Projections and clusterings

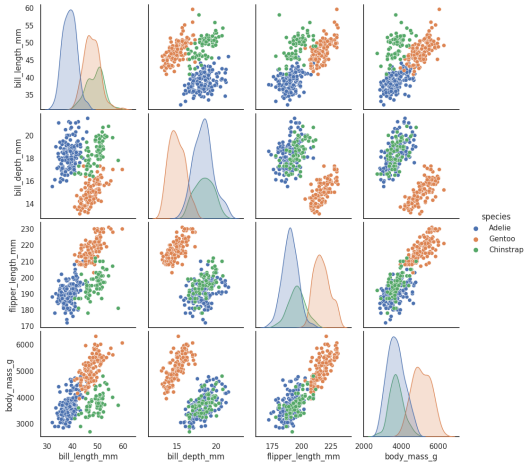
AI for ecologists

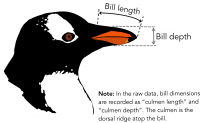
Paul Tresson

21/05/25

Introduction

Visualize what is happening in higher dimensions





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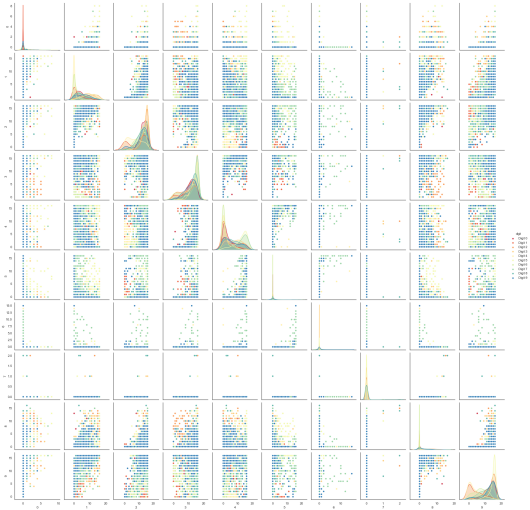

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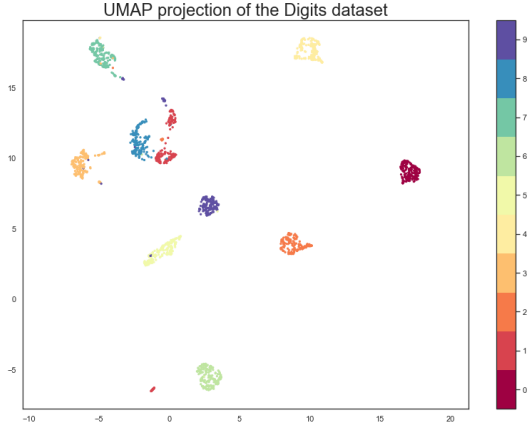
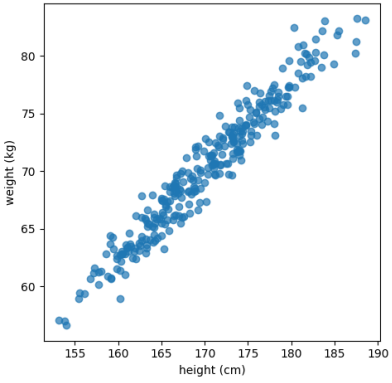


Projections

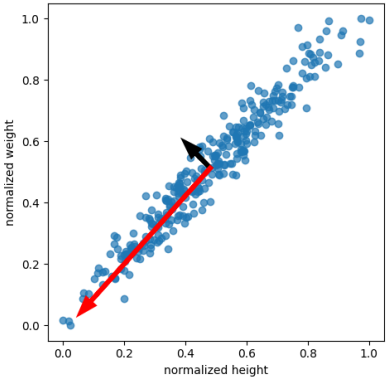
Projections

PCA

PCA


weight (kg)
80
75
70
65
60
155
160
165
170
175
180
185
190
height (cm)

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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Drawbacks

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

Non linear data

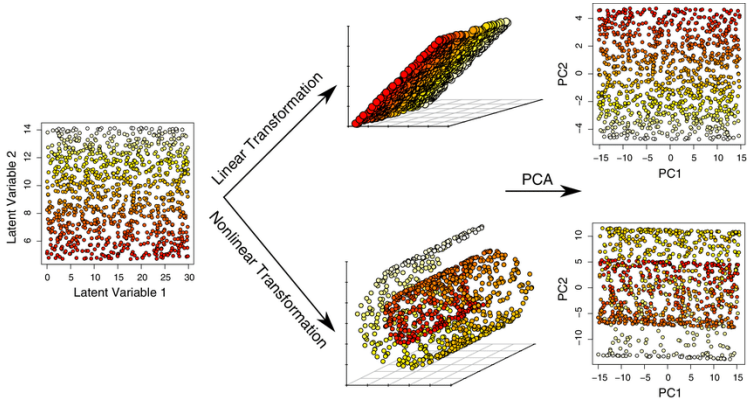

Figure from Du, 2019

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

Classics

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

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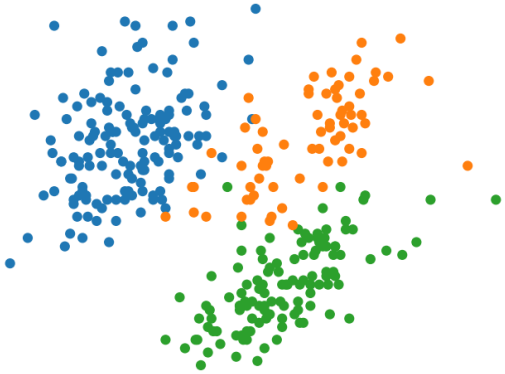
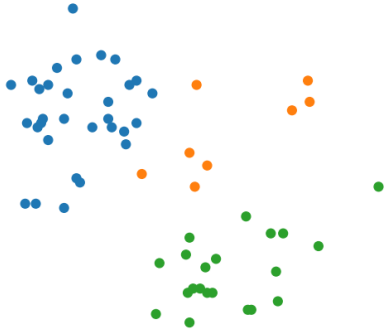
- **UMAP** (Uniform Manifold Approximation and Projection) McInnes et al., 2018

