浙江大学爱丁堡大学联合学院

ZJU-UoE Institute

Clustering and Machine Learning

ADS2, Lecture 2.13

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Semester 2, 2023/24

Pre-lecture version

This lecture contains questions that I will ask you to think about before class. Providing the answers beforehand would defeat that purpose.

Therefore, the version of the slides available to you before the lecture will not contain all of the information that is presented in the lecture.

A complete version will be uploaded to Blackboard Learn after the lecture. In the meantime, here is a famous Scottish painting called ‘The Skating Minister’.

This lecture is about...

- How to teach a computer to cluster data ("unsupervised machine learning") **and**
- How to teach a computer to classify data ("supervised machine learning")

Learning objectives

After this lecture, you should be able to:

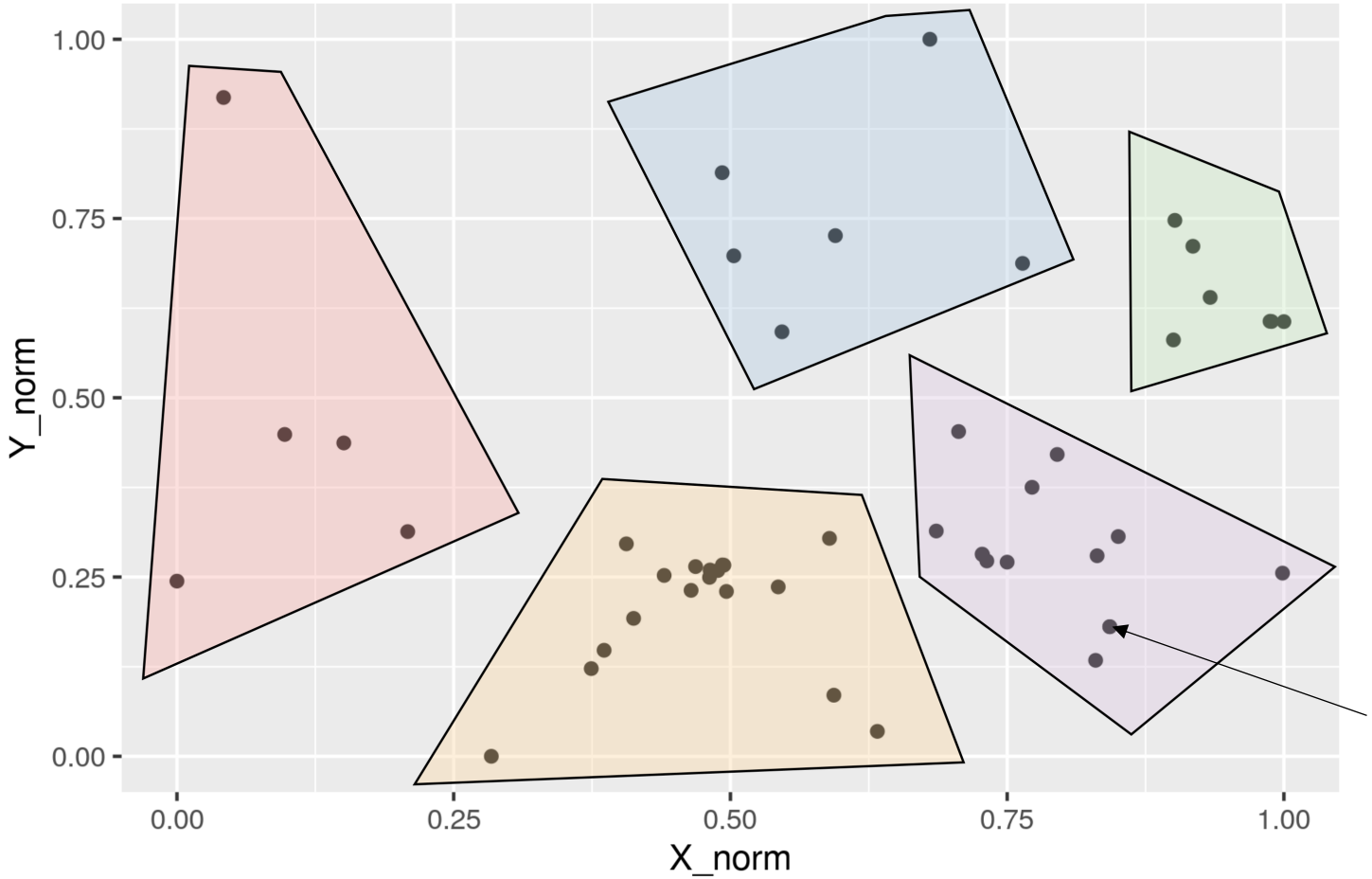
- Explain how clustering works (k-means, hierarchical clustering)
- Discuss the choices that need to be made when tackling a clustering problem
- Explain how supervised machine learning works (classification)
- How to simply evaluate a classification method

Outline

1. **What is clustering?**
2. k-means clustering
3. Hierarchical clustering
4. Machine learning

What exactly did you do?

What exactly happens when we cluster data? How would you explain it to a computer?



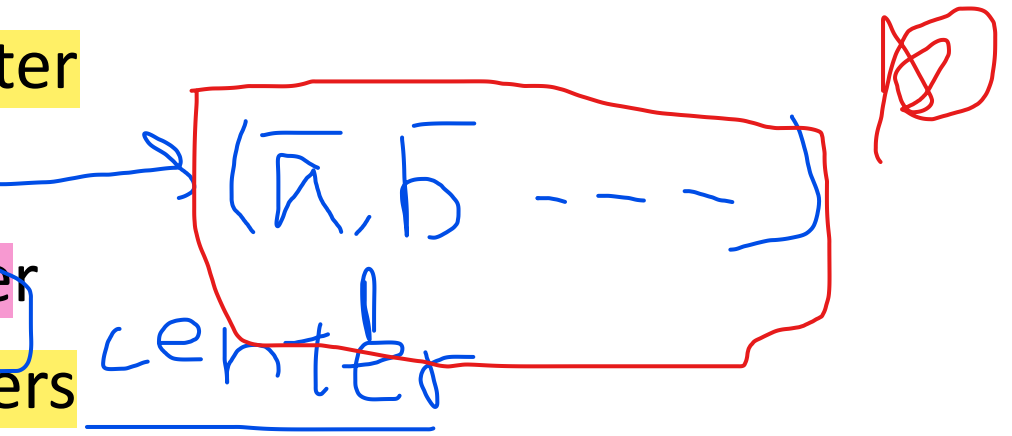
Outline

1. **What is clustering?**
2. **k-means clustering**
3. Hierarchical clustering
4. Machine learning

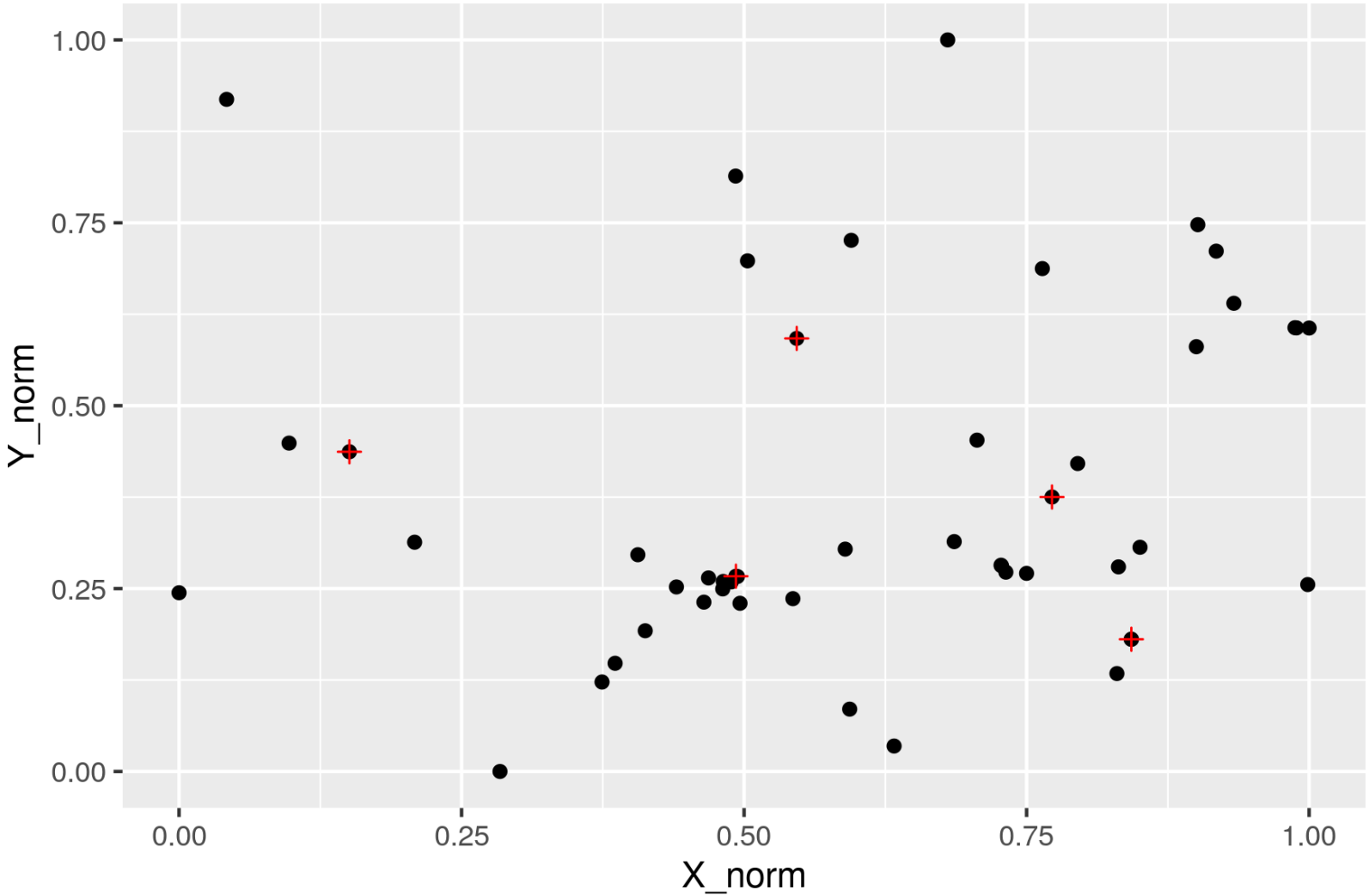
k-means clustering

This idea behind this is that you:

- Decide beforehand on the number of clusters you want (*k*)
- Select *k* data points at random, and make them the *k* cluster centres
- Assign each data point to the nearest cluster
- Re-compute the centre of each cluster
- Re-assign data points to the nearest cluster
- Repeat until this converges to stable clusters



k-means clustering



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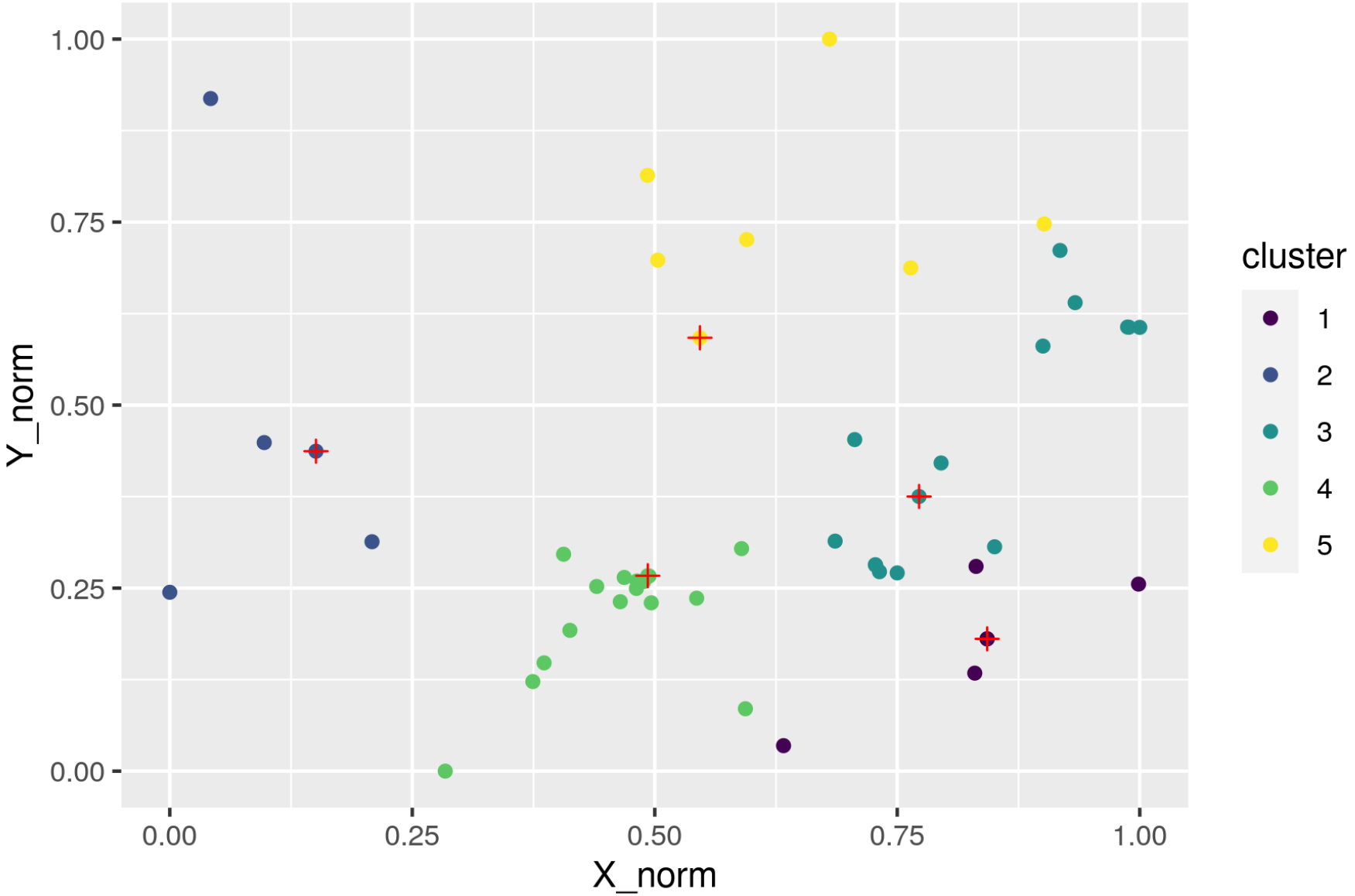

