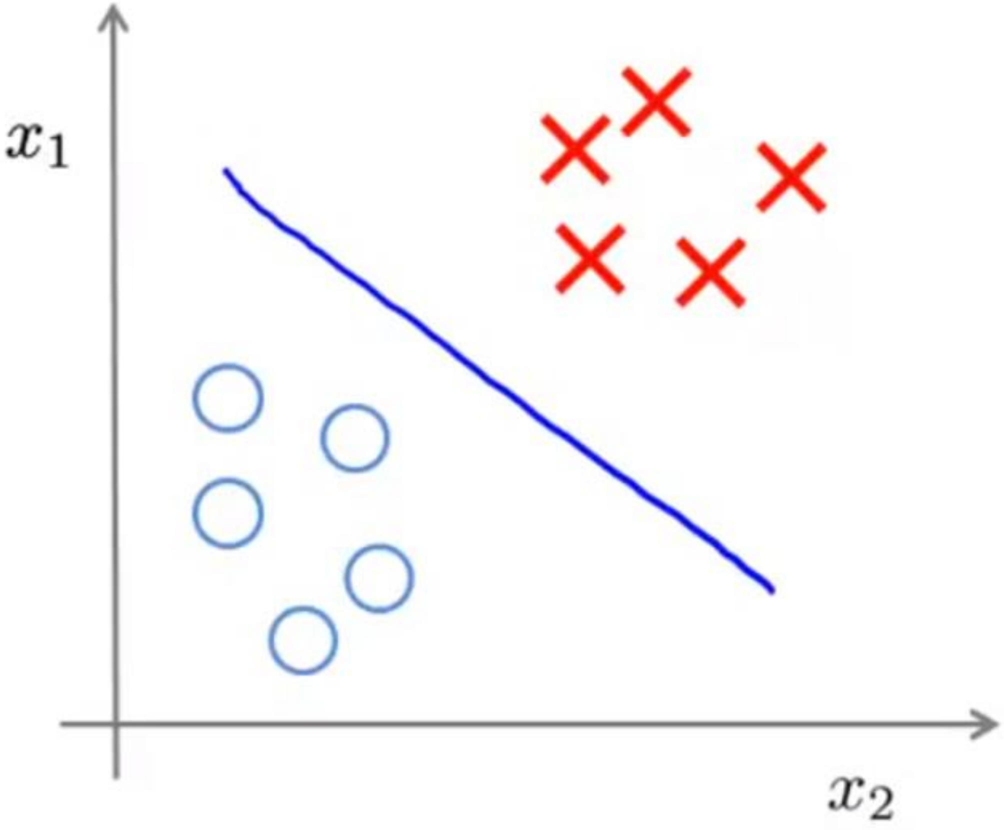
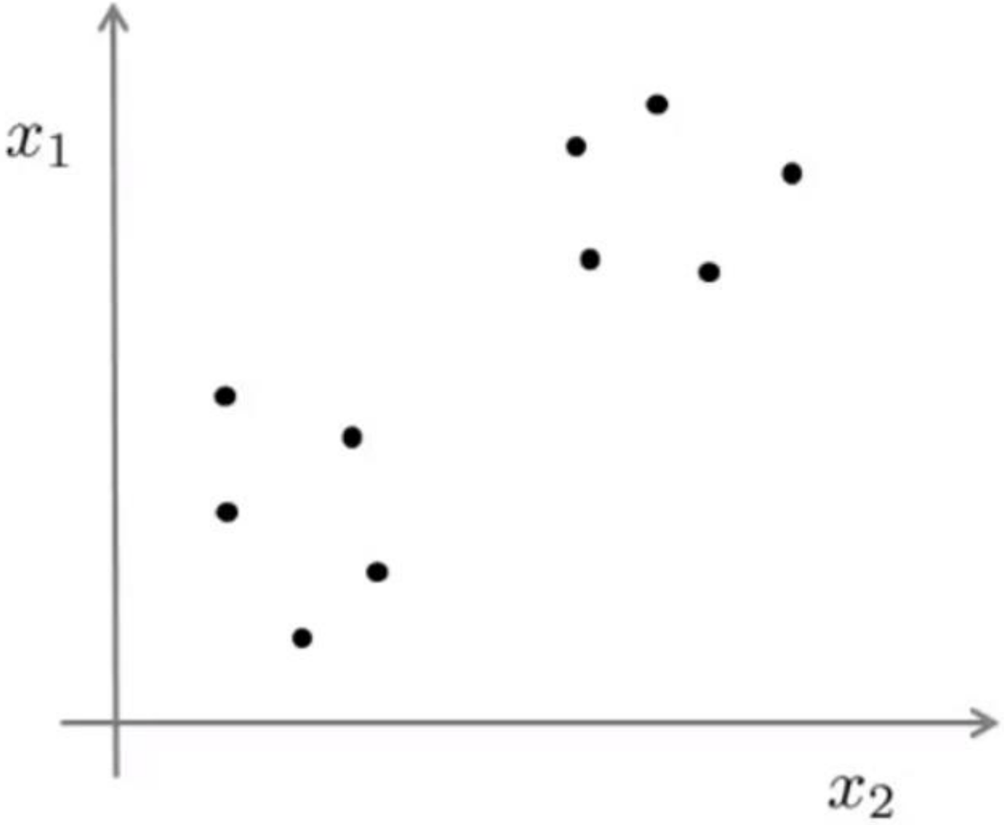
Unsupervised Learning: Clustering with K-Means