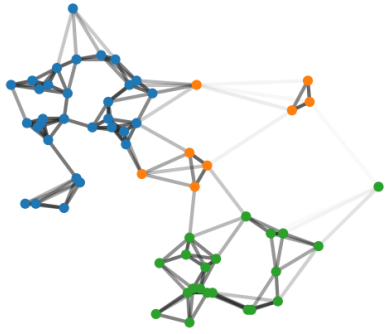
UMAP : Finding high dimension graph



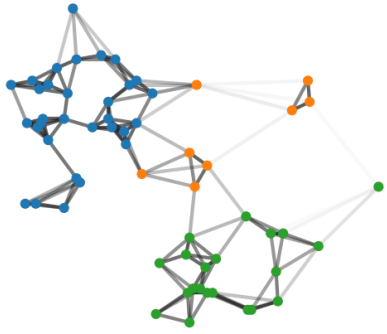
UMAP : Finding high dimension graph



UMAP : Finding high dimension graph



UMAP : Fitting low dimensional representation



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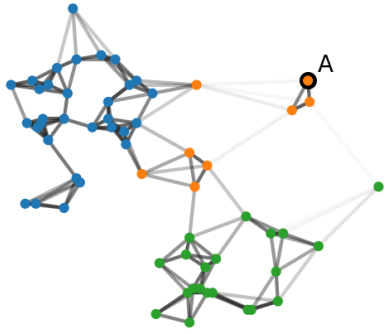

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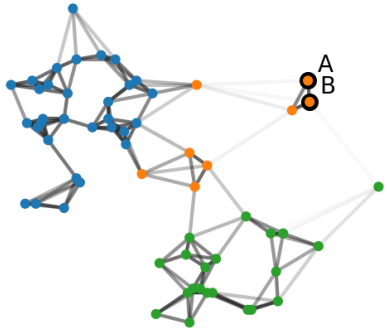

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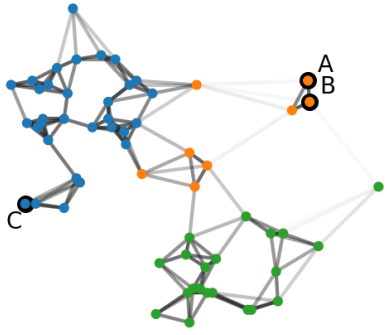

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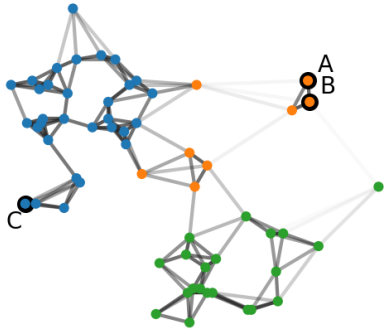

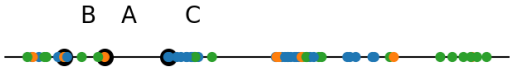

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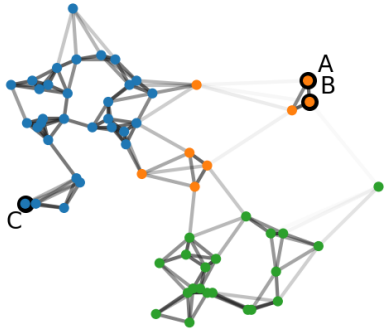

