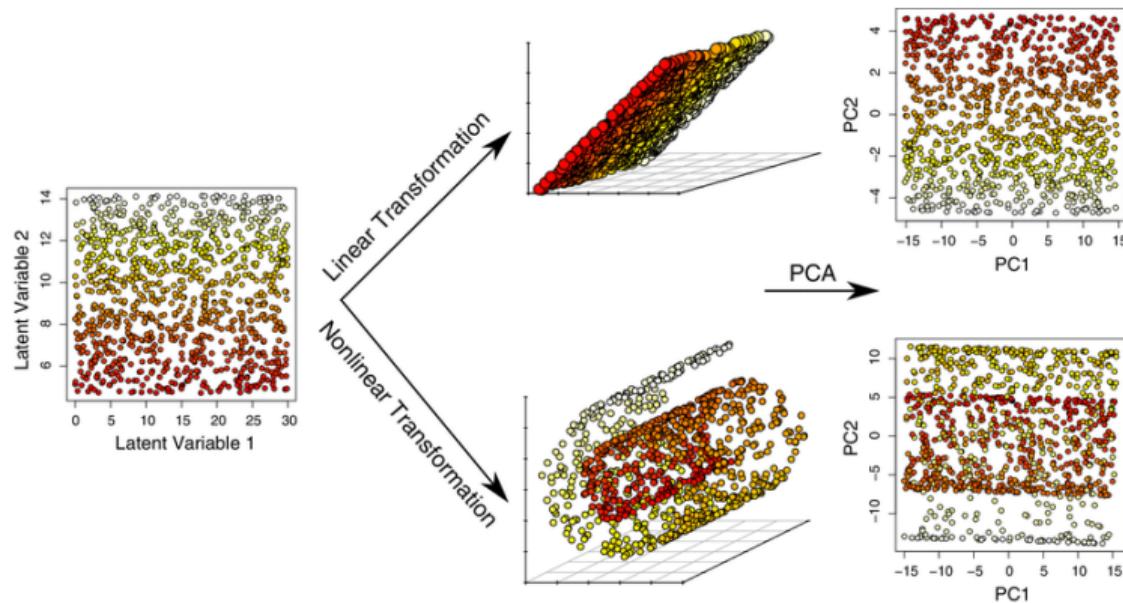


Figure from Du, 2019

Projections

UMAP

How to work with non linear data

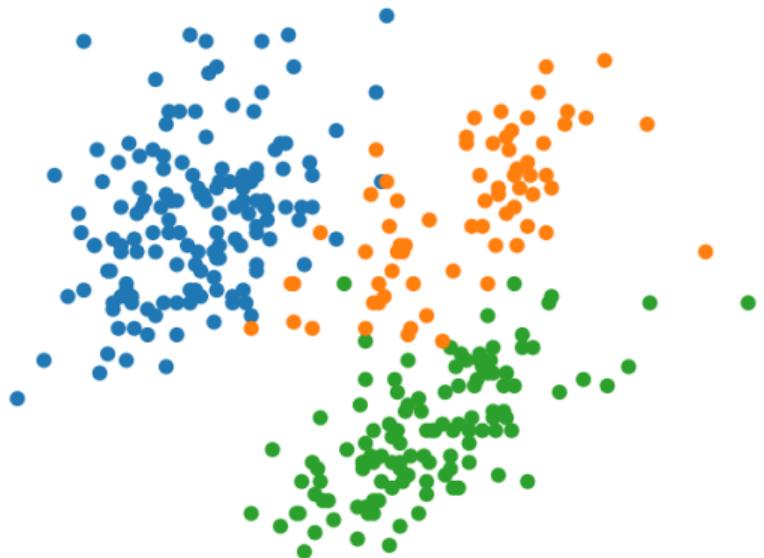
1. Find a good representation of the data in high dimension
2. Fit a good representation of in low dimension

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

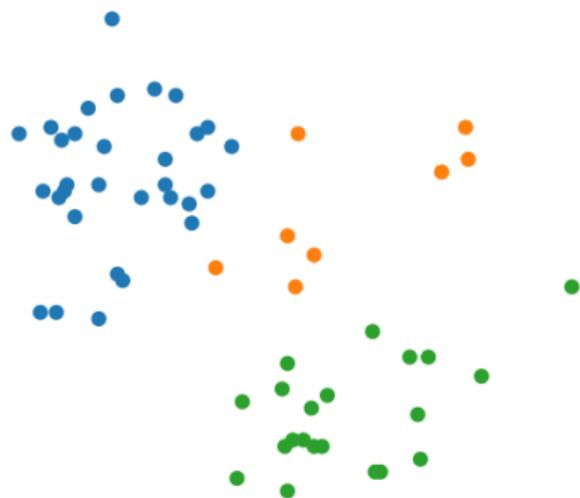
- **SNE** (Stochastic Neighbor Embedding) Hinton and Roweis, 2002
- **T-SNE** (T-distributed SNE) Van der Maaten and Hinton, 2008

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

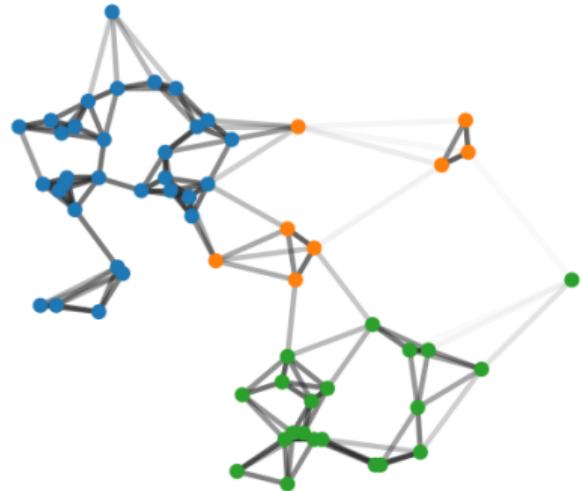
UMAP : Finding high dimension graph



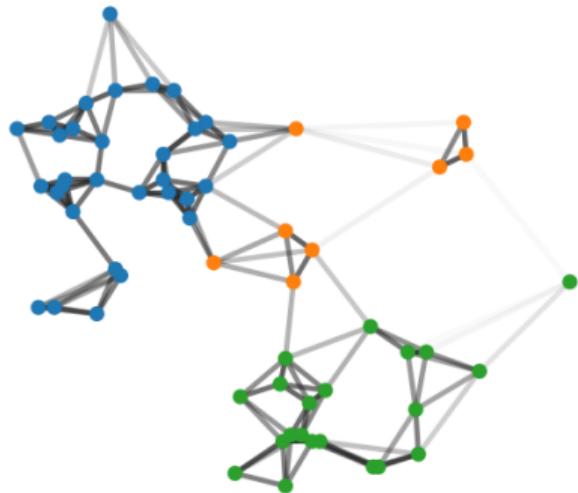
UMAP : Finding high dimension graph



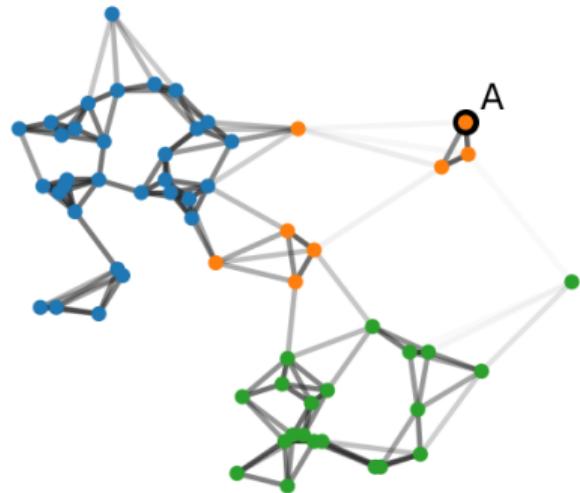
UMAP : Finding high dimension graph



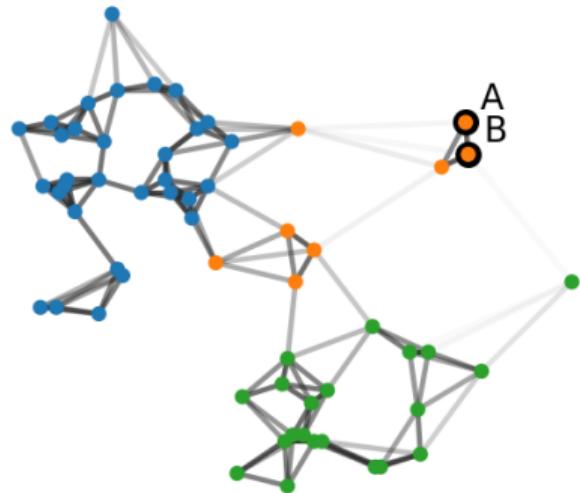
UMAP : Fitting low dimensional representation



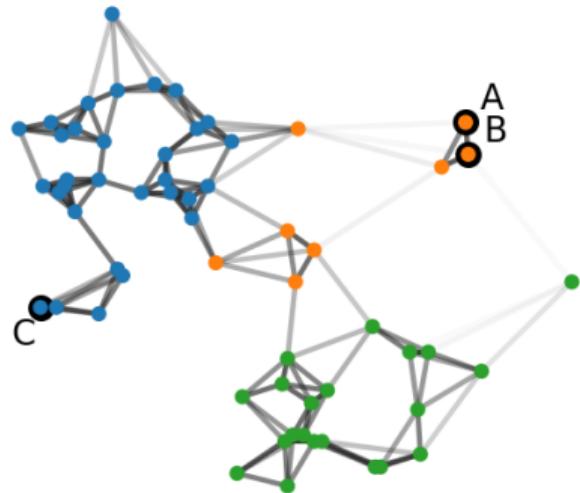
UMAP : Fitting low dimensional representation



