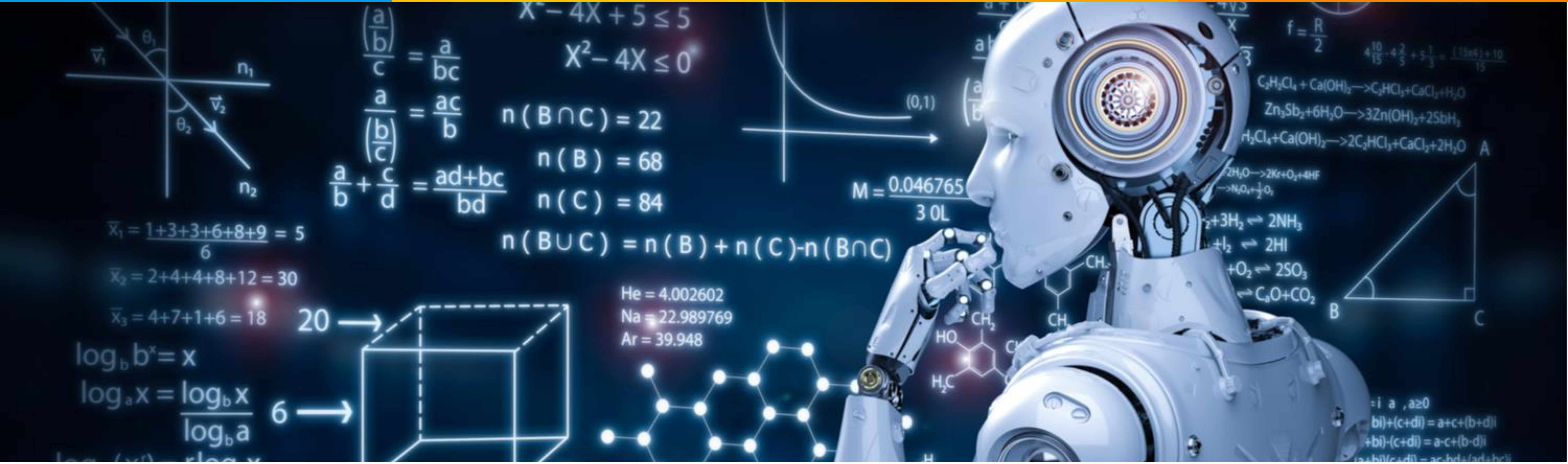
Duration: 60 min

Srikanth Shenoy

AML 5102

M.E. AI & ML



Lecture 12: Clustering 101

Recap

- Multivariate Gaussian distributions
  - Mahalanobis distance
  - Minimum Covariance Determinant
- Using Bayes Rule for generative ML
- Different kind of decision boundaries & corresponding covariance matrix

AML class logistics for next week

- ALA portion for sessional 1 completed
- Using ALA next week hours for AML
  - Tuesday – 11-12 as usual
  - Thursday - 9-10, 11-12

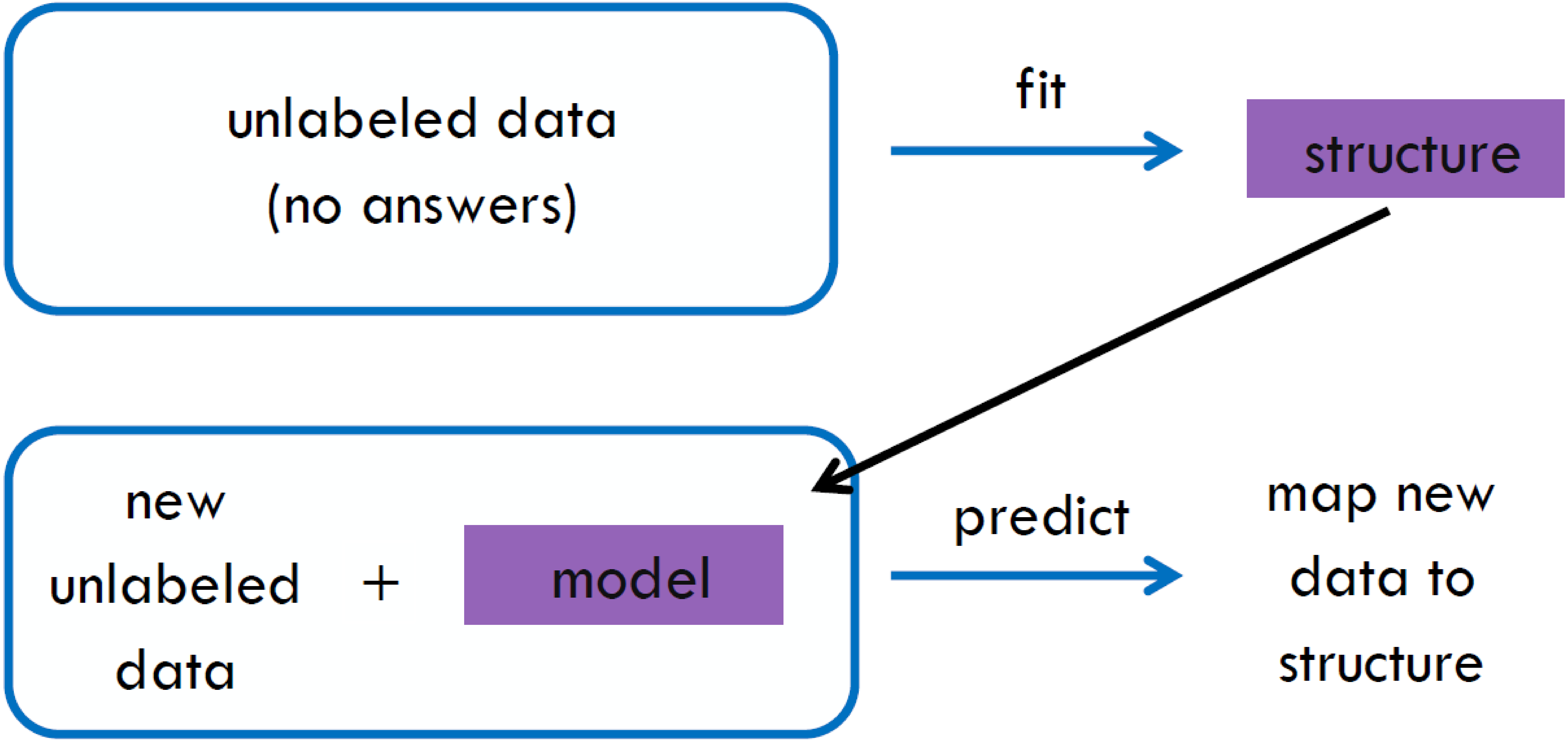
Sessional 1 – Theory

- 20 marks:10+ questions objective type: +2/-1
- 30 marks: No negative marks
  - Problems
  - 1-2 sentences answer of type “why/justify”
  - Given a formula, why is it the best choice?
  - Complexity of algorithm
- Disclaimer: There may be some variations

Sessional 1 – Lab

- 30 minutes: No API (from scratch) coding on paper
  - 1 of 3 algorithms (definitely a variation)
    - NearestCentroid, KNN, Kmeans – with CV
  - Using class, methods
  - Submit at 30 minutes
- 60 minutes: Coding on computer
  - Dataset will be given
  - Sklearn pipelining for EDA and fit/predict
  - Can use sklearn if your code does not work

Clusters, properties & basic metrics



unlabeled data

(no answers)

fit

structure

new

unlabeled

data

+

model

predict

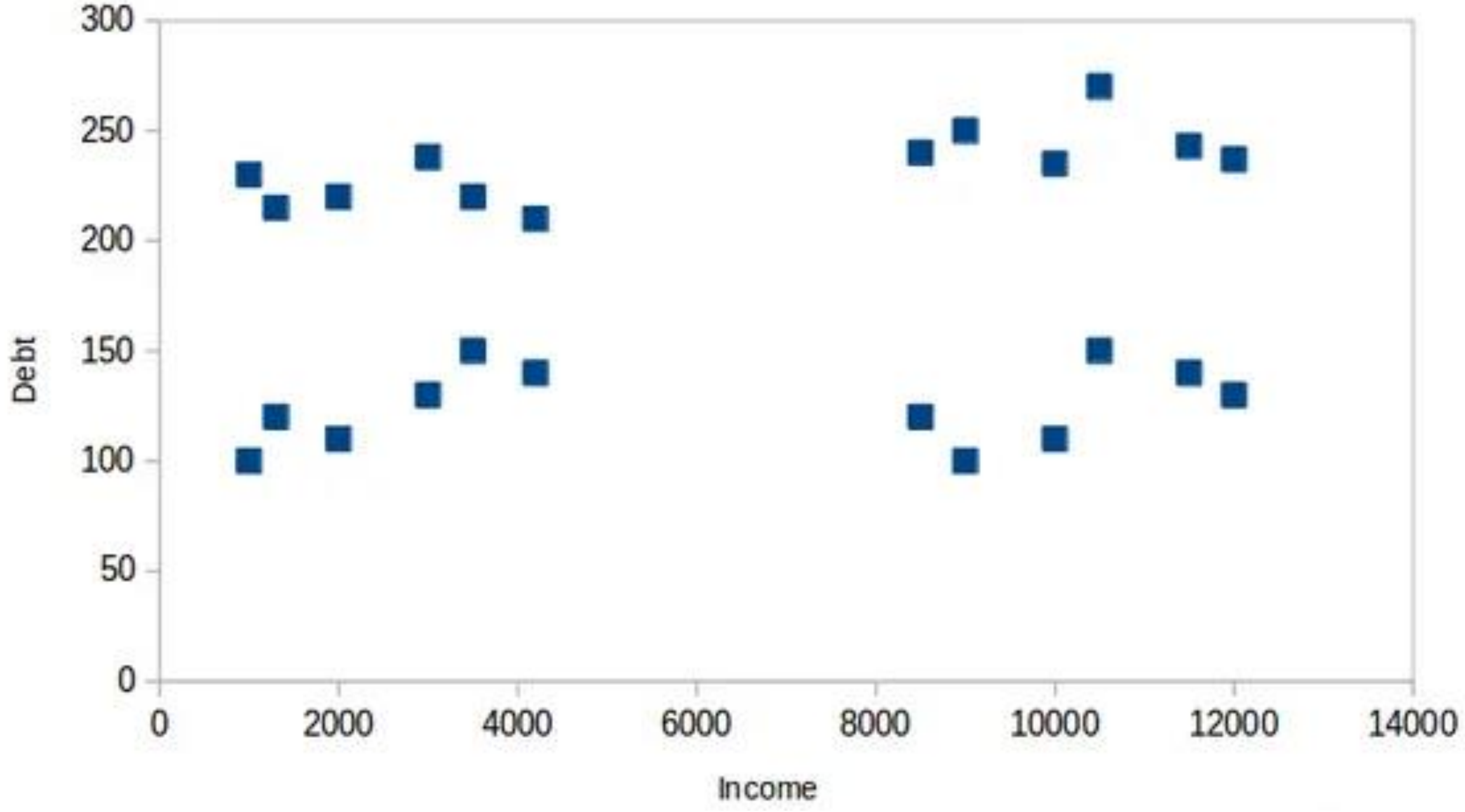
map new

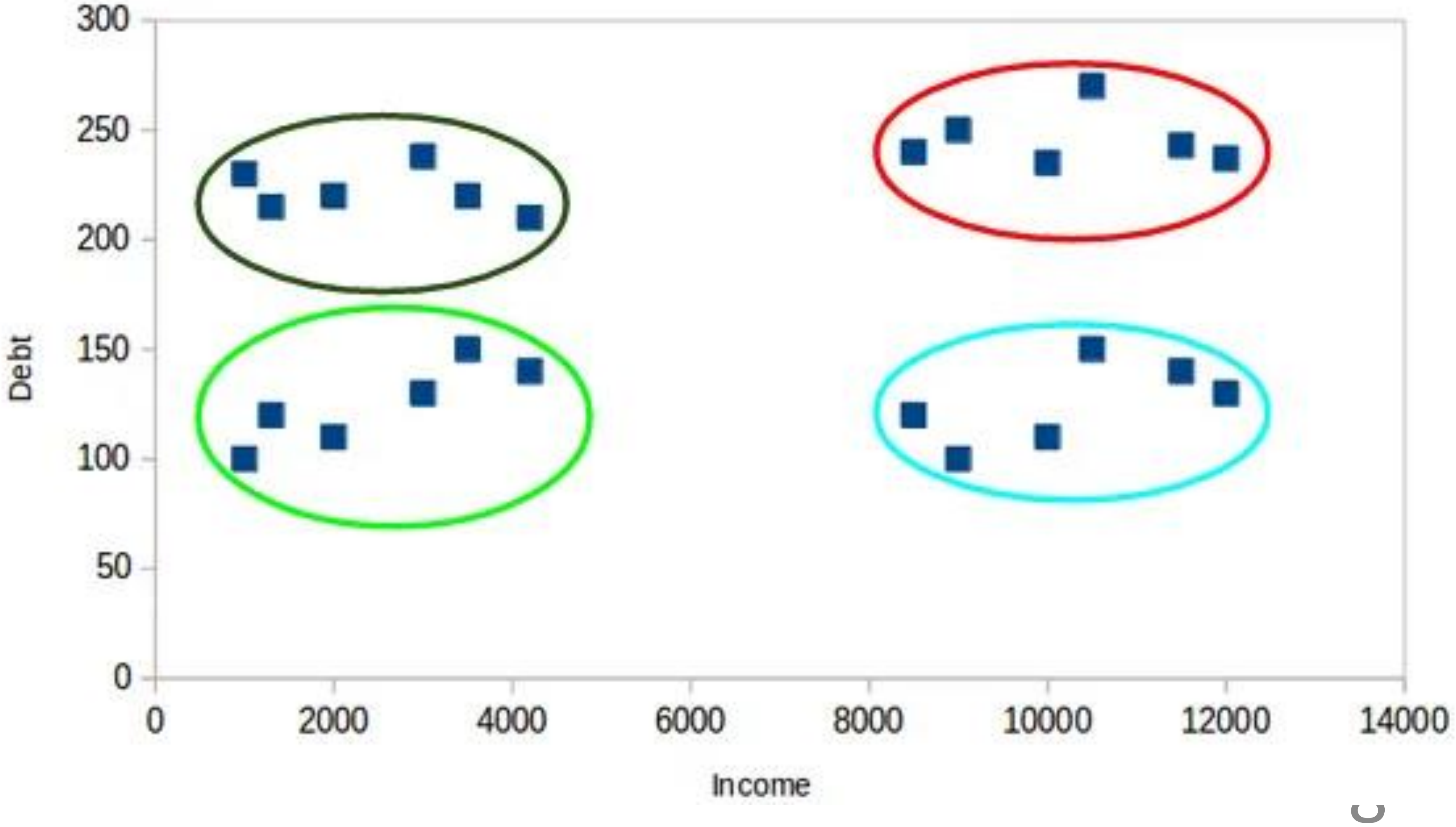
data to

structure

Clustering Intro

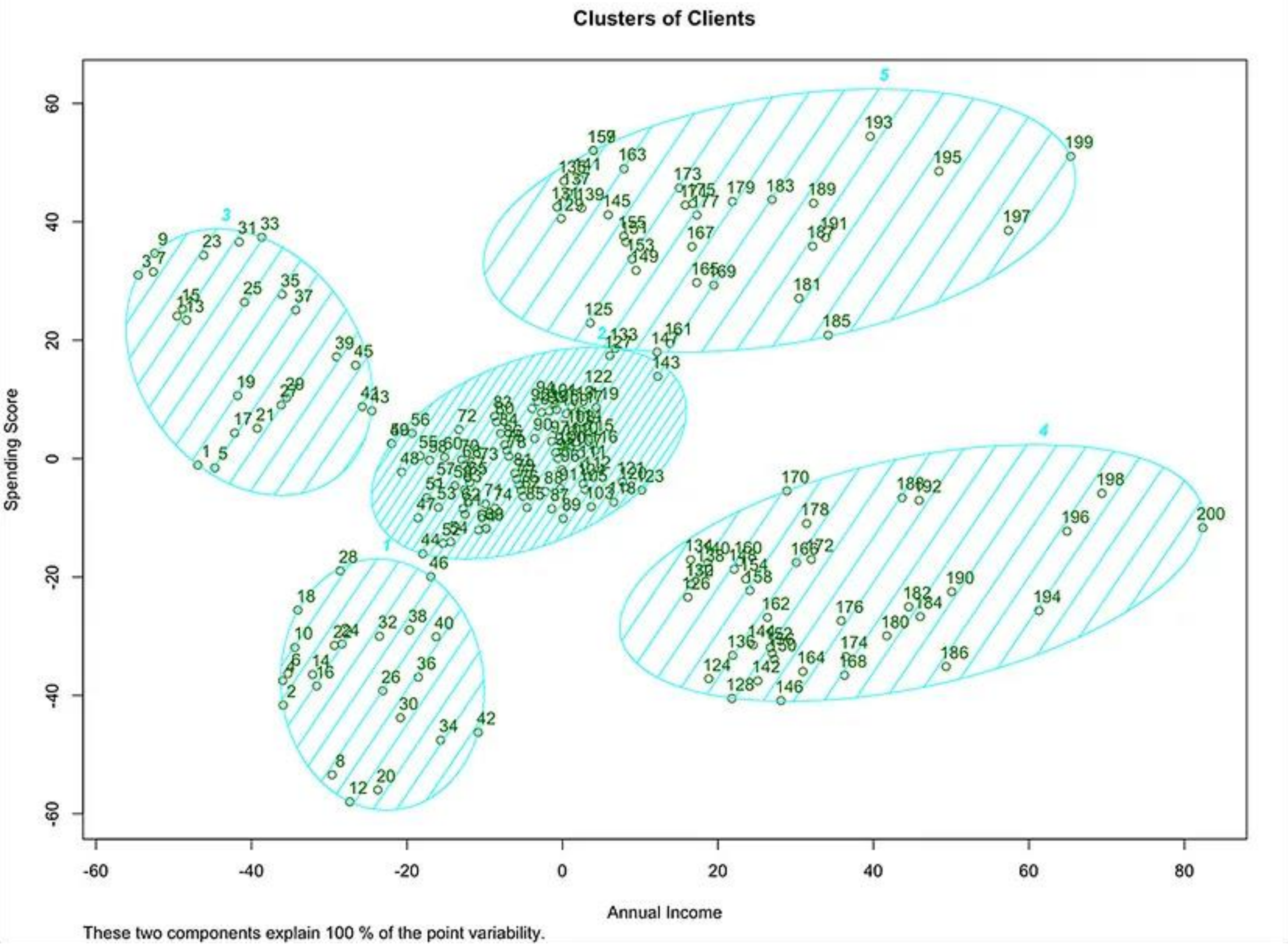
- Unsupervised Learning
  - No labels. Only data
- Dividing data into groups based on some underlying pattern