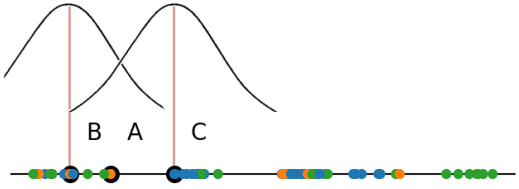

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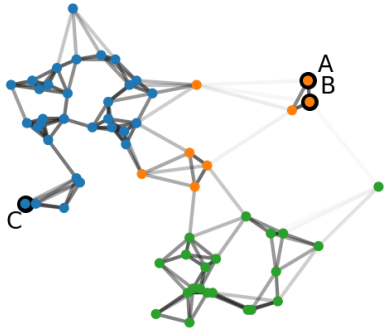
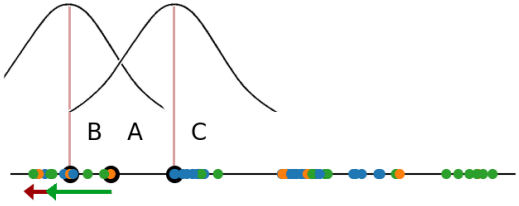
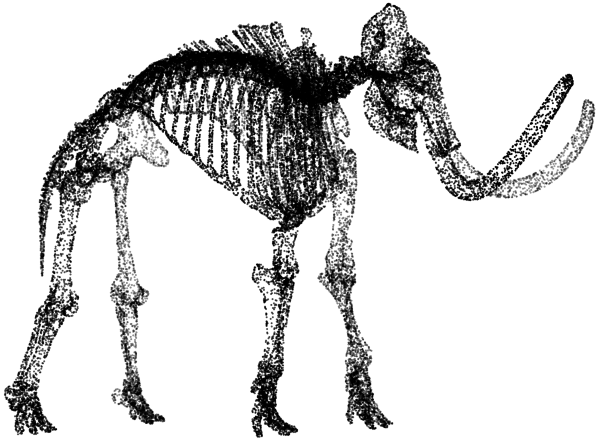
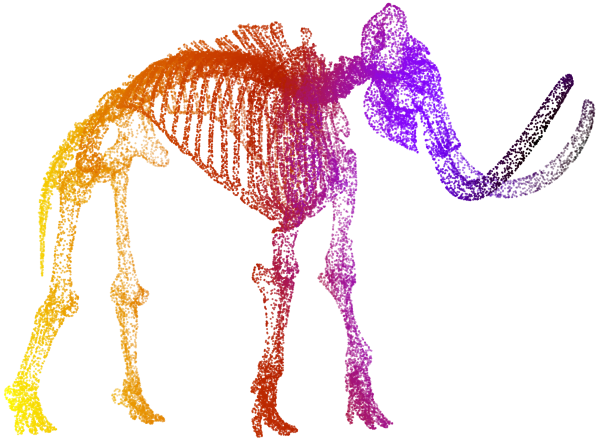




Mammoth example

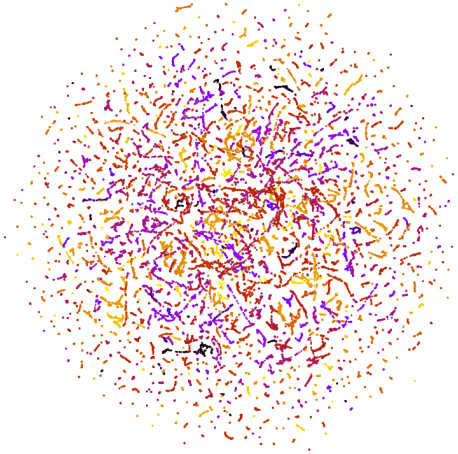


Mammoth example

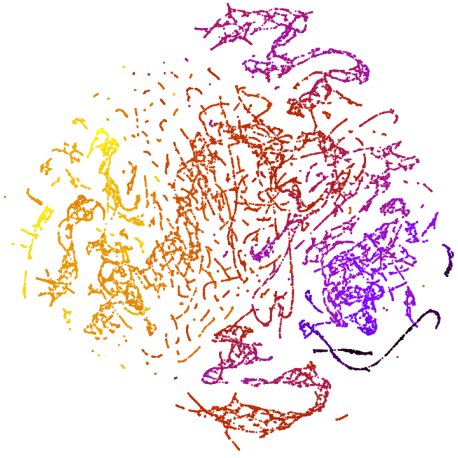


Mammoth example - PCA

Mammoth example - UMAP



Mammoth example - UMAP



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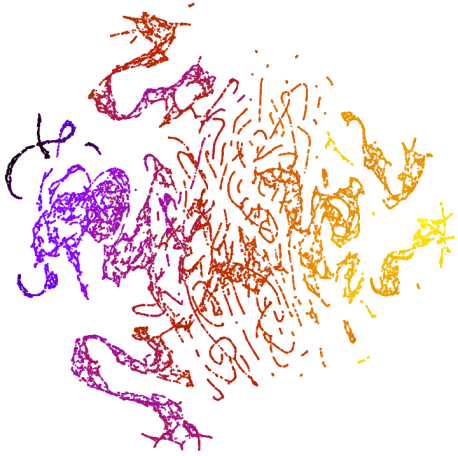

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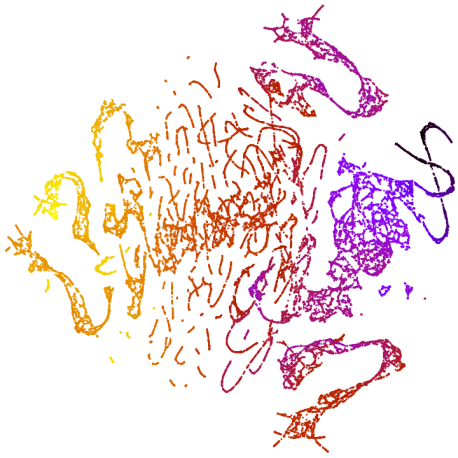

