COMP9321:
Data services engineering

Week 9: Clustering

Term1, 2023

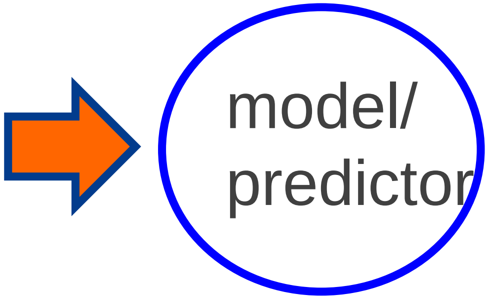
By Mortada Al-Banna, CSE UNSW

Supervised learning

label

label_1

label_3



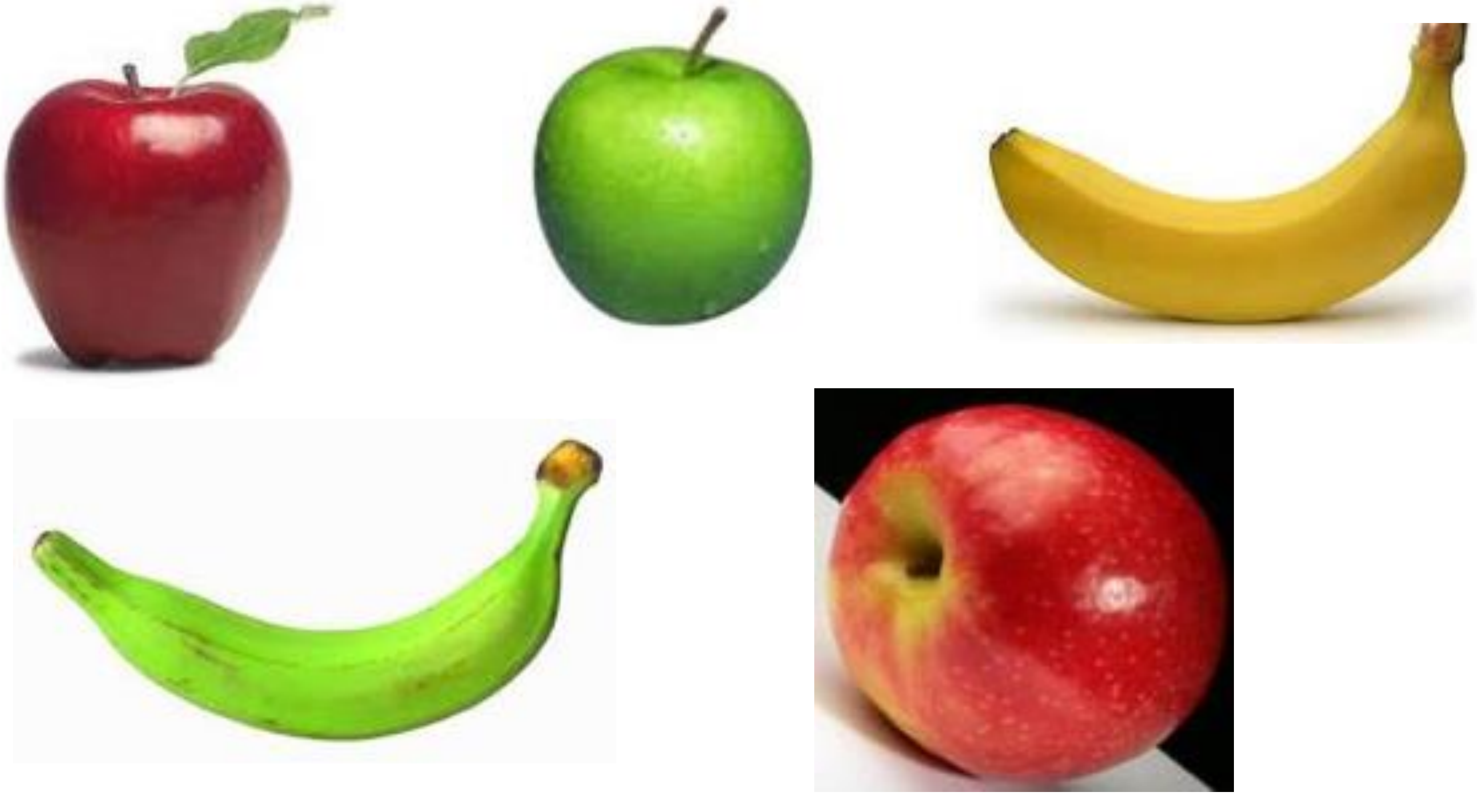
model/
predictor

label_4

label_5

Supervised learning: given labeled examples

Unsupervised learning



Unupervised learning: given data, i.e. examples, but no labels

Unsupervised Learning

Definition of Unsupervised Learning:

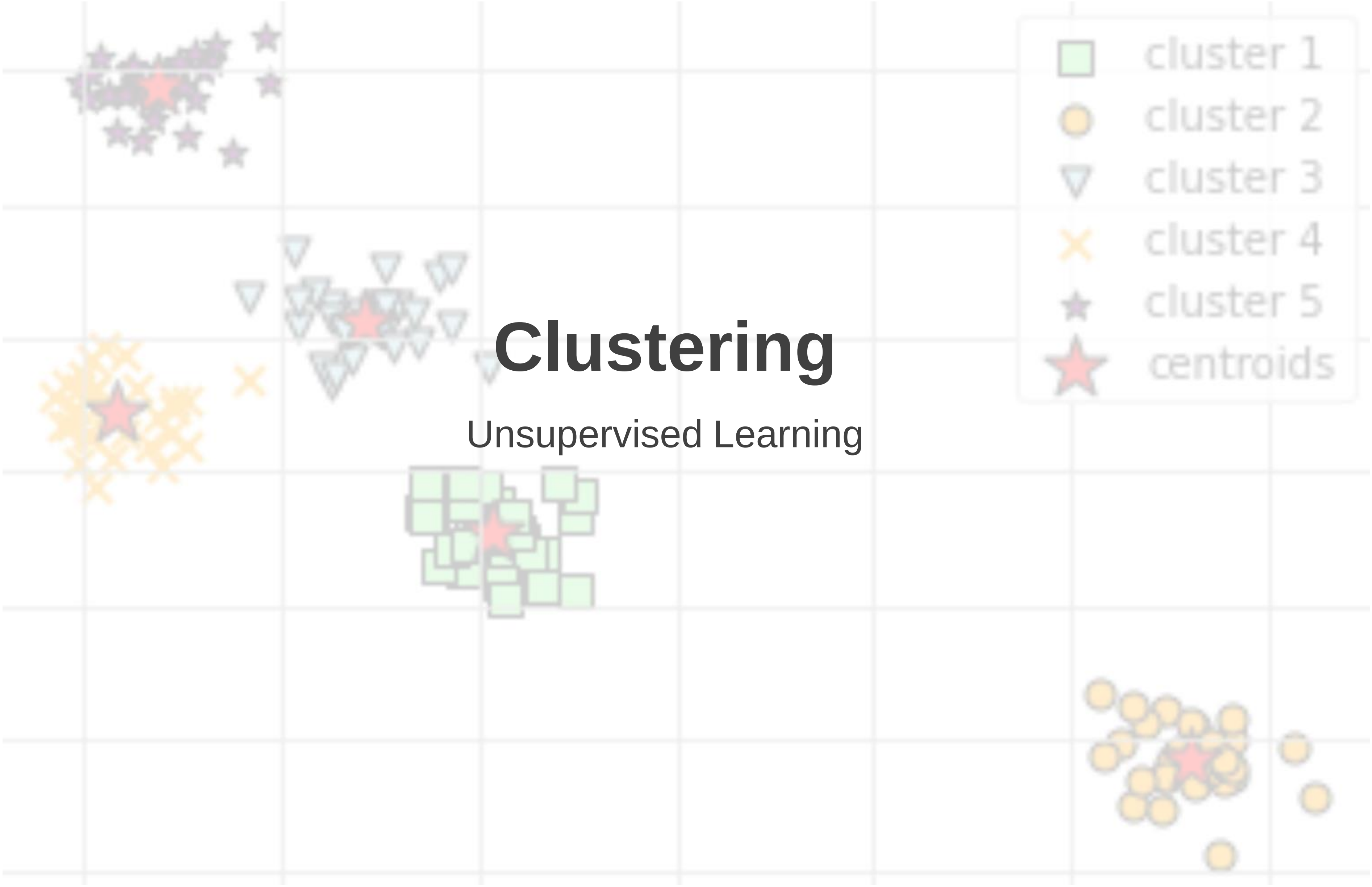
> Learning useful structure *without* labeled classes, optimization criterion, feedback signal, or any other information beyond the raw data

Unsupervised Learning

- Unsupervised learning involves operating on datasets without labelled responses or target values.
- The goal is to capture a structure of interest of useful information (e.g., relationships)
- Unsupervised learning good be used in:
  - ❑Visualizing the structure of a complex dataset
  - ❑Compressing and summarising the data (e.g, image compression)
  - ❑Extracting features for supervised learning
  - ❑Discover groups or outliers

Clustering

Unsupervised Learning



Clustering

– Unsupervised learning

– Requires data, but no labels

– Detect patterns

Motivations of Clustering

- Exploratory data analysis

– understanding general characteristics of data

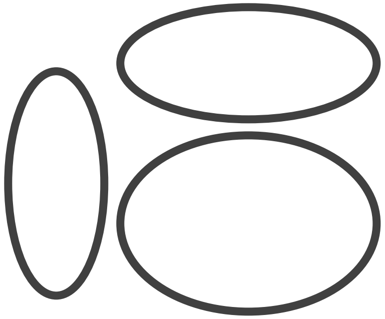
– visualizing data

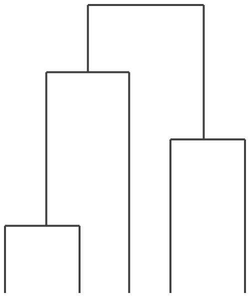
- Generalization – infer something about an instance (e.g. a gene) based on how it relates to other instances

Paradigms

Flat algorithms

- Usually start with a random (partial) partitioning
- Refine it iteratively
  - *K* means clustering
  - Model based clustering
- Spectral clustering





Hierarchical algorithms

- Bottom-up, agglomerative
- Top-down, divisive

Paradigms

Hard clustering: Each example belongs to exactly one cluster

Soft clustering: An example can belong to more than one cluster (probabilistic)

- Makes more sense for applications like creating browsable hierarchies
- You may want to put a pair of sneakers in two clusters: (i) sports apparel and (ii) shoes

