Data Driven Engineering I: Machine Learning for Dynamical Systems

Analysis of Static Datasets II: Clustering

Institute of Thermal Turbomachinery
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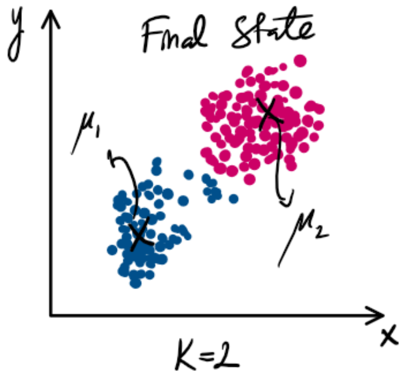

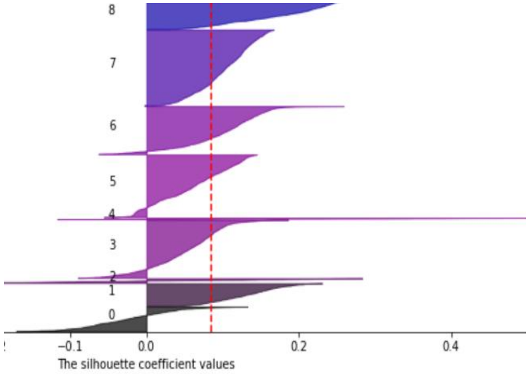

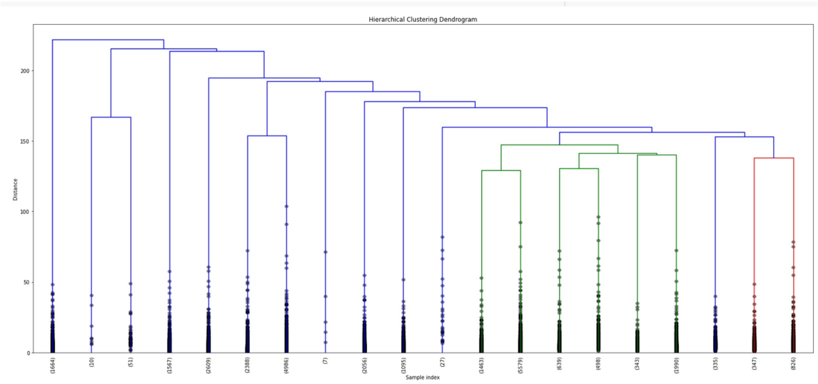

Today's Agenda

Basic Steps to Follow:

0.) Understand the business / task.
1.) Understand the data.
2.) Explore & prepare the data.
3.) Shortlist candidate models.
4.) ~~Training the model~~
5.) Evaluate the model predictions
6.) "Serve" the model!

Still valid

⇒ 4 major types

↪ Tricky!

#0 Understanding the task

- **Problem**: Manufacturing error in a production line
- **Modified sensory input:** 28 variables including sensory input
- 280,000 instances, where only a **small fraction** (~500) of products are **defective**.
- **Heuristic**: <0.5% is defective

A similar example for you:

“Bosch Production Line Performance
Reduce manufacturing failures”

#1 Understanding the data

- ❑ Check the data source: understand what the data refers to

- ❑ Objective: understand the characteristics of the data

- ❑ Look at the feature columns:
  - ❑ Any missing values?
  - ❑ Any features with NaN values?
  - ❑ Uniqueness of the dataset? (“cardinality”)

```
 23   S23      284807 non-null  float64
 24   S24      284807 non-null  float64
 25   S25      284807 non-null  float64
 26   S26      284807 non-null  float64
 27   S27      284807 non-null  float64
 28   S28      284807 non-null  float64
 29   Class    284807 non-null  object
dtypes: float64(29), object(1)
memory usage: 65.2+ MB
time: 54.5 ms
```

	Time	S1	S2	S3	S4	S5	S6
count	284807.000000	2.848070e+05	2.848070e+05	2.848070e+05	2.848070e+05	2.848070e+05	2.848070e+05
mean	94813.859575	1.758743e-12	-8.252298e-13	-9.636929e-13	8.316157e-13	1.591952e-13	4.247354e-13
std	47488.145955	1.958696e+00	1.651309e+00	1.516255e+00	1.415869e+00	1.380247e+00	1.332271e+00
min	0.000000	-5.640751e+01	-7.271573e+01	-4.832559e+01	-5.683171e+00	-1.137433e+02	-2.616051e+01
25%	54201.500000	-9.203734e-01	-5.985499e-01	-8.903648e-01	-8.486401e-01	-6.915971e-01	-7.682956e-01
50%	84692.000000	1.810880e-02	6.548556e-02	1.798463e-01	-1.984653e-02	-5.433583e-02	-2.741871e-01
75%	139320.500000	1.315642e+00	8.037239e-01	1.027196e+00	7.433413e-01	6.119264e-01	3.985649e-01
max	172792.000000	2.454930e+00	2.205773e+01	9.382558e+00	1.687534e+01	3.480167e+01	7.330163e+01

