

Clustering

Introduction to Clustering

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N

ANTIHEDEN UND
DOPPELMORAL



SCHARFER HUMOR UND
DUNKLE VERBRECHEN



GEFÄHRliche WELTEN
UND TIEFGREIFENDE
KONSEQUENZEN



COMING-OF-AGE
GESCHICHTEN

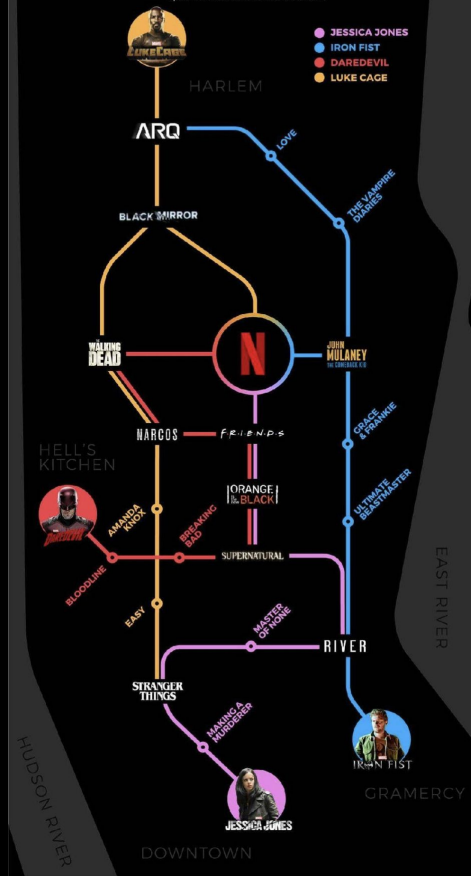


MARVEL

NETFLIX

DER WEG ZU MARVEL'S DEFENDERS

Auf dem Weg zum Marvel-Binge gibt es einige unerwartete Haltepunkte, aber die Reise durch die Serienwelt bringt genauso viel Spaß wie die Ankunft bei den Defenders.





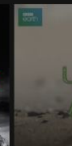
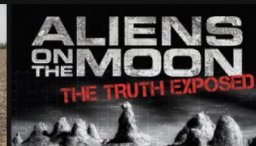
Netflix Originals



Derzeit beliebt



Weil Ihnen „Unser Kosmos: Die Reise geht weiter“ gefallen hat

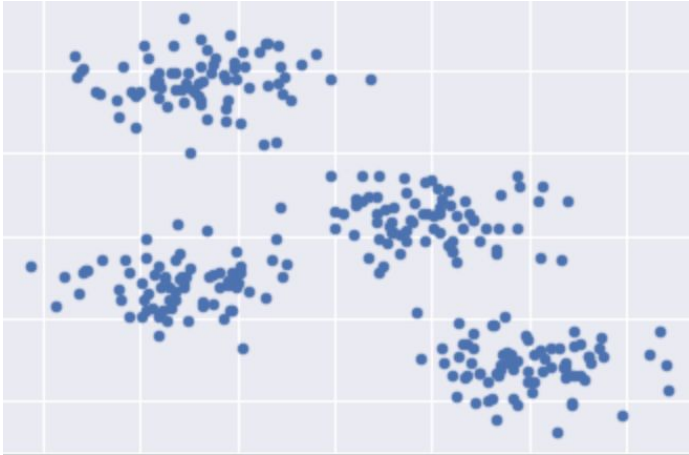


Beliebt auf Netflix

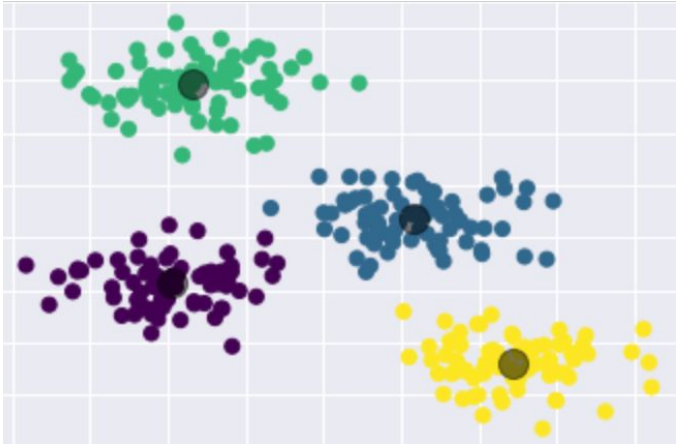


Discover unknown
subgroups in data.

Unlabeled examples (observations)



Grouping unlabeled examples is called clustering.



Clustering is **unsupervised learning**

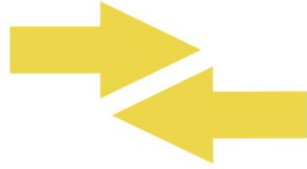
The goal is to discover interesting things about the observations:

- is there an informative way to **visualize** the data?
- Can we **discover subgroups** among the variables or among the observations?