Clustering: Image Segmentation

Break up the image into meaningful or perceptually similar regions

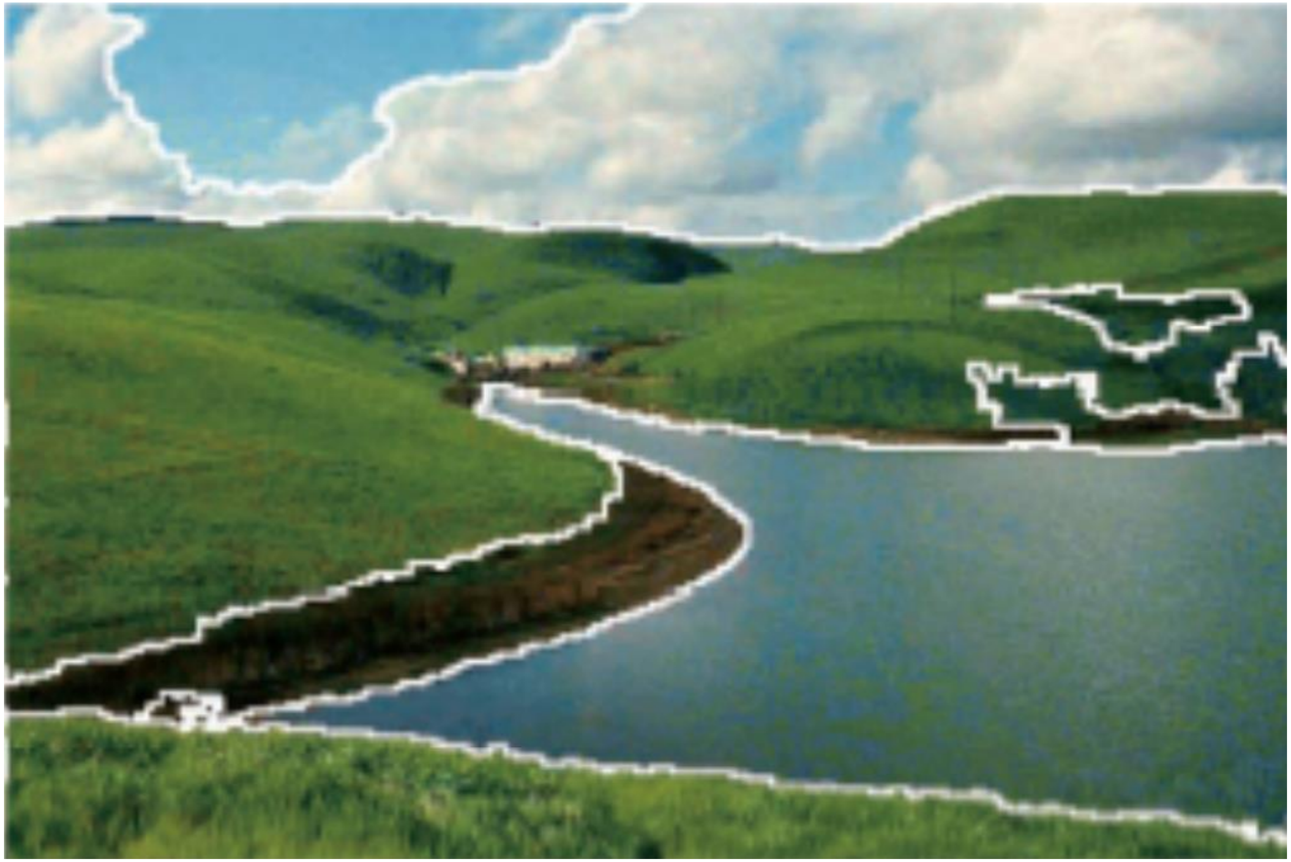


Figure from: James Hayes

Clustering: Edge Detection

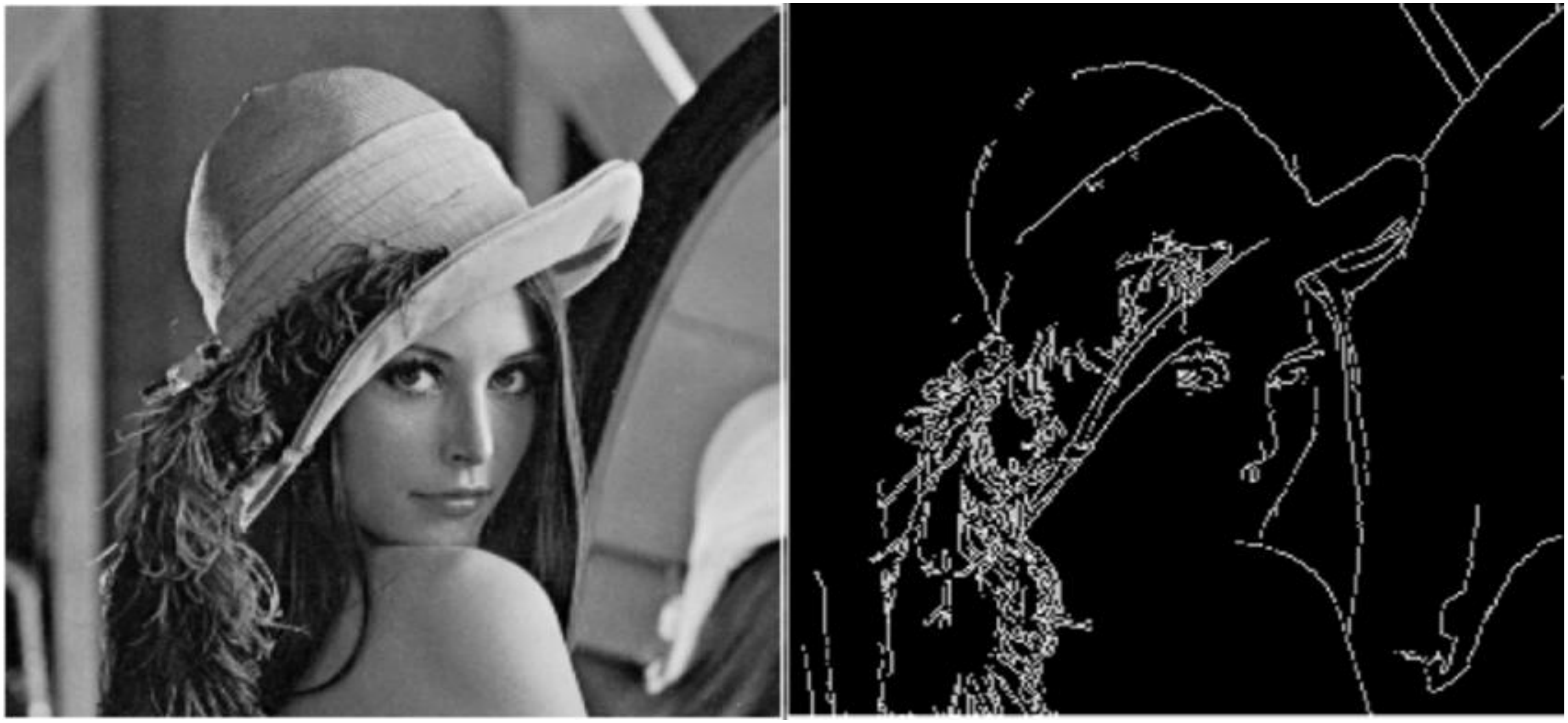
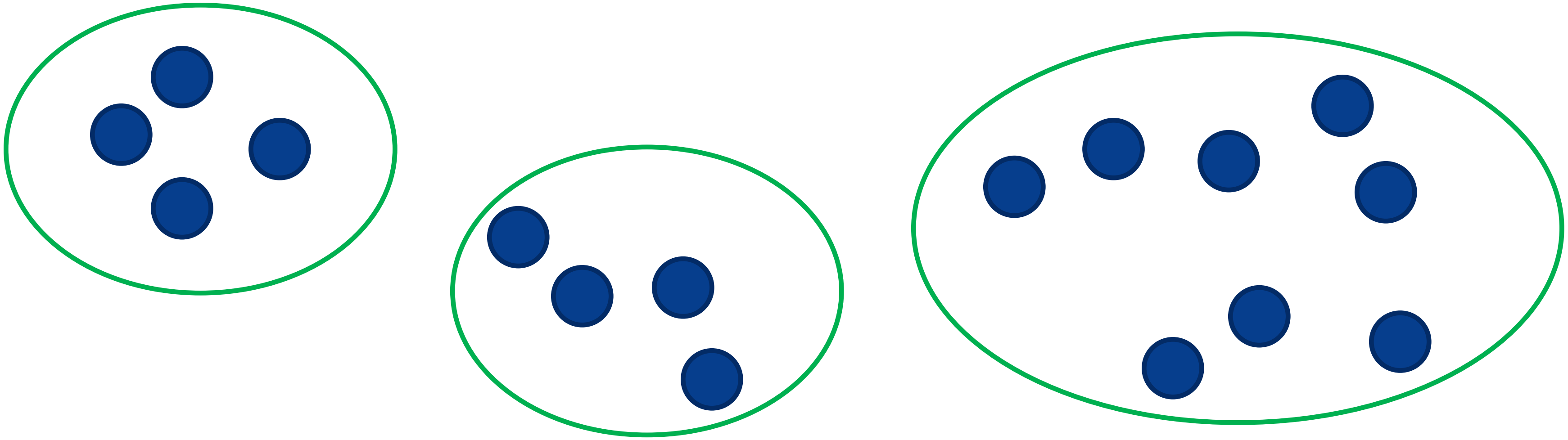
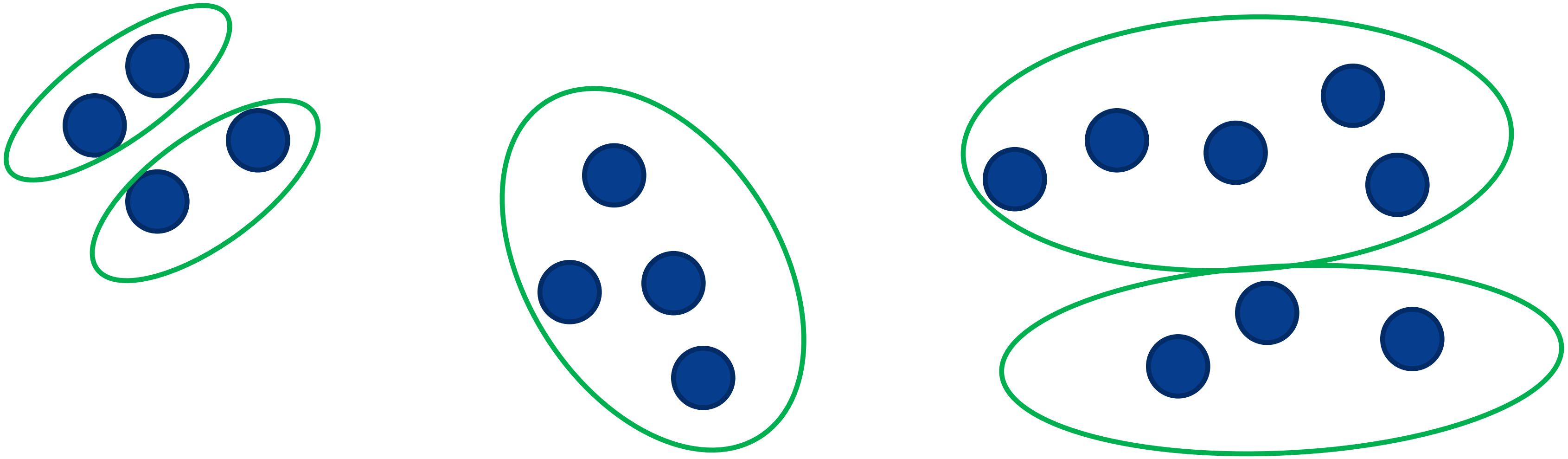


Figure from: James Hayes

Basic Idea of Clustering



Basic Idea of Clustering



Basic Idea of Clustering

Group together similar data points (instances)

- How to measure the similarity?

✓ What could similar mean?

- How many clusters do we need?

K-means

Most well-known and popular clustering algorithm:

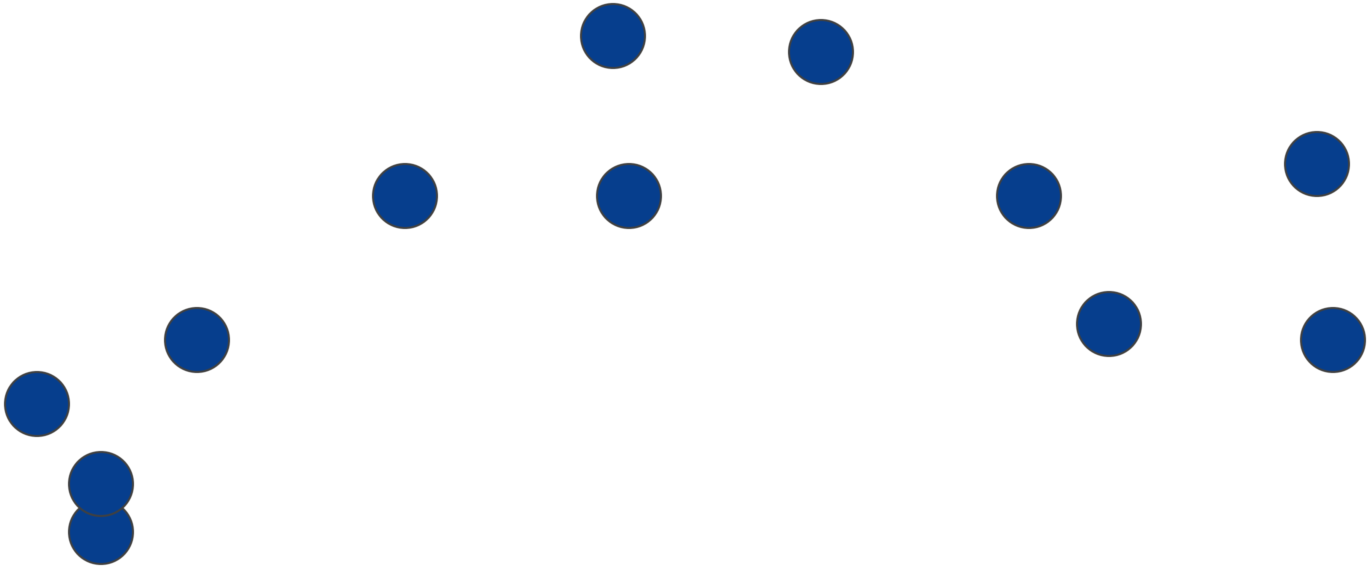
Step 1. Start with some initial cluster centers (k random points)

Step 2. Iterate:

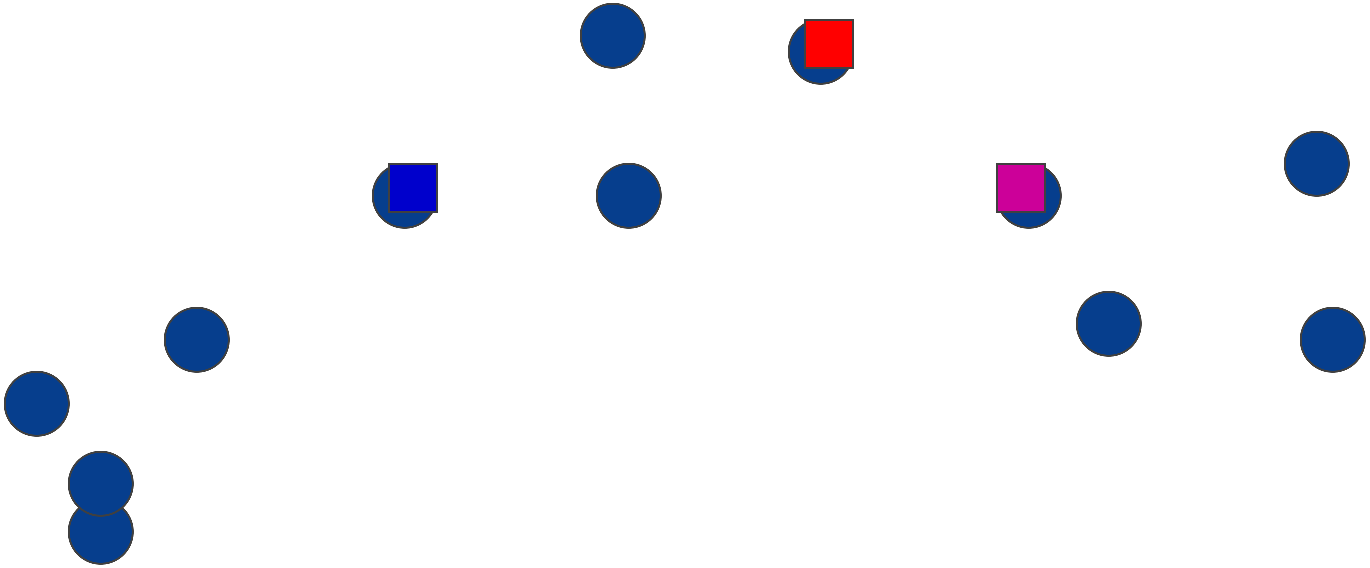
- Assign/cluster each example to closest center
- Recalculate and change centers as the mean of the points in the cluster.