time: 447 ms

=> Colab


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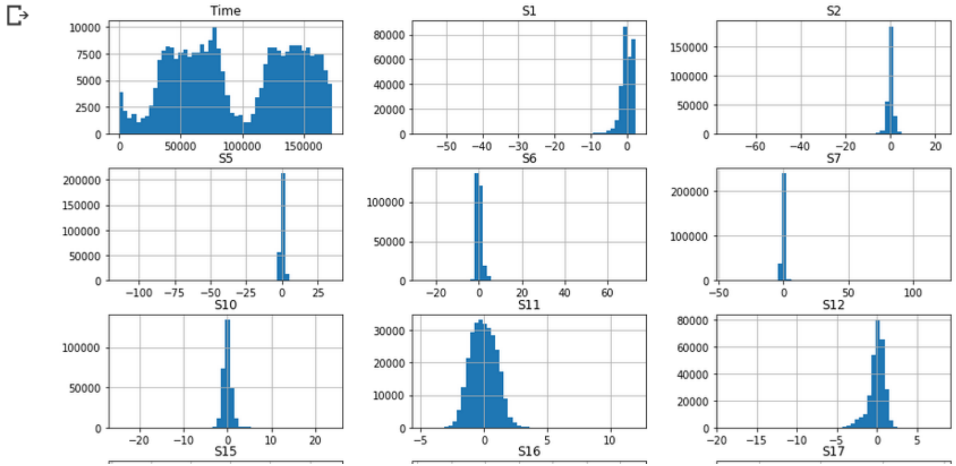
#2 Exploring the data

- ❑ **Objective**: generate a data quality report

- ❑ Using standard statistical measures of central tendency and variation
  - ❑ tabular data and visual plots
  - ❑ mean, mode, and median
  - ❑ standard deviation and percentiles
  - ❑ bars, histograms, box and violin plots



- ✓ Missing values,
- ✓ Irregular cardinality problems,
  - 1 or comparably small
- ✓ Outliers
  - invalid outliers and valid outliers

#2 Exporing the data: Correlation Matrix

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- Shows the correlation between each pair of features

$$Cov(\underset{\text{Features}}{a,b}) = \frac{1}{n-1}\sum_{i=1}^{n}\left[(a_i - \underset{\text{mean}}{\bar{a}}) \times (b_i - \underset{\text{mean}}{\bar{b}})\right]$$

i: instance

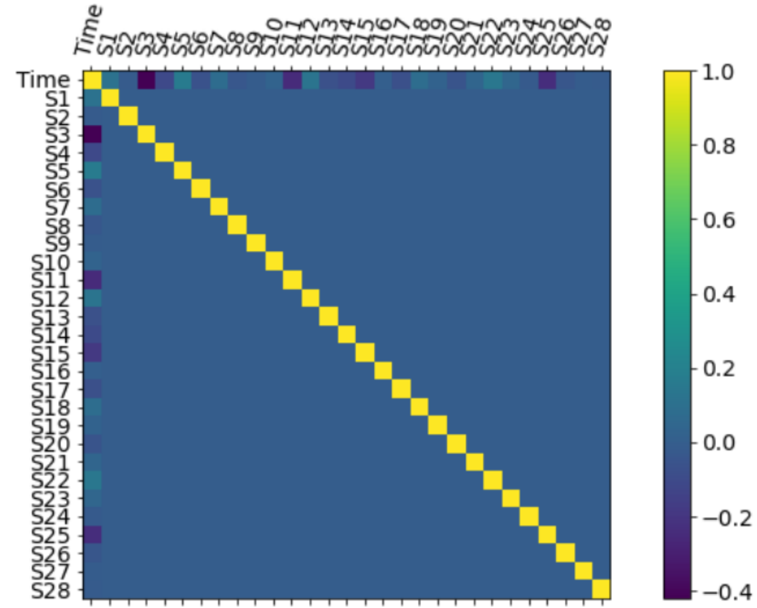
- Normalized form of "covariance"