Use cases for cluster analysis

- **Customer segmentation** (understanding different customer segments to devise marketing strategies)
- **Recommender systems** (grouping together users with similar viewing patterns on Netflix, in order to recommend similar content)
- **Anomaly detection** (fraud detection, detecting defective mechanical parts)

To cluster your data, you'll follow these steps:



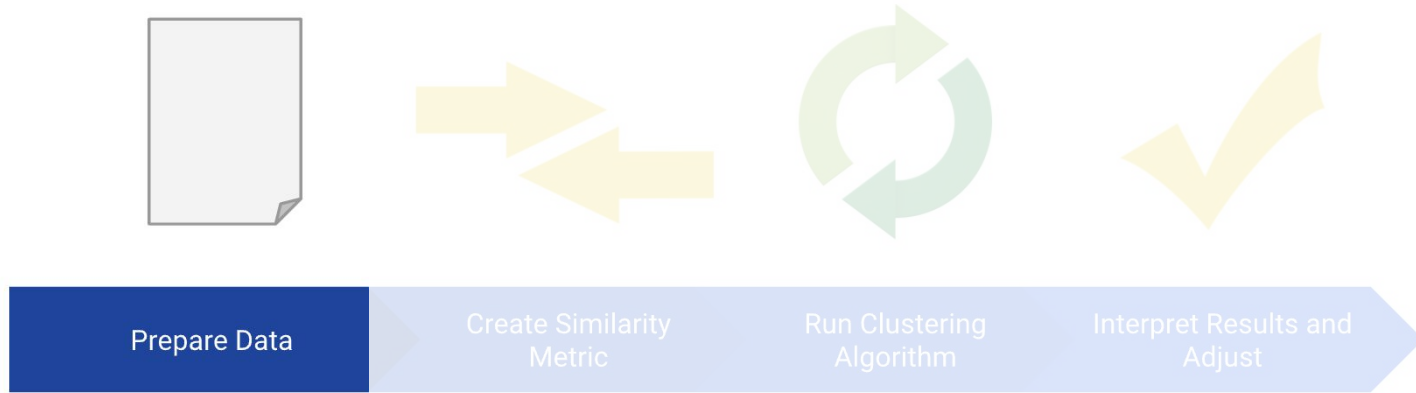
Prepare Data

Create Similarity
Metric

Run Clustering
Algorithm

Interpret Results and
Adjust

To cluster your data, you'll follow these steps:



Exclude all missing values and outliers

Normalizing data

If you only have a few values, you could use this simple rule:

$$x' = \frac{x}{\max(x)}$$

Normalizing data by rescaling (min-max normalization)

Typically, we use rescaling like this:

Rescaling results in a range [0, 1]

$$x' = \frac{x - \min(x)}{\max(x) - \min(x)}$$

Standardization with **z-score**

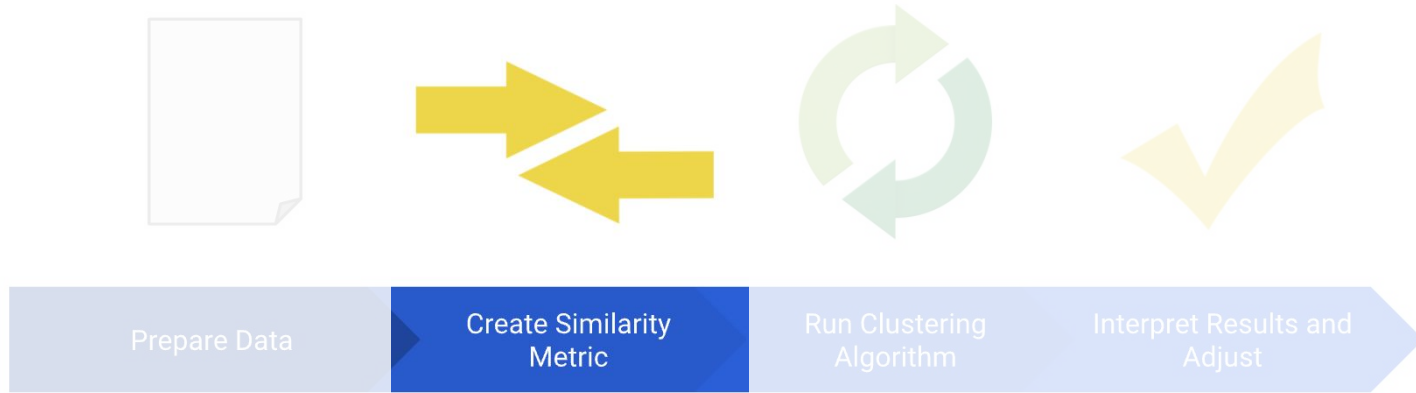
Another alternative:

$$x' = (x - \mu) / \sigma$$

where: μ = mean

σ = standard deviation

To cluster your data, you'll follow these steps:



How to create a similarity measure for a numeric feature?

- Feature X_1 : shoe size

Shoe A



size: 8

Shoe B



size: 11

How to create a similarity measure for a numeric feature?

