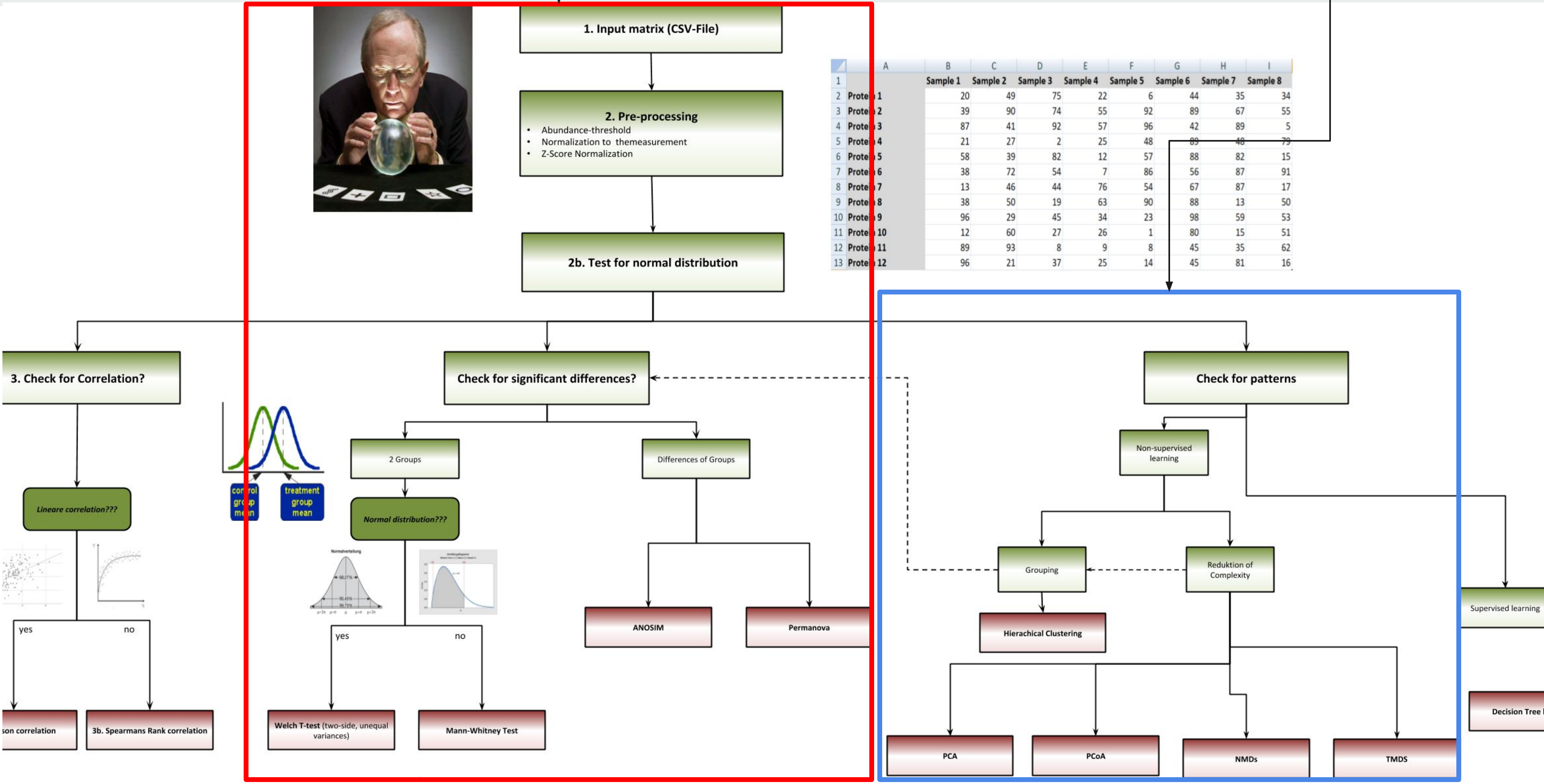
Multivariate Methods

CLASSIFICATION & ORDINATION

roadmap

First Tutorial

Second Tutorial



1. Input matrix (CSV-File)

2. Pre-processing
- Abundance-threshold
- Normalization to themeasurement
- Z-Score Normalization

2b. Test for normal distribution

3. Check for Correlation?

Lineare correlation???

yes

no

son correlation

3b. Spearmans Rank correlation

Check for significant differences?

2 Groups

Normal distribution???

yes

no

Welch T-test (two-side, unequal variances)

Mann-Whitney Test

Differences of Groups

ANOSIM

Permanova

Check for patterns

Non-supervised learning

Grouping

Reduktion of Complexity

Hierachical Clustering

PCA

PCoA

NMDs

TMDS

Supervised learning

Decision Tree

	A	B	C	D	E	F	G	H	I
1		Sample 1	Sample 2	Sample 3	Sample 4	Sample 5	Sample 6	Sample 7	Sample 8
2	Protein 1	20	49	75	22	6	44	35	34
3	Protein 2	39	90	74	55	92	89	67	55
4	Protein 3	87	41	92	57	96	42	89	5
5	Protein 4	21	27	2	25	48	89	48	79
6	Protein 5	58	39	82	12	57	88	82	15
7	Protein 6	38	72	54	7	86	56	87	91
8	Protein 7	13	46	44	76	54	67	87	17
9	Protein 8	38	50	19	63	90	88	13	50
10	Protein 9	96	29	45	34	23	98	59	53
11	Protein 10	12	60	27	26	1	80	15	51
12	Protein 11	89	93	8	9	8	45	35	62
13	Protein 12	96	21	37	25	14	45	81	16

GOALS :

Overview : Normalization & Group Comparison

Moving Ahead - Multivariate Methods : Supervised Learning & Unsupervised Learning, Ordination & Clustering

Ordination: PCA, PCoA & NMDS

Grouping: Clustering

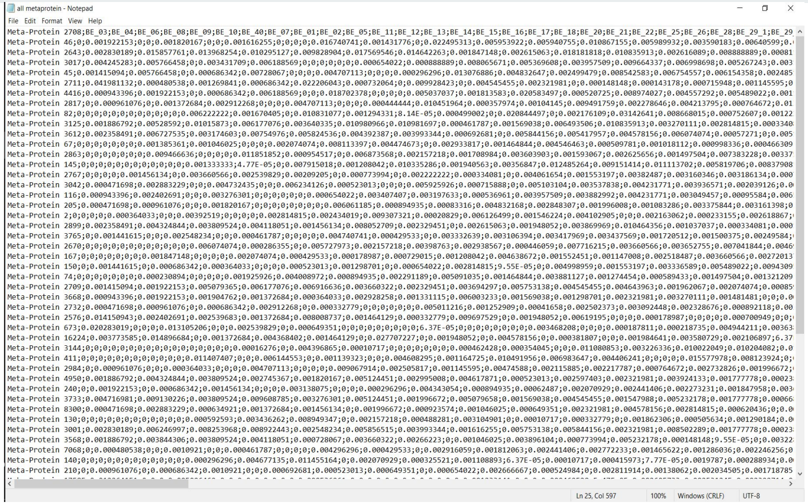
OVERVIEW

- what are we upto?
- keywords

  NORMALIZATION? GROUP COMPARISON? WHY ALL THE FUSS?
- previously unclarified

  p-value, w-value, Bonferoni Correction T-Test, Benjamin Hochberger Correction T-Test

what are we upto?



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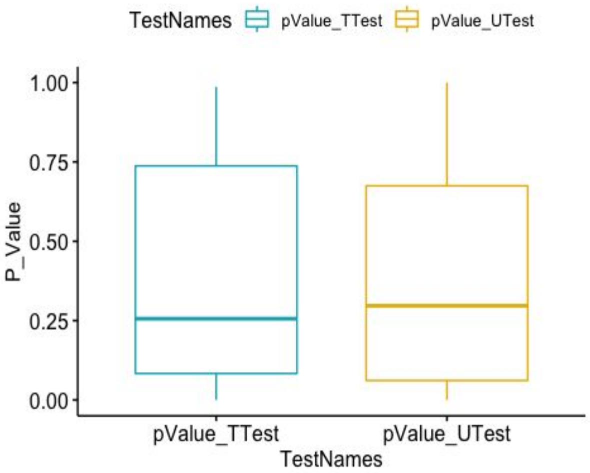


why?

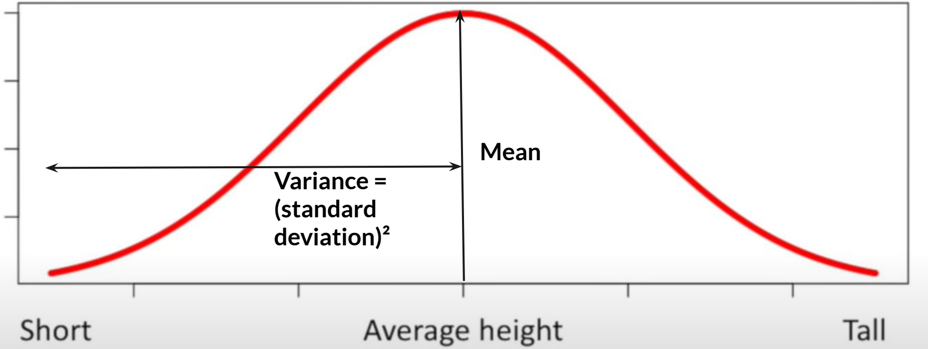
to **visualize** large amounts of complex **data** is easier than poring over spreadsheets or reports. ... **Data visualization** can also: **Identify areas that need attention or improvement.**

how?

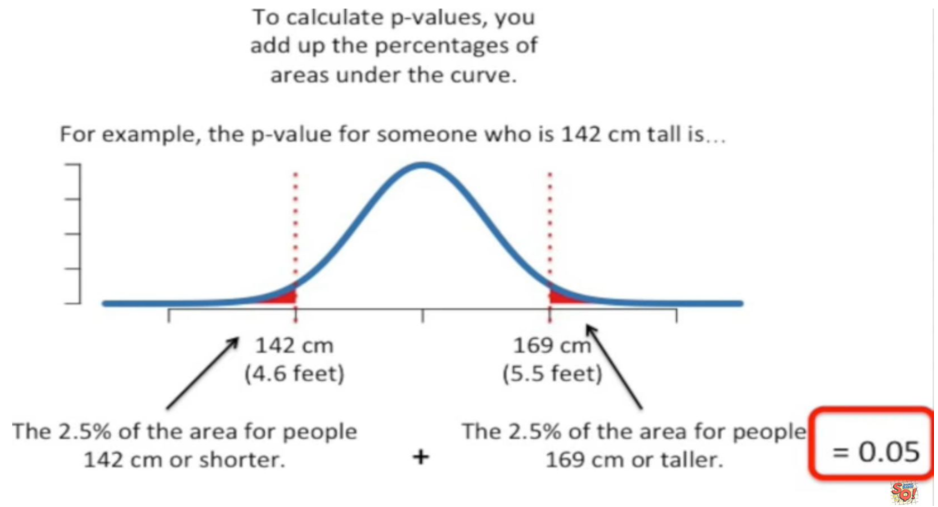
Statistical Tools through **R :**

- Normalization
- Group Comparison **(T-Test, PERMANOVA etc.)**
- Multivariate Methods **(Clustering, Ordination)**

keyword : normalization



p-value


To calculate p-values, you add up the percentages of areas under the curve.

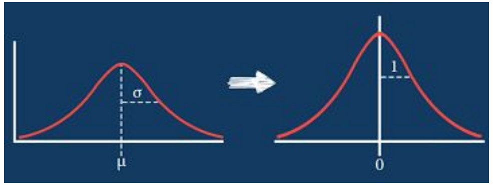
For example, the p-value for someone who is 142 cm tall is…

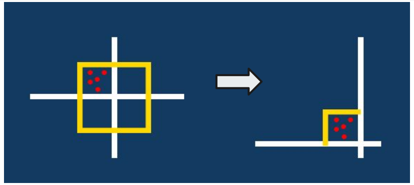
The 2.5% of the area for people 142 cm or shorter. + The 2.5% of the area for people 169 cm or taller. = 0.05

why bother?

- Robust **visualization** of a data or data variable - possible to create null hypothesis and test them
- **data normalization** when seeking for **relations**
- as part of data preparation for **machine learning**. The goal of **normalization** is to change the values of numeric columns in the dataset to a common scale, without distorting differences in the ranges of values
- Easy to **compare** data or data variables

how?

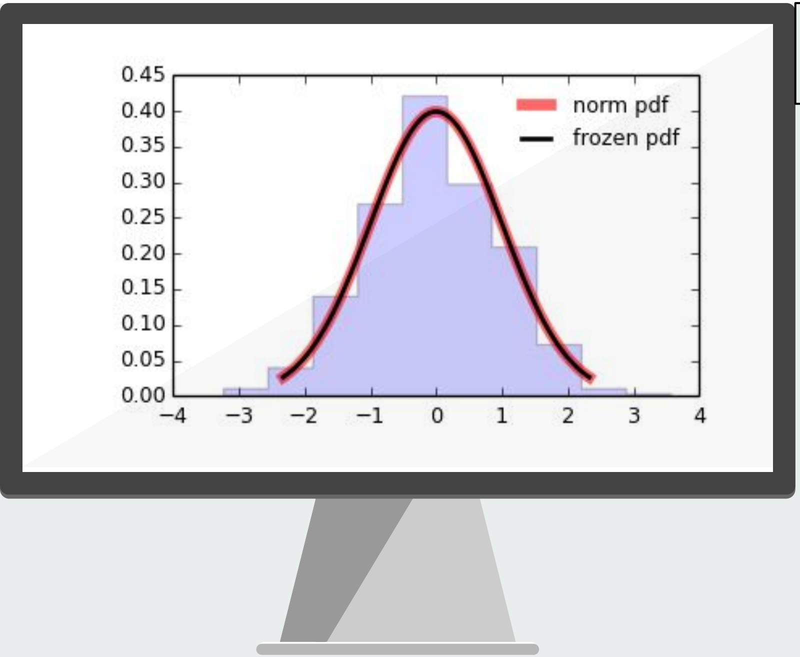


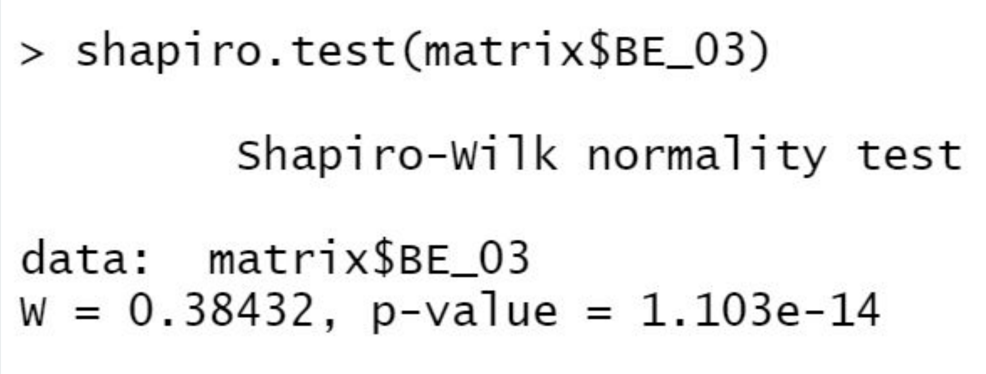


Name(ID)	**Age**	**Height**	**Gender** (1=f, 2=m, 3=other)	**Education Level** (0=Bachelor, 1= Master, 2= Post Doc)	**Class Label : Teacher(1) or Student(0)**
Robert	30	6.1	m(2)	Post Doc(2)	Teacher(1)
Julian	26	6.3	m(2)	Master(1)	Student(0)
Danial	25	5.8	m(2)	Master(1)	Student(0)
Max	26	5.9	m(2)	Master(1)	Student(0)
Faizan	23	6.0	m(2)	Master(1)	Student(0)
Abdullah	27	5.8	m(2)	Master(1)	Student(0)
Ammar	26	5.9	m(2)	Master(1)	Student(0)
Rahul	25	5.8	m(2)	Master(1)	Student(0)
Mean	**26**	**5.95**	**2**	**1.125**	

Name(ID)	**Age**		**Height**		**Gender** (1=f, 2=m, 3=other)	**Education Level** (0=Bachelor, 1= Master, 2= Post Doc)	**Class Label : Teacher(1) or Student(0)**
Robert	30	1	6.1	3/5	m(2)	Post Doc(2)	Teacher(1)
Julian	26	3/7	6.3	1	m(2)	Master(1)	Student(0)
Danial	25	2/7	5.8	0	m(2)	Master(1)	Student(0)
Max	26	3/7	5.9	1/5	m(2)	Master(1)	Student(0)
Faizan	23	0	6.0	2/5	m(2)	Master(1)	Student(0)
Abdullah	27	4/7	5.8	0	m(2)	Master(1)	Student(0)
Ammar	26	3/7	5.9	1/5	m(2)	Master(1)	Student(0)
Rahul	25	2/7	5.8	0	m(2)	Master(1)	Student(0)
Mean	**26**	3/7	**5.95**	0.3	**2**	**1.125**	

