UNIVERSITY AT ALBANY
STATE UNIVERSITY OF NEW YORK

CSI 436/536 (Fall 2024)

Machine Learning

Lecture 18: Clustering

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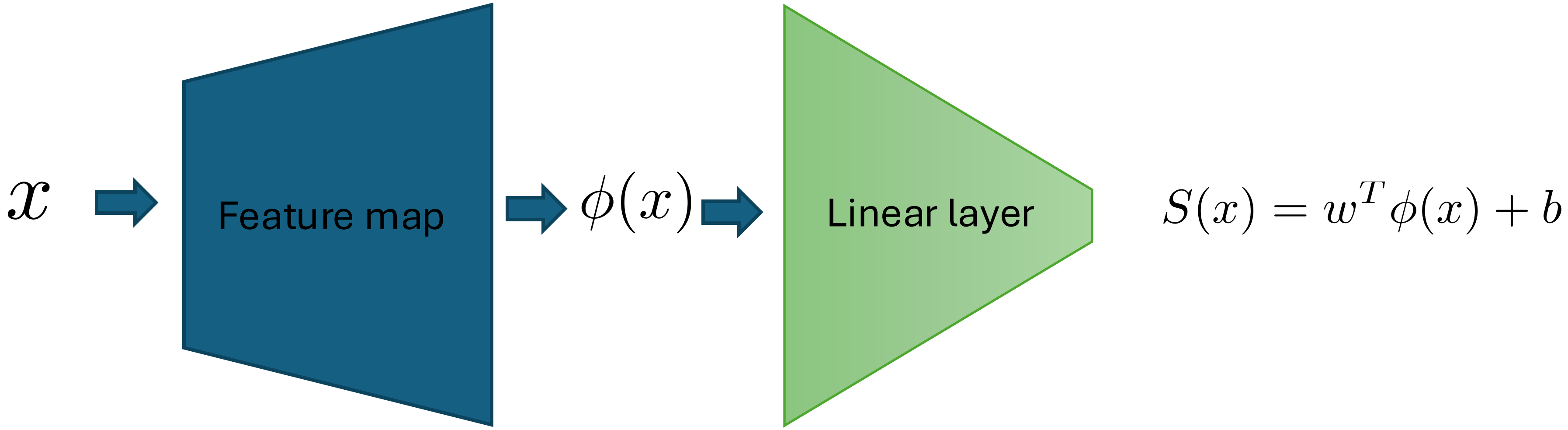
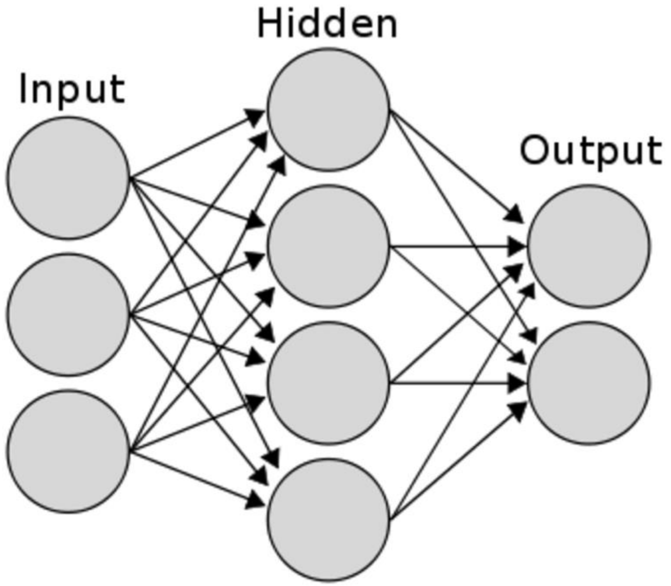
Recap: From kernels to neural networks



Recap: Two-layer neural networks

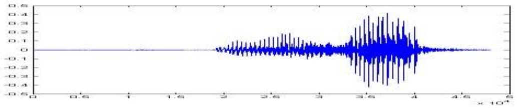
- Neural network: $S(x) \; = \; w_2^T(W_1 x + \boldsymbol{b}_1) + b_2$
  - Still a linear model at the end of the day, so let's add a nonlinearity σ!

- Two-layer MLP: $S(x) \; = \; w_2^T \sigma(W_1 x + \boldsymbol{b}_1) + b_2$
  - Linear model w.r.t. to a learnable feature map



Recap: Learning ≈ Configuring the learnable function so it behaves as instructed.

- Speech Recognition

$f\Big($  $\Big) =$ “Hello!”

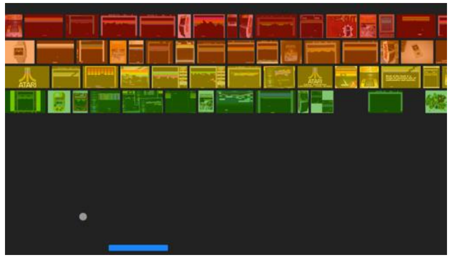
- Handwritten Recognition

$f\Big($  $\Big) =$ “2”

- Weather forecast

$f\Big($ Thursday $\Big) =$ “  Saturday”

- Play video games

$f\Big($  $\Big) =$ “move left”