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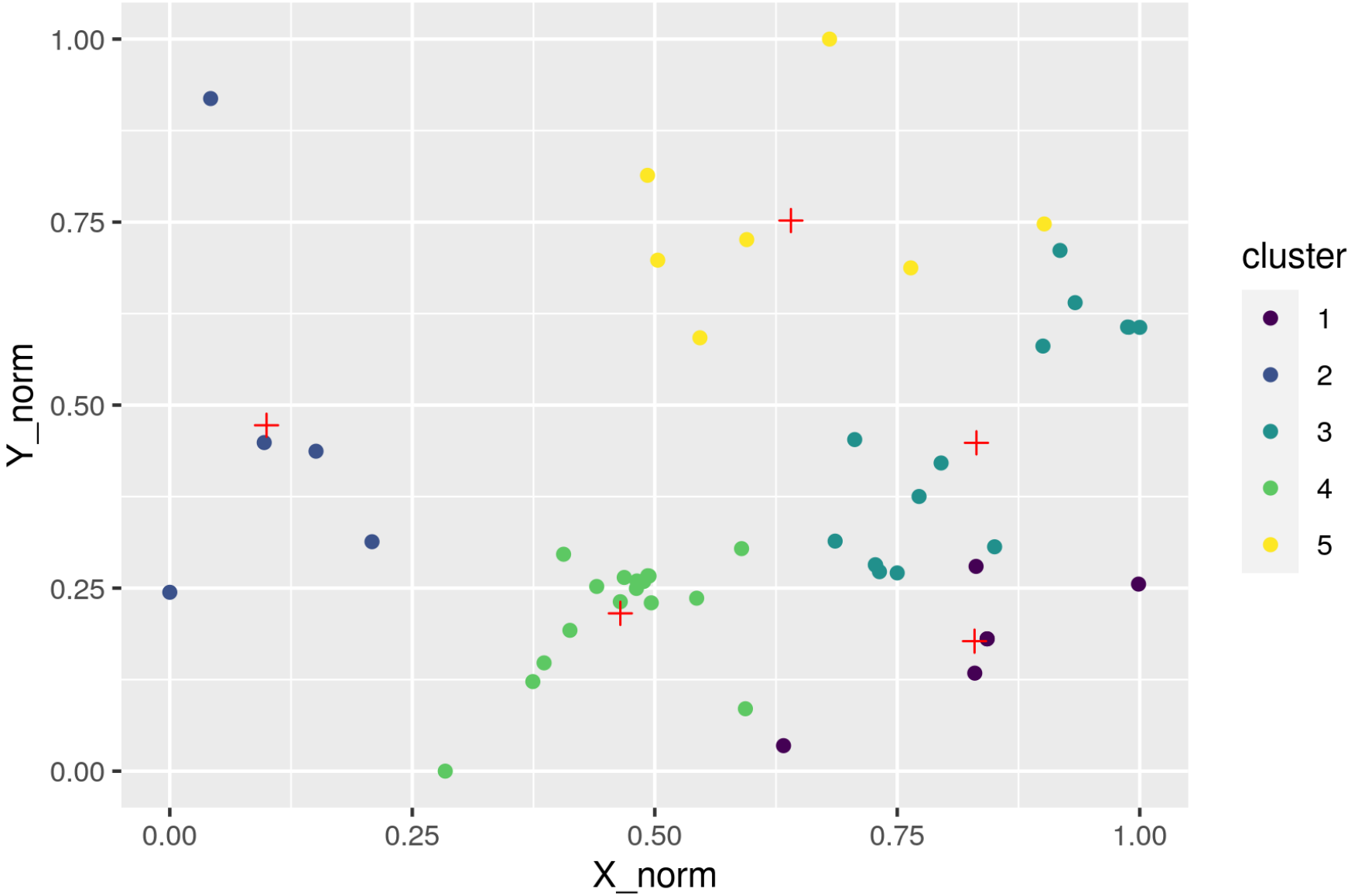

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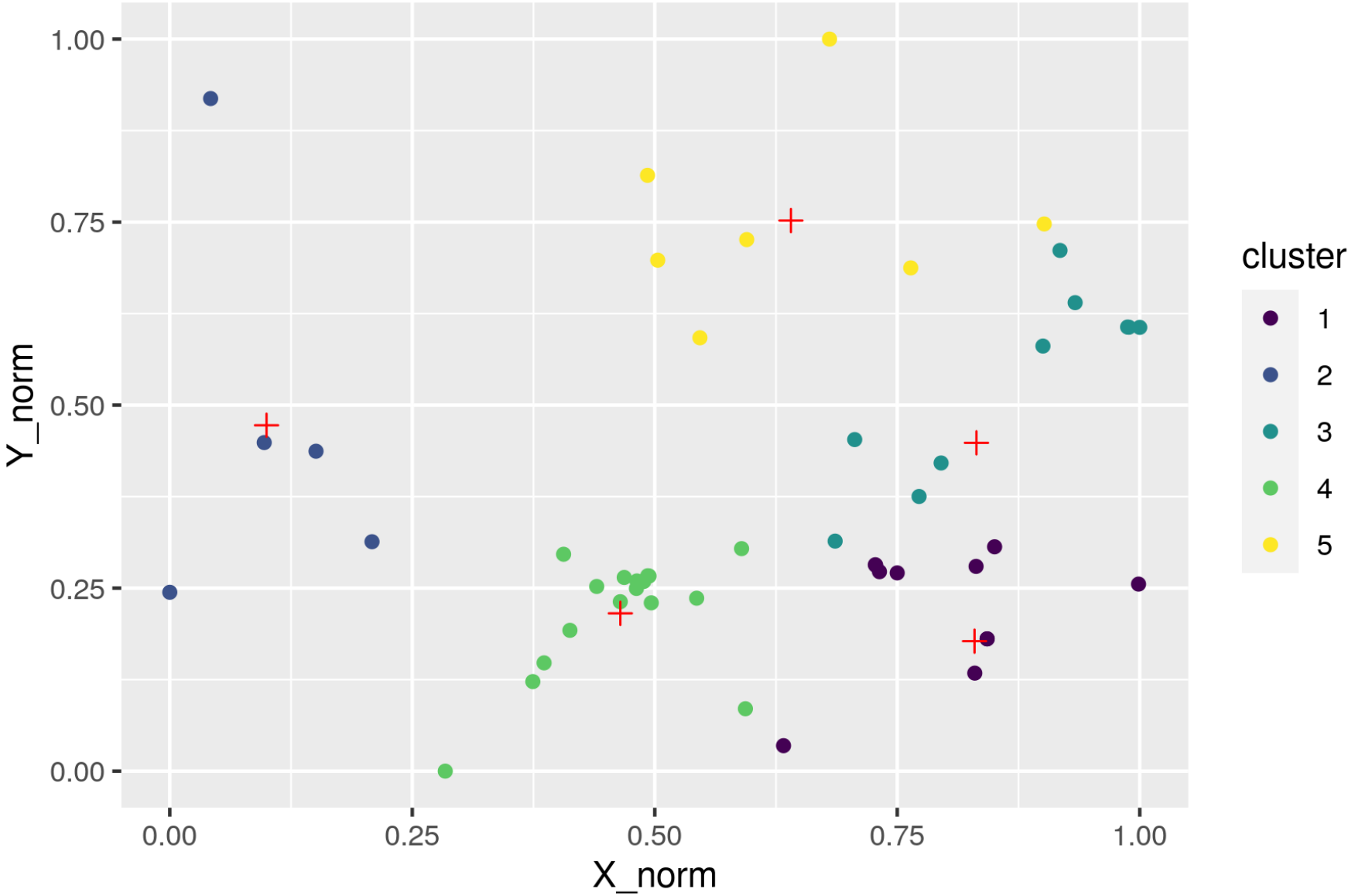

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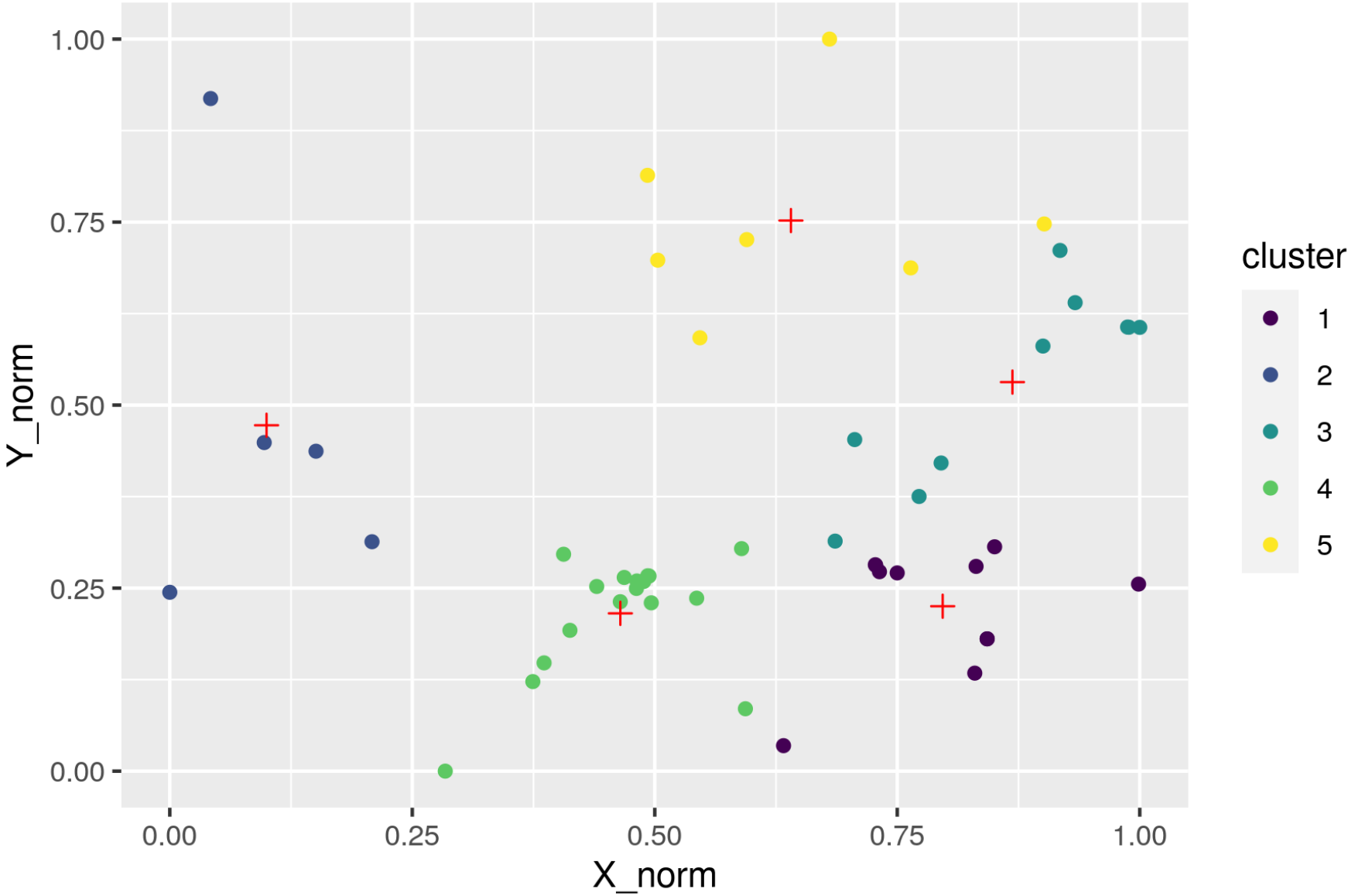

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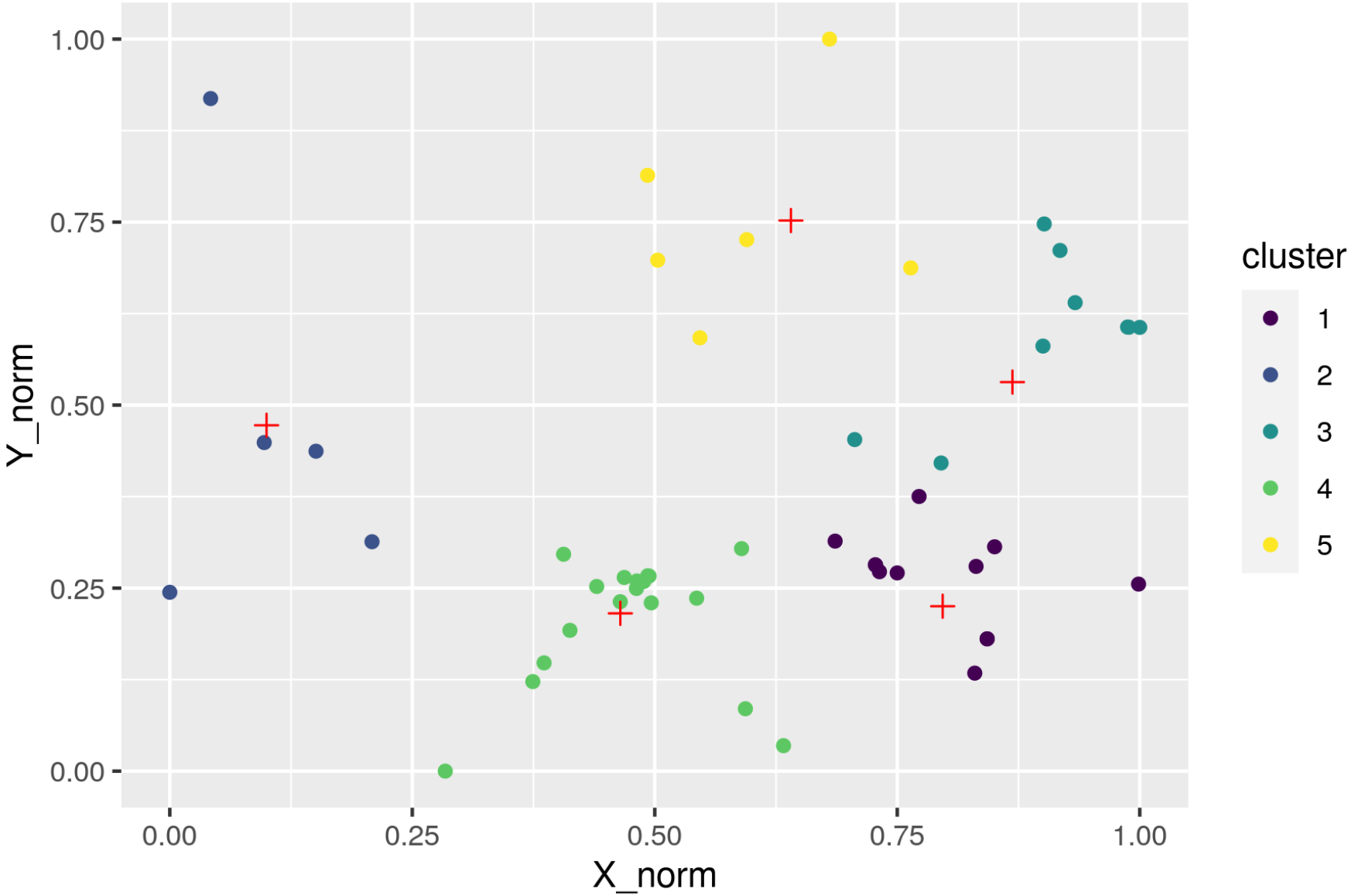