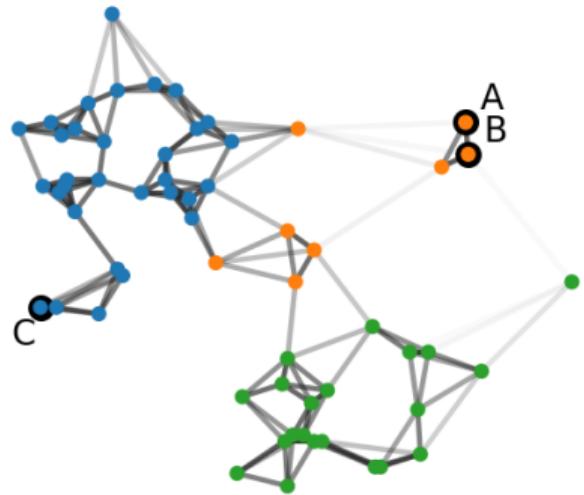
UMAP : Fitting low dimensional representation



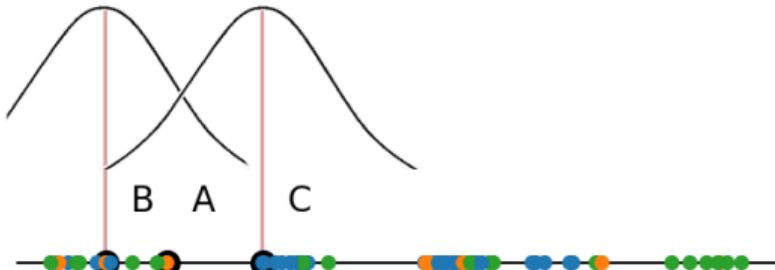
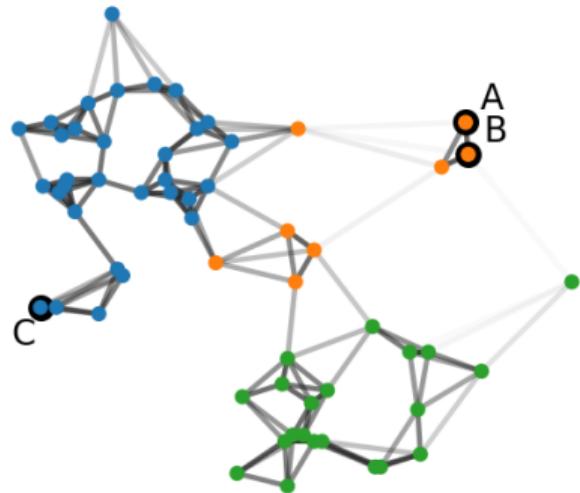
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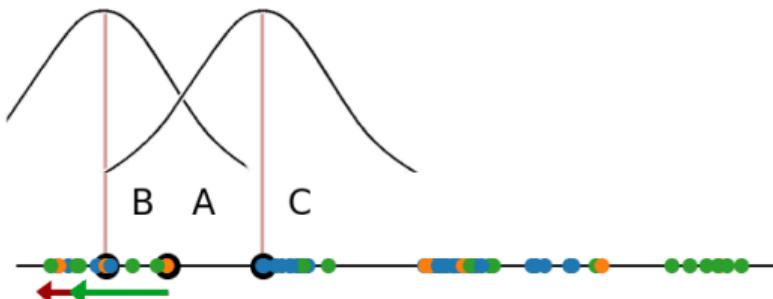
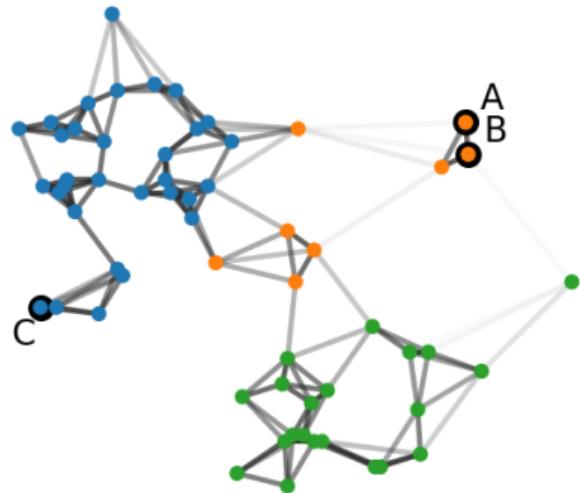
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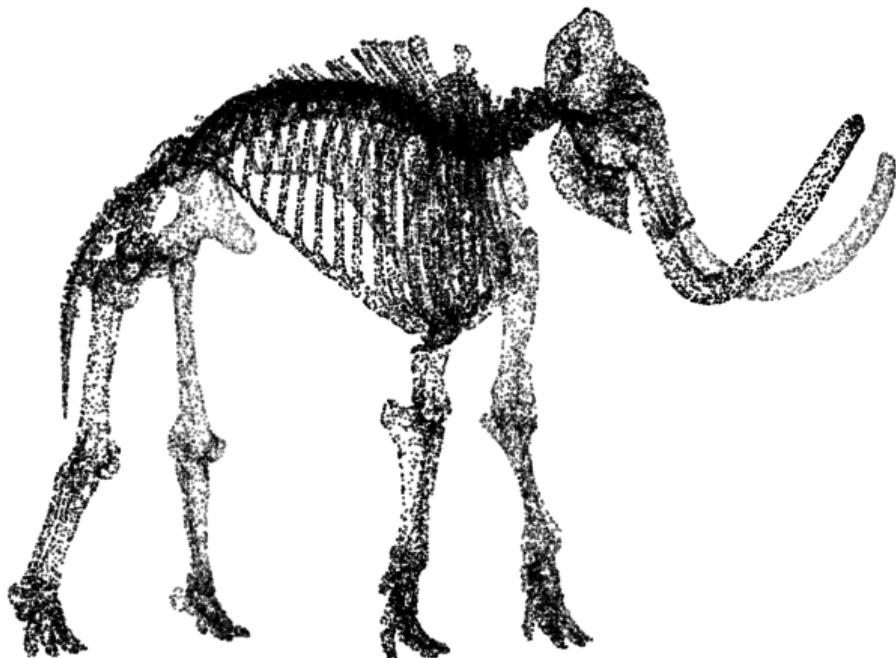
UMAP : Fitting low dimensional representation



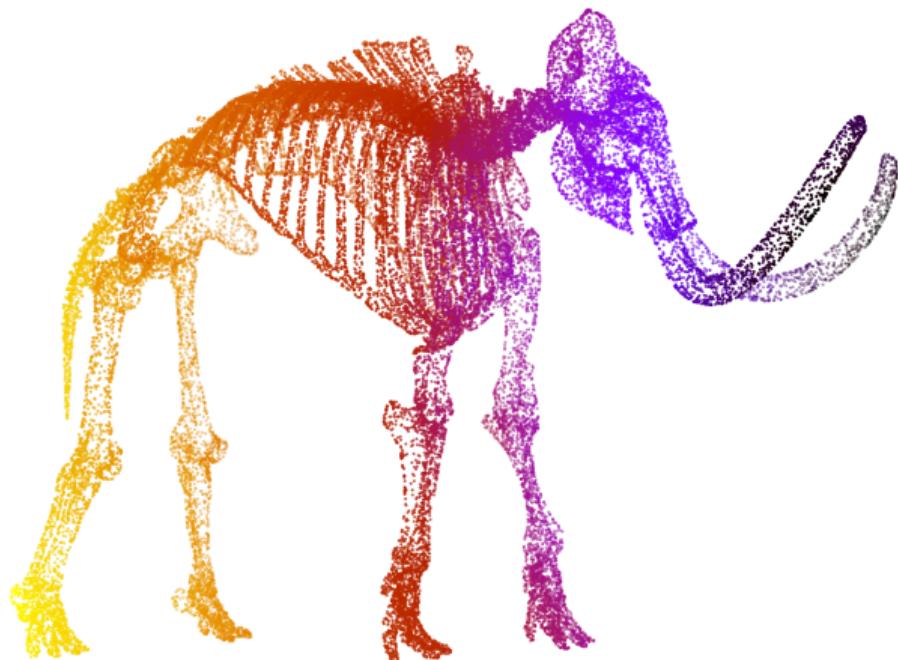
UMAP : Fitting low dimensional representation