Supervised learning

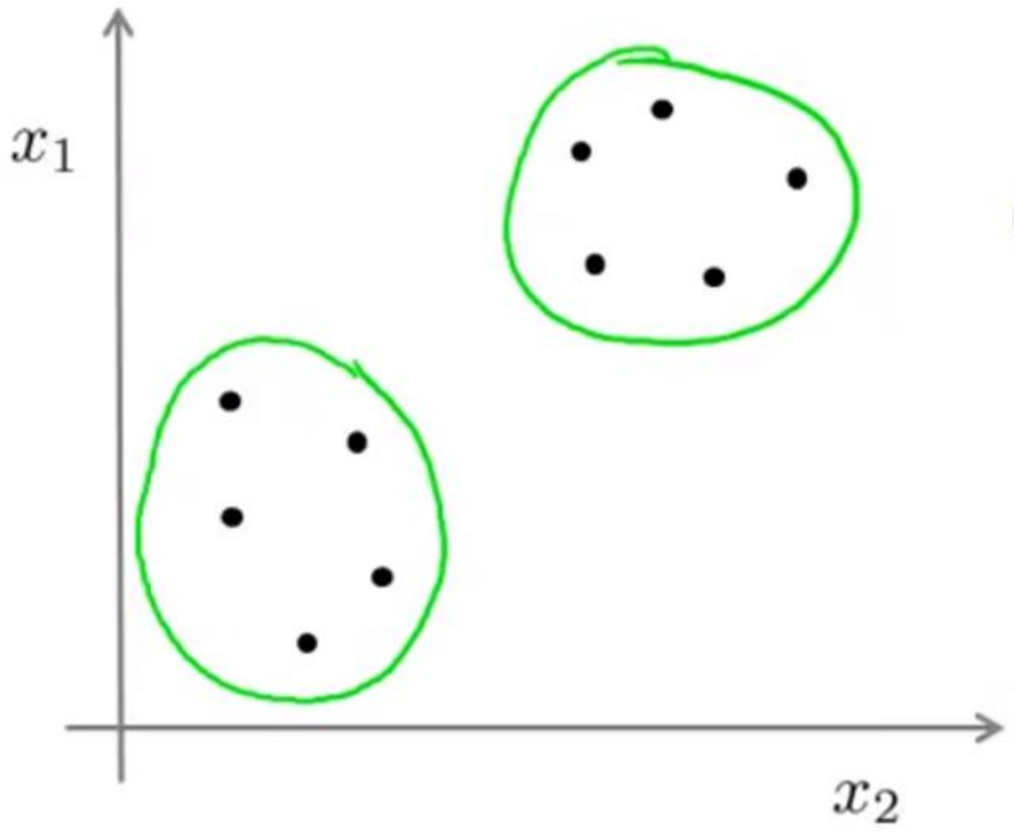


Unsupervised learning



Training set: $\{x^{(1)}, x^{(2)}, x^{(3)}, \ldots, x^{(m)}\}$ $\leftarrow$

Unsupervised learning



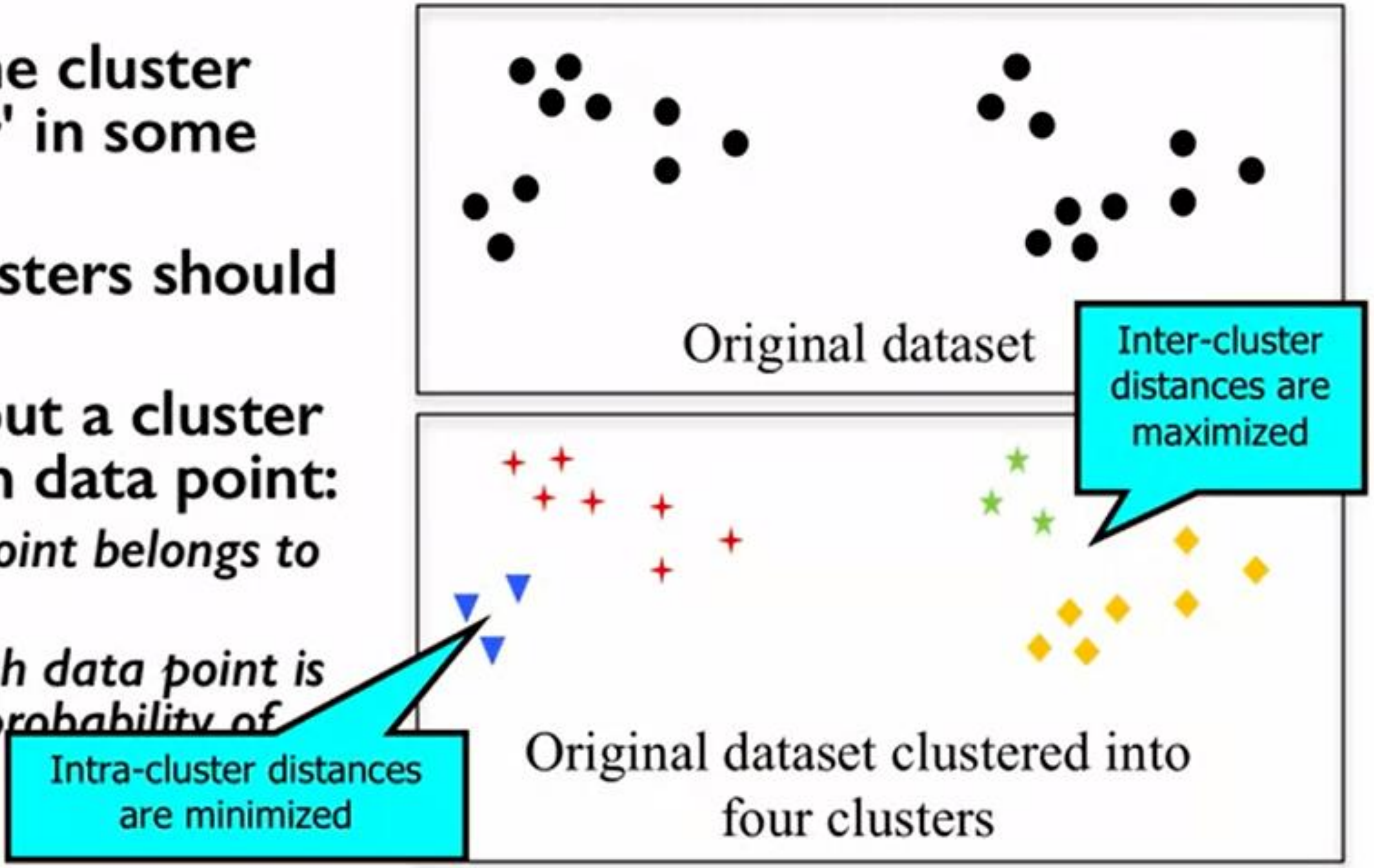
Clustering algorithm

Training set: $\{x^{(1)}, x^{(2)}, x^{(3)}, \ldots, x^{(m)}\}$ $\leftarrow$

Clustering:

Finding a way to divide a dataset into groups ('clusters')

- Data points within the same cluster should be 'close' or 'similar' in some way.
- Data points in different clusters should be 'far apart' or 'different'
- Clustering algorithms output a cluster membership index for each data point:
  - *Hard clustering: each data point belongs to exactly one cluster*
  - *Soft (or fuzzy) clustering: each data point is assigned a weight, score, or probability of membership for each cluster*



K-means Clustering

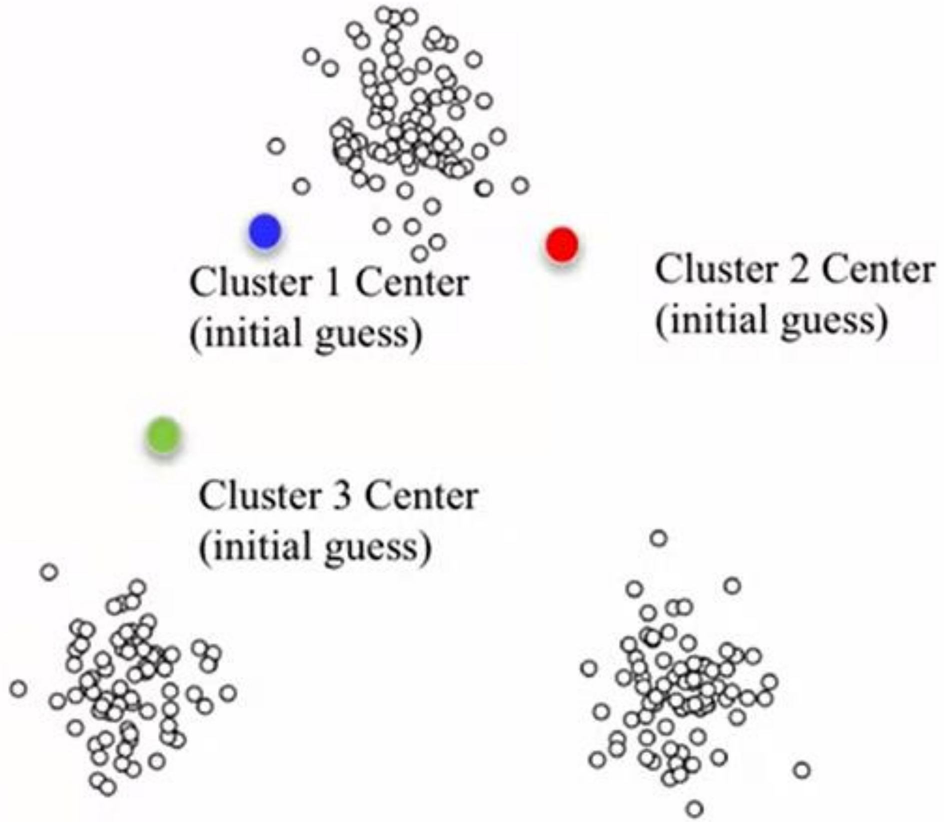
The k-means algorithm

Initialization Pick the number of clusters *k* you want to find. Then pick *k random* points to serve as an initial guess for the cluster centers.

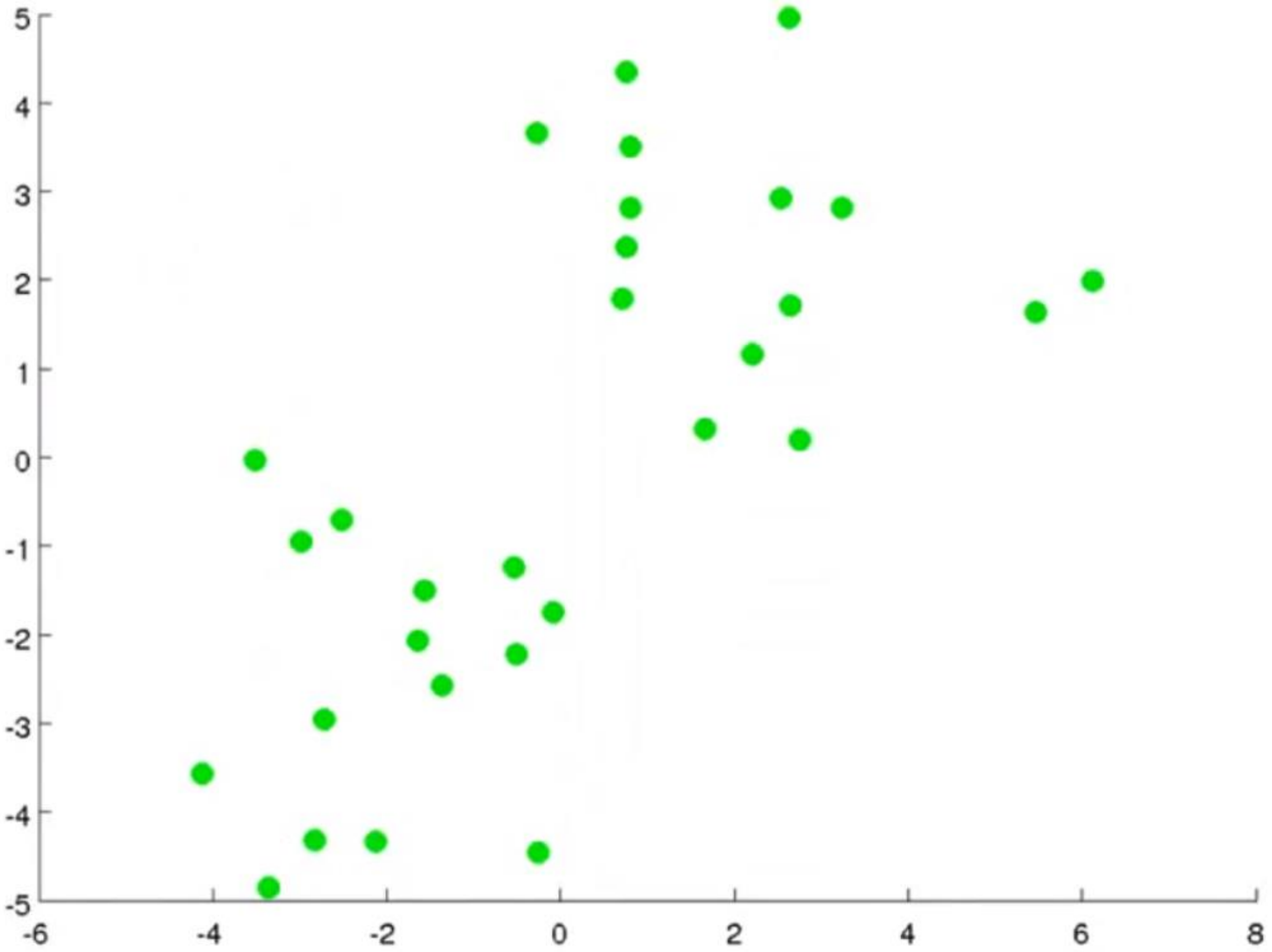
Step A Assign each data point to the nearest cluster center.