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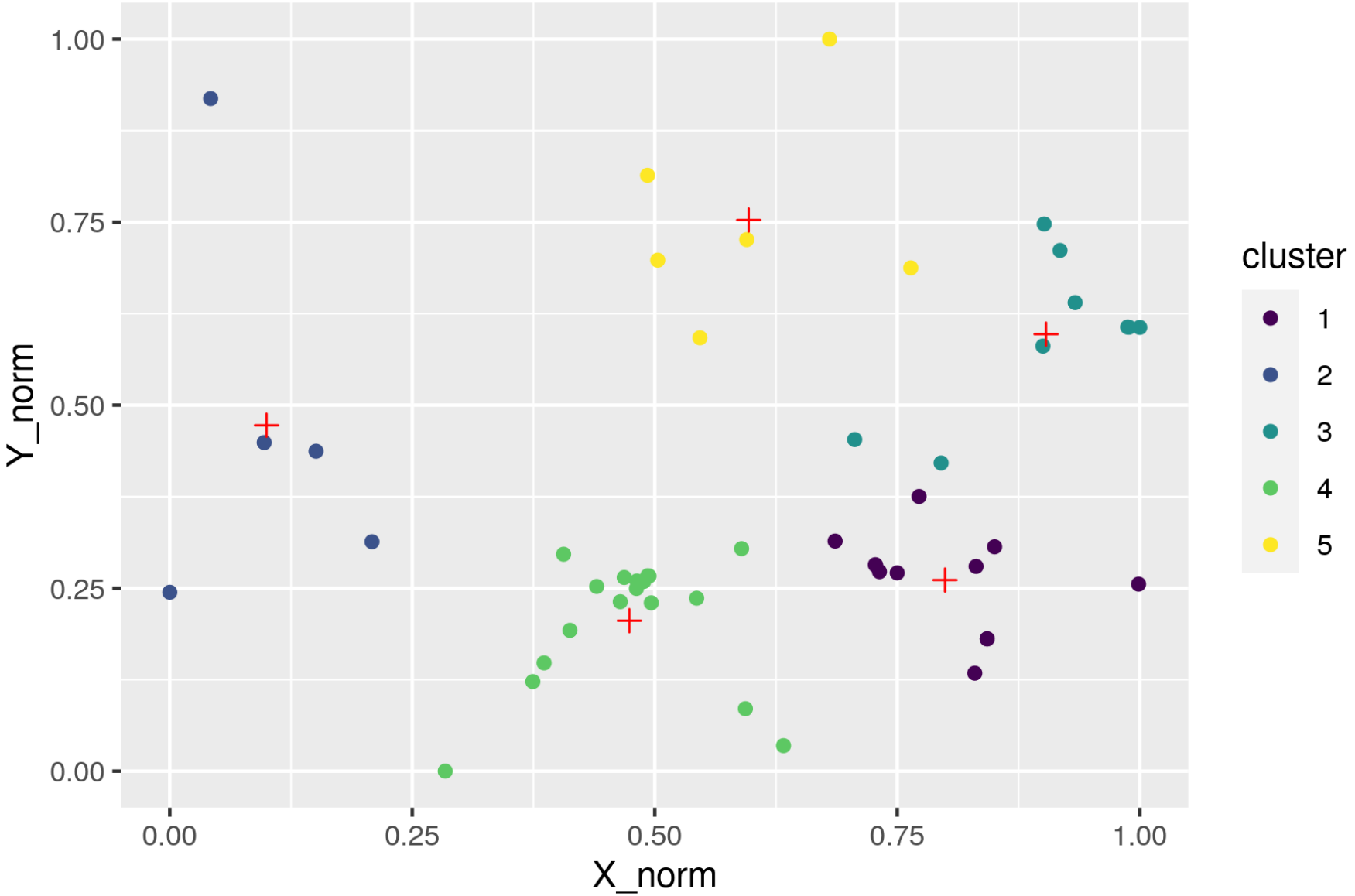

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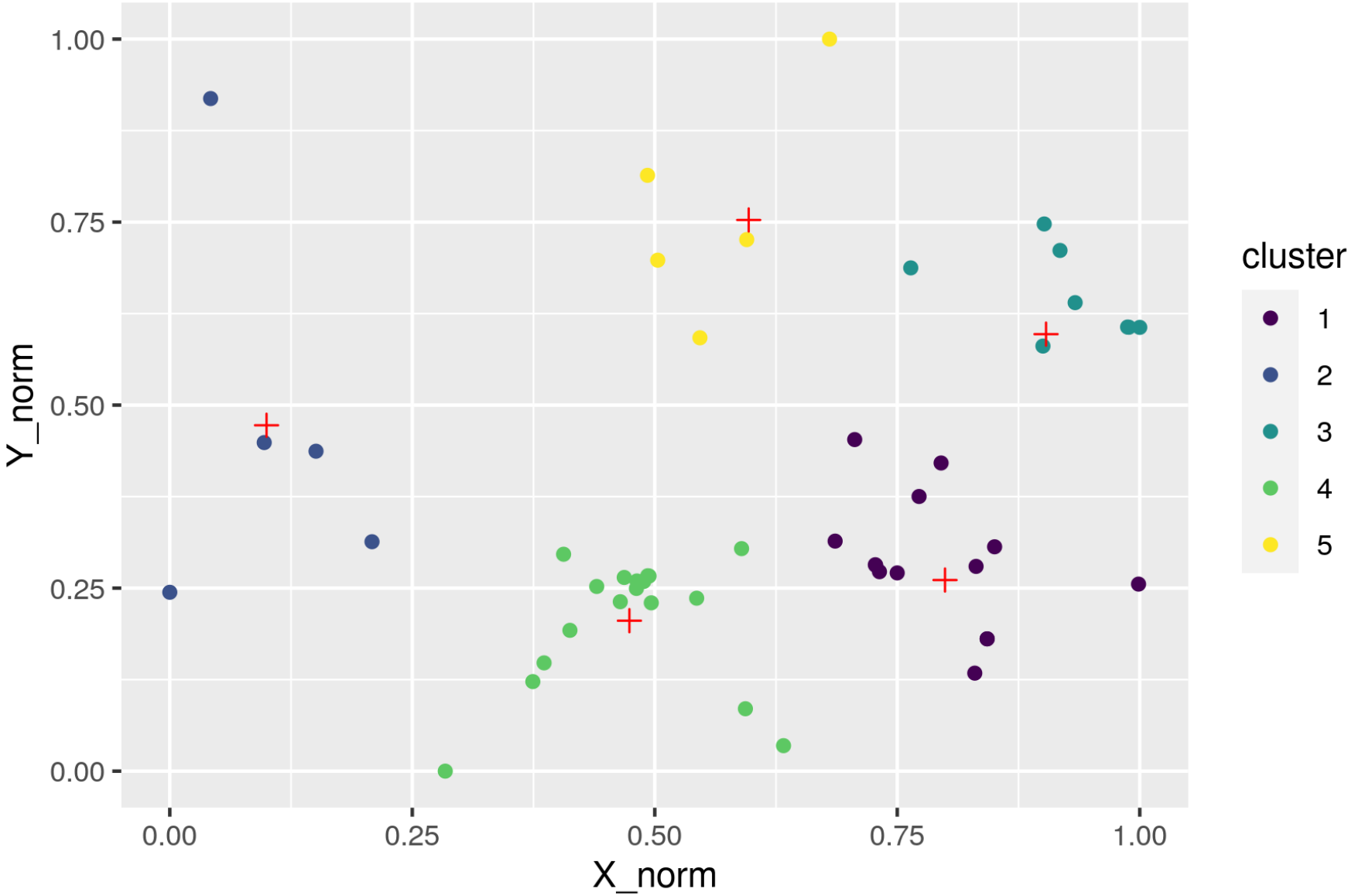

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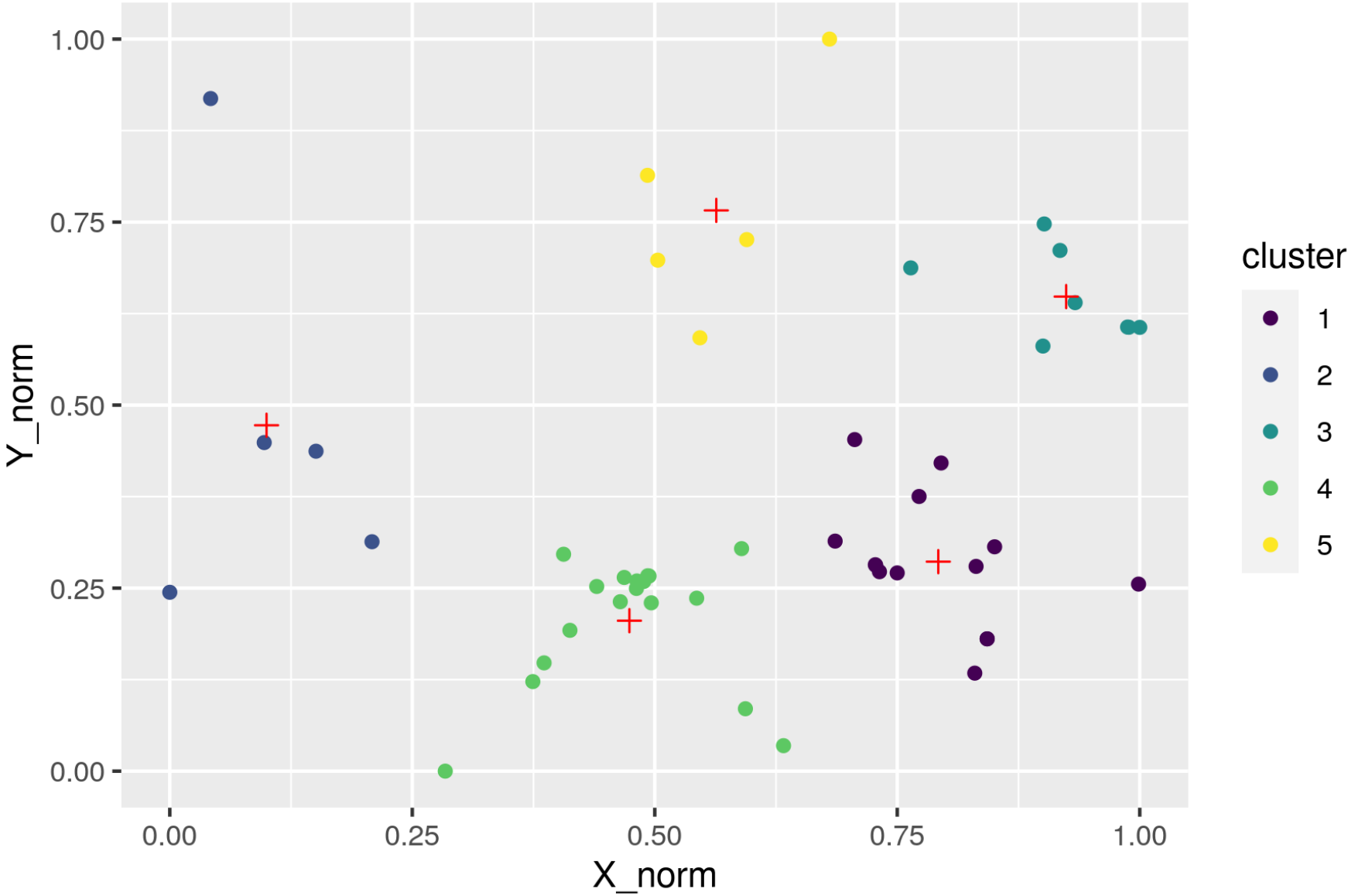

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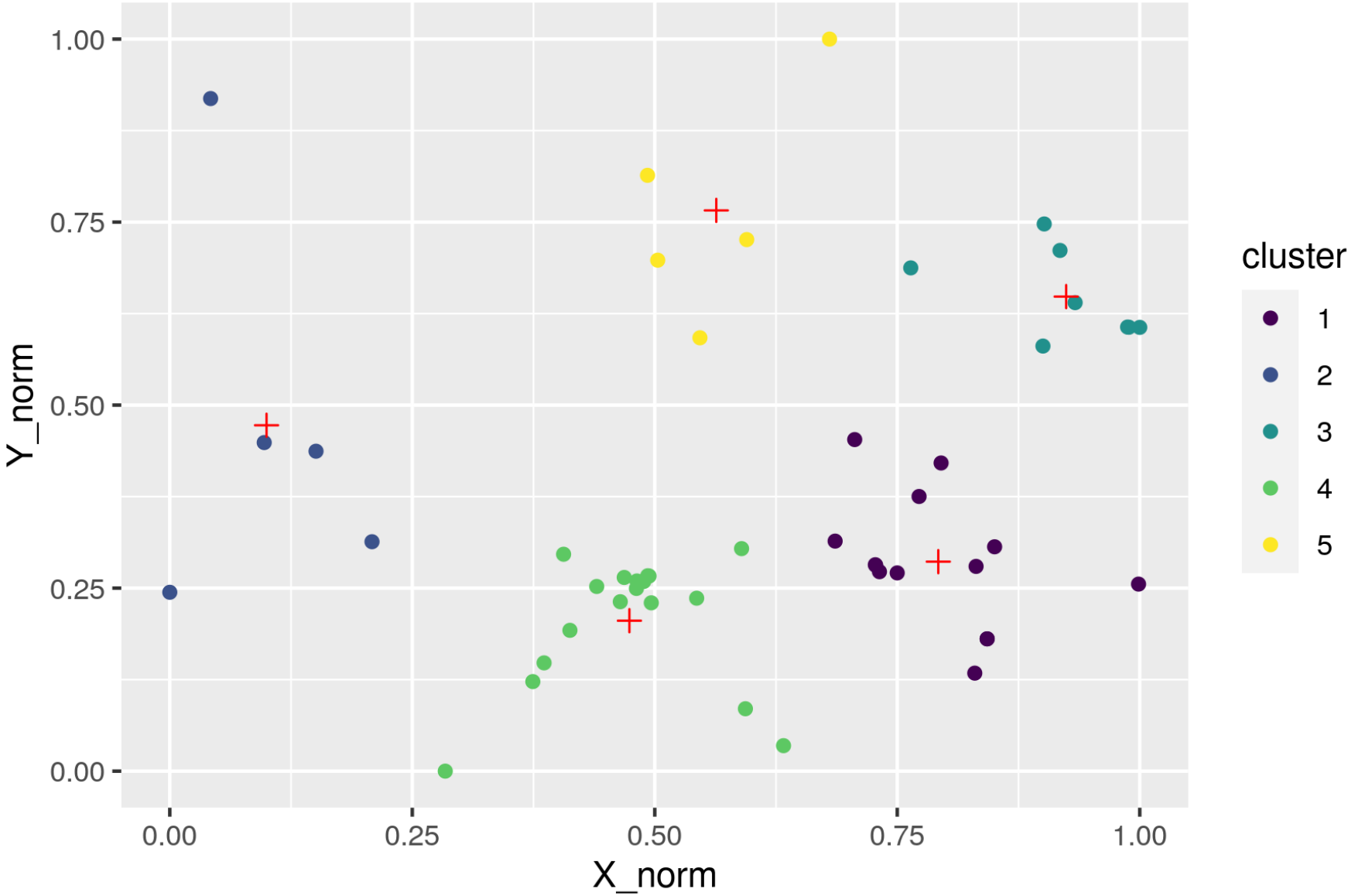