Clustering used in

- Customer segmentation
  - Targeted marketing & advertising
- Document clustering
- A computationally easy way for image segmentation
- Recommender systems


Clusters of Clients
Spending Score
Annual Income
60
40
20
0
-20
-40
-60
-60
-40
-20
0
20
40
60
80
1
2
3
4
5
9
31
33
23
3
7
15
11
13
25
35
37
39
45
19
29
27
17
21
41
43
1
5
159
163
135
141
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183
189
193
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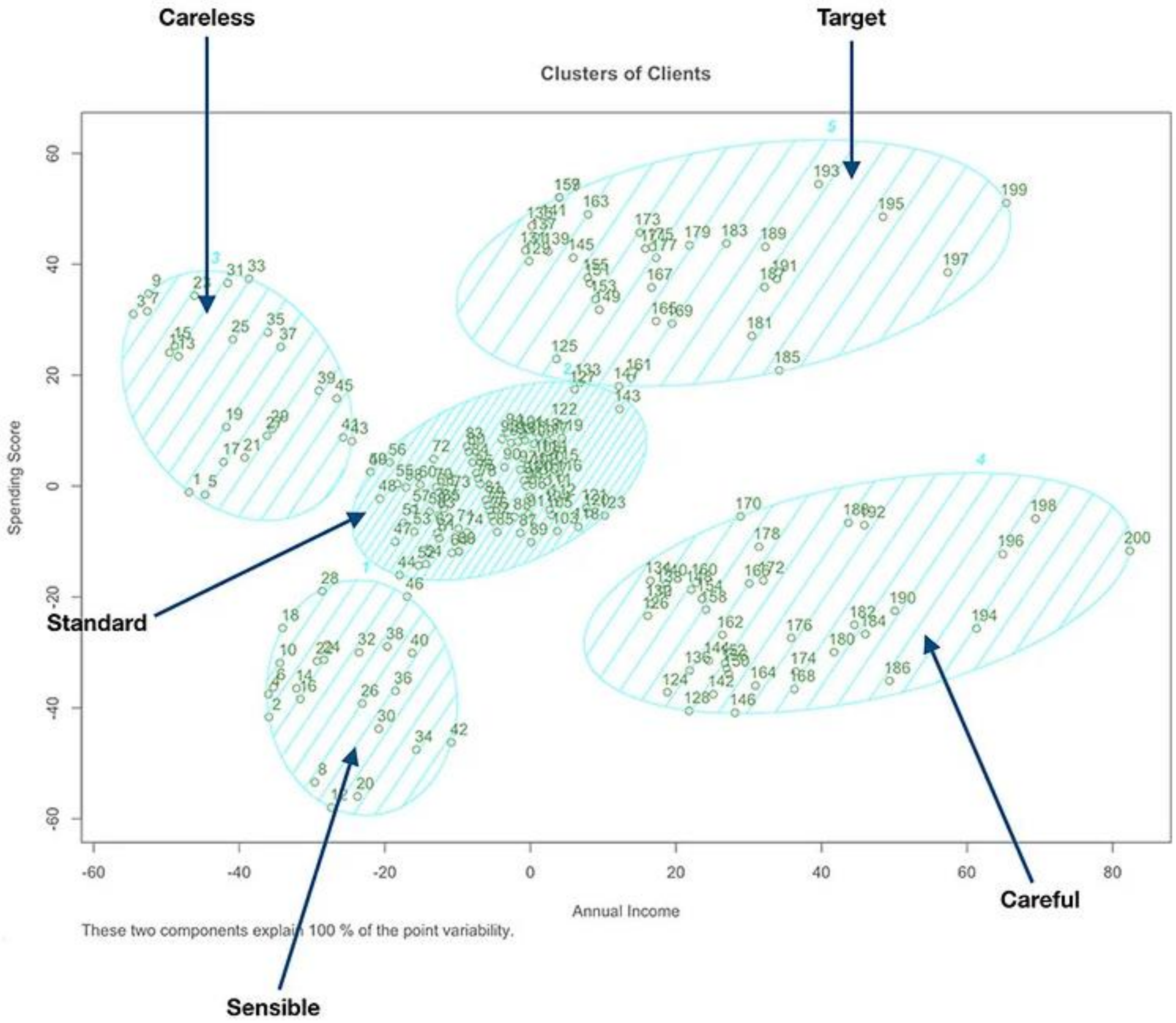
174
124
142
164
168
186
128
146
28
46
44
18
10
22
24
32
38
40
6
4
14
16
2
26
36
30
34
42
8
20
12
These two components explain 100 % of the point variability.



Careless

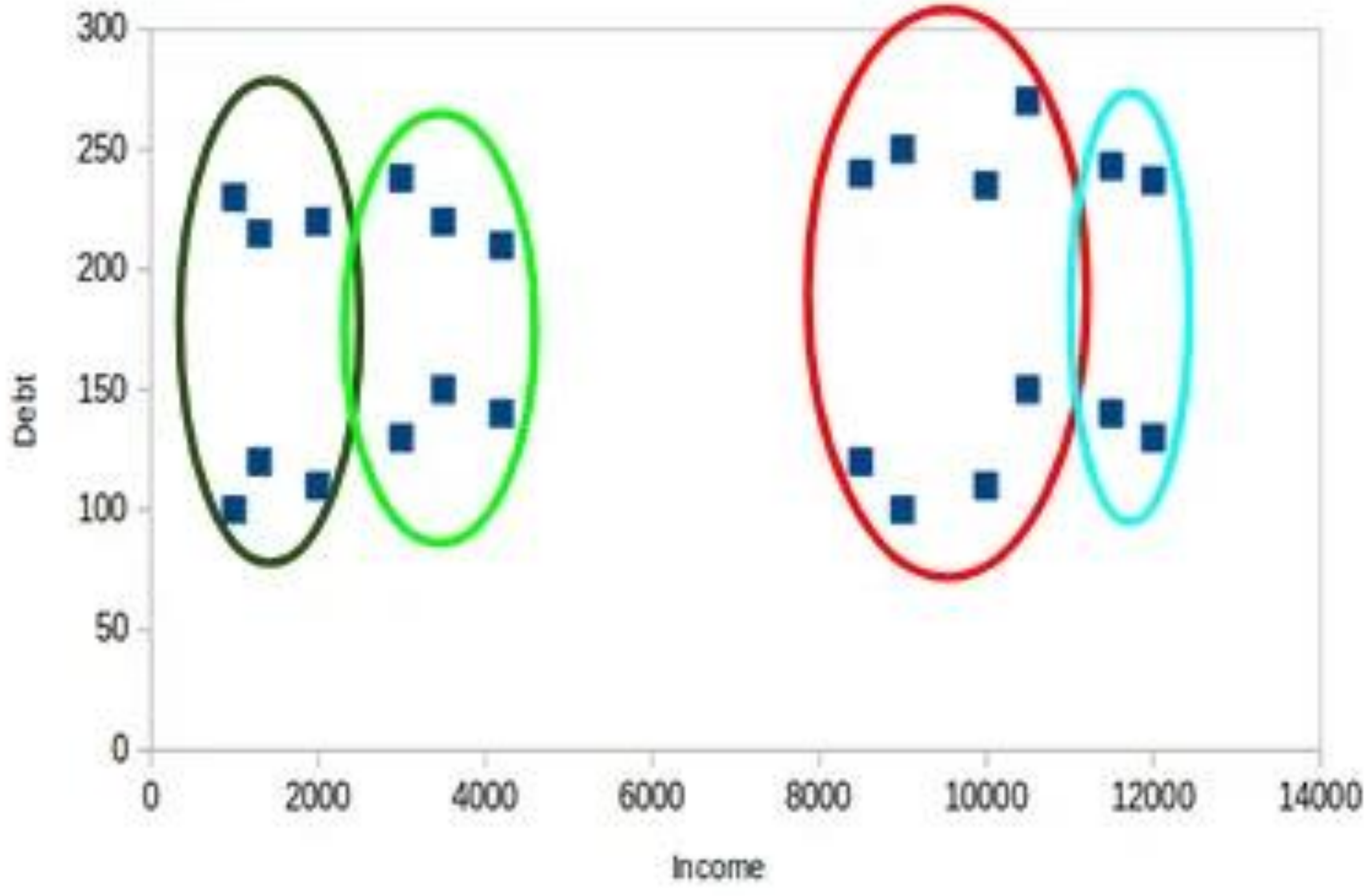
Target

Standard

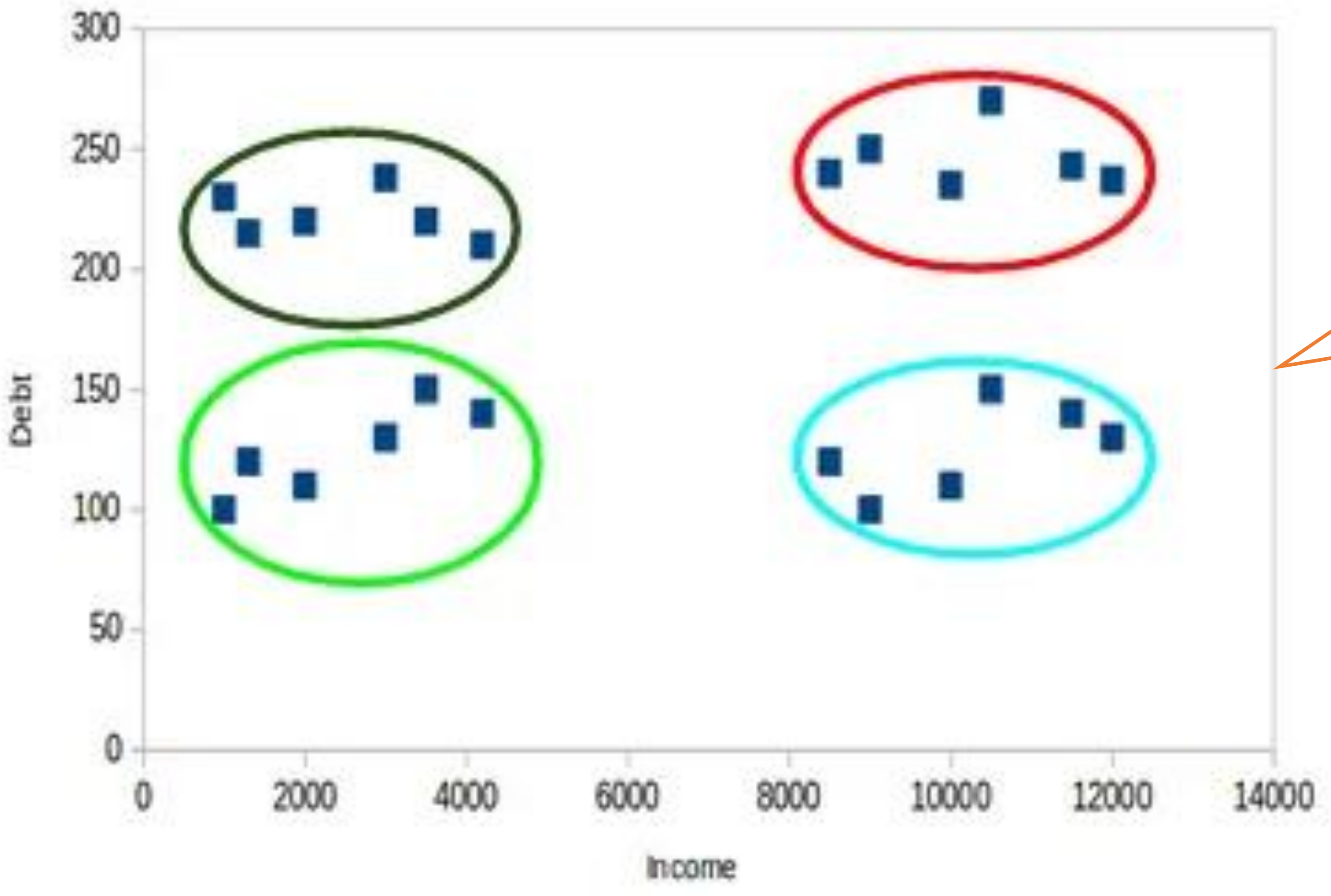
Careful

Sensible

Cluster properties



Case - I



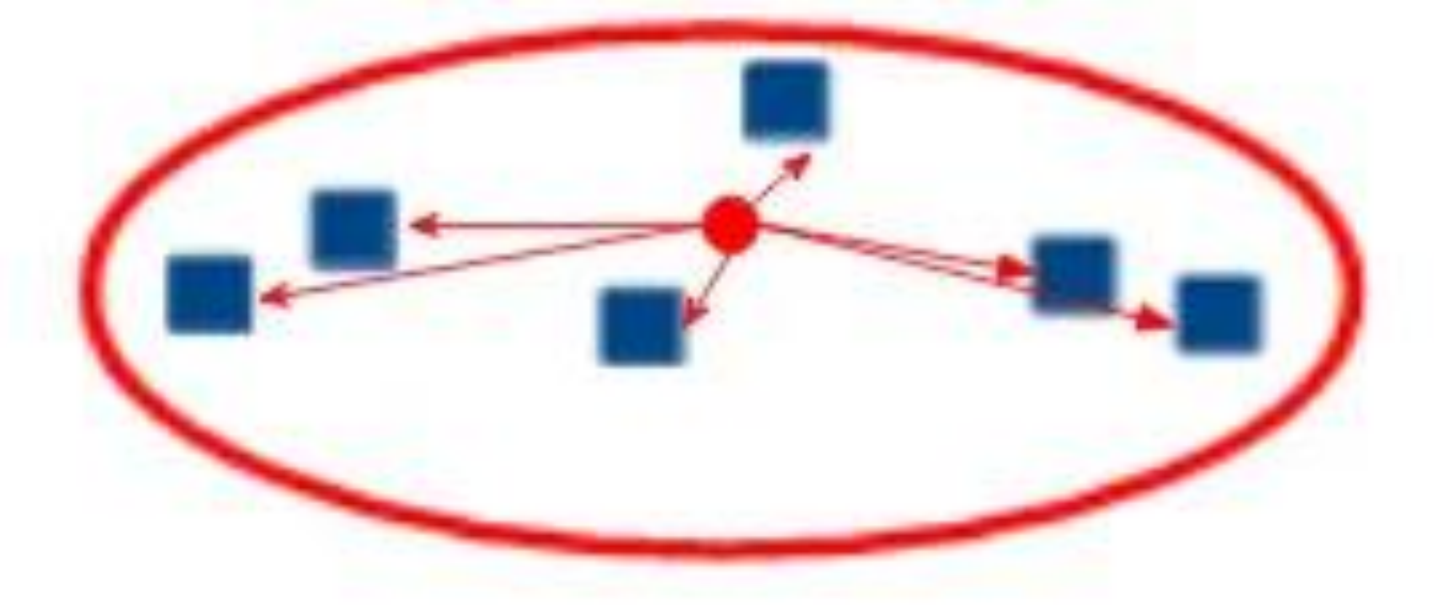
Case - II

Which is better cluster?