- Feature X_1 : shoe size



Create a manual **similarity measure** for two numeric features

- Feature X_1 : shoe size (numeric)
- Feature X_2 : price (numeric)



size: 8
price: 120



size: 11
price: 150

Create a manual similarity measure for two numeric features

- Feature X_1 : shoe size (numeric)
- Feature X_2 : price (numeric)



Create a manual similarity measure for two numeric features

Since we don't have enough data, we'll simply scale the data without normalizing

Action	Method
Scale the size.	Assume a maximum possible shoe size of 20. Divide 8 and 11 by the maximum size 20 to get 0.4 and 0.55.
Scale the price.	Divide 120 and 150 by the maximum price 150 to get 0.8 and 1.
Find the difference in size.	$0.55 - 0.4 = 0.15$
Find the difference in price.	$1 - 0.8 = 0.2$
Find the RMSE.	$\sqrt{\frac{0.2^2 + 0.15^2}{2}} = 0.17$

$$x' = \frac{x}{\max(x)}$$

Create a manual similarity measure for two numeric features

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Create a manual similarity measure for a categorical feature

- Feature X_3 : color (categorical)



color: black



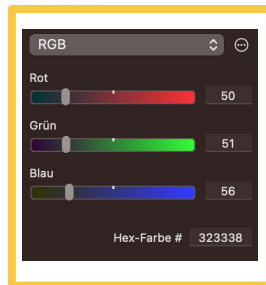
color: blue

Create a manual similarity measure for a categorical feature

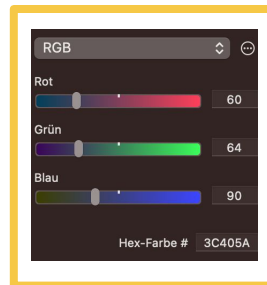
- Feature X_o : color (categorical)



color: black



color: blue



Create a manual **similarity** measure for a **categorical** feature

Feature with **multiple levels** (multivalent)

- Movie genres:
 - comedy,
 - action,
 - drama,
 - non-fiction,
 - biographical
- Can be "action" and "comedy" simultaneously, or just "action"

How to measure similarity?

1: [comedy, action]



A

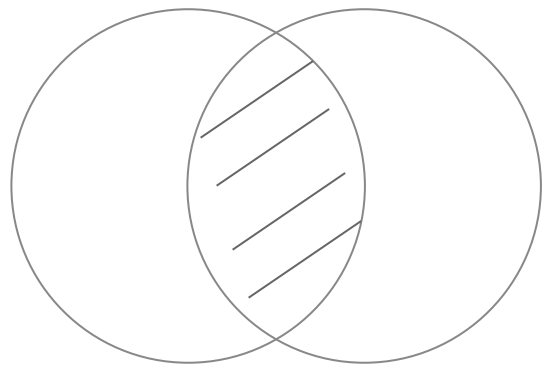
2: [action, drama]



B

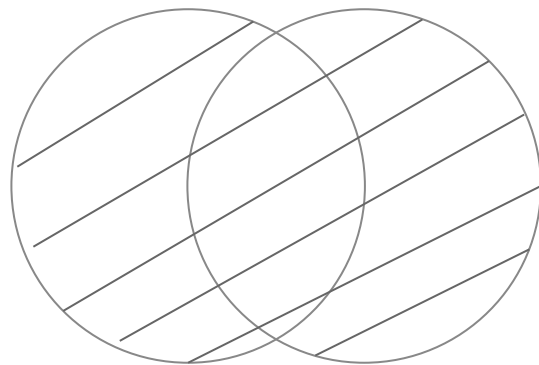
Intersection & union

Intersection



$A \cap B$

Union

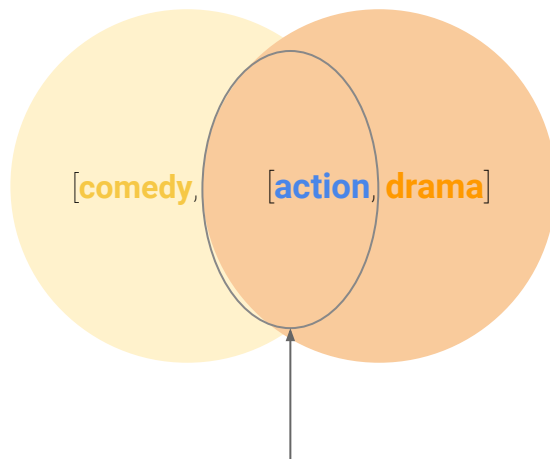


$A \cup B$

Jaccard distance

[comedy, action]

[action, drama]



Union:
[comedy, action, drama]

Intersection:
action

Jaccard distance

Intersection

action

Union

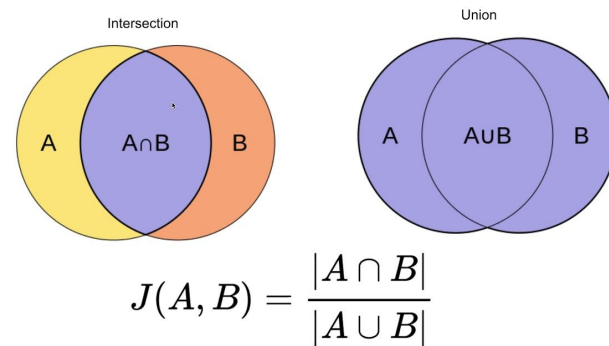
[comedy, action, drama]

