Lecture: K-Means Clustering

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Cal Poly State University, May 26th

Slides and Code

https://github.com/rocanaan/k-means

Types of Machine Learning

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- **Supervised Learning**

Learning to predict values or classify objects based on labeled data

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- Human labeling is expensive!

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- Generate examples that look like the data
- Label data for downstream tasks

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- **Visual Processing**

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- **Science**

Create a taxonomy of phenomena (e.g. stars) based on their observed properties (magnitude, spectrum, distance…)

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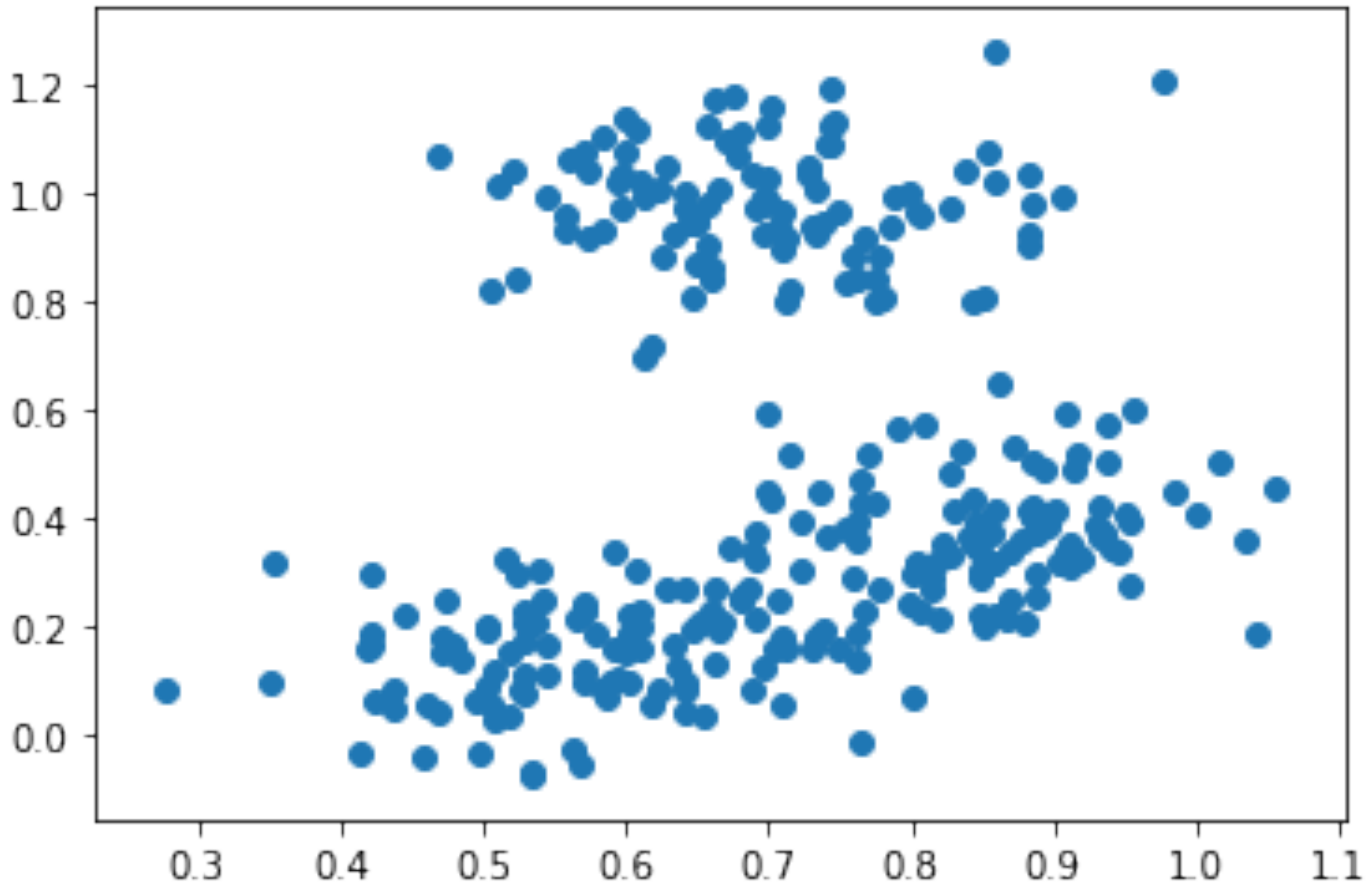
Clustering - Visual Example

Before clustering



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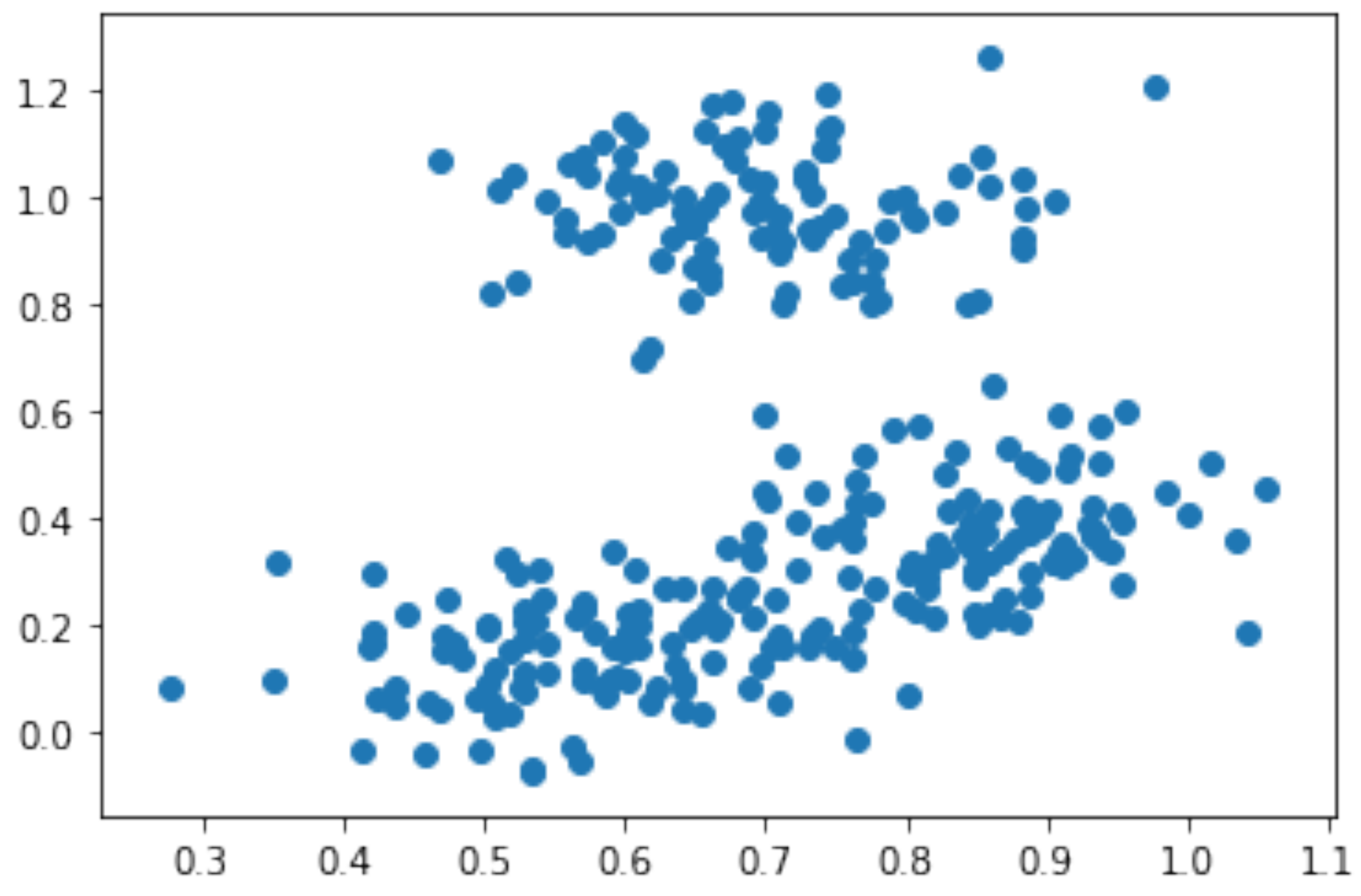
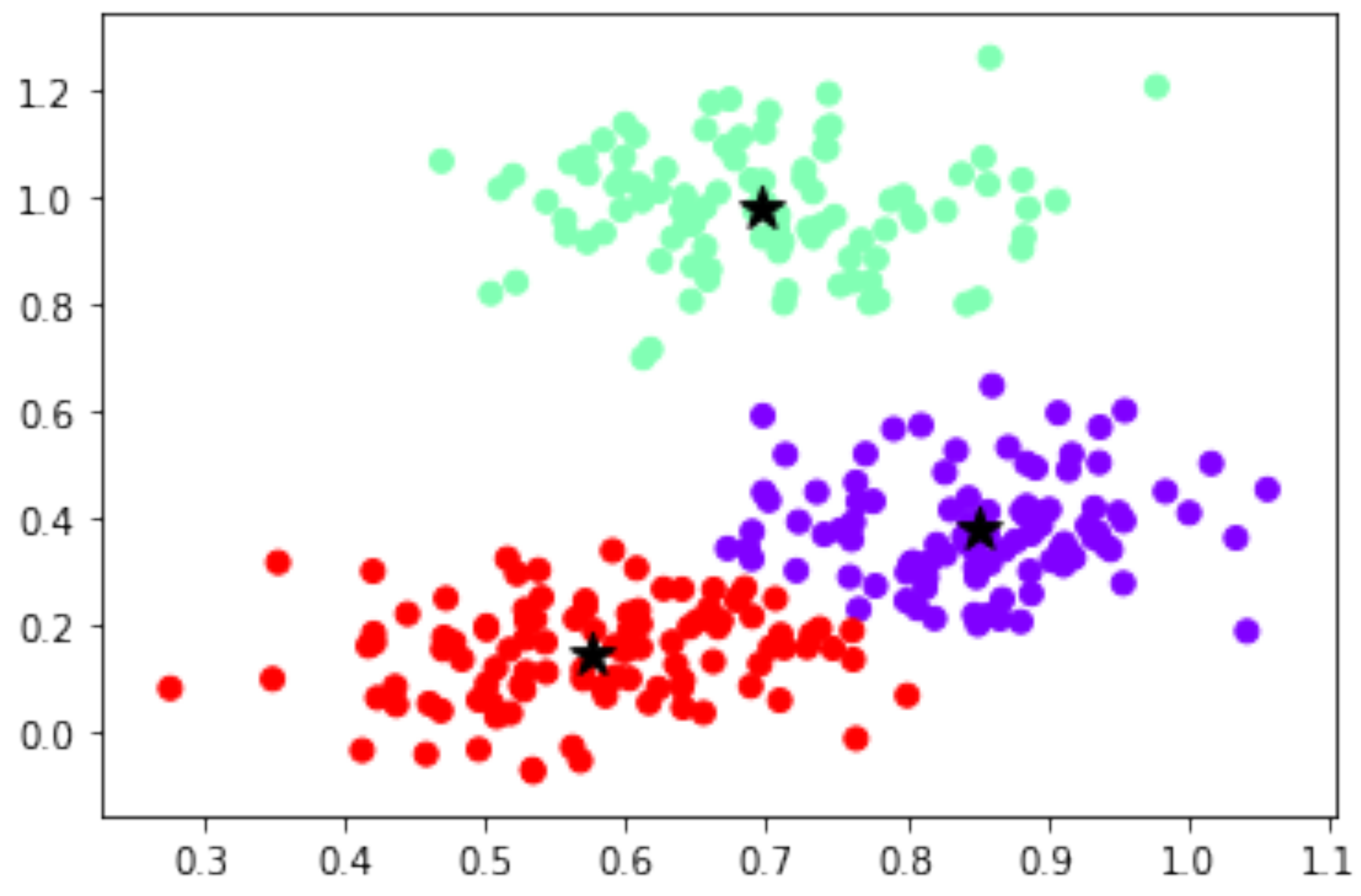