- Data points in cluster should have as many similar properties as possible (compactness)
- Data points in different clusters should be as different as possible (separation)

Cluster properties – Similar data points

- Data points in cluster should have as many similar properties as possible
- How to quantify this?
  - Distance between intra-cluster points should be as low as possible



Intra cluster distance

- Sum/avg of Euclidean distances from centroid

$$\frac{1}{|C_i|}\sum_{x\in C_i}(x-\mu_i)^2$$

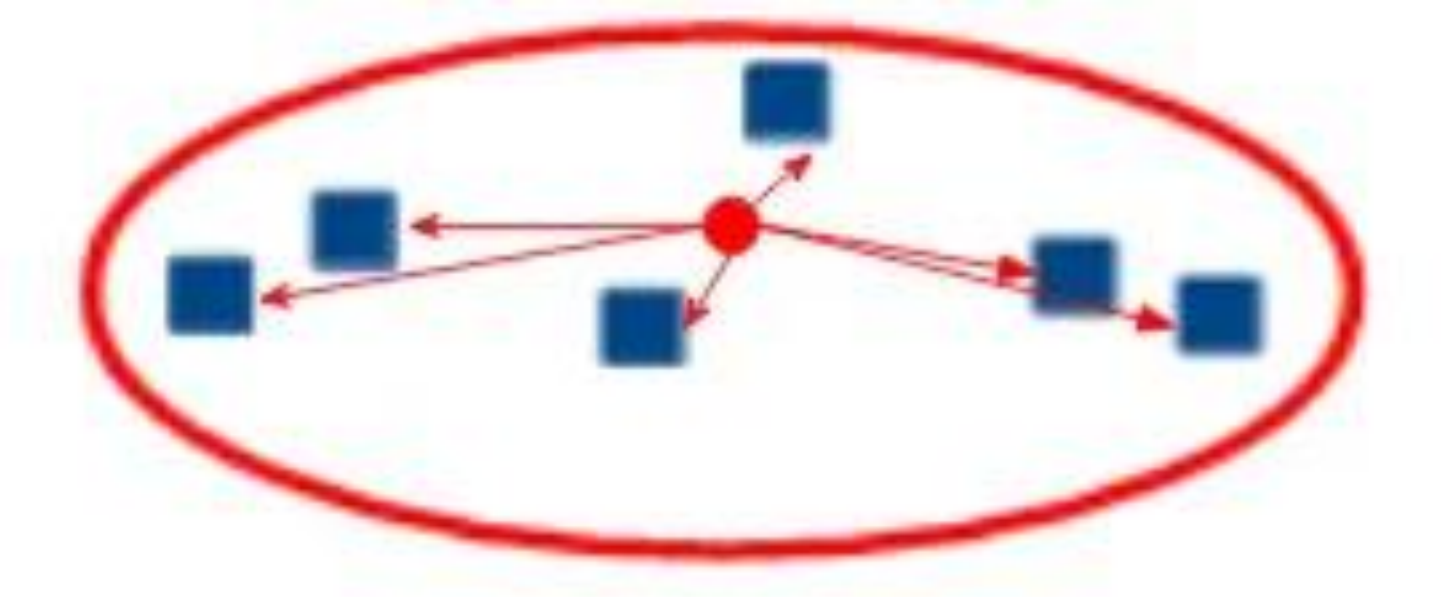
- This is nothing but variance
- Variance is a metric!

Cluster metric – Inertia

- How far the points are within a cluster

Optional normalizing term

$$\frac{1}{|C_i|}\sum_{x\in C_i}(x-\mu_i)^2$$



Intra cluster distance

- Across all clusters

$$Inertia = \frac{1}{k}\sum_{i=1}^{k}\frac{1}{|C_i|}\sum_{x\in C_i}(x-\mu_i)^2$$

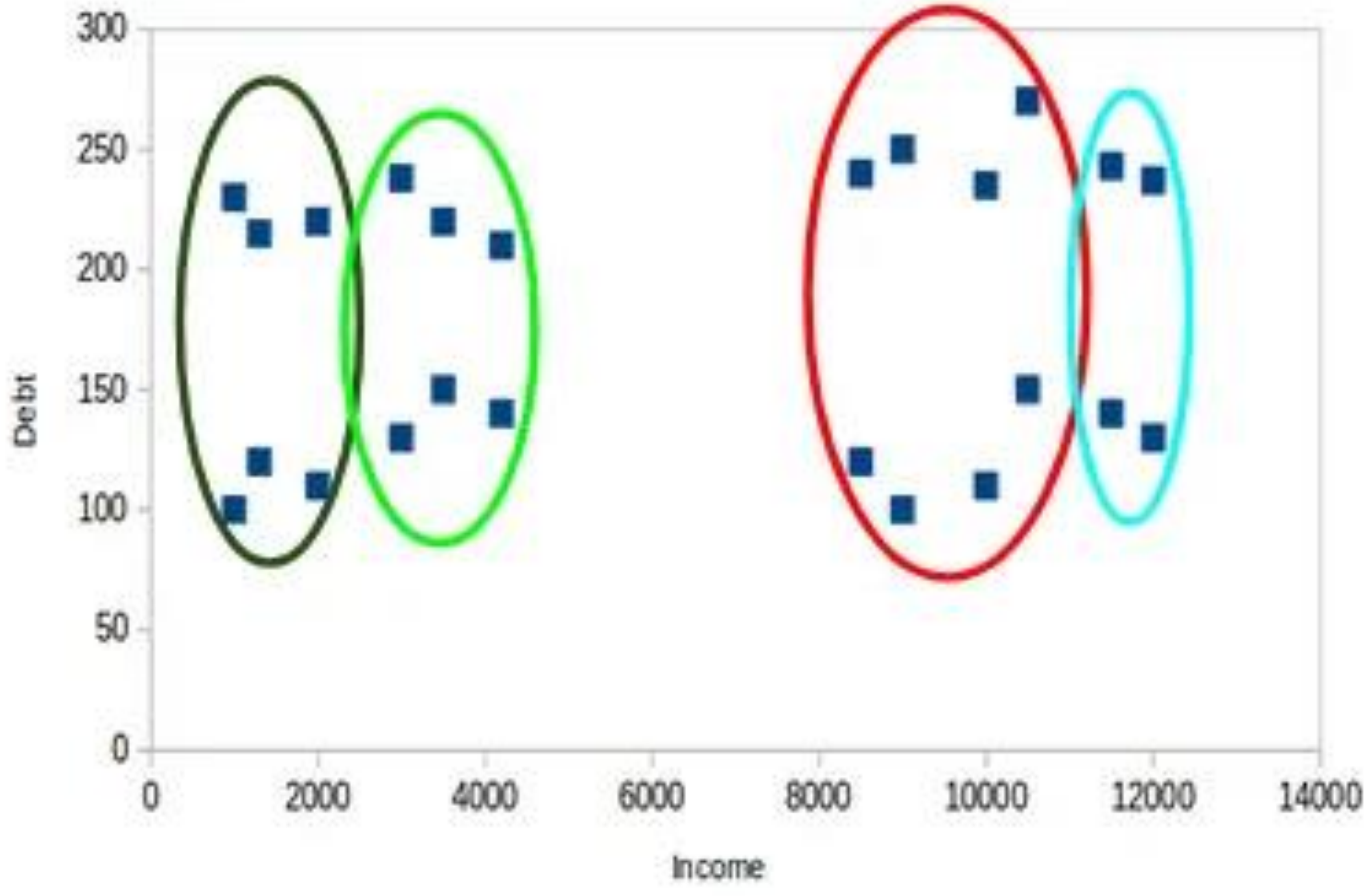
Also an optional normalizing term

$$\sum_{i=1}^{k}\sum_{x\in C_i}(x-\mu_i)^2$$

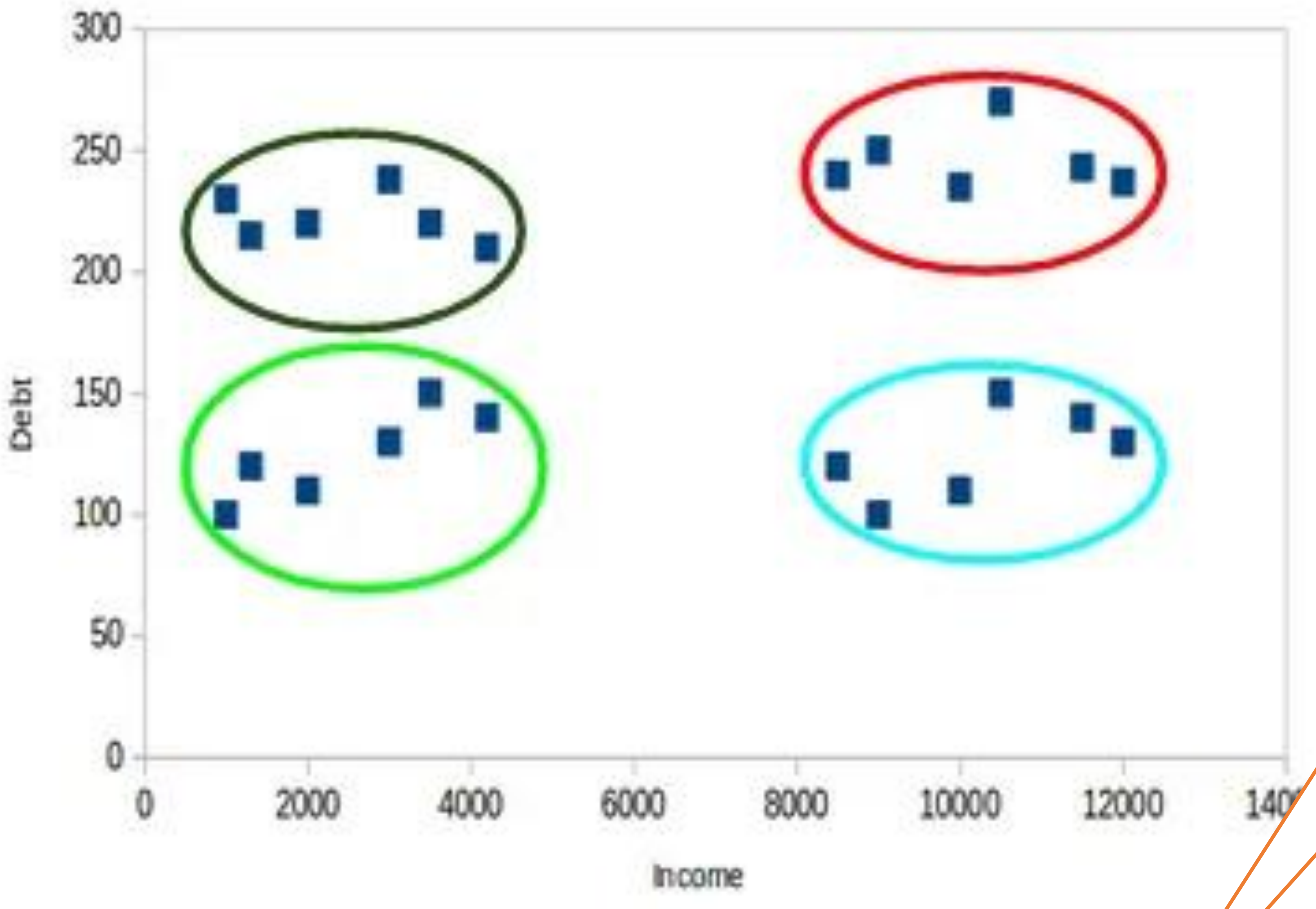
Sklearn calculates inertia without normalizing term

- Inertia also known as WCSS (Within cluster sum of squares)
- Low inertia = better cluster

Cluster metric - Recap



Case - I



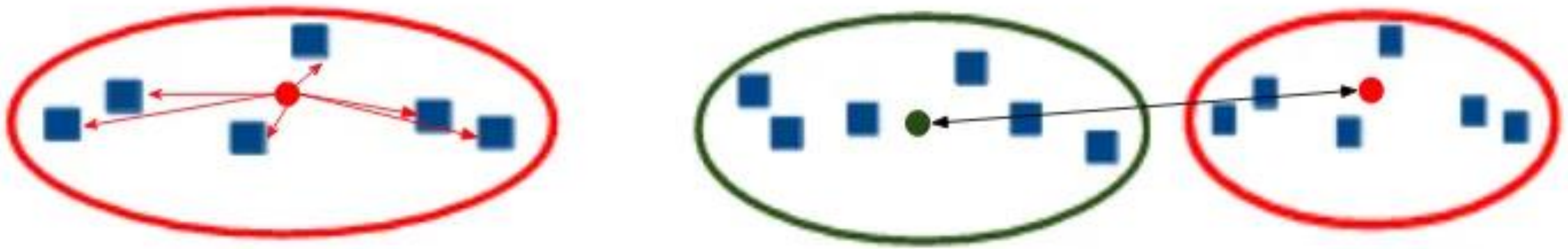
Case - II

Inertia only accounted for this

What about this?

- Data points in cluster should have as many similar properties as possible
- Data points in different clusters should be as different as possible

Cluster metric – Dunn Index

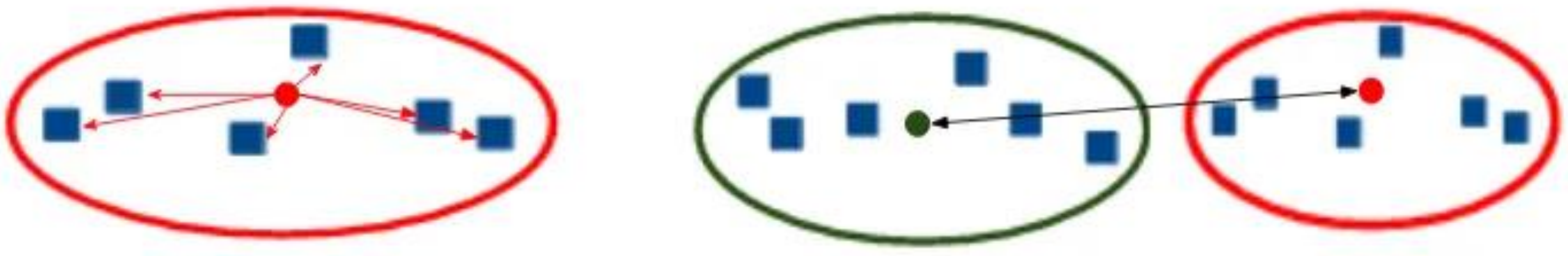


Intra cluster distance

Inter cluster distance

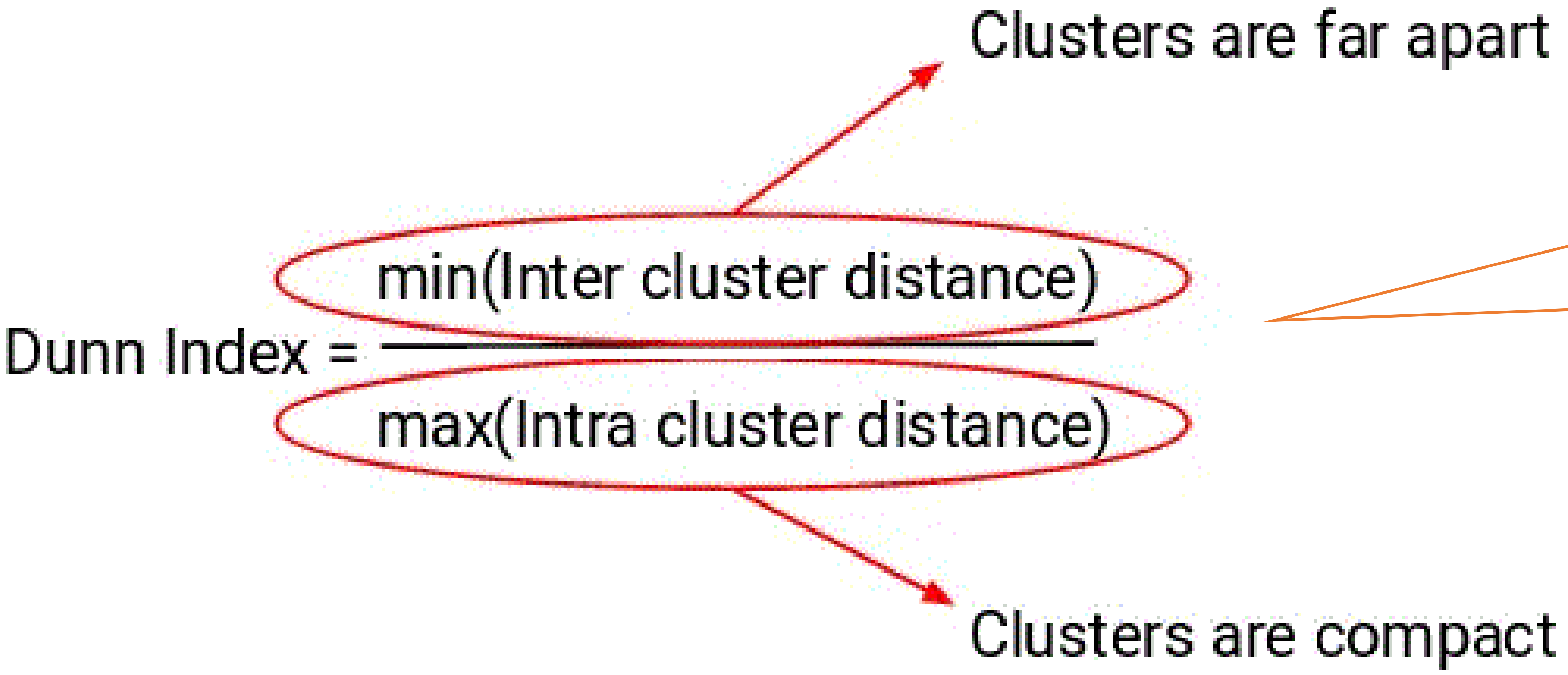
$$\text{Dunn Index} = \frac{\min(\text{Inter cluster distance})}{\max(\text{Intra cluster distance})}$$

Cluster metric – Dunn Index (one of many)



Intra cluster distance

Inter cluster distance



Clusters are far apart

$$\text{Dunn Index} = \frac{\text{min(Inter cluster distance)}}{\text{max(Intra cluster distance)}}$$