Step B Update each cluster center by replacing it with the mean of all points assigned to that cluster (in step A).

Repeat steps A and B until the centers converge to a stable solution.



Demo: https://www.naftaliharris.com/blog/visualizing-k-means-clustering/



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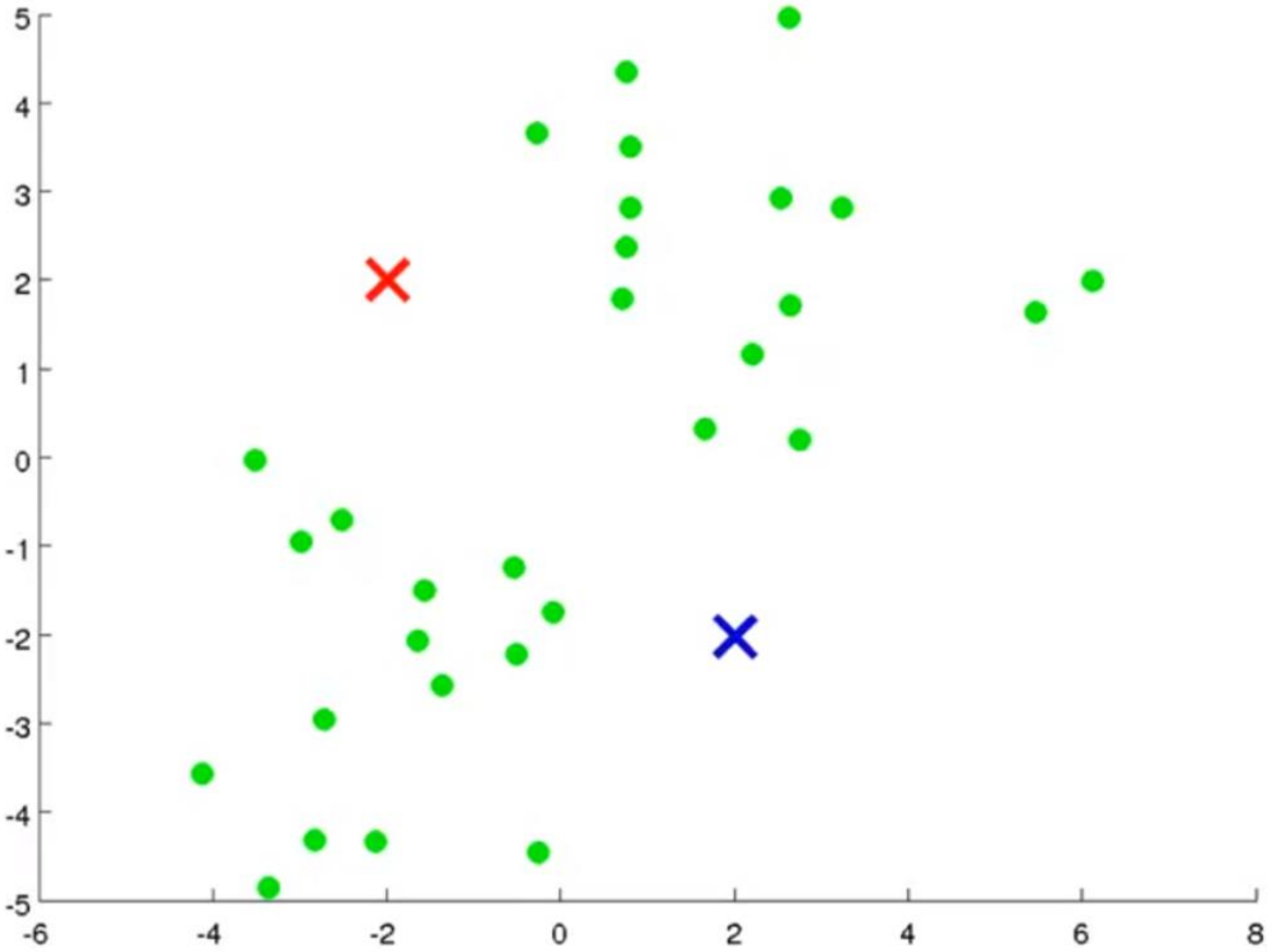

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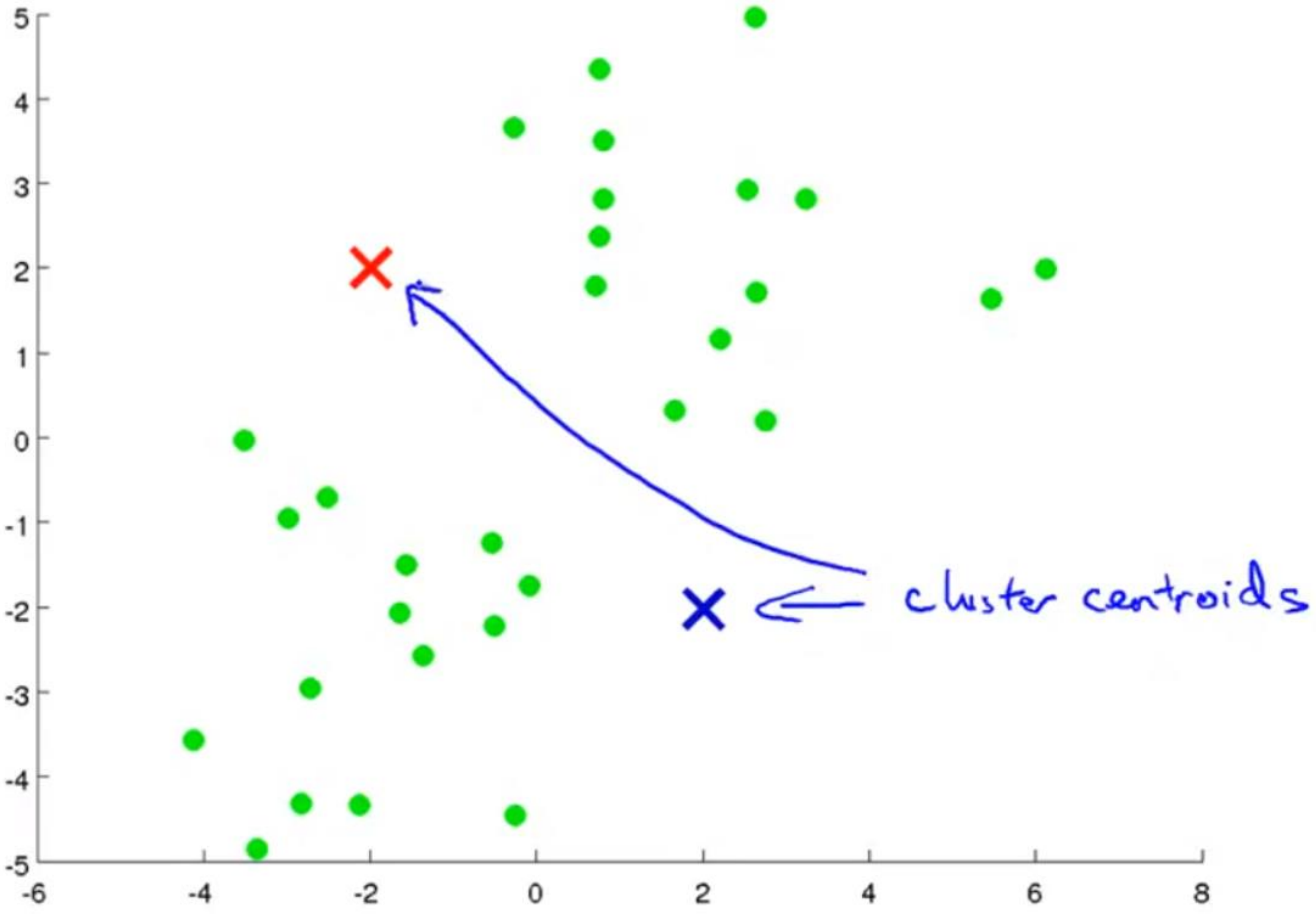