$A \cap B$

$A \cup B$

Create a manual similarity measure for a categorical feature

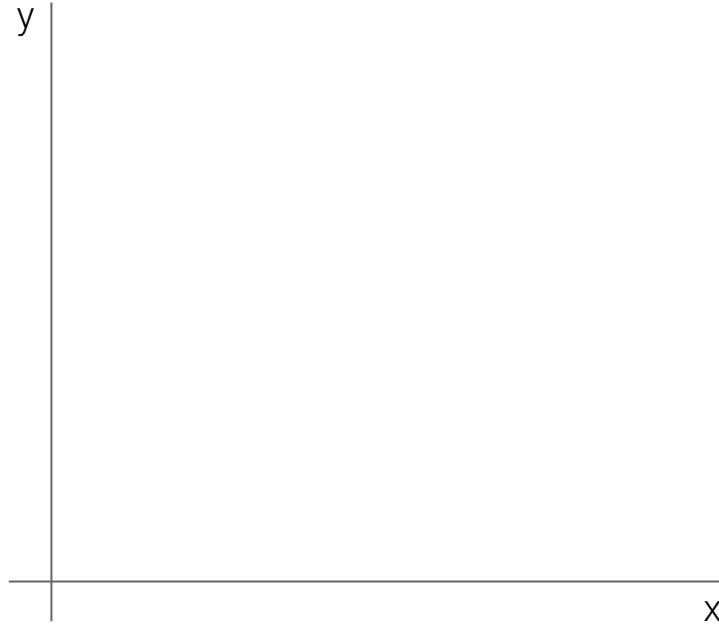
- A: ["comedy","action"] and B: ["comedy","action"] = 1
- A: ["comedy","action"] and B: ["action"] = $\frac{1}{2}$
- A: ["comedy","action"] and B: ["action", "drama"] = $\frac{1}{3}$
- A: ["comedy","action"] and B: ["non-fiction","biographical"] = 0



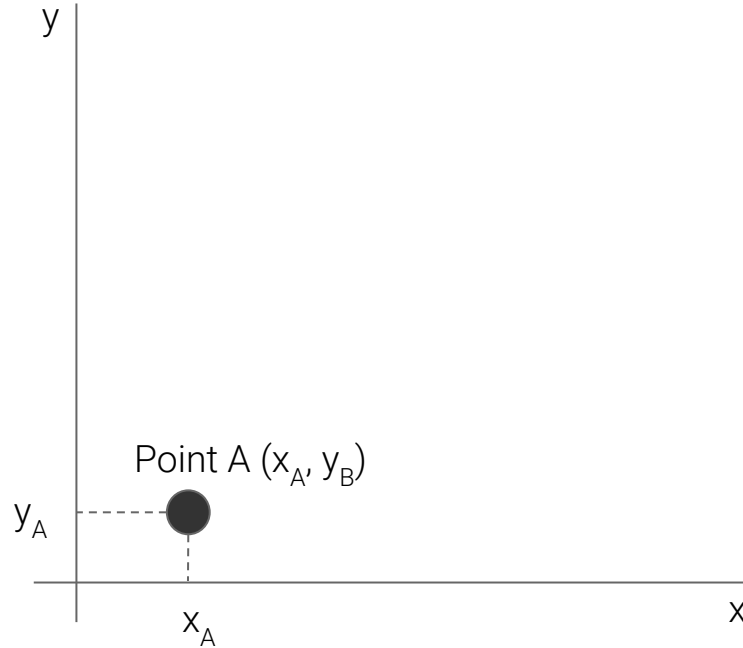
- **Jaccard similarity.** Calculate similarity using the ratio of common values
- **Jaccard distance.** Calculate distance using (1- Jaccard similarity)

Popular distance metrics for numerical features

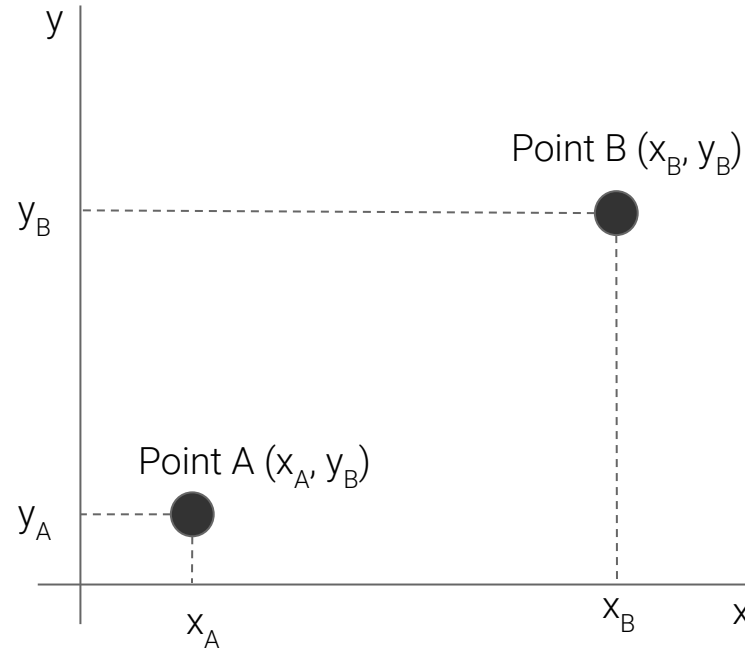
Let's start with a simple coordinate system (CS)