Step 3. Stop when no points' assignments change

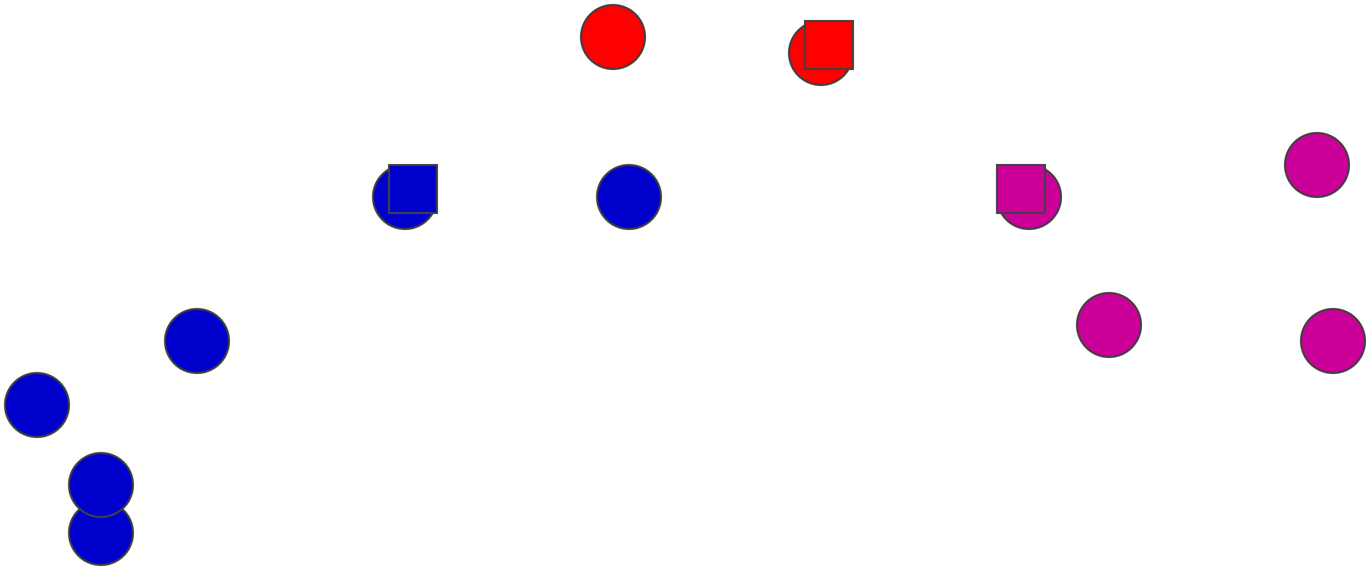
K-means: an example



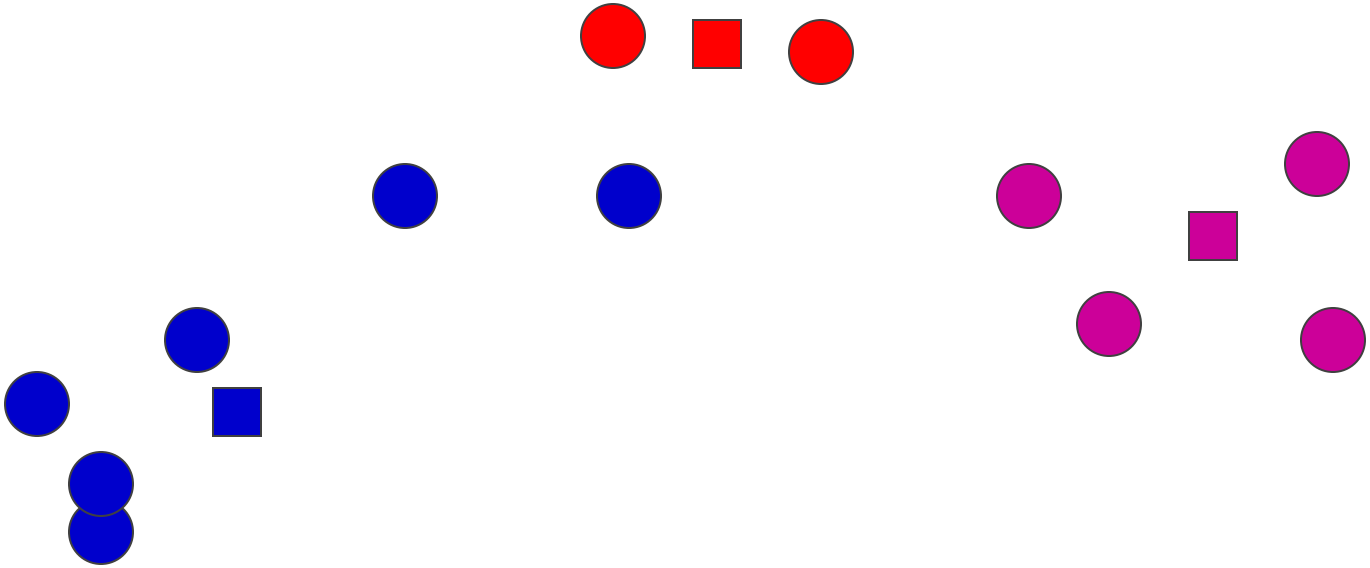
K-means: Initialize centers randomly



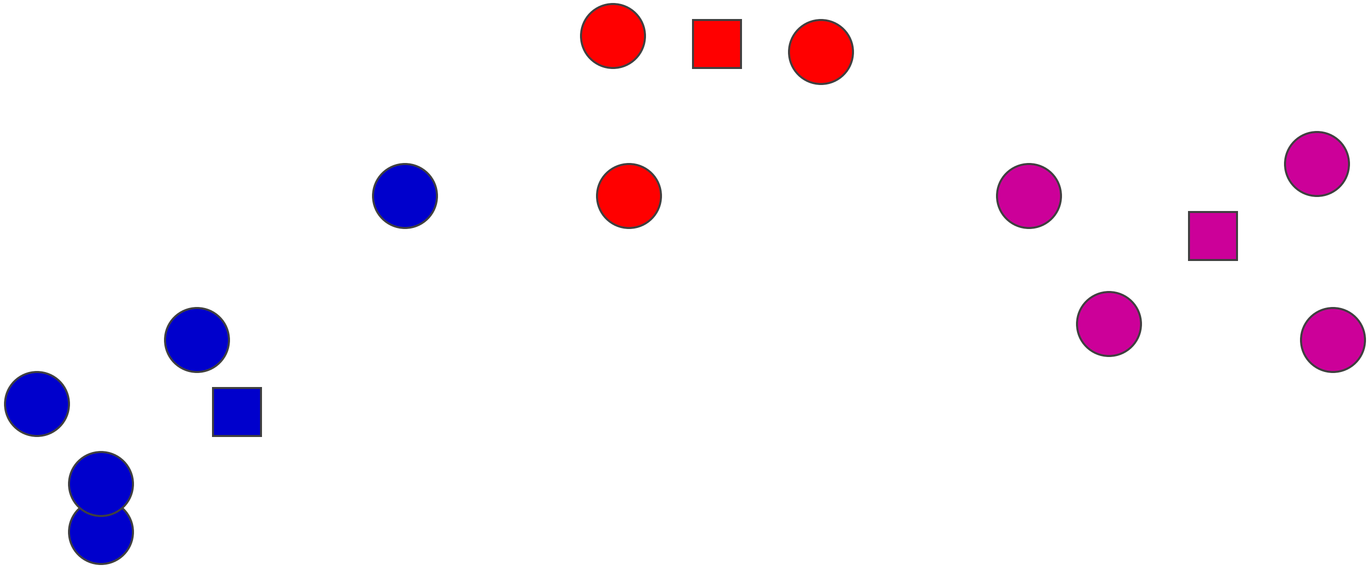
K-means: assign points to nearest center



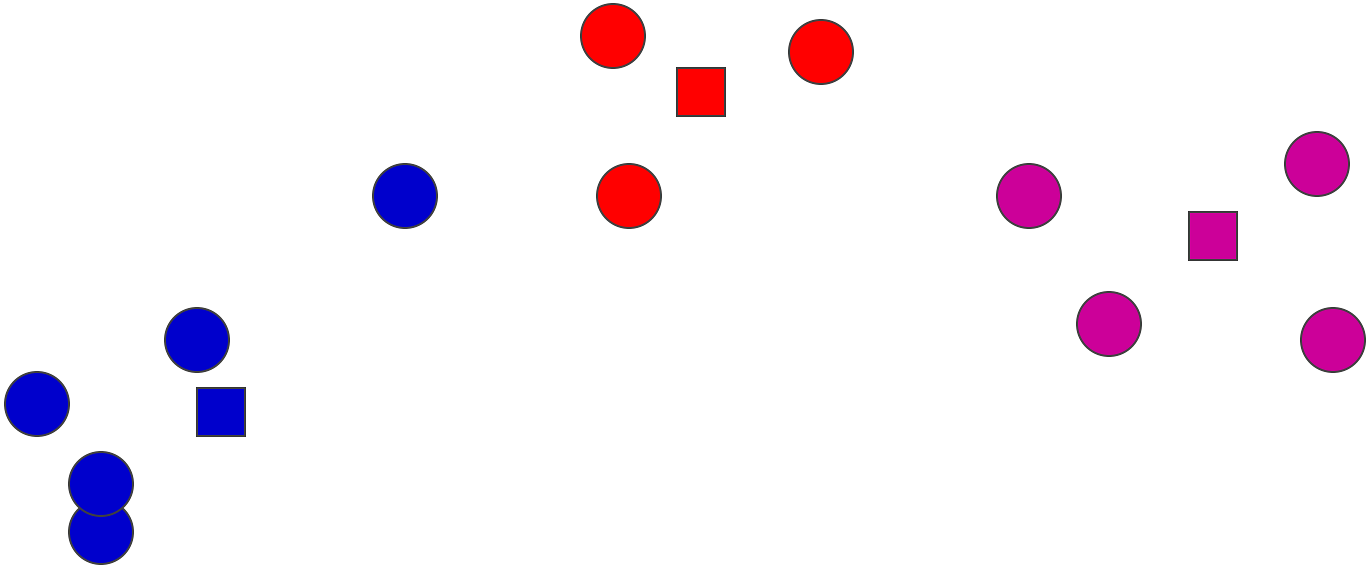
K-means: readjust centers



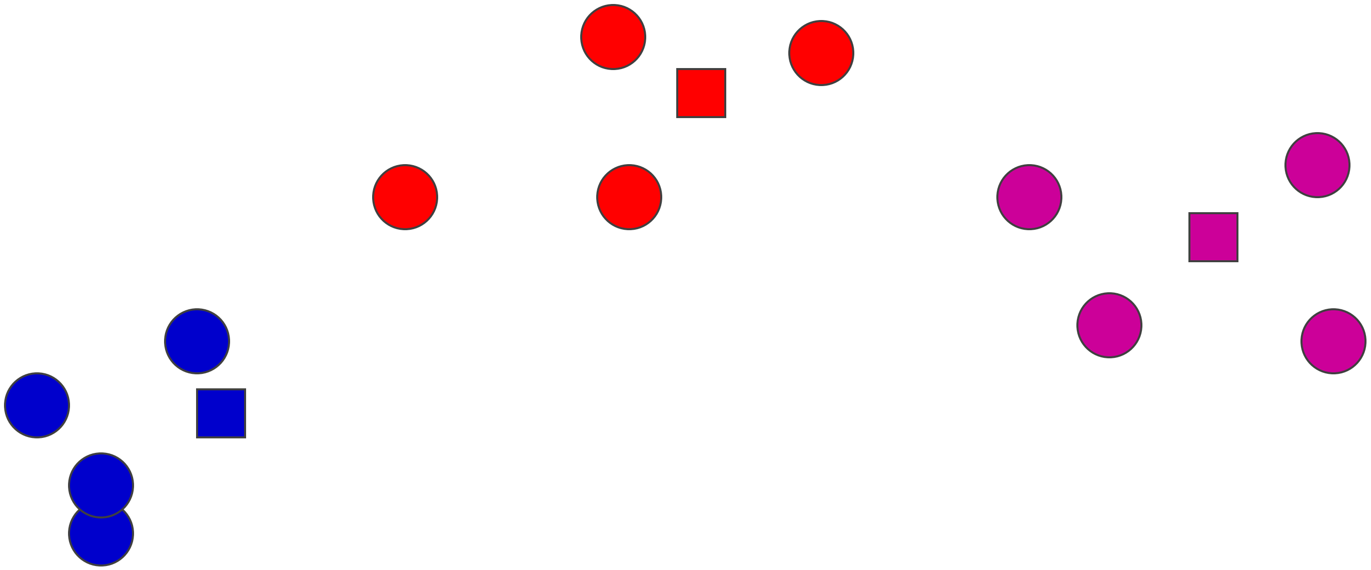
K-means: assign points to nearest center



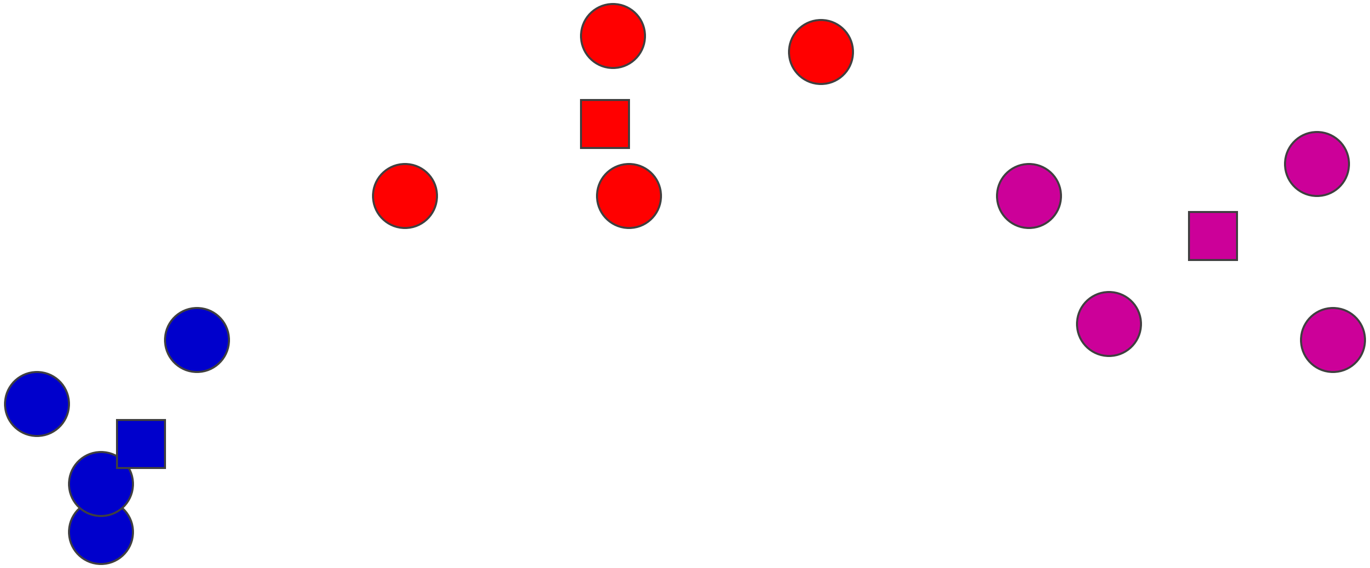
K-means: readjust centers



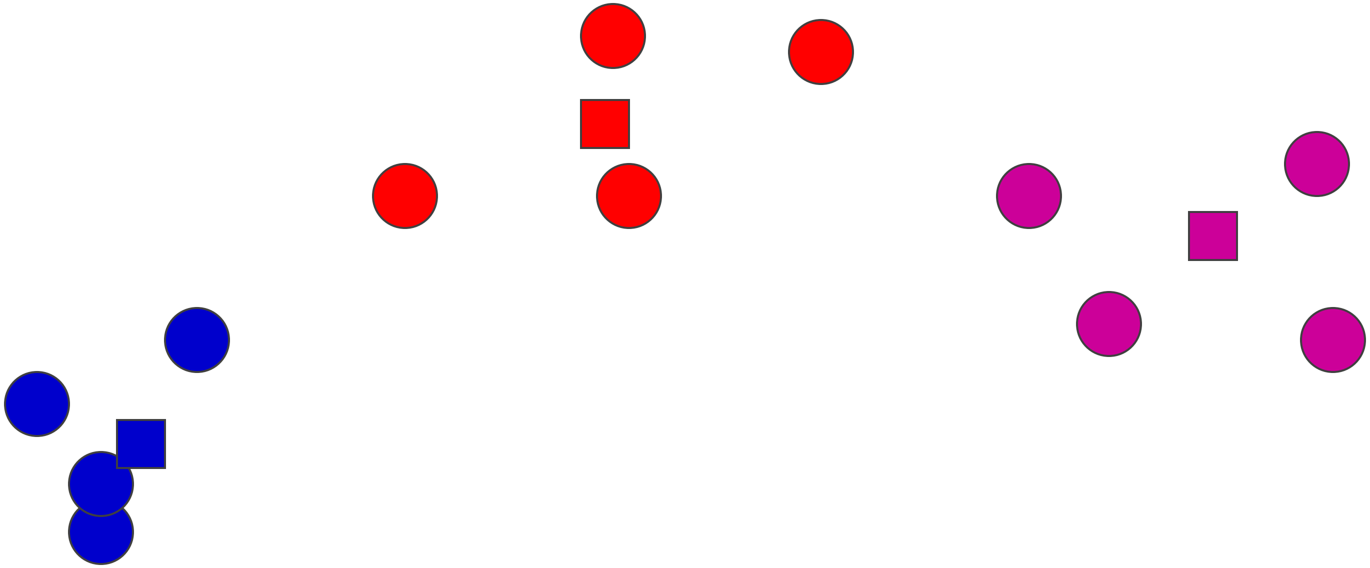
K-means: assign points to nearest center



K-means: readjust centers



K-means: assign points to nearest center

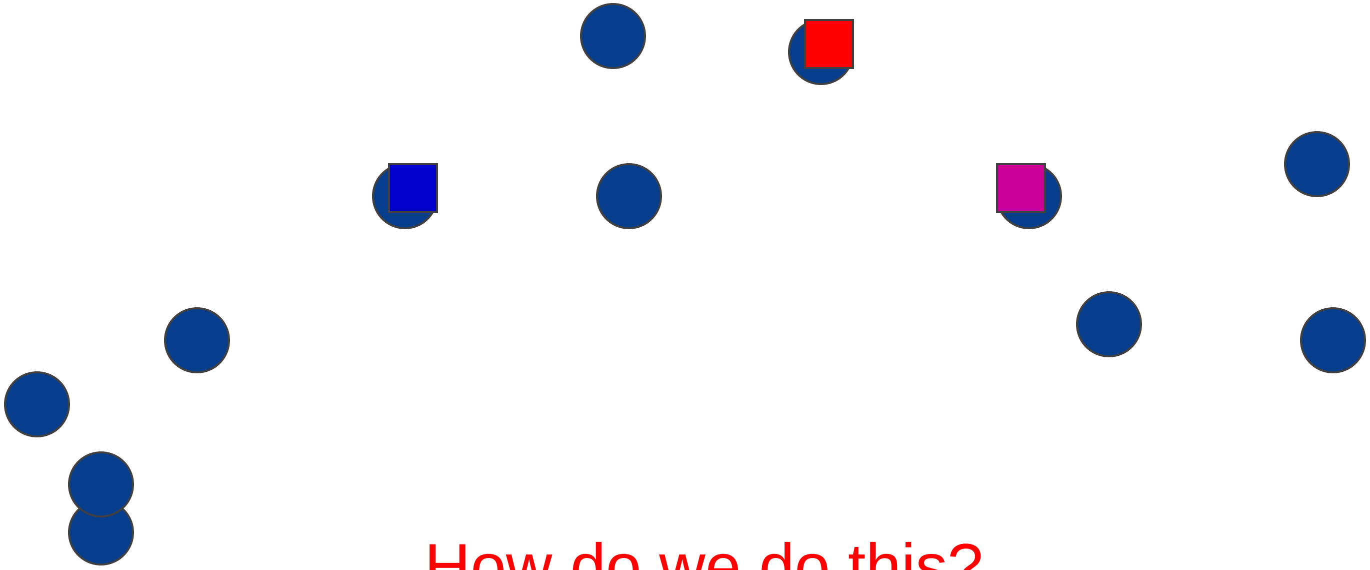


No changes: Done

K-means

Iterate:

- **Assign/cluster each example to closest center**
- Recalculate centers as the mean of the points in a cluster



How do we do this?