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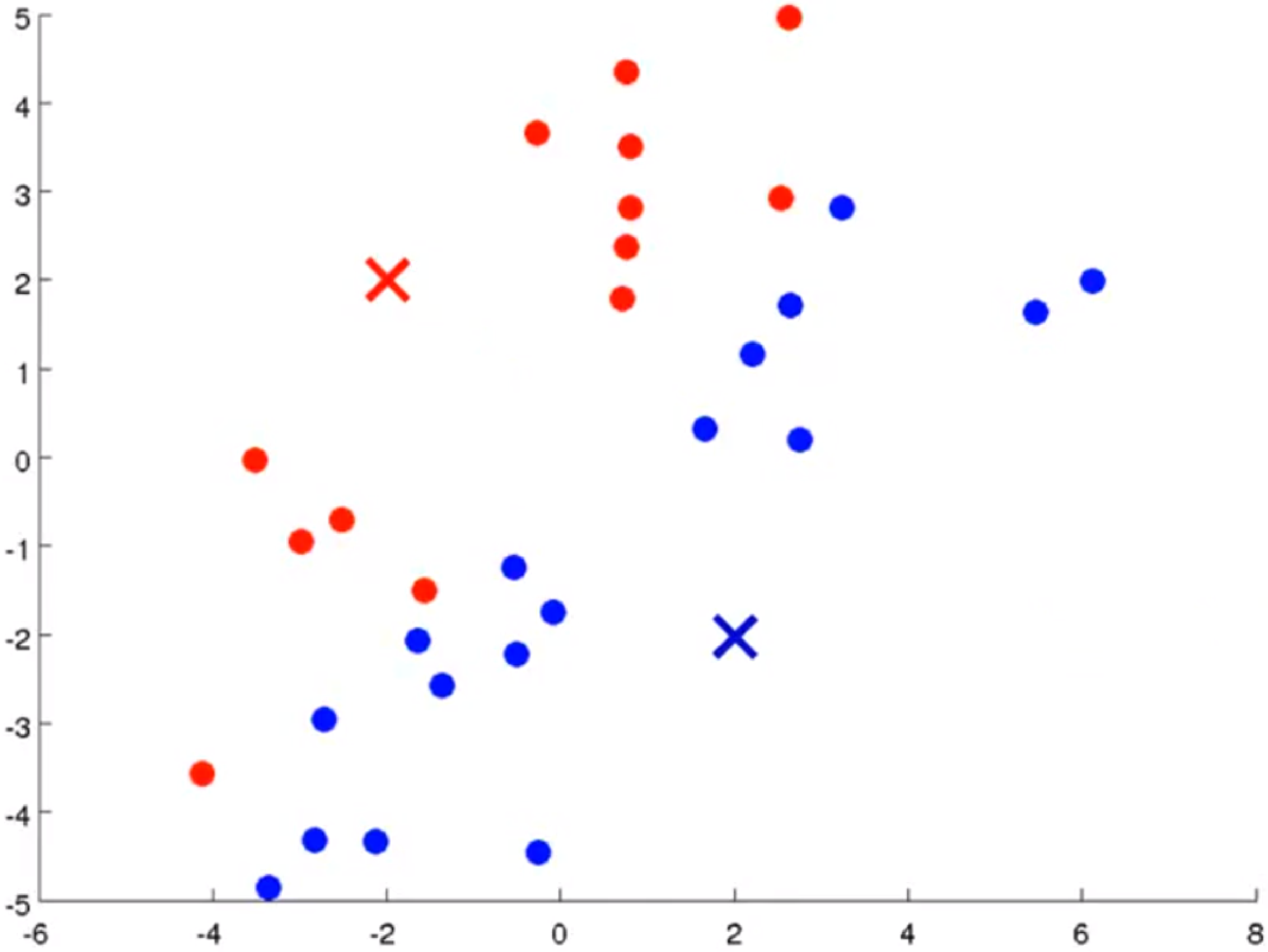
cluster centroids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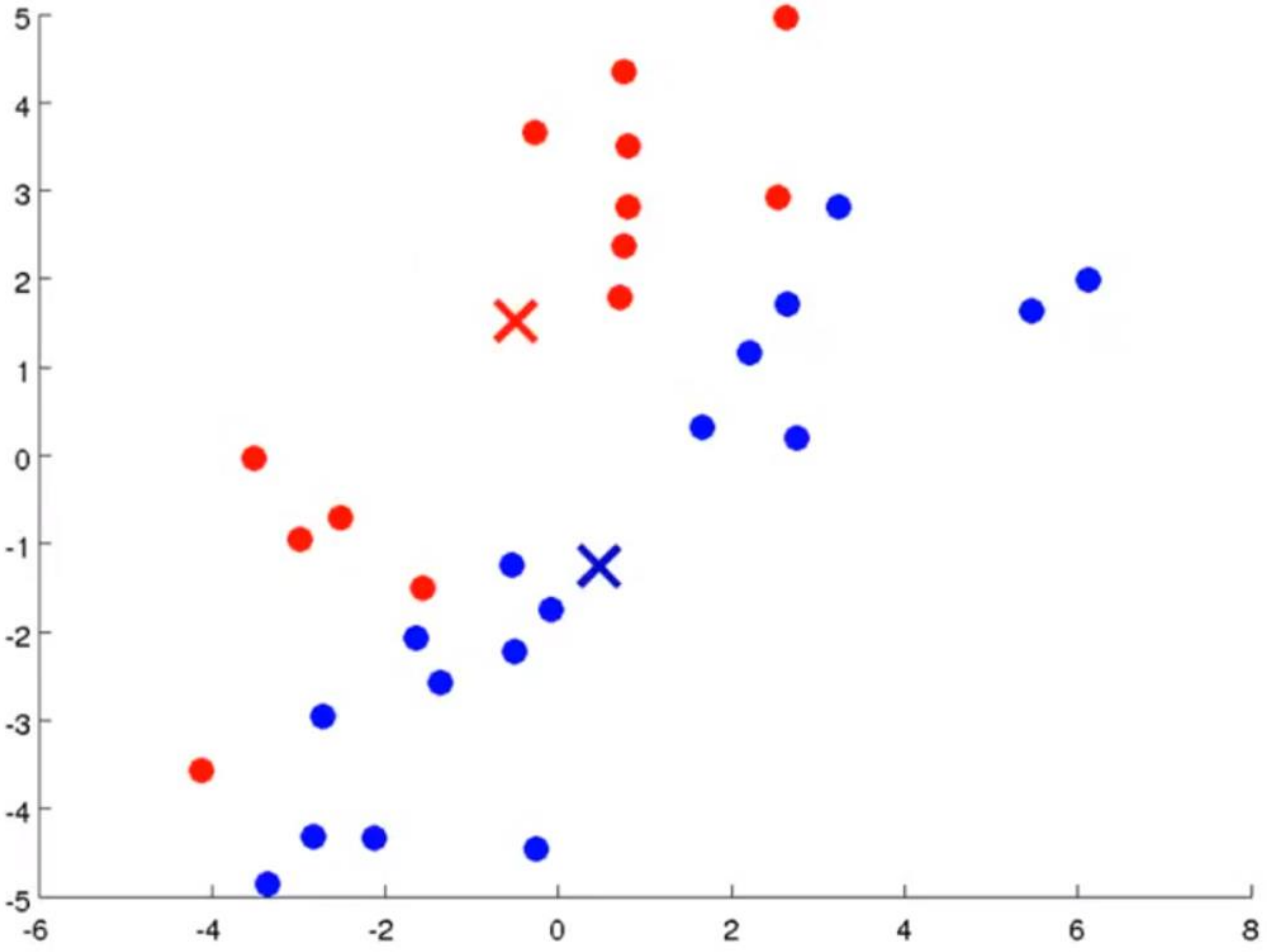