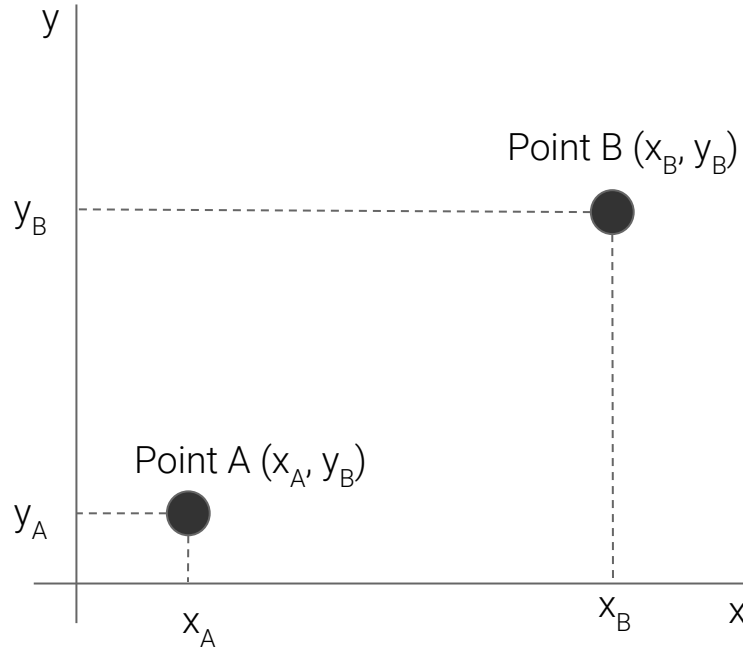
We include one observation “A”



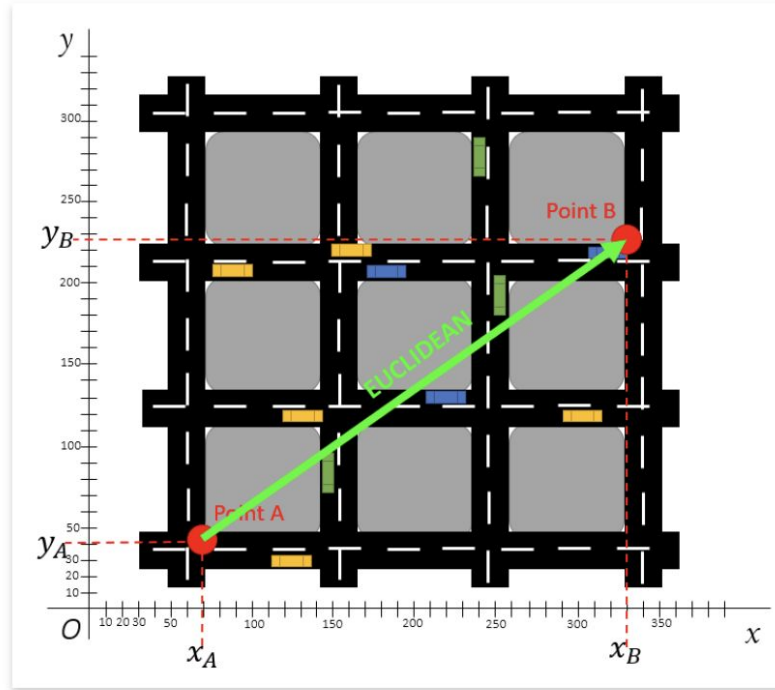
And another observation "B"



How can we measure the distance between A and B?