Clusters are compact

Dunn Index considers worst case of Davis Bouldin index

Cluster metrics recap

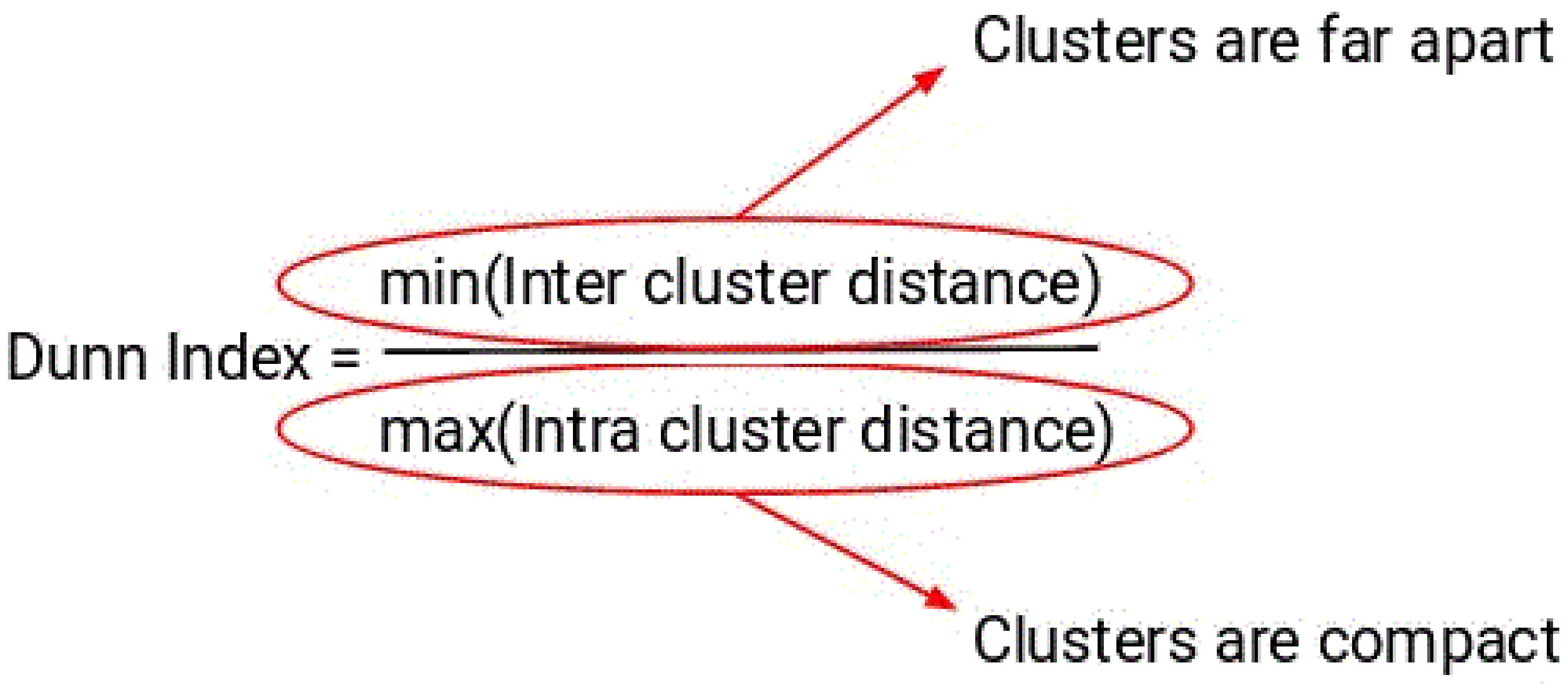
- Inertia (WCSS) – Lower the better

$$Inertia = \frac{1}{k}\sum_{i=1}^{k}\frac{1}{|C_i|}\sum_{x\in C_i}(x-\mu_i)^2$$

Used for choosing K

- Dunn Index – Higher the better

Used for cluster evaluation



$$\text{Dunn Index} = \frac{\text{min(Inter cluster distance)}}{\text{max(Intra cluster distance)}}$$

Clusters are far apart

Clusters are compact

Selecting the best K for clustering

- Selecting by Cross validation with one of:
  - Elbow method
  - Silhouette score
  - Gap Statistic (not part of syllabus)
- Davis-Bouldin Index, Dunn Index not used
- Cluster Validation Indices (CVI)
  - Internal Validation Indices
  - External Validation Indices
  - Relative Validation Indices

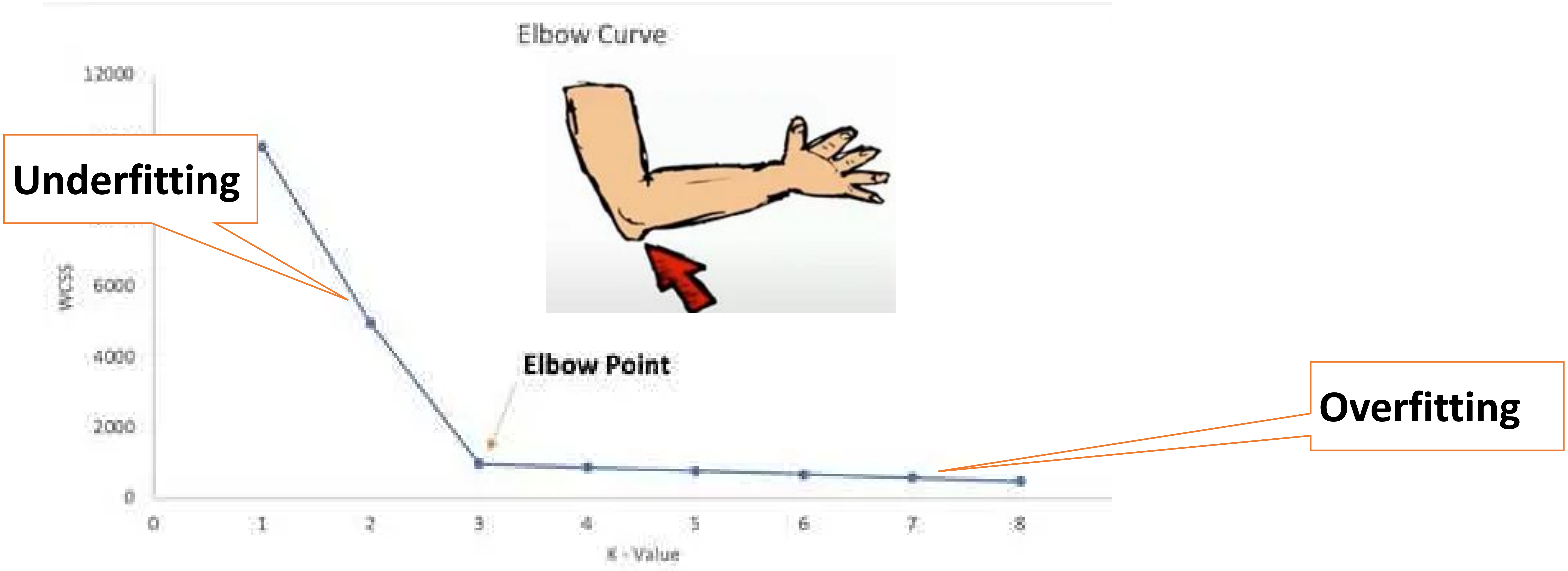
Relies on cluster goodness labels to measure clustering efficacy

Relies on labels to measure clustering efficacy

For choosing K, Internal validation index should also function as a good relative validation index

Selecting the best k with elbow method

Elbow plot

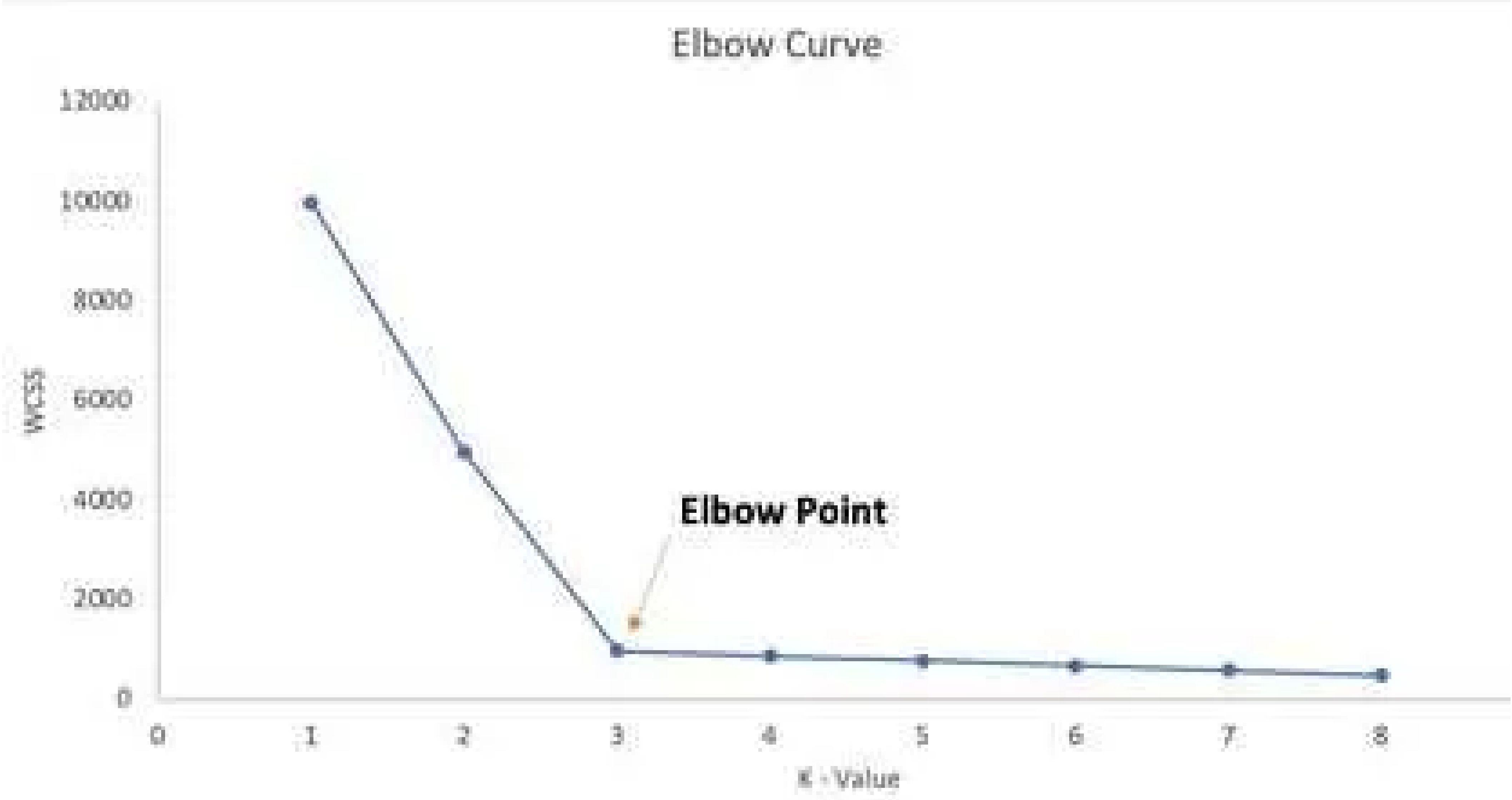


Underfitting

Overfitting

- Increasing k decreases inertia. But is it worth it?
- Cost of tuning parameter is no longer worth the benefit

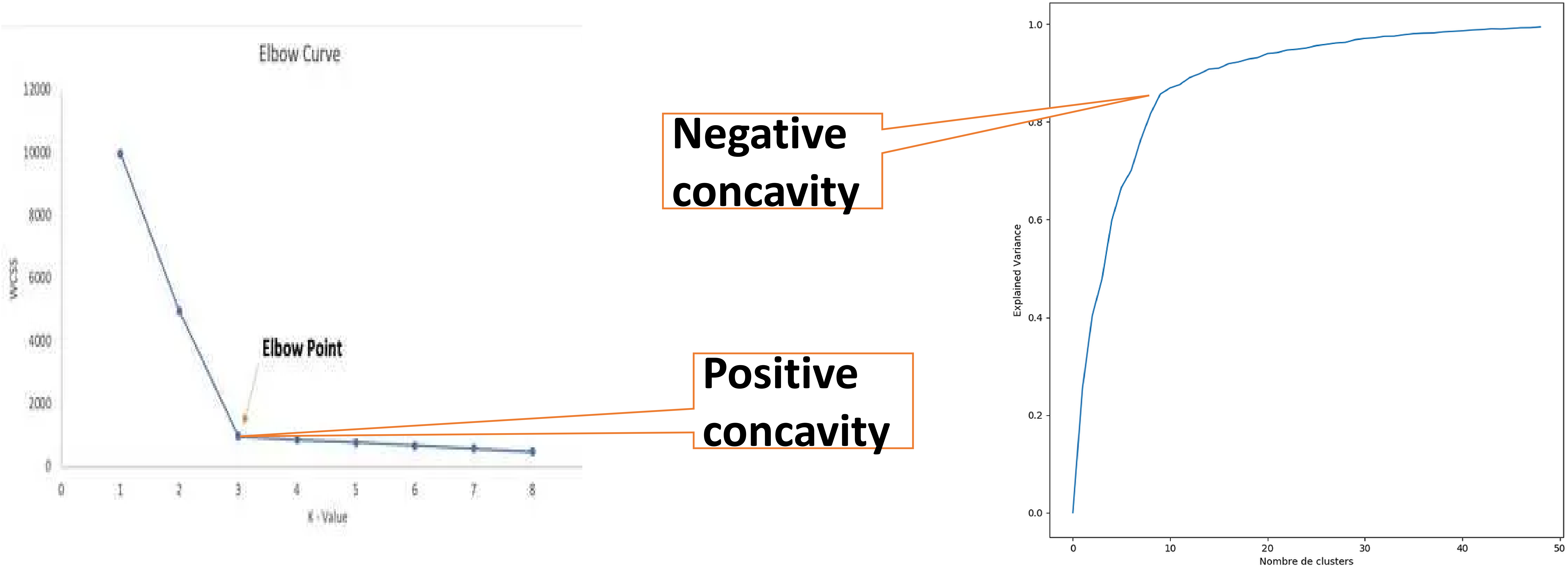
Elbow plot: Cons



- Needs visual examination
- Not possible in automated environments

Knees & Elbows

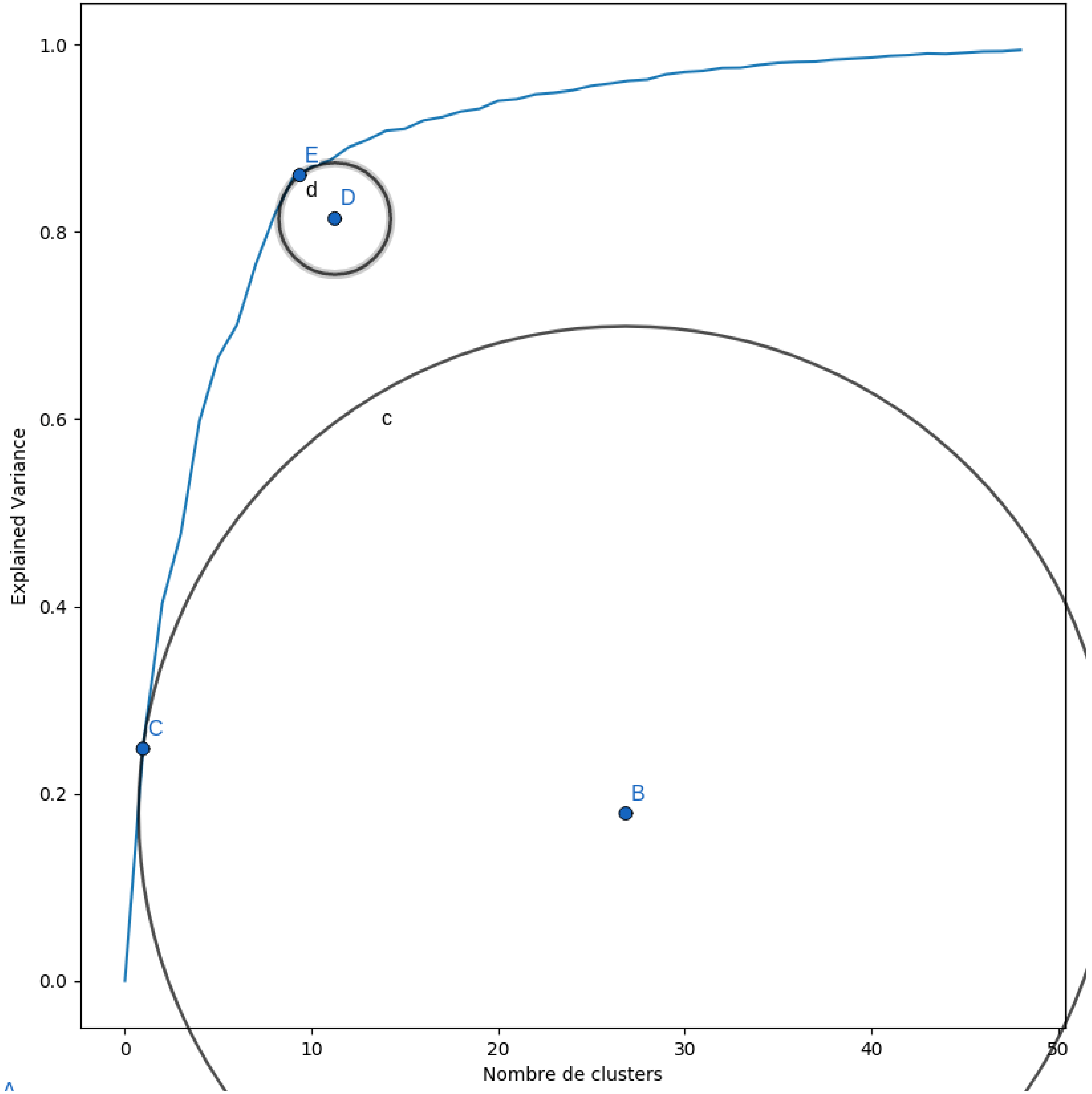
- Automated detection based on curvature
- Elbow – Decrease in rate of decrease of WCSS
- Knee – Decrease in rate of increase of “explained variance”