K-means

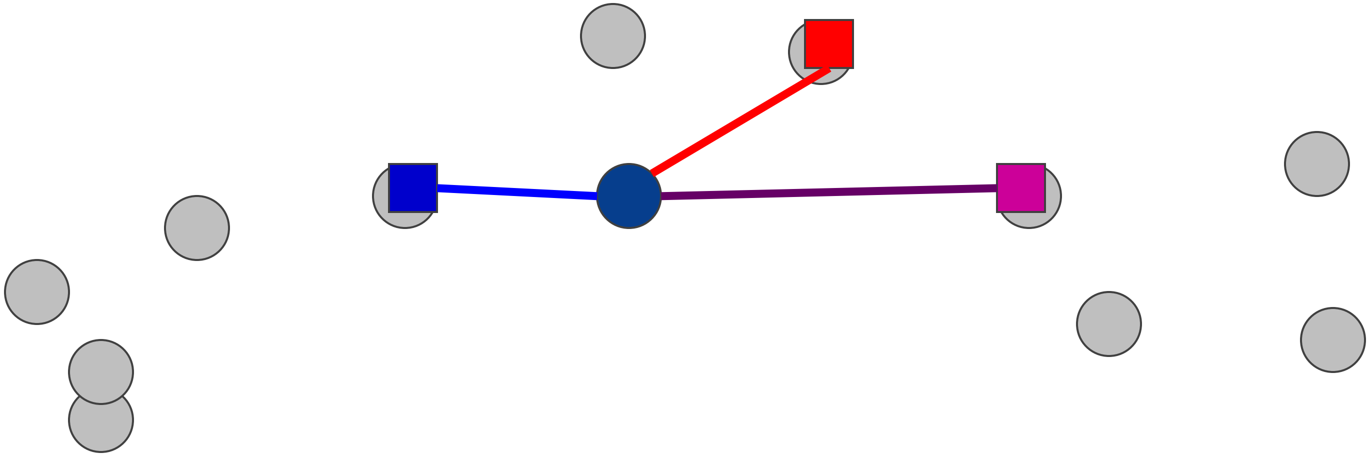
Iterate:

- **Assign/cluster each example to closest center**

  iterate over each point:

  - get distance to each cluster center
  - assign to closest center (hard cluster)

- Recalculate centers as the mean of the points in a cluster



K-means

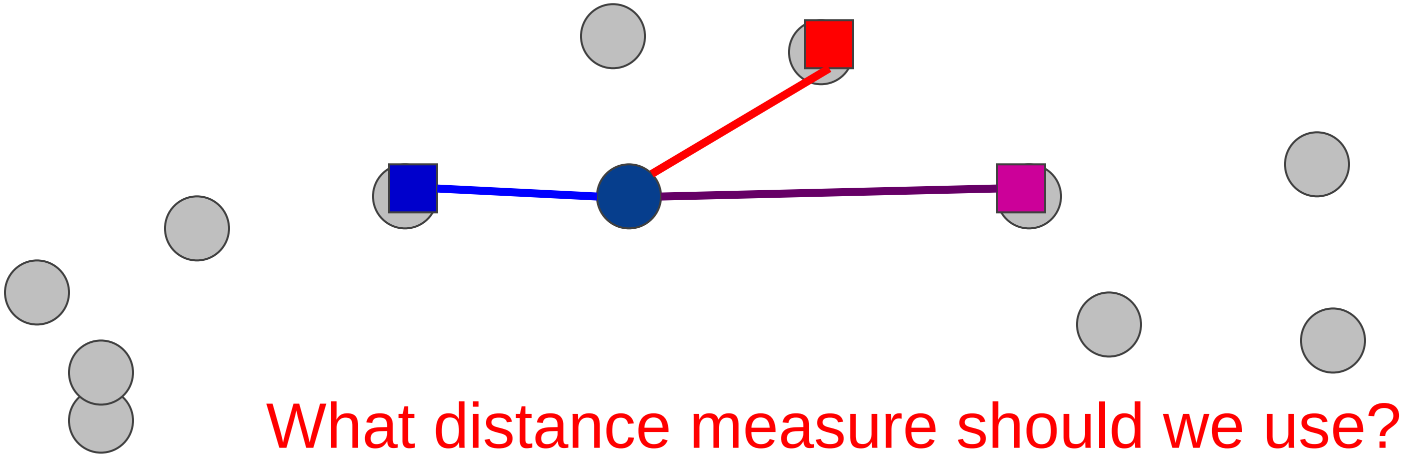
Iterate:

- **Assign/cluster each example to closest center**

  iterate over each point:

  - get **distance** to each cluster center
  - assign to closest center (hard cluster)

- Recalculate centers as the mean of the points in a cluster



What distance measure should we use?

Distance measures

Euclidean:

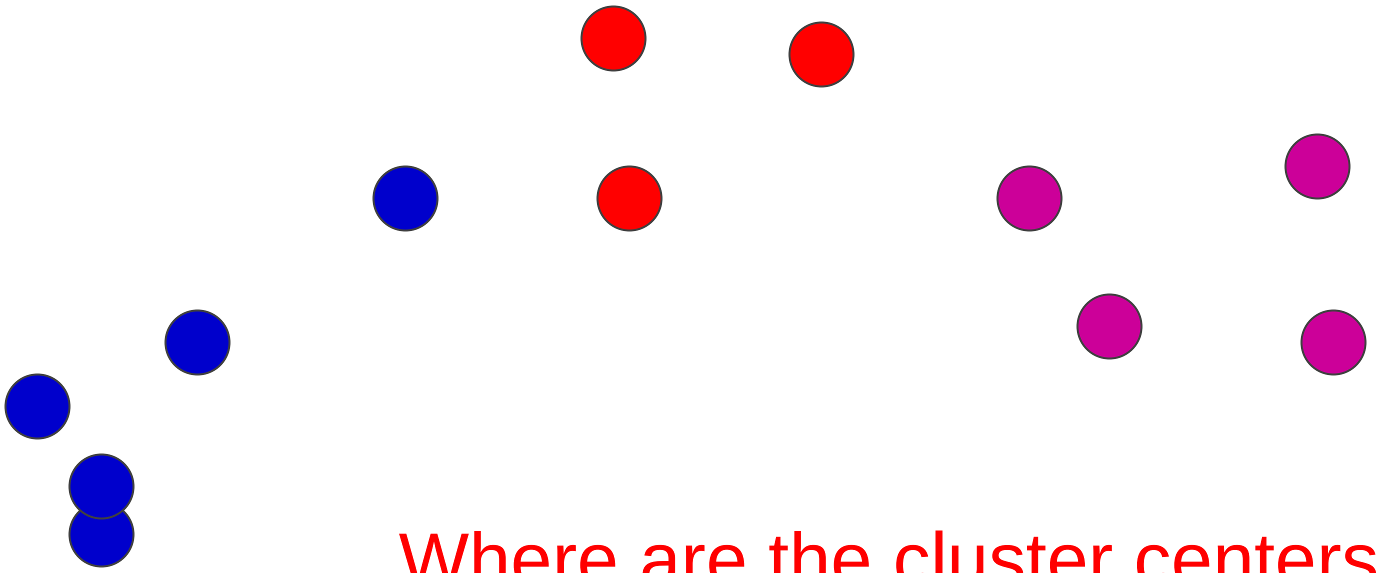
$$d(x,y) = \sqrt{\text{å}_{i=1}^{n}(x_i - y_i)^2}$$

good for spatial data

K-means

Iterate:

- Assign/cluster each example to closest center
- Recalculate centers as the mean of the points in a cluster

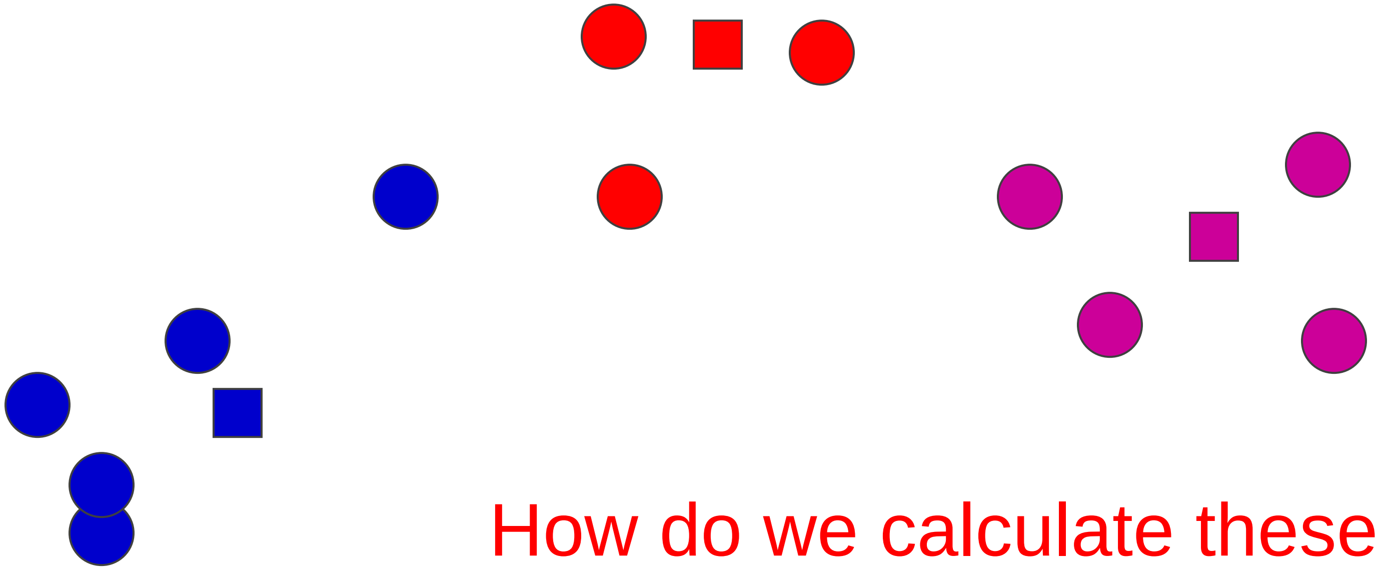


Where are the cluster centers?

K-means

Iterate:

- Assign/cluster each example to closest center
- Recalculate centers as the mean of the points in a cluster



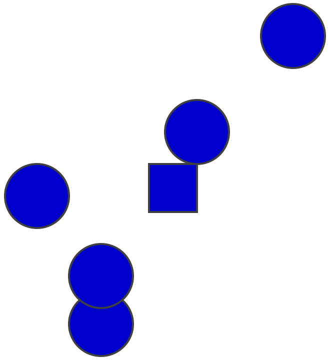
How do we calculate these?

K-means

Iterate:

- Assign/cluster each example to closest center
- Recalculate centers as the mean of the points in a cluster

e.g., for a set of instances that have been assigned to a cluster , we c_j -compute the mean of the cluster as follow



$$\mu(c_j) = \frac{\sum_{\vec{x}_i \in c_j} \vec{x}_i}{|c_j|}$$

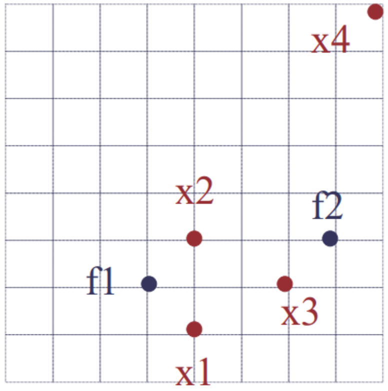
K-means

```
given : a set $X = \{\vec{x}_1 \ldots \vec{x}_n\}$ of instances
select $k$ initial cluster centers $\vec{f}_1 \ldots \vec{f}_k$
while stopping criterion not true do
    for all clusters $c_j$ do
        // determine which instances are assigned to this cluster
        $c_j = \left\{ \vec{x}_i \mid \forall f_l \ \mathrm{dist}\left(\vec{x}_i, \vec{f}_j\right) < \mathrm{dist}\left(\vec{x}_i, \vec{f}_l\right) \right\}$
    for all means $\vec{f}_j$ do
        // update the cluster center
        $\vec{f}_j = \mu(c_j)$
```

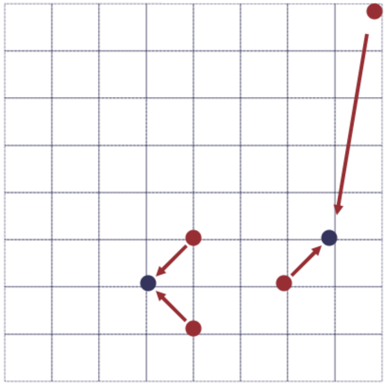
Run an example together ~~

Initialization: 4 points, 2 clusters and distance function

$$\mathrm{dist}(x_i, x_j) = \sum_e \left| x_{i,e} - x_{j,e} \right|$$

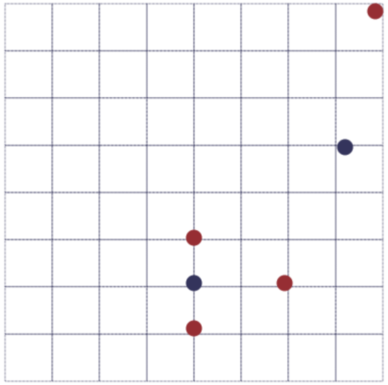


$$
\begin{aligned}
&dist(x_1, f_1) = 2, \quad dist(x_1, f_2) = 5\\
&dist(x_2, f_1) = 2, \quad dist(x_2, f_2) = 3\\
&dist(x_3, f_1) = 3, \quad dist(x_3, f_2) = 2\\
&dist(x_4, f_1) = 11, \quad dist(x_4, f_2) = 6
\end{aligned}
$$

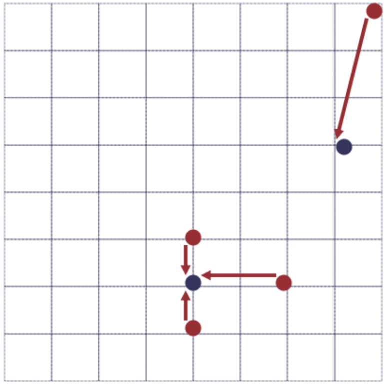


$$f_1 = \left\langle \frac{4+4}{2}, \frac{1+3}{2} \right\rangle = \langle 4,2 \rangle$$

$$f_2 = \left\langle \frac{6+8}{2}, \frac{2+8}{2} \right\rangle = \langle 7,5 \rangle$$



$$
\begin{aligned}
&dist(x_1, f_1) = 1, \quad dist(x_1, f_2) = 7\\
&dist(x_2, f_1) = 1, \quad dist(x_2, f_2) = 5\\
&dist(x_3, f_1) = 2, \quad dist(x_3, f_2) = 4\\
&dist(x_4, f_1) = 10, \quad dist(x_4, f_2) = 4
\end{aligned}
$$



$$f_1 = \left\langle \frac{4+4+6}{3}, \frac{1+3+2}{3} \right\rangle = \langle 4.67,2 \rangle$$

$$f_2 = \left\langle \frac{8}{1}, \frac{8}{1} \right\rangle = \langle 8,8 \rangle$$

Properties of K-means

Guaranteed to converge in a finite number of iterations

Running time per iteration

1. Assign data points to closest cluster center O(KN) time
2. Change the cluster center to the average of its assigned points O(N)

K-means variations/parameters

Start with some initial cluster centers

Iterate:

- Assign/cluster each example to closest center
- Recalculate centers as the mean of the points in a cluster

What are some other variations/parameters we haven’t specified?