Mammoth example - UMAP

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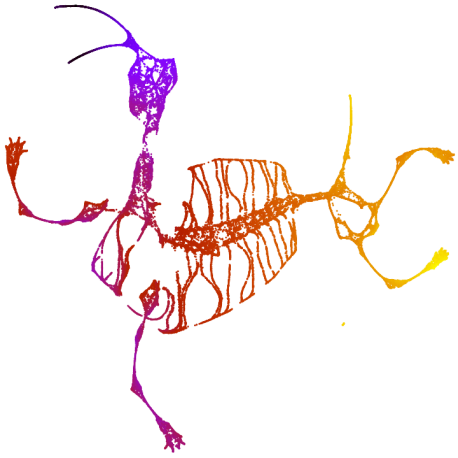
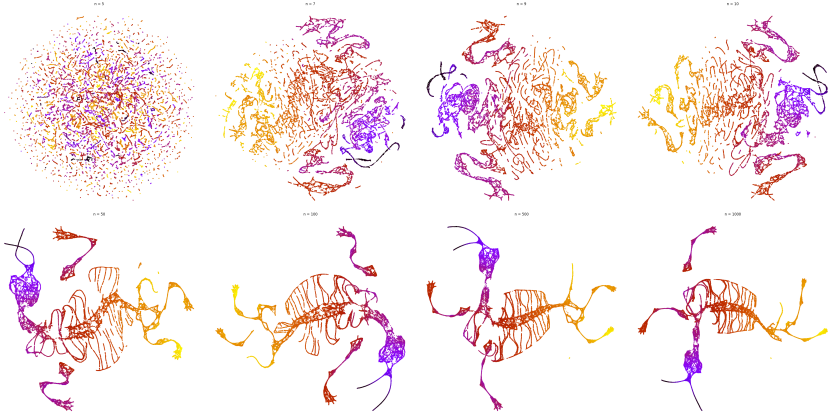


Mammoth example - UMAP

Mammoth example - Number of neighbors



UMAP vs. T-SNE

UMAP

- graph theory, fuzzy logic

T-SNE

- probabilities

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- determinist initialization

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- random initialization

UMAP vs. T-SNE

UMAP

- graph theory, fuzzy logic
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T-SNE

- probabilities
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- gaussian distribution similarity

UMAP vs. T-SNE

UMAP

- graph theory, fuzzy logic
- determinist initialization
- log_2 similarity scores
- update by pairs

$\rightarrow$ scales well for large datasets

T-SNE

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

scales less

Scaling

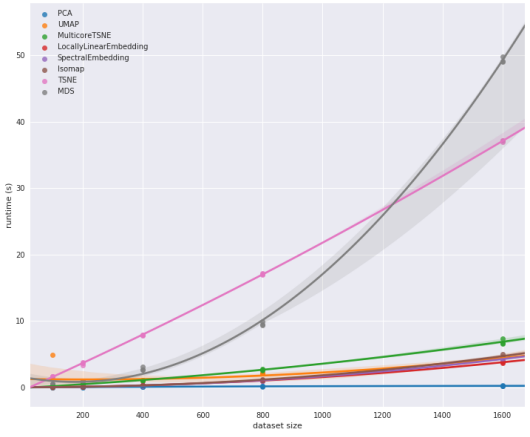


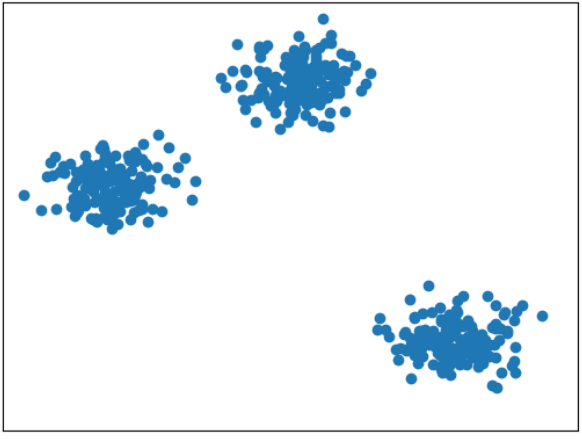
Figure from umap-learn documentation

Clustering

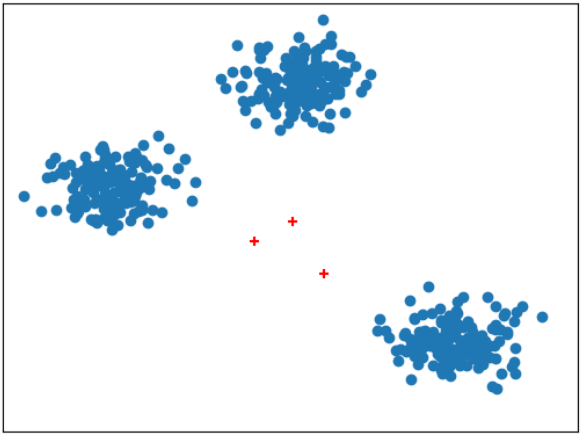
Clustering

K-means

K-means



K-means



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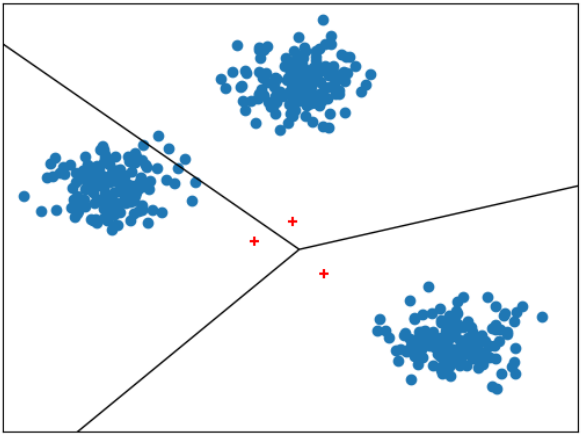