$$Corr(a,b) = \frac{Cov(a,b)}{SD(a) \times SD(b)}$$

* Normalized
* Dimensionless

Easy to interpret

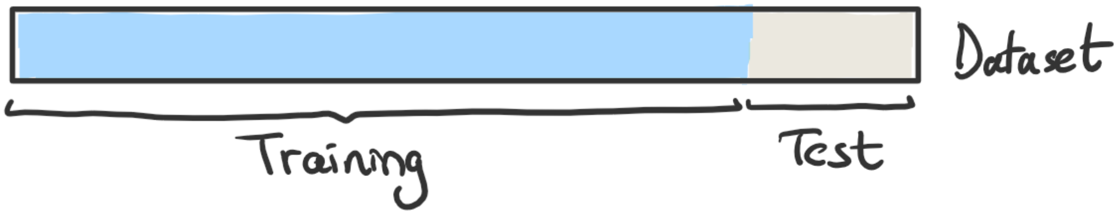
- Ranges between −1 and +1



time: 975 ms

#2 Preparing the Data

- Clustering >> unsupervised >> **training & test split not needed**



- We will use it to **reduce the volume of the data** when needed:

```
[ ]  X_train, X_test, y_train, y_test = train_test_split(dataX,
     dataY, test_size=0.9,
     random_state=2020, stratify=dataY)

     time: 188 ms
```

#3 Candidate models: k-Means

Clustering :

* Grouping similar objects together.

input → Model → Output

↙ Partitional Clustering ↘ Hierarchical Clustering

Partitional Clustering

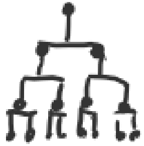
I	II	III
•	△	□
•	△	□
	△	

* $\tilde{O}(m \cdot n)$

(−) Need to know "k"

(−) Sensetive to initial cond.

Hierarchical Clustering

* 

"nested tree"

* $\tilde{O}(n^2 \log(n))$

(+) does not need "k" at the begining

(−) Always work even for white noise!

#3 Candidate models: k-Means 2

k-means :

* partitioning n observation into 'k' clusters.

(–) 'k' is typically unknown ⇒ parametric analysis

* define a similarity distance.

* k-means is iterative & depends on its initialization

#3 Candidate models: k-Means 3

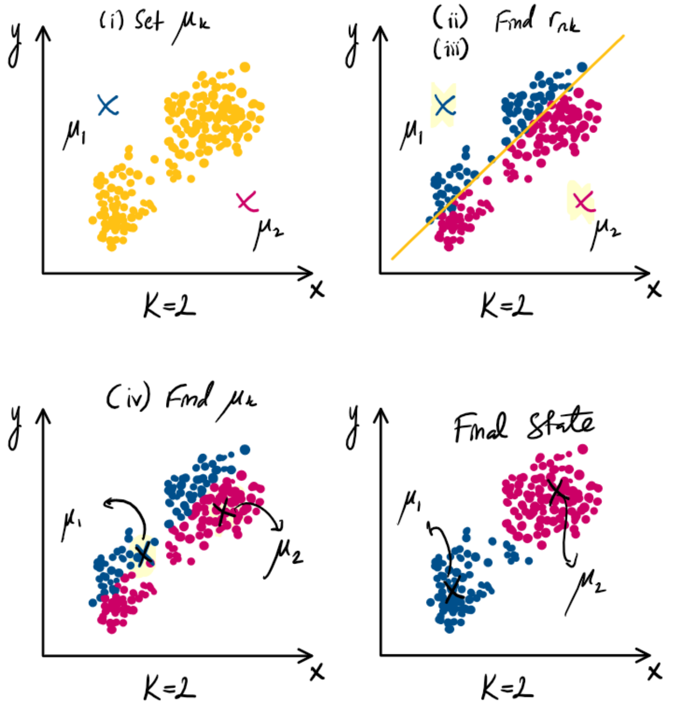
Algorithm:

(i) Assume a center of cluster for k cluster: μ_k.

(ii) Compute the distance between each observation X & μ

(iii) Label each observation as belonging to the nearest cluster.