K-means variations/parameters

Initial (seed) cluster centers

Convergence

- A fixed number of iterations
- partitions unchanged
- Cluster centers don’t change

K!

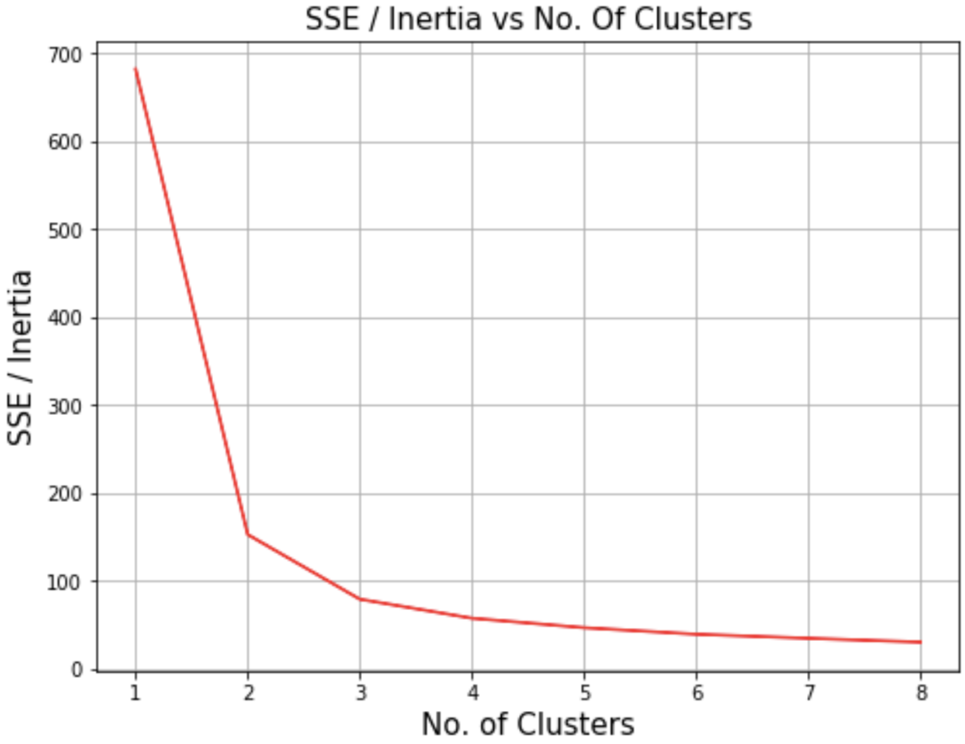
K-means Choosing K

Using the Elbow Method:

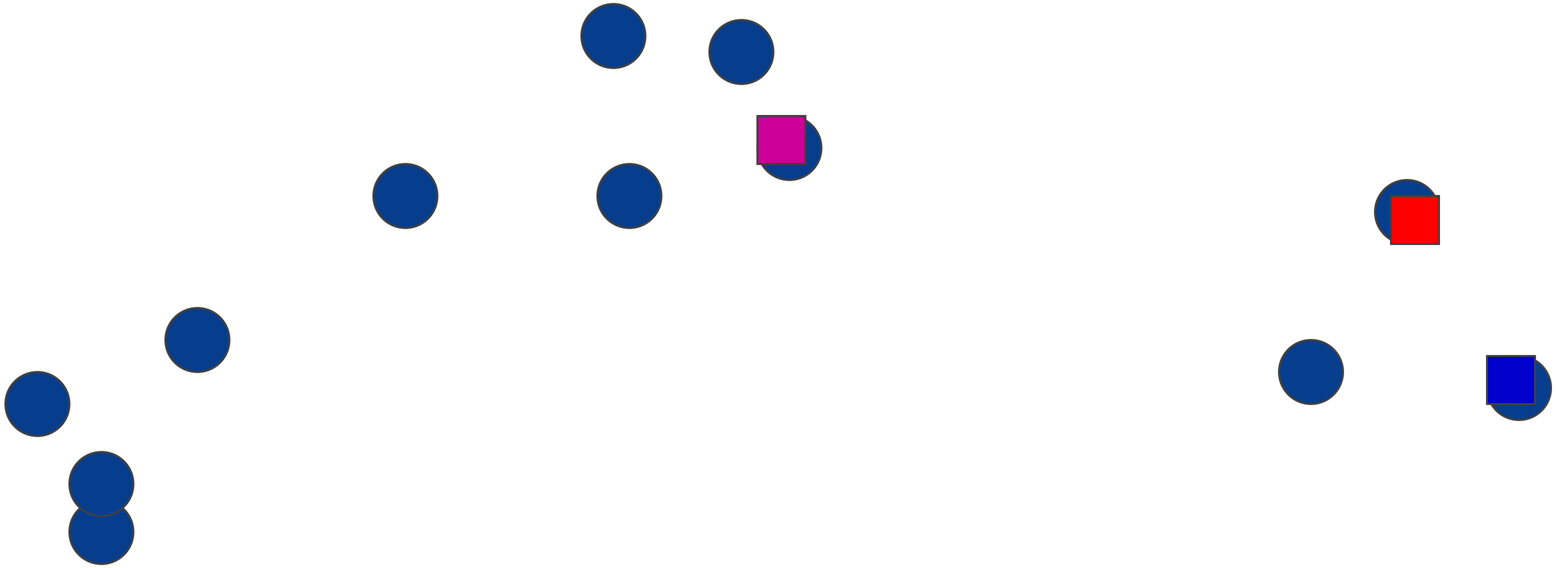
- Elbow method is one of the most popular method used to select the optimal number of clusters by fitting the model with a range of values for K in K-means algorithm.
- Elbow method requires drawing a line plot between SSE (Sum of Squared errors) vs number of clusters and finding the point representing the “elbow point” (the point after which the SSE or inertia starts decreasing in a linear fashion).

Choosing K with Elbow Method

$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2 (m_i, x)$$



K-means: Initialize centers randomly



What would happen here?

Seed selection ideas?

Seed choice

Results can vary drastically based on random seed selection

Some seeds can result in poor convergence rate, or convergence to sub-optimal clustering

Common heuristics

- Random centers in the space
- Randomly pick examples
- Points least similar to any existing center (furthest centers heuristic)
- **Try out multiple starting points**
- Initialize with the results of another clustering method

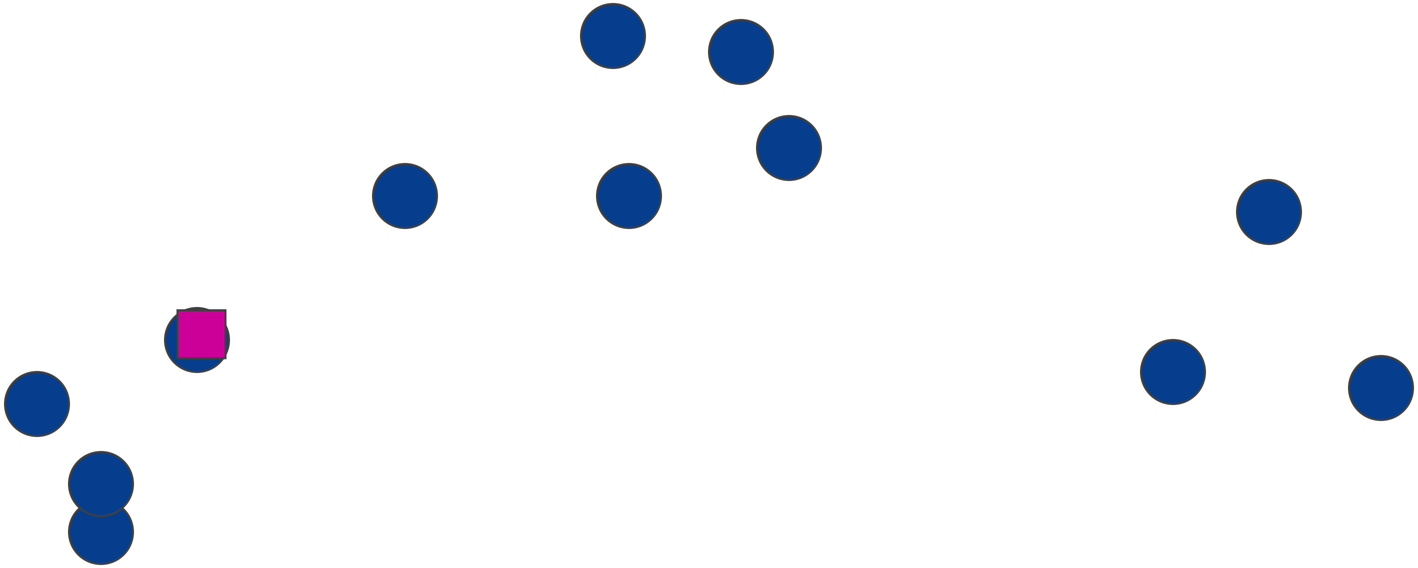
Furthest centers heuristic

```
μ$_1$ = pick random point

for i = 2 to K:
    μ$_i$ = point that is furthest from **any** previous centers
```

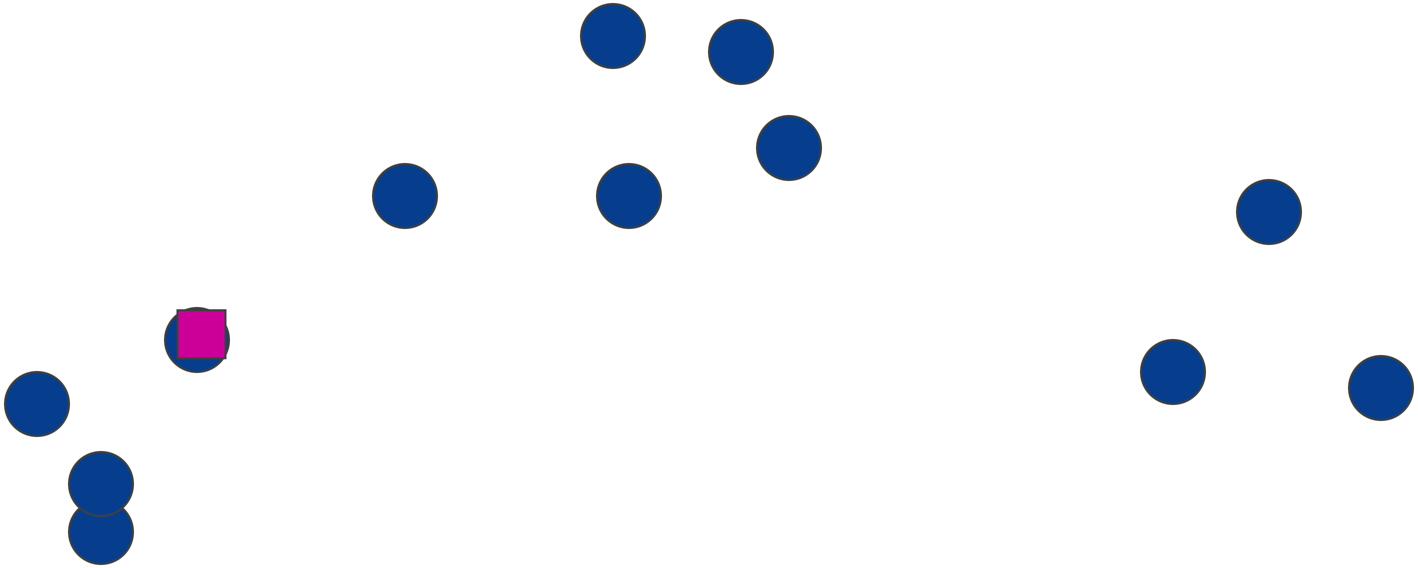
$$m_i = \underbrace{\arg\max_{x}}_{\text{point with the largest distance to any previous center}} \underbrace{\min_{m_j : 1 < j < i}}_{\text{smallest distance from x to any previous center}} d(x, m_j)$$

K-means: Initialize furthest from centers



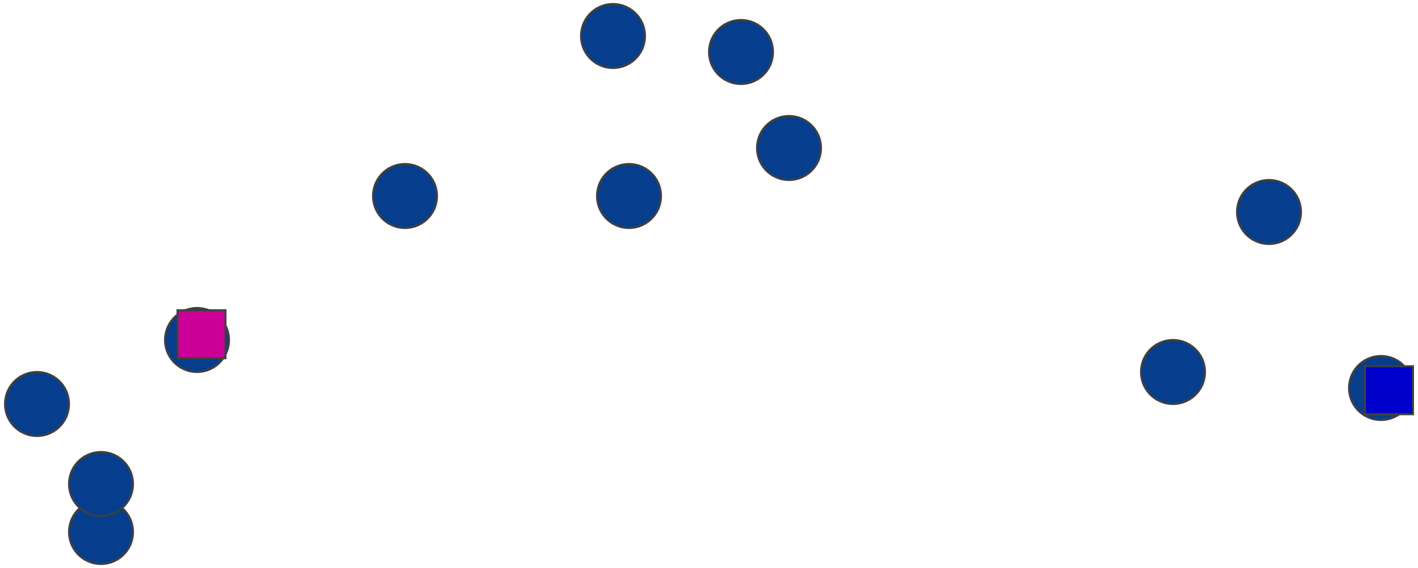
Pick a random point for the first center

K-means: Initialize furthest from centers



What point will be chosen next?