Test for Normality: Shapiro-Wilk Test





```
> shapiro.test(matrix$BE_03)

        Shapiro-Wilk normality test

data:  matrix$BE_03
W = 0.38432, p-value = 1.103e-14
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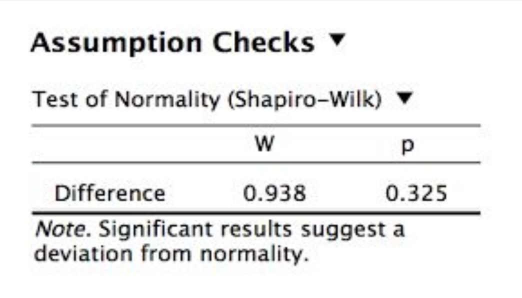


Assumption Checks ▼

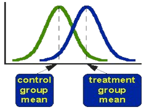
Test of Normality (Shapiro-Wilk) ▼

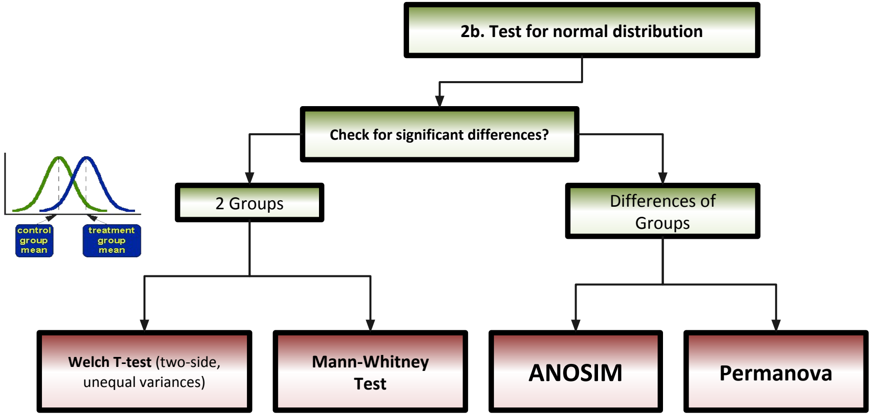
	W	p
Difference	0.938	0.325

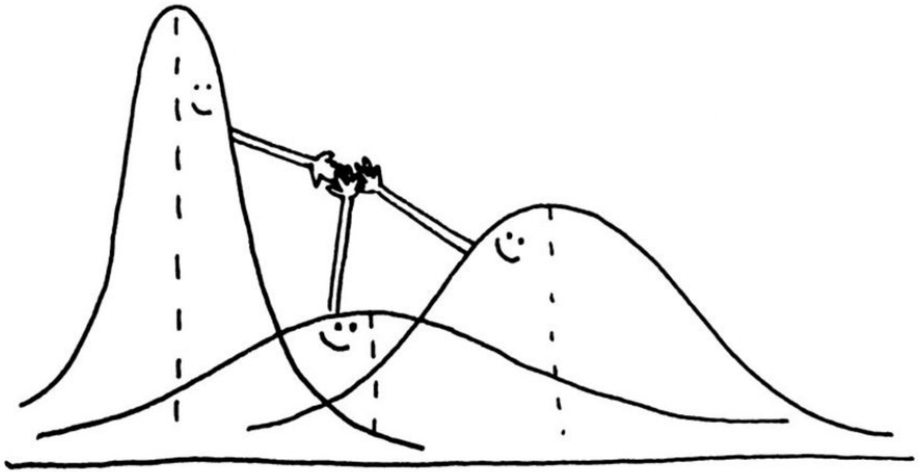
Note. Significant results suggest a deviation from normality.

- Using w-value, we create a NULL hypothesis
  - *if W is very small then the distribution is probably not normally distributed*
- If P < 0.05 , we reject the NULL Hypothesis

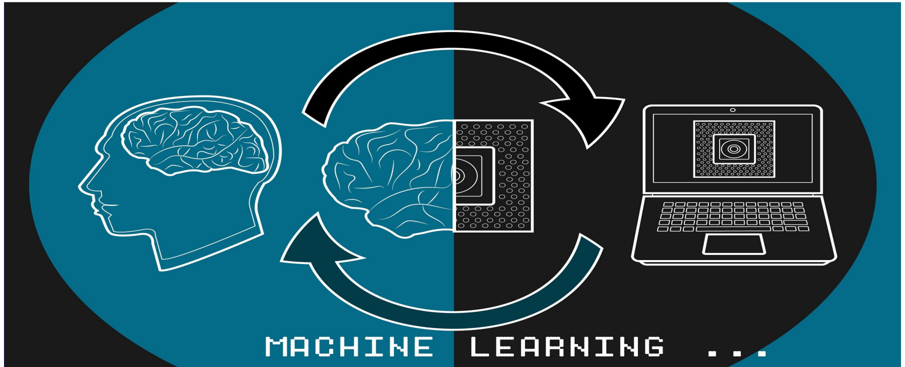
So now that we have data(normalized), what next?




2b. Test for normal distribution
Check for significant differences?
2 Groups
Differences of Groups
Welch T-test (two-side, unequal variances)
Mann-Whitney Test
ANOSIM
Permanova



- check for **Significant Differences (Group Comparison)**
  - between 2 or more groups
    - T-Test & U-Test
    - ANOSIM & PERMANOVA
    - ANOVA & Kruskal-Walis Test
- infer **Knowledge** out of dataset and/or **prove hypothesis**



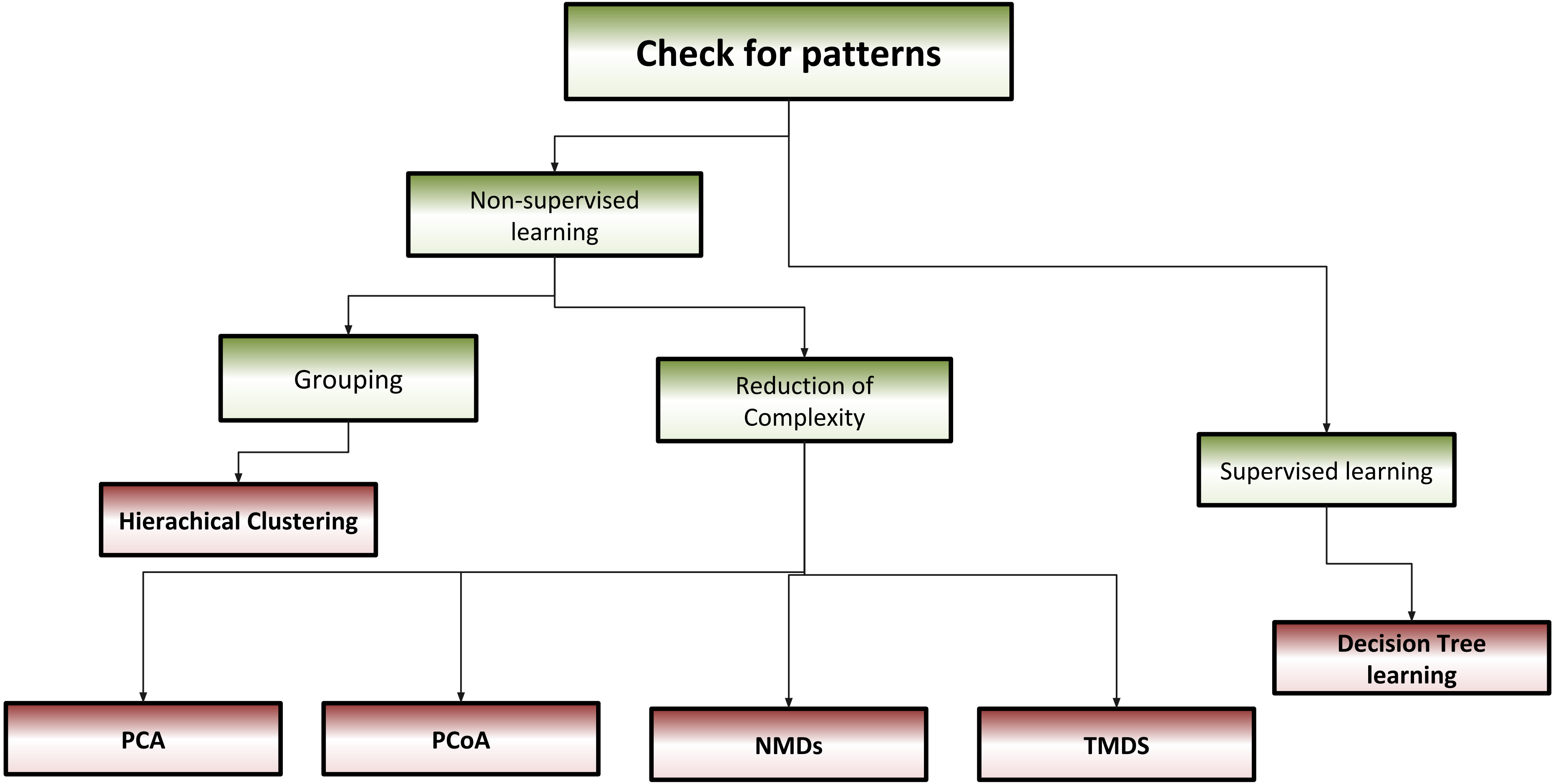
and why is this important?

can DATA be NOT Normalized & still make sense??

Multivariate Methods : Ordination & Classification

- **unsupervised learning** vs **supervised learning**
- Ordination
  - Grouping
    - Clustering
  - Dimension/Complexity Reduction
    - PCA
    - PCoA
    - NMDS
    - CCA

roadmap



Check for patterns

Non-supervised learning

Grouping

Hierachical Clustering

Reduction of Complexity

PCA

PCoA

NMDs

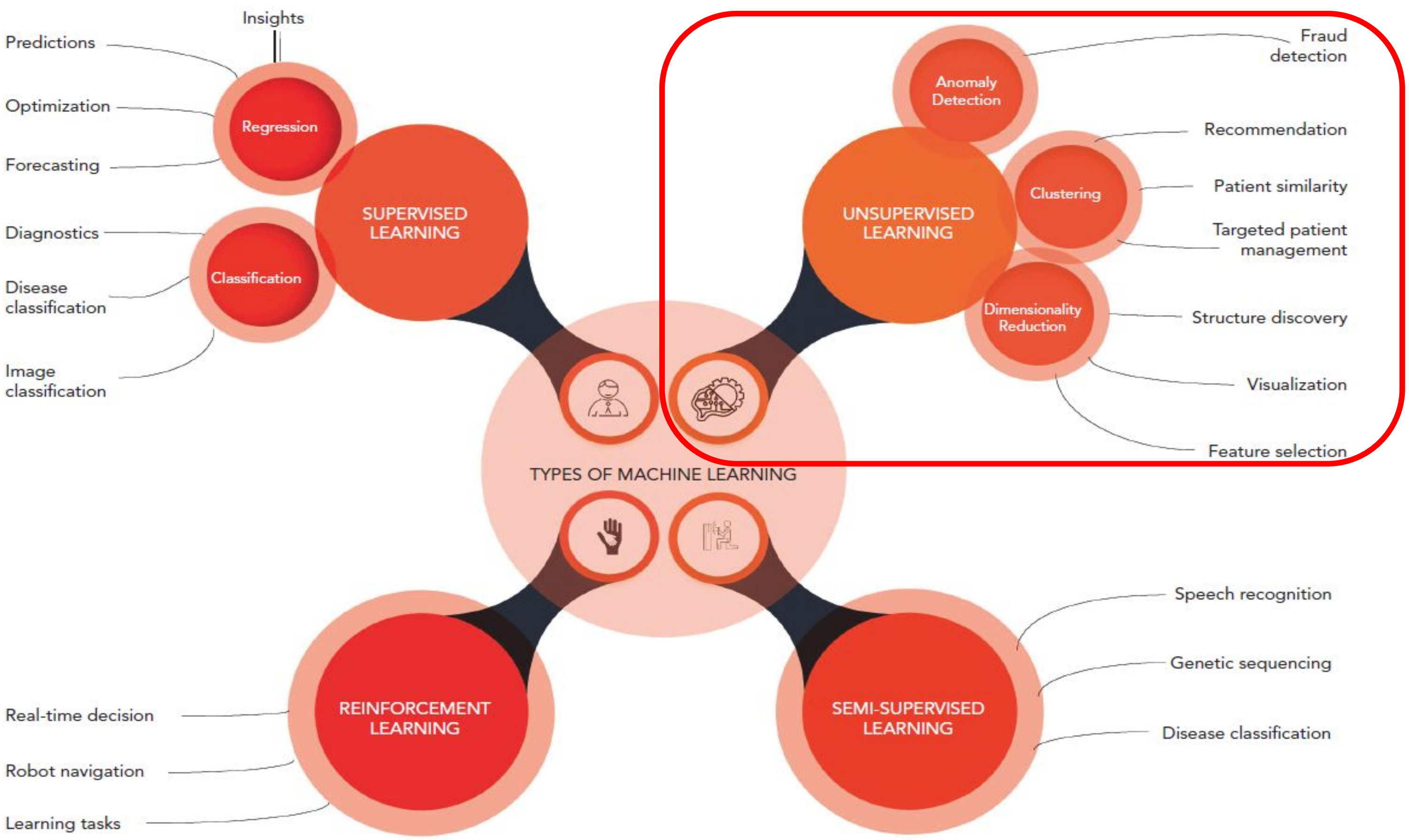
TMDS

Supervised learning

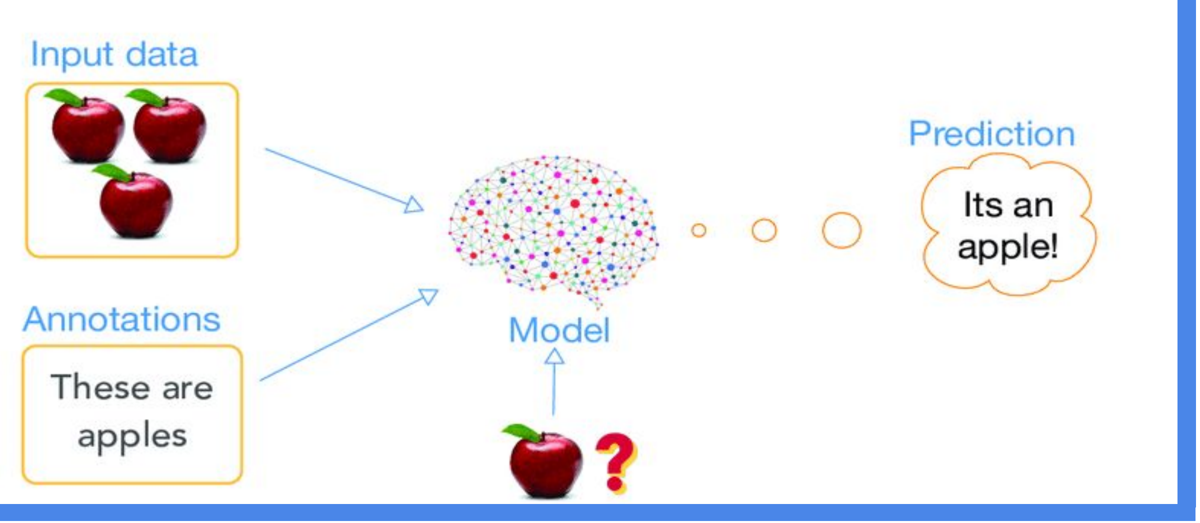
Decision Tree learning

types of Machine Learning

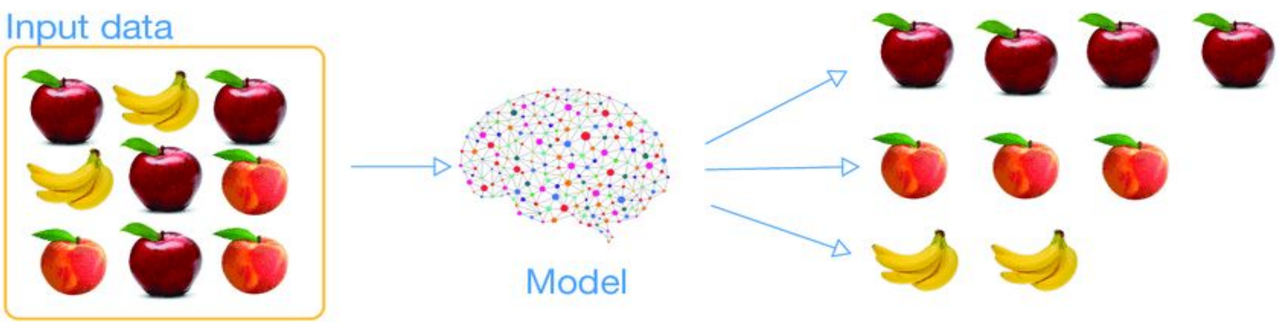
Figure 1: Types of Machine Learning with Examples of Respective Use

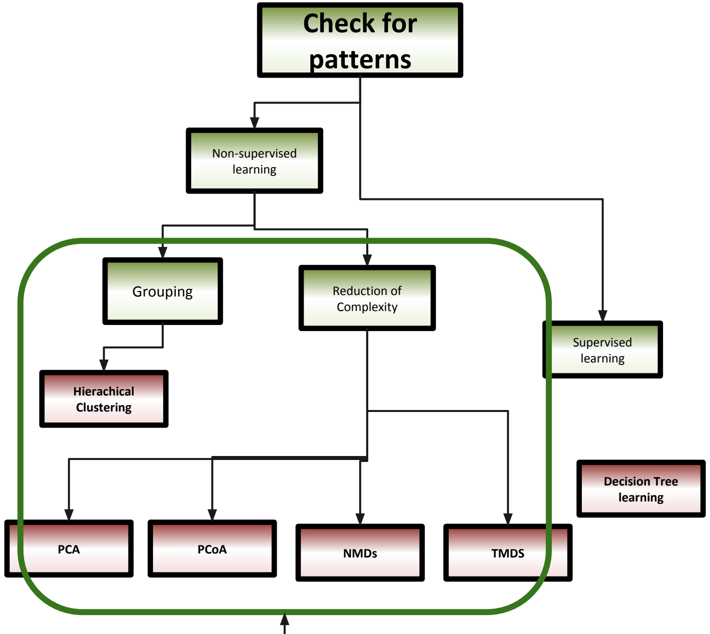


supervised learning