Mammoth example



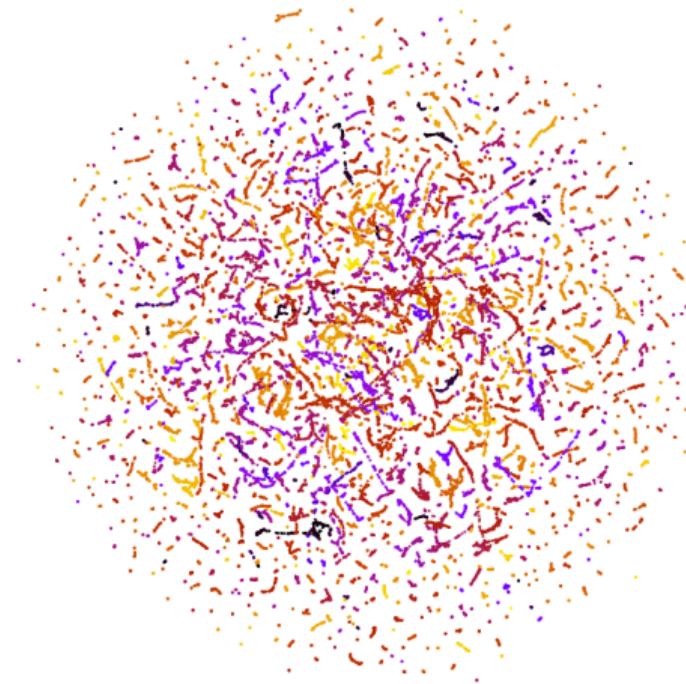
Mammoth example



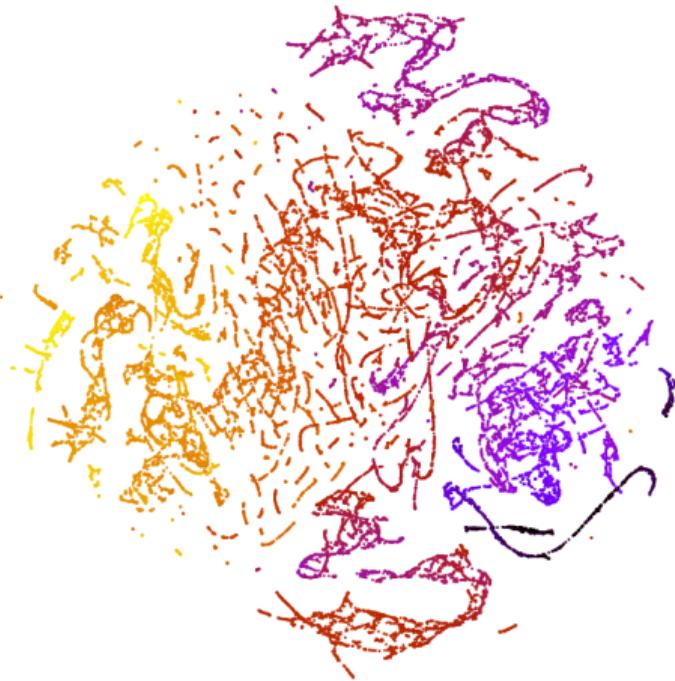
Mammoth example - PCA



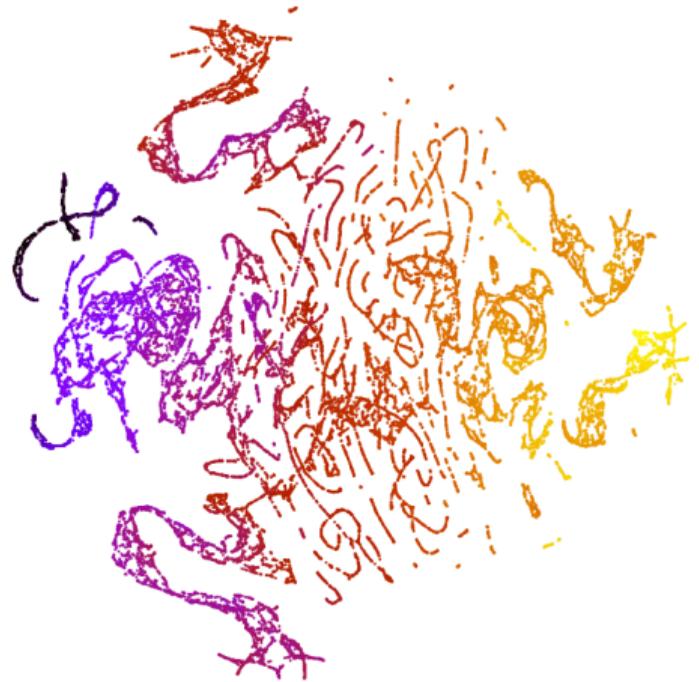
Mammoth example - UMAP



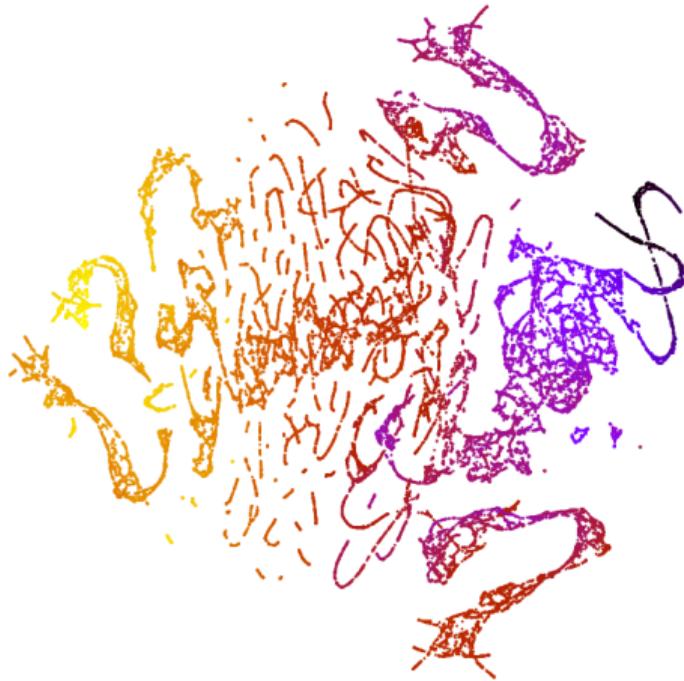
Mammoth example - UMAP



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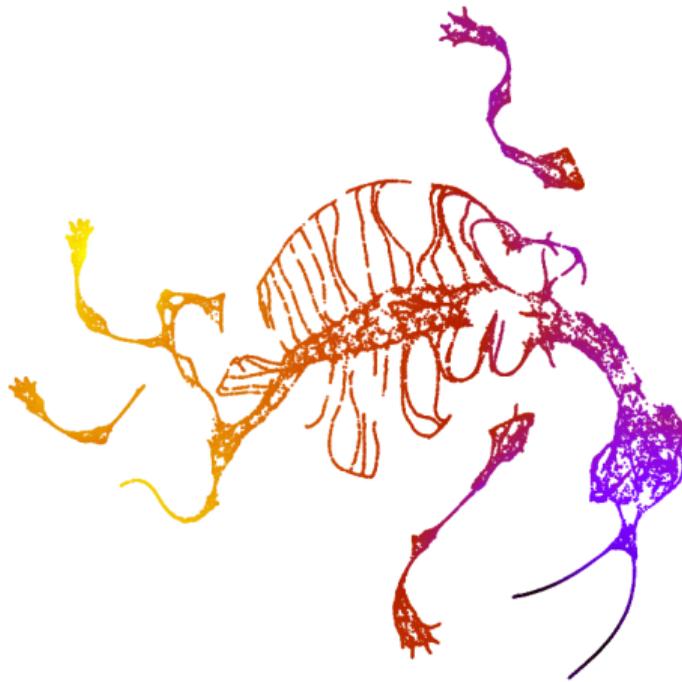
Mammoth example - UMAP



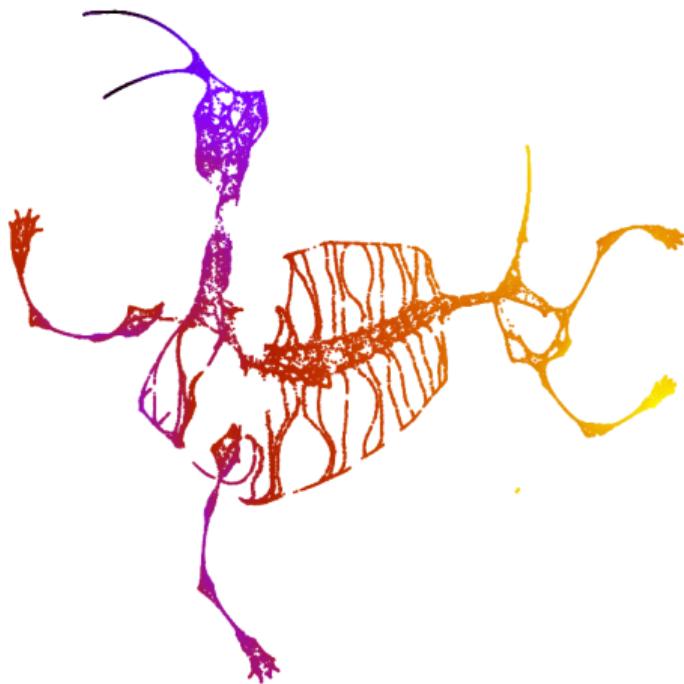
Mammoth example - UMAP



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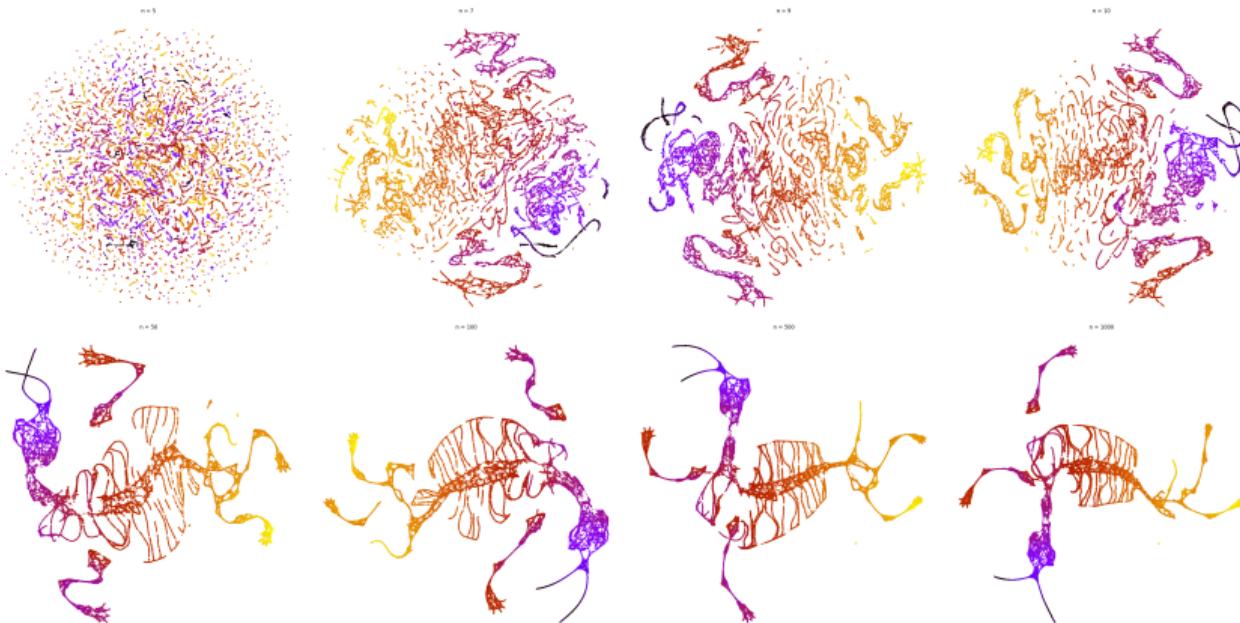
Mammoth example - UMAP