(iv) Find the "center of mass" for each cluster $\longrightarrow \mu_k$



#3 Candidate models: k-Means 4

* Objective Function: $J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \| x_n - \mu_k \|^2$

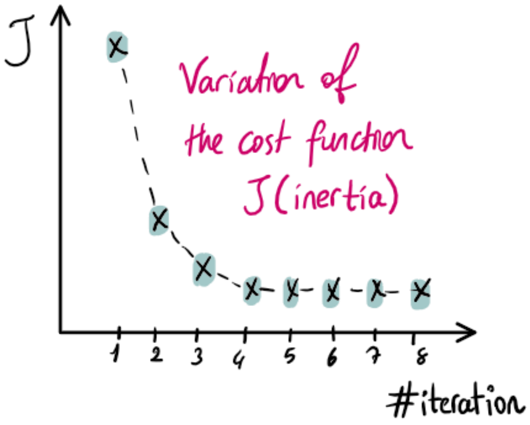
$r_{nk} = 1 \; ; \text{if } n \to k$

$r_{nk} = 0 \; ; \text{if } n \not\to k$

find r_{nk} & μ_k minimizing J

① $r_{nk} = \begin{cases} 1, & \text{if } \; k = \arg\min_j \| x_n - \mu_j \|^2 \\ 0, & \text{otherwise} \end{cases}$ given $\mu_j \to r_{nk}$

② $\dfrac{\partial J}{\partial \mu_k} = 0 \Rightarrow 2 \sum_{n=1}^{N} r_{nk} (x_n - \mu_k) = 0 \Rightarrow \mu_k = \dfrac{\sum_n r_{nk} x_n}{\sum_n r_{nk}}$ "K means"



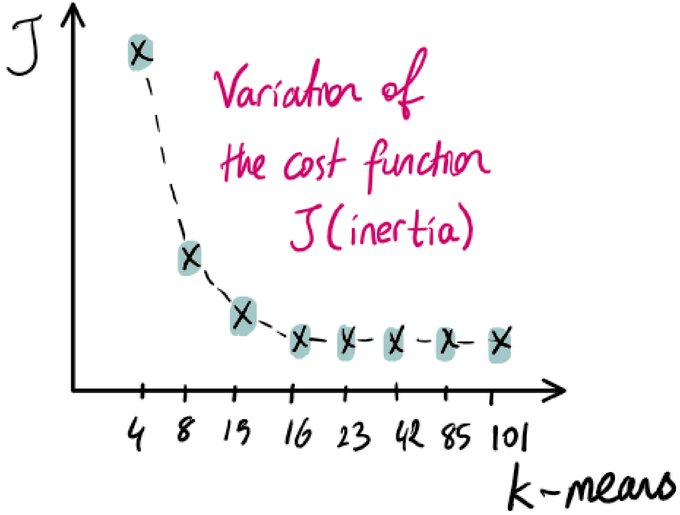
#3 Candidate models: k-Means 5

Deciding on the # Clusters

(i) Find J with increasing #k.

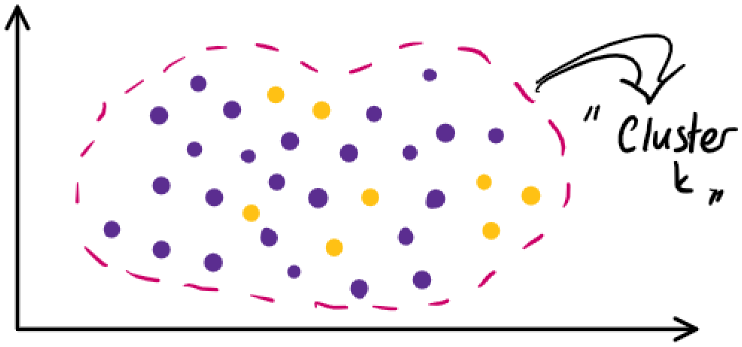
(ii) Look at the variation.

(iii) Pick a reasonable k value.



#5 Evaluate model predictions

Predictive Accuracy



* Do you know a set of examples with labels?

(1) There is not any labelled data.

Silhouette Score:

* Relative distances between instances.

(2) There are some labelled data

Homogeneity (Purity):

#5 Evaluate model predictions 2

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Silhouette Score:

* Relative distances between instances.