unsupervised learning





ORDINATION

unsupervised learning vs/& supervised learning

what is DATA to a Machine??

unsupervised learning

- grouping
  - **Clustering**
- reduction of Dimension and/or Complexity
  - Principal Component Analysis **(PCA)**
  - Principal Coordinate Analysis **(PCoA)**
  - Non Metric MultiDimensional Scaling **(NMDS)**
  - Canonical Correspondence Analysis **(CCA)**

why?

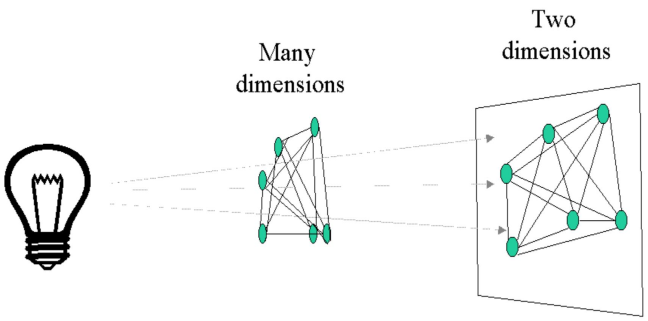
to find **Similarities** & **Recommendations**

Structure Discovery, Feature Selection & **Visualization**

how?

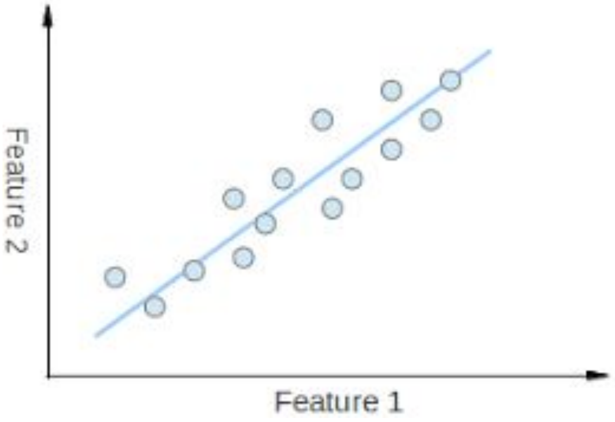
ordination (an unsupervised approach)

Ordination is a collective term for multivariate techniques which summarize a multidimensional dataset in such a way that when it is projected onto a low dimensional space, any intrinsic pattern the data may possess becomes apparent upon visual inspection.



why?

Ordination can be used on the analysis of any set of multivariate objects.

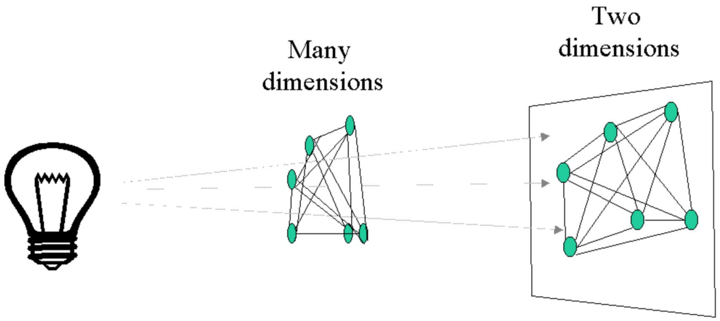


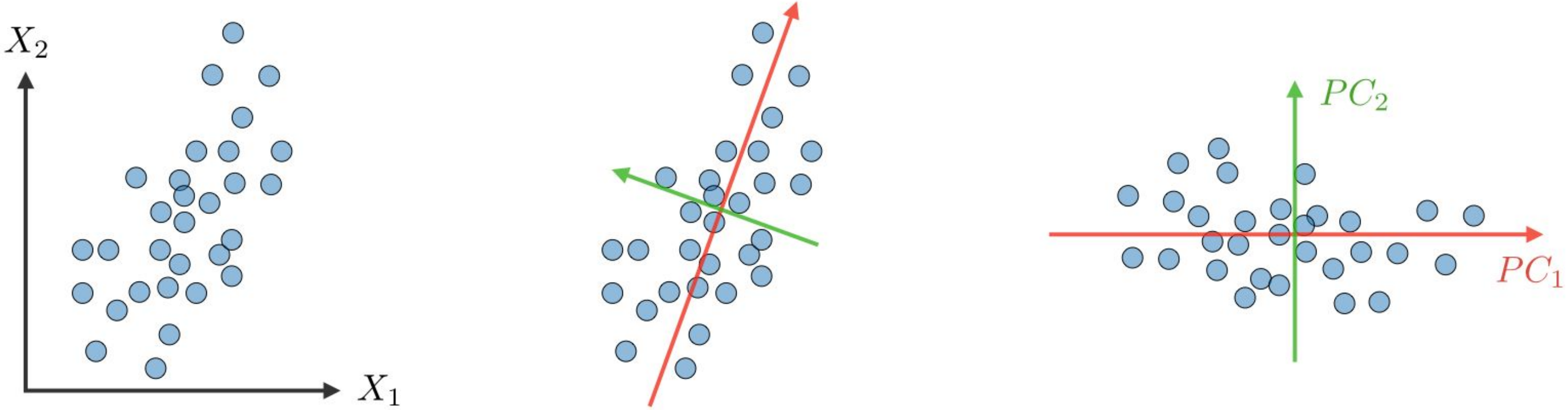
how?

Ordination

- Dimension Reduction
    - **PCA** (Principal Component Analysis)
    - **PCoA** (Principal Coordinates Analysis)
    - **NMDS** (Non metric Multidimensional Scaling)

PCA (Principal Component Analysis)

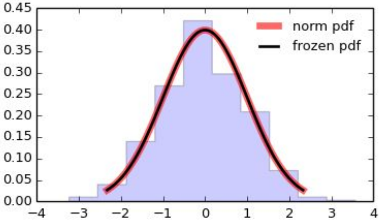


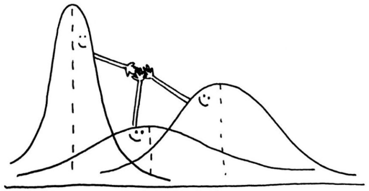


Data in feature space → Find principal components → Data in **p**rincipal **c**omponents space

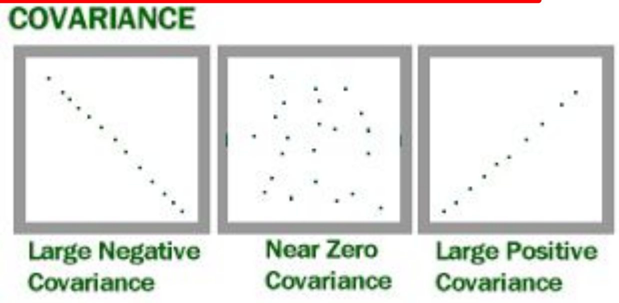
Steps (PCA)

1. Normalize the **Dataset**

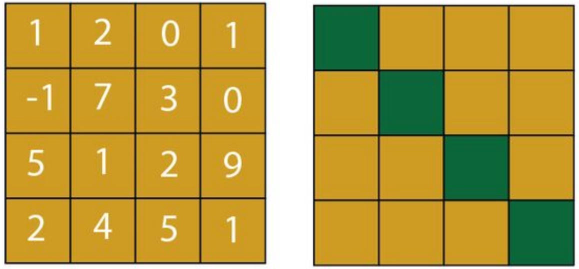




2. Compute **Covariance Matrix**

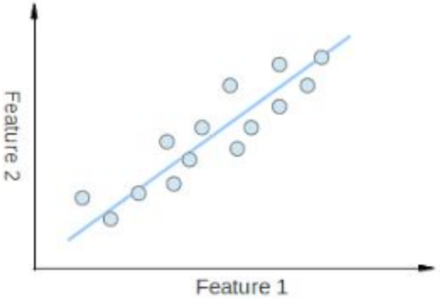


3. Perform **Eigen Decomposition**

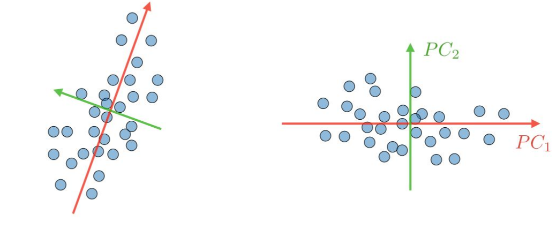


1	2	0	1
-1	7	3	0
5	1	2	9
2	4	5	1

4. Determine **Principal Component**



4. Compute **Transformation**



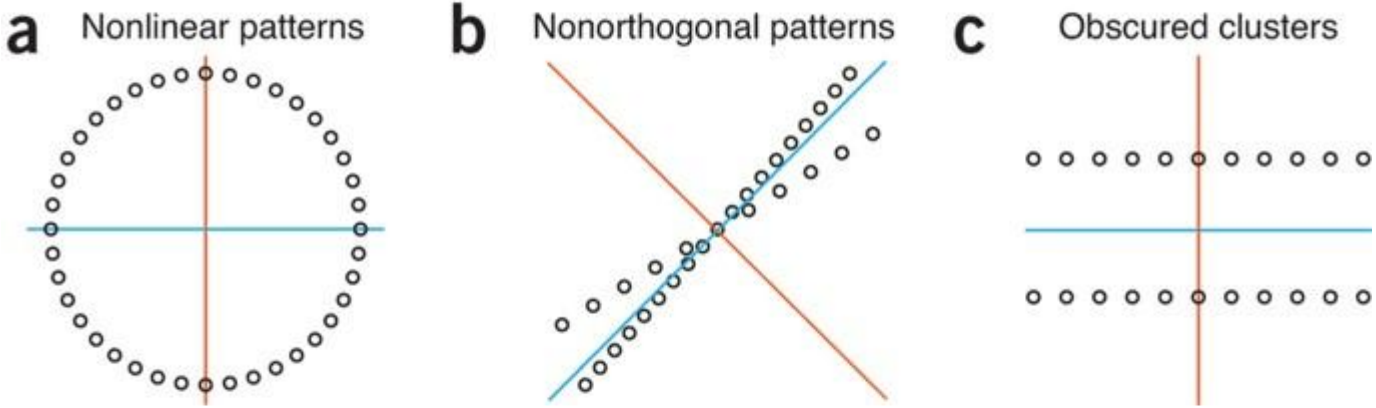
Find principal components → Data in principal components space

6. VISUALIZATION

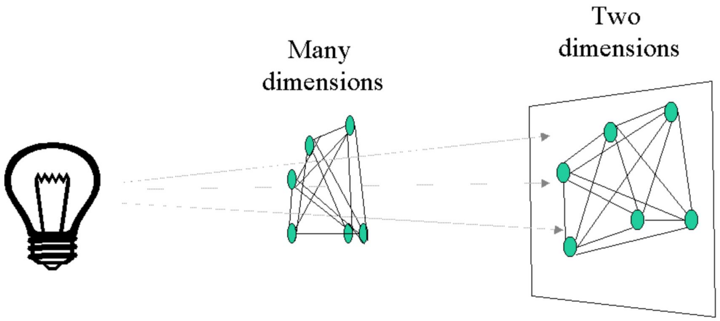
importance(PCA)