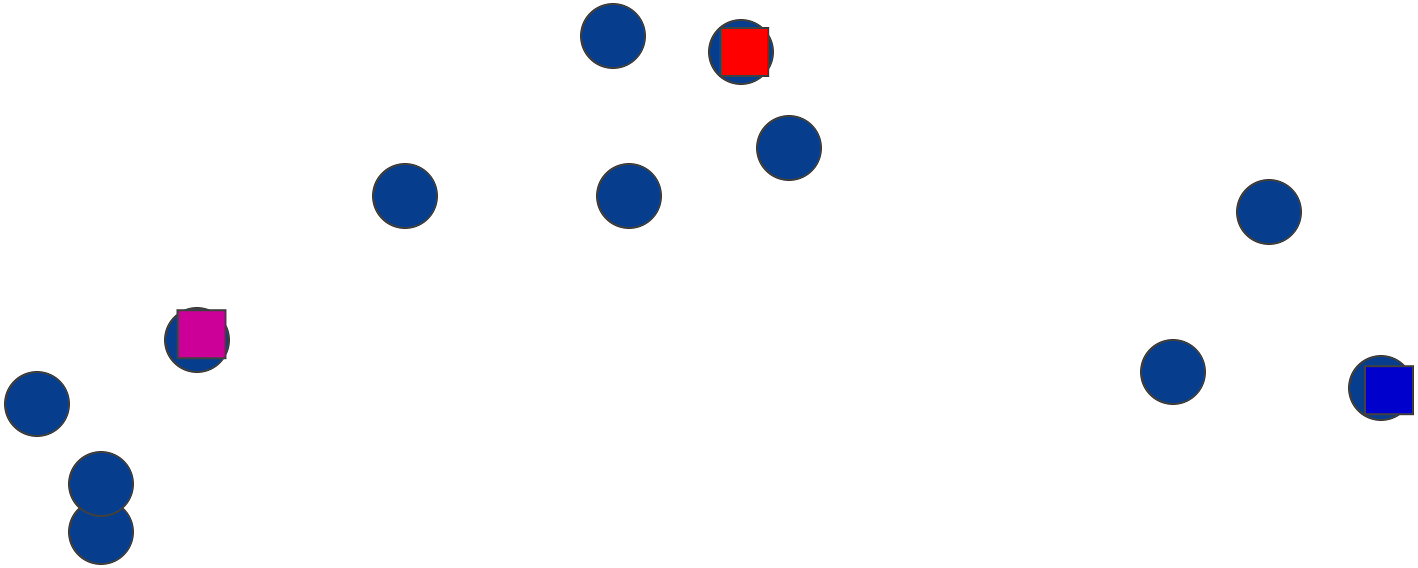
K-means: Initialize furthest from centers



Furthest point from center

What point will be chosen next?

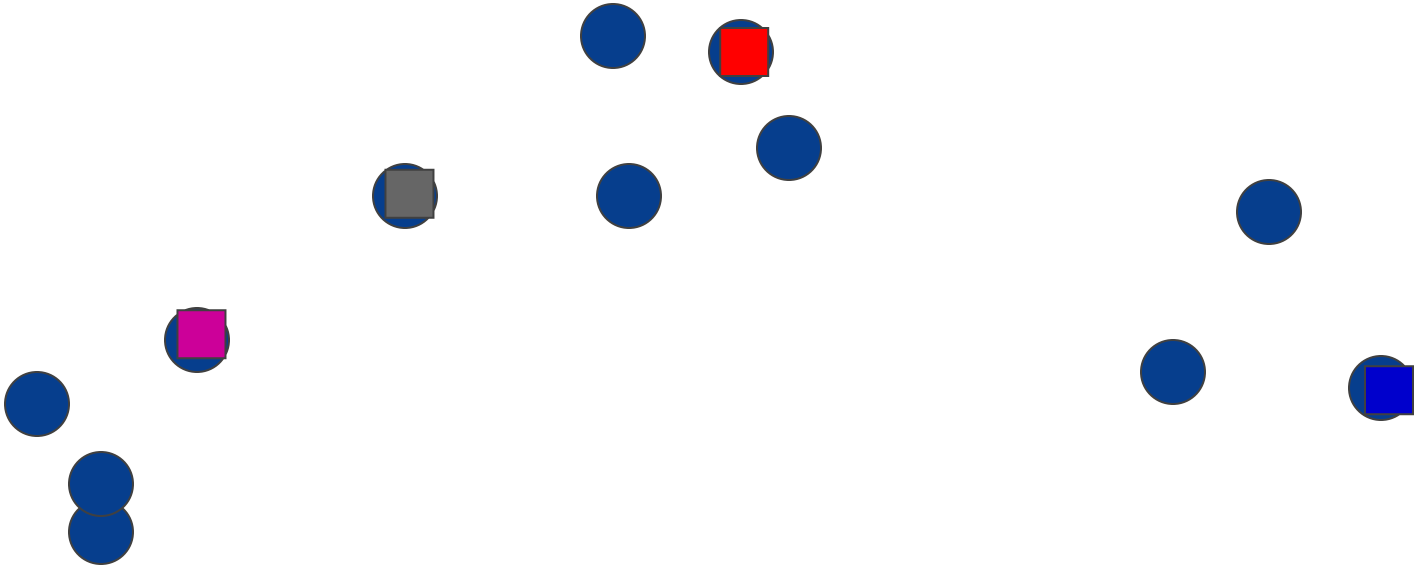
K-means: Initialize furthest from centers



Furthest point from center

What point will be chosen next?

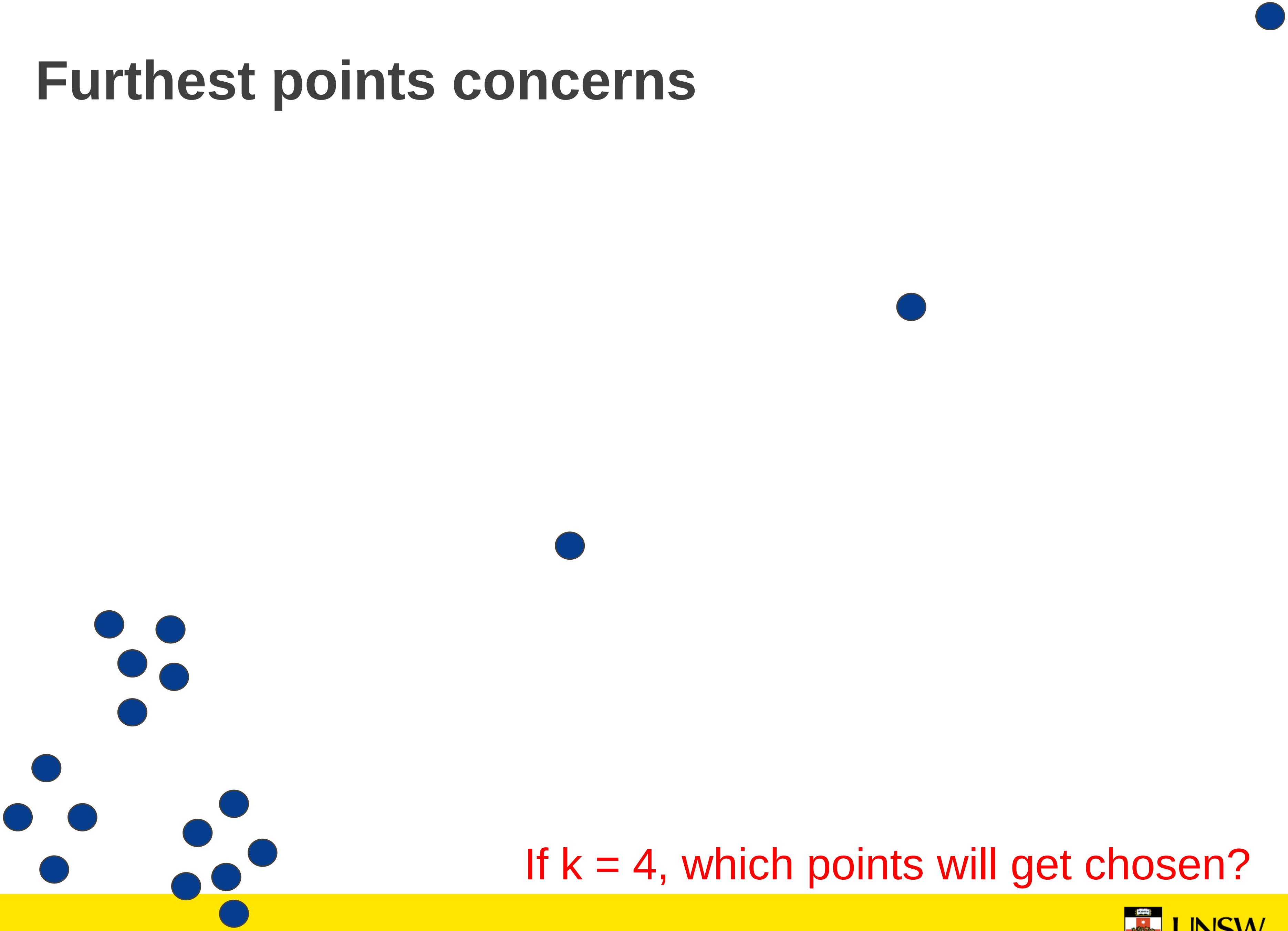
K-means: Initialize furthest from centers



Furthest point from center

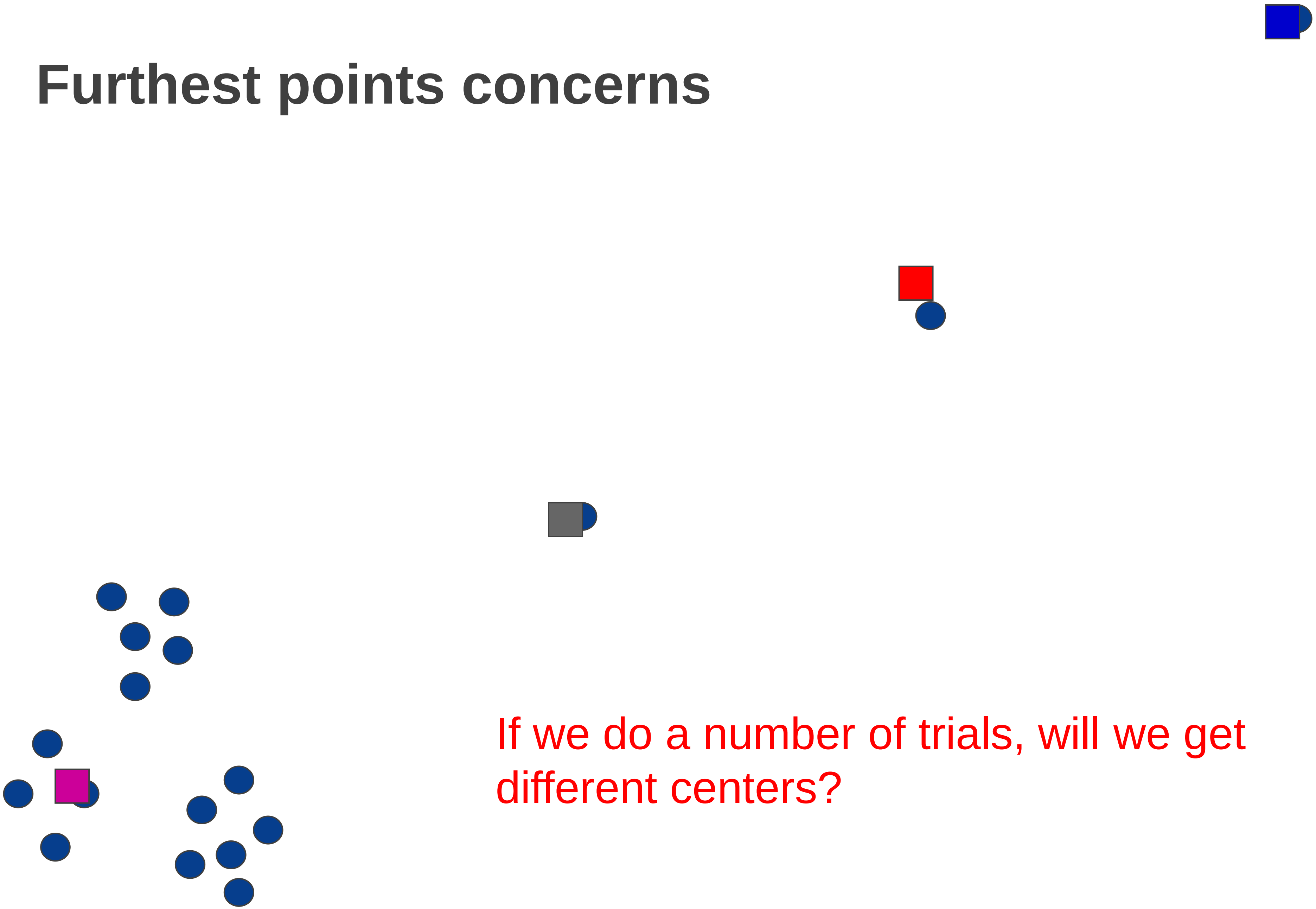
Any issues/concerns with this approach?

Furthest points concerns



If k = 4, which points will get chosen?

Furthest points concerns



If we do a number of trials, will we get different centers?

K-means++

1. Choose one center uniformly at random from among the data points.
2. For each data point x, compute D(x), the distance between x and the nearest center that has already been chosen.
3. Choose one new data point at random as a new center, using a weighted probability distribution where a point x is chosen with probability proportional to $D(x)^2$
4. Repeat Steps 2 and 3 until k centers have been chosen.
5. Now that the initial centers have been chosen, proceed using standard k-means clustering.

http://ilpubs.stanford.edu:8090/778/1/2006-13.pdf

K-means++

```
$\mu_1$ = pick random point

for k = 2 to K:
    for i = 1 to N:
        $s_i$ = min d($x_i$, $\mu_{1...k-1}$) // smallest distance to any center

    $\mu_k$ = randomly pick point proportionate to s
```

How does this help?

K-means++

```
$\mu_1$ = pick random point
for k = 2 to **K**:
    for i = 1 to **N**:
        $s_i = \min d(x_i, \mu_{1 \ldots k-1})$ // smallest distance to any center
    $\mu_k$ = randomly pick point ***proportionate*** to ***s***
```

- Makes it possible to select other points
  - if #points >> #outliers, we will pick good points
- Makes it non-deterministic, which will help with random runs
- Nice theoretical guarantees!

What Is A Good Clustering?

Internal criterion: A good clustering will produce high quality clusters in which:

- the intra-class (that is, intra-cluster) similarity is high
- the inter-class similarity is low
- The measured quality of a clustering depends on both the document representation and the similarity measure used

Clustering Evaluation

- Intra-cluster cohesion (compactness):

– Cohesion measures how near the data points in a cluster are to the cluster centroid.