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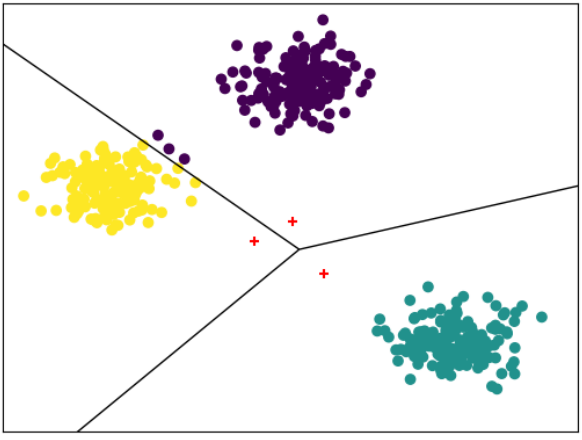

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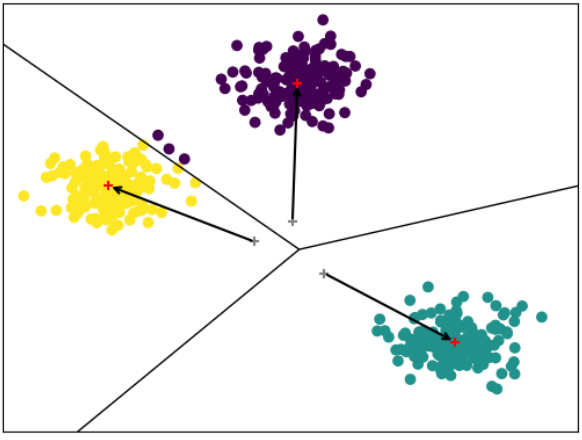

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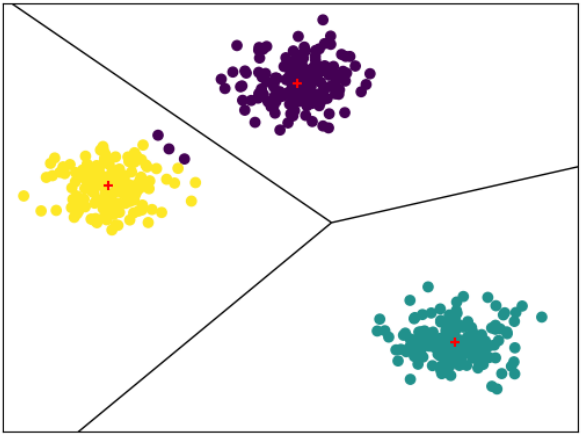

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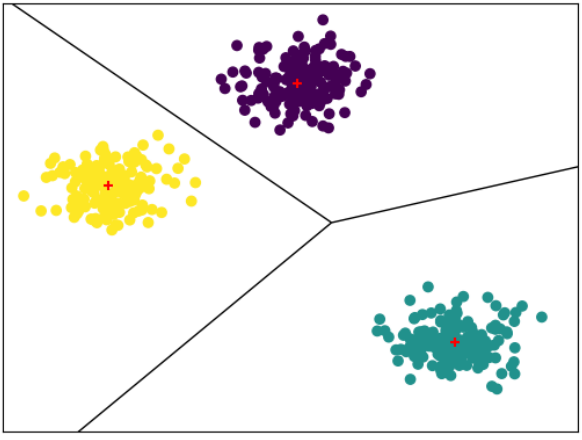


Determine the good K ? Elbow method

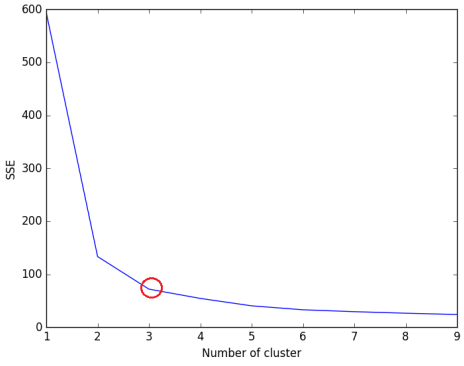
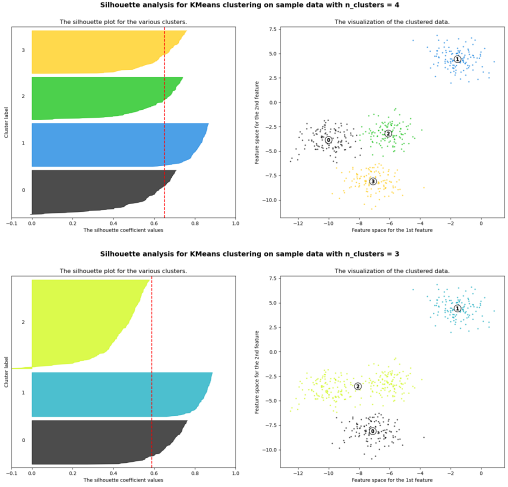


Figure from SO

Determine the good K ? Silouhette



Figures from scikit-learn documentation

K-means advantages and drawbacks

Advantages

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Drawbacks

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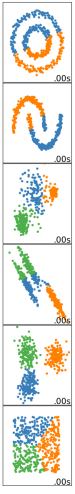

K-means advantages and drawbacks

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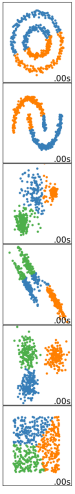
$\rightarrow$ Density based clustering