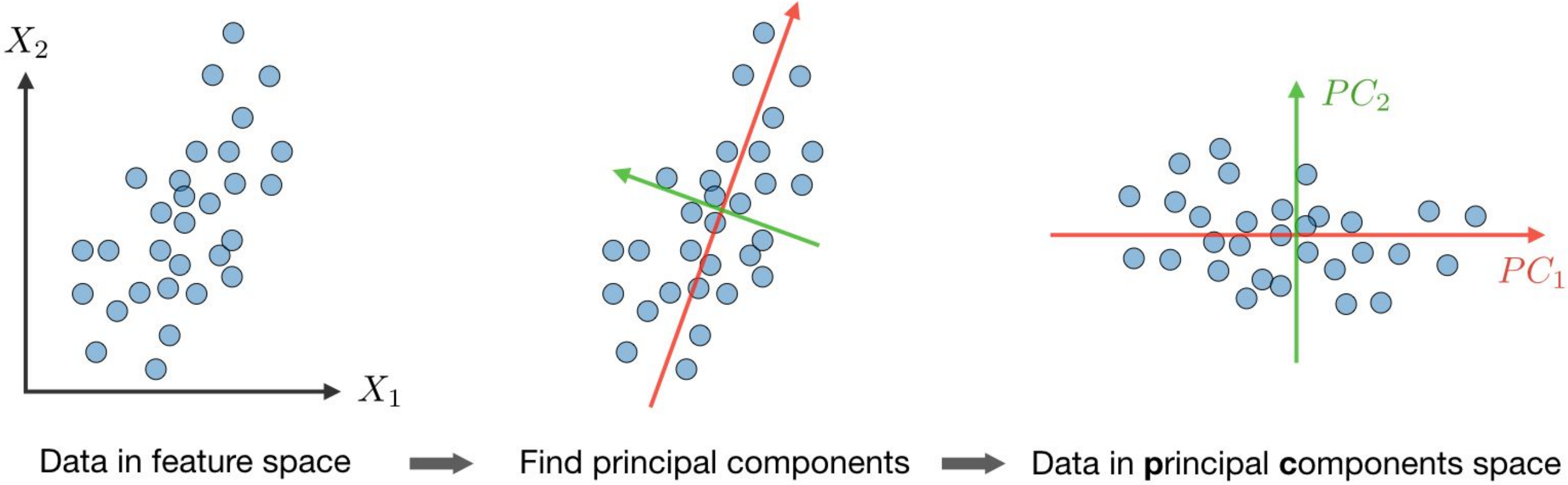
PCA helps you discover correlations & interpret your data, but it will not always find the important patterns.

Principal component analysis (PCA) **simplifies the complexity in high-dimensional data while retaining trends and patterns.** It does this by transforming the data into fewer dimensions, which act as summaries of features

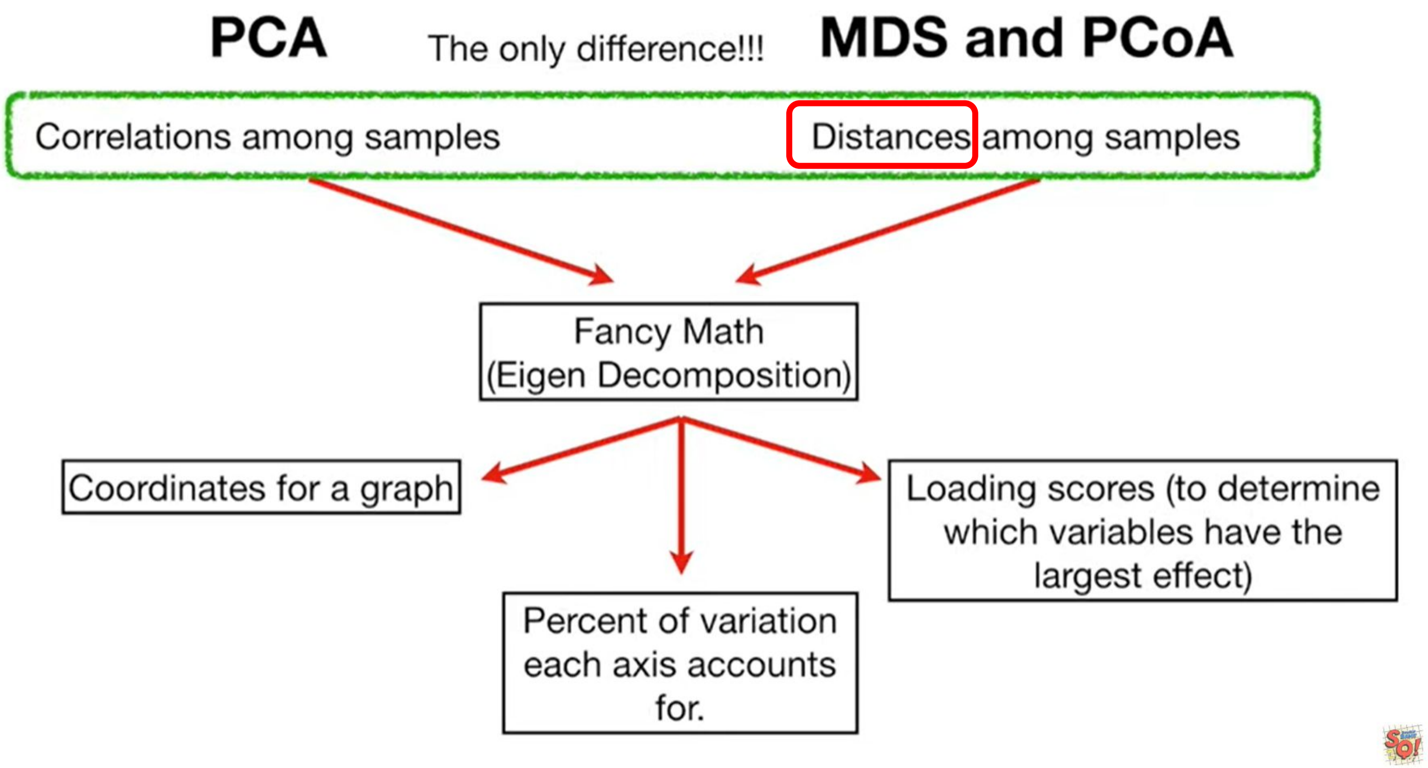


PCoA (Principal Component Analysis)/ metric multidimensional scaling





PCoA vs PCA



PCA The only difference!!! **MDS and PCoA**

Correlations among samples

Distances among samples

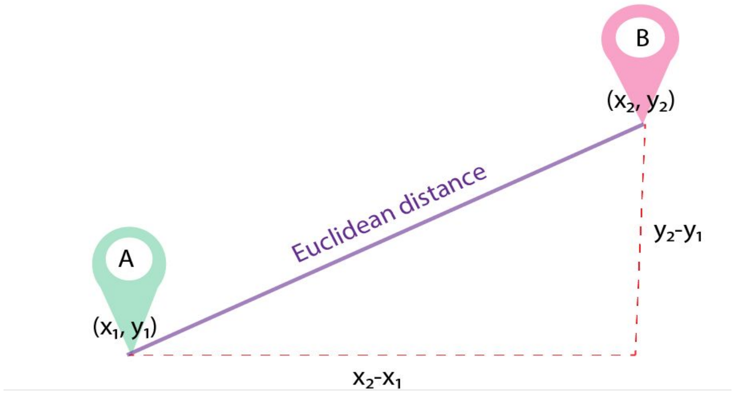
Fancy Math
(Eigen Decomposition)

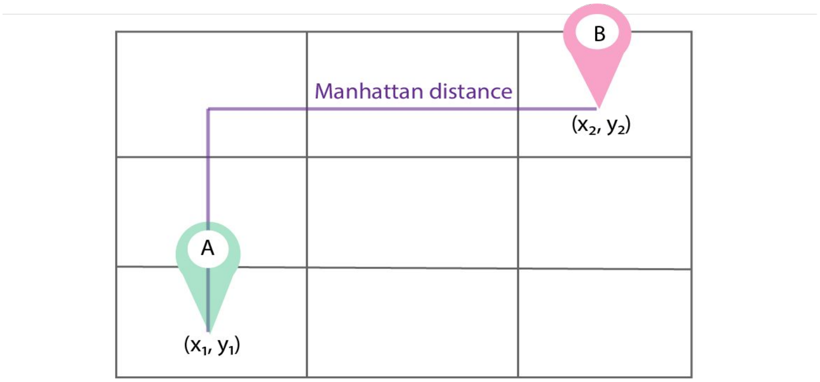
Coordinates for a graph

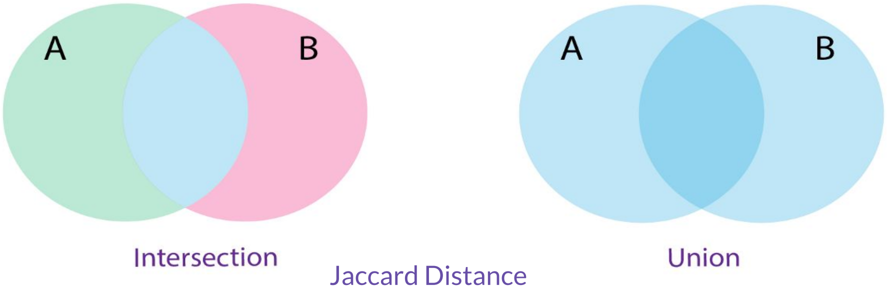
Percent of variation each axis accounts for.

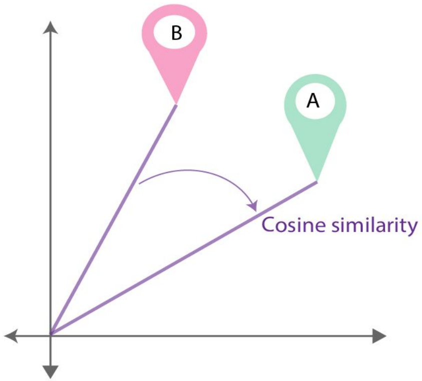
Loading scores (to determine which variables have the largest effect)

Distance/ Proximity Measures



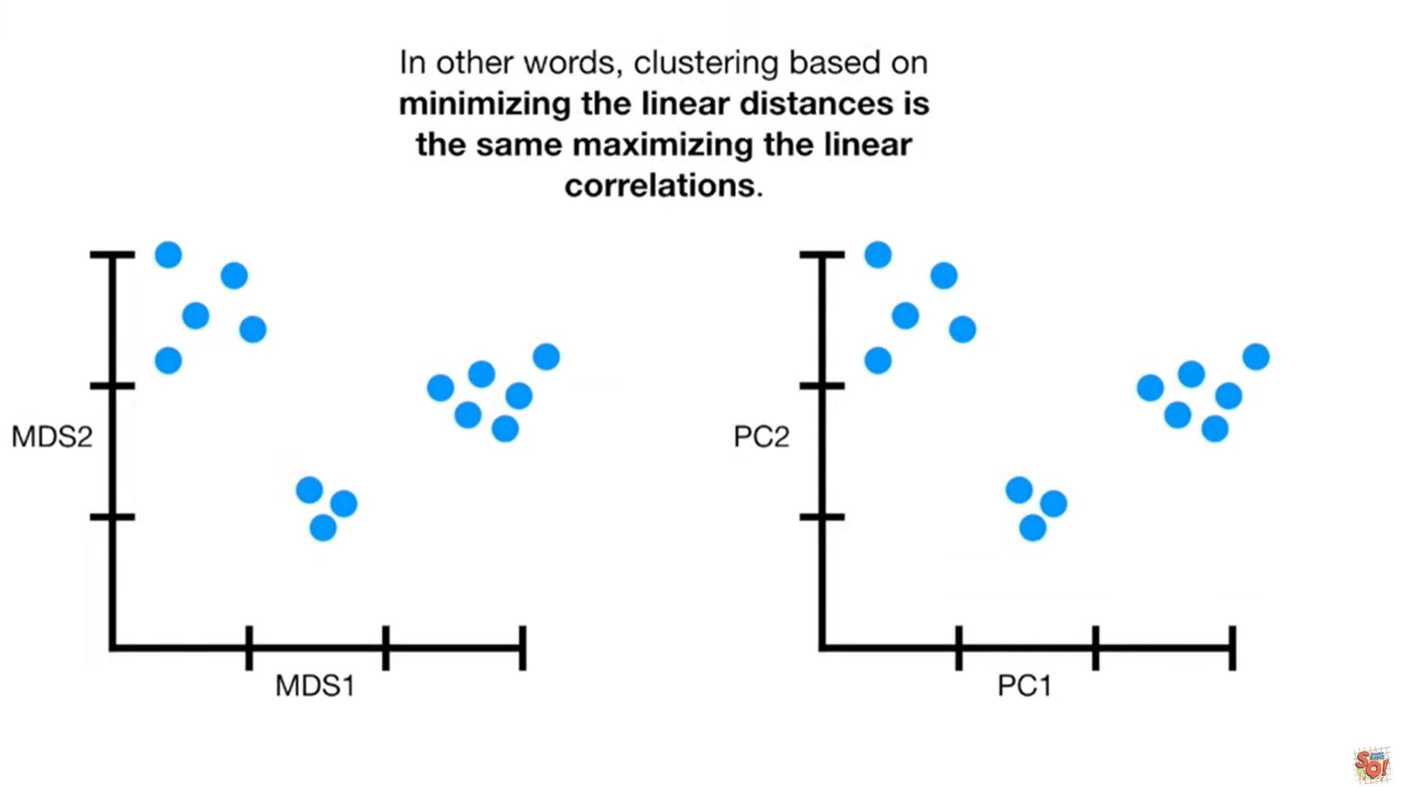






PCoA vs PCA

IF we use Euclidean Distance in PCoA, the graph would be similar to a PCA graph



In other words, clustering based on **minimizing the linear distances is the same maximizing the linear correlations.**

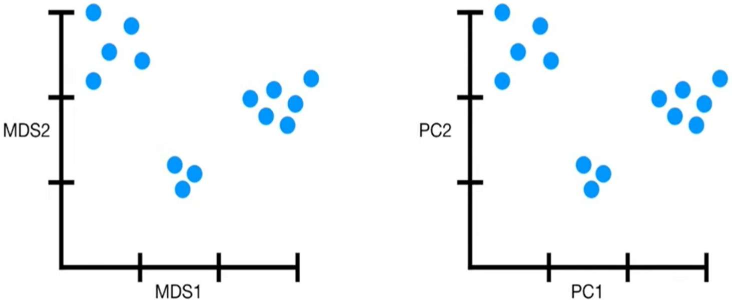
importance(PCoA)

As with other ordination techniques such as PCA and CA, PCoA produces a set of uncorrelated (orthogonal) axes to summarise the variability in the data set.

While PCoA is suited to handling a wide range of data, information concerning the original variables cannot be recovered.

How do I interpret a PCA/PCoA plot?

Interpreting the plots



1. There is Principal Component/Coordinate for each dimensions

   a. If we have “n” variables, we would have “n” Principal Components/Coordinates

2. PC1/PCoA1 would span the direction of most variation

   PC2/PCoA2 would span in the direction of 2nd most variation

   .

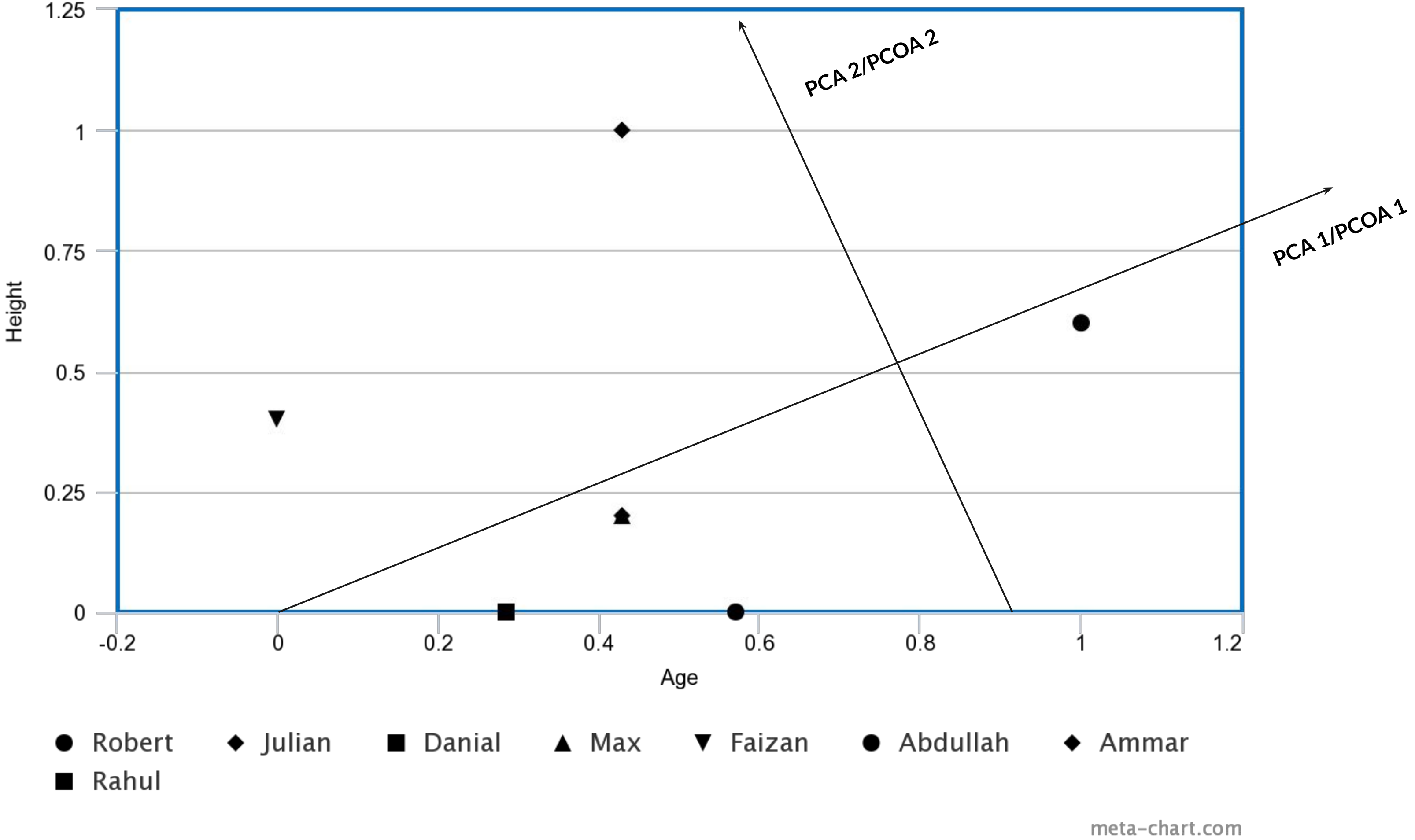
   .

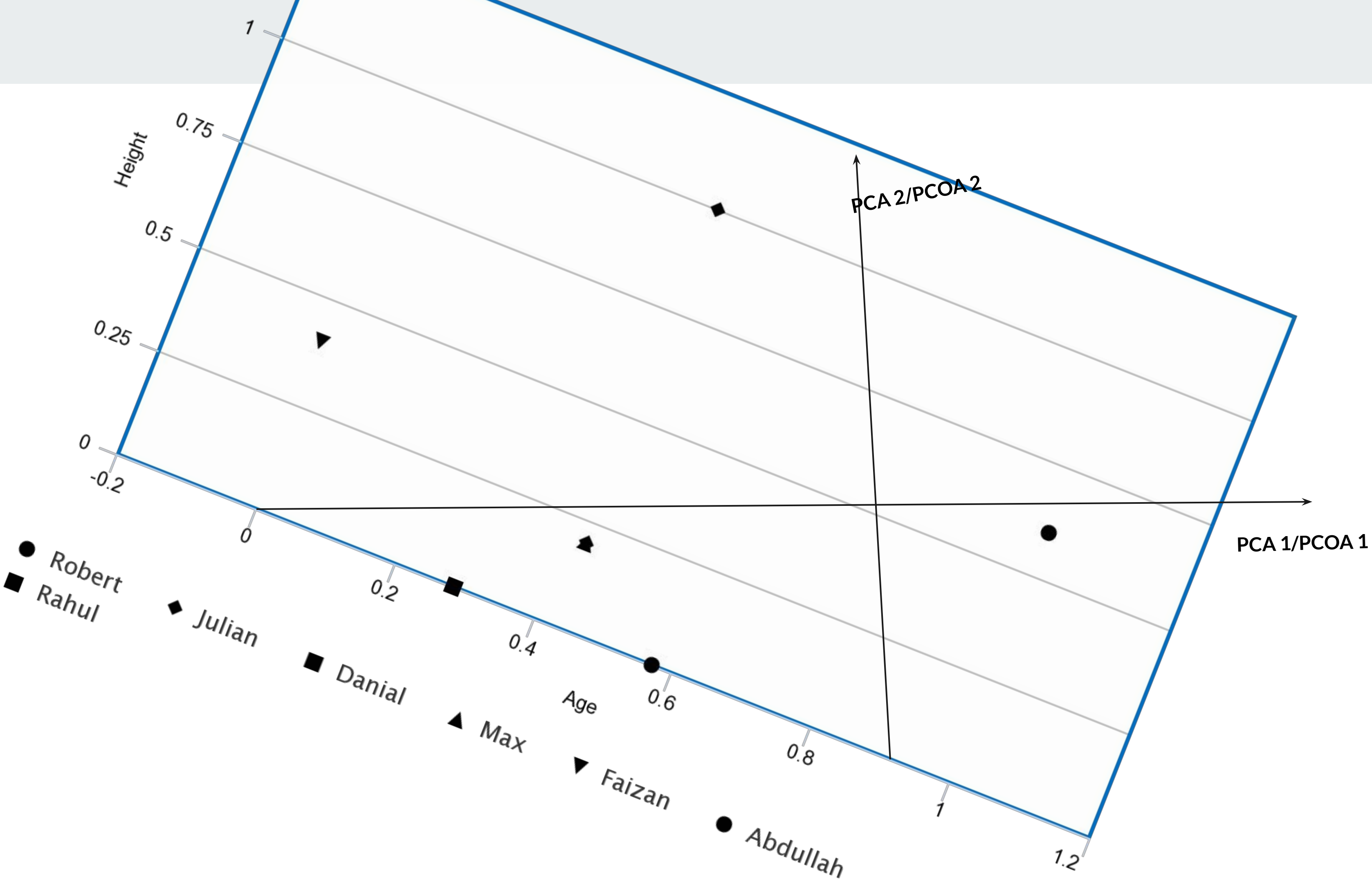
   .

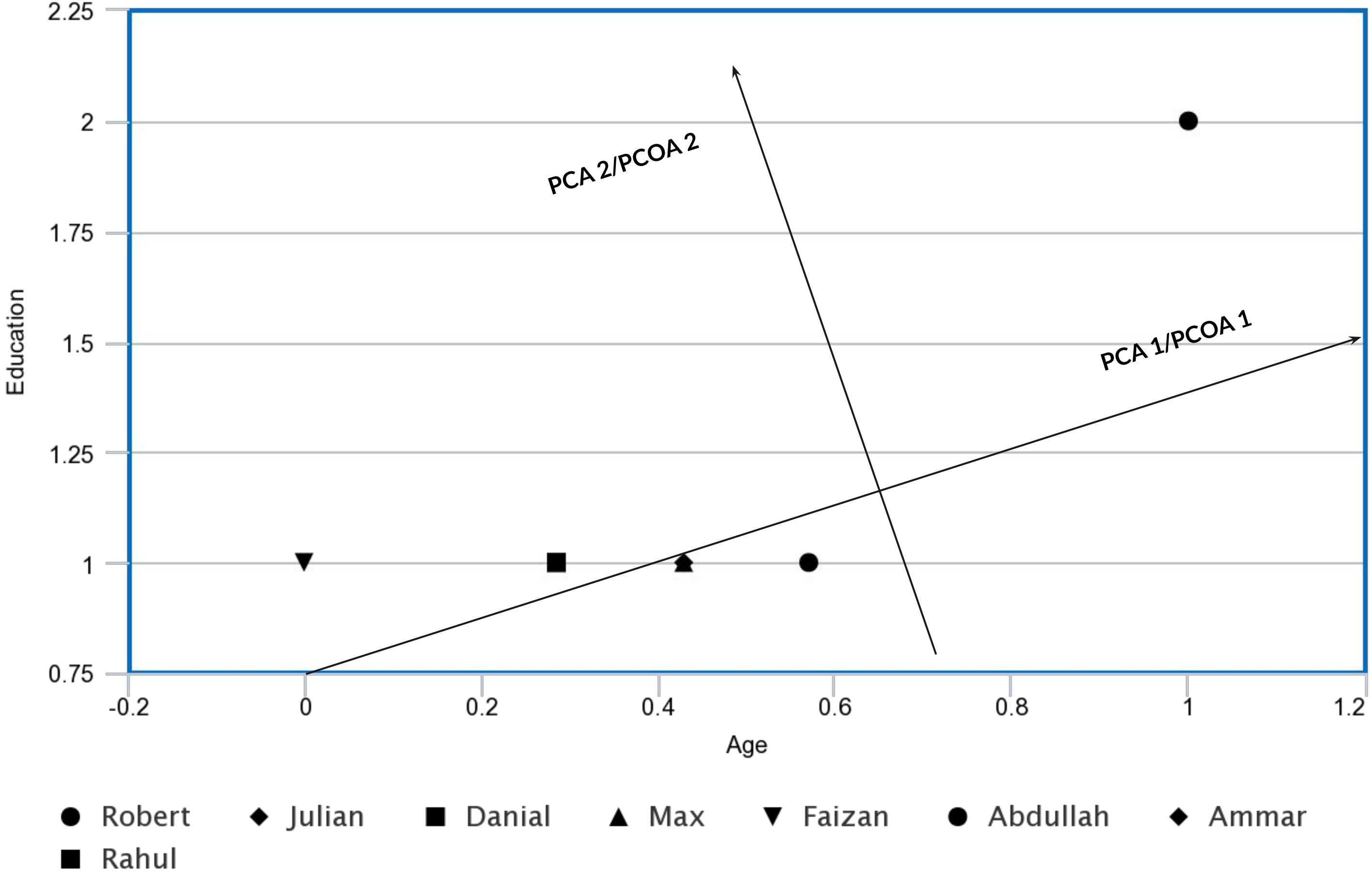