After k-means Clustering (k=3)



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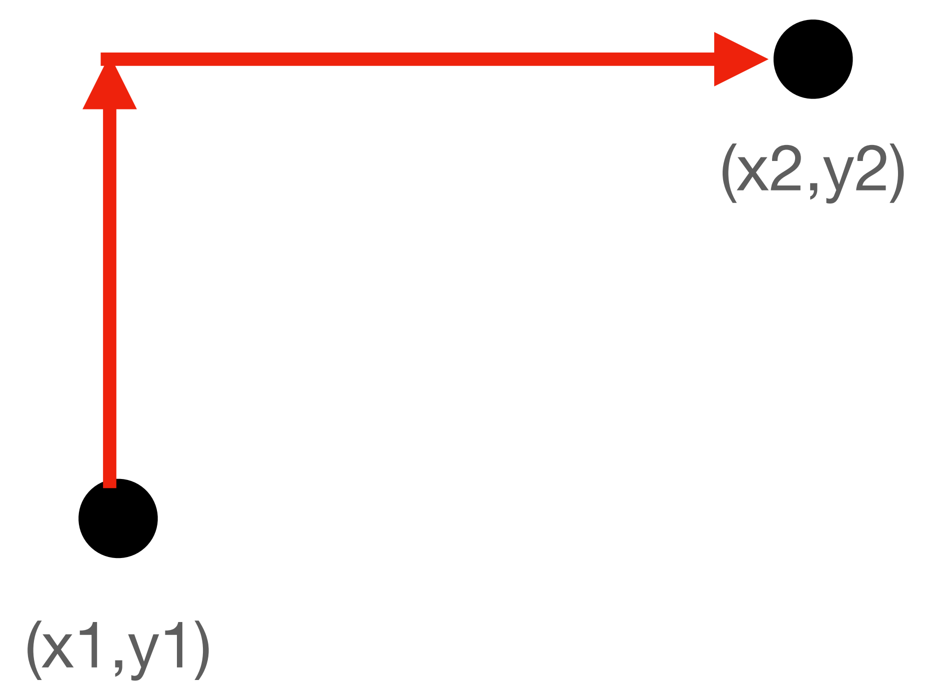
Examples (in 2-dimensions)

Manhattan Distance



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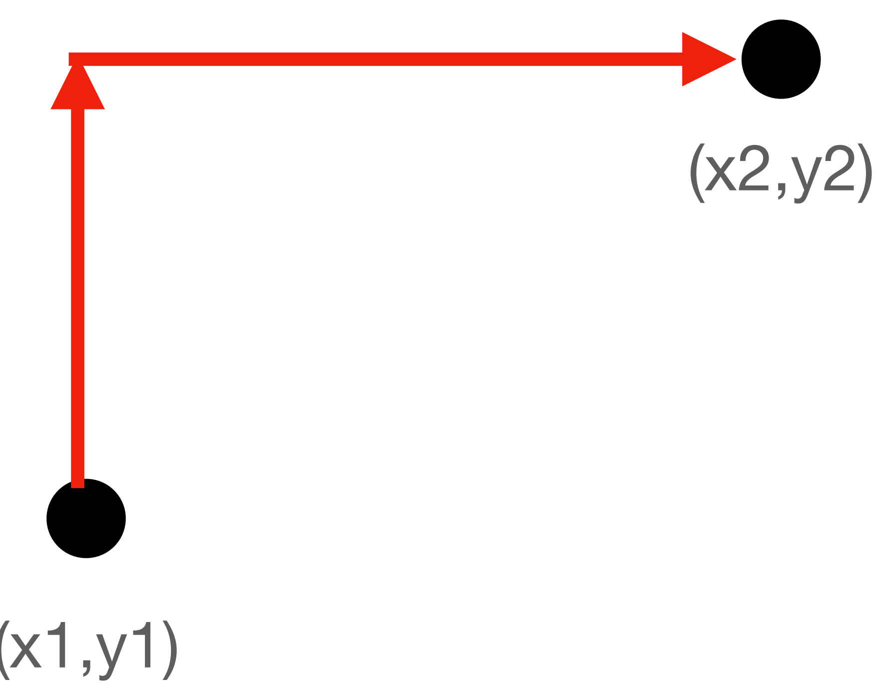

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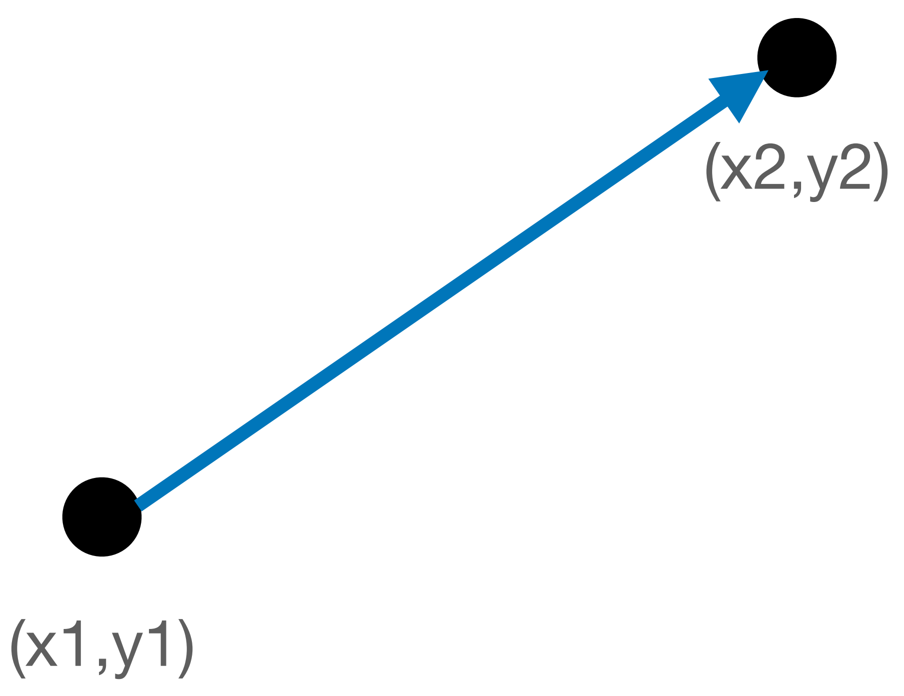
Euclidean Distance



$$D_E = \sqrt{(x2 - x1)^2 + (y2 - y1)^2}$$

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Examples:

- Within-Cluster Sum of Squares (WCSS)
- Average Distance from Centroid
- Maximum Distance from Centroid

What is the simplest-possible clustering algorithm?