Negative concavity

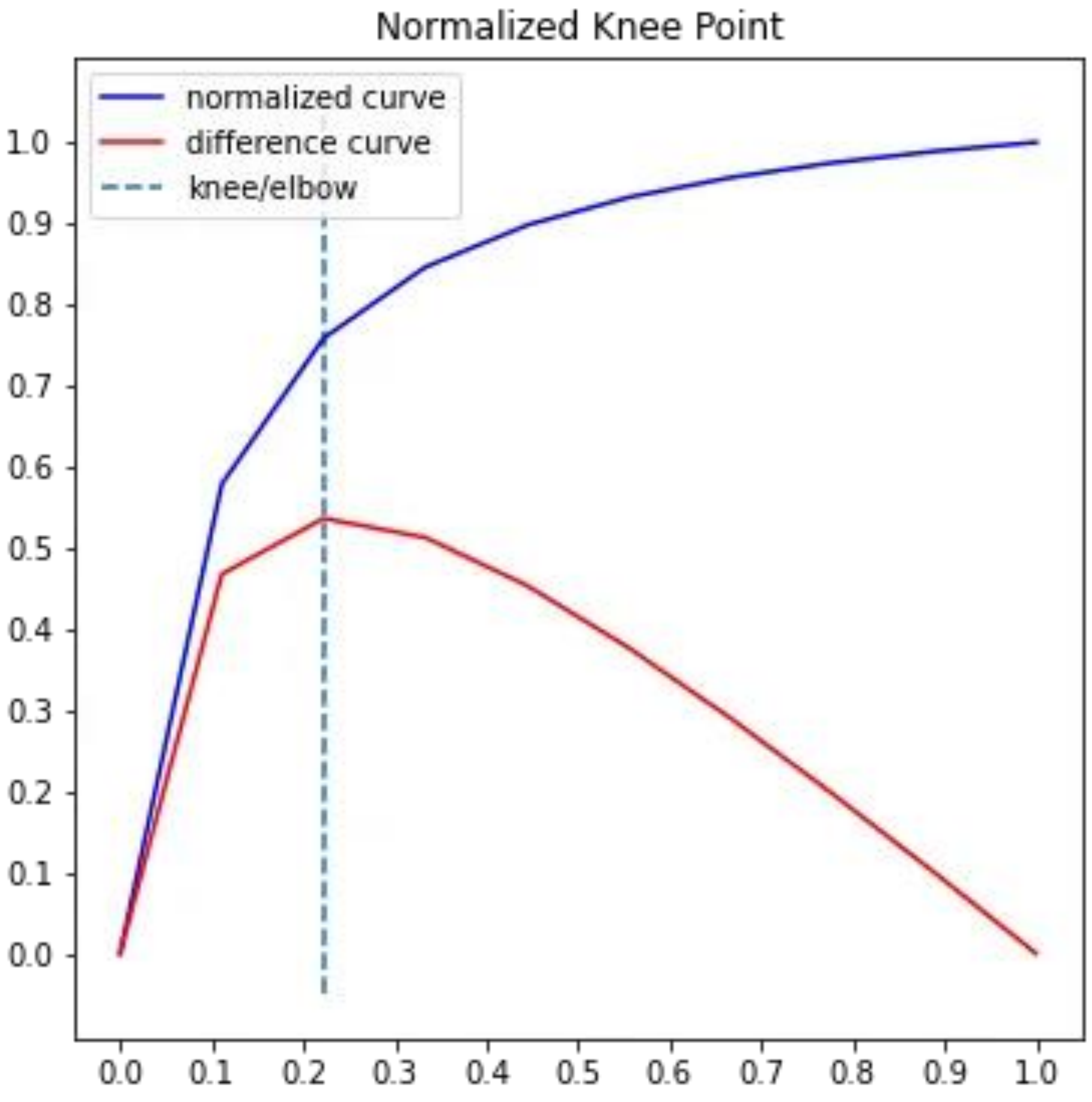
Positive concavity

Curvature at Knees & Elbows



- Curvature: Draw **largest** circle where the tangent touches the curve
    - Such that circle touches the curve only at one point
- Smaller the circle, larger the curvature
- Knees & elbows – Region where curvature is most drastic

Curvature at Knees & Elbows conceptually

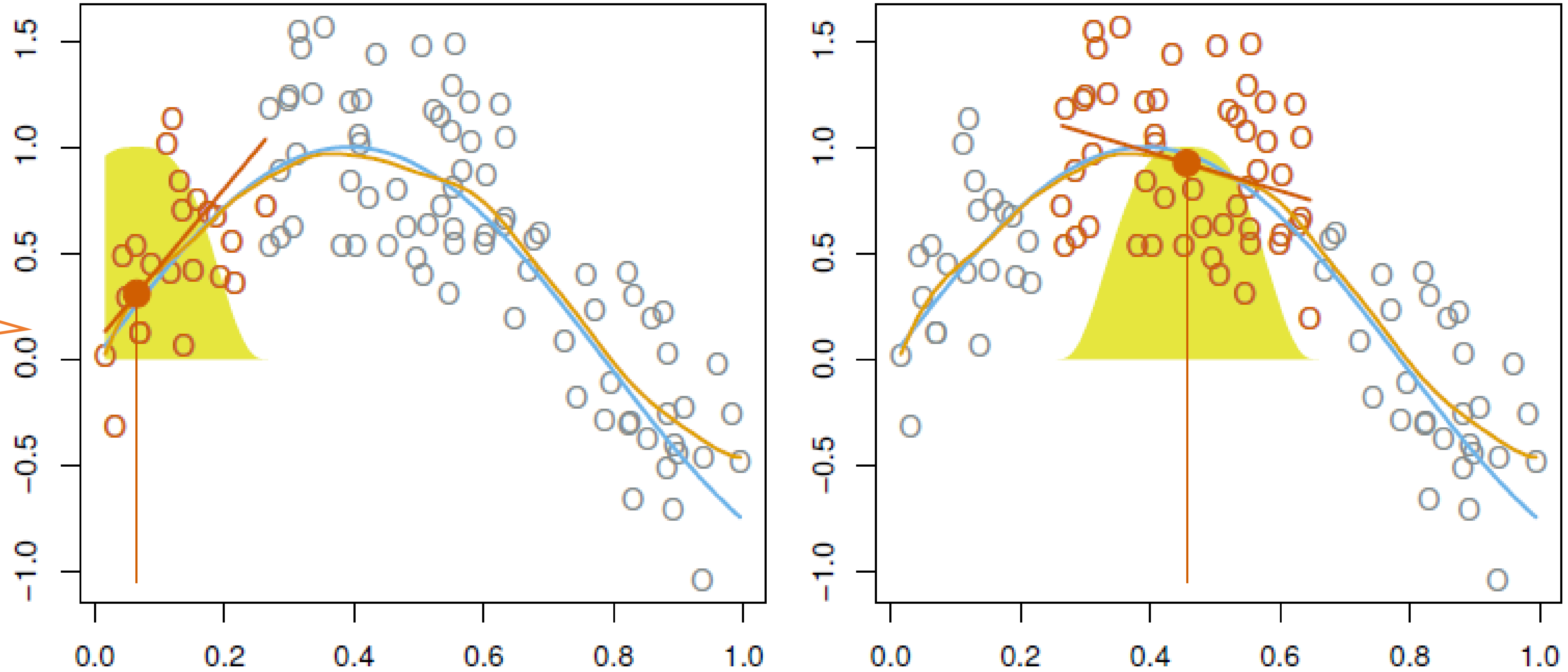


- Second derivative
- Knee – Maxima of second derivative
- Elbow – Minima of second derivative
- Kneed library available
- Based on paper IEEE
- Finding a Kneedle in haystack
- Paper is slightly more involved than simple second derivative

Problems to address in applying kneedle

- Need to find second derivative. Knots aren't differentiable
- Smoothing spline should be applied first
- Smoothing spline = Regression Spline + Regularization
- Regression Spline = Piecewise continuous polynomial regression

Learn more about spline in Intro to Statistical Learning in Gareth, Tibshirani etal.



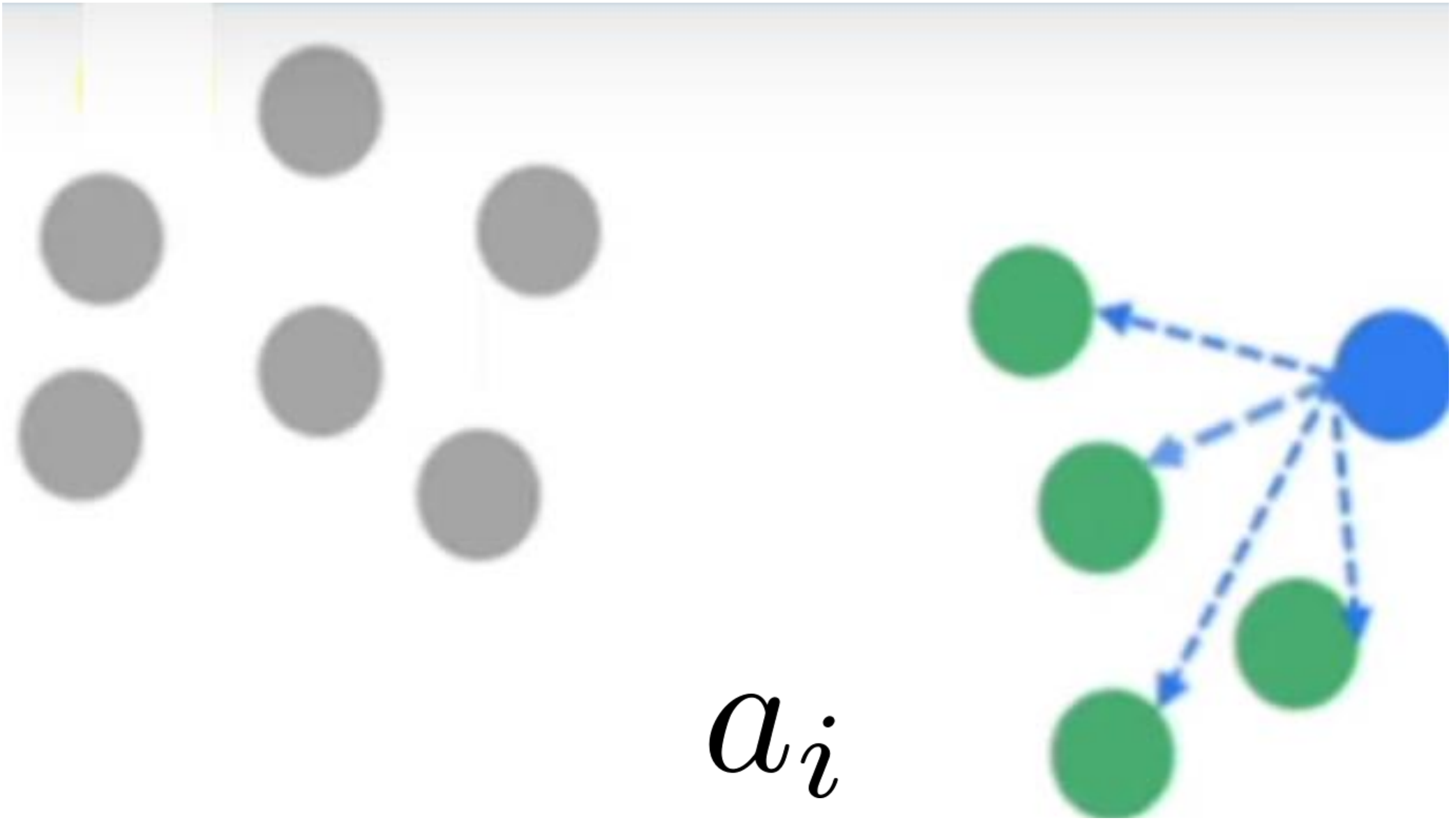
Selecting the best k with Silhouette score

Silhouette score intuition

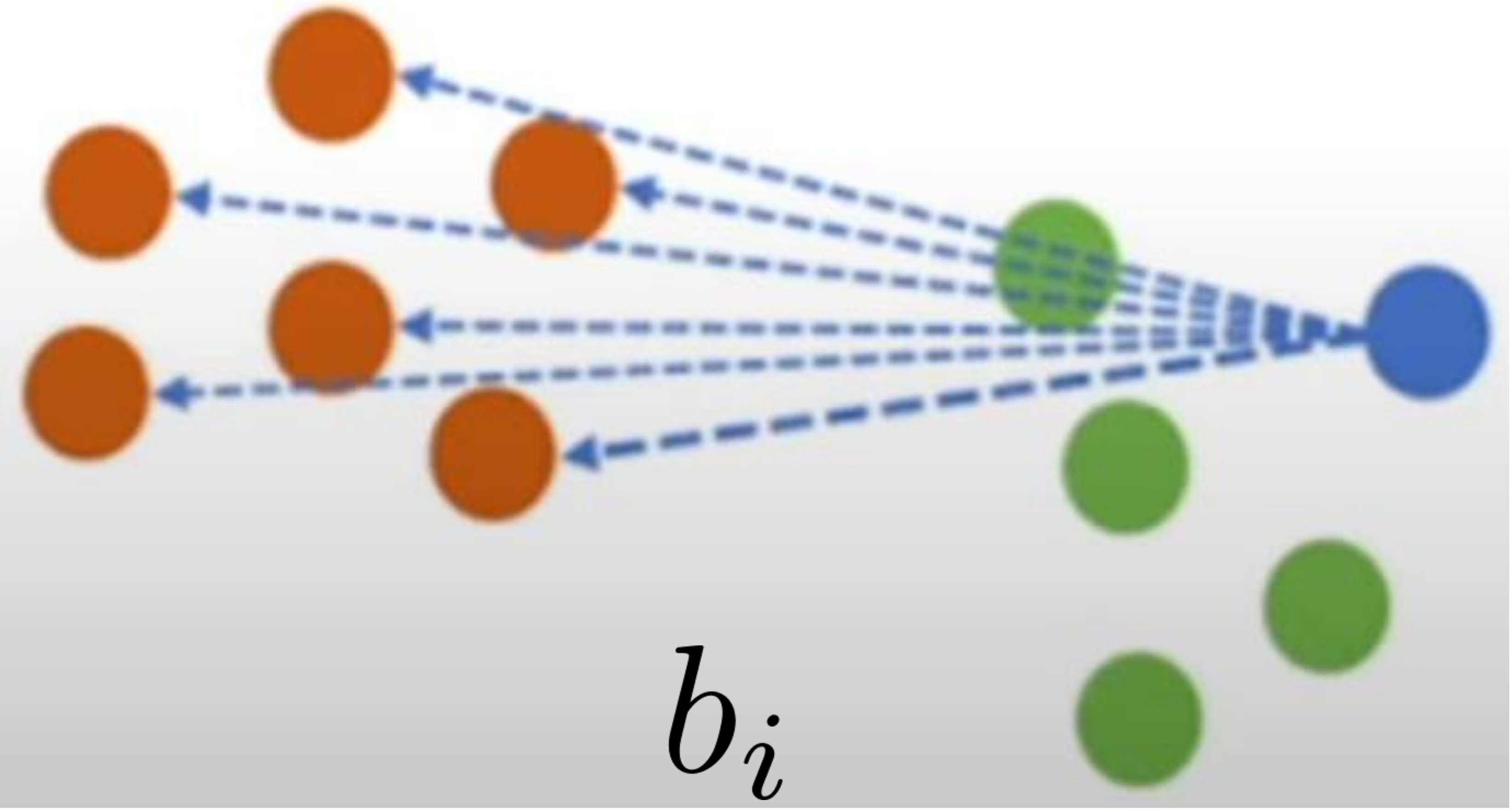
- Overall representative score of clustering using
  - Compactness of individual clusters (intra cluster distance)
  - Separation between clusters (inter cluster distance)
- Uses both intra cluster cohesion & inter cluster separation