(1) $SC = b - a / \max(a, b)$

where;

a → mean intra-cluster distance

b → mean distance to the instances of the next closest cluster

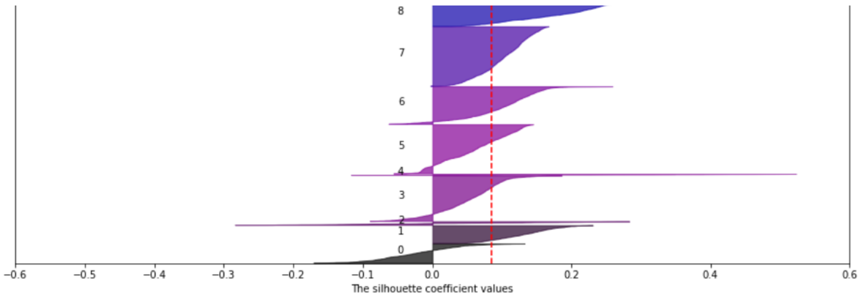
(2) Plot every instances Sil. coeff;

⇒ Silhouette Diagram

SC = +1 ⇒ Well inside in its own cluster
Away from others
$\sim b/b = 1.0$

SC = −1 ⇒ Wrong Cluster ($-a/a \sim -1$)

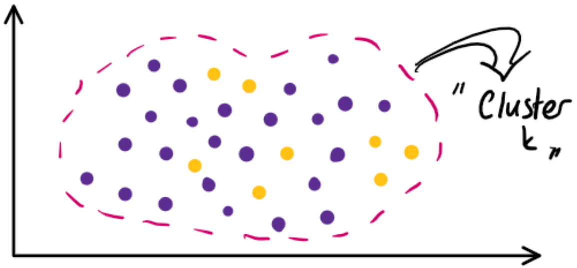
SC ≈ 0 ⇒ Near the cluster boundary ($a \sim b$)

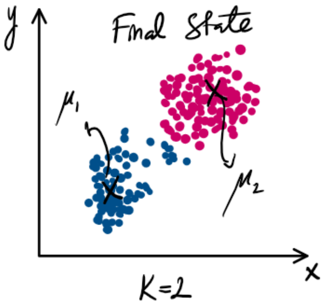


#5 Evaluate model predictions 3

Homogeneity (Purity):

* k: cluster index $(1, 2, \dots, K)$
* j: class index $(0, 1)$





(1) N_{kj} = # instances in cluster k belonging class j

(2) N_k = # instances in cluster k

(3) $H_{kj} = N_{kj} / N_k$ } homog. of cluster k for class j

(4) $H_k := \max(H_{kj})$ ⇒ homo. of cluster k

(5) $H = \sum_{k=1}^{K} N_k/N \, H_k$ ⇒ Overall homog.

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#3 Candidate Models: Hierarchical Clustering

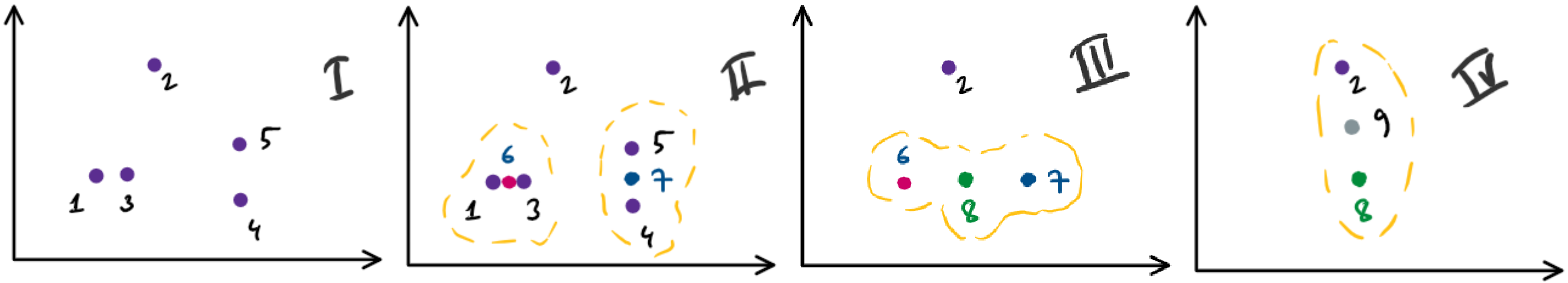
Hierarchical Clustering

* Clusters are nested:

(i) Bottom-up (agglomerative)

(ii) Top-down (divisive)

$$\begin{bmatrix}1\\2\\3\\4\\5\end{bmatrix} \rightarrow \begin{bmatrix}6\\4\\5\\2\end{bmatrix} \rightarrow \begin{bmatrix}6\\7\\2\end{bmatrix} \rightarrow \begin{bmatrix}8\\2\end{bmatrix} \rightarrow \begin{bmatrix}9\end{bmatrix}$$