Mammoth example - UMAP



Mammoth example - Number of neighbors



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

Scaling

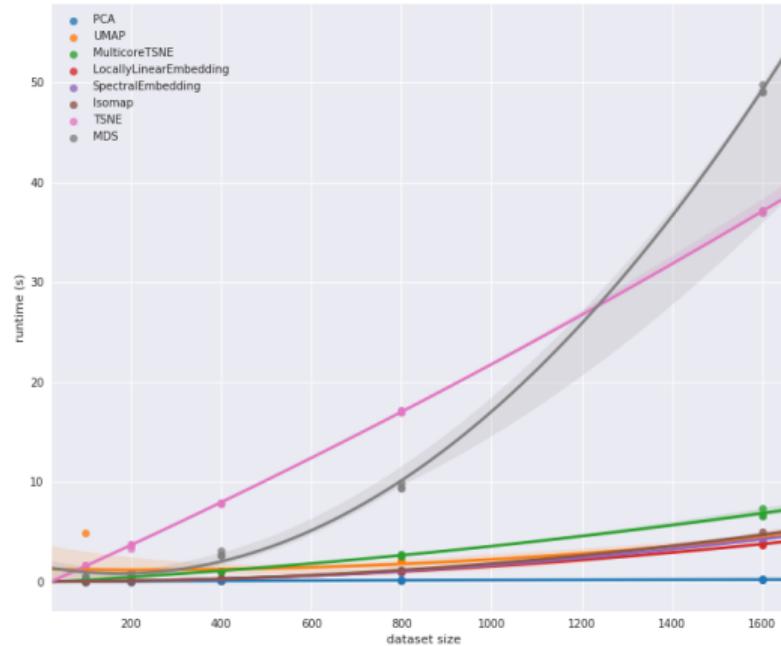


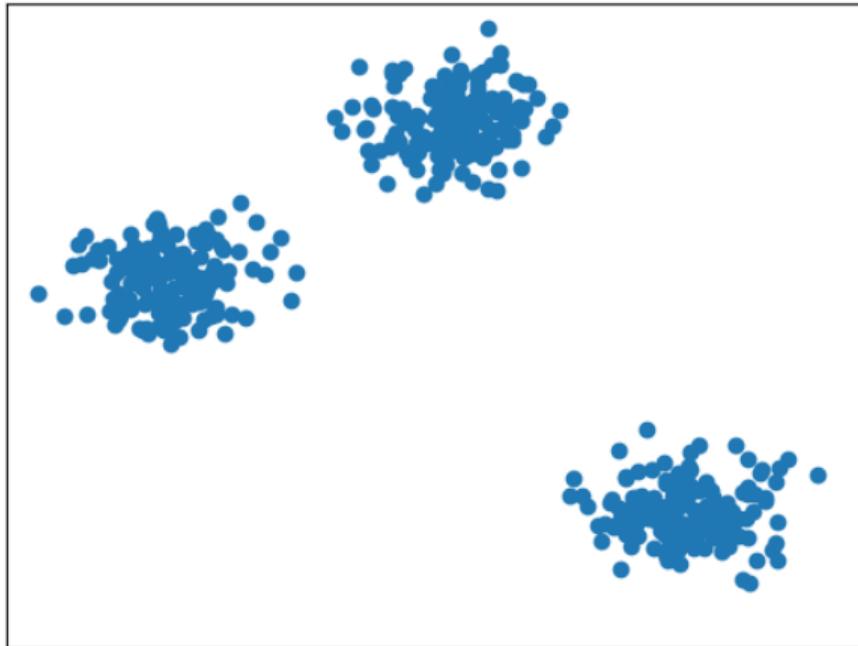
Figure from umap-learn documentation

Clustering

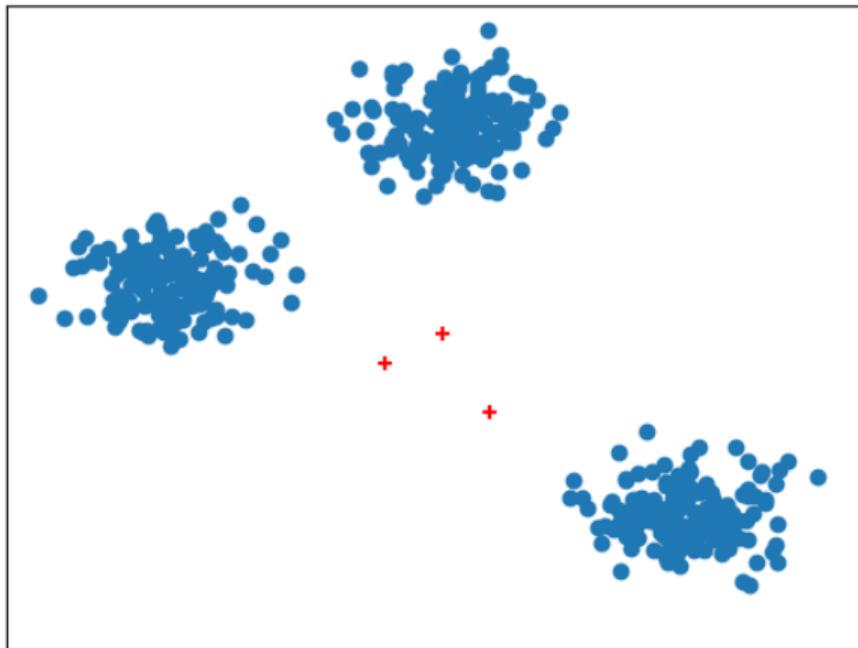
Clustering

K-means

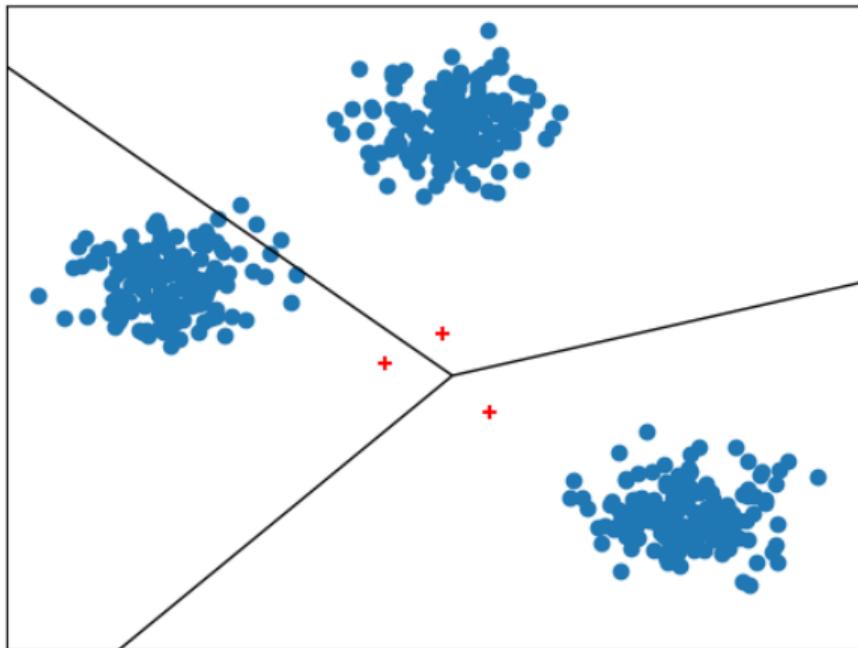
K-means



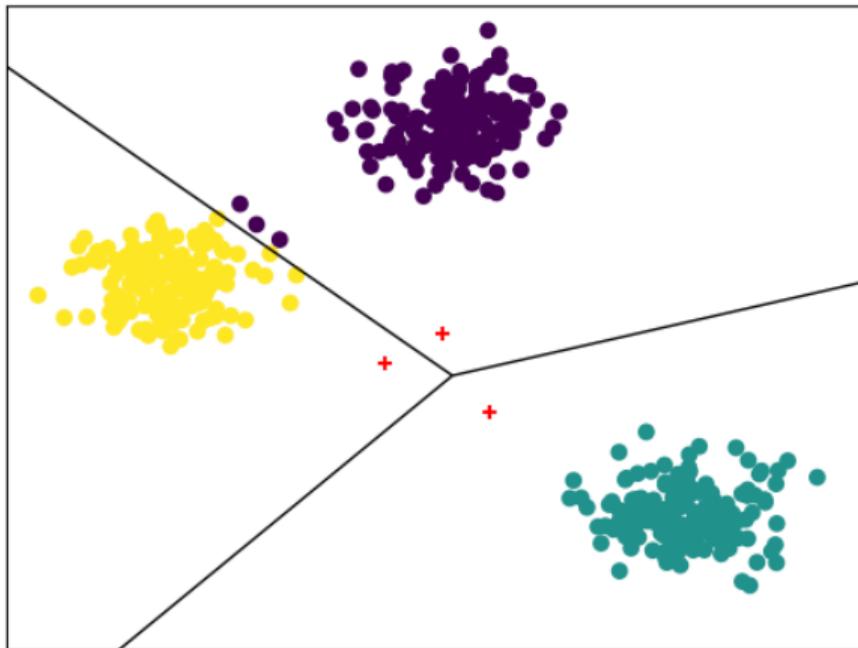
K-means



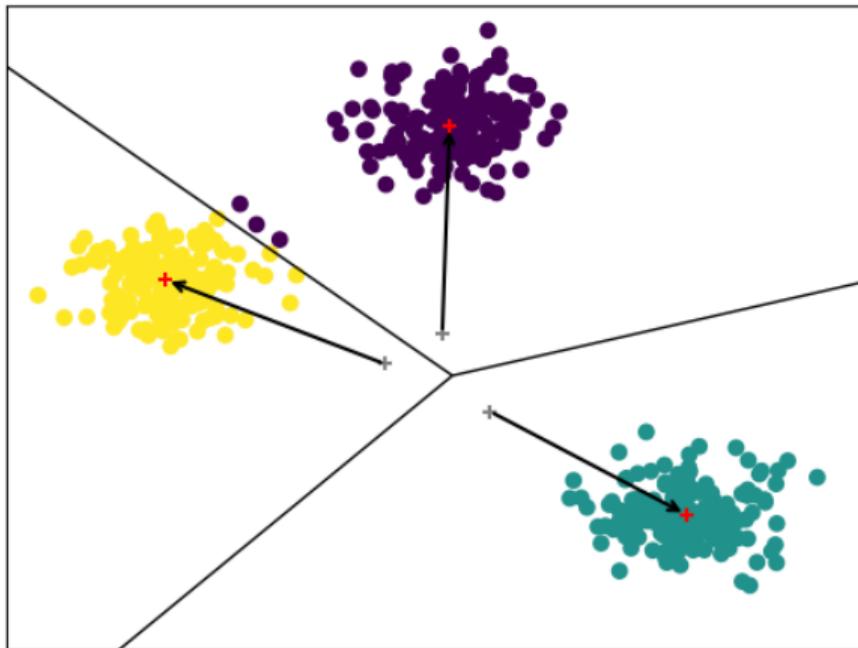
K-means



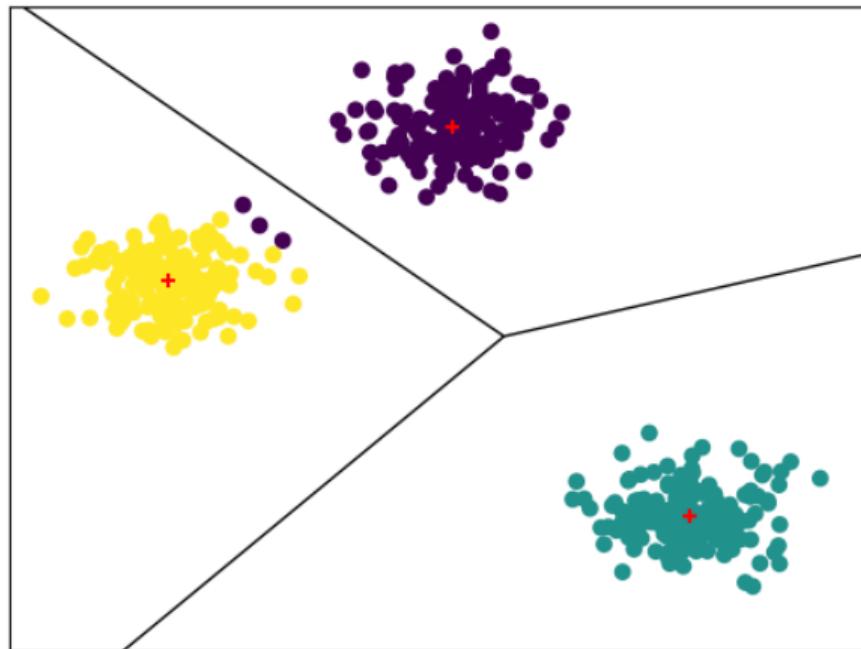
K-means



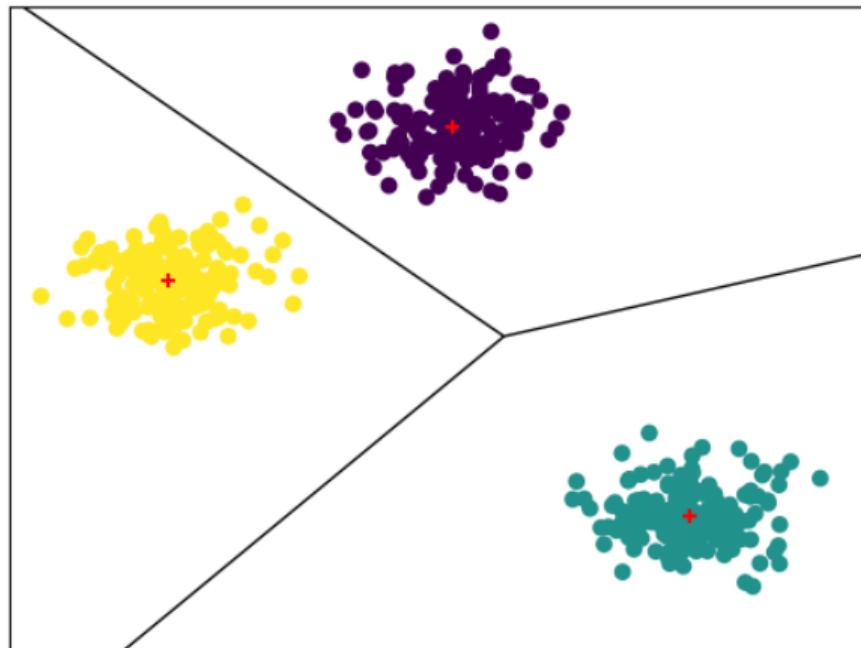
K-means



K-means



K-means



Determine the good K ? Elbow method

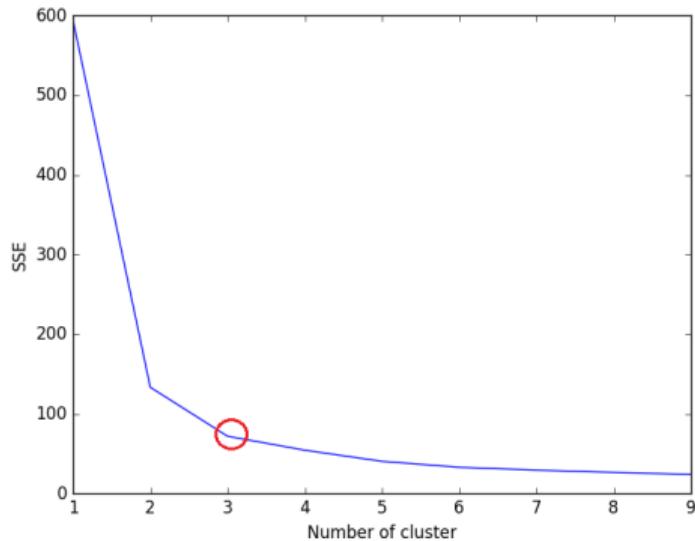
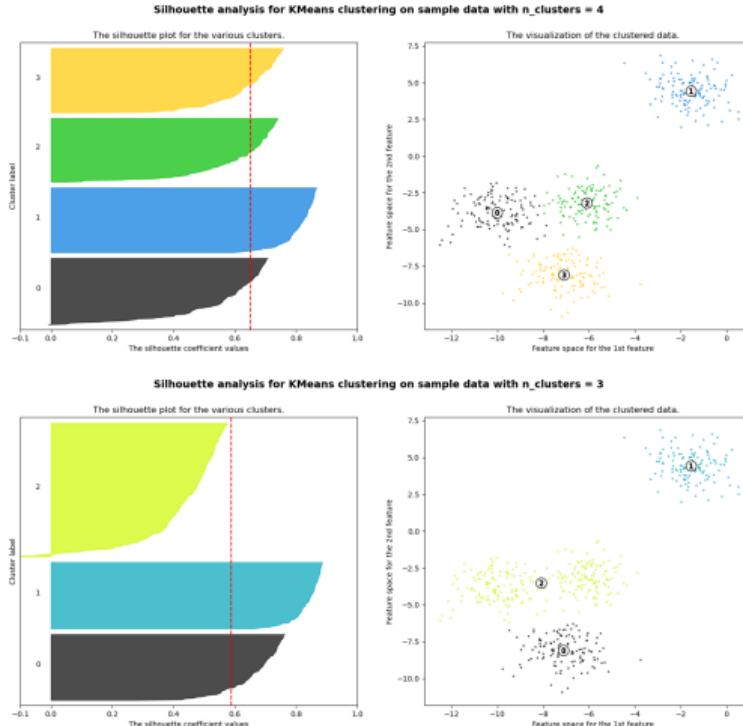


Figure from SO

Determine the good K ? Silhouette



Figures from scikit-learn documentation