$$s_i = \frac{b_i - a_i}{max(b_i, a_i)}$$

Silhouette score intuition



Avg distance between i & data points in same cluster

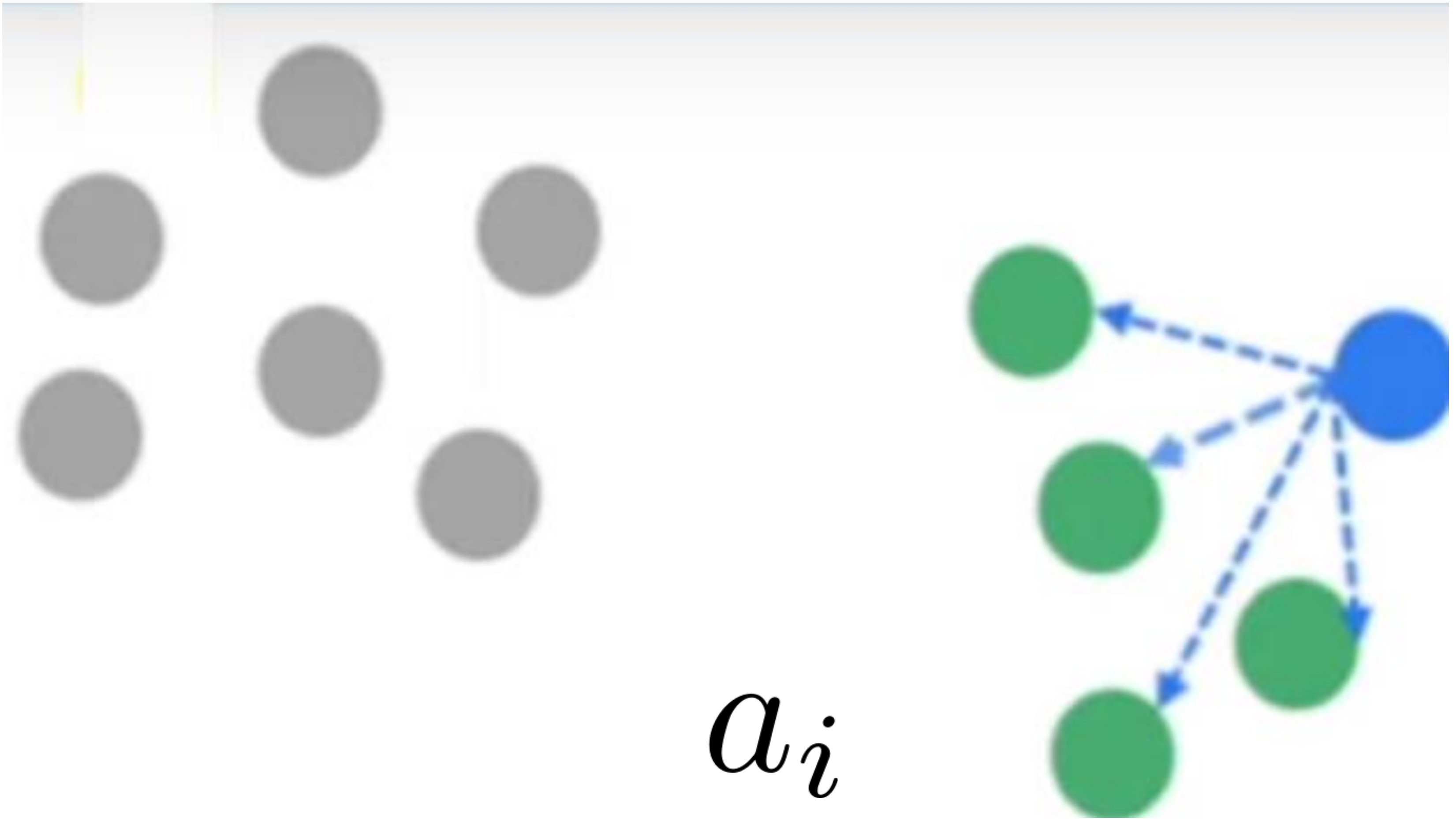


Avg distance between i & data points in other clusters

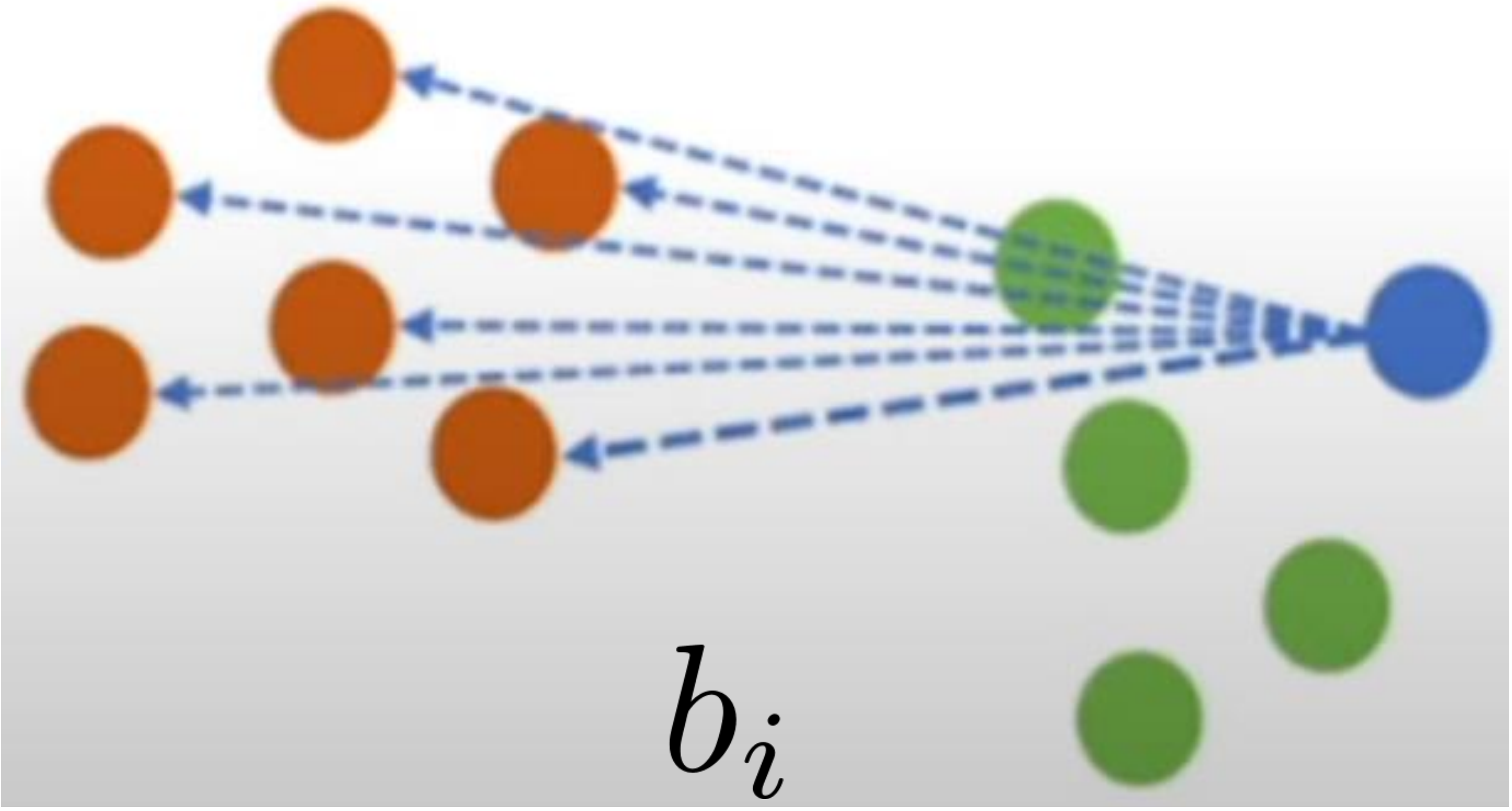
$$s_i = \frac{b_i - a_i}{max(b_i, a_i)}$$

- Measured for each data point
- Between -1 and +1

Silhouette score intuition (contd.)



Avg distance between i & data points in same cluster



Avg distance between i & data points in other clusters

$$s_i = \frac{b_i - a_i}{max(b_i, a_i)}$$

$$Silhouette - Score = \frac{1}{n}\sum_{i=1}^{n} s_i$$

Silhouette score summary

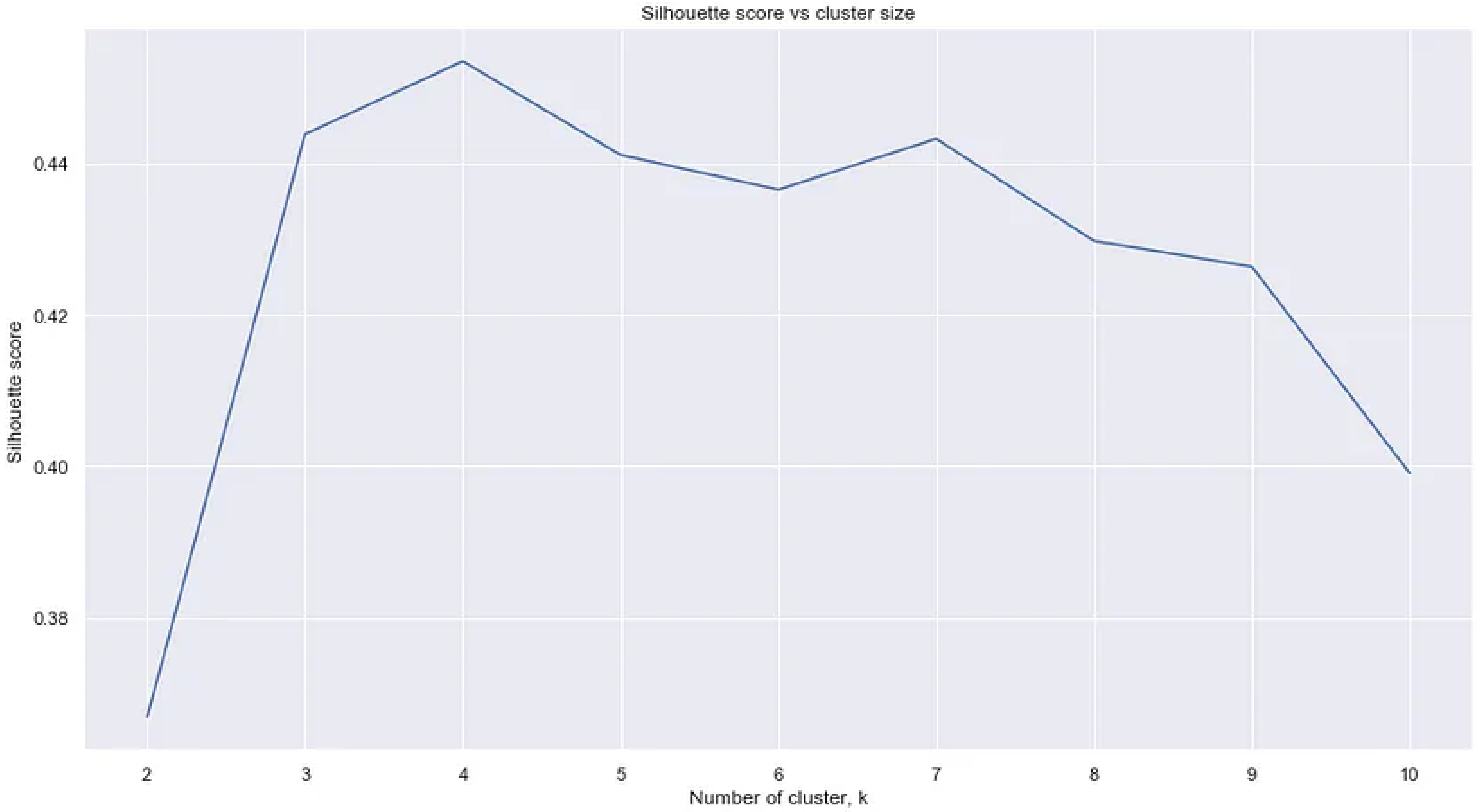
$$s_i = \frac{b_i - a_i}{max(b_i, a_i)}$$

$$a_i = \frac{1}{|C_i| - 1} \sum_{j \in C_i, i \neq j} d(i, j) \qquad b_i = \min_{k \neq i} \frac{1}{|C_k|} \sum_{j \in C_k} d(i, j)$$

$$Silhouette - Score = \frac{1}{n} \sum_{i=1}^{n} s_i$$

- Implementation available in sklearn

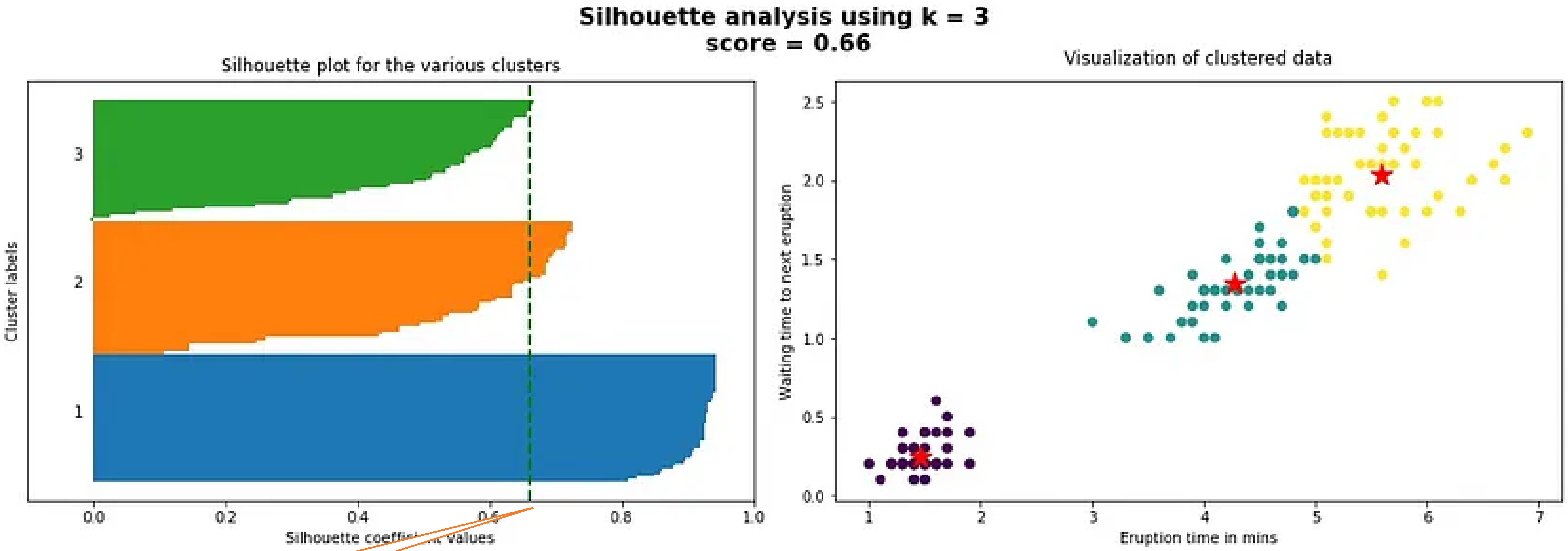
Silhouette score plot



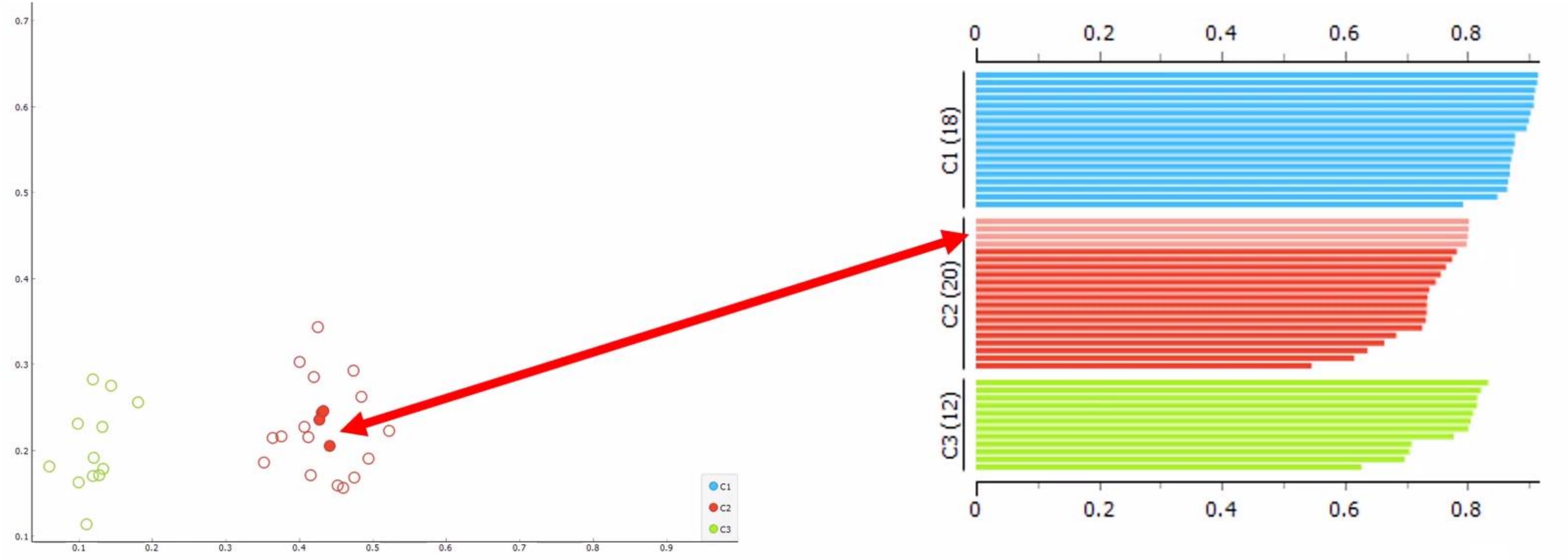
- Choose k with largest Silhouette score

Silhouette analysis with silhouette plot

- How to read a silhouette plot?