#3 Candidate Models: Hierarchical Clustering

Hierarchical Clustering

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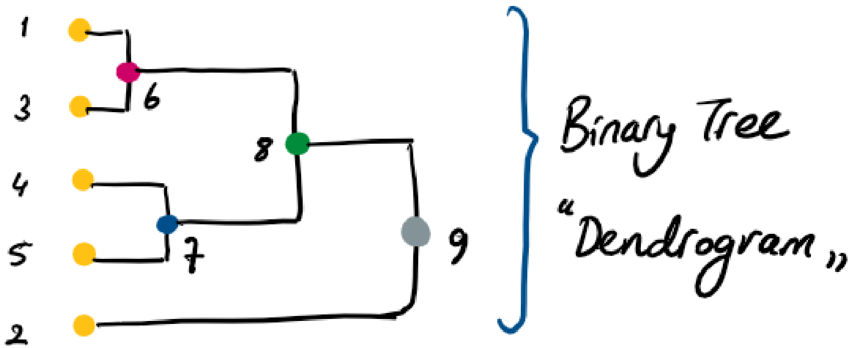
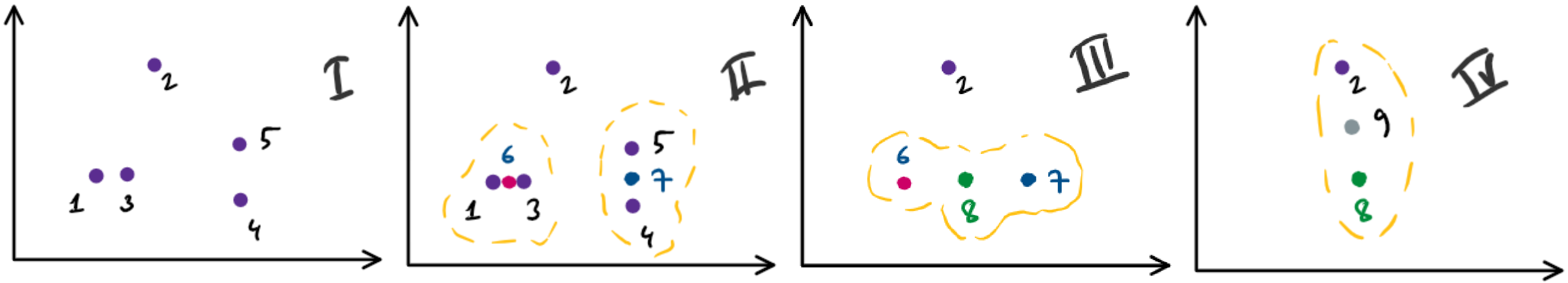
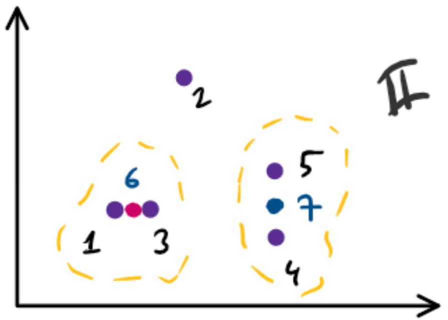




#3 Candidate Models: Hierarchical Clustering 2



Distance Calculation btw. Clusters: $\begin{bmatrix} 2 \\ 6 \\ 7 \end{bmatrix}$

* There are three options here for distance calculation:

① Single Link ⇒ nearest neighbour clustering

(✓) Distance $:= \min(d_{ij})$

$\}$ $\tilde{O}(n^2)$ time

② Complete Link ⇒ furthest neigh. clustering

(✓) Distance $:= \max(d_{ij})$

$\}$ $\tilde{O}(n^3)$ time, Compact Clusters

③ ✓ Average link ⇒ mean distance

(✓) Distance $:= \dfrac{1}{n_i\, n_j} \sum_i \sum_j d_{ij}$

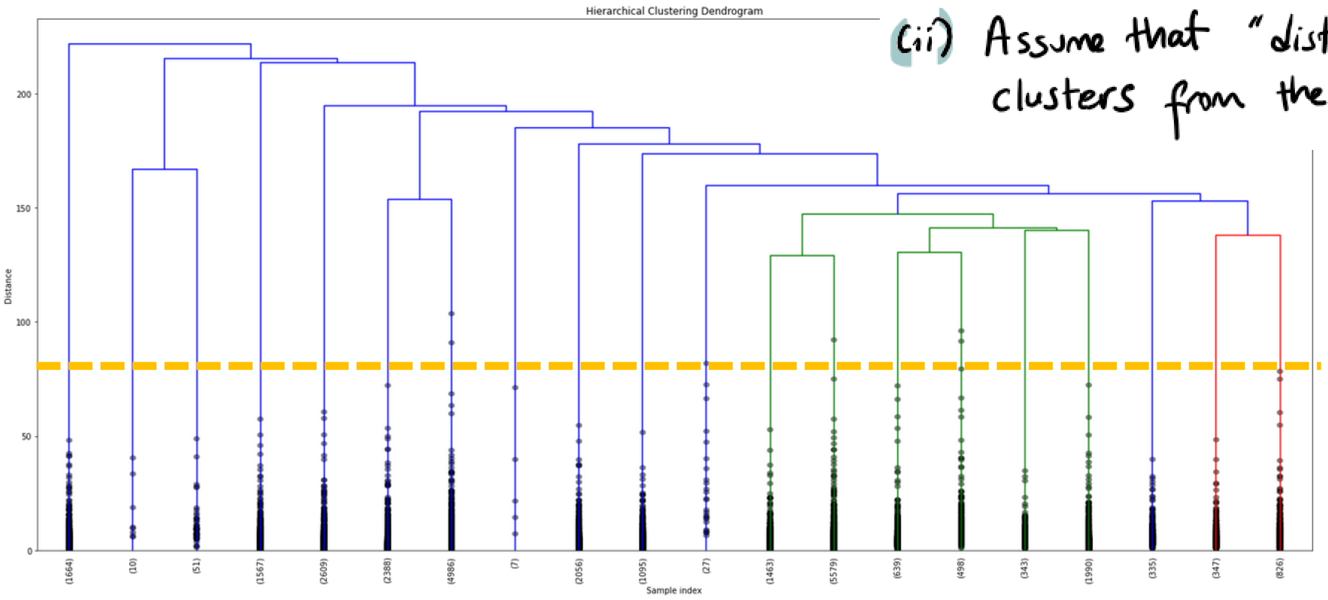
$\}$ $\tilde{O}(n^3)$ time, feature scaling is important

#3 Candidate Models: Hierarchical Clustering 3

* Deciding on # cluster:

(i) Select a threshold value that separates clusters in the dendrogram

(ii) Assume that "distance" segragates natural clusters from the unnatural ones.



* Alternative:

"Bayesian Hier. Clustering"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#3 Candidate Models: DBSCAN

Density-based Clustering: DBSCAN

* Groups points that are closely packed together
  → [points with many neighbours]

* Outliers ⇒ "Low density" regions

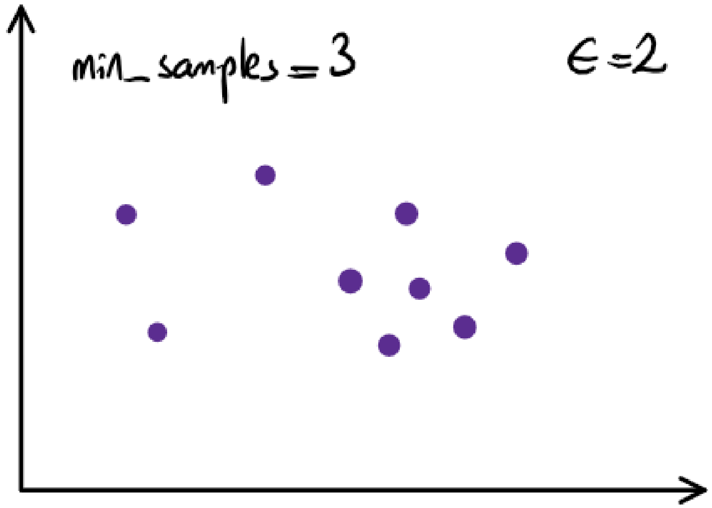
* In k-Means ⇒ all instances are assigned to a cluster k.

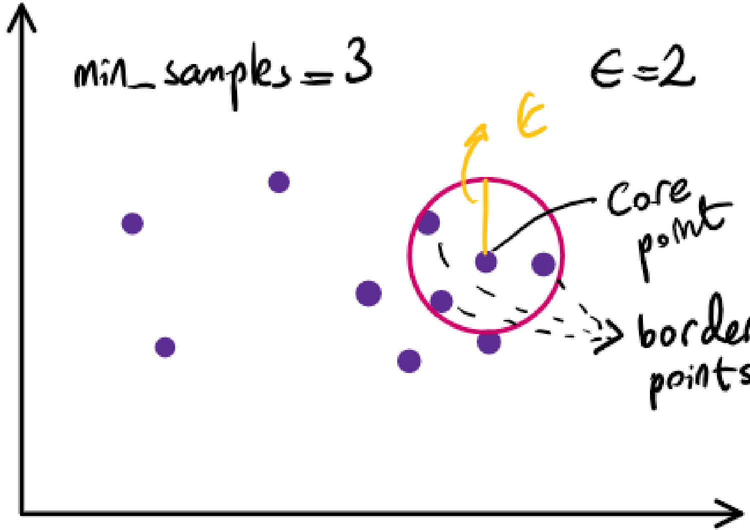
* In DBSCAN ⇒ • k is not needed ⇒ There is also noise class.