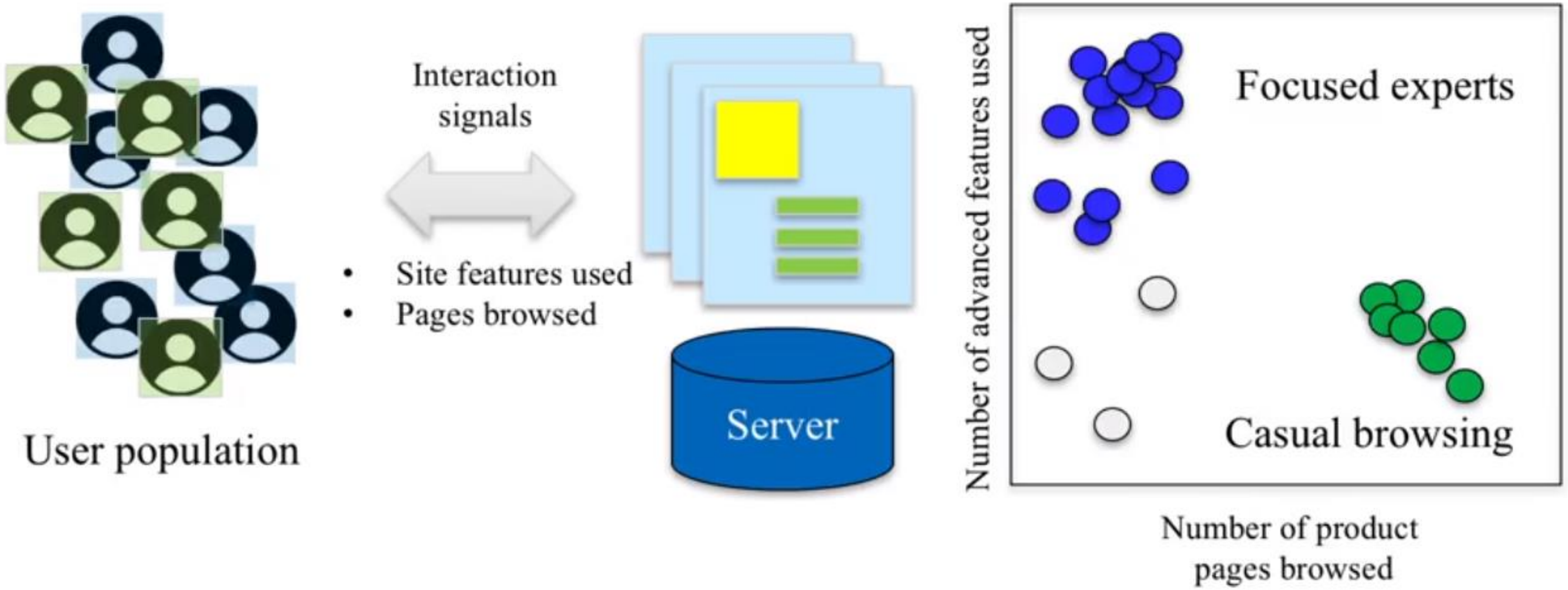
– Sum of squared error (SSE) is a commonly used measure.

- Inter-cluster separation (isolation):

– Separation means that different cluster centroids should be far away from one another.

- In most applications, expert judgments are still the key

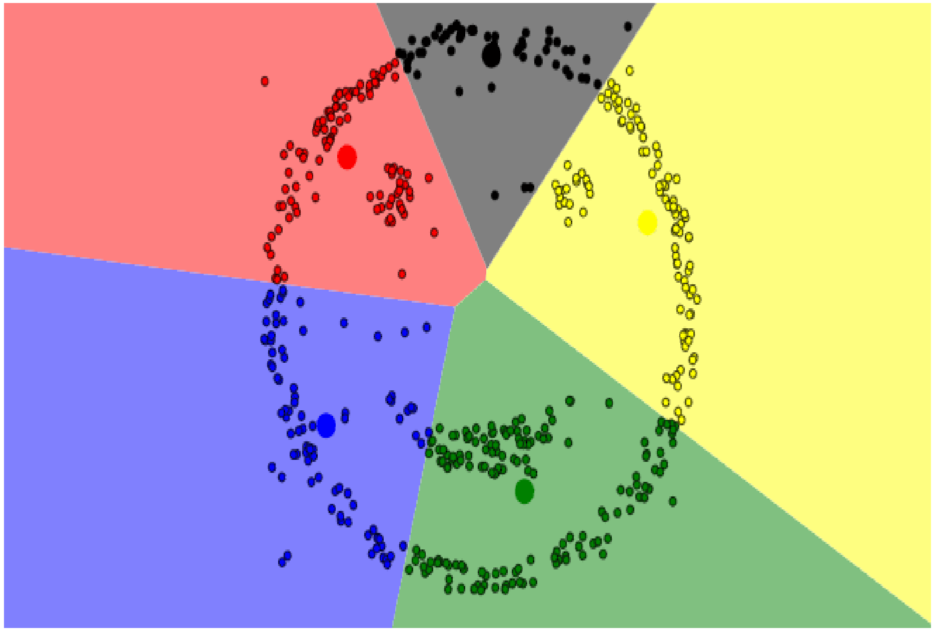
Web Clustering Examples



https://www.coursera.org/learn/python-machine-learning

Limitations of k-means

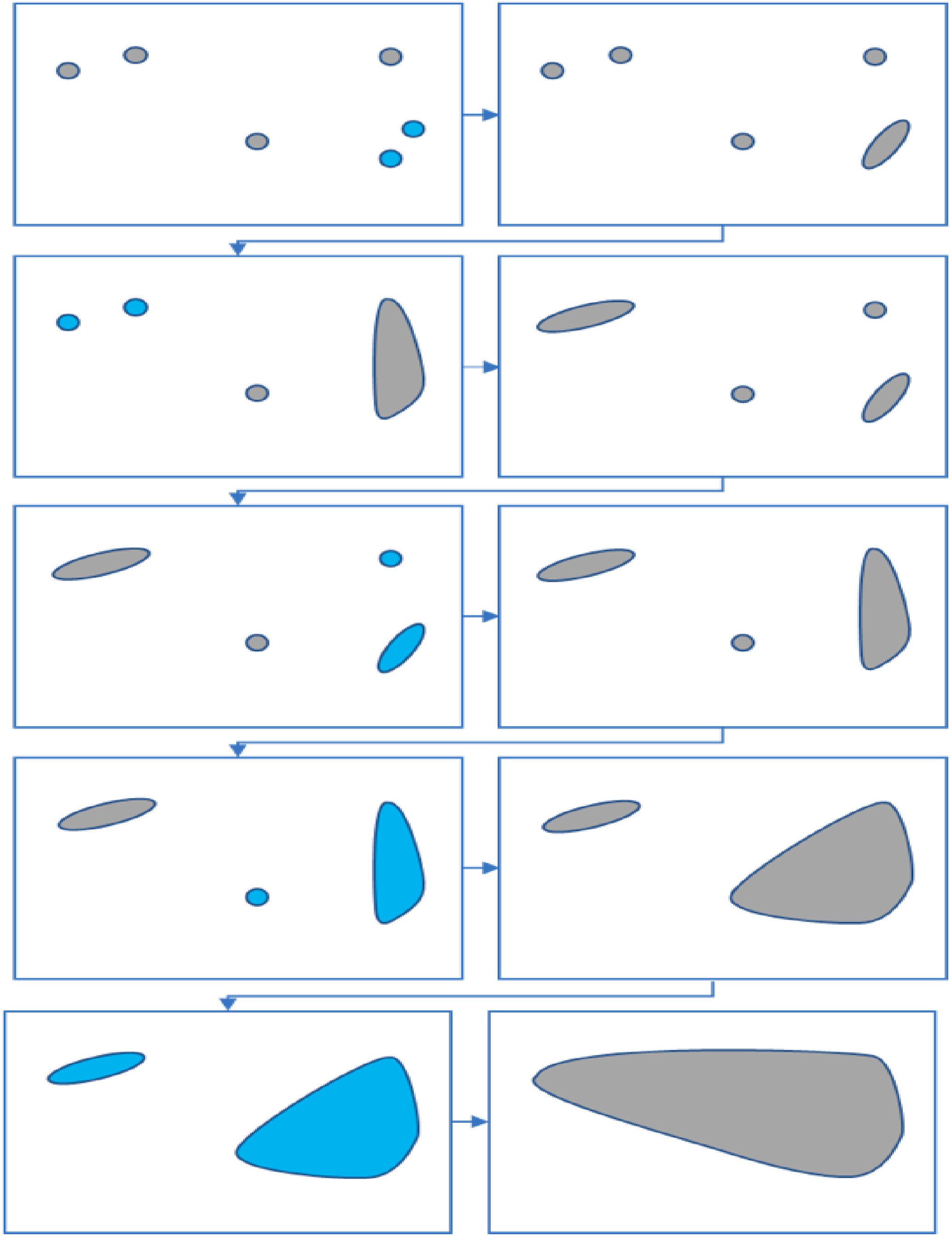
- Sometime the number of clusters is difficult to determine
- Does not do well with irregular or complex clusters.
- Has a problem with data containing outliers



http://arogozhnikov.github.io/2017/07/10/opera-clustering.html

Hierarchal Clustering

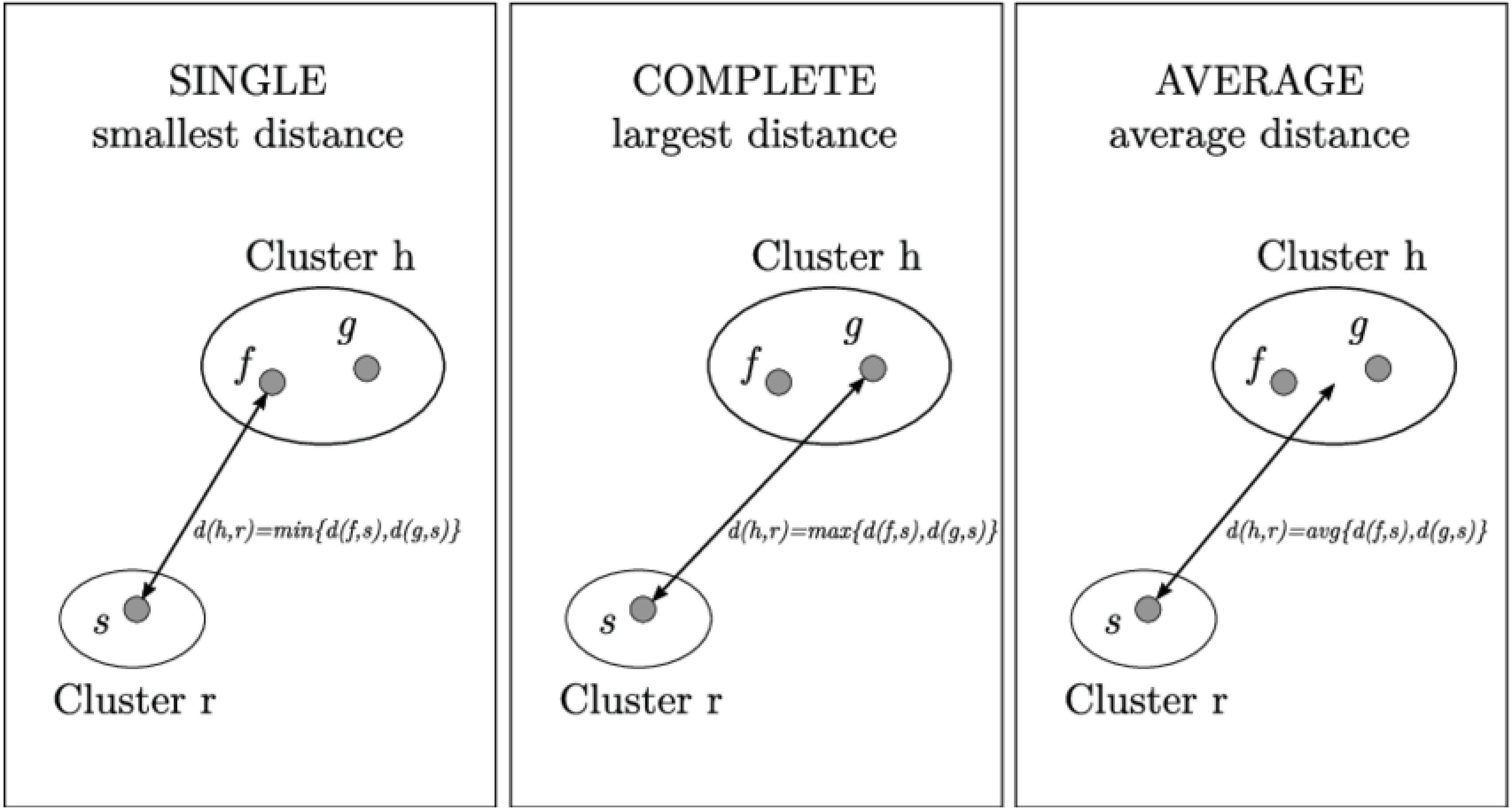
- What is it?
  - ➢ Unsupervised machine learning.
  - ➢ It is essentially building a hierarchy of clusters
- Types of Hierarchal Clustering
  - ➢ Agglomerative hierarchical clustering
  - ➢ Divisive Hierarchical clustering



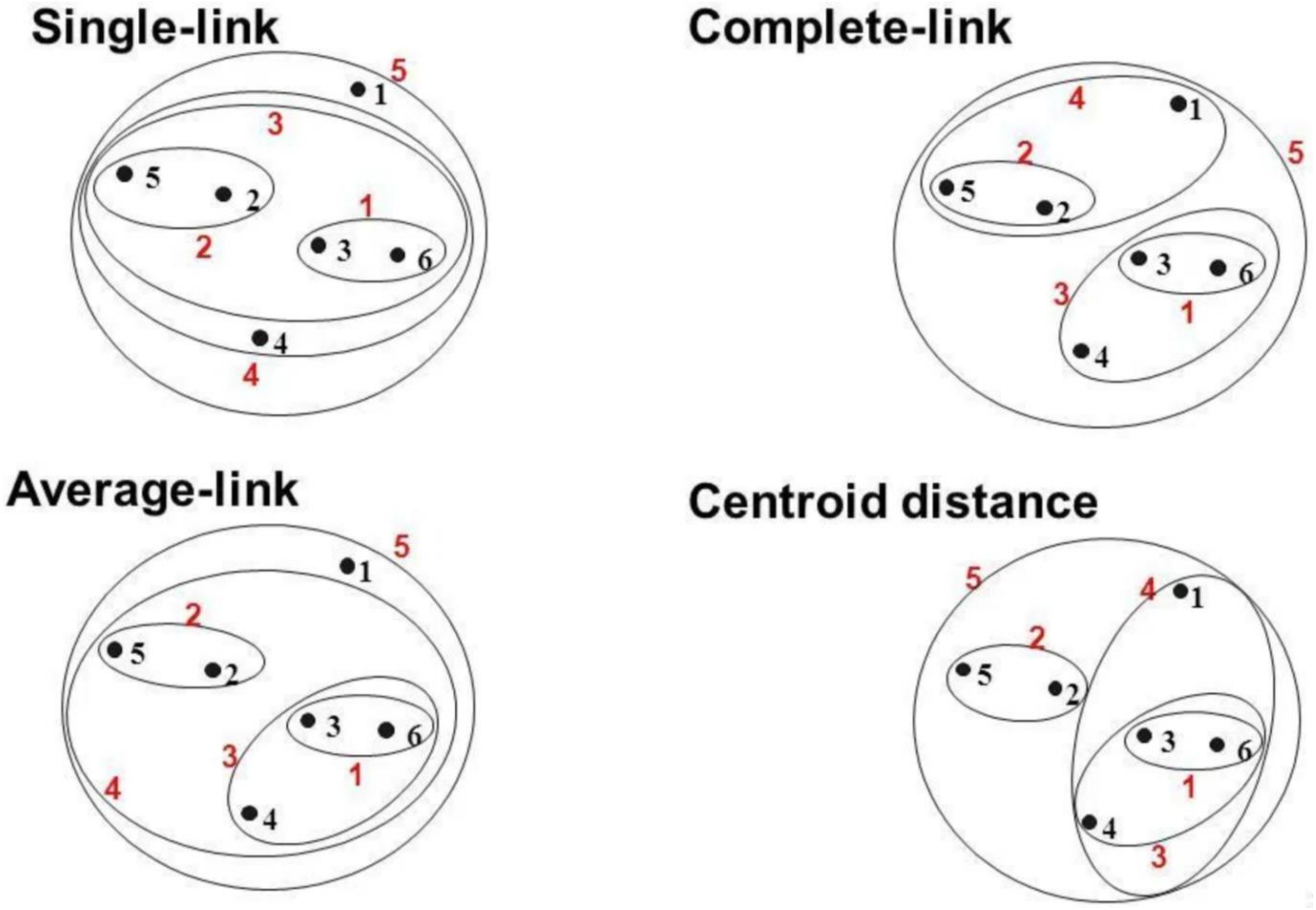
Linkage Criteria

- It is necessary to determine from where distance is computed in cluster.
- Your options
  - ➢It can be computed between the two most similar parts of a cluster (*single-linkage*)
  - ➢the two least similar bits of a cluster (*complete-linkage*)
  - ➢the center of the clusters (*mean* or *average-linkage*)
  - ➢or some other criterion