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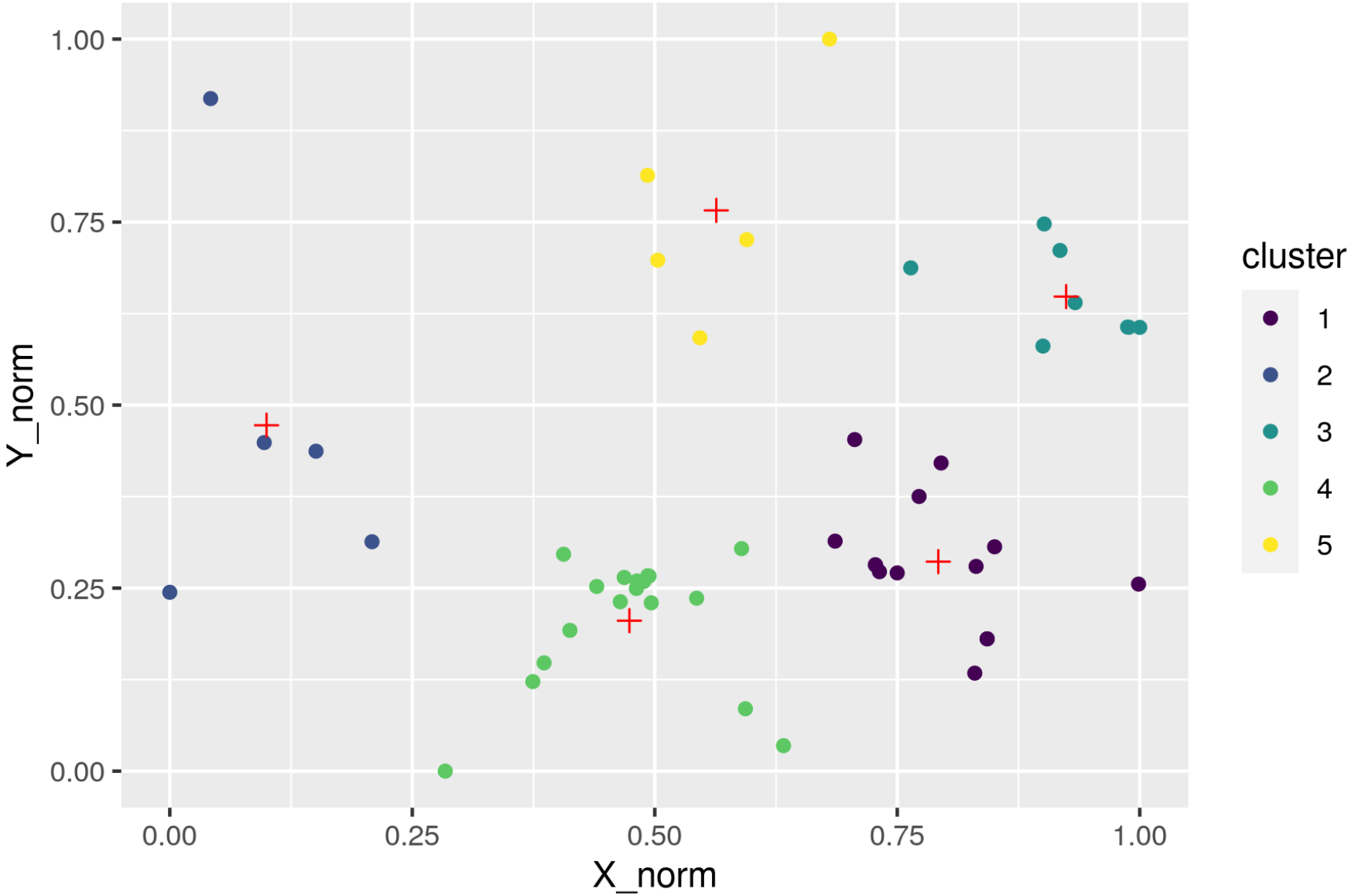
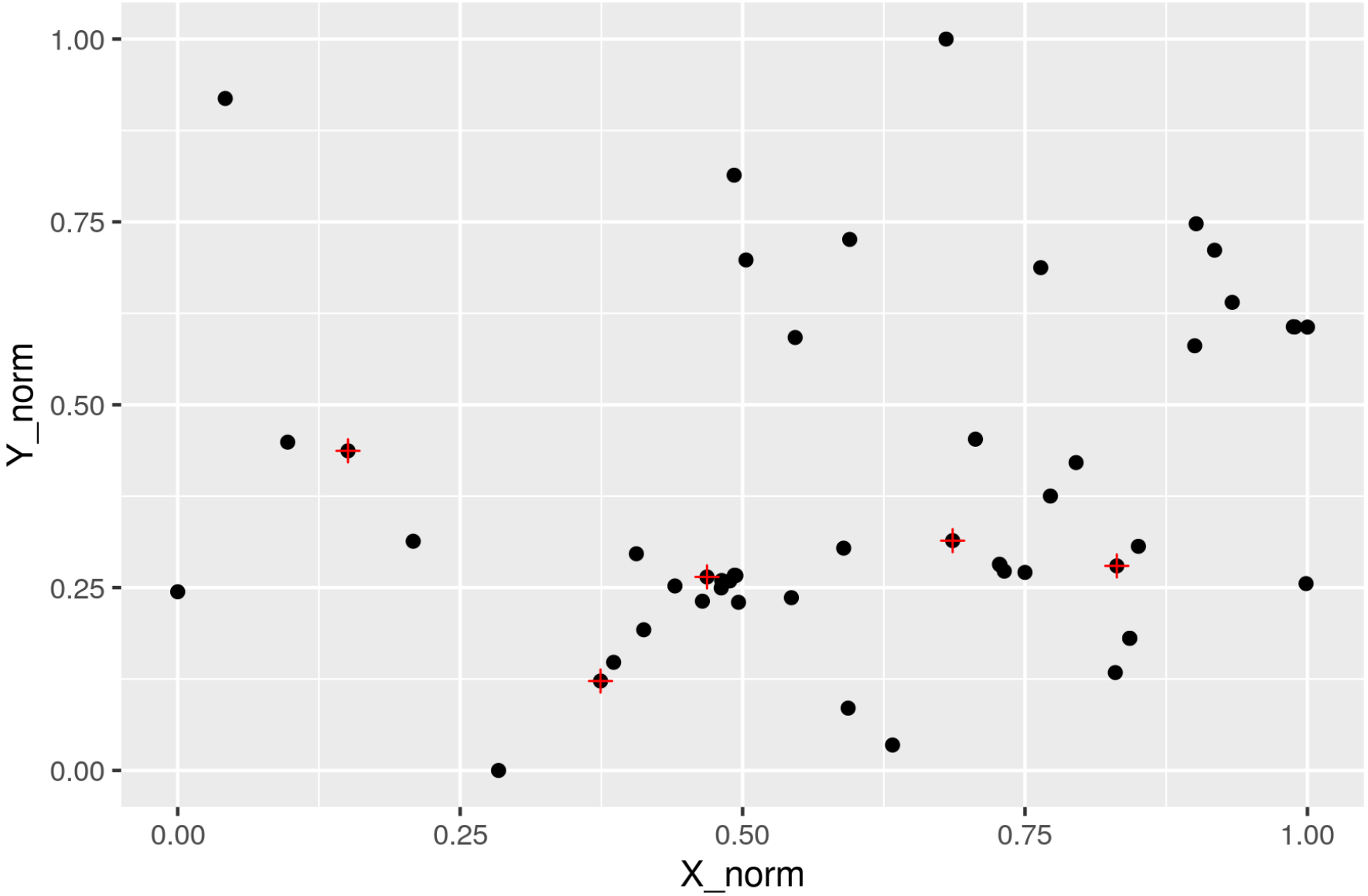


k-means clustering

What questions do you have? (Or what problems may there be?)

k-means clustering



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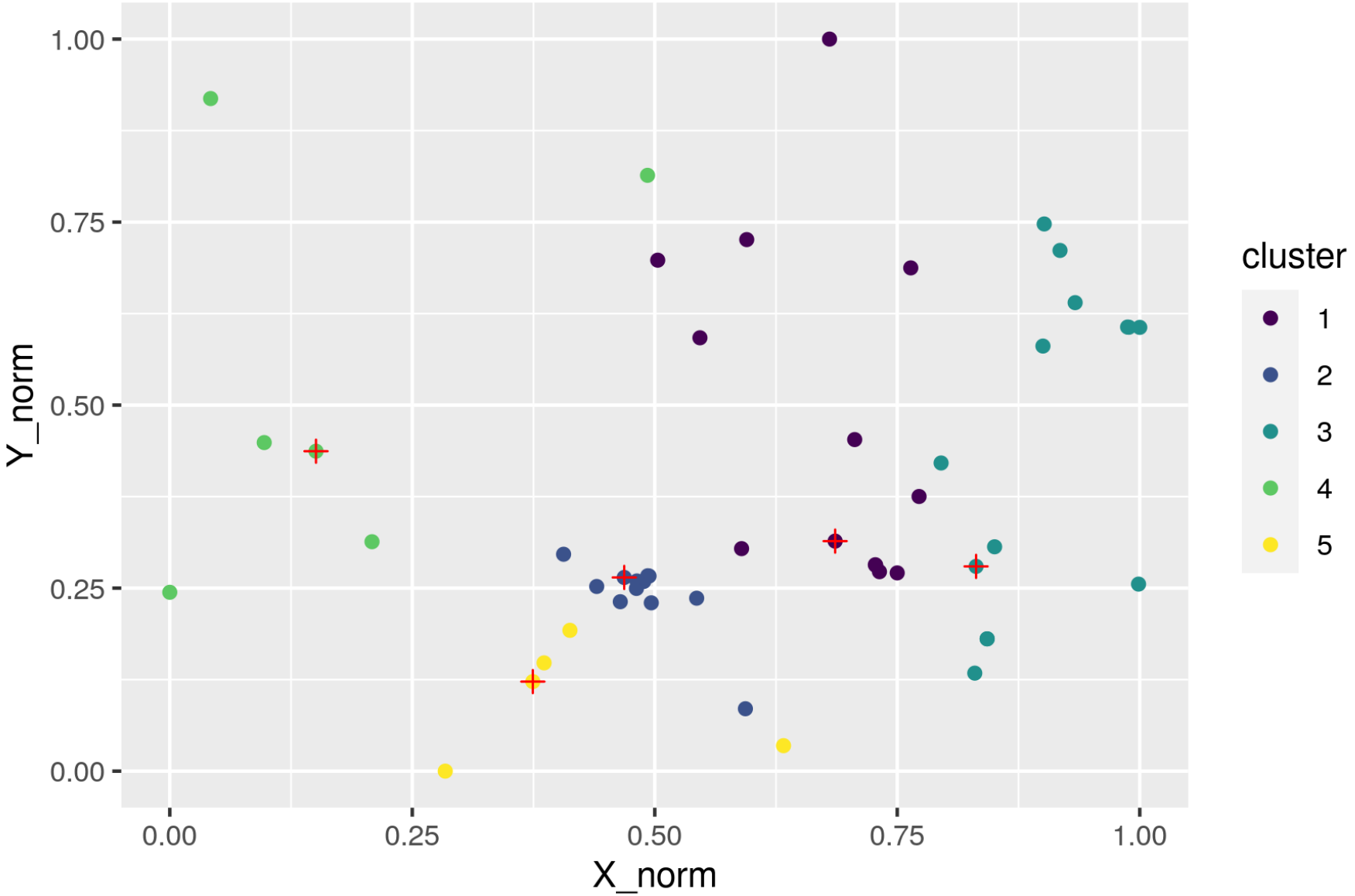

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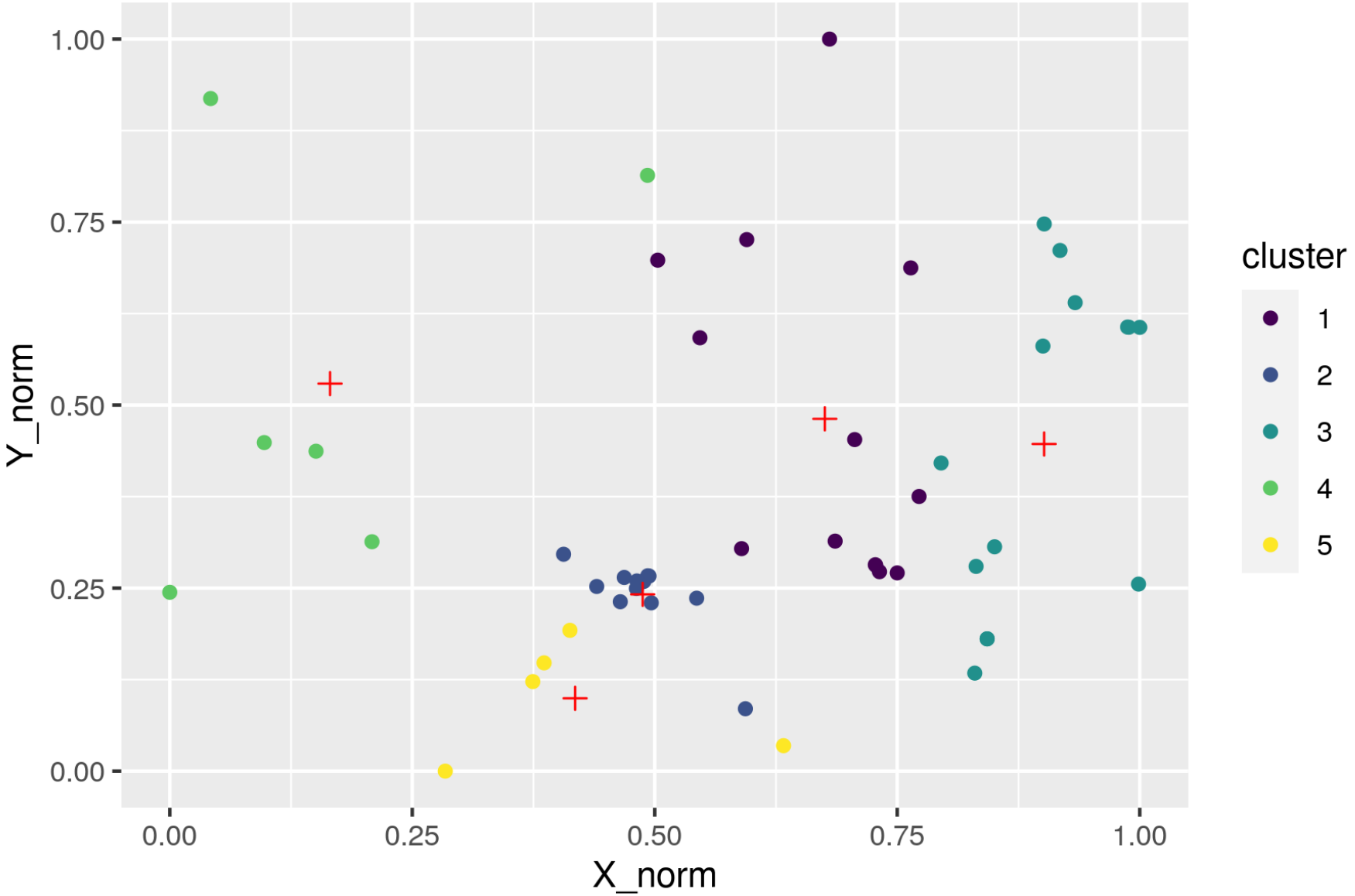