   PC”n”/PCoA”n” would span in the direction of “n”th most variation

3. Each axis has an eigenvalue whose magnitude indicates the amount of variation captured in that axis

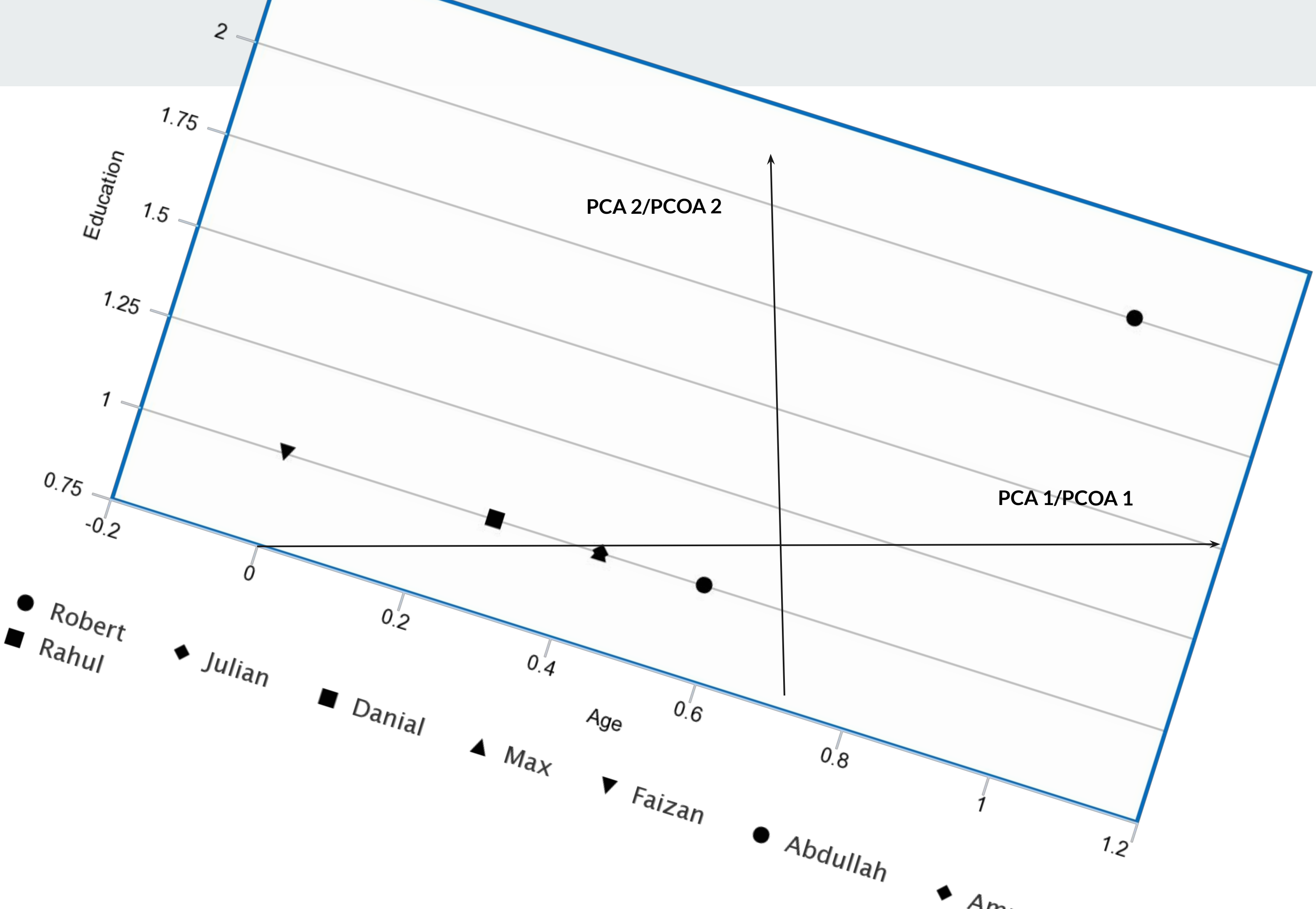
Name(ID)	**Age**		**Height**		**Gender** (1=f, 2=m, 3=other)	**Education Level** (0=Bachelor, 1= Master, 2= Post Doc)	**Class Label : Teacher(1) or Student(0)**
Robert	30	1	6.1	3/5	m(2)	Post Doc(2)	Teacher(1)
Julian	26	3/7	6.3	1	m(2)	Master(1)	Student(0)
Danial	25	2/7	5.8	0	m(2)	Master(1)	Student(0)
Max	26	3/7	5.9	1/5	m(2)	Master(1)	Student(0)
Faizan	23	0	6.0	2/5	m(2)	Master(1)	Student(0)
Abdullah	27	4/7	5.8	0	m(2)	Master(1)	Student(0)
Ammar	26	3/7	5.9	1/5	m(2)	Master(1)	Student(0)
Rahul	25	2/7	5.8	0	m(2)	Master(1)	Student(0)
Mean	**26**	3/7	**5.95**	0.3	**2**	**1.125**	


1.25
1
0.75
0.5
0.25
0
Height
-0.2
0
0.2
0.4
0.6
0.8
1
1.2
Age
PCA 2/PCOA 2
PCA 1/PCOA 1
● Robert
◆ Julian
■ Danial
▲ Max
▼ Faizan
● Abdullah
◆ Ammar
■ Rahul
meta-chart.com


Height
1
0.75
0.5
0.25
0
-0.2
0
0.2
0.4
0.6
0.8
1
1.2
Age
PCA 2/PCOA 2
PCA 1/PCOA 1
● Robert
■ Rahul
◆ Julian
■ Danial
▲ Max
▼ Faizan
● Abdullah

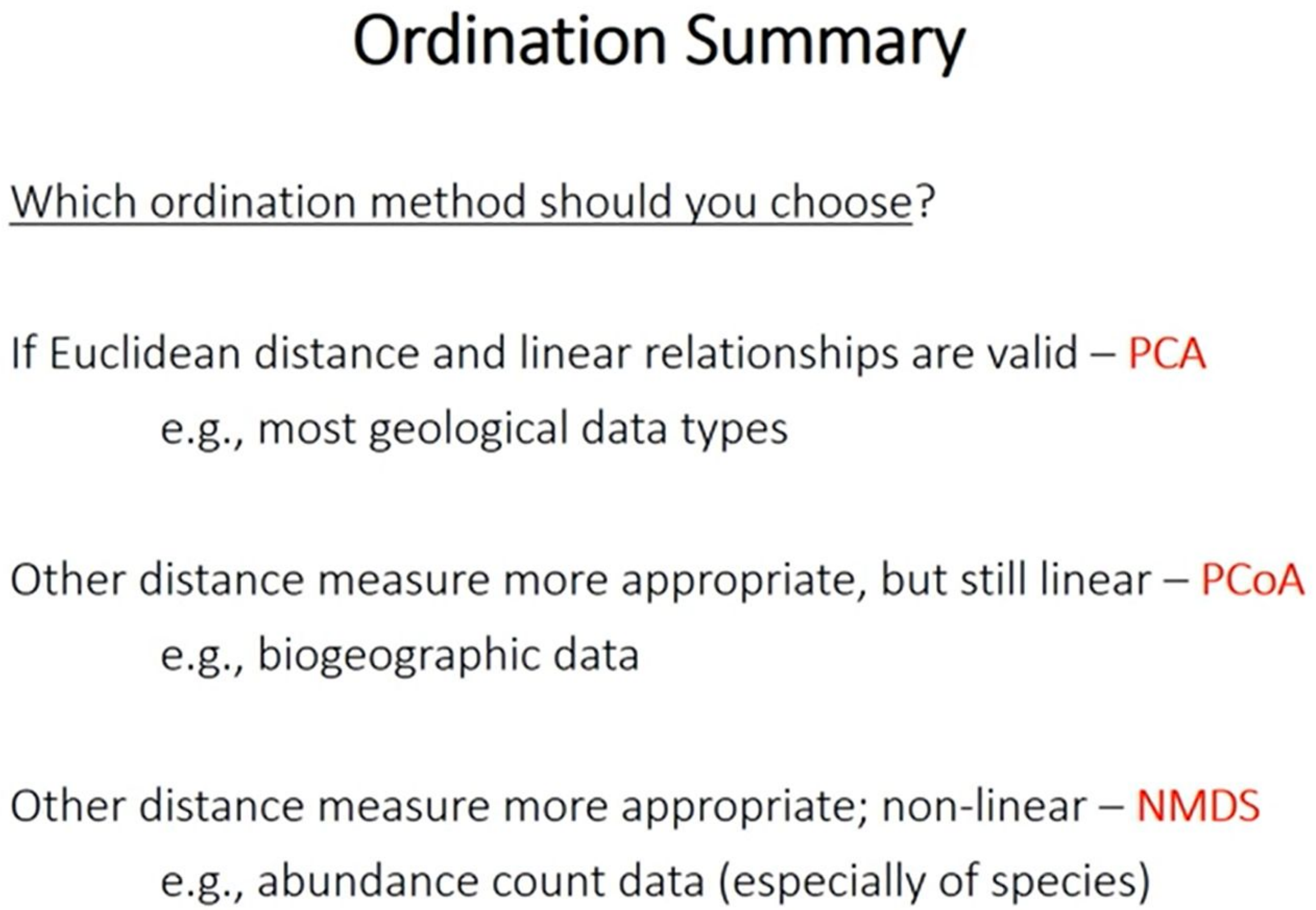


meta-chart.com


PCA 2/PCOA 2
PCA 1/PCOA 1
Education
2
1.75
1.5
1.25
1
0.75
-0.2
0
0.2
0.4
0.6
0.8
1
1.2
Age
Robert
Rahul
Julian
Danial
Max
Faizan
Abdullah
Am

Questions?

NMDS (Non-metric Multidimensional Scaling)



Ordination Summary

Which ordination method should you choose?

If Euclidean distance and linear relationships are valid – PCA

e.g., most geological data types

Other distance measure more appropriate, but still linear – PCoA

e.g., biogeographic data

Other distance measure more appropriate; non-linear – NMDS

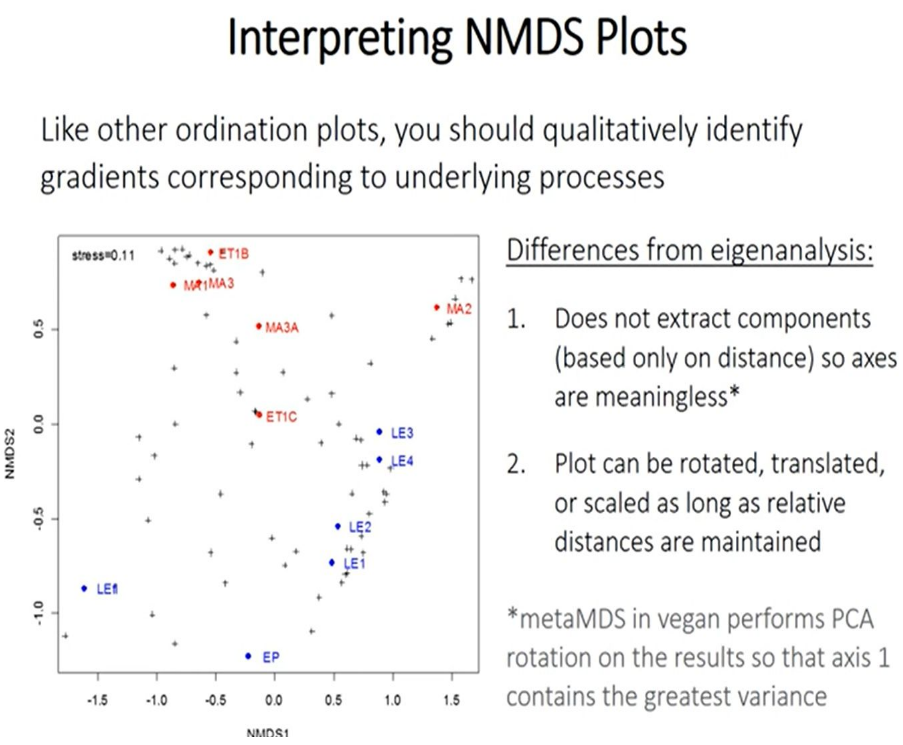
e.g., abundance count data (especially of species)

NMDS (Non-metric Multidimensional Scaling)

- Fundamentally different than PCA, CA (and DCA); more robust : **produces an ordination based on a distance or dissimilarity matrix.**
- Ordination based on ranks rather than distance **rather than object A being 2.1 units distant from object B and 4.4 units distant from object C, object C is the "first" most distant from object A while object C is the "second" most distant.**
- Avoids assumption of linear relationships among variables

Placing Objects Initially

- Random Placement
- **Placement according to a PCA result**
- Placement according to geographic distances
- Placement by moving from high to low dimensionality



Interpreting NMDS Plots

Like other ordination plots, you should qualitatively identify gradients corresponding to underlying processes

Differences from eigenanalysis:

1. Does not extract components (based only on distance) so axes are meaningless*
2. Plot can be rotated, translated, or scaled as long as relative distances are maintained

*metaMDS in vegan performs PCA rotation on the results so that axis 1 contains the greatest variance

NMDS (Non-metric Multidimensional Scaling)

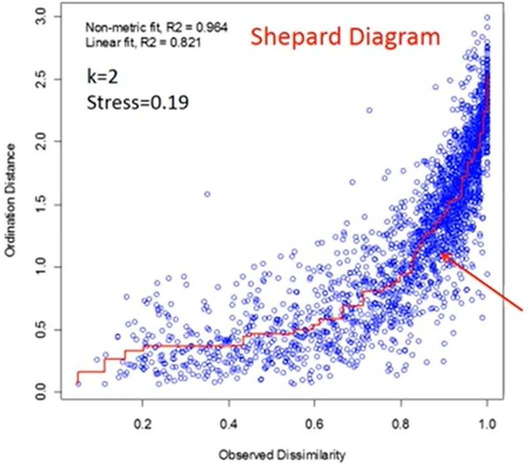
Stress

NMDS **Maximizes rank-order correlation** between **distance measures** and **distance in ordination space**. Points are **iteratively moved** to **minimize "stress"**. Stress is a **measure of the mismatch between the two kinds of distance.**

Think of optimizing stress as: “Pulling on all points a little **bit so no single point is completely wrong**, **all points are a little off compared to distances**”

NMDS Goodness-of-Fit

Goodness-of-fit is measured by “stress” – a measure of rank-order disagreement between observed and fitted distances

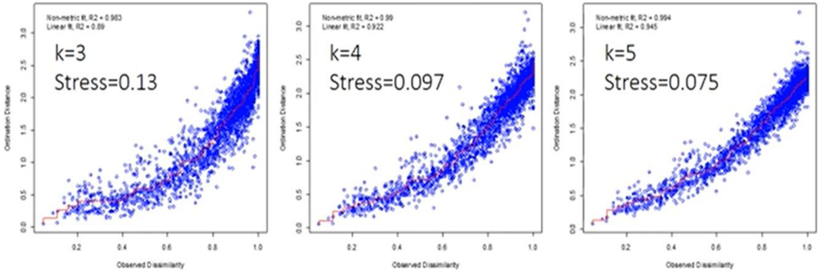


Stress calculated from residuals around monotone regression line

Ideally, all points should fall on monotonic line (increasing ordination distance = increasing observed distance)

NMDS Goodness-of-Fit

Stress *always* decreases with increasing dimensionality *k*

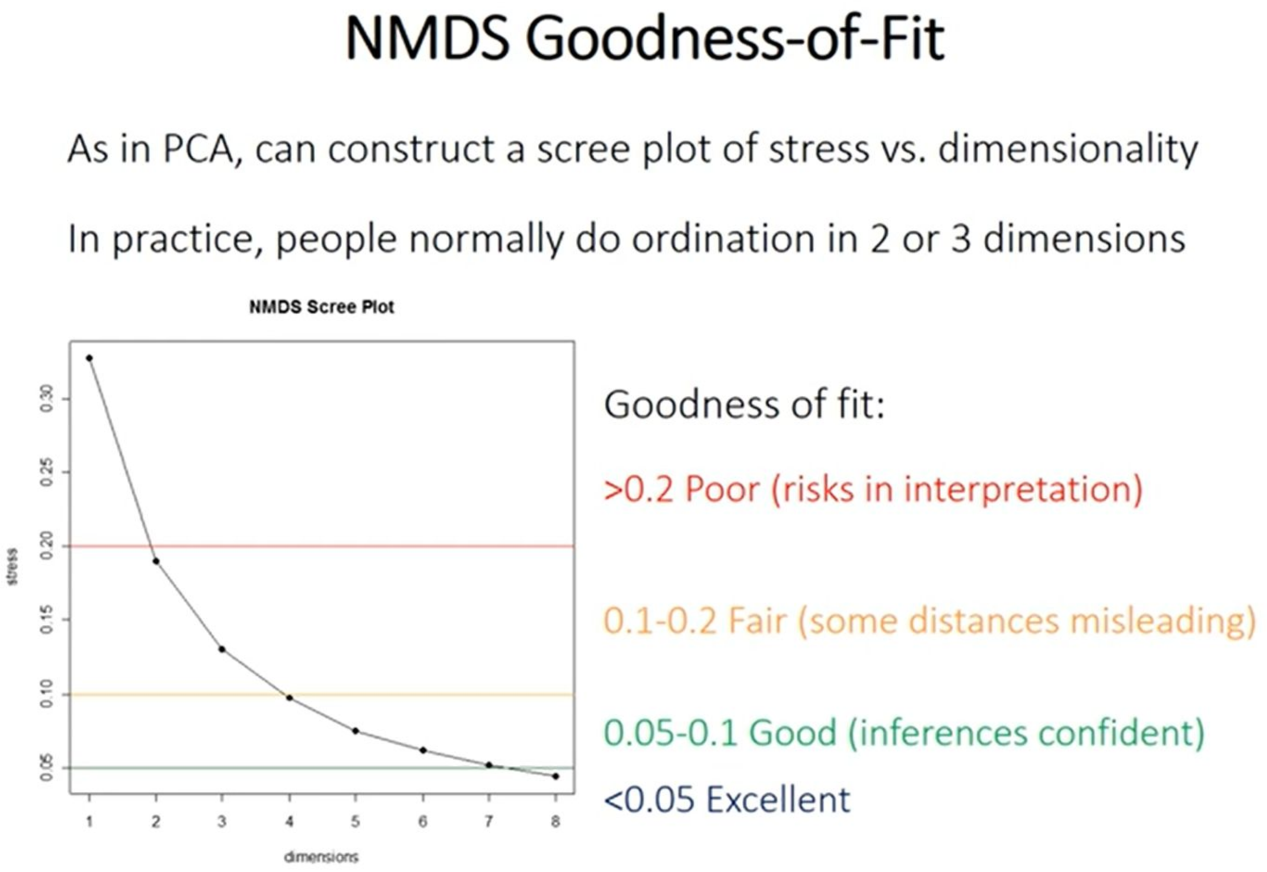


Remember that a 2D solution is not a projection of higher-dimensional solutions (as in PCA)

Shepard Diagram

NMDS (Non-metric Multidimensional Scaling)

Scree Plot



NMDS Goodness-of-Fit

As in PCA, can construct a scree plot of stress vs. dimensionality

In practice, people normally do ordination in 2 or 3 dimensions

Goodness of fit:

>0.2 Poor (risks in interpretation)

0.1-0.2 Fair (some distances misleading)

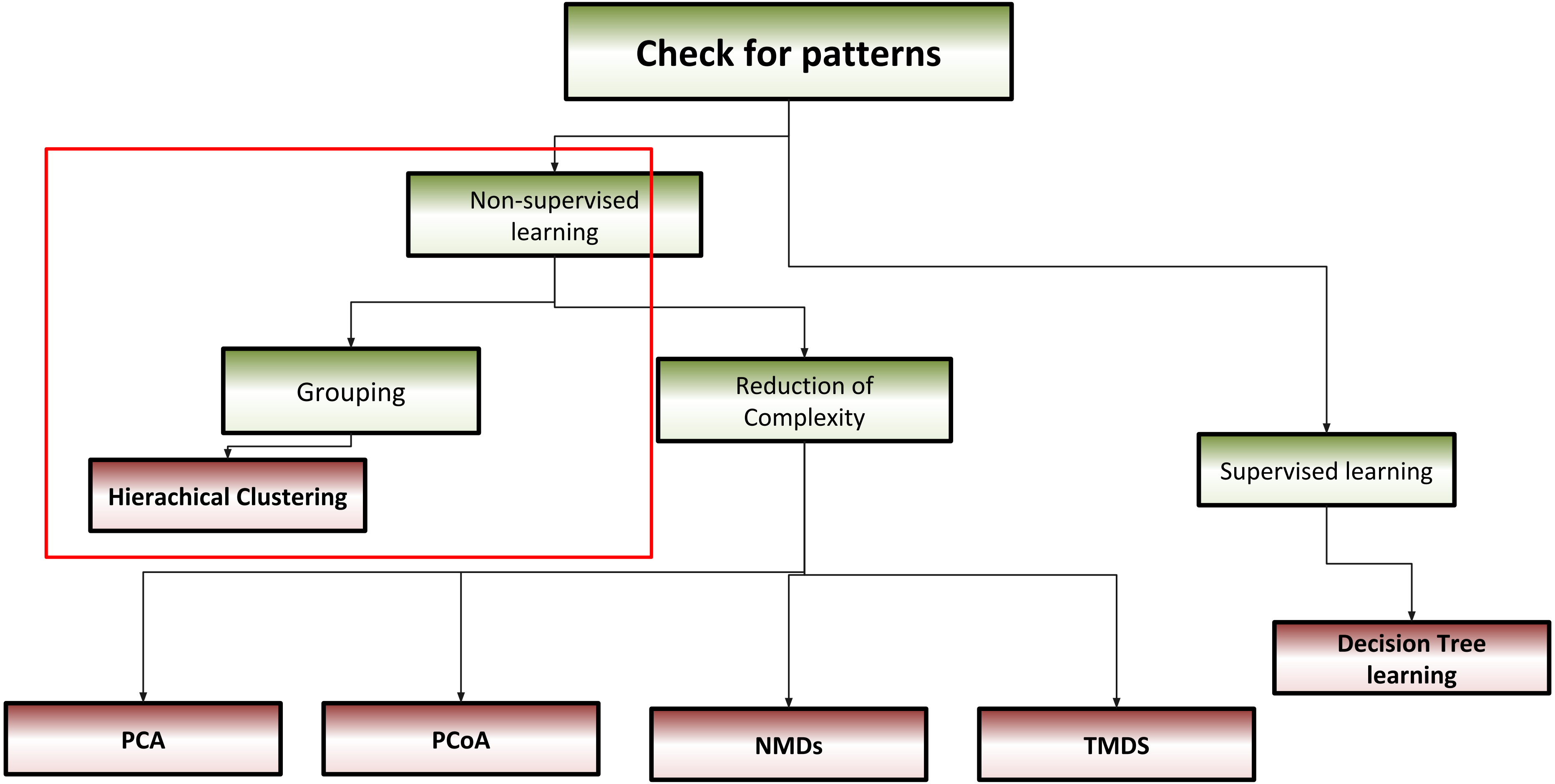
0.05-0.1 Good (inferences confident)

<0.05 Excellent

Grouping

- Clustering
    - Centroid Based
        - **K-Means**
    - Density Based
        - **DBSCAN**
    - Hierarchical
        - **Agglomerative**
- Dendrograms & Heatmaps

roadmap



Check for patterns

Non-supervised learning

Grouping

Hierachical Clustering

Reduction of Complexity

Supervised learning

Decision Tree learning

PCA

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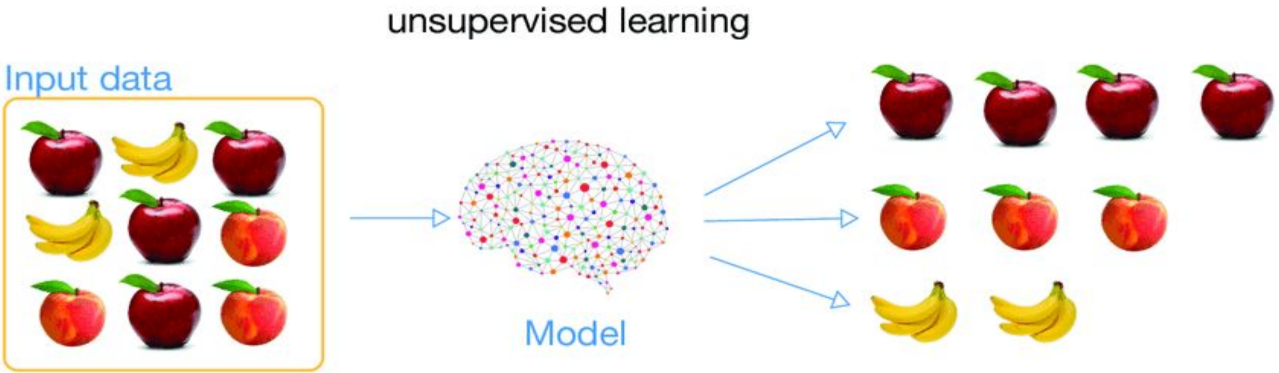
NMDs

TMDS

Clustering



finding a ***structure*** in a collection of **unlabeled data** i.e. the process of **organizing objects into groups** whose members are similar in some way

why?

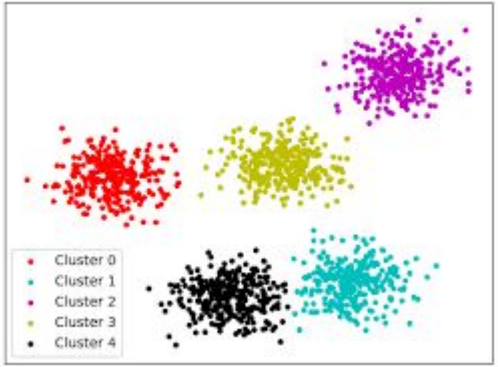
finding representatives for

- homogeneous groups (***data reduction***),
- in finding "natural clusters" and describe their unknown properties (***"natural" data types***),
- in finding useful and suitable groupings (***"useful" data classes***) or
- in finding unusual data objects (***outlier detection***)

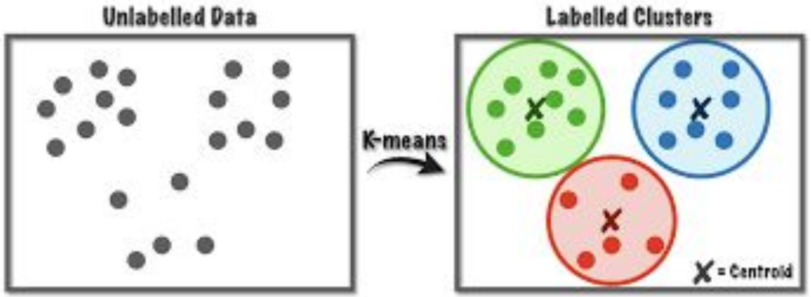
how?

- Centroid based : **K-Means**
- Density based : **DBSCAN**
- Hierarchical : **Agglomerative**

what?



Centroid Based Clustering



K-Means

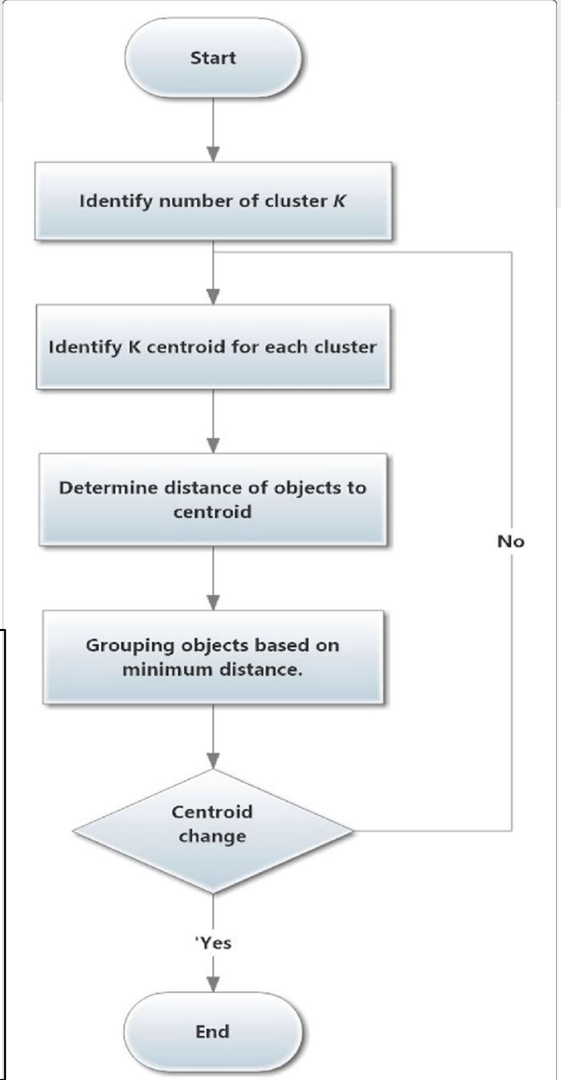
Centroid

The middle of a cluster i.e. a multidimensional average of a cluster

why & why not?

- + simple
- + guarantees convergence
- + scales to large data set
- - clustering goodness depends on initialization
- - sensitive to outliers
- - troubled with clusters of varying size & density

how?



Start

Identify number of cluster *K*

Identify K centroid for each cluster

Determine distance of objects to centroid

Grouping objects based on minimum distance.

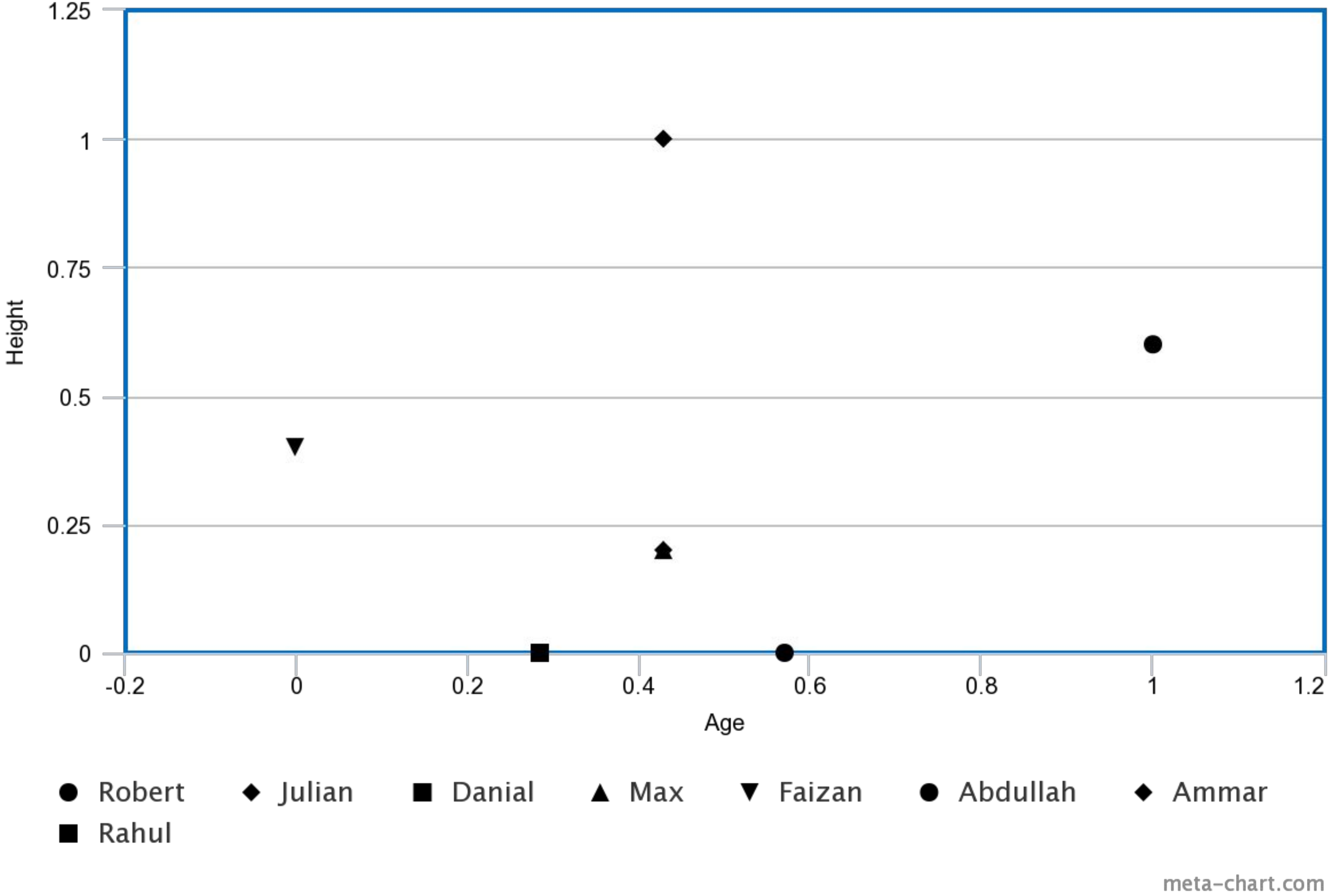