Clustering by exhaustive enumeration

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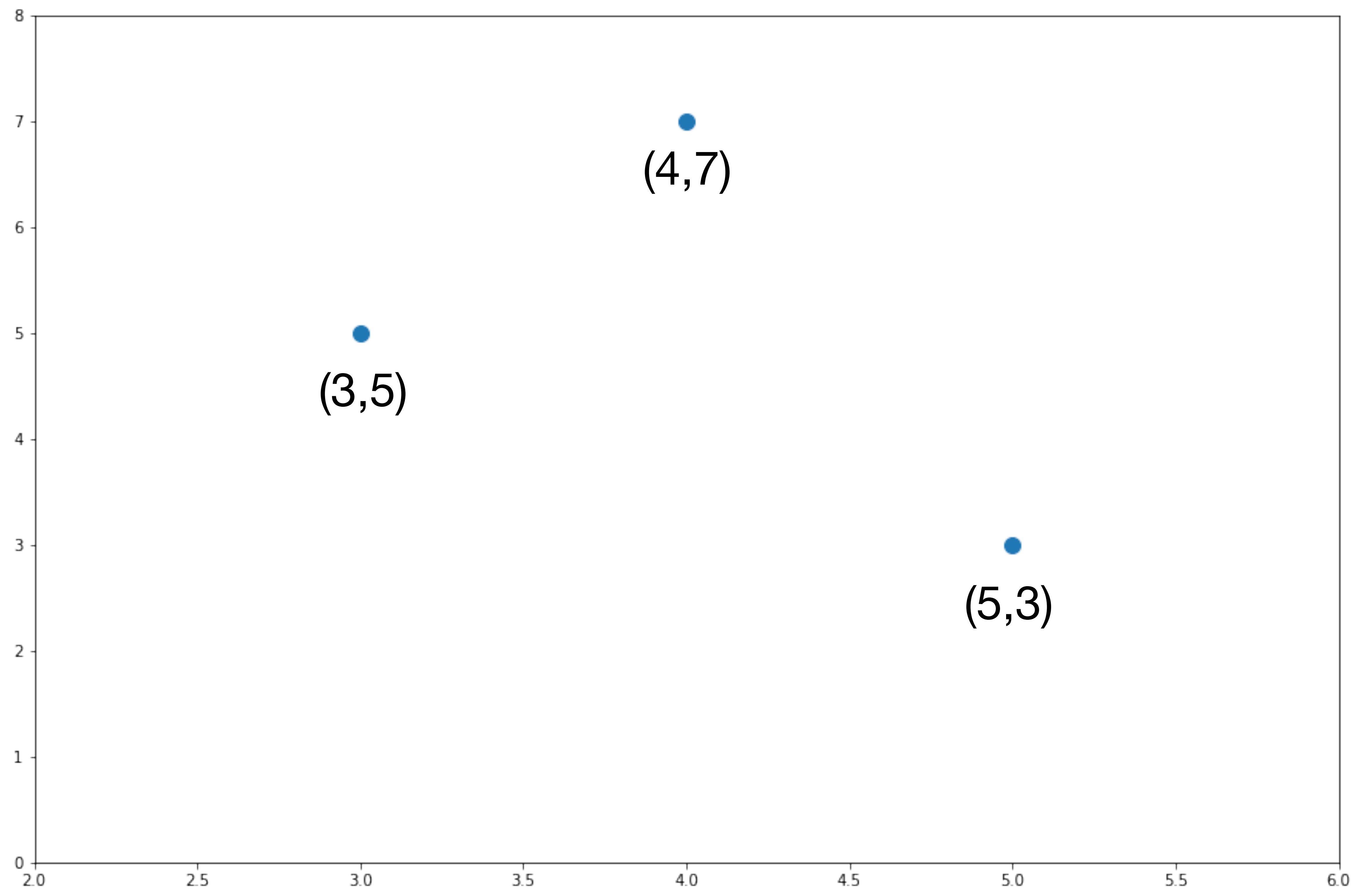
Example: assign each point to cluster with nearest centroid

Centroid Calculation



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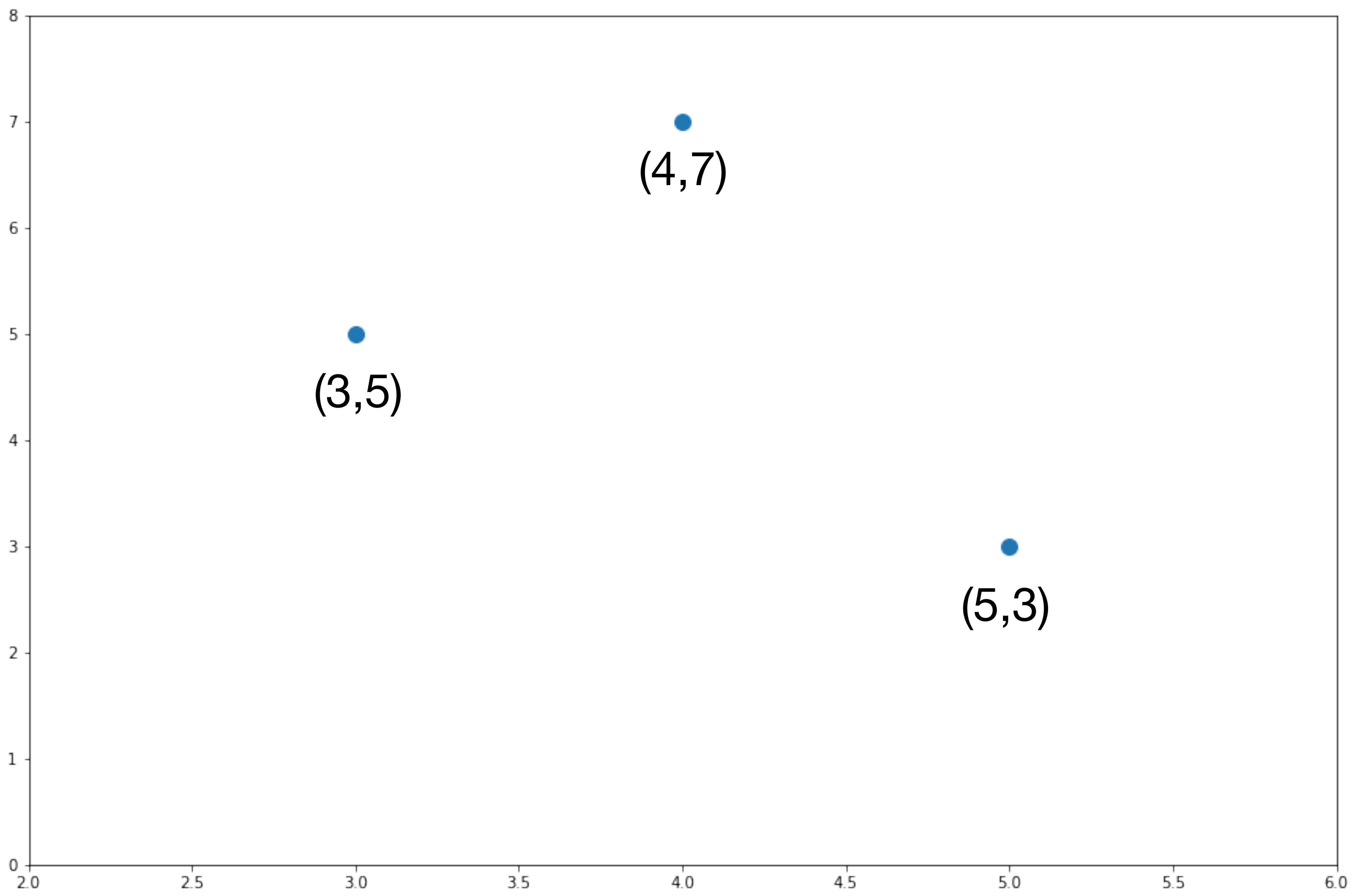