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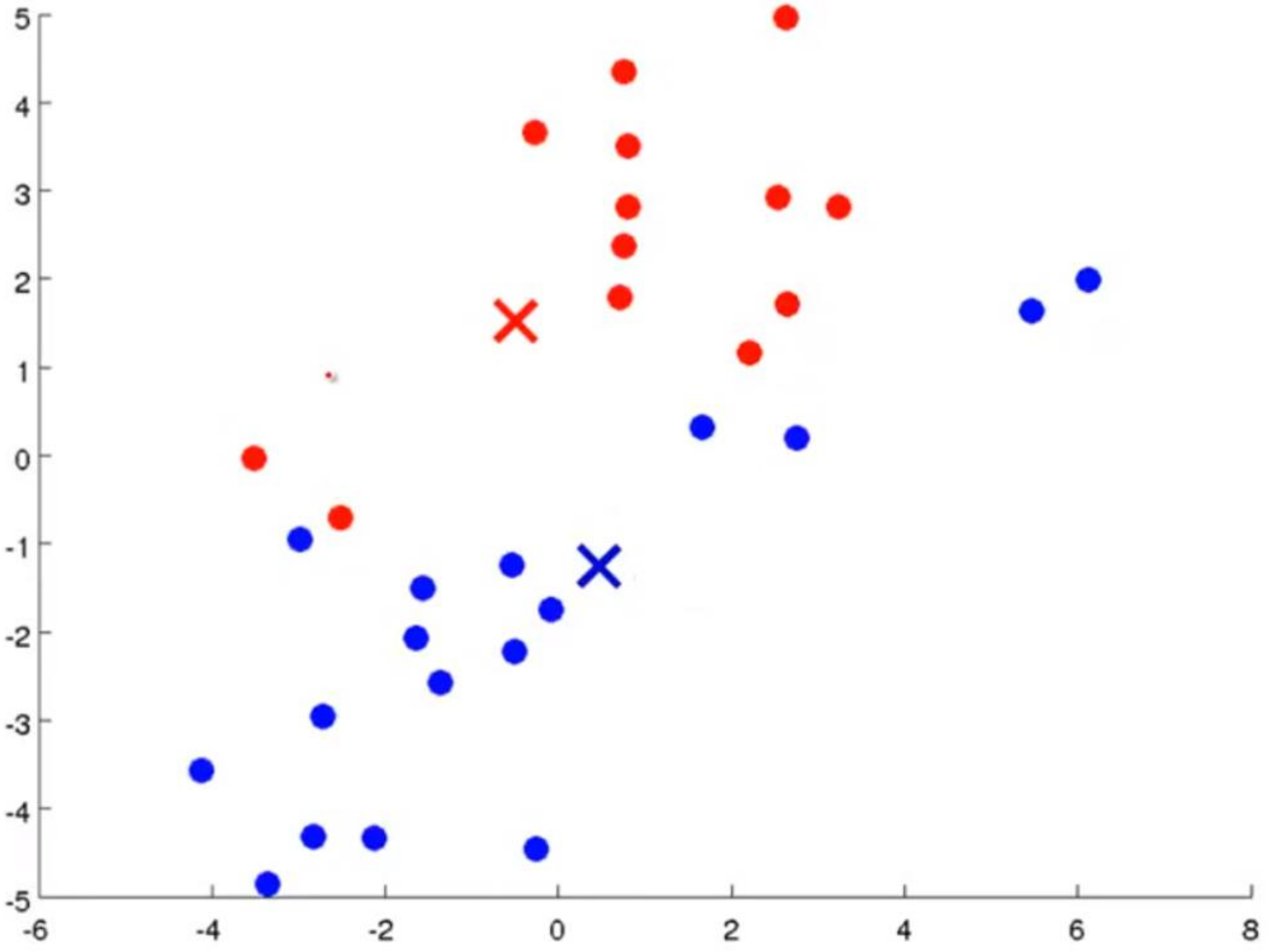

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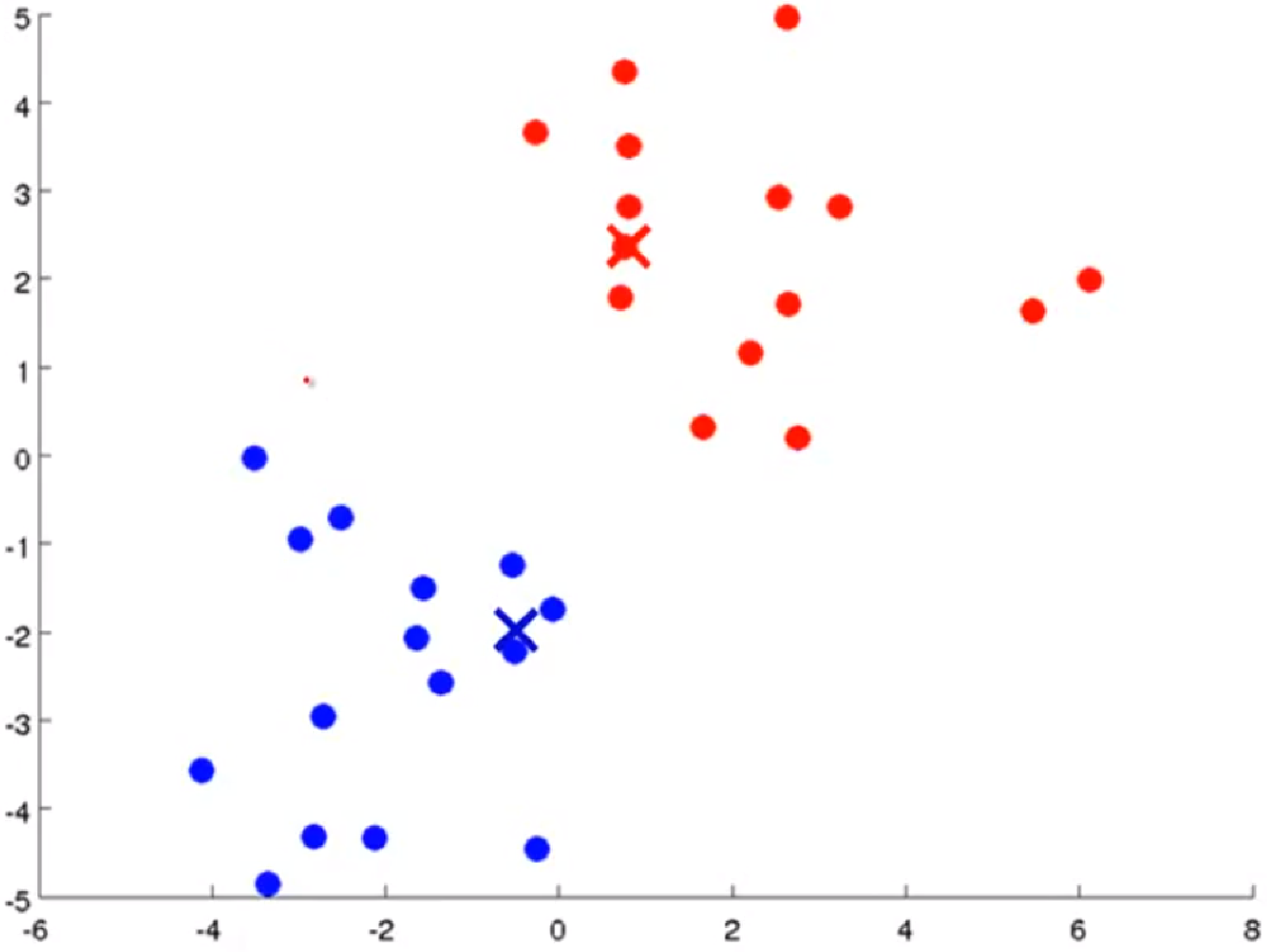