Linkage Criteria



Linkage Criteria Comparison



Single-link

Complete-link

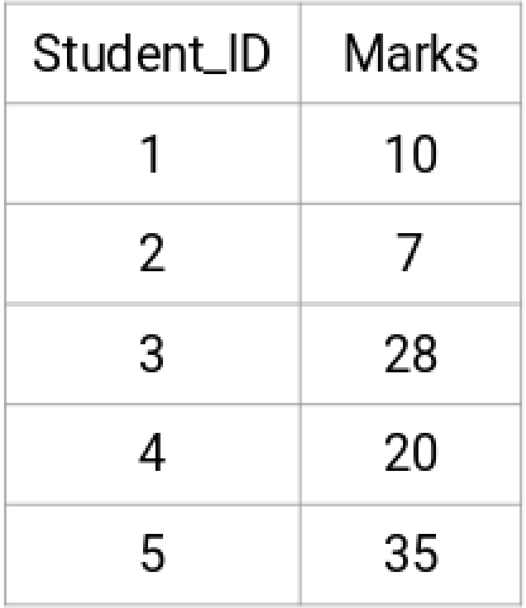
Average-link

Centroid distance

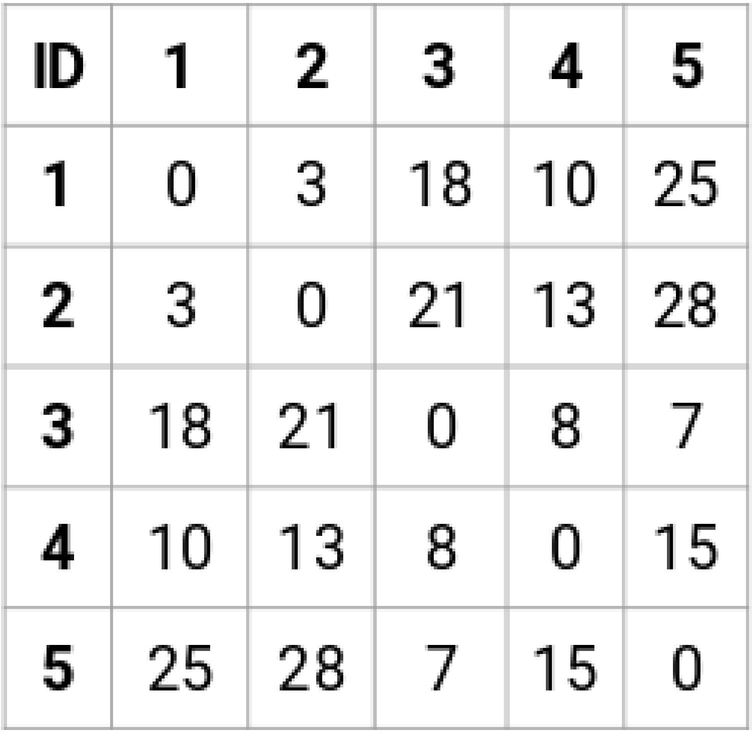
Agglomerative Clustering Algorithm

1. Compute the proximity matrix
2. Let each data point be a cluster
3. Repeat: Merge the two closest clusters and update the proximity matrix
4. Until only a single cluster remains

Agglomerative Clustering Example



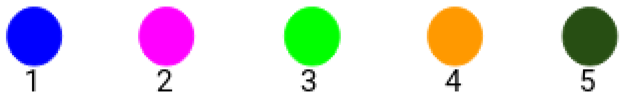
Student_ID	Marks
1	10
2	7
3	28
4	20
5	35

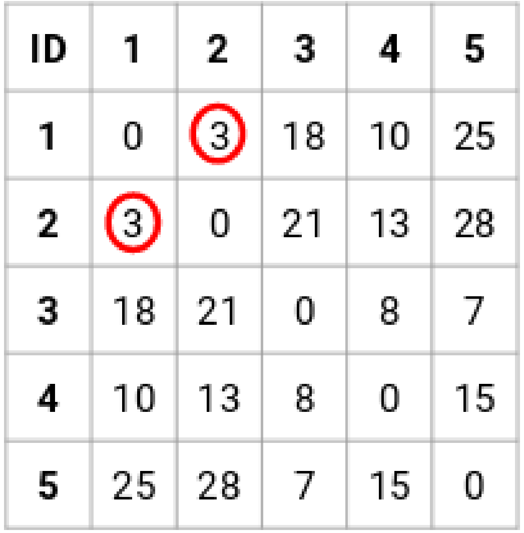


ID	1	2	3	4	5
1	0	3	18	10	25
2	3	0	21	13	28
3	18	21	0	8	7
4	10	13	8	0	15
5	25	28	7	15	0

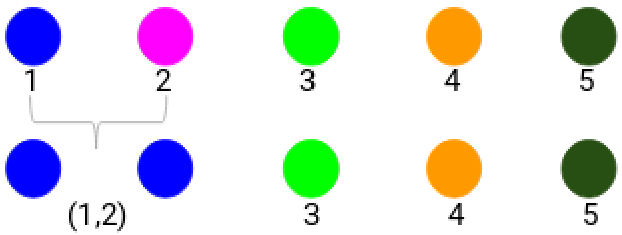
Proximity Matrix

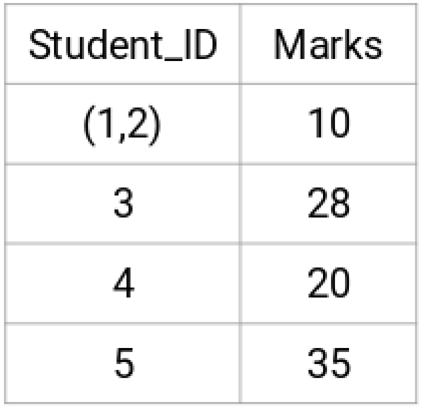
Agglomerative Clustering Example





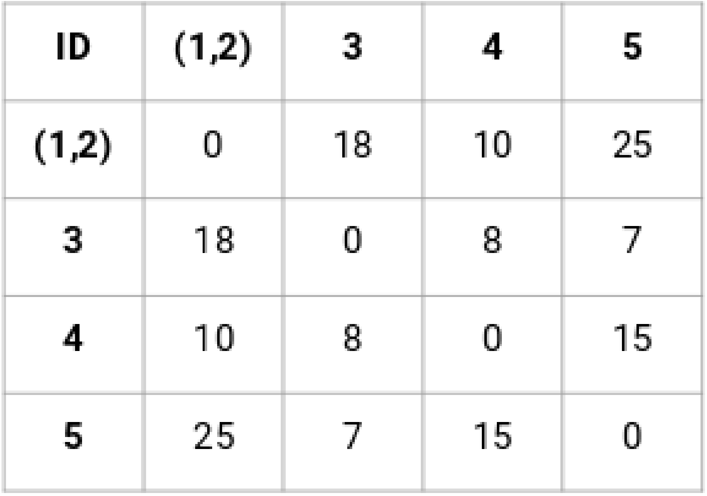
ID	1	2	3	4	5
1	0	3	18	10	25
2	3	0	21	13	28
3	18	21	0	8	7
4	10	13	8	0	15
5	25	28	7	15	0



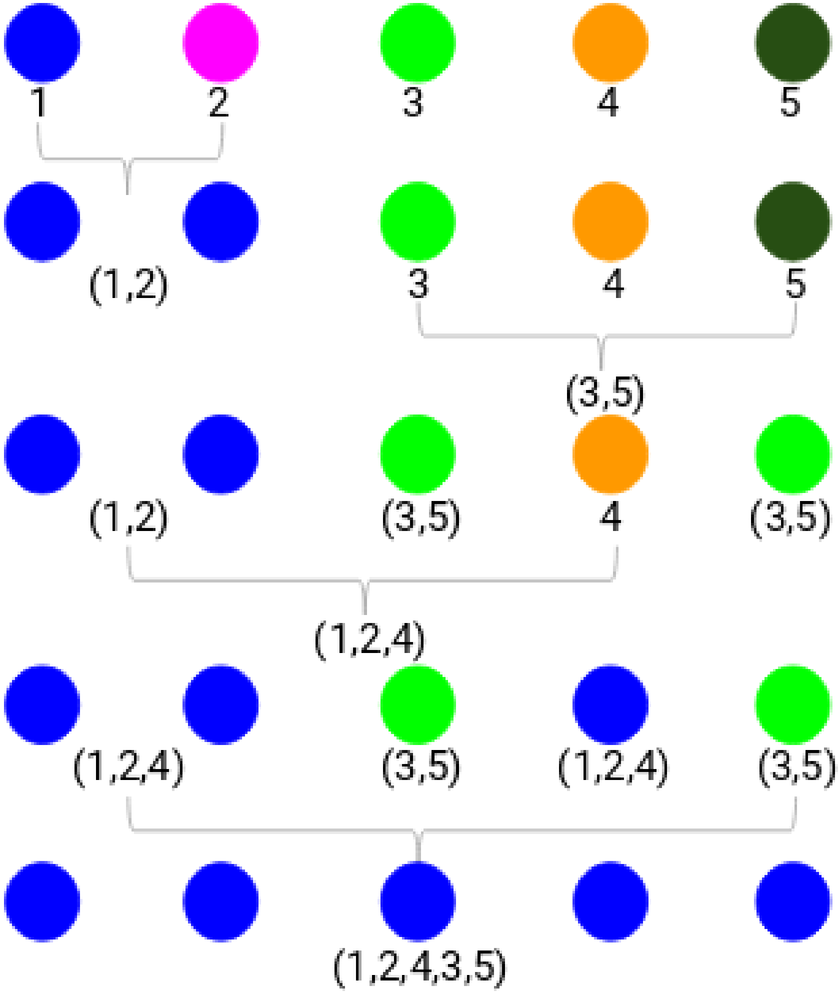


Student_ID	Marks
(1,2)	10
3	28
4	20
5	35

Agglomerative Clustering Example



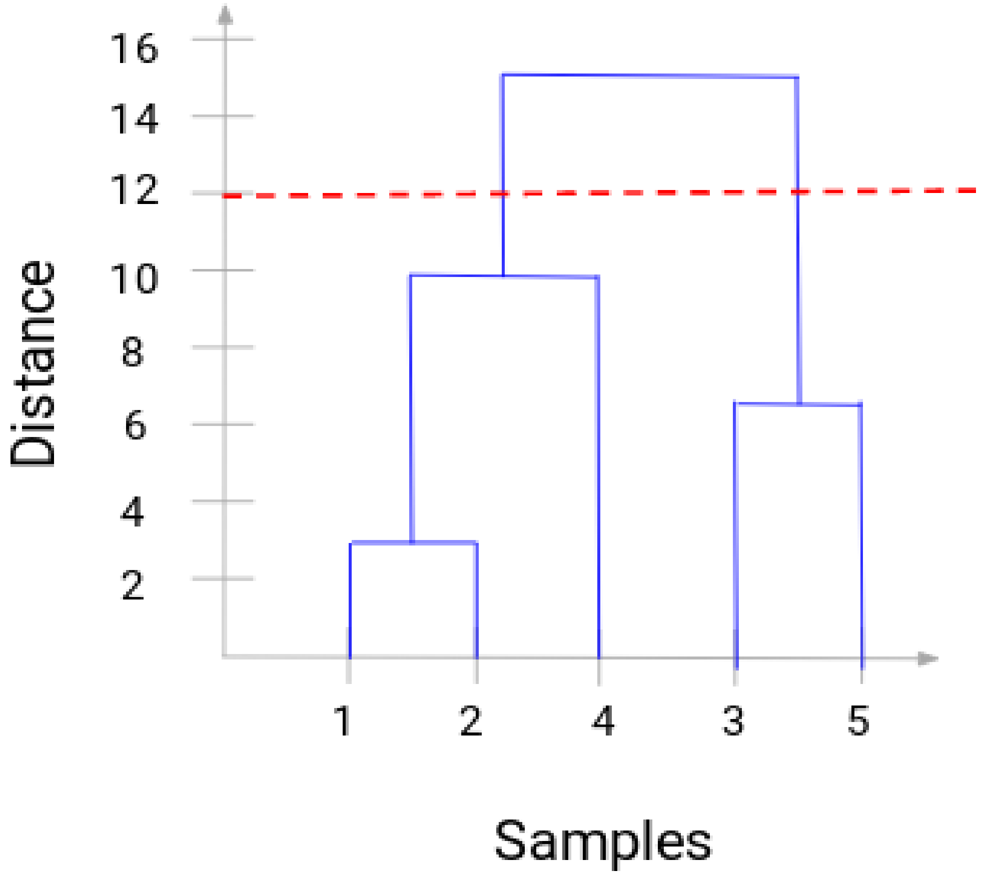
ID	(1,2)	3	4	5
(1,2)	0	18	10	25
3	18	0	8	7
4	10	8	0	15
5	25	7	15	0



How Can we Choose the Number of Clusters?

- Using a Dendrogram
- A dendrogram is a tree-like diagram that records the sequences of merges or splits
- Whenever two clusters are merged, we will join them in this dendrogram and the height of the join will be the distance between these points
- We set a threshold distance and draw a horizontal line (try to set the threshold in such a way that it cuts the tallest vertical line)
- The number of clusters will be the number of vertical lines which are being intersected by the line drawn using the threshold

How Can we Choose the Number of Clusters?



Advantages and Disadvantages of Hierarchal Clustering

- Advantages
  - ➢ Easy to Implement
  - ➢ No Need to decide the number of clusters beforehand.
- Disadvantages
  - ➢ Not suitable for large datasets
  - ➢ Sensitive to Outliers
  - ➢ Initial Seeds have strong impact of final results
  - ➢ Linkage criteria and Distance measure are selected most of the time arbitrary.

Useful Resources

- https://www.datacamp.com/community/tutorials/k-means-clustering-python
- https://realpython.com/k-means-clustering-python/
- https://developers.google.com/machine-learning/clustering/algorithm/advantages-disadvantages
- https://towardsdatascience.com/understanding-the-concept-of-hierarchical-clustering-technique-c6e8243758ec

Q&A