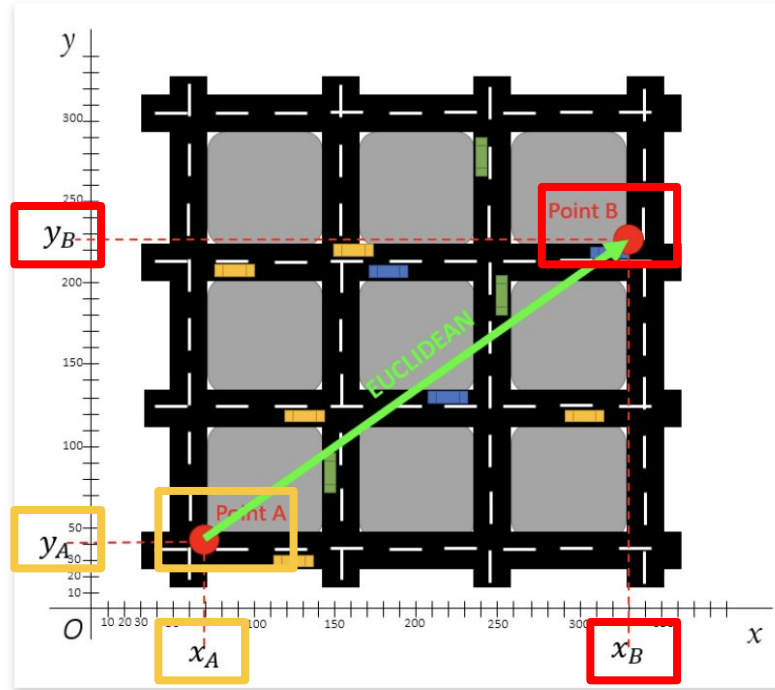
Imagine there are streets on the CS



This would be the shortest distance

$$d(A, B) = \sqrt{\sum_{i=1}^n (A_i - B_i)^2}$$

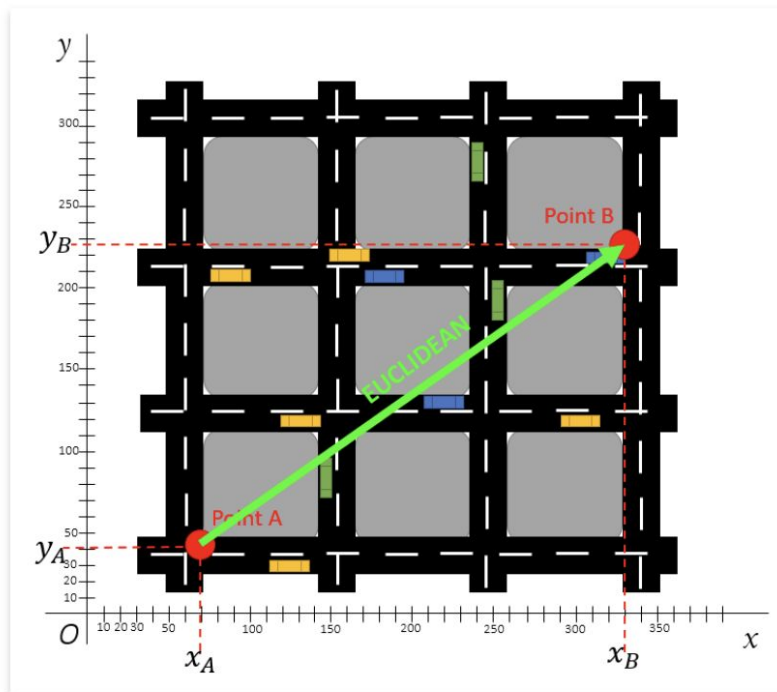
- $x_A = 70$
- $x_B = 330$
- $y_A = 40$
- $y_B = 228$



Euclidean distance (L_2 distance)

$$d(A, B) = \sqrt{\sum_{i=1}^n (A_i - B_i)^2}$$

- $x_A = 70$
- $x_B = 330$
- $y_A = 40$
- $y_B = 228$



$$d(A, B) = \sqrt{(x_A - x_B)^2 + (y_A - y_B)^2}$$

$$d(A, B) = \sqrt{(70 - 330)^2 + (40 - 228)^2}$$

$$d(A, B) = \sqrt{(-260)^2 + (-188)^2}$$

$$d(A, B) = \sqrt{(76600 + 35344)}$$

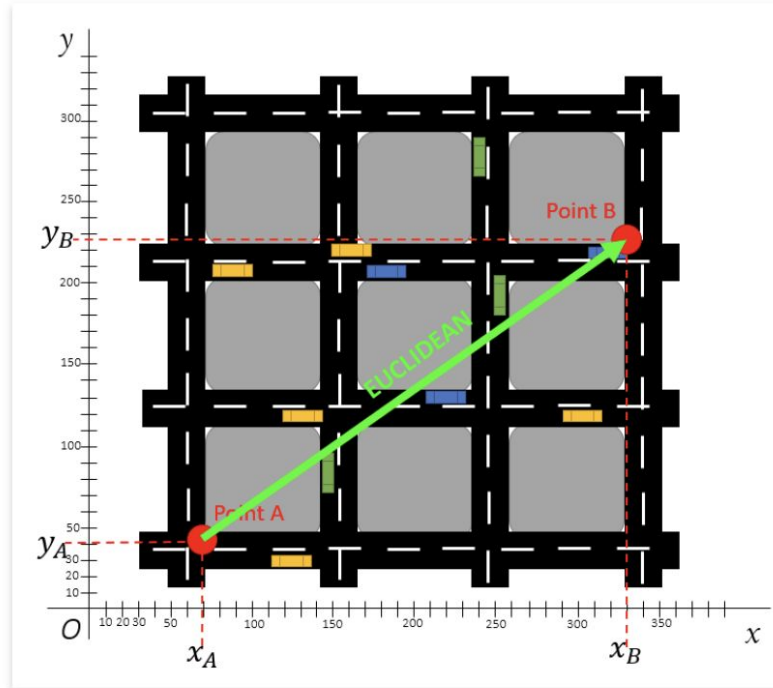
$$d(A, B) = \sqrt{112225}$$

$$d(A, B) = 335$$

Squared Euclidean distance (L_2)