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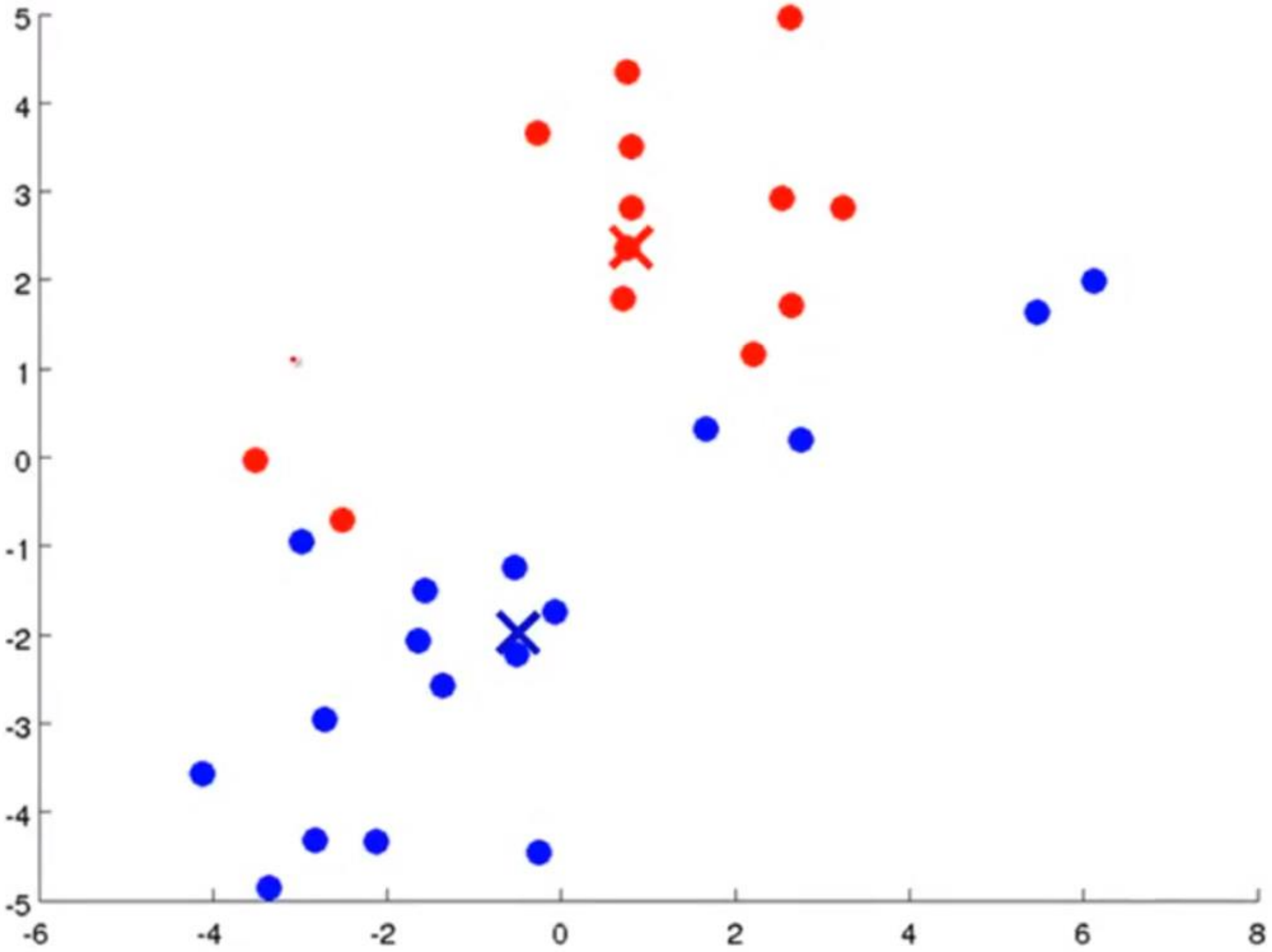
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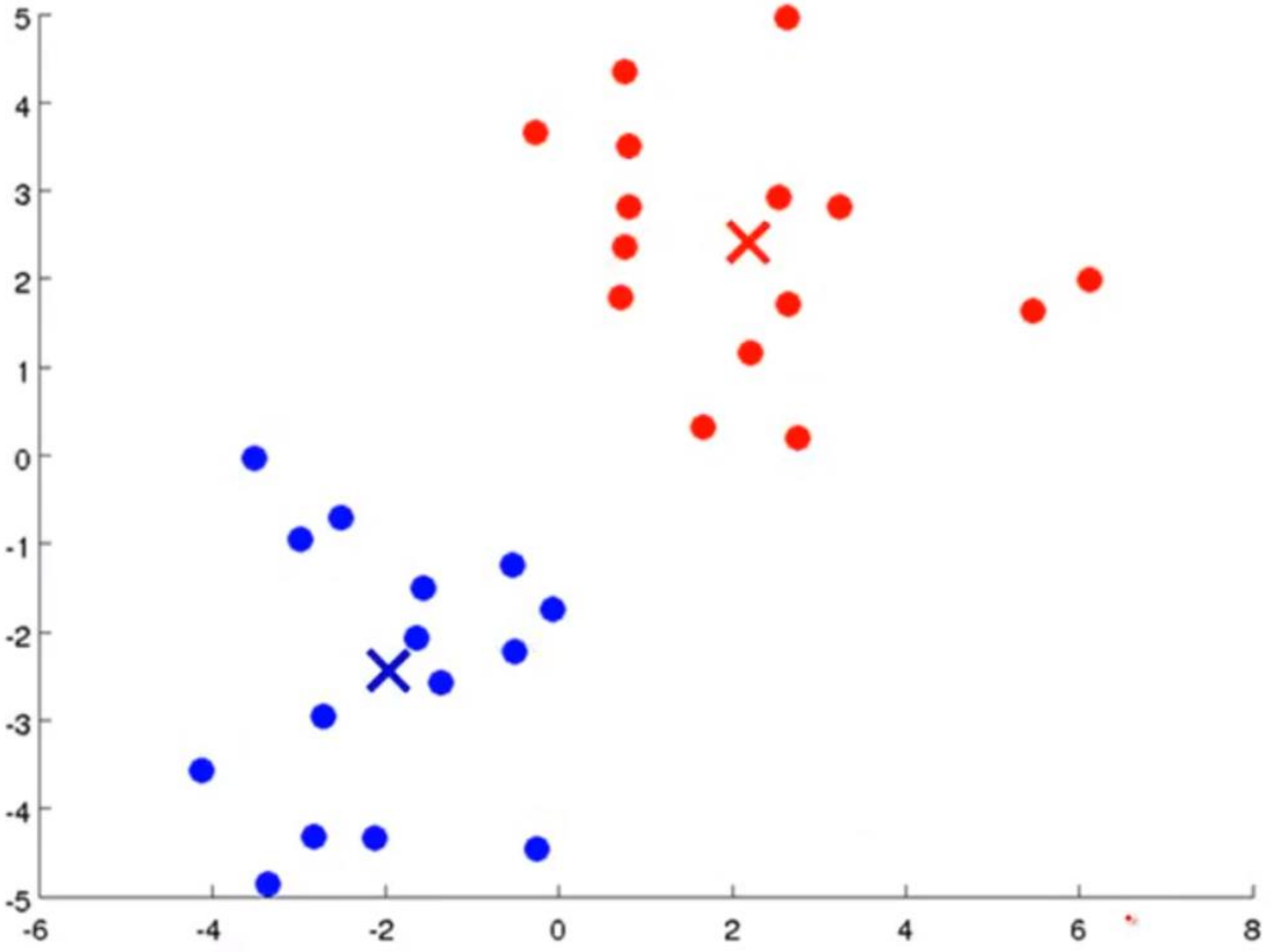

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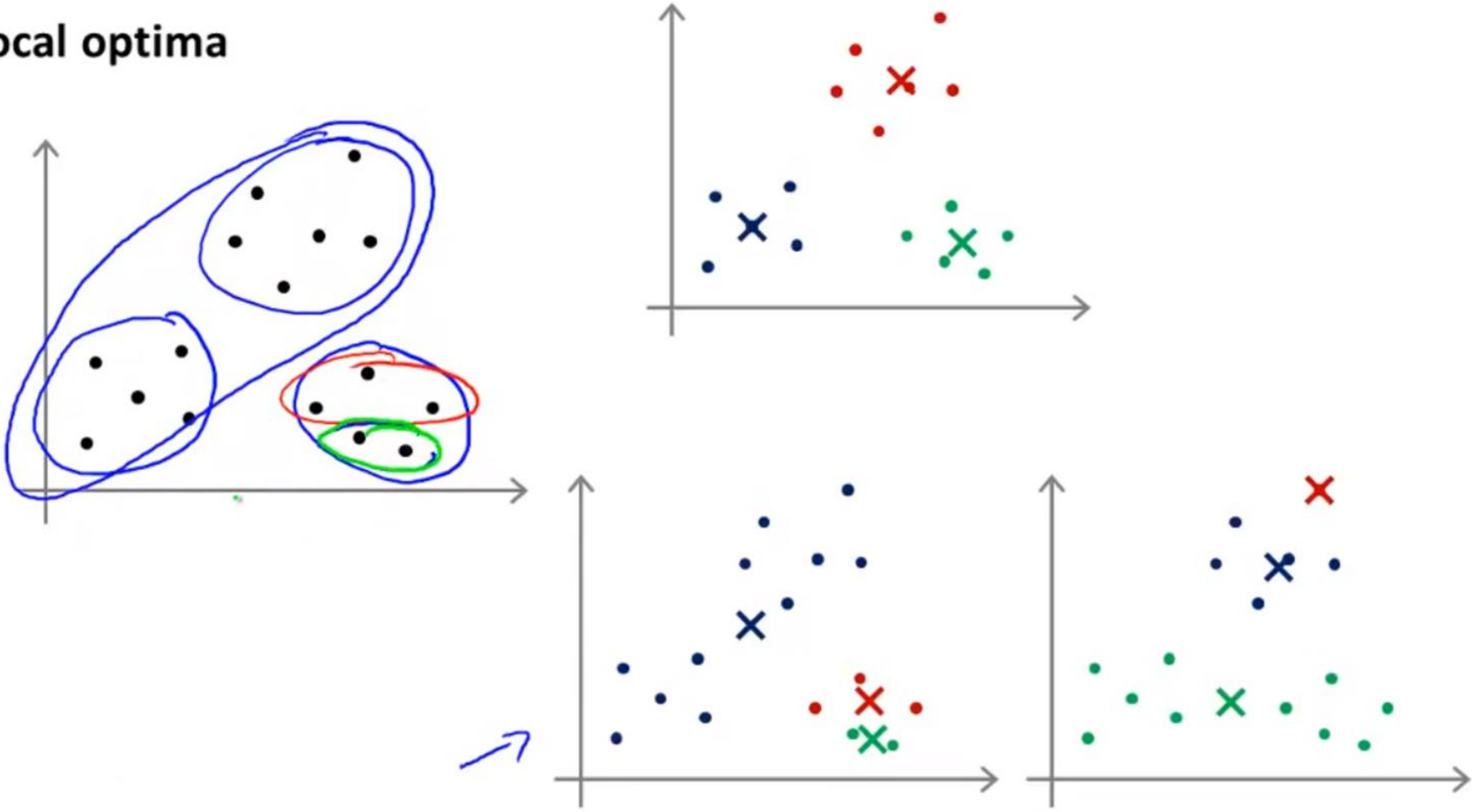
Local optima



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Random initialization

For i = 1 to 100 {

Randomly initialize K-means.

Run K-means. Get $c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K$.