You need: {
- min # points to be considered as a dense cluster.
- a distance measure to locate neighbours (ϵ)

#3 Candidate Models: DBSCAN 2

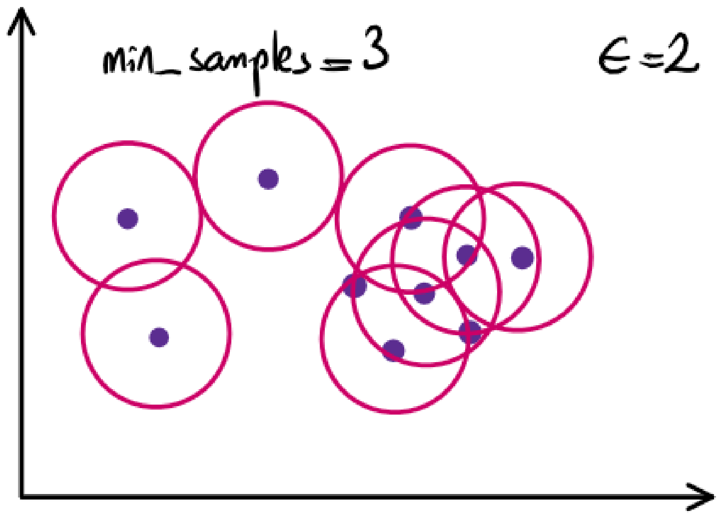
Density-based Clustering: DBSCAN

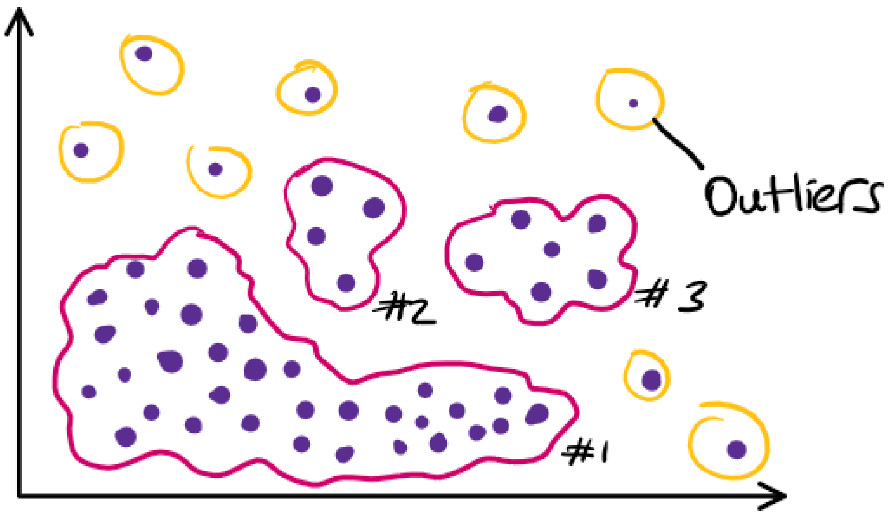




#3 Candidate Models: DBSCAN 2

Density-based Clustering: DBSCAN





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#3 Candidate Models: Gaussian Mixtures

Mixture Models:

* Idea: Observation is constituted by P (Gaussian) processes

mean variance

$\underbrace{\text{variance}}_{\text{uncertainity}}$?

$$f_i = \sum_{p=1}^{k} \alpha_p f_p$$

PDF

weight

$$f_i = \sum_{p=1}^{k} \alpha_p \mathcal{N}(x_i, \mu_p, \sigma_p)$$

Gaussian MM

#3 Candidate Models: Gaussian Mixtures 2

Mixture Models:

* Uses expectation – maximization (EM) algorithm
* Similar to k-Means: Define "k".
* Bayesian Gaussian Mixture: probabilistic interpretation
  Cluster # Optimization

Hint: EM algorithm is much slower than k-Means. Therefore, you can use k-means to determine the better initial conditions for GMM.

Additional Notes