K-means advantages and drawbacks

Advantages

- fast

Drawbacks

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- scales well

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K-means advantages and drawbacks

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- fast
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K-means advantages and drawbacks

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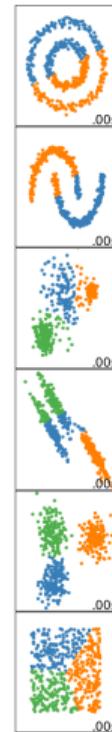
K-means advantages and drawbacks

Advantages

- fast
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- robust

Drawbacks

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



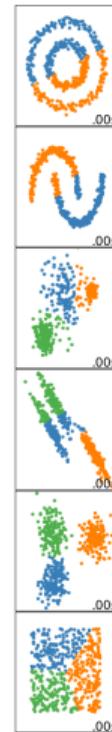
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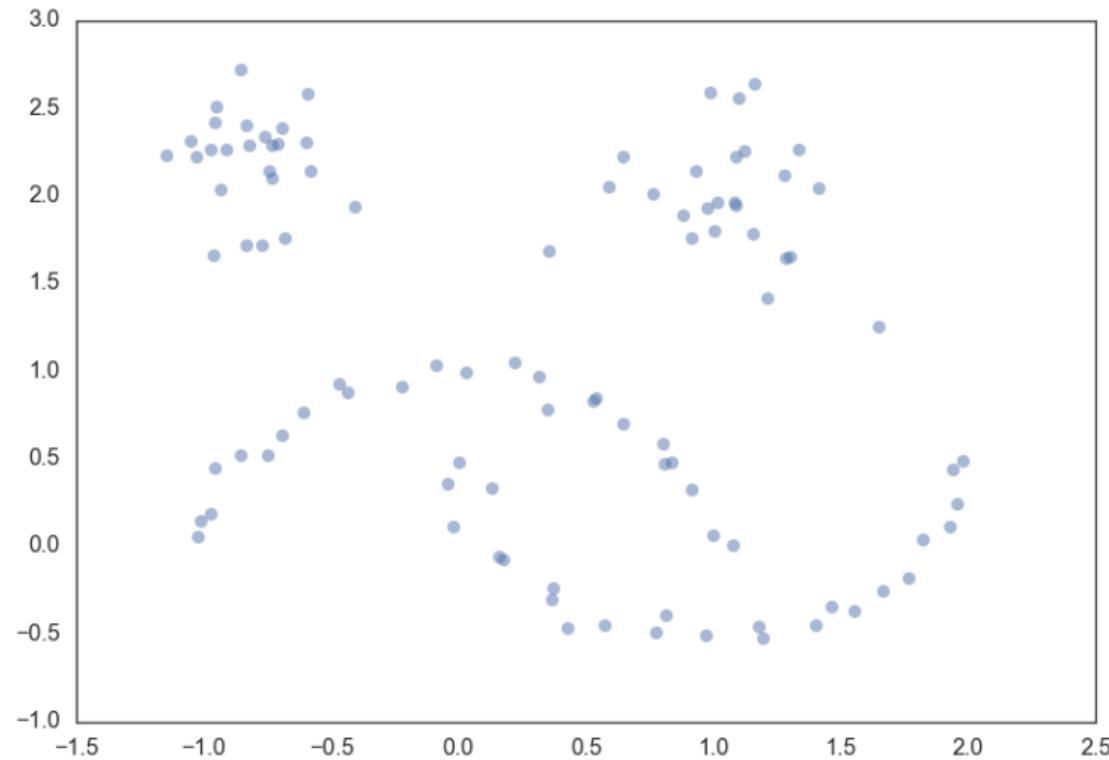
- **not suited for non-linear data**
→ Density based clustering



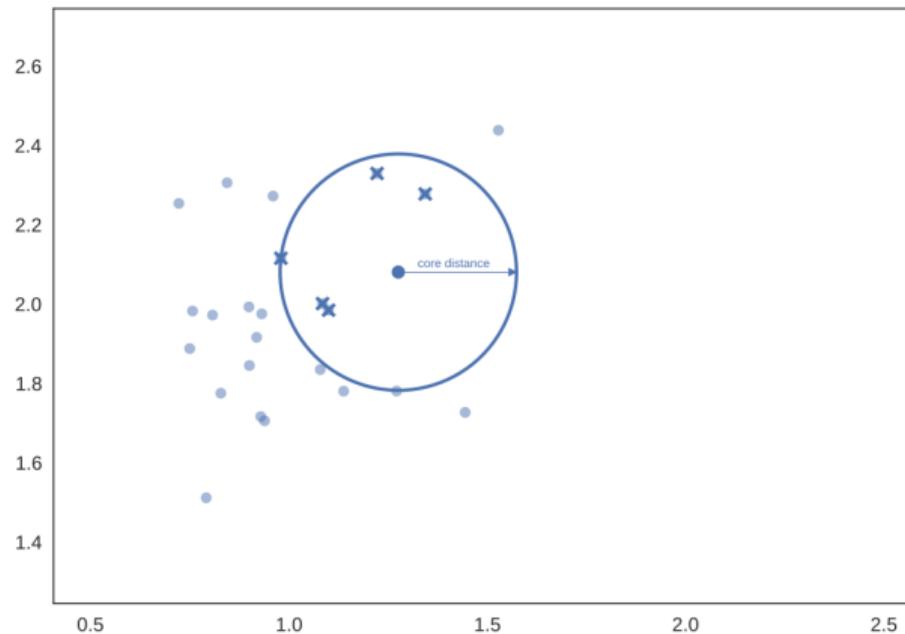
Clustering

HDBSCAN

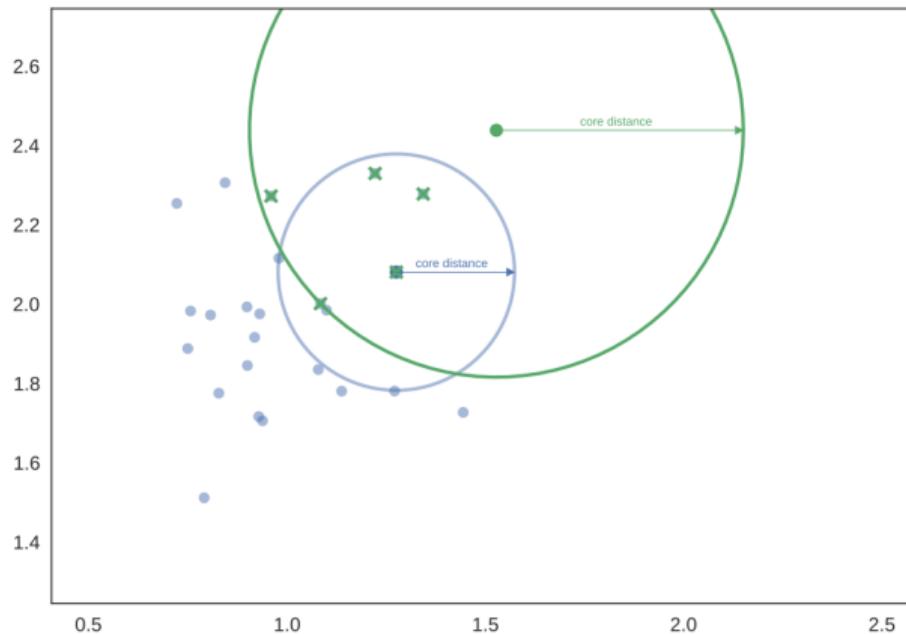
HDBSCAN



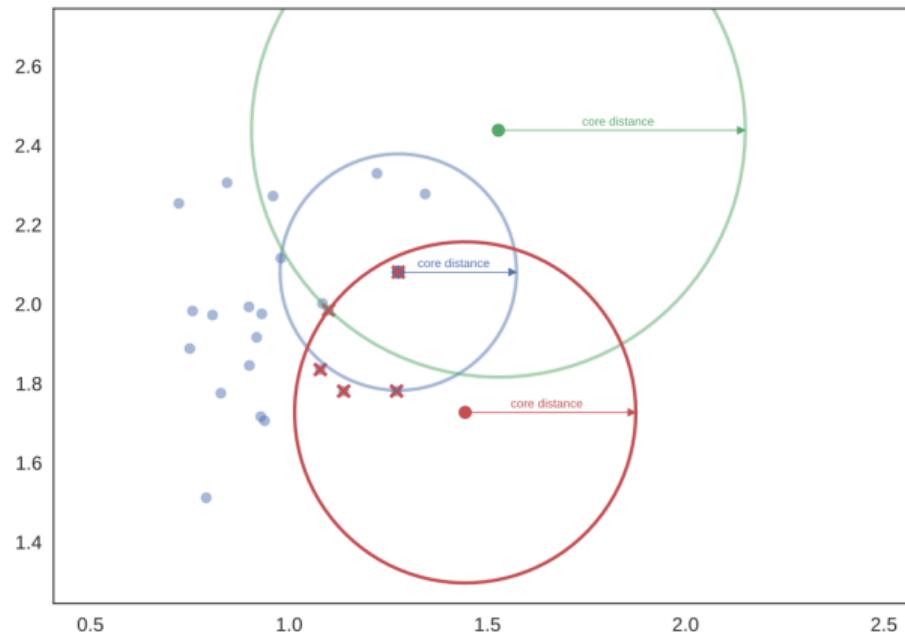
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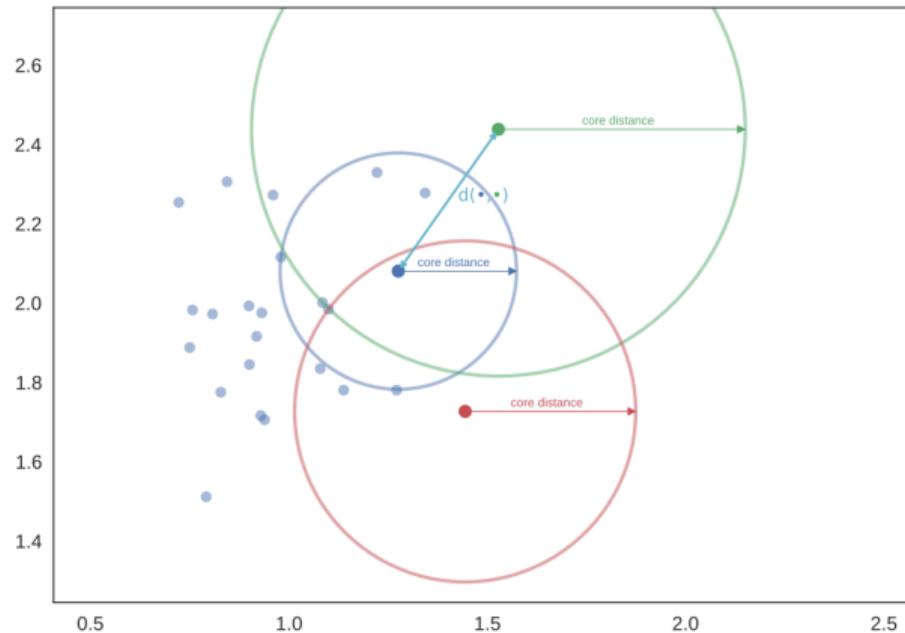
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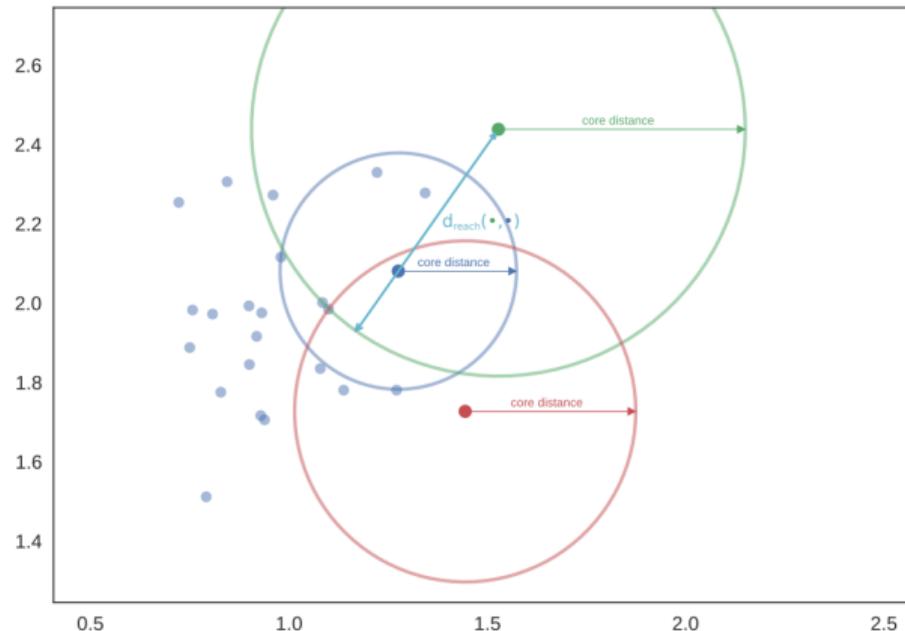
HDBSCAN



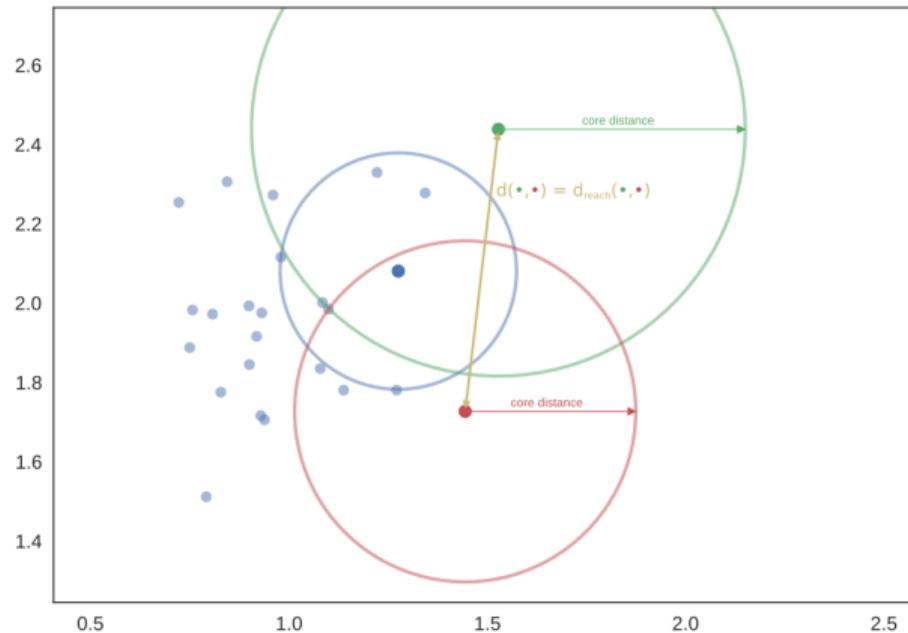
HDBSCAN



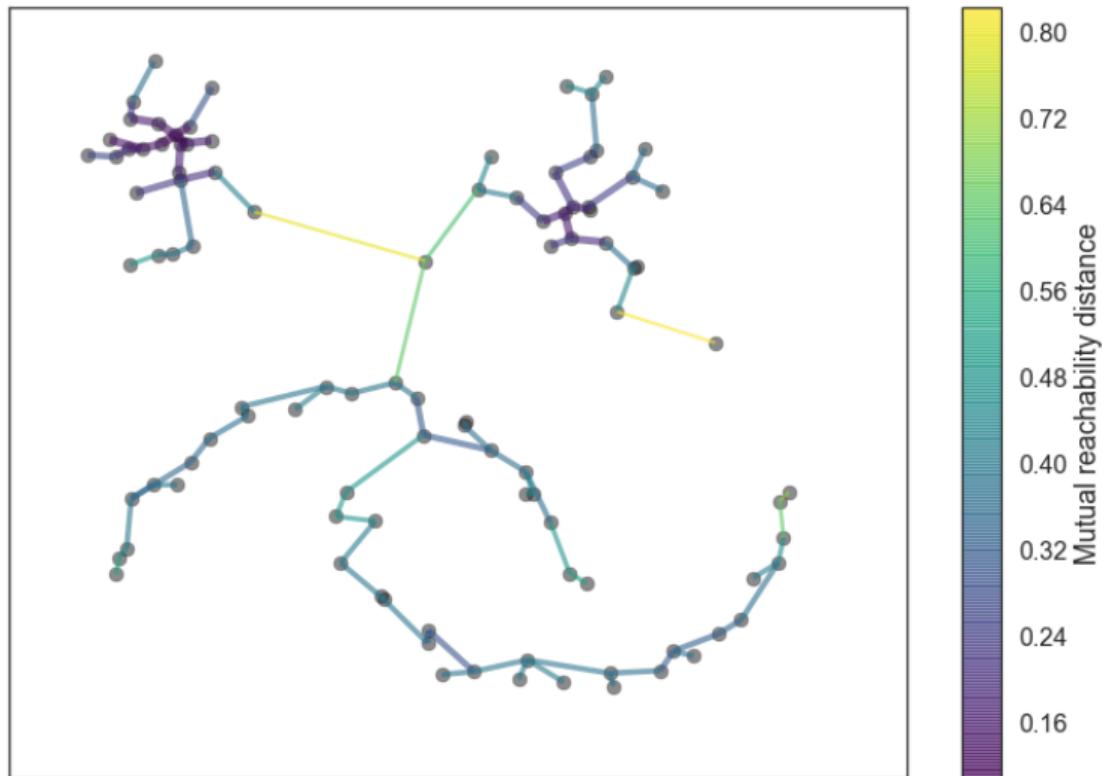
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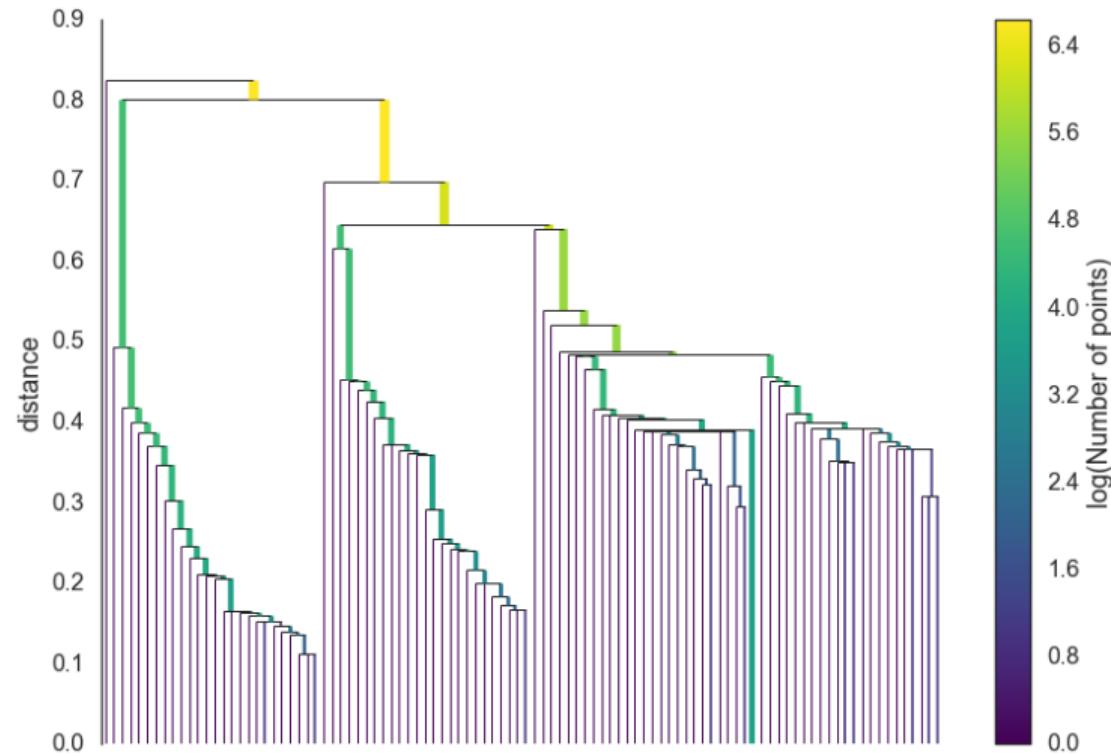
HDBSCAN