Clustering

HDBSCAN

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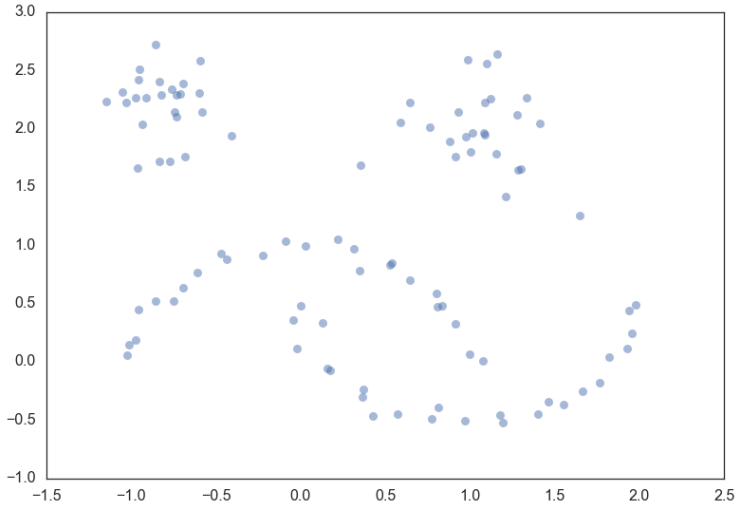
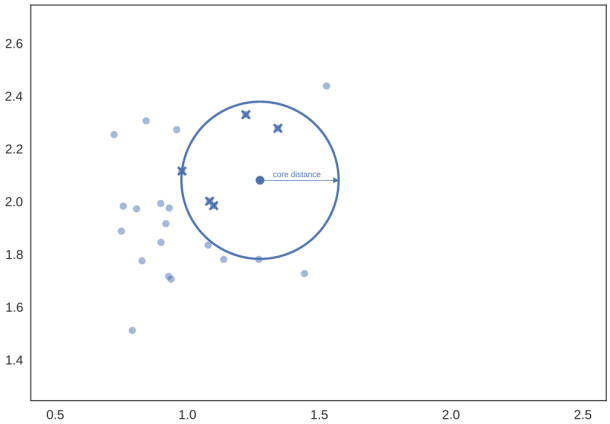


HDBSCAN



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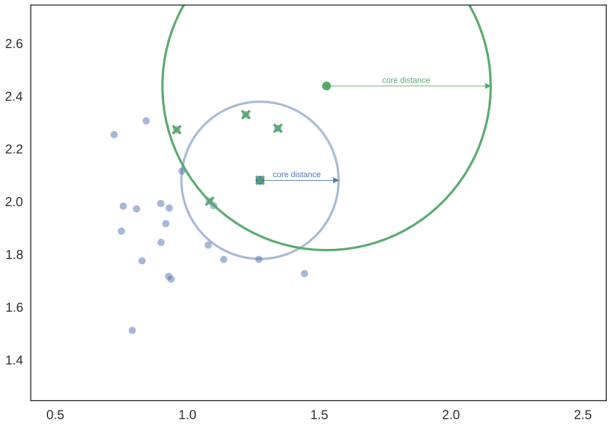

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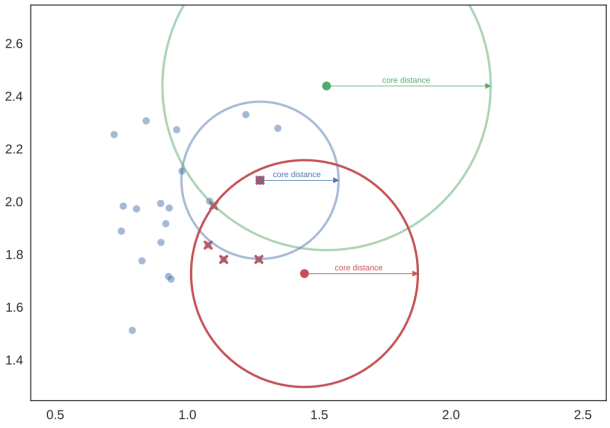
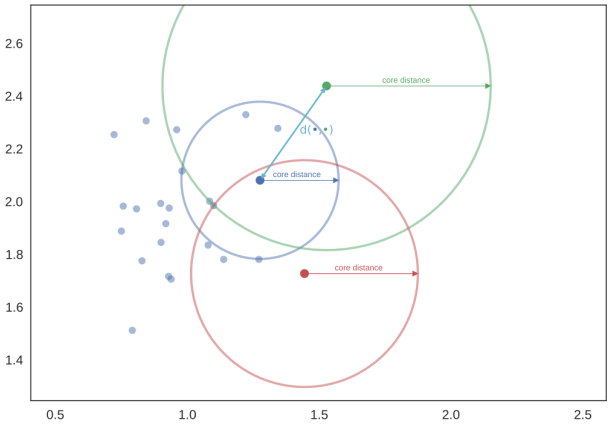
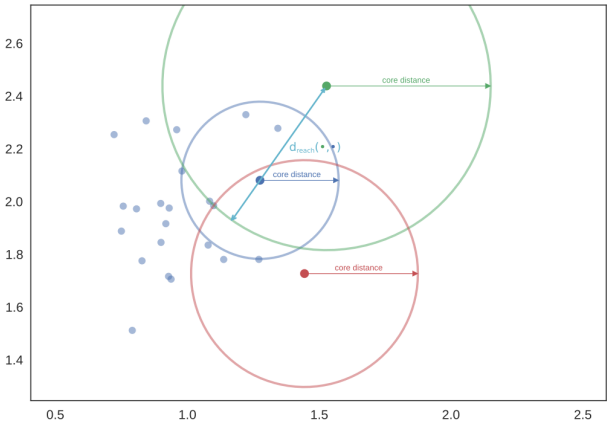

core distance
core distance
core distance
2.6
2.4
2.2
2.0
1.8
1.6
1.4
0.5
1.0
1.5
2.0
2.5