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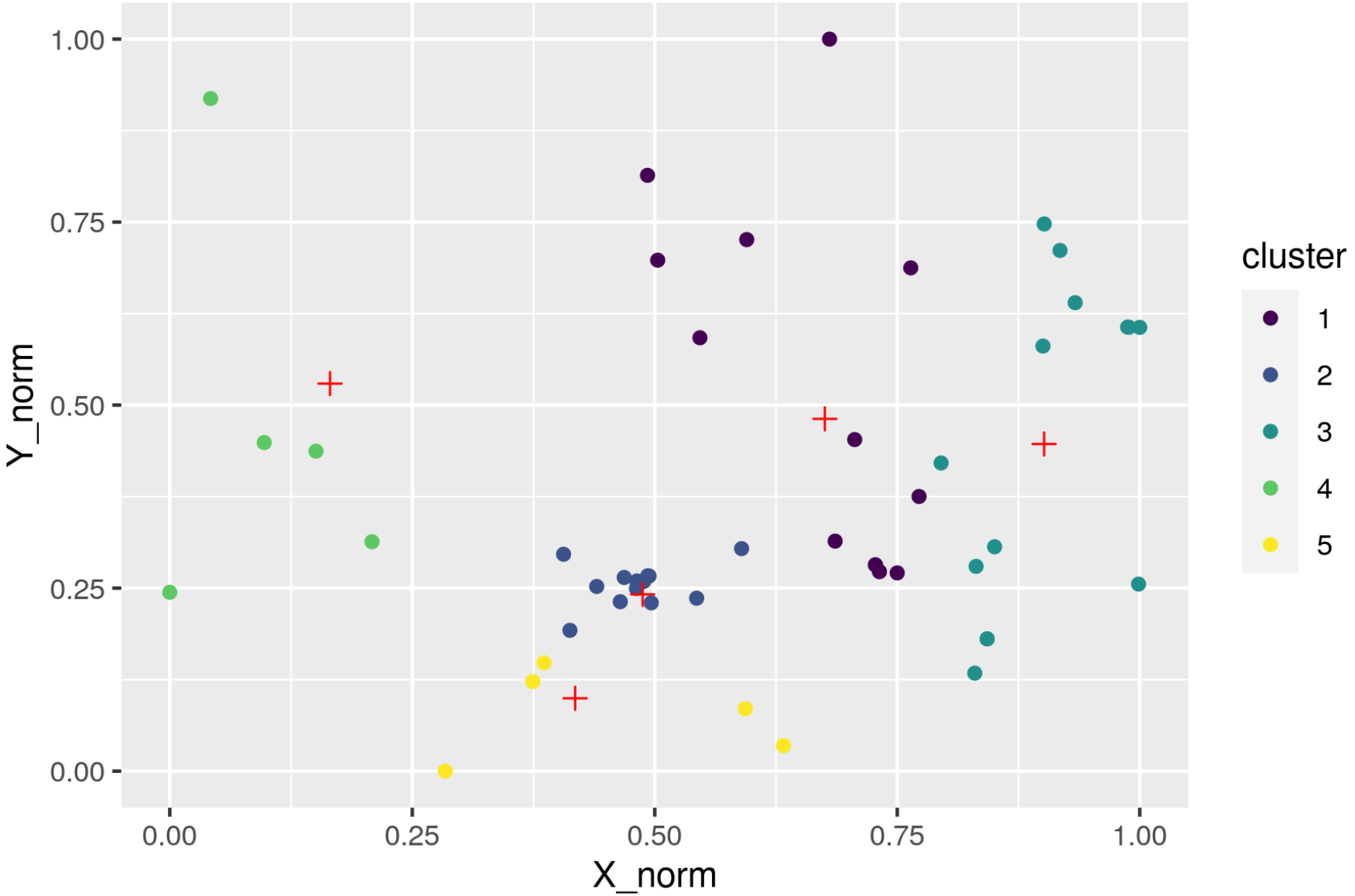

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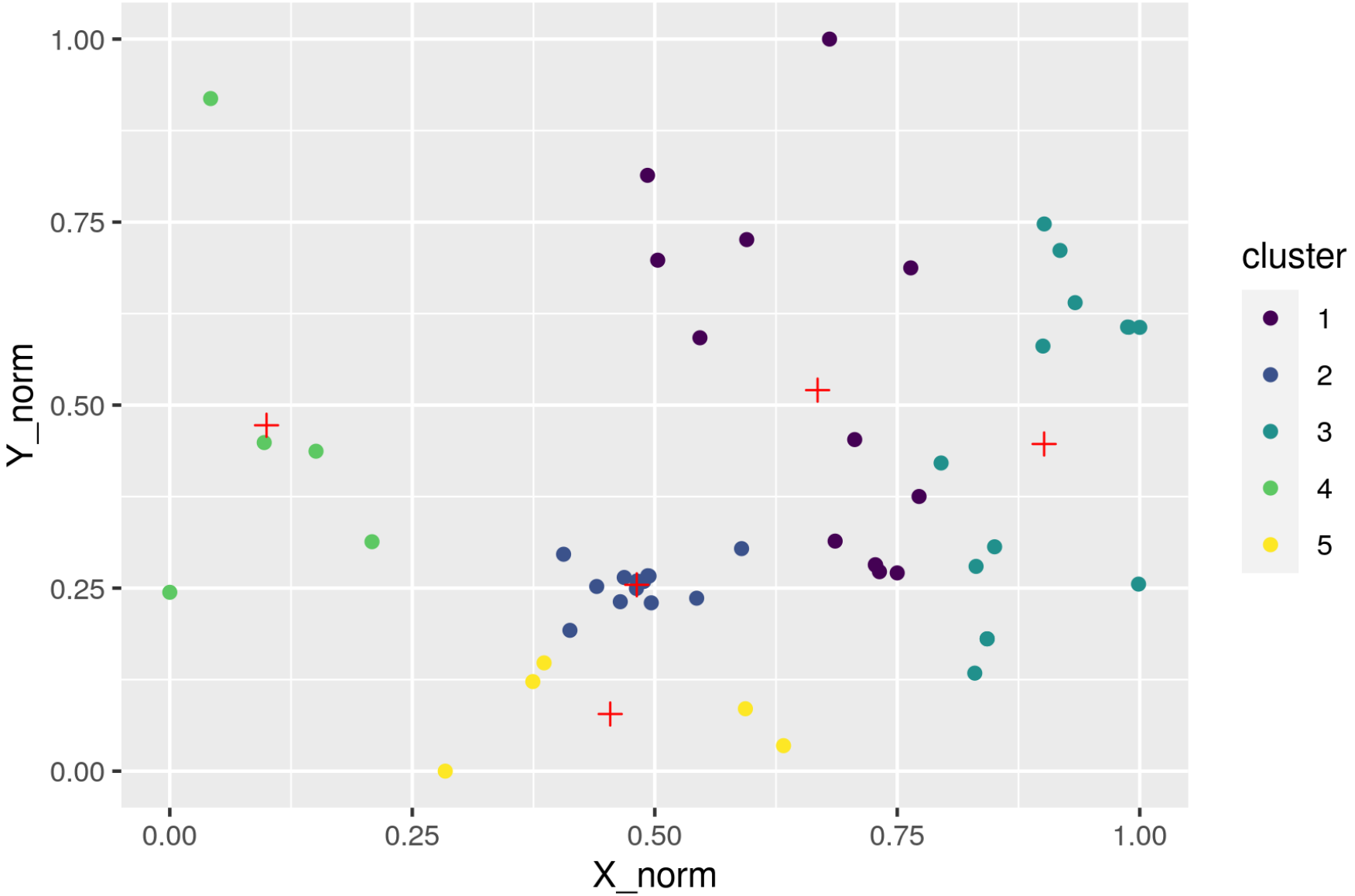

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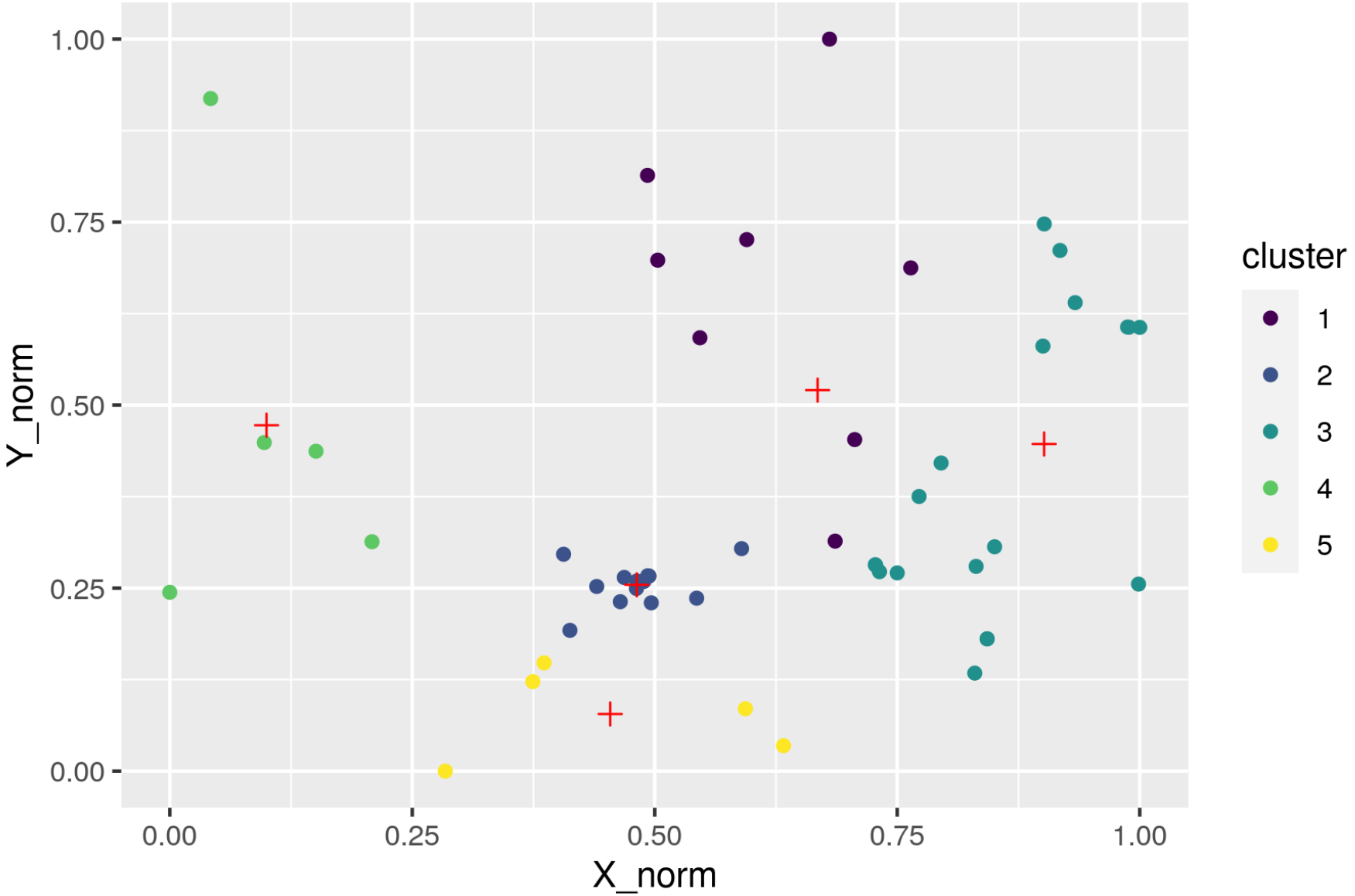

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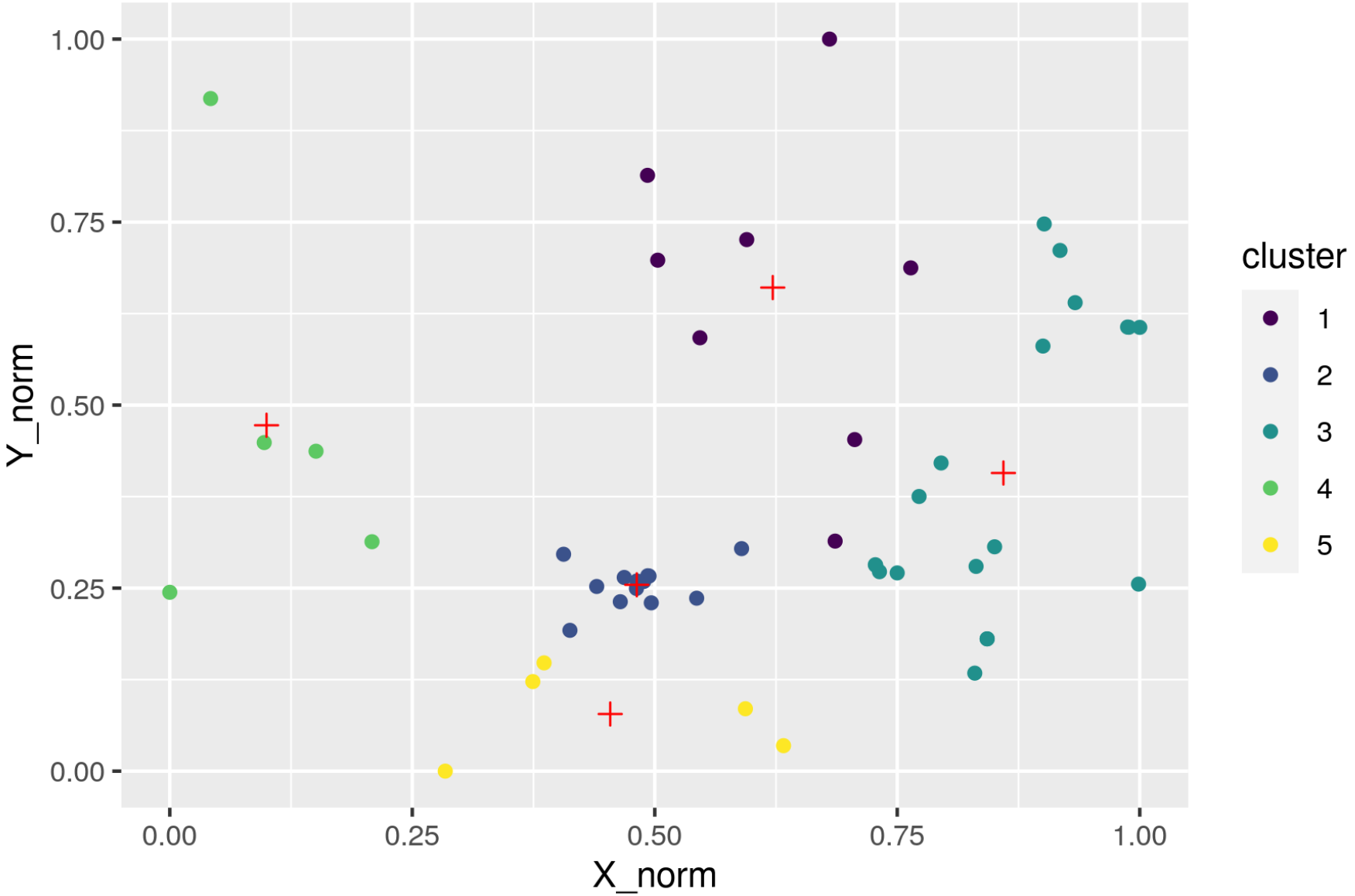