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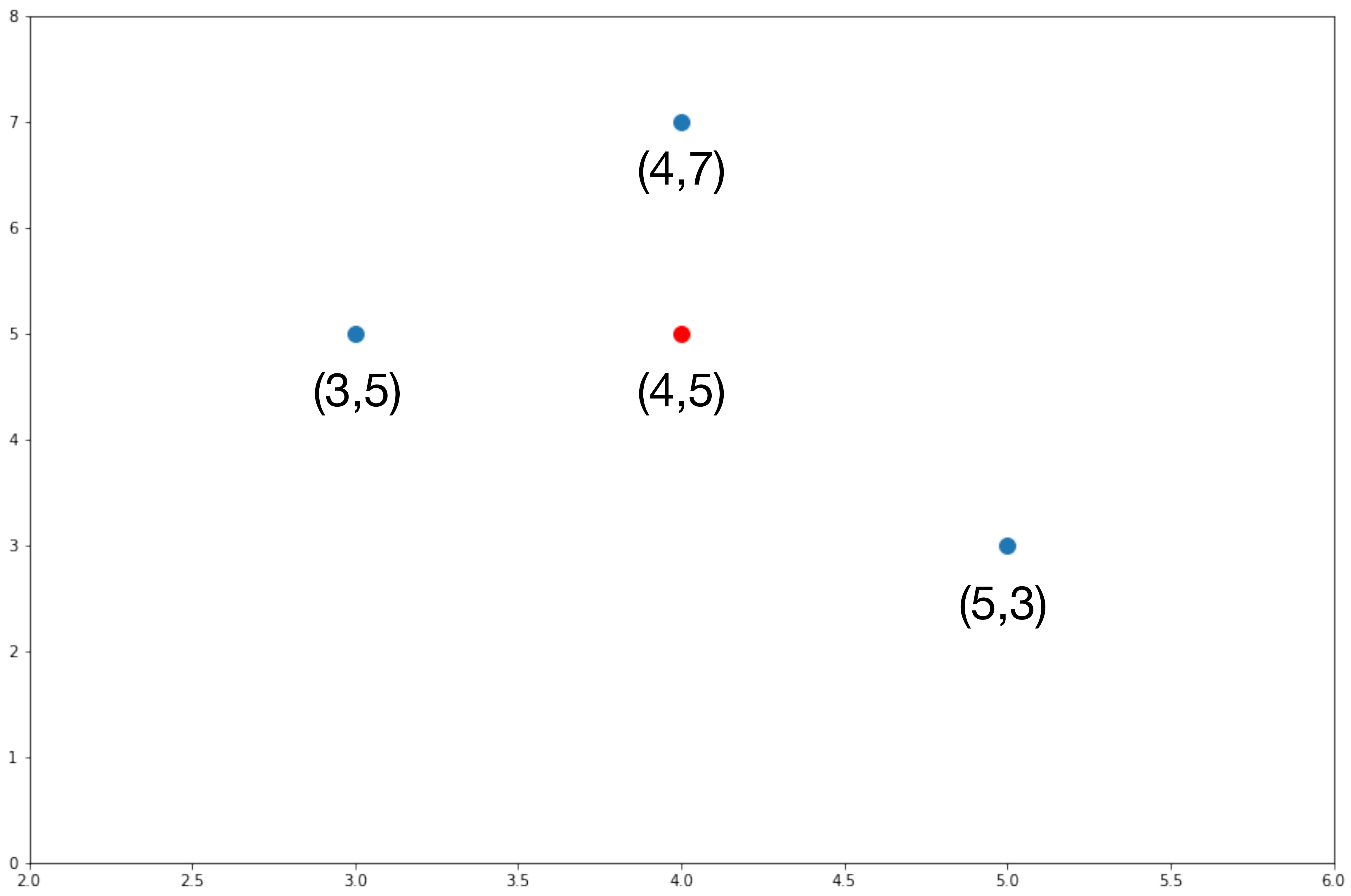

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Centroid = (4,5)

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4. **Repeat (2, 3) until no re-assignments**
   Alternatively, up to some maximum number of epochs

(Naive) K-Means Pseudo-Code

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- Other options: see comparative study by (Celebi et al., 2013)

K-Means Initialization Pseudo-Code

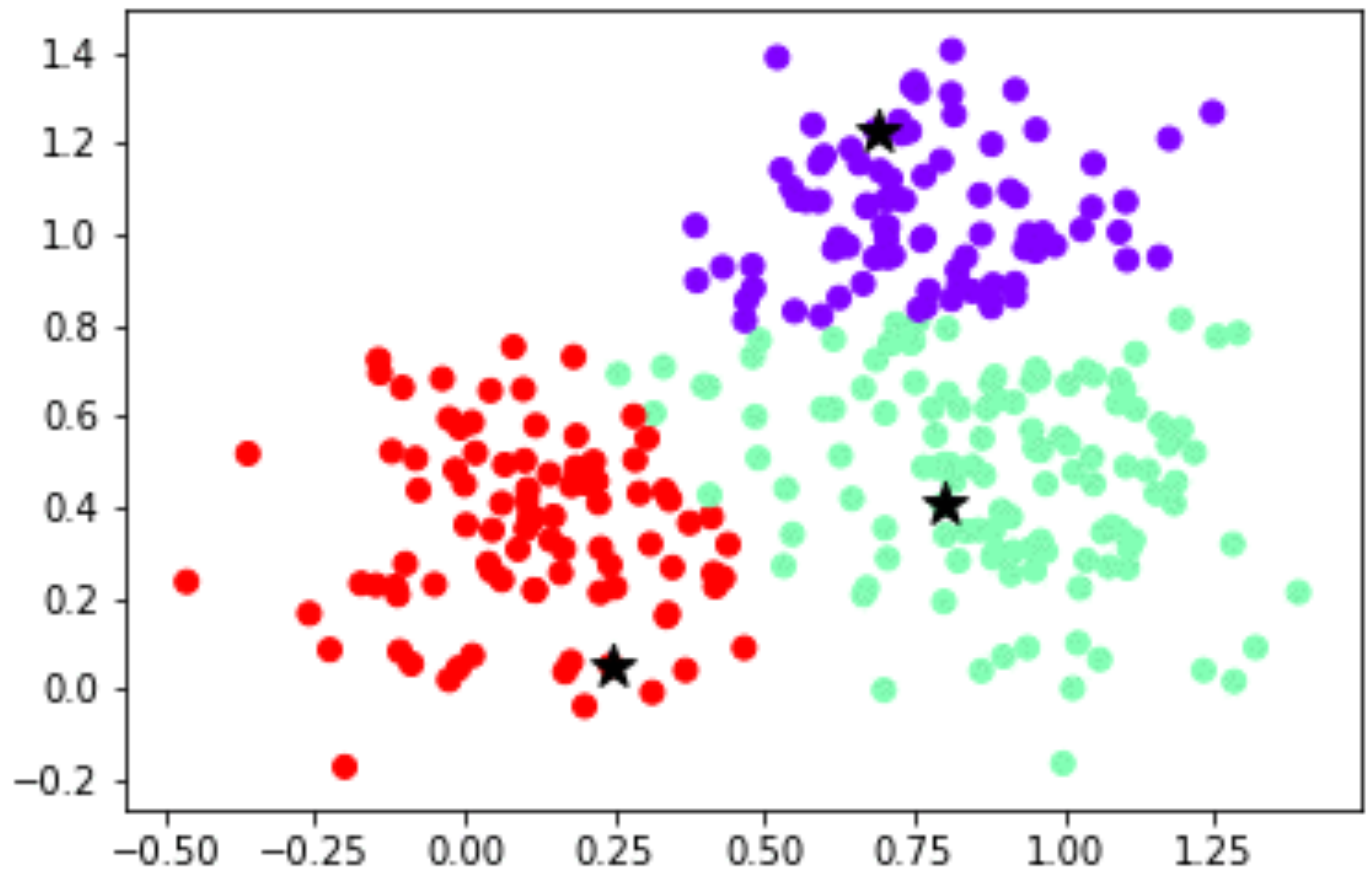
```
# Initial assignment of labels can be done in the main algorithm itself!
Function initialize_partitions(data,k)
    P <- empty_partition(k)
    P.centroids <- sample_without_replacement(data,k) # get k points from data
Endfunction

#OR

# Random Partition initialization
# Assign each point to a random label, then compute centroids
Function initialize_partitions(data,k)
    P <- empty_partition(k)
    for d in data
        label <- random_uniform(k)
        P.add_element(d,label)
    Endfor
    P.compute_centroids()
    return P
Endfunction
```