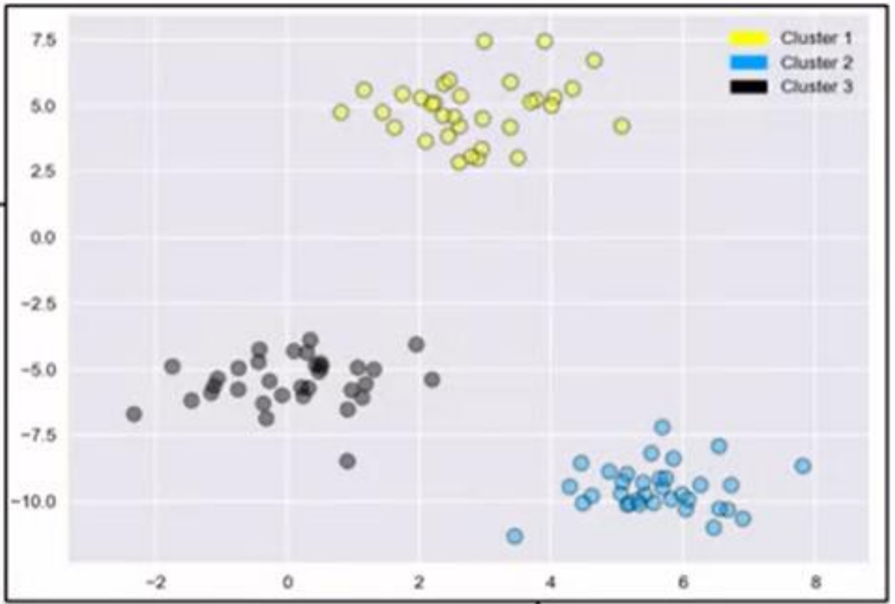
Compute cost function (distortion)

$$J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$$

}

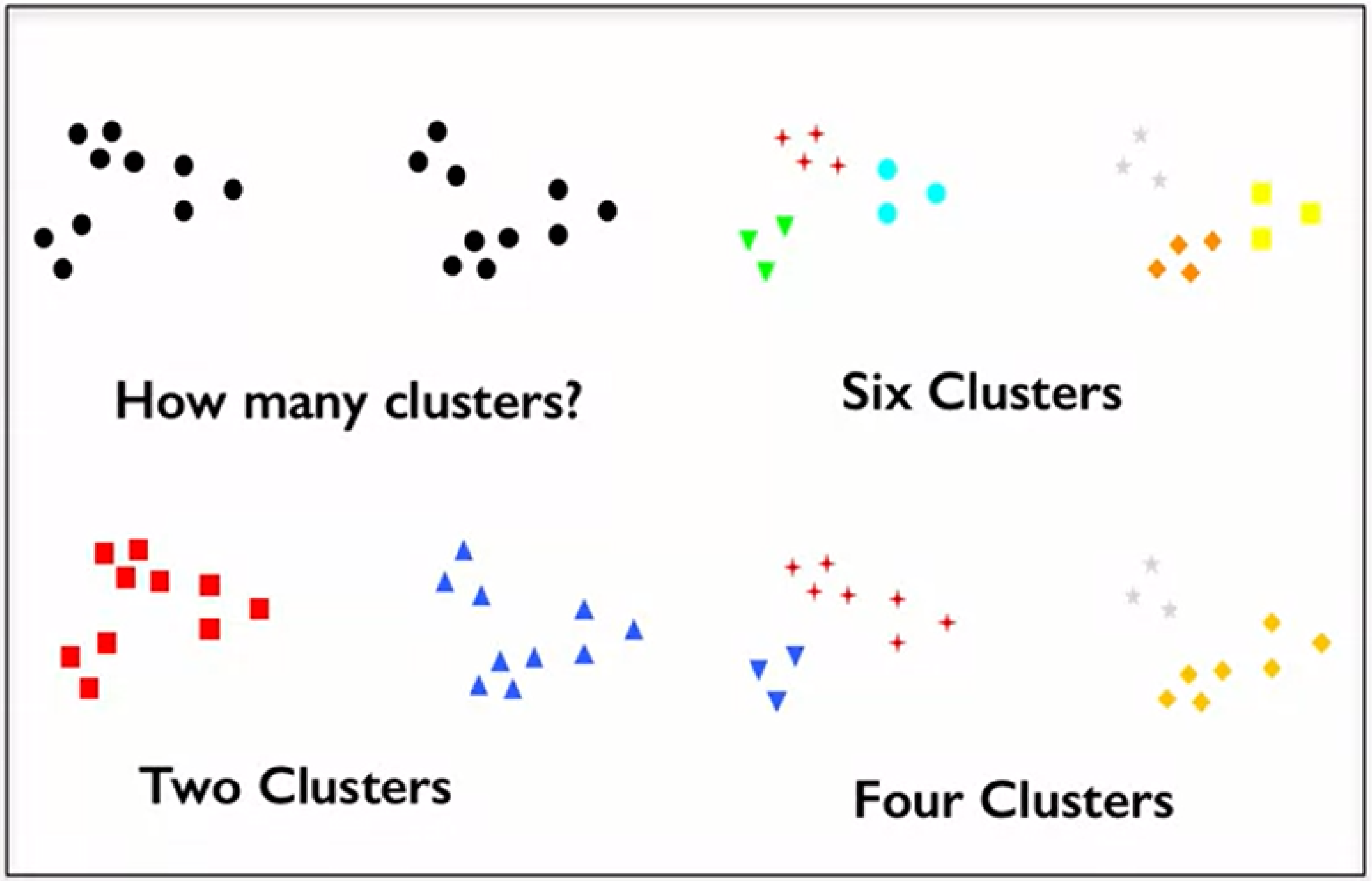
k-means Example in Scikit-Learn

```
from sklearn.datasets import make_blobs
from sklearn.cluster import KMeans
from adspy_shared_utilities import plot_labelled_scatter

X, y = make_blobs(random_state = 10)

kmeans = KMeans(n_clusters = 3)
kmeans.fit(X)

plot_labelled_scatter(X, kmeans.labels_, ['Cluster 1', 'Cluster 2', 'Cluster 3'])
```



Clustering Evaluation

- With ground truth, existing labels can be used to evaluate cluster quality.
- Without ground truth, evaluation can difficult: multiple clusterings may be plausible for a dataset.
- Consider task-based evaluation: Evaluate clustering according to performance on a task that does have an objective basis for comparison.
- Example: the effectiveness of clustering-based features for a supervised learning task.
- Some evaluation heuristics exist (e.g. silhouette) but these can be unreliable.

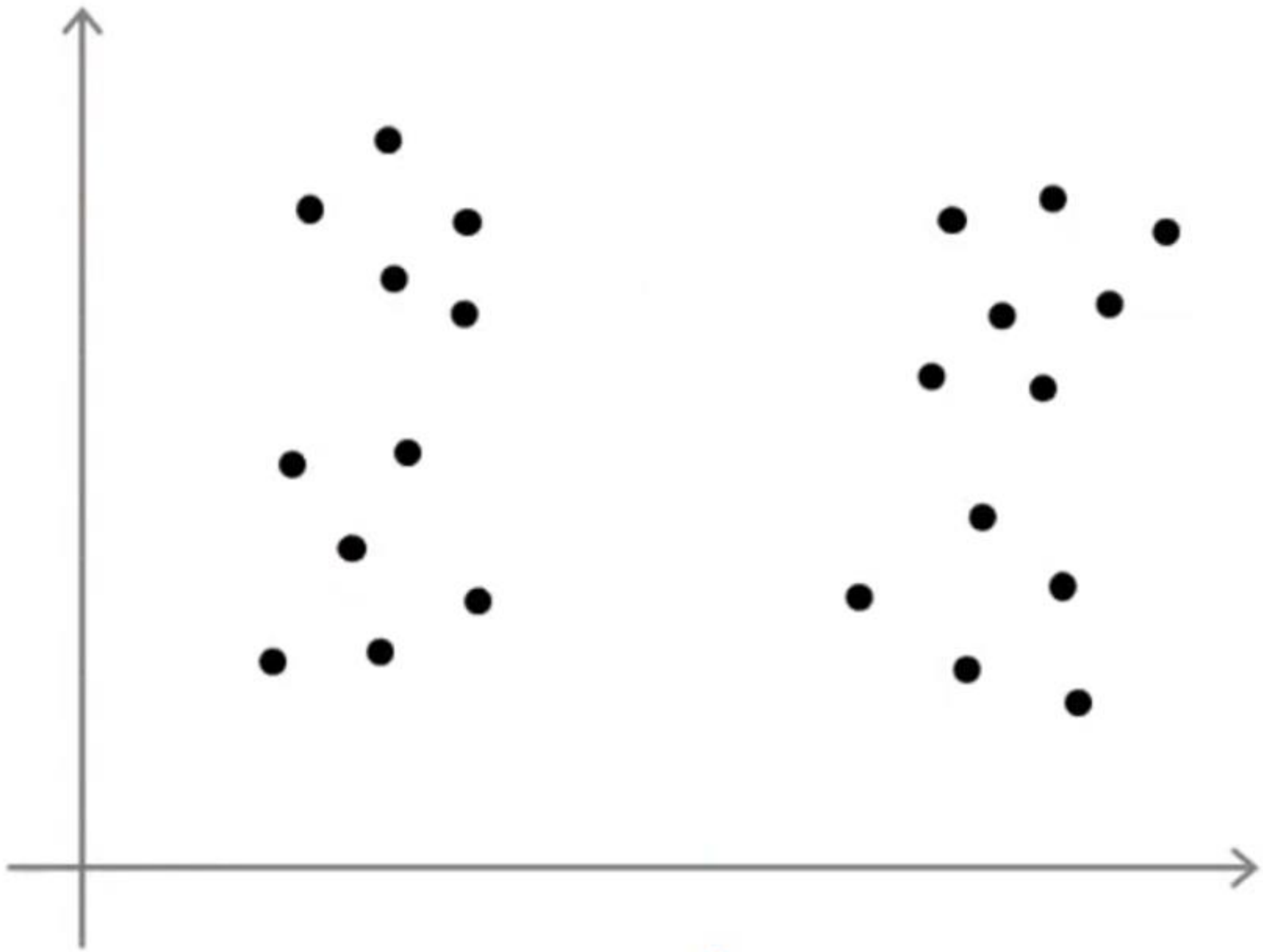


Choosing K

Clustering

Unsupervised Learning

What is the right value of K?