$$d^2(A, B) = \sum_{i=1}^n (A_i - B_i)^2$$

- $x_A = 70$
- $x_B = 330$
- $y_A = 40$
- $y_B = 228$



$$d^2(A, B) = (x_A - x_B)^2 + (y_A - y_B)^2$$

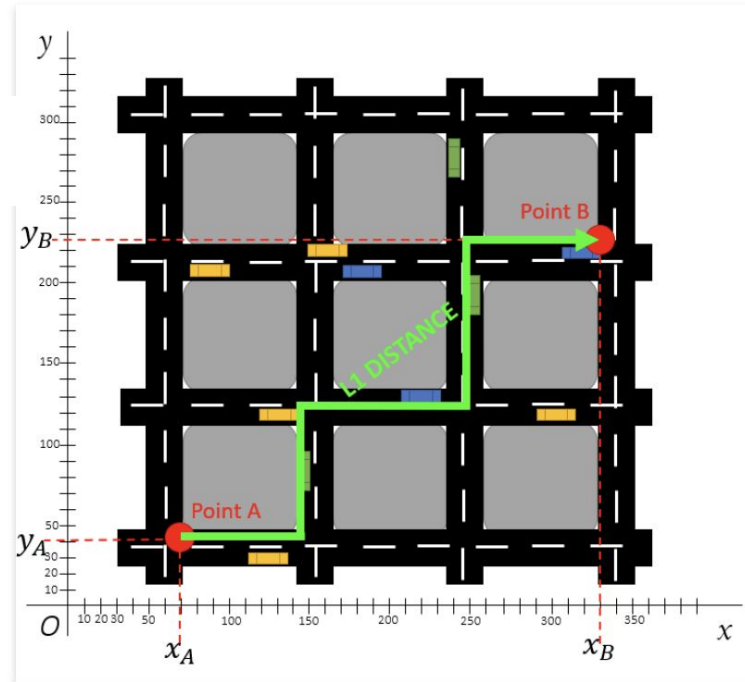
$$d^2(A, B) = (70 - 330)^2 + (40 - 228)^2$$

$$d^2(A, B) = 112225$$

L_1 distance (Manhattan distance)

$$d(A, B) = \sum_i |A_i - B_i|$$

- $x_A = 70$
- $x_B = 330$
- $y_A = 40$
- $y_B = 228$



$$d(A, B) = |x_A - x_B| + |y_A - y_B|$$

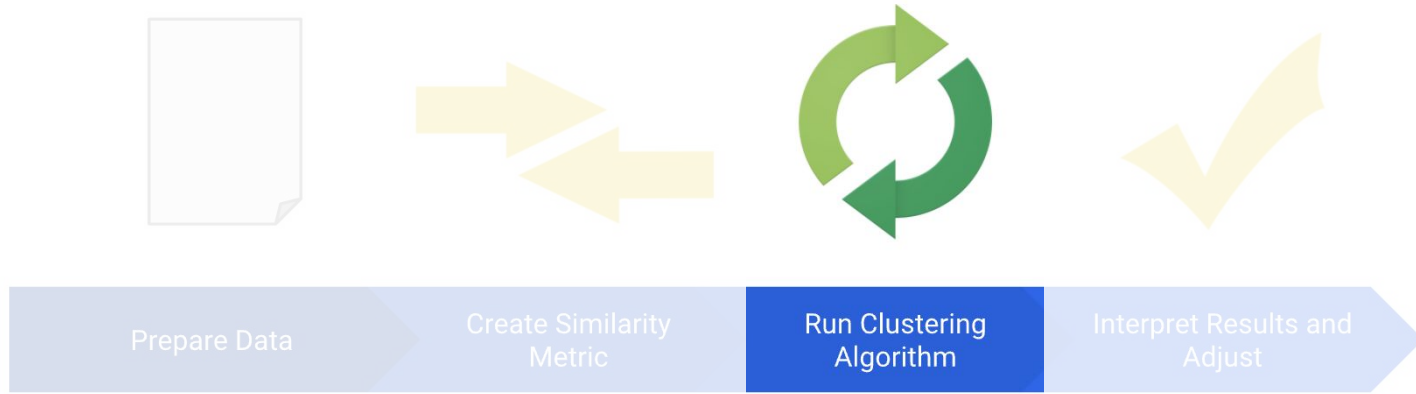
$$d(A, B) = |70 - 330| + |40 - 228|$$

$$d(A, B) = |-260| + |-188|$$

$$d(A, B) = 260 + 188$$

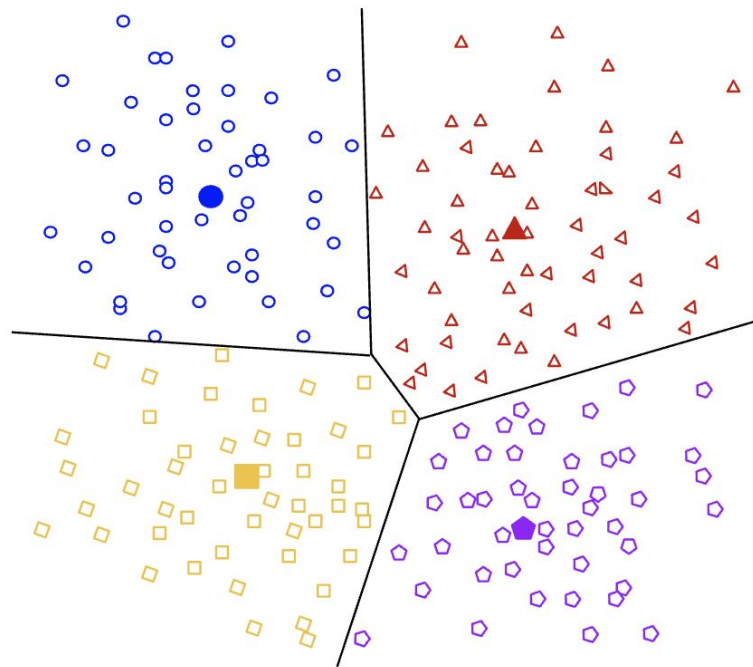
$$d(A, B) = 448$$

To cluster your data, you'll follow these steps:



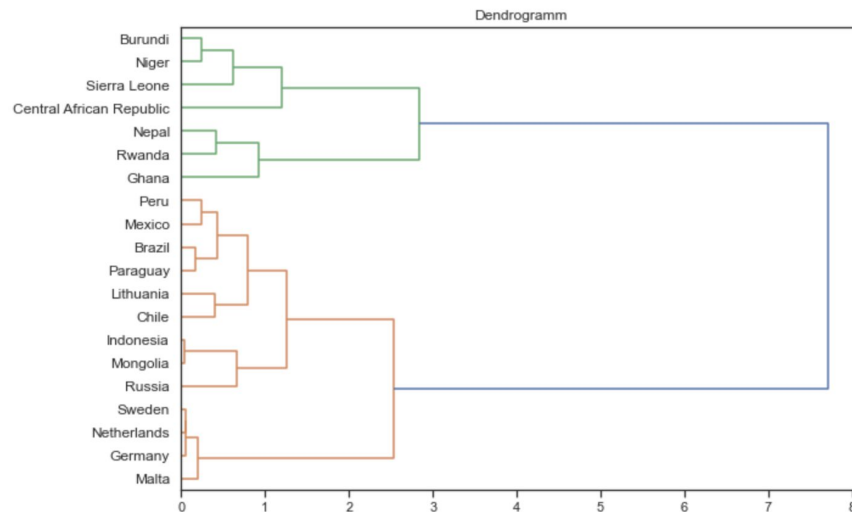
Centroid-based Clustering

- Centroid-based algorithms are **efficient**
- But sensitive to **initial conditions** and **outliers**.
- **k-means** is the most widely-used centroid-based clustering algorithm.



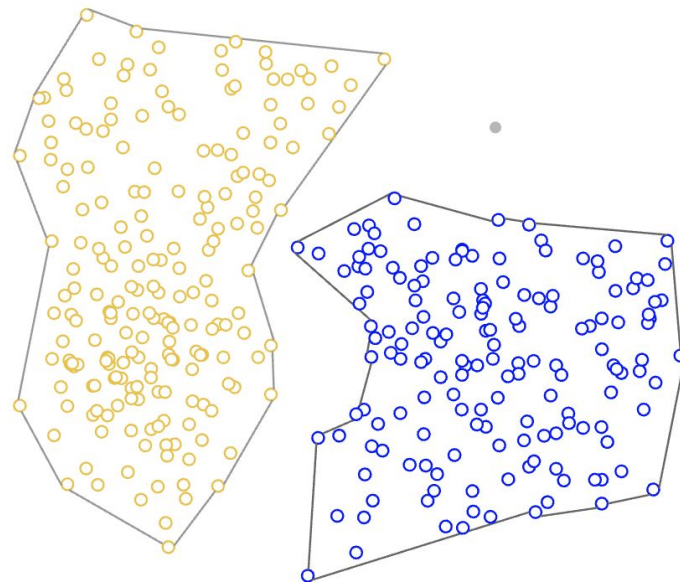
Hierarchical Clustering

- Hierarchical clustering creates a **tree** of clusters.
- One advantage is that any number of clusters can be chosen by cutting the tree at the right level.

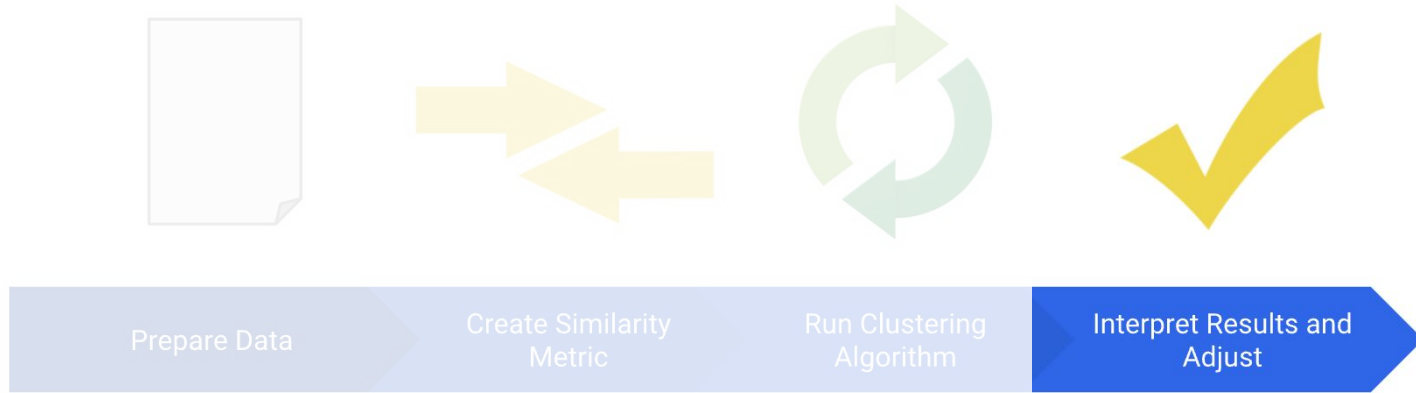


Density-based Clustering

- Density-based clustering connects areas of high example **density** into clusters
- Advantage:
 - they do not assign outliers to clusters.
- Disadvantage:
 - have difficulty with data of varying densities and high dimensions.



To cluster your data, you'll follow these steps:



Because clustering is unsupervised, no “truth” is available to verify results

- It mainly depends on the **subjective interpretability**
- We have some kind of quality measures for some algorithms (like k-Means)