Silhouette score (avg)


0.7
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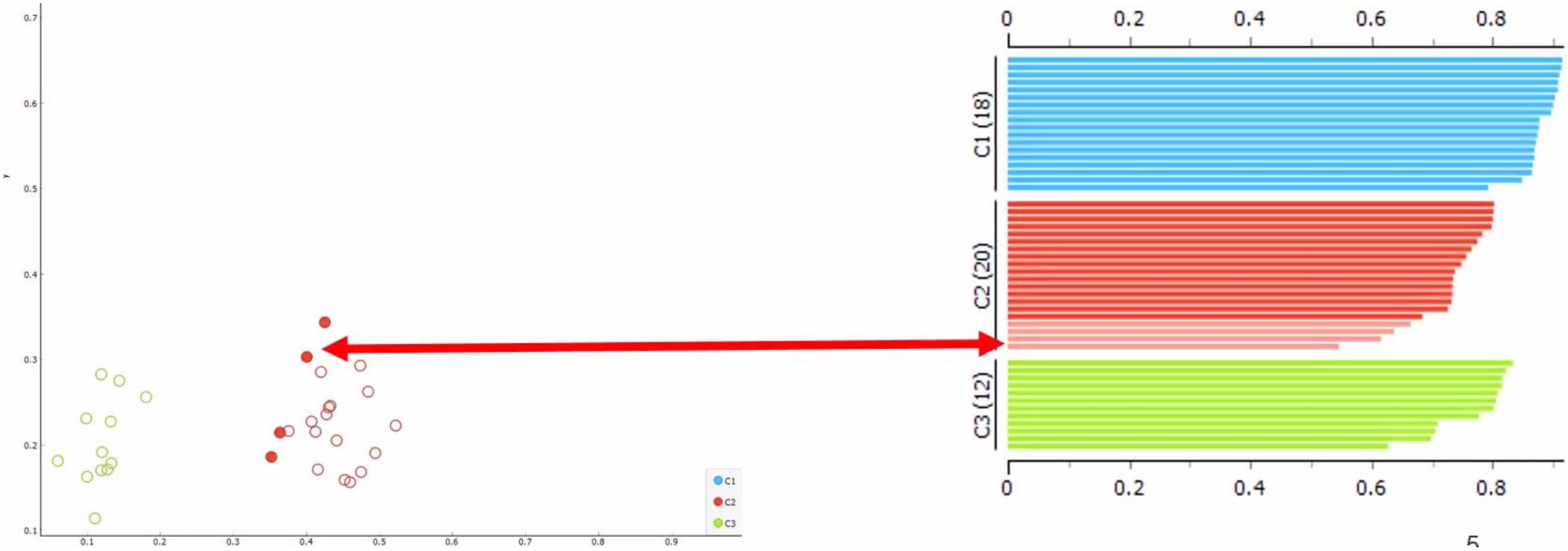
0.5
0.4
0.3
0.2
0.1
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
C1
C2
C3
0
0.2
0.4
0.6
0.8
C1 (18)
C2 (20)
C3 (12)
0
0.2
0.4
0.6
0.8



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C1
C2
C3
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C1 (18)
C2 (20)
C3 (12)
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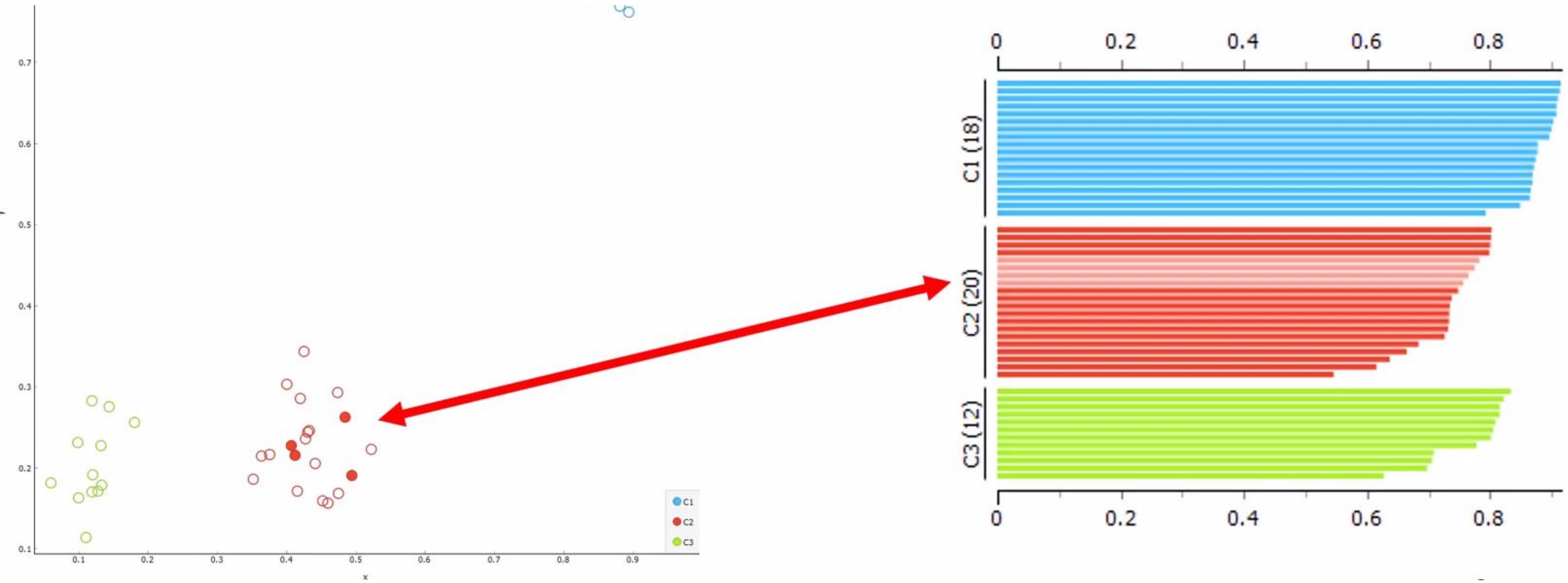
5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C1
C2
C3
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C1 (18)
C2 (20)
C3 (12)
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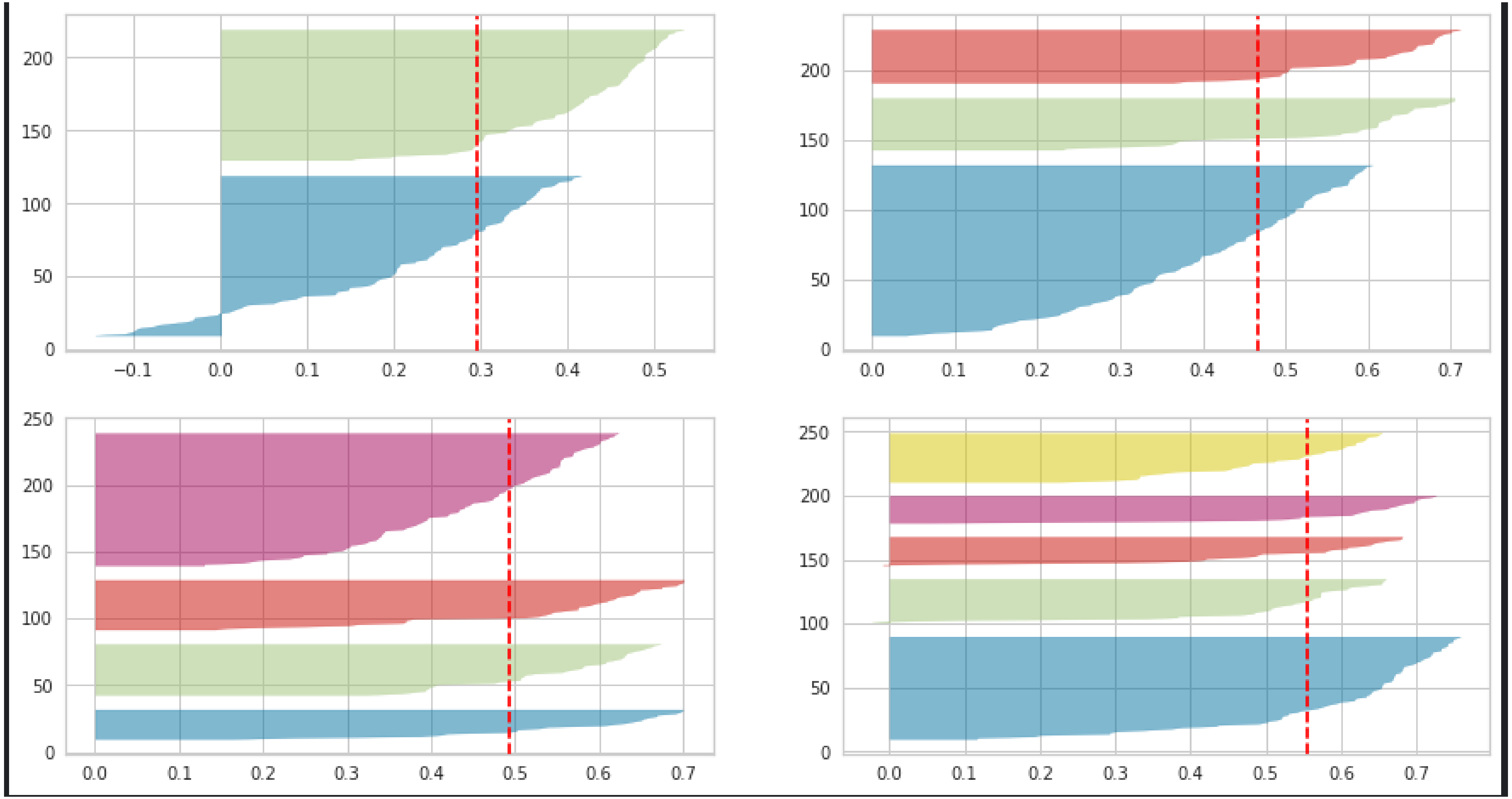
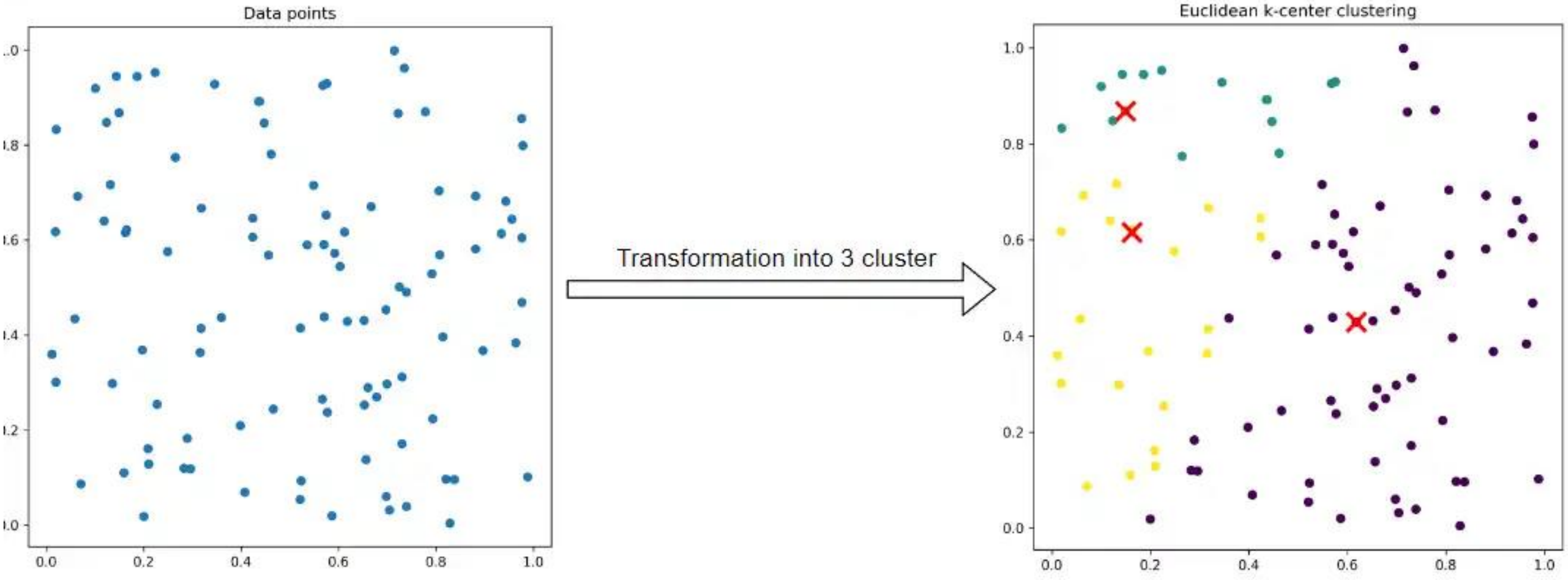


- Sub optimal cluster will show
  - Clusters below avg. score
  - Wide fluctuation in plot

P, NP, NP-hard, NP-complete refresher & clustering complexity

K-means demo

What is the cost of K-Center Clustering?

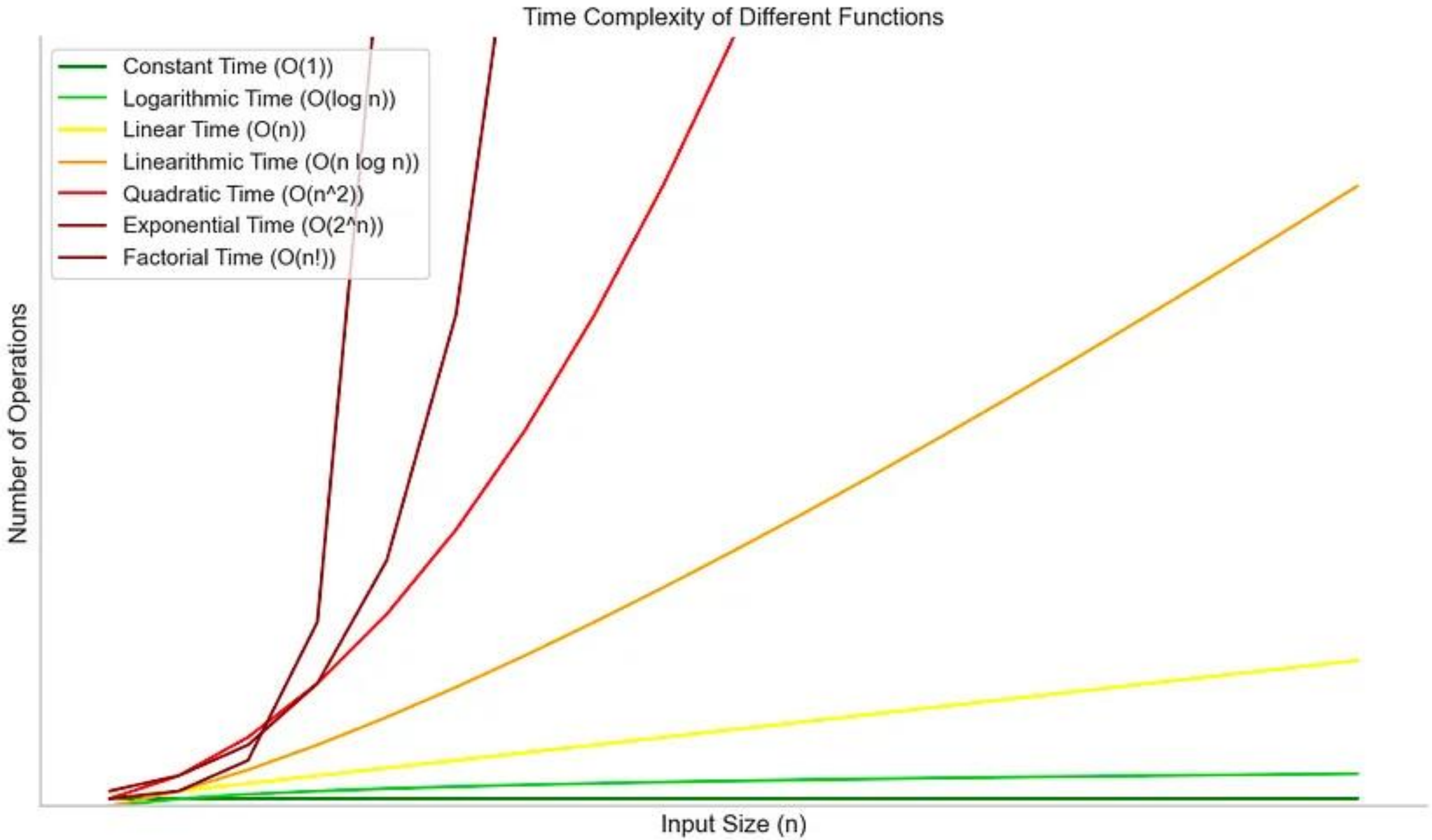


Transformation into 3 cluster

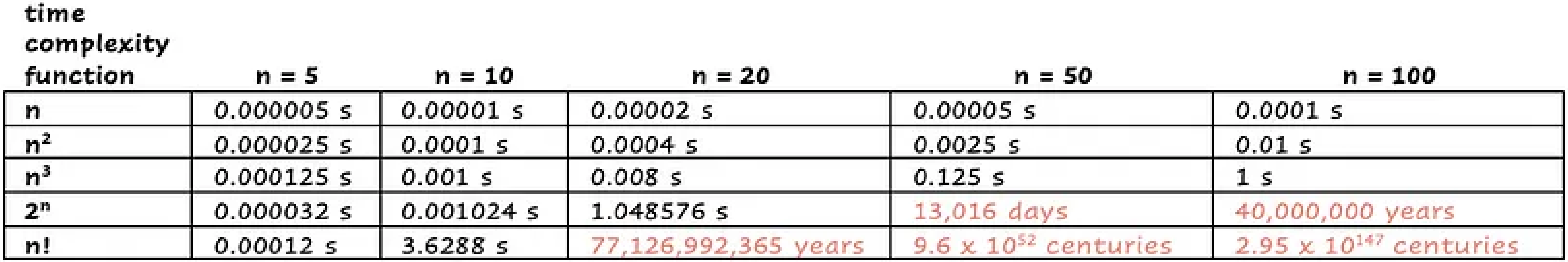
$$\binom{100}{3} = \frac{100!}{3!\ \ 97!}$$

$$\binom{n}{k} = \frac{n!}{k!\ \ (n-k)!}$$

Analyzing time complexity



Analyzing time complexity of K-Centers



time complexity function	n = 5	n = 10	n = 20	n = 50	n = 100
n	0.000005 s	0.00001 s	0.00002 s	0.00005 s	0.0001 s
n^2	0.000025 s	0.0001 s	0.0004 s	0.0025 s	0.01 s
n^3	0.000125 s	0.001 s	0.008 s	0.125 s	1 s
2^n	0.000032 s	0.001024 s	1.048576 s	13,016 days	40,000,000 years
n!	0.00012 s	3.6288 s	77,126,992,365 years	9.6×10^{52} centuries	2.95×10^{147} centuries