Demo

Forgy Method, k=3



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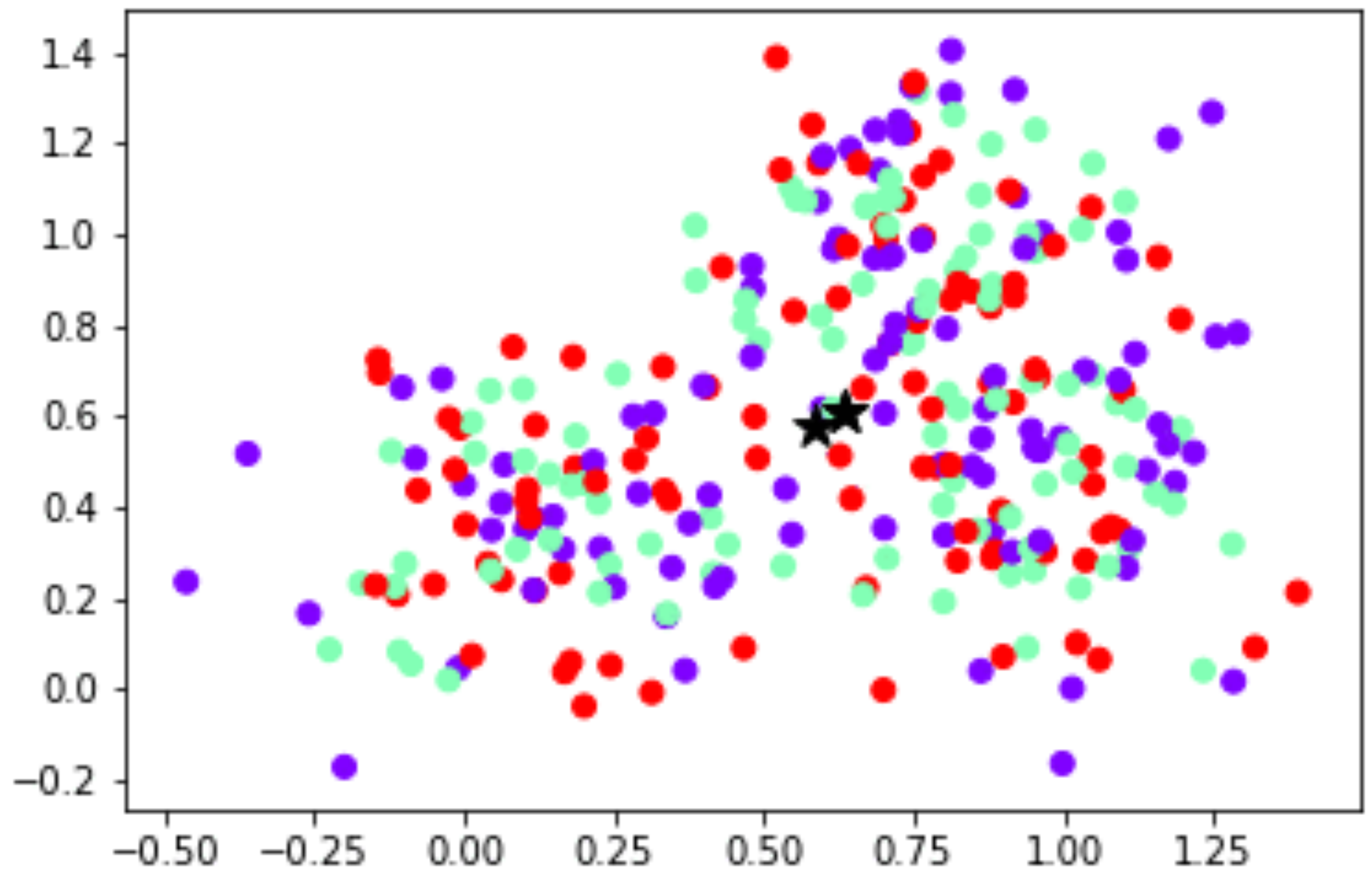

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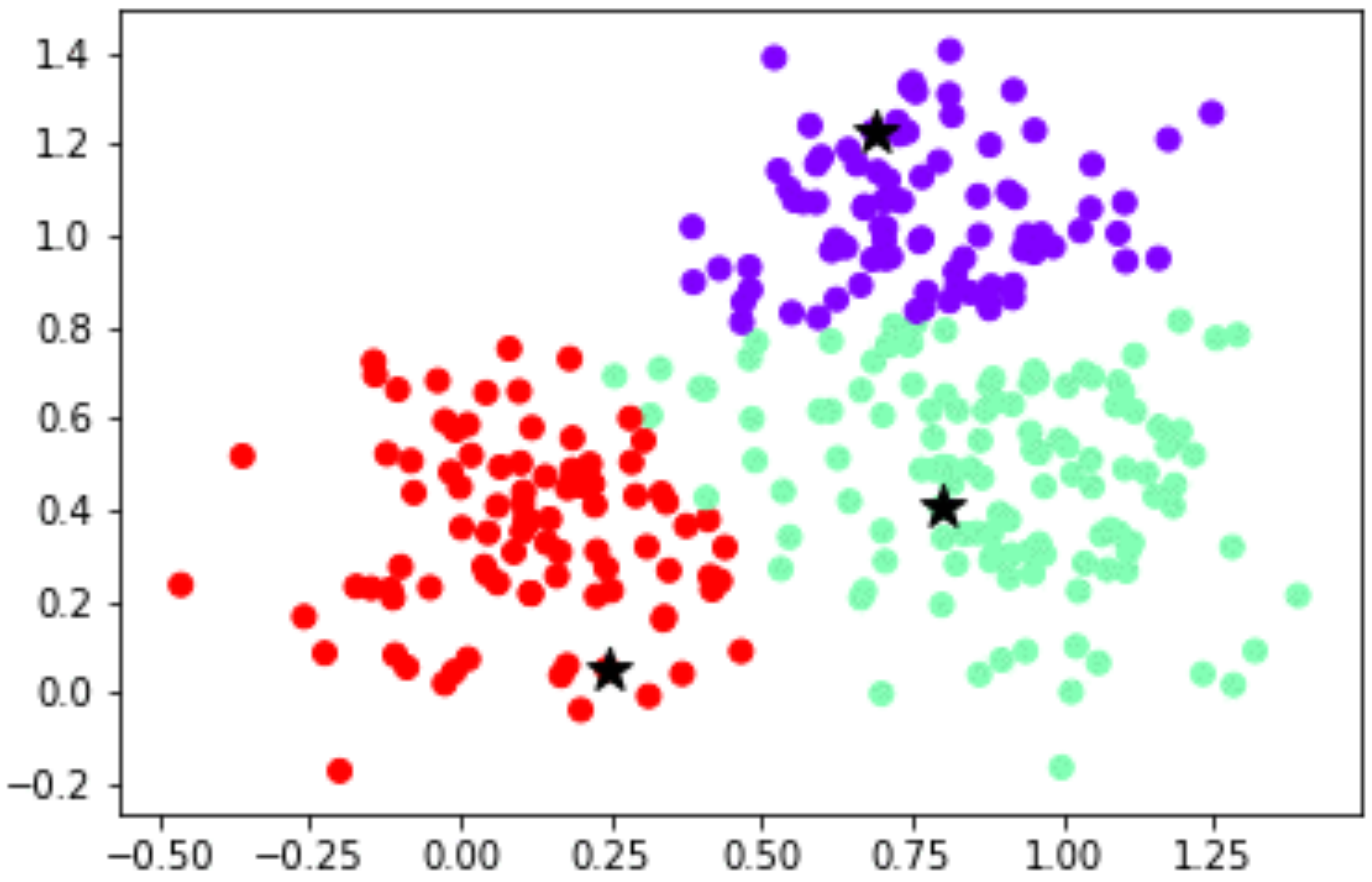

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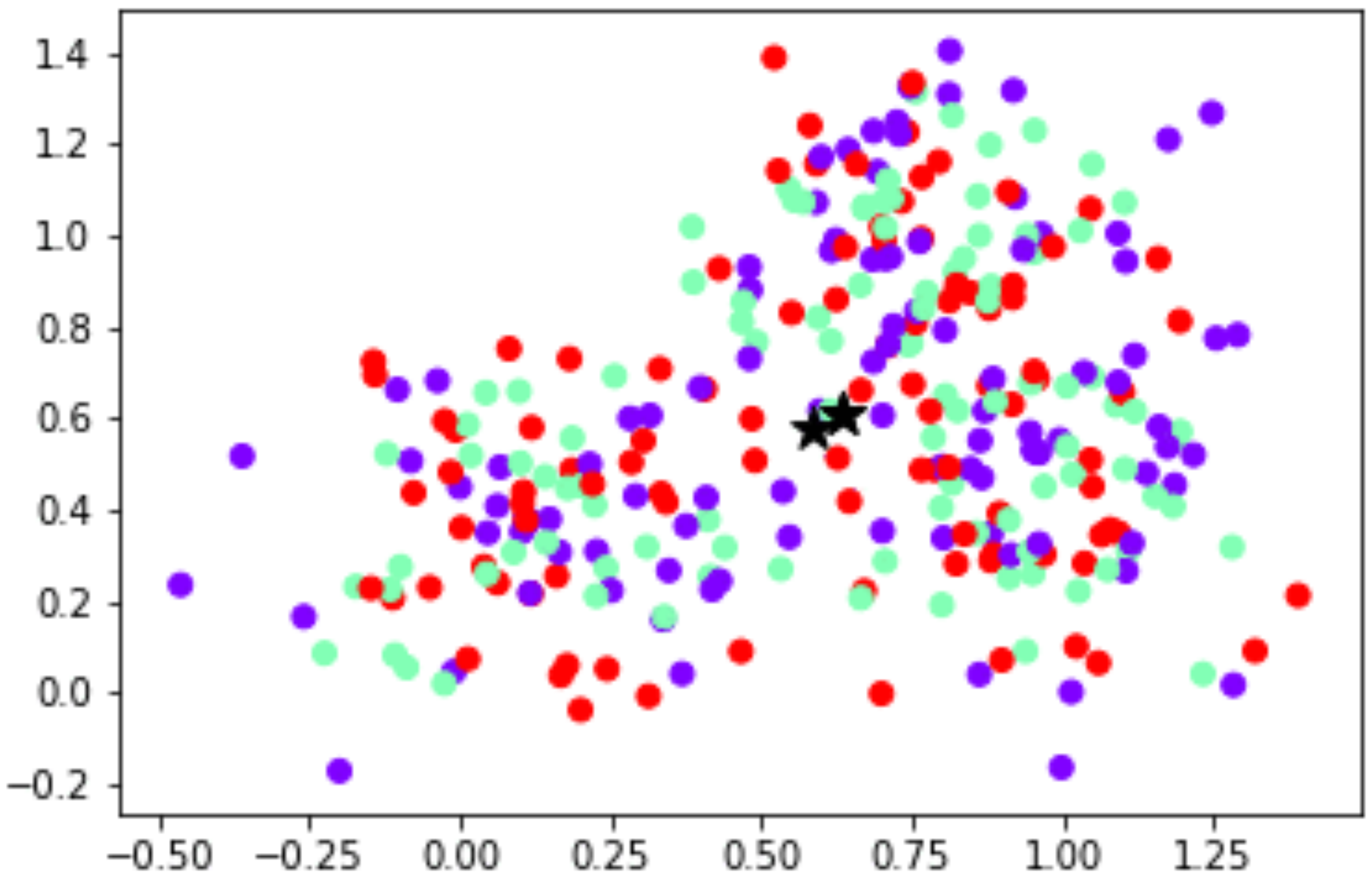

Advantages and Disadvantages

(Naive) K-Means Disadvantages

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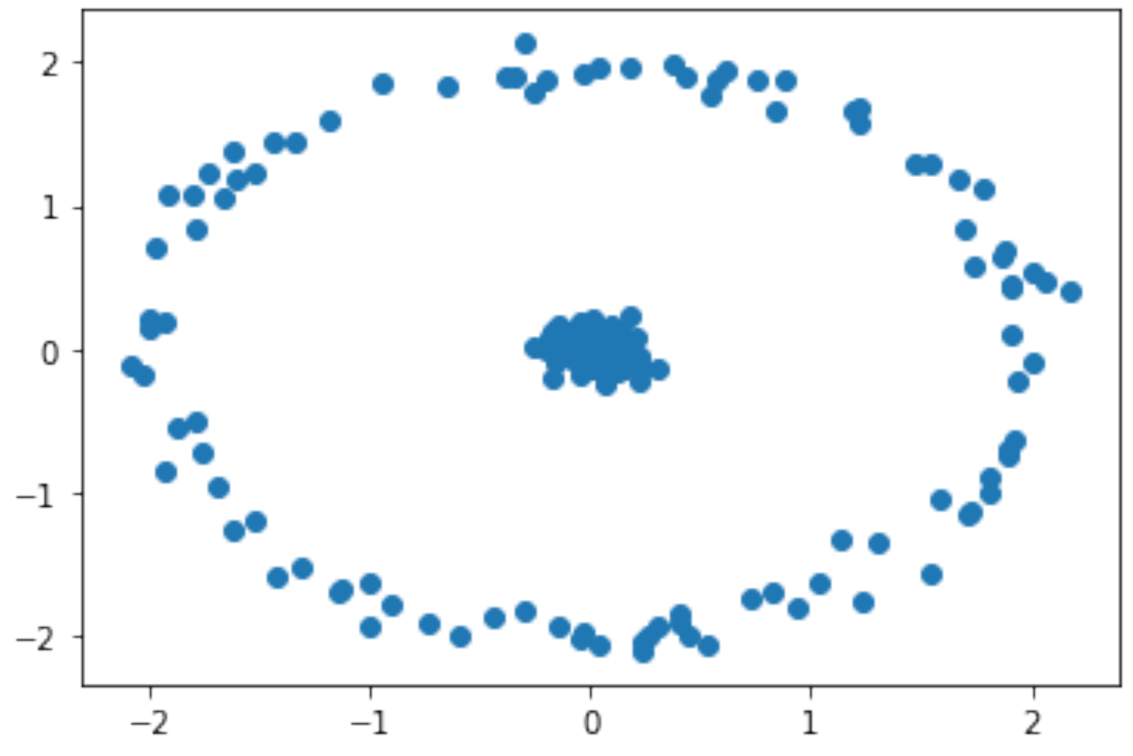
- **Struggles with some data shapes, sizes and outliers**

Non-Convex Clusters



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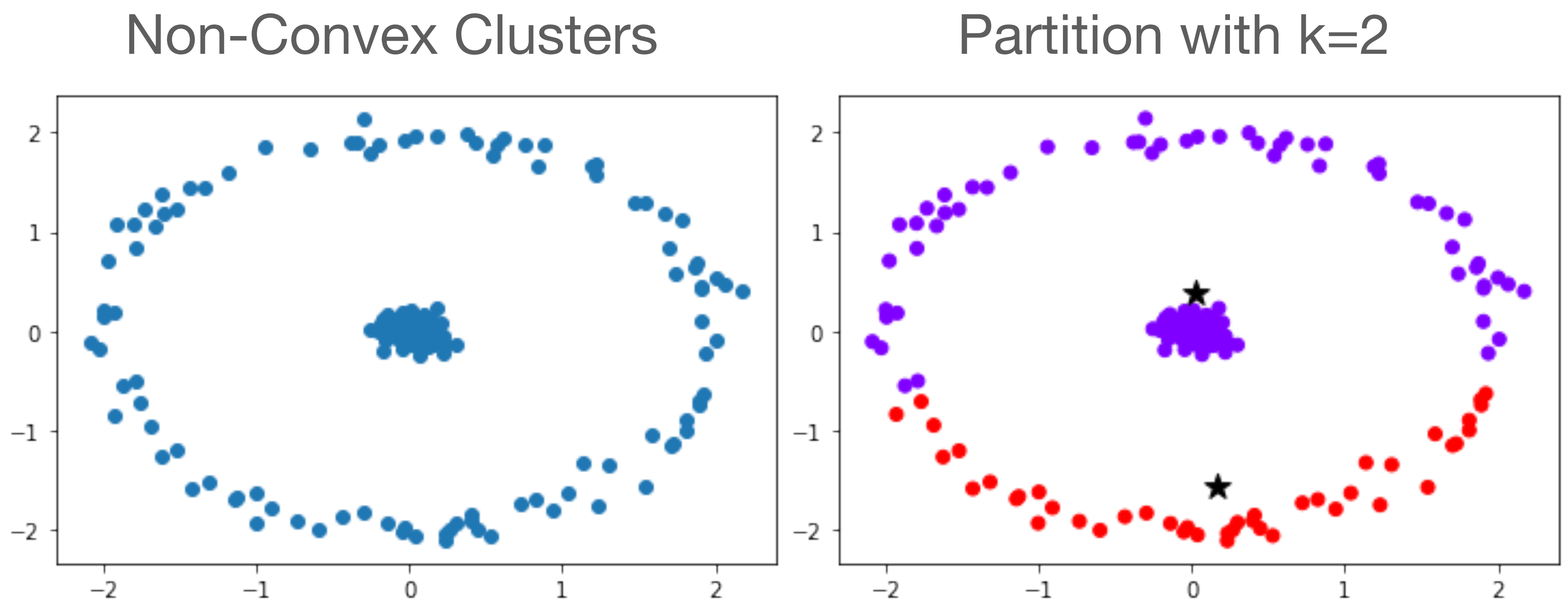

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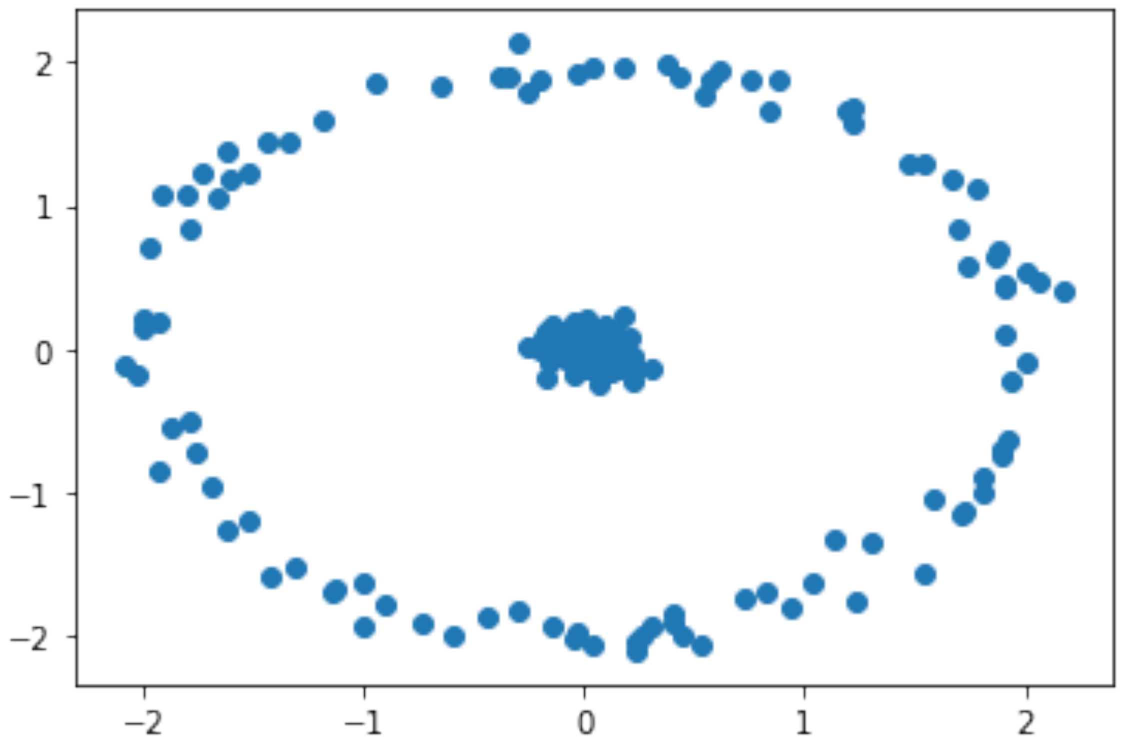
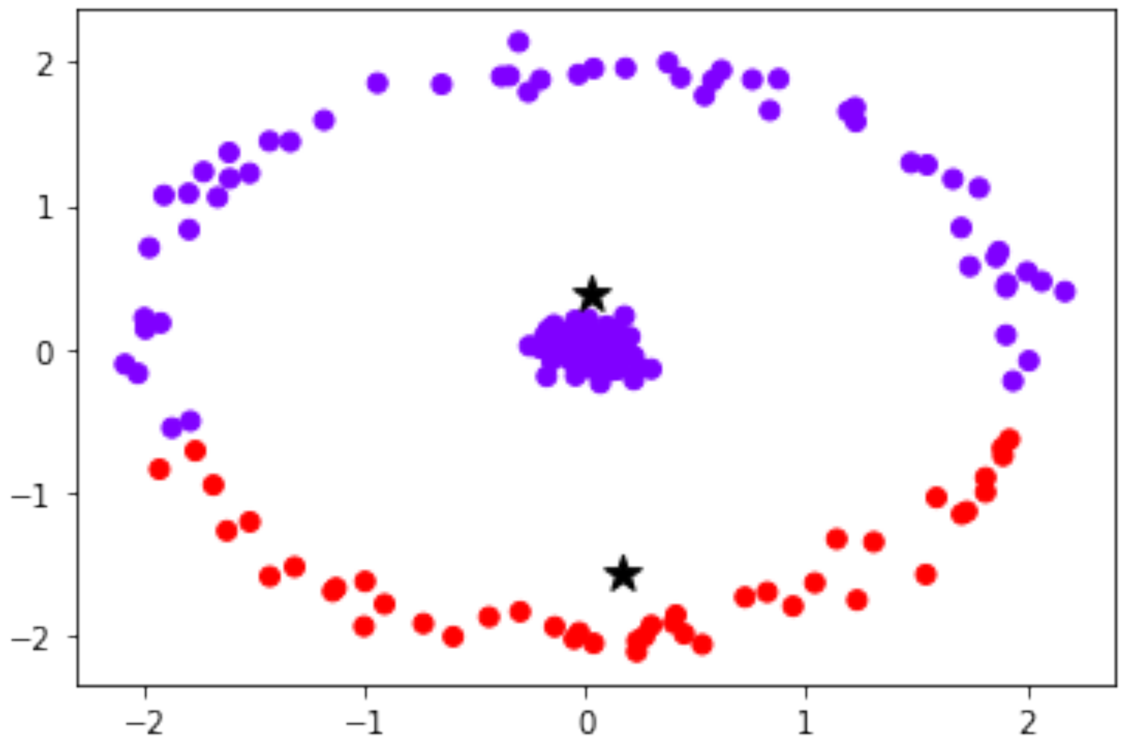
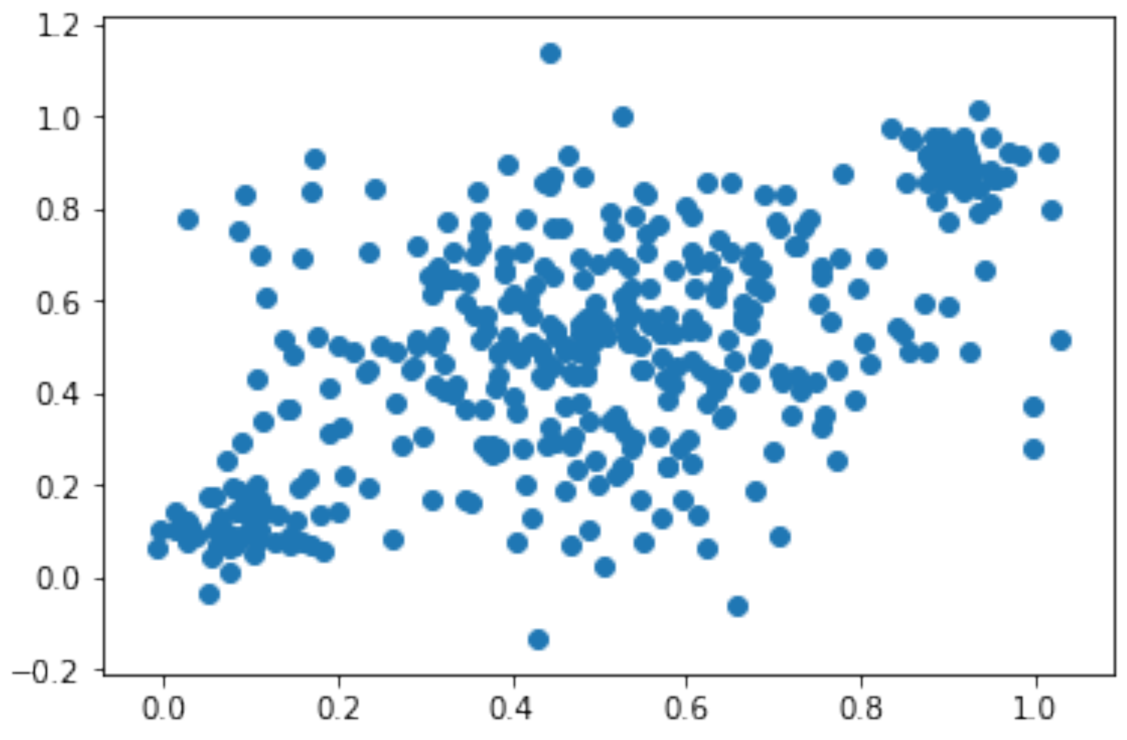


Partition with k=2



Clusters of different sizes



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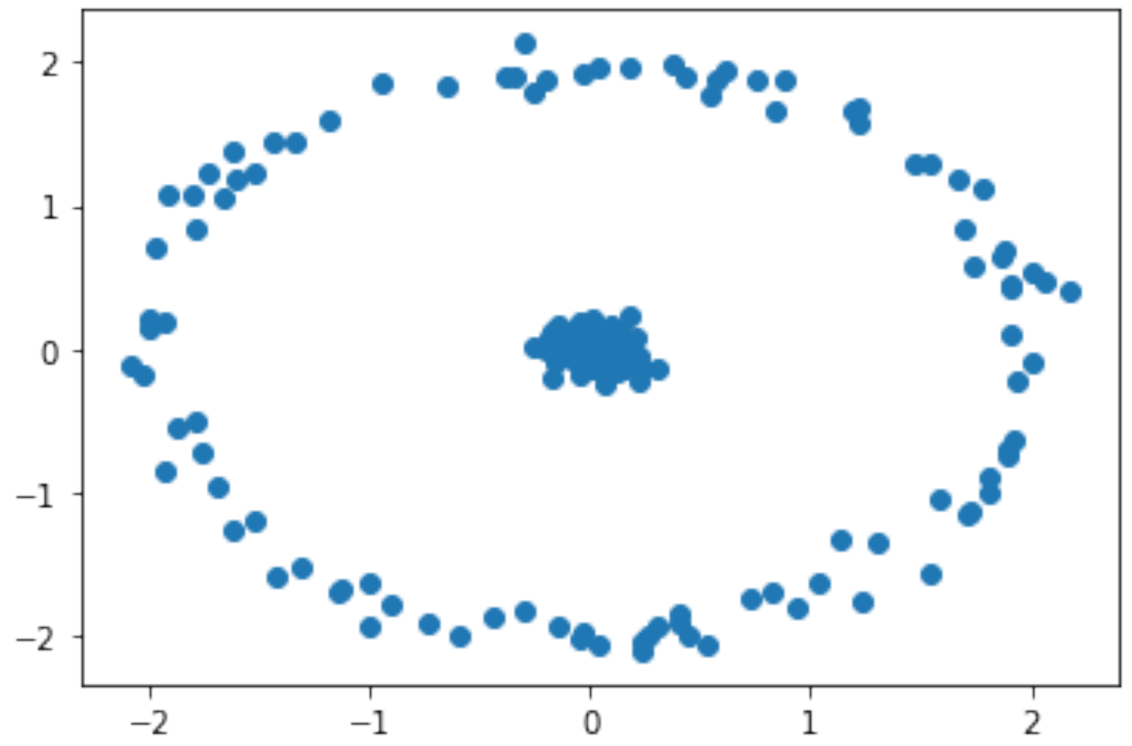

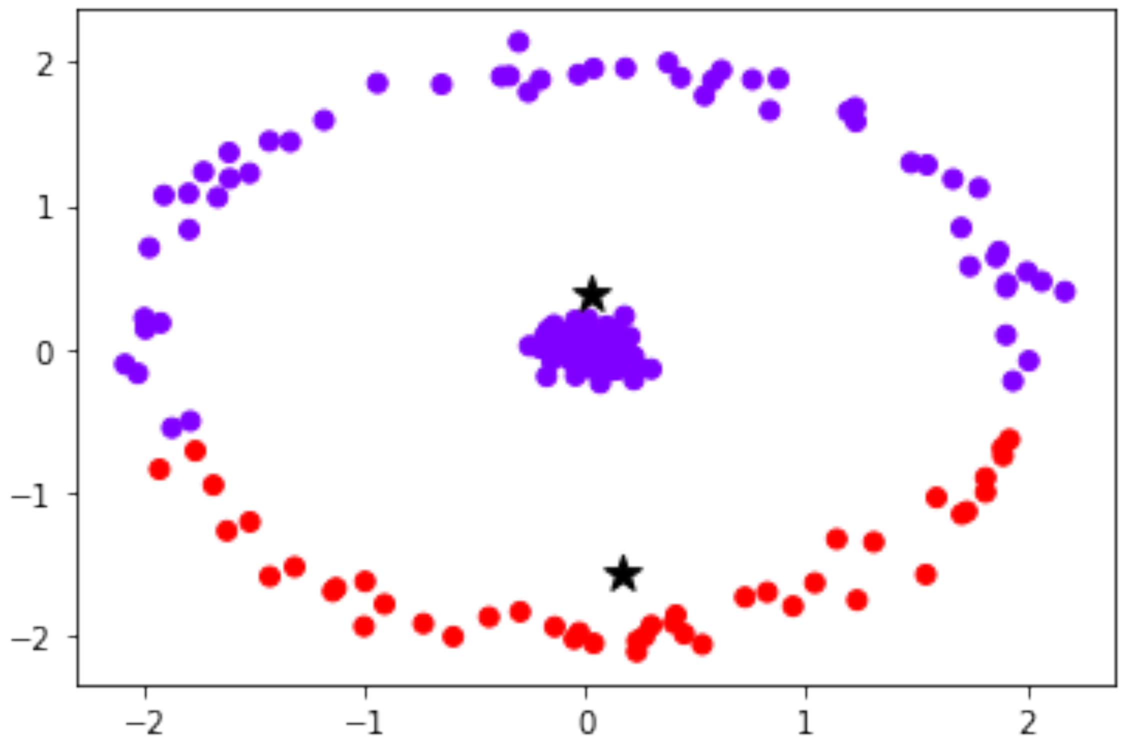

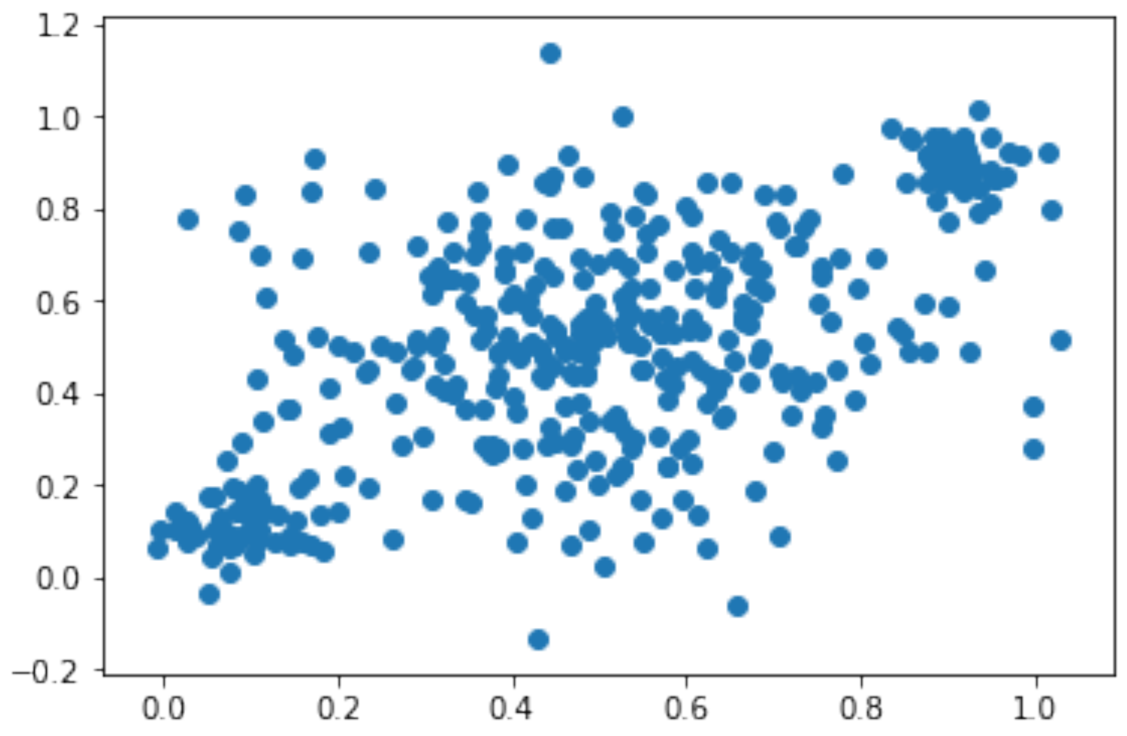

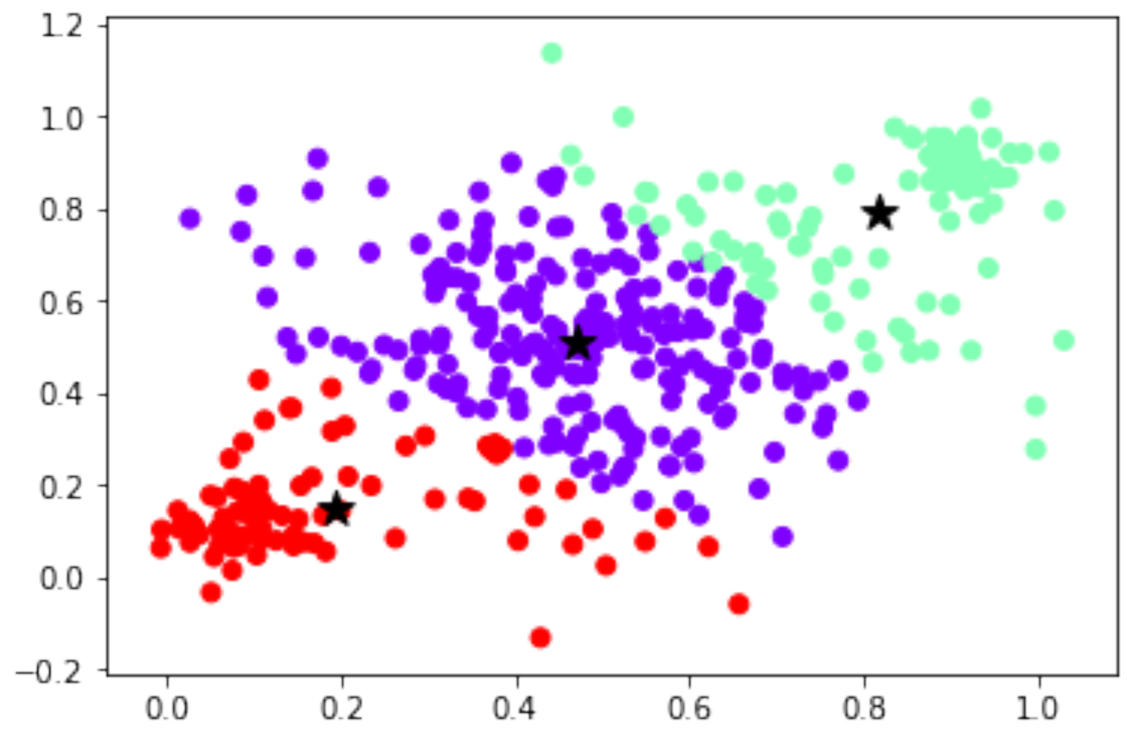

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- Worst-case time complexity?

Time Complexity

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O(k)

Note: number of epochs e is hard to estimate, can be big in worst case

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- **Struggles with categorical data**
- **Guaranteed convergence only to local (not global optimum)**
- **Need to specify *k* in advance**
- **“Curse of dimensionality”**
- **High worst-case time complexity**

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  Examples: k-medians, k-modes, k-medoids, hierarchical clusterings, kernel methods, dimensionality reduction…

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- **Performance can be improved by non-naive implementations**

  Example: using k-d trees to select initial centroids

Thank you!

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rocanaan@gmail.com
@rocanaan

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