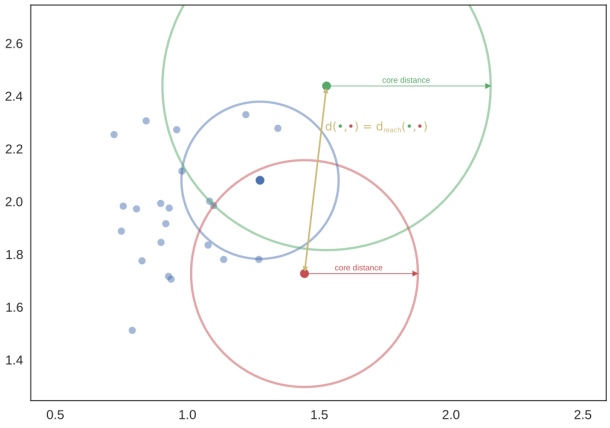
HDBSCAN


2.6
2.4
2.2
2.0
1.8
1.6
1.4
0.5
1.0
1.5
2.0
2.5
core distance
d(•, •)
core distance
core distance

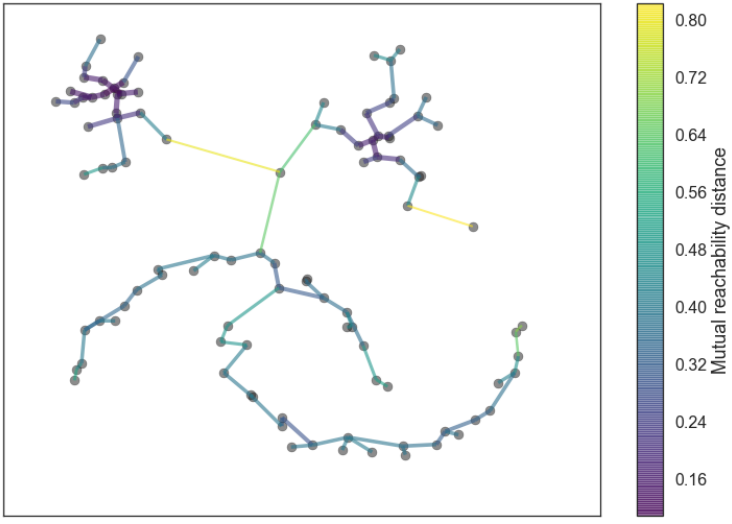
HDBSCAN


2.6
2.4
2.2
2.0
1.8
1.6
1.4
0.5
1.0
1.5
2.0
2.5
core distance
core distance
core distance
$d_{reach}(\bullet, \bullet)$

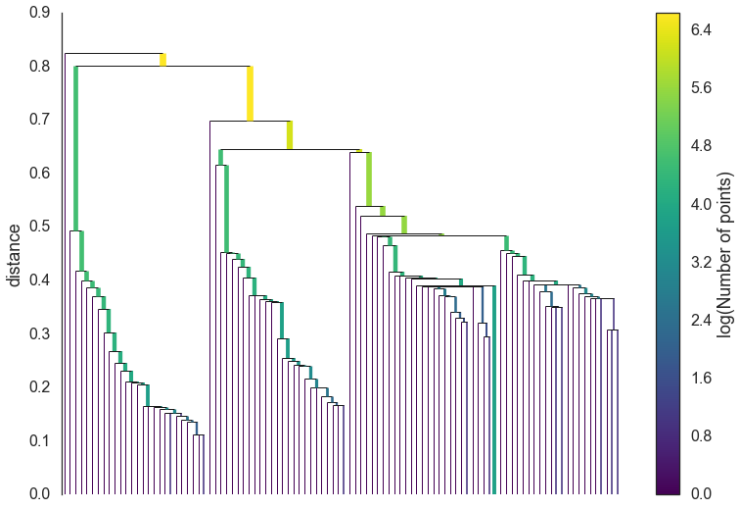
HDBSCAN


core distance
d(•, •) = d_mach(•, •)
core distance
2.6
2.4
2.2
2.0
1.8
1.6
1.4
0.5
1.0
1.5
2.0
2.5