- It didn’t take us centuries to execute K-Means. Why?
- We used non-deterministic algorithm
  - Expectation-Maximization (EM)
  - K-centers is NP-Complete problem with deterministic approach
  - We used heuristic (initial centroid selection)

P versus NP decision problem

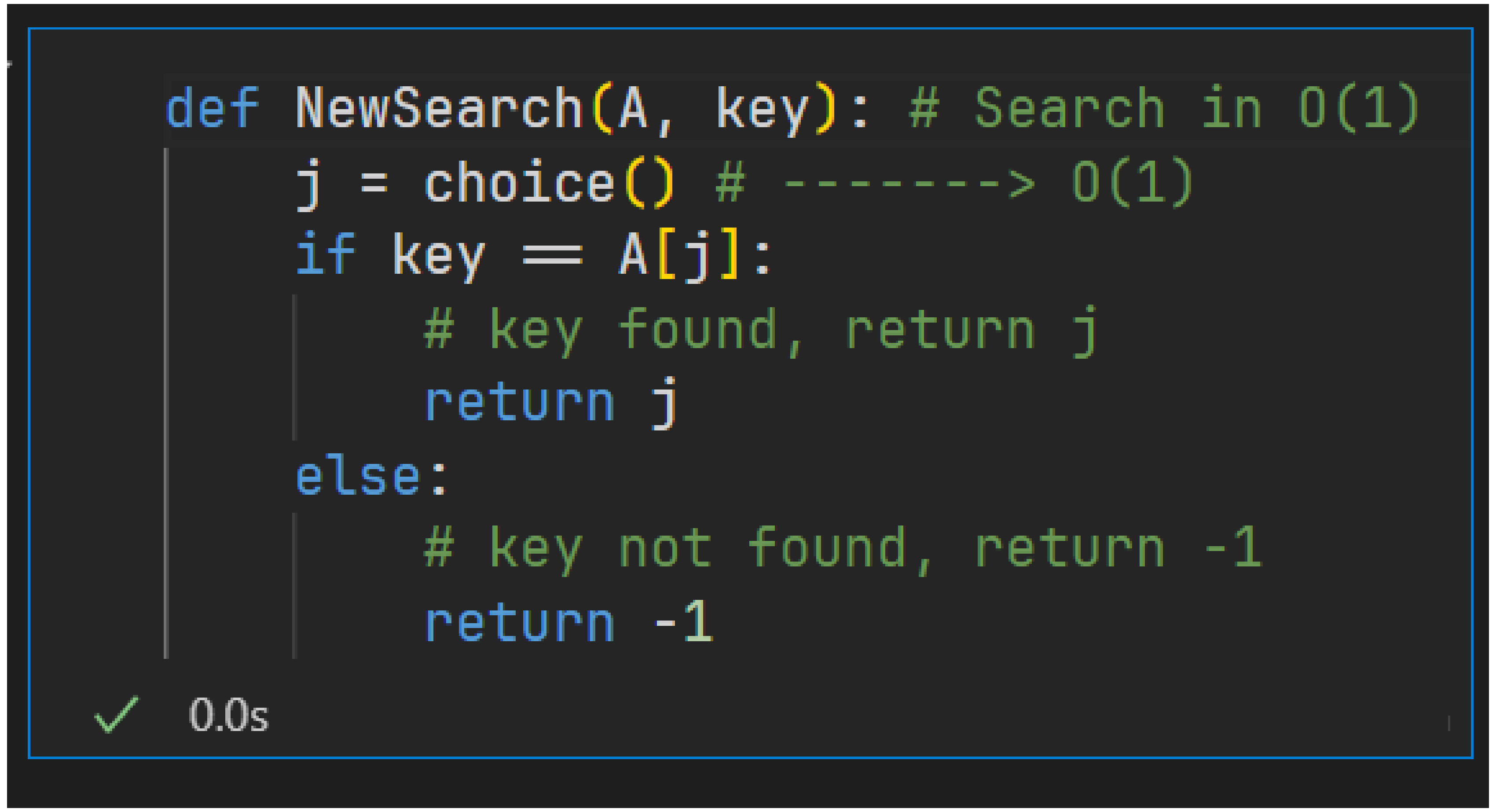
P	NP
Solvable in polynomial time	Solvable in exponential time
Linear search – n Binary search – log n Bubble sort – n^2 Merge sort – n logn Matrix multiplication – n^3	0/1 Knapsack Travelling salesman Hamiltonian cycle CNF
Verified in polynomial time	Verified in polynomial time
Deterministic in polynomial time	Non-deterministic in polynomial time

- What is non-deterministic?

Non-deterministic

- Deterministic: We clearly know how every statement we code behaves
- Non Deterministic: Most of the statements in algorithm may be deterministic. Some may be non deterministic

- A = [10, 15, 20, 2, 4, 6]
- key = 20
- Returns j = 2 in O(1)
- How?
    - We don’t know (yet)

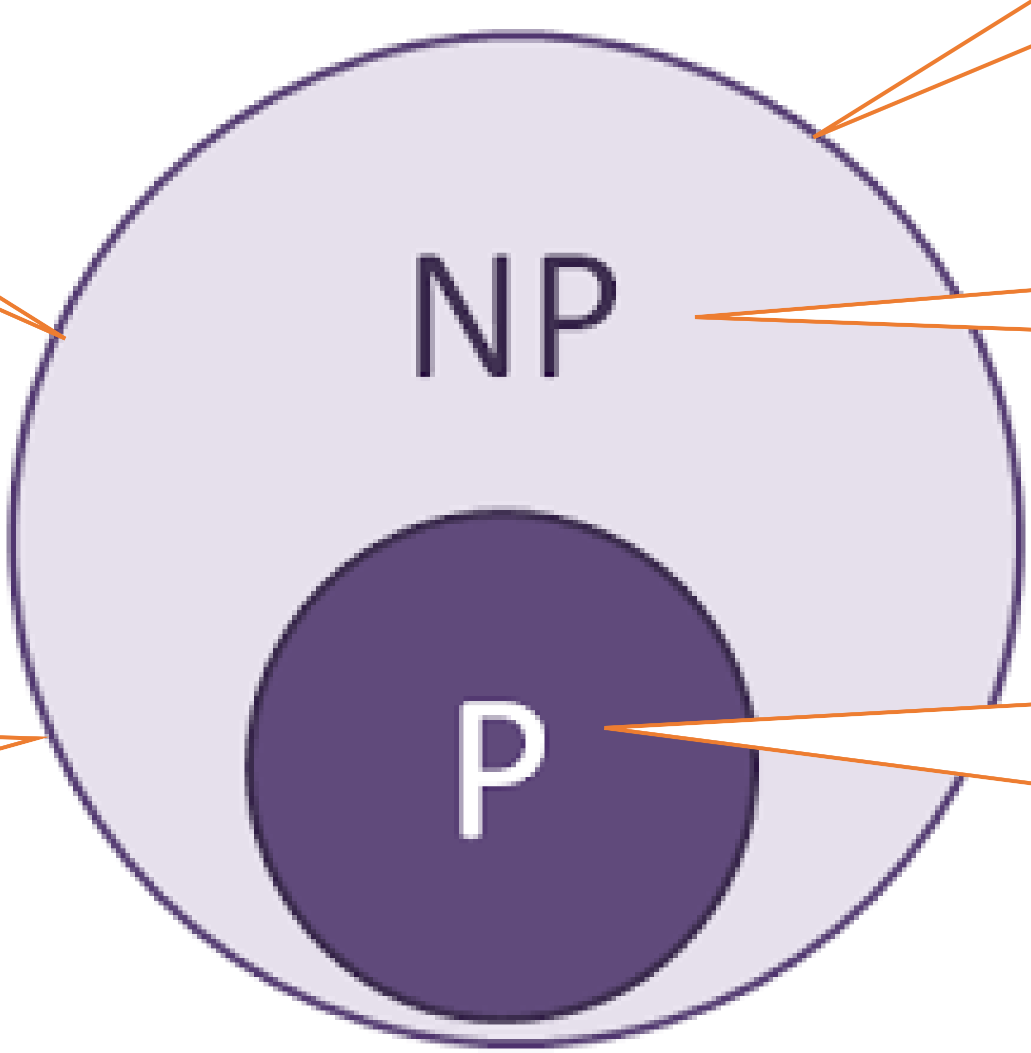


```
def NewSearch(A, key): # Search in O(1)
    j = choice() # -------> O(1)
    if key == A[j]:
        # key found, return j
        return j
    else:
        # key not found, return -1
        return -1
```

✓ 0.0s

NP becoming P

- Before the advent of Binary search
  - Search was O(n)



Why is P subset of NP?

Both verifiable in polynomial time

Sudoku (NP) can be verified in P time

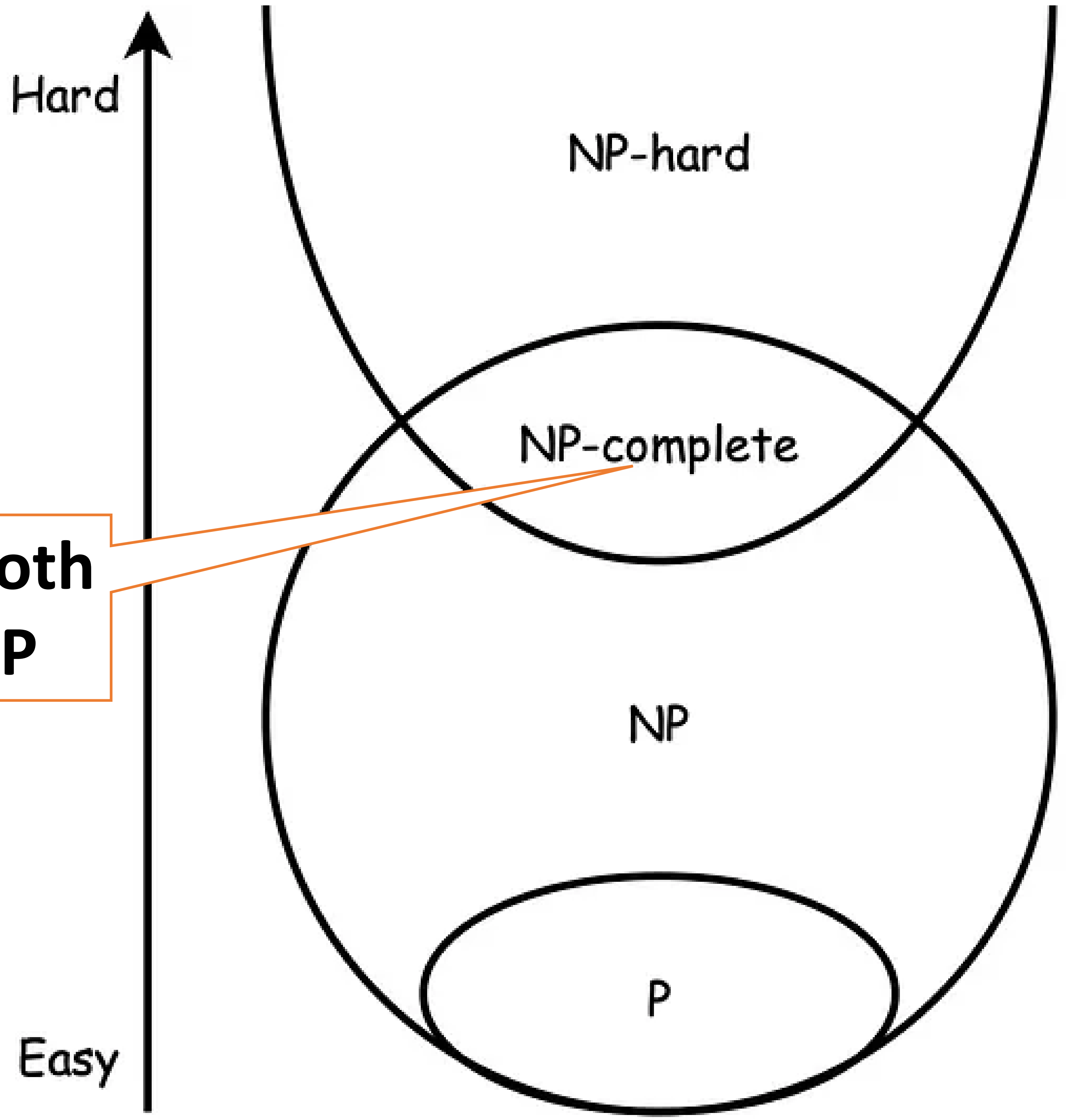
Non deterministic v/s deterministic in polynomial time

Sort (P) can be verified in P time (in addition to solving in P time)

NP-hard NP-complete

- NP-hard problem: Any problem that is at least as hard as the hardest problem in NP
- NP-complete problem is NP-hard that can be verified in polynomial time.
  - E.g. Sudoku, K-centers
- How to determine NP-hard v/s NP-complete
- Reducing NP-hard problems
  - Take a base problem. E.g. CNF

NP-complete is both in NP-hard and NP

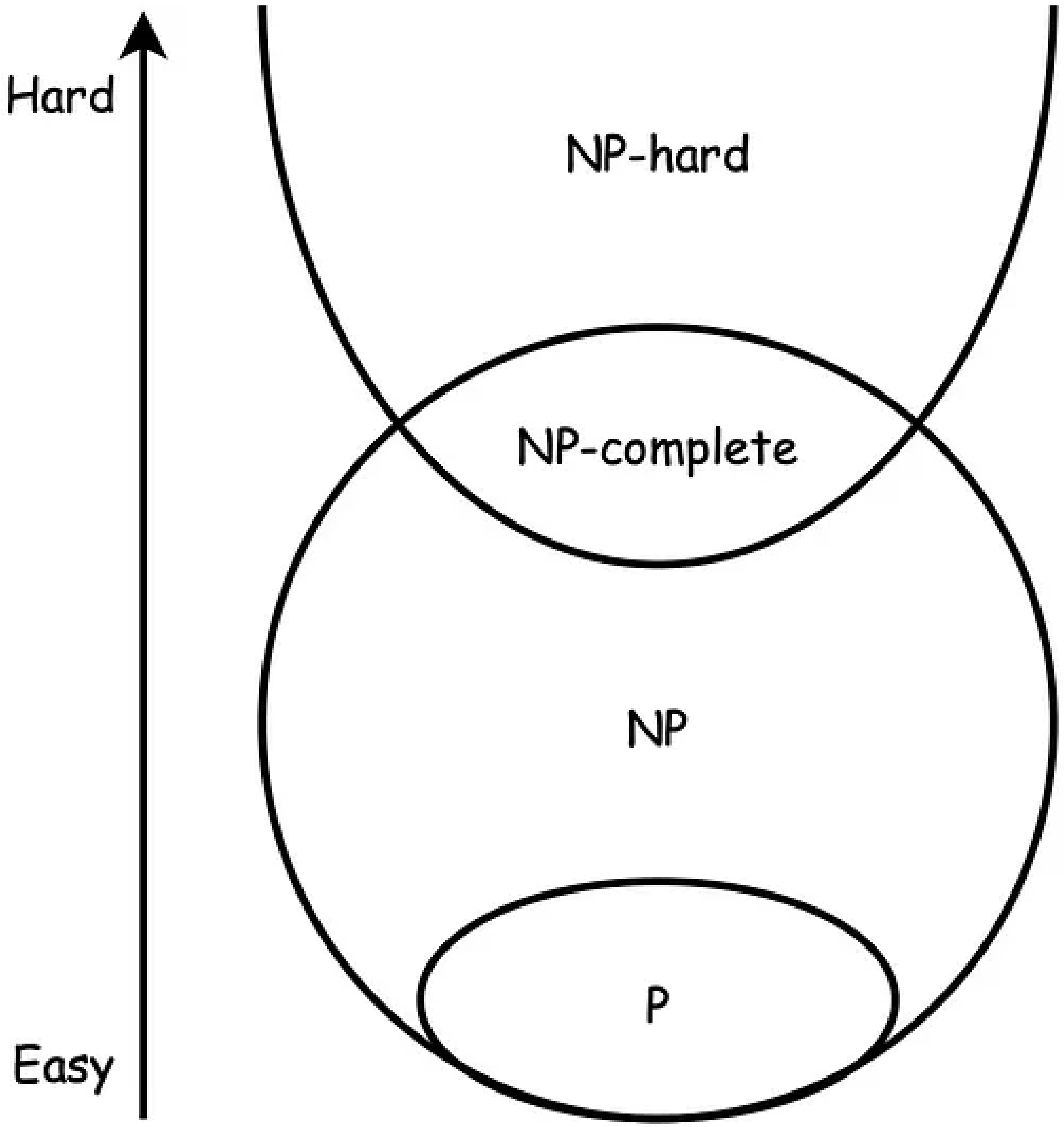


NP-hard NP-complete (contd.)

- CNF – Conjugate Normal Form
- Express logical operations using propositional logic

$$(\neg x_1 \vee x_2 \vee x_3) \wedge (x_2 \vee x_3 \vee \neg x_4)$$

- What values of x1, x2, x3, x4 satisfy this?
- Solve in 2^4 time. Verify in O(n)
- NP-complete problem
- K-centers can be reduced to planar 3-SAT



QUESTIONS