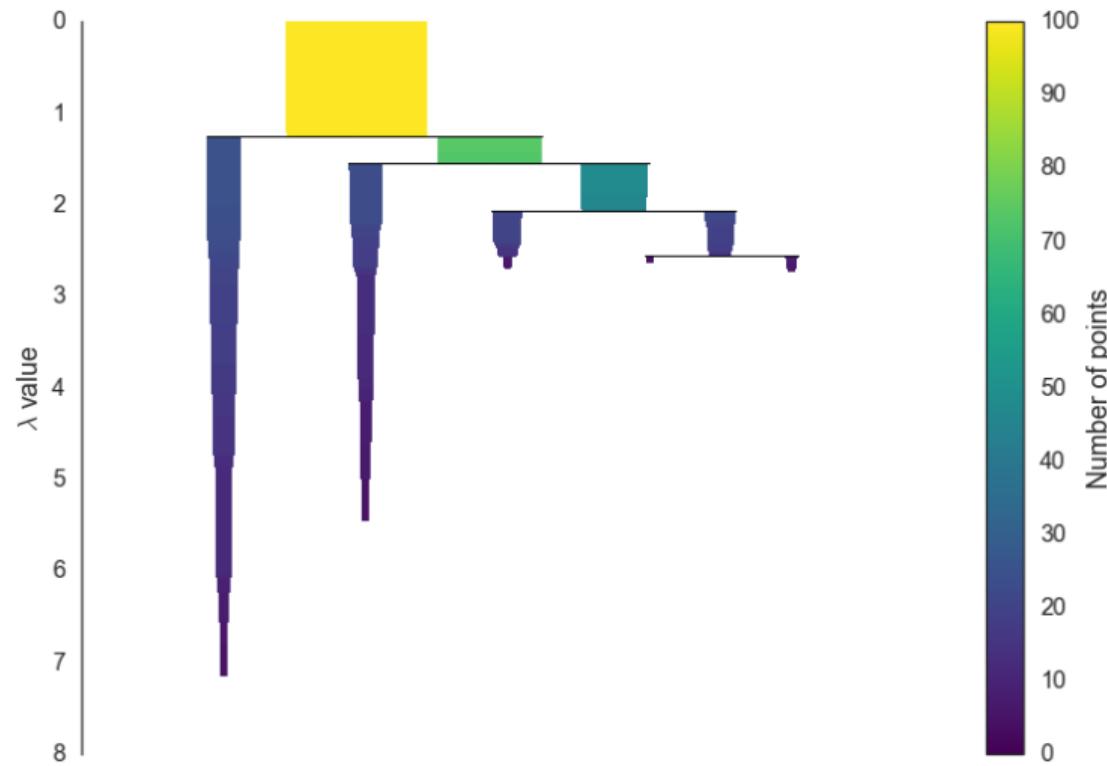
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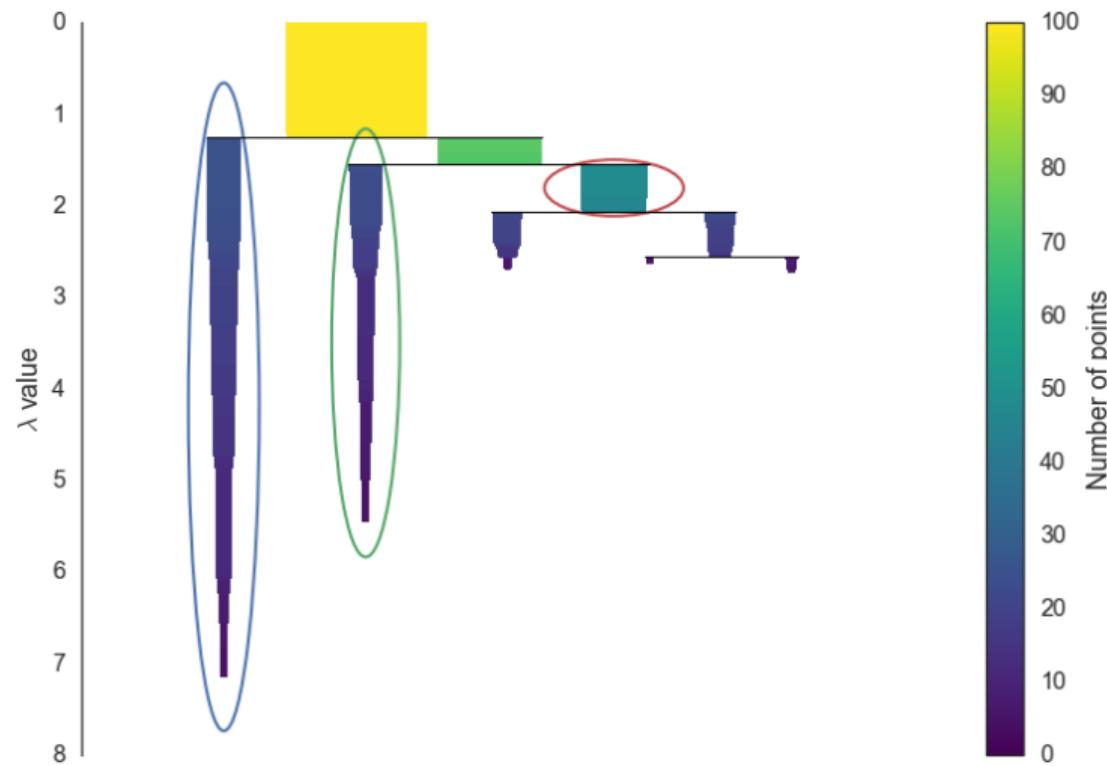
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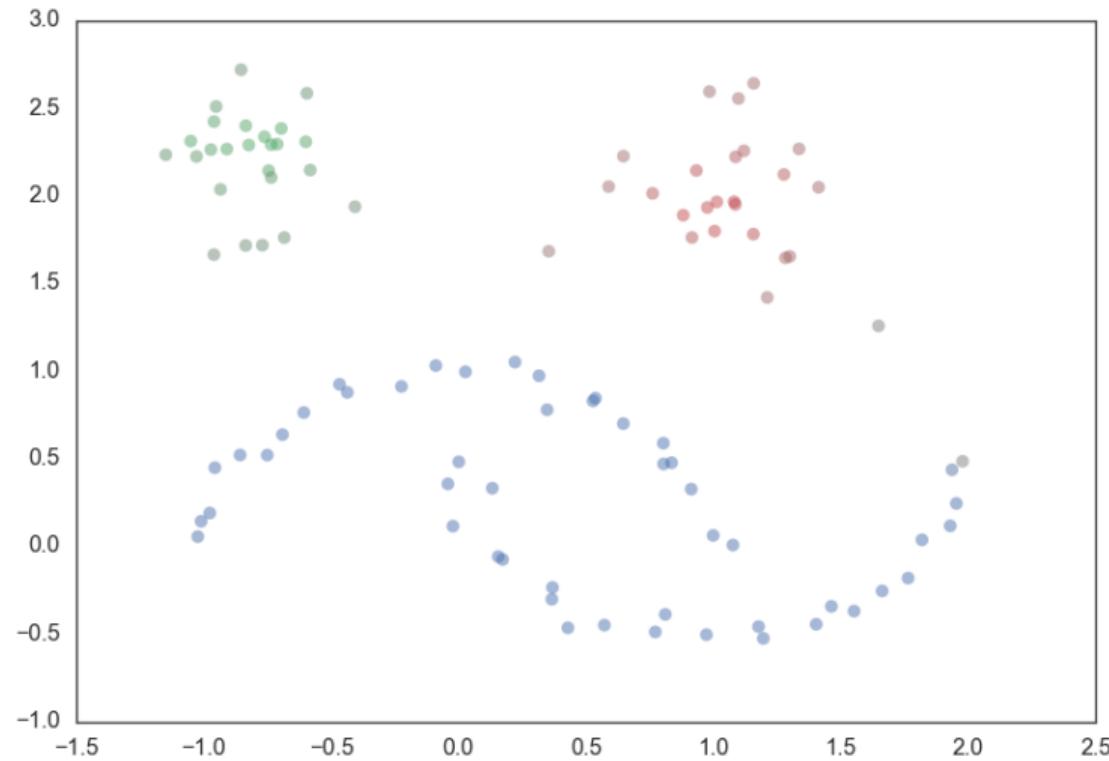
HDBSCAN



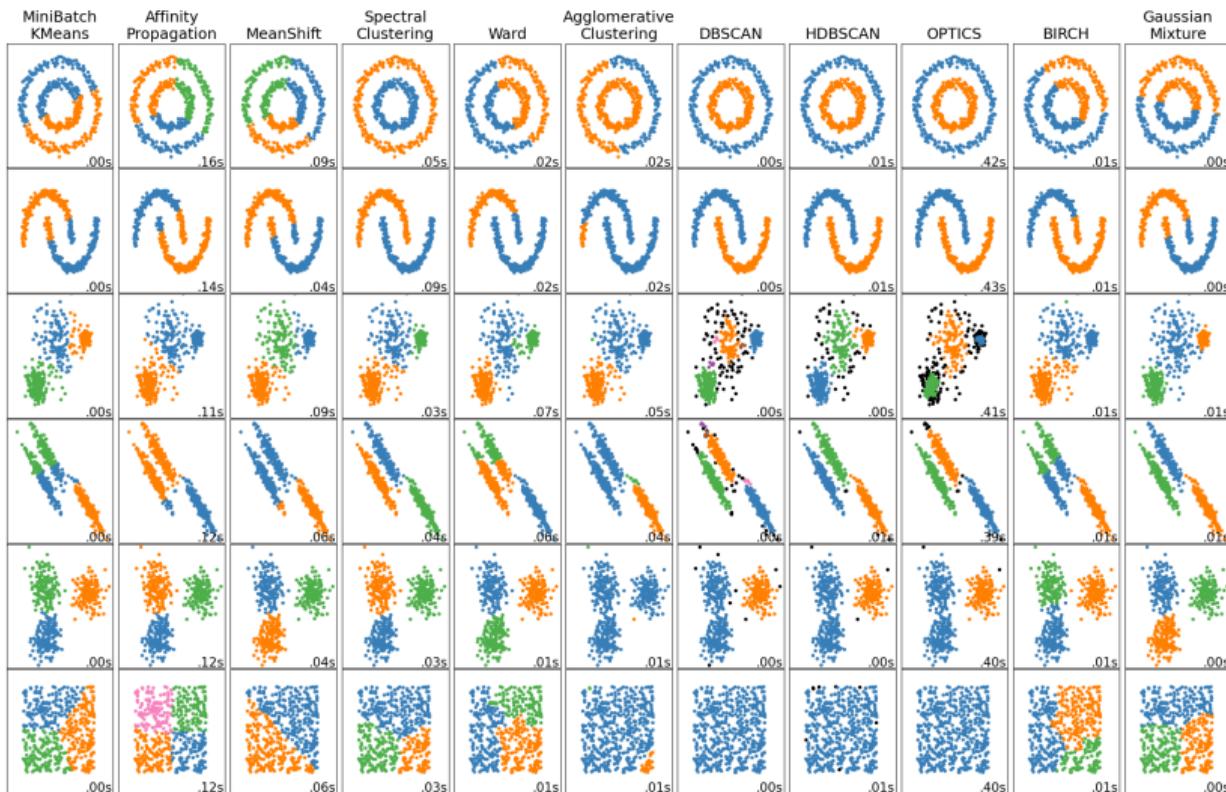
HDBSCAN



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.
- Hinton, Geoffrey E and Sam Roweis (2002). “**Stochastic neighbor embedding**”. In: *Advances in neural information processing systems* 15.
- McInnes, Leland, John Healy, and James Melville (2018). “**Umap: Uniform manifold approximation and projection for dimension reduction**”. In: *arXiv preprint arXiv:1802.03426*.
- Van der Maaten, Laurens and Geoffrey Hinton (2008). “**Visualizing data using t-SNE**”. In: *Journal of machine learning research* 9.11.