Centroid change

No

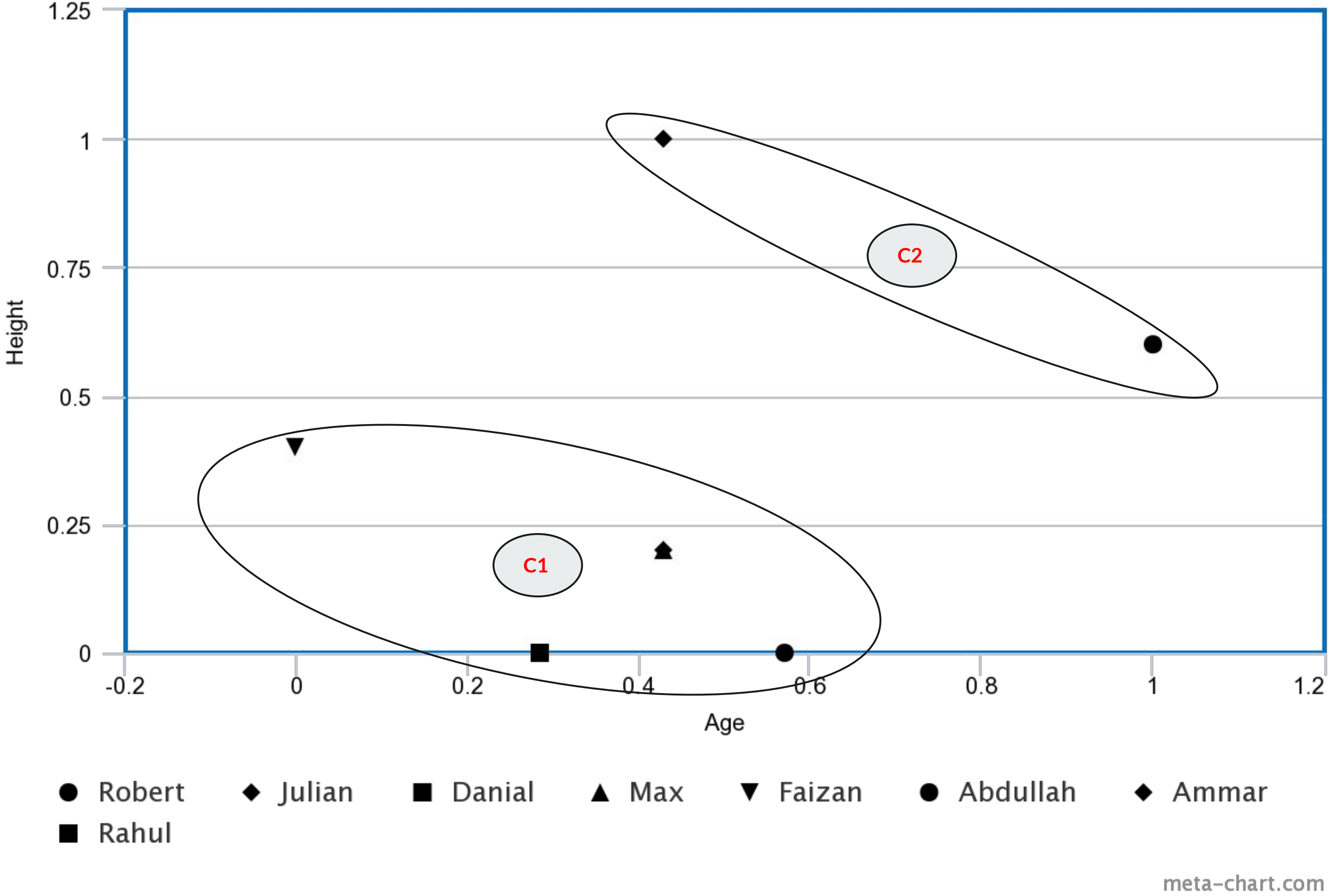
'Yes

End

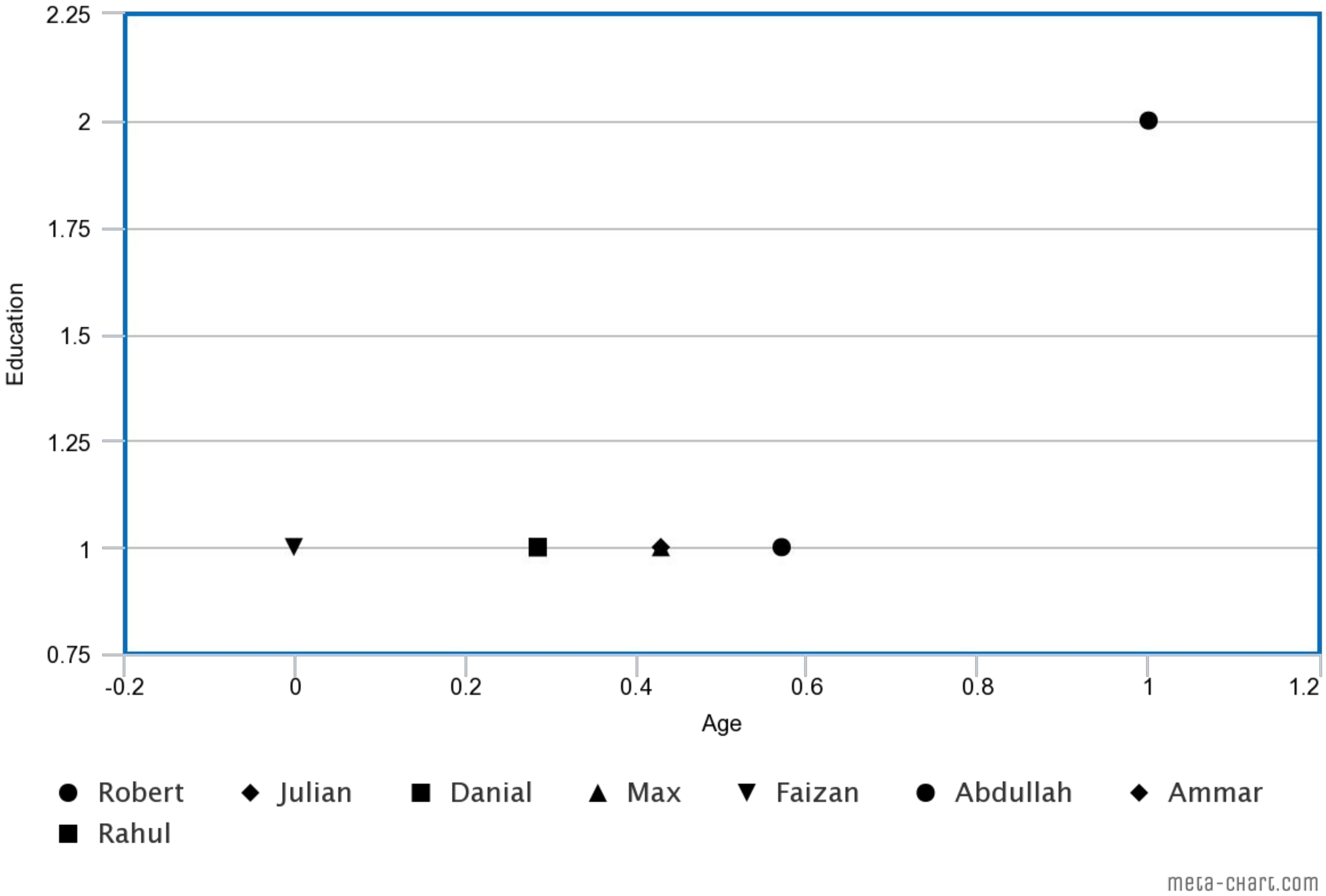
Centroid Based Clustering: K-Means



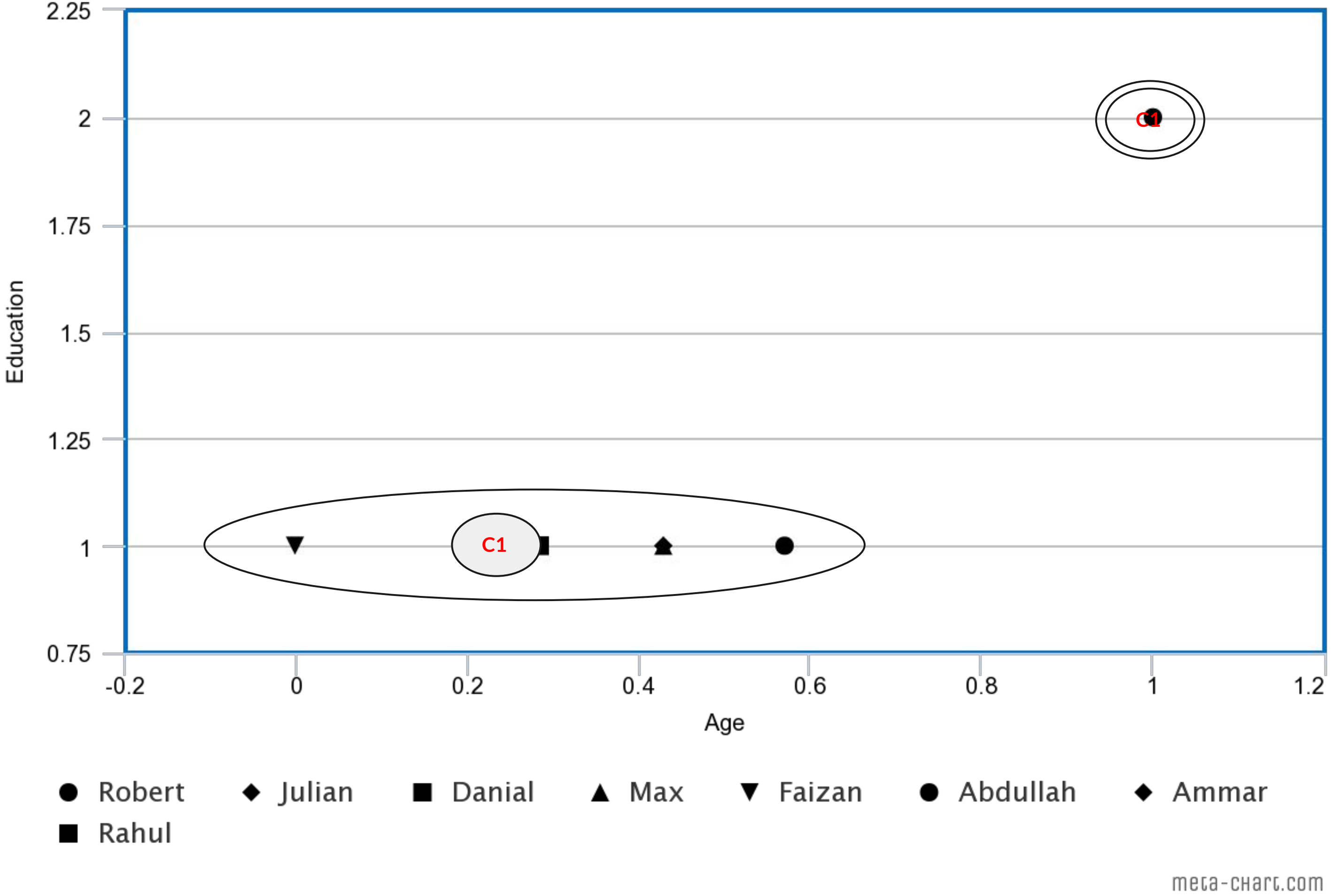
Centroid Based Clustering: K-Means



Centroid Based Clustering: K-Means

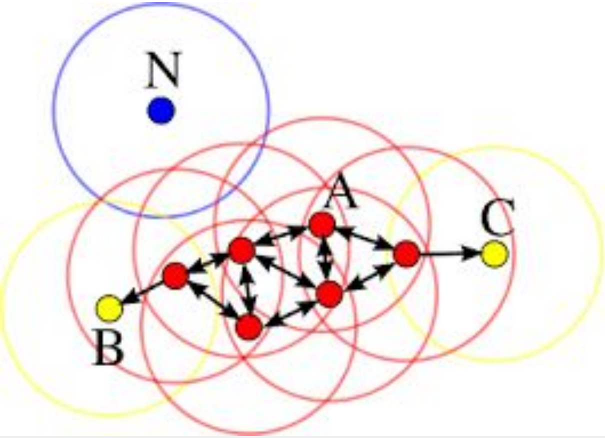


Centroid Based Clustering: K-Means

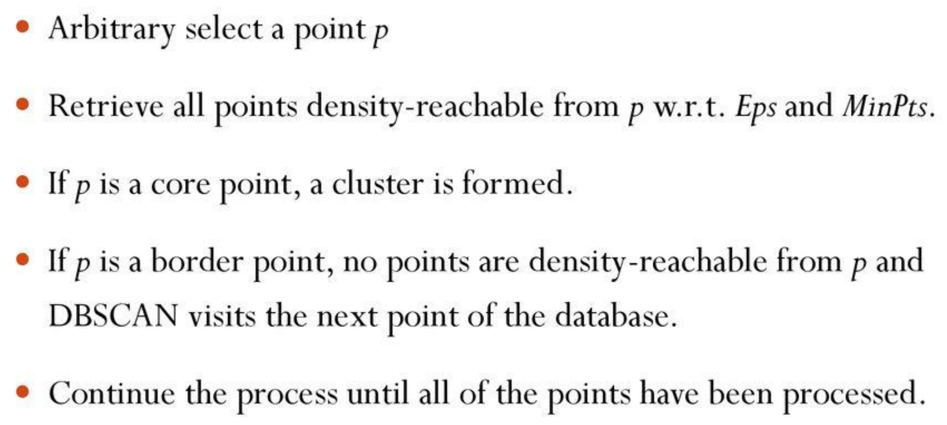


Questions?

Density Based Clustering: DBSCAN

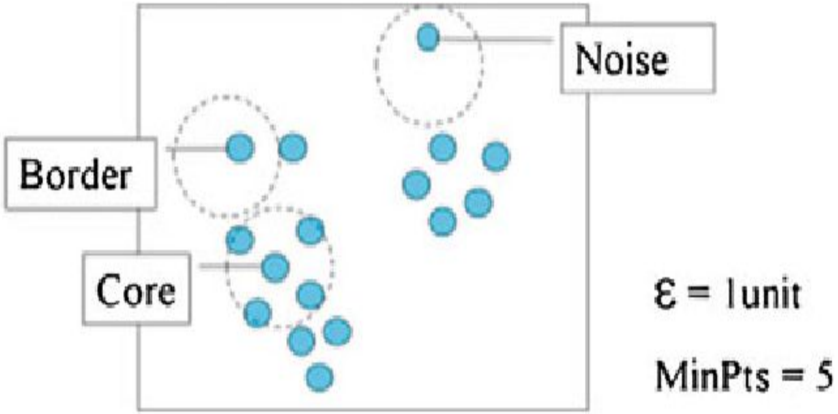


how?



- Arbitrary select a point *p*
- Retrieve all points density-reachable from *p* w.r.t. *Eps* and *MinPts*.
- If *p* is a core point, a cluster is formed.
- If *p* is a border point, no points are density-reachable from *p* and DBSCAN visits the next point of the database.
- Continue the process until all of the points have been processed.

core, border & noise points

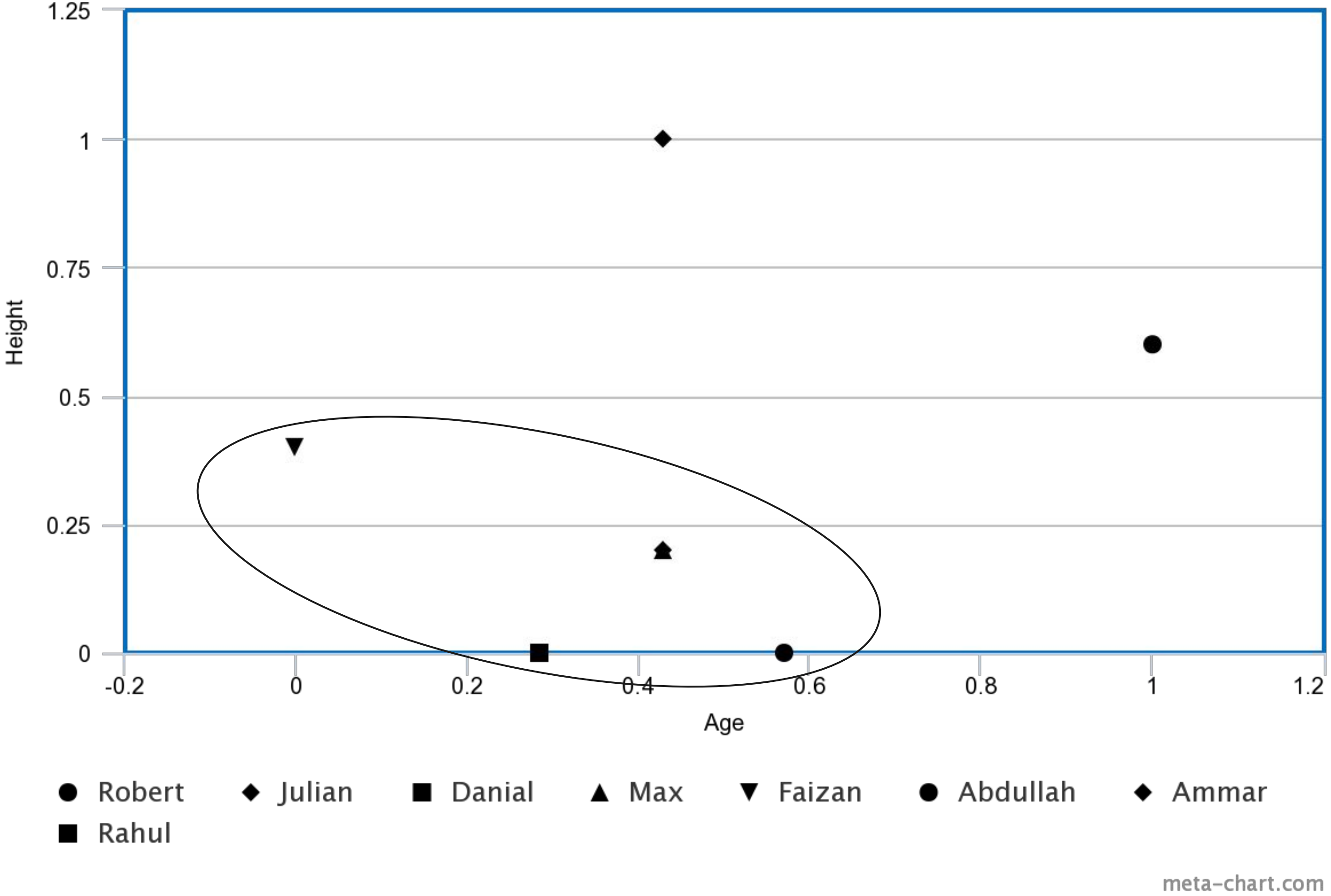


why & why not?

- + can handle varying density
- + good with outliers
- - does not work well at similar densities
- - struggles with high dimensional data

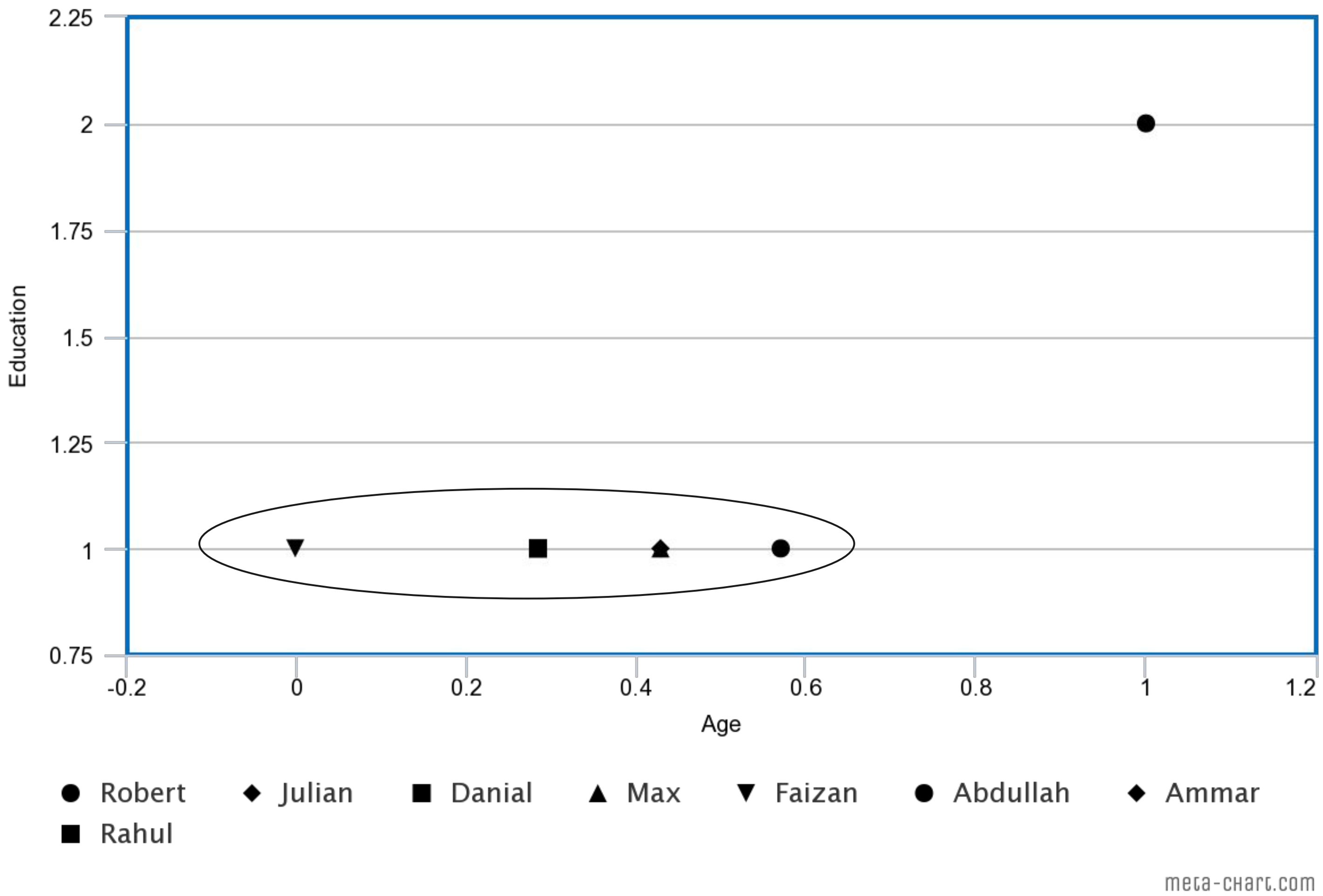
Density Based Clustering: DBSCAN

epsilon: 0.5
minPts: 2

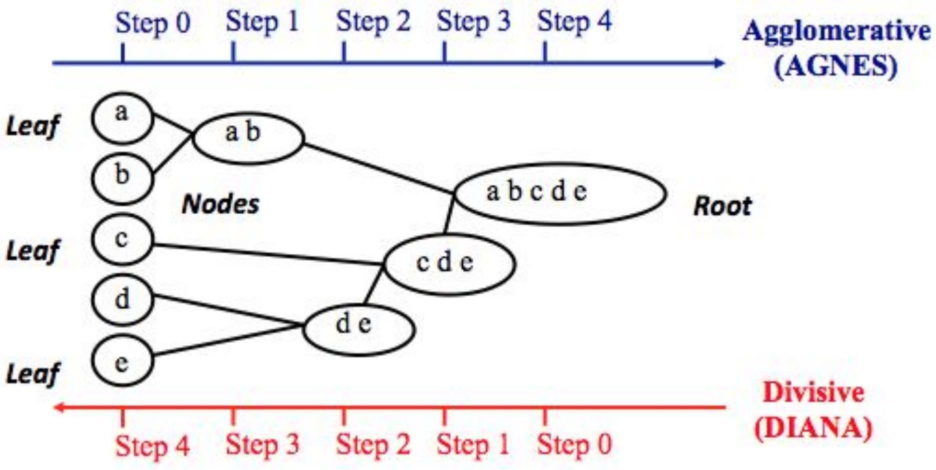


Density Based Clustering: DBSCAN

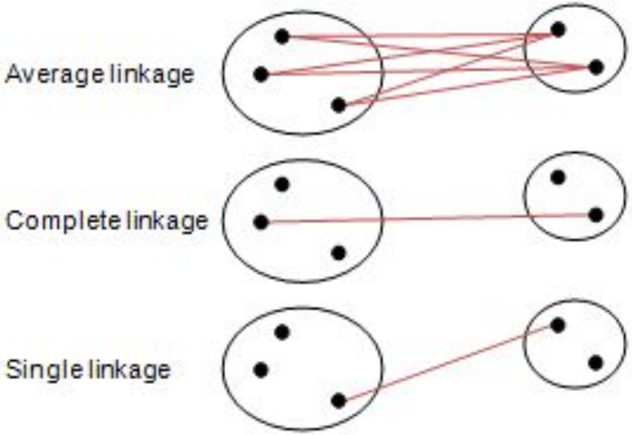
epsilon: 0.5
minPts: 2



Hierarchical Clustering: Agglomerative



linkage criterion

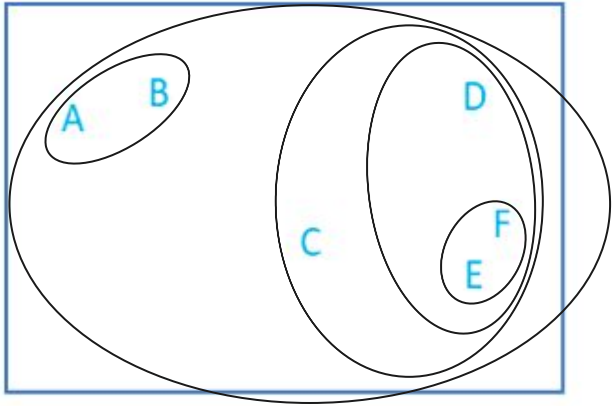


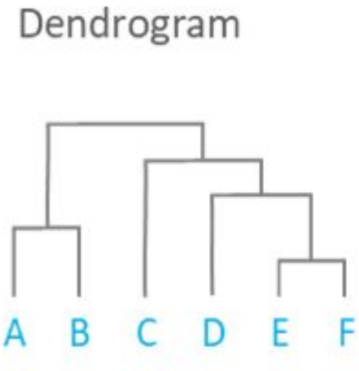
why & why not?

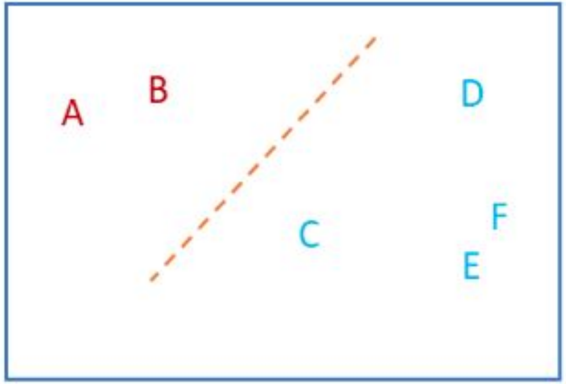
- + easy to do & understand
- + possibilities to choose from a hierarchy of clusters
- - possible to misinterpret
- - expensive

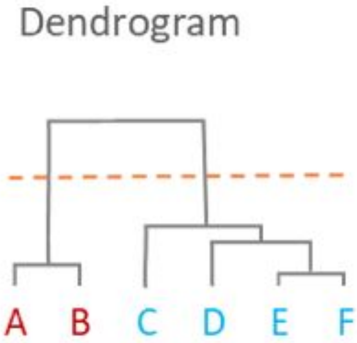
Hierarchical cluster analysis is an algorithmic approach to find discrete groups with varying degrees of (dis)similarity in a data set represented by a (dis)similarity matrix. These groups are hierarchically organised as the algorithms proceed and may be presented as a **dendrogram**

Hierarchical Clustering: Dendrogram




Dendrogram
A
B
C
D
E
F




Dendrogram
A
B
C
D
E
F