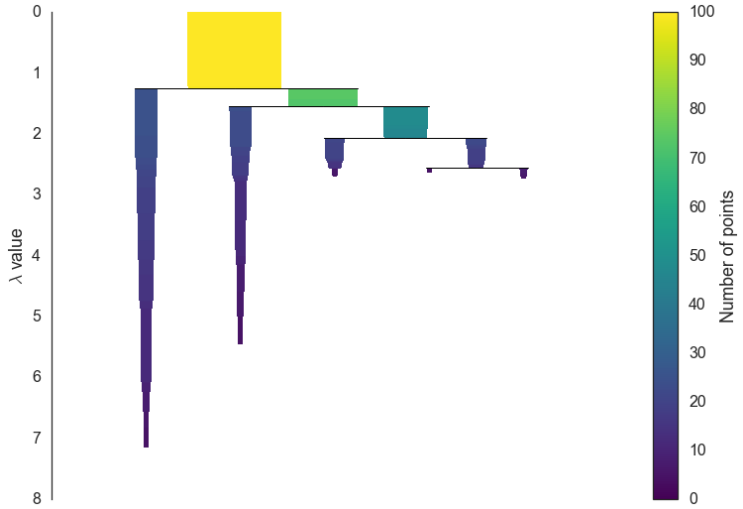
HDBSCAN


0.80
0.72
0.64
0.56
0.48
0.40
0.32
0.24
0.16
Mutual reachability distance

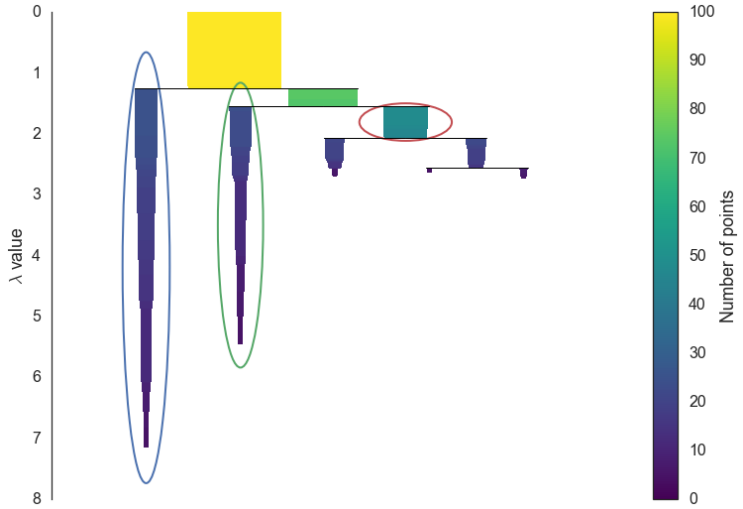
HDBSCAN


distance
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
log(Number of points)
6.4
5.6
4.8
4.0
3.2
2.4
1.6
0.8
0.0

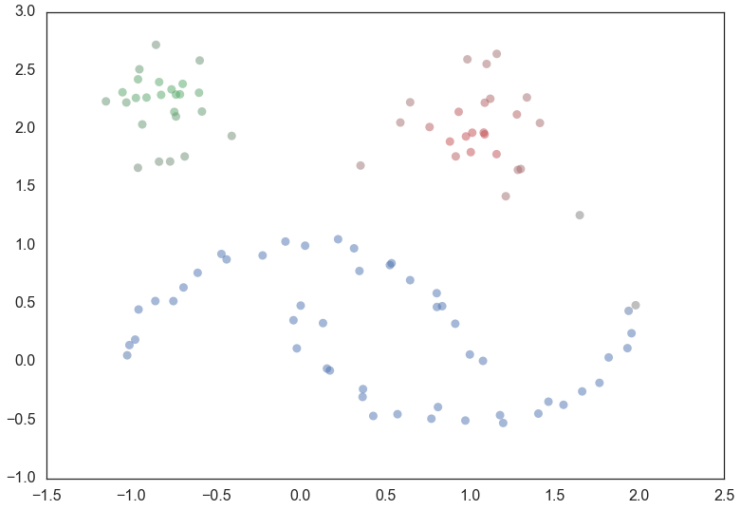
HDBSCAN


0
1
2
3
4
5
6
7
8
λ value
100
90
80
70
60
50
40
30
20
10
0
Number of points

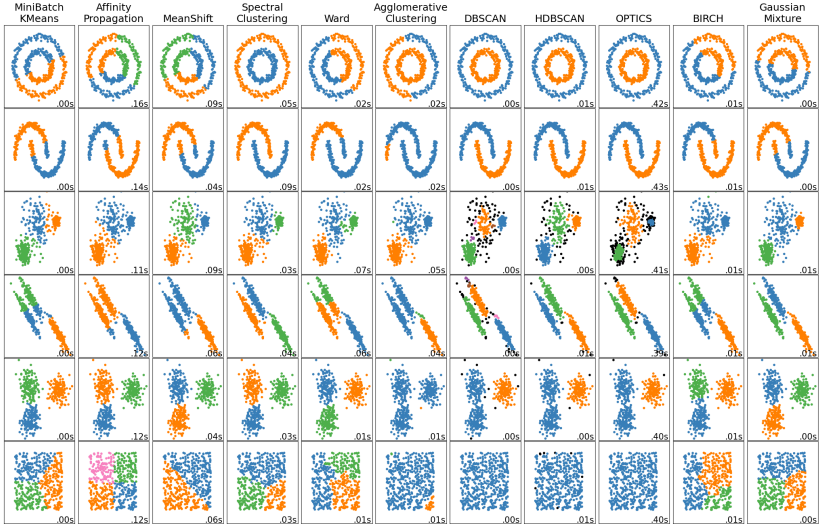
HDBSCAN


0
1
2
3
4
5
6
7
8
λ value
100
90
80
70
60
50
40
30
20
10
0
Number of points

HDBSCAN



A lot of options !



Useful ressources

- `scikit-learn` docs !
- deepia
- StatQuest

Thanks for you attention !

Let's practice !

References i

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Hinton, Geoffrey E and Sam Roweis (2002). **"Stochastic neighbor embedding".** In: *Advances in neural information processing systems* 15.

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Van der Maaten, Laurens and Geoffrey Hinton (2008). **"Visualizing data using t-SNE.".** In: *Journal of machine learning research* 9.11.