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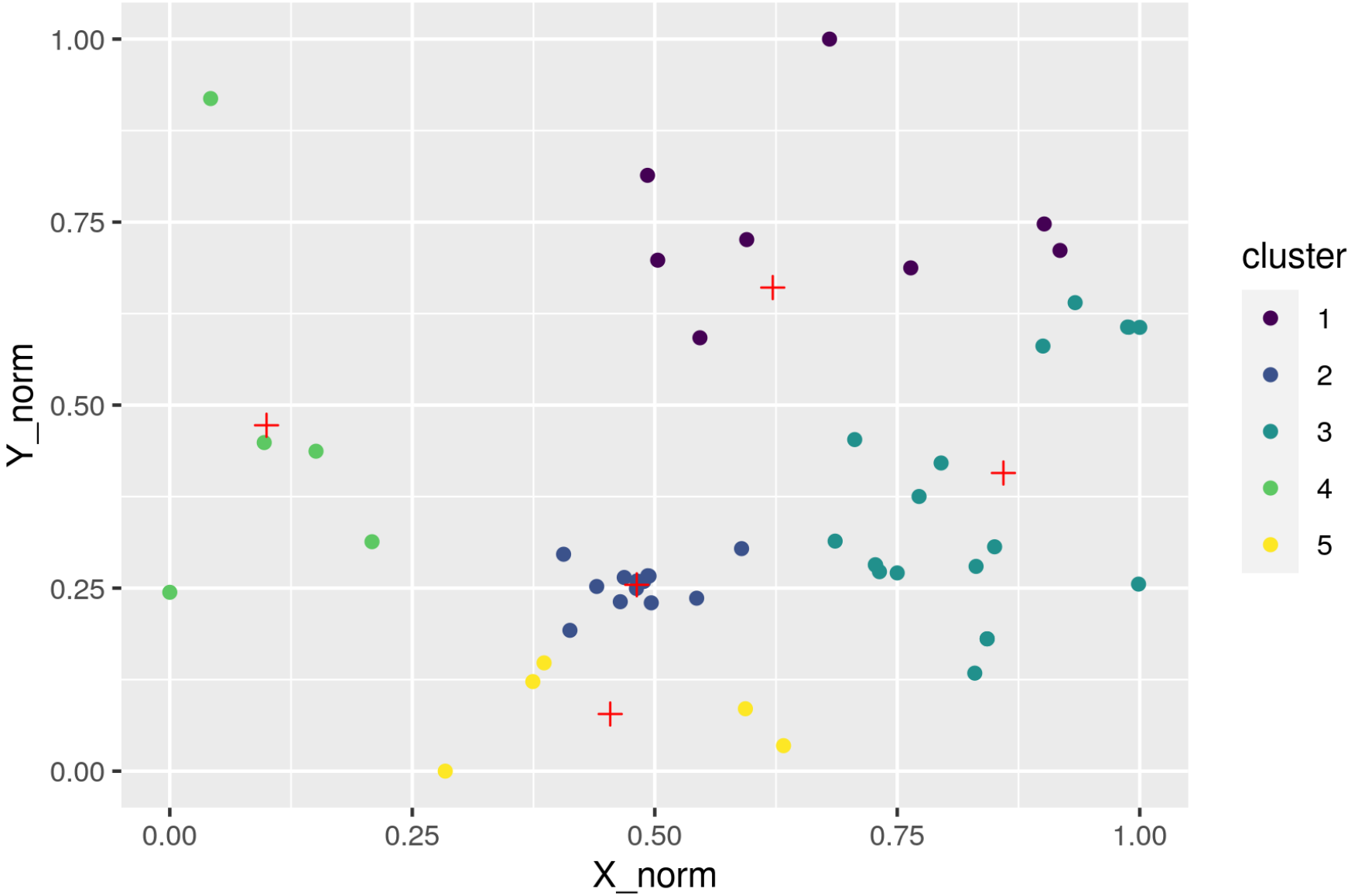

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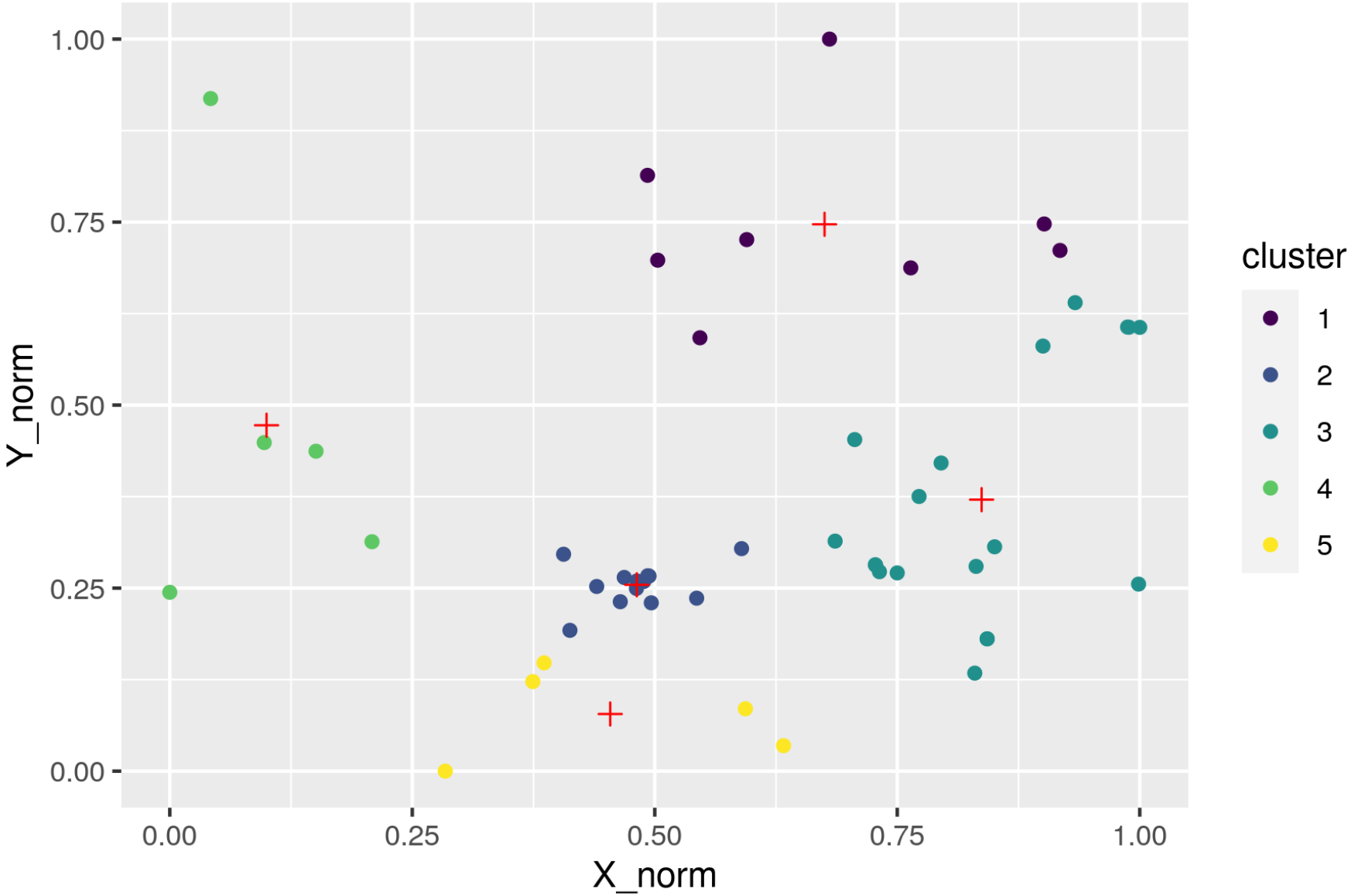

k-means clustering
Outcome depends on initial conditions

k-means clustering

- What do we mean by ‘centre’?
  Most often: *centroid* (mean coordinate along every axis)
  or *medoid* (‘median’ data point).
- Will this always converge?
  Ish. Most of the time it does, and quite quickly. You may need a way to break ties if a data point is equally far away from two centroids.
- Doesn’t it depend on what points are initially chosen?
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k-means clustering

Can we just minimise within-cluster variance to see what *k* is best?

k-means clustering

But what if I really, really don’t want to choose a *k*?

Outline

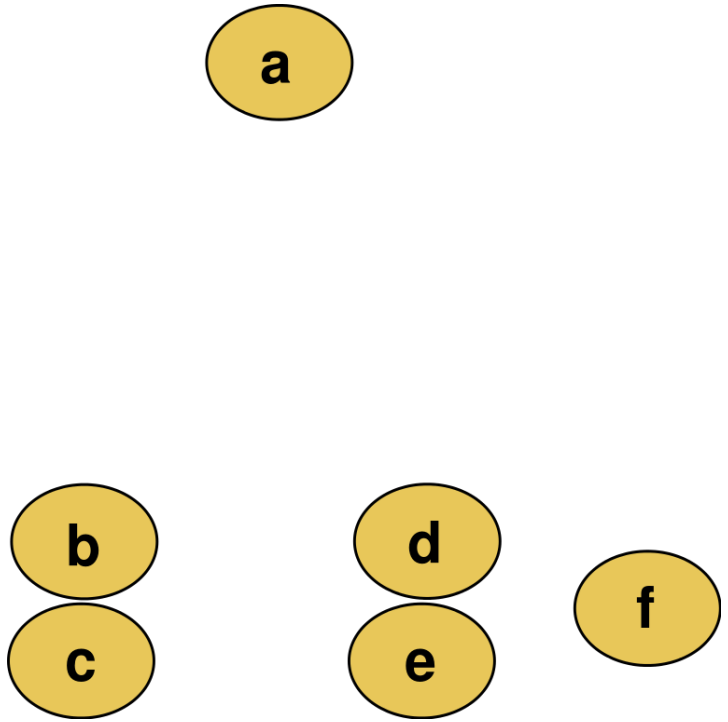
1. What is clustering?
2. k-means clustering
3. **Hierarchical clustering**
4. Machine learning

Hierarchical clustering

- Basic idea:

- No prior ideas about cluster sizes – we will just to *every* cluster size!
- Start by putting every individual data point in its own cluster
- **Group the two closest clusters** together in a common cluster
- Repeat until you have only one big cluster

Hierarchical clustering



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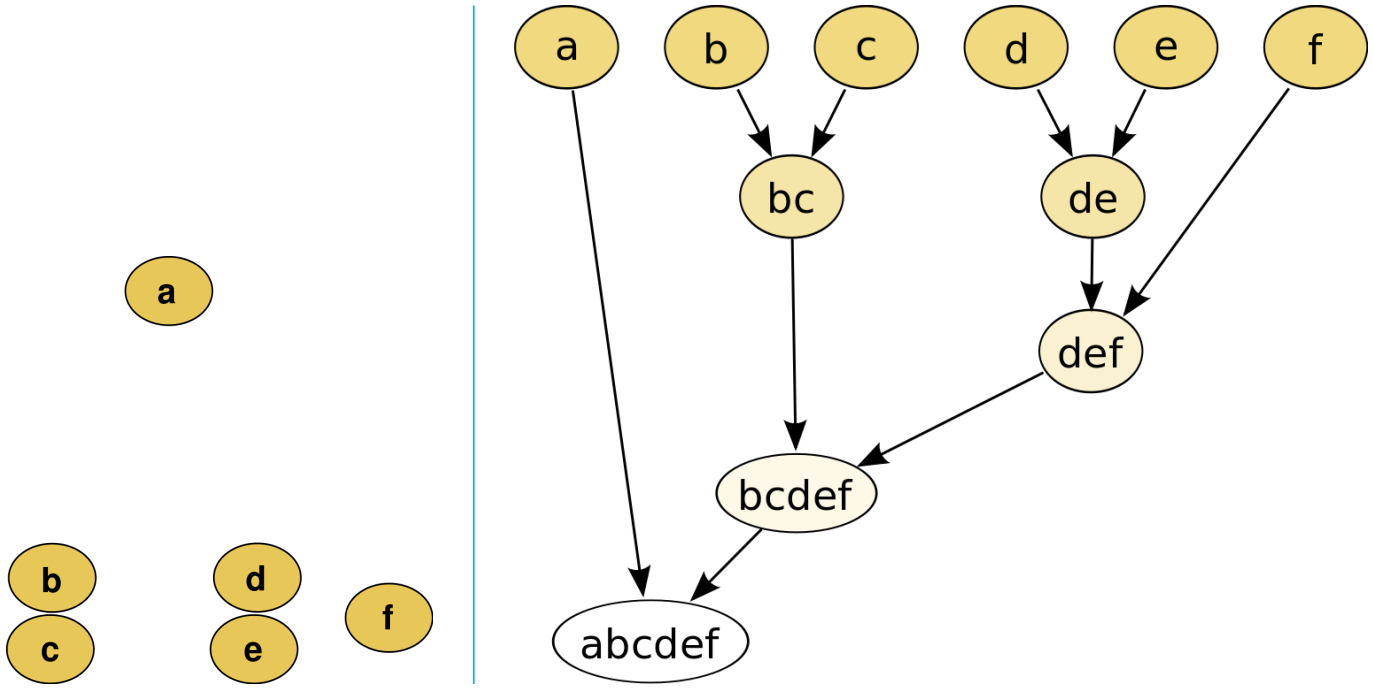


Hierarchical clustering

What questions do you have?

Hierarchical clustering

- How do we define ‘closest together’?

Hierarchical clustering

- How do we define ‘closest together’?

- Several methods exist:
  - Shortest distance between points of two clusters (single-linkage clustering)
  - Longest distance between points of two clusters (complete-linkage clustering)
  - Mean distance between points of two clusters (average linkage cluster)
  - …

Hierarchical clustering

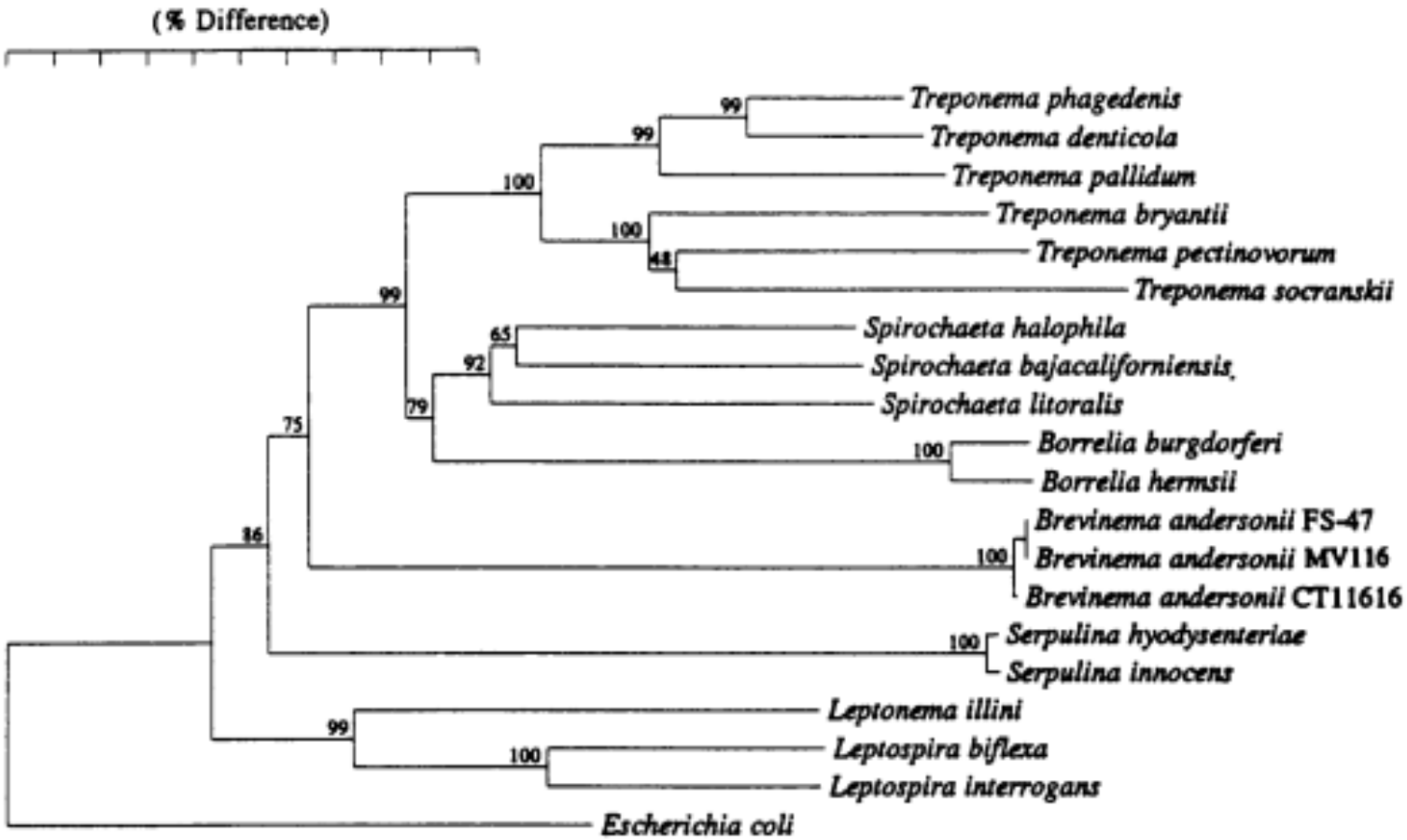
- Does the outcome depend on initial choices, like for k-means?
  No (apart from the distance measure chosen)

Hierarchical clustering

- Does the outcome depend on initial choices of points, like for k-means?
  No (apart from the distance measure chosen)

- Why are we doing this?
  It produces a phylogeny that is useful to choose possible cluster numbers, cluster sizes, etc. The phylogeny is also closely related to evolutionary analysis.

Hierarchical clustering



Hierarchical vs k-means clustering

Which one would you pick?

Outline

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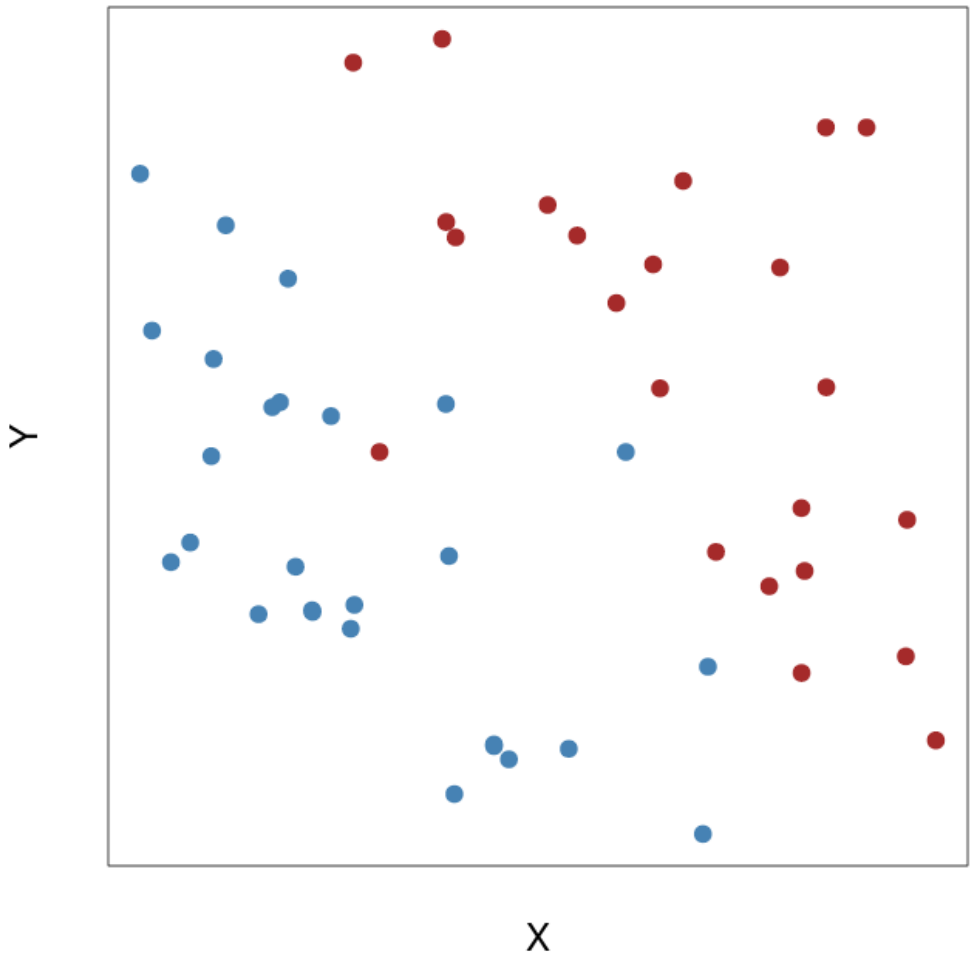
- A third kind of machine learning – ‘reinforcement learning’
  - Also need some interactive *supervisor*
  - i.e. we get some feedback from the environment to adjust our actions
  - e.g. robot control in catching things, self-driving cars

Two types of supervised learning

- Classification
  - The data are with discrete labels
  - e.g. 50 hospitals labelled with grades (‘Edinburgh’, ‘Glasgow’, …), pictures labelled as dog or cat

- Regression
  - The data are with continuous labels
  - e.g. 50 hospitals labelled with some score range from 0 to 100, patients’ blood pressure in some mmHg, patients’ temperature in some degrees Celsius

Example: classification



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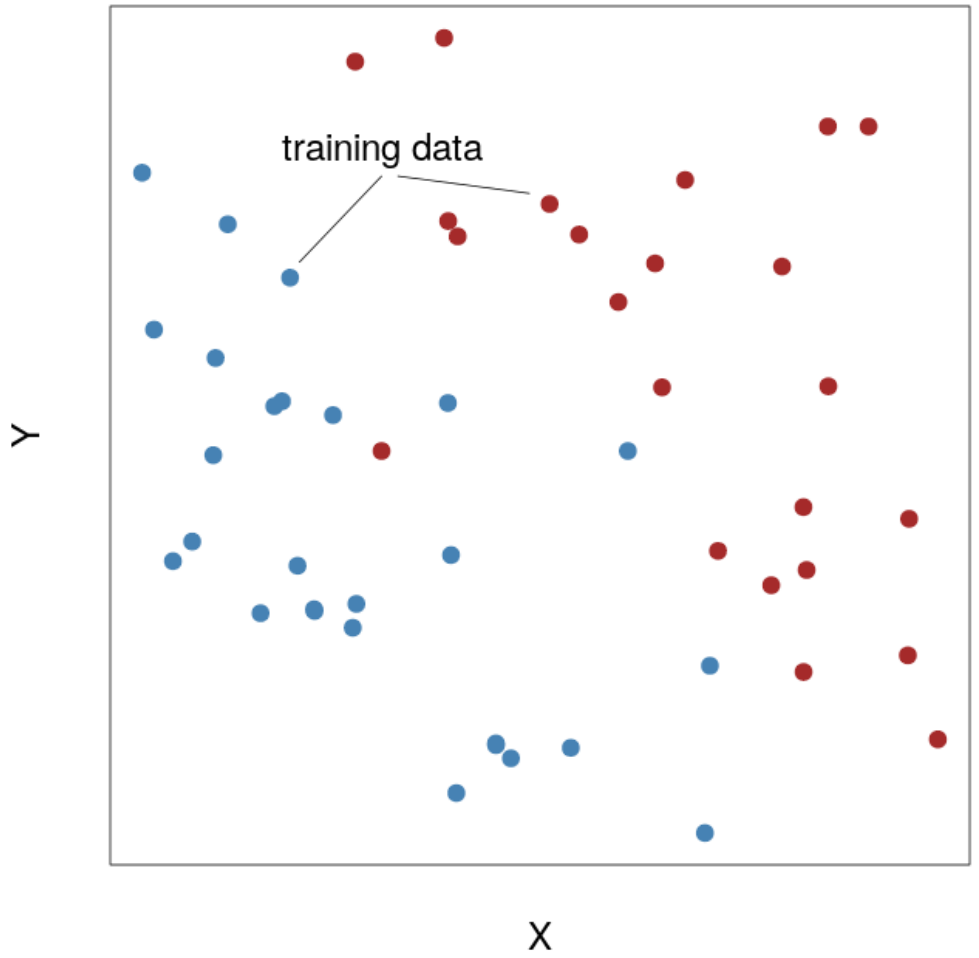

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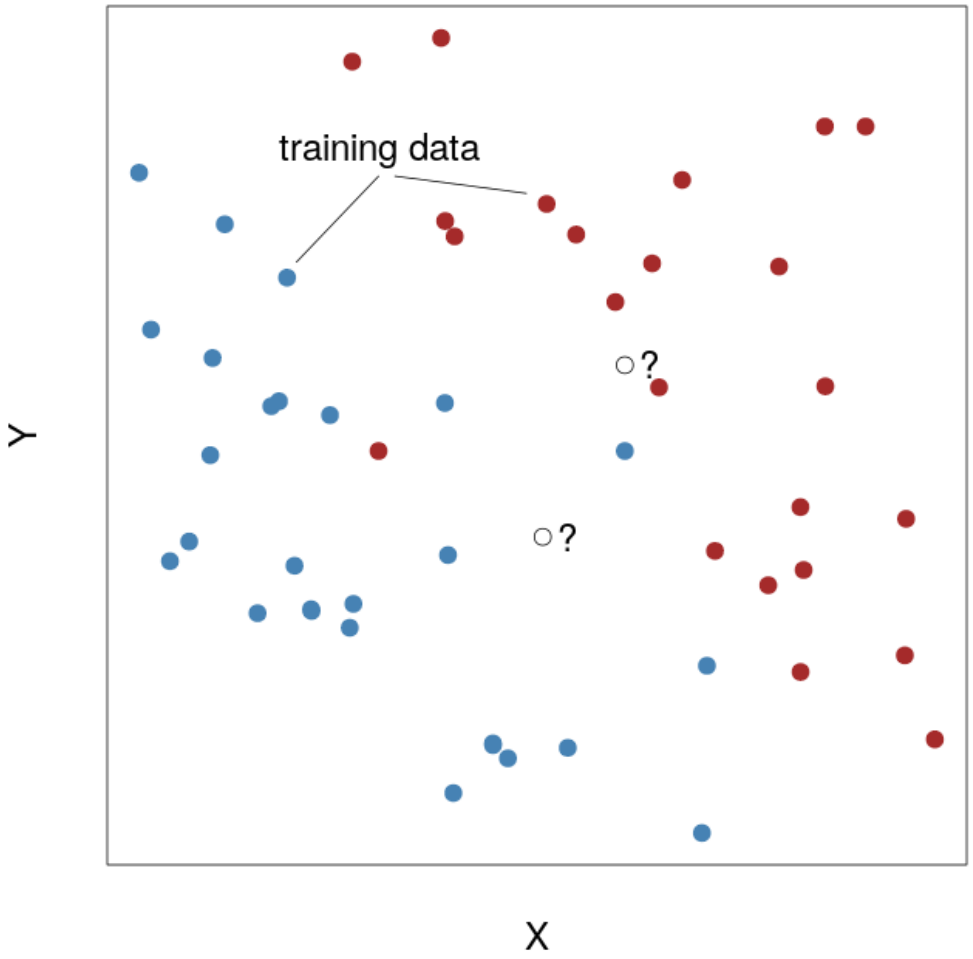

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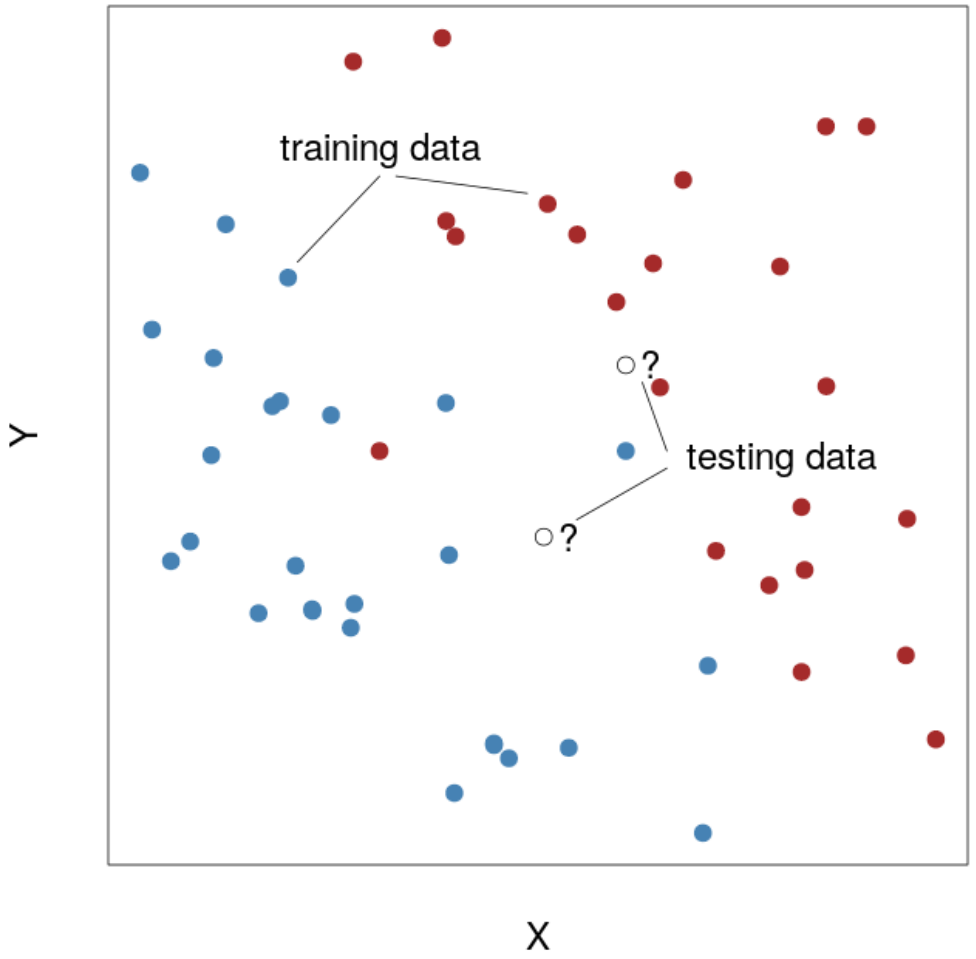

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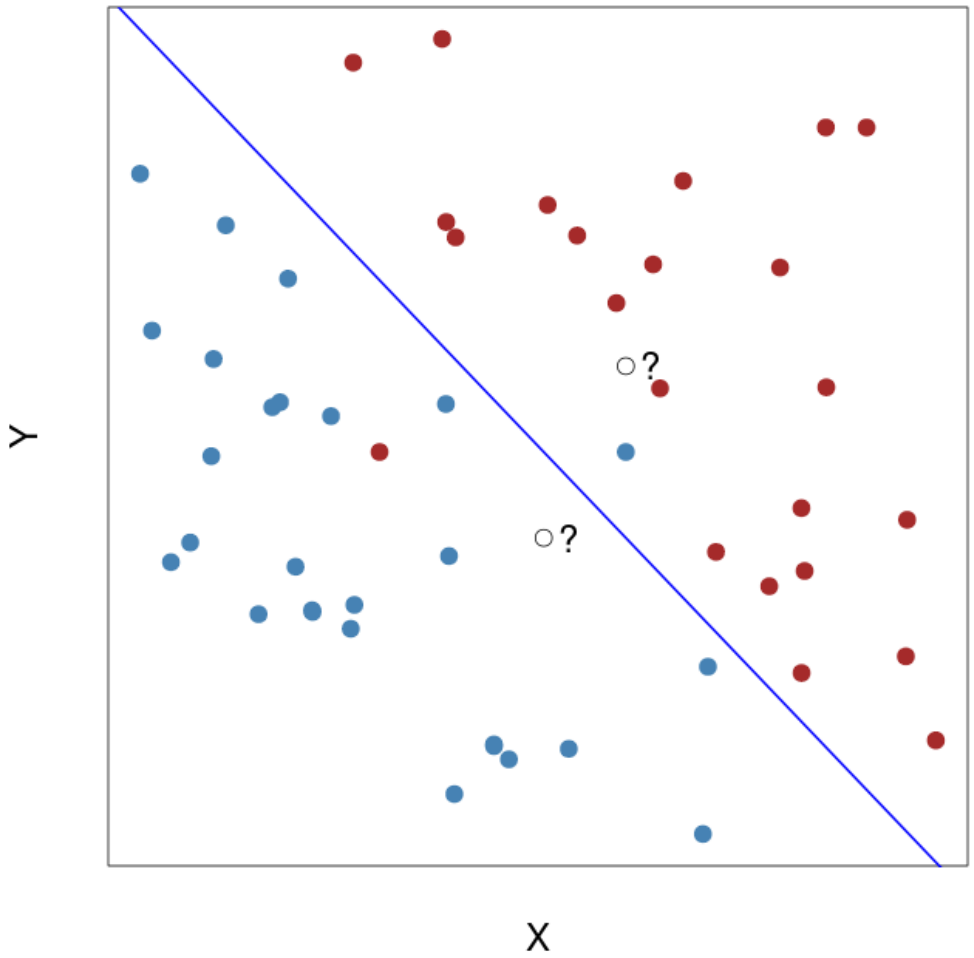

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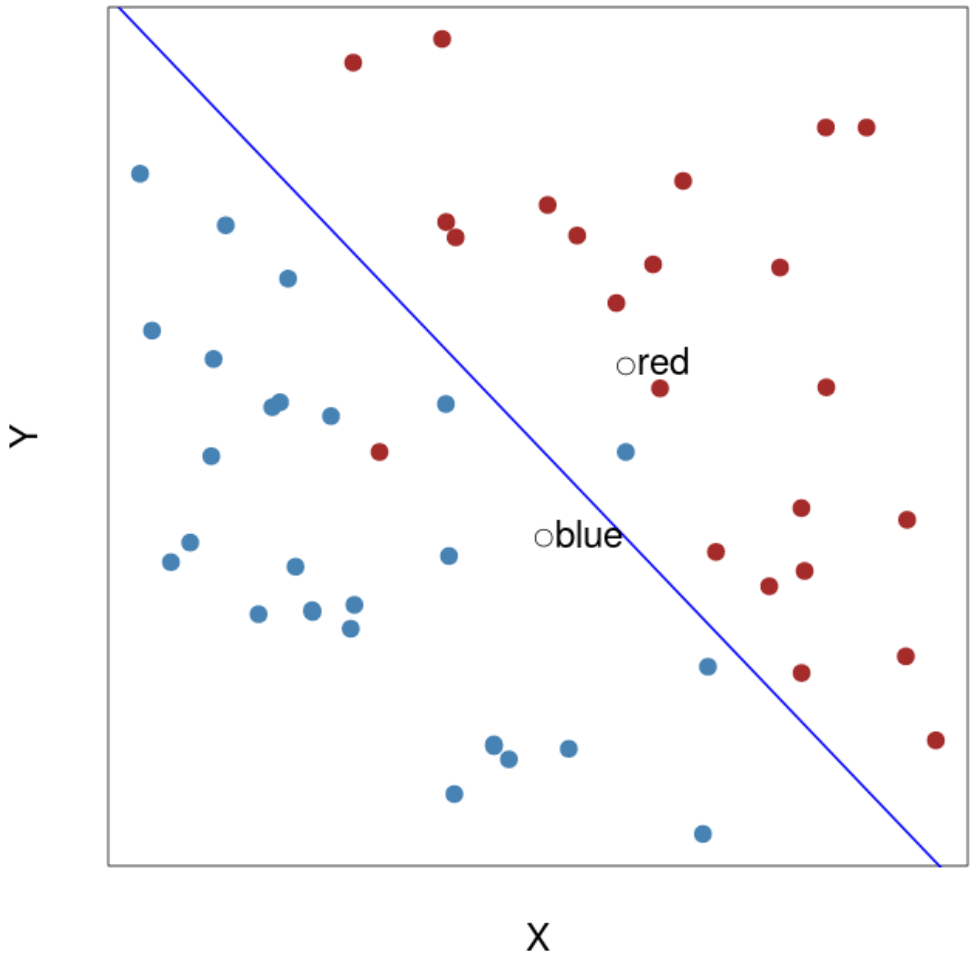

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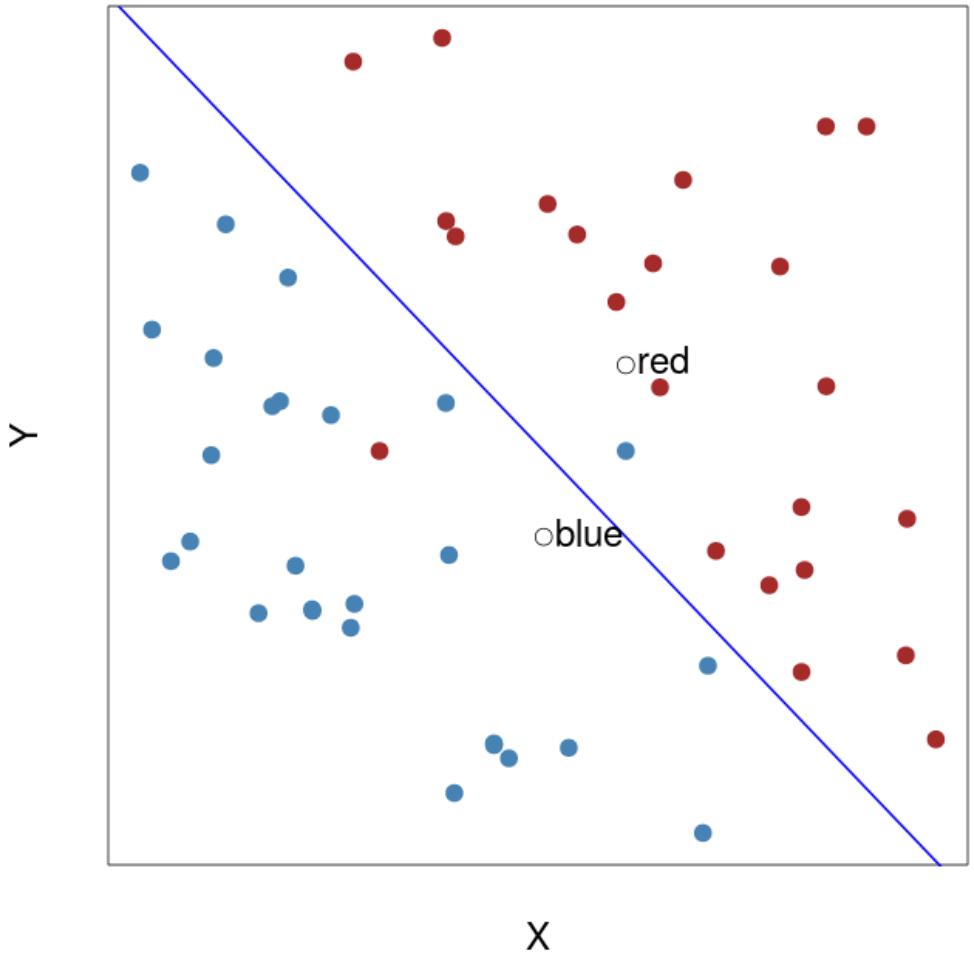

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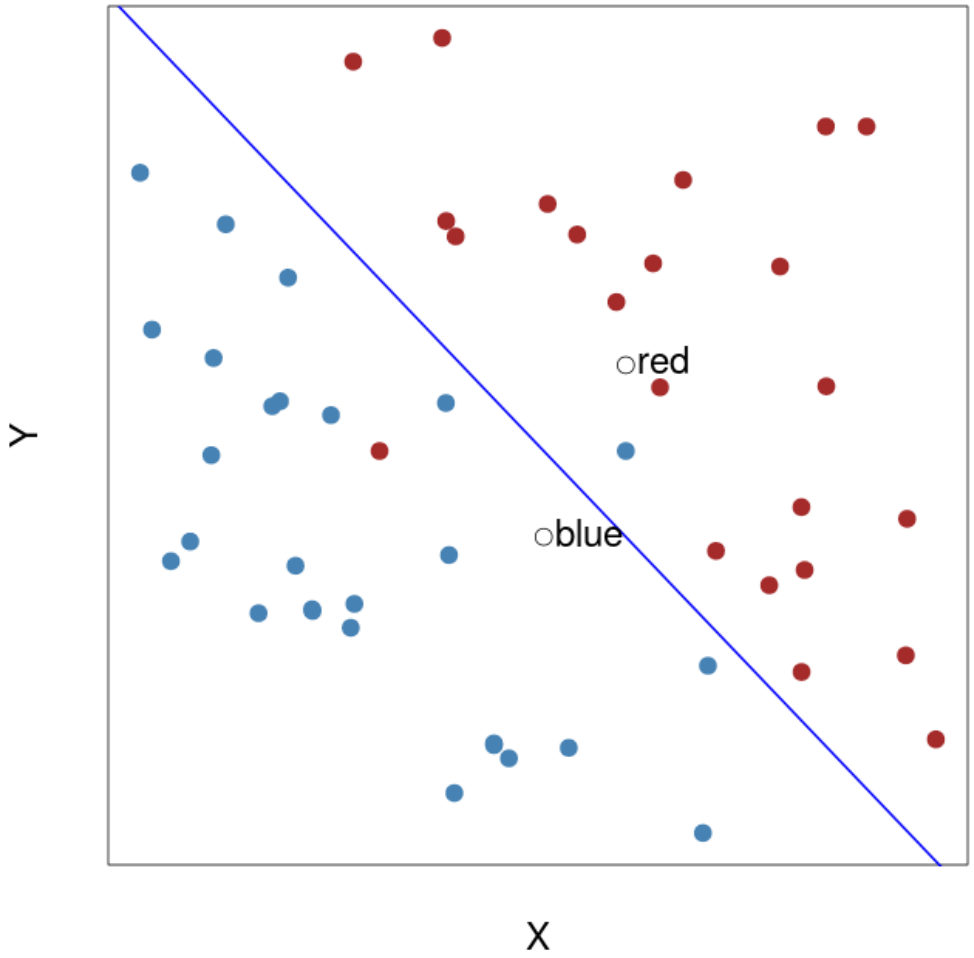
Measuring the quality of a classification model



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Measuring the quality of a classification model

- Proportion of data correctly classified:

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}}$$

- Proportion of positive data correctly classified

$$\text{Sensitivity} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

- Proportion of negative data correctly classified

$$\text{Specificity} = \frac{TN}{TN + FP}$$

- Proportion of true positive in the data classified as 'positive'

$$\text{Positive Predictive Value (PPV)} = \frac{TP}{TP + FP}$$

- What are these measures in our classification example?

Learning objectives

Now, you should be able to:

- Explain how clustering works (k-means, hierarchical clustering)
- Discuss the choices that need to be made when tackling a clustering problem
- Explain how supervised machine learning works (classification)
- How to simply evaluate a classification method

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Clustering and Machine Learning Any questions?

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