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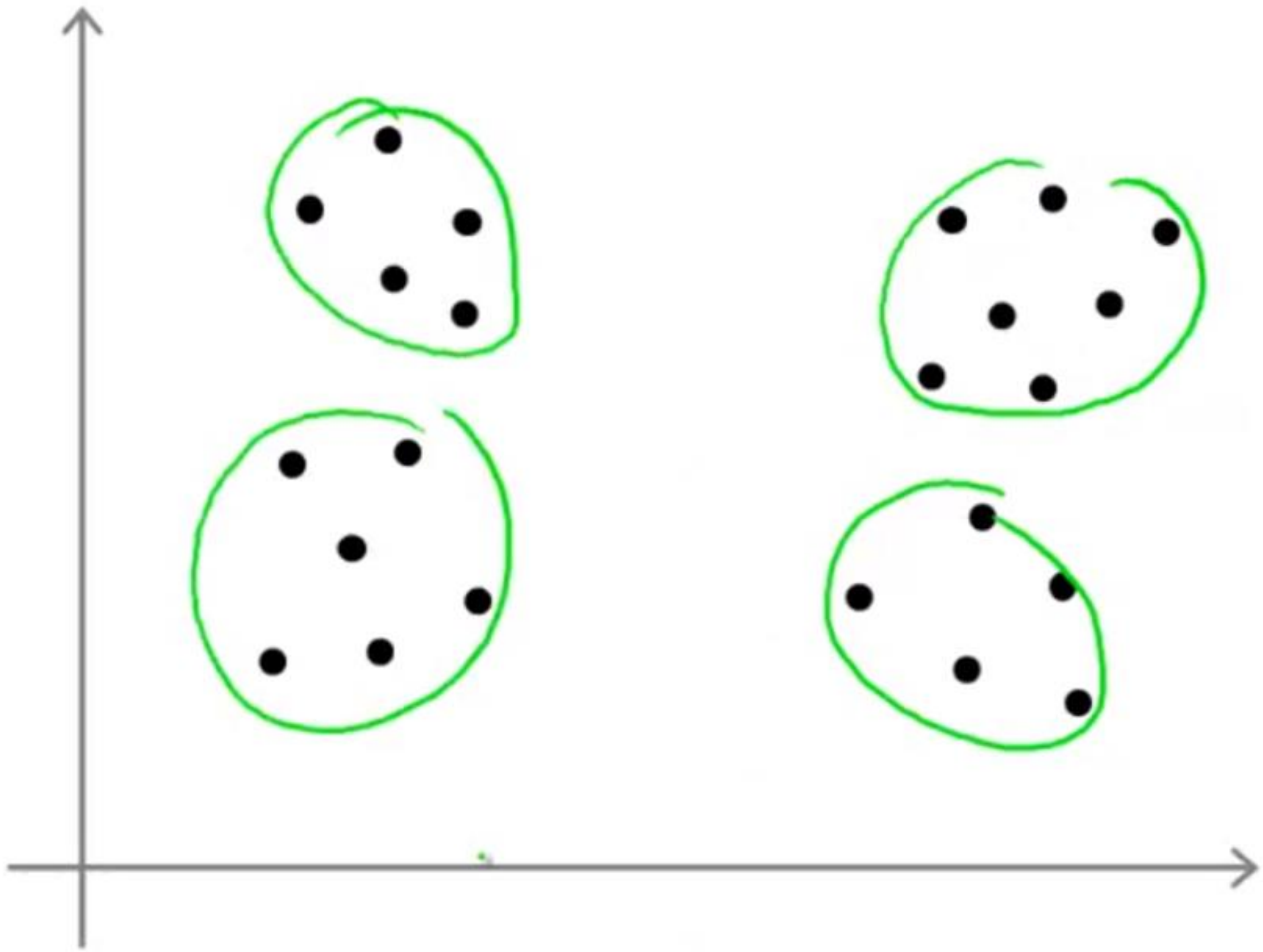

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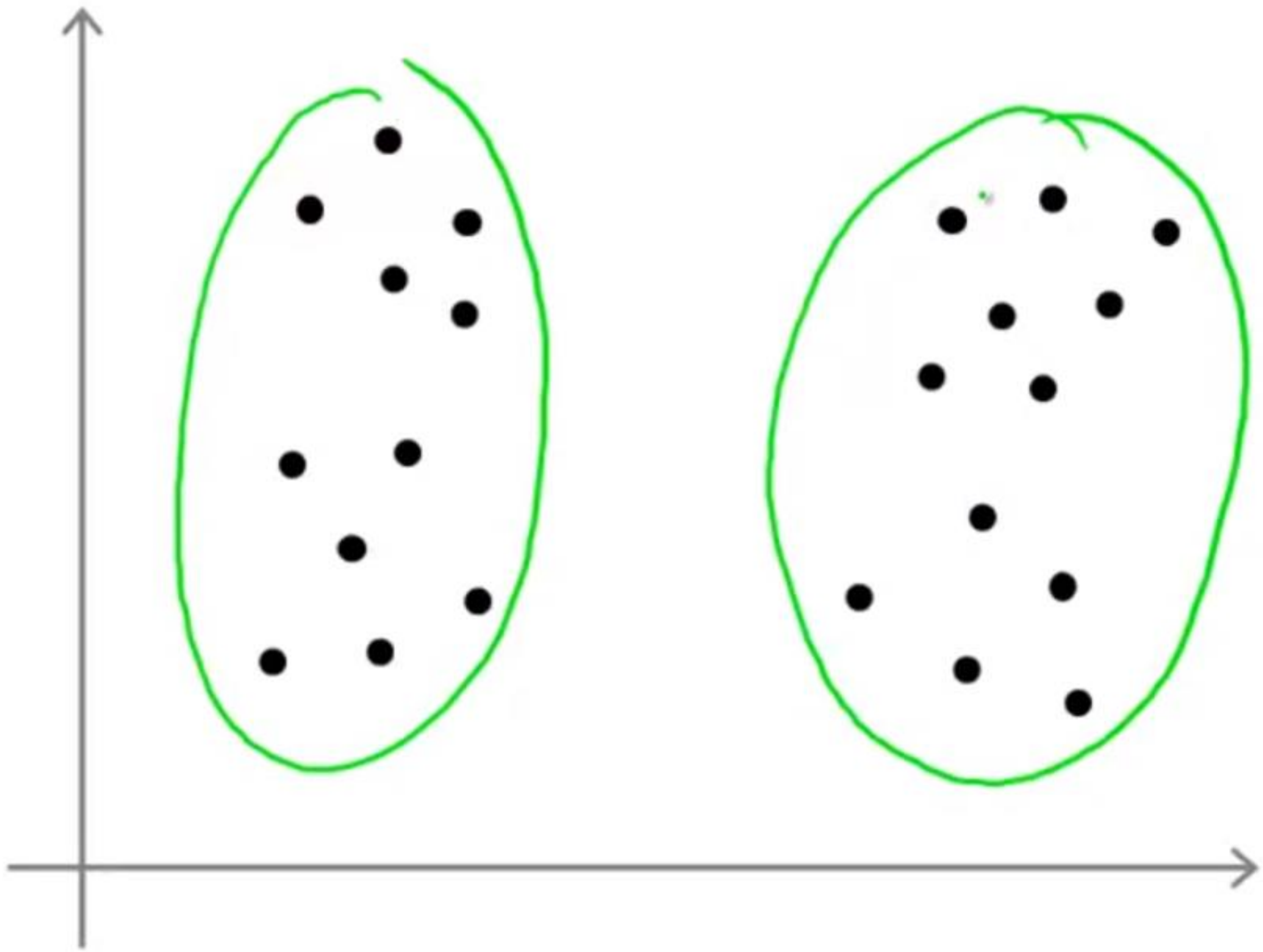

Choosing the value of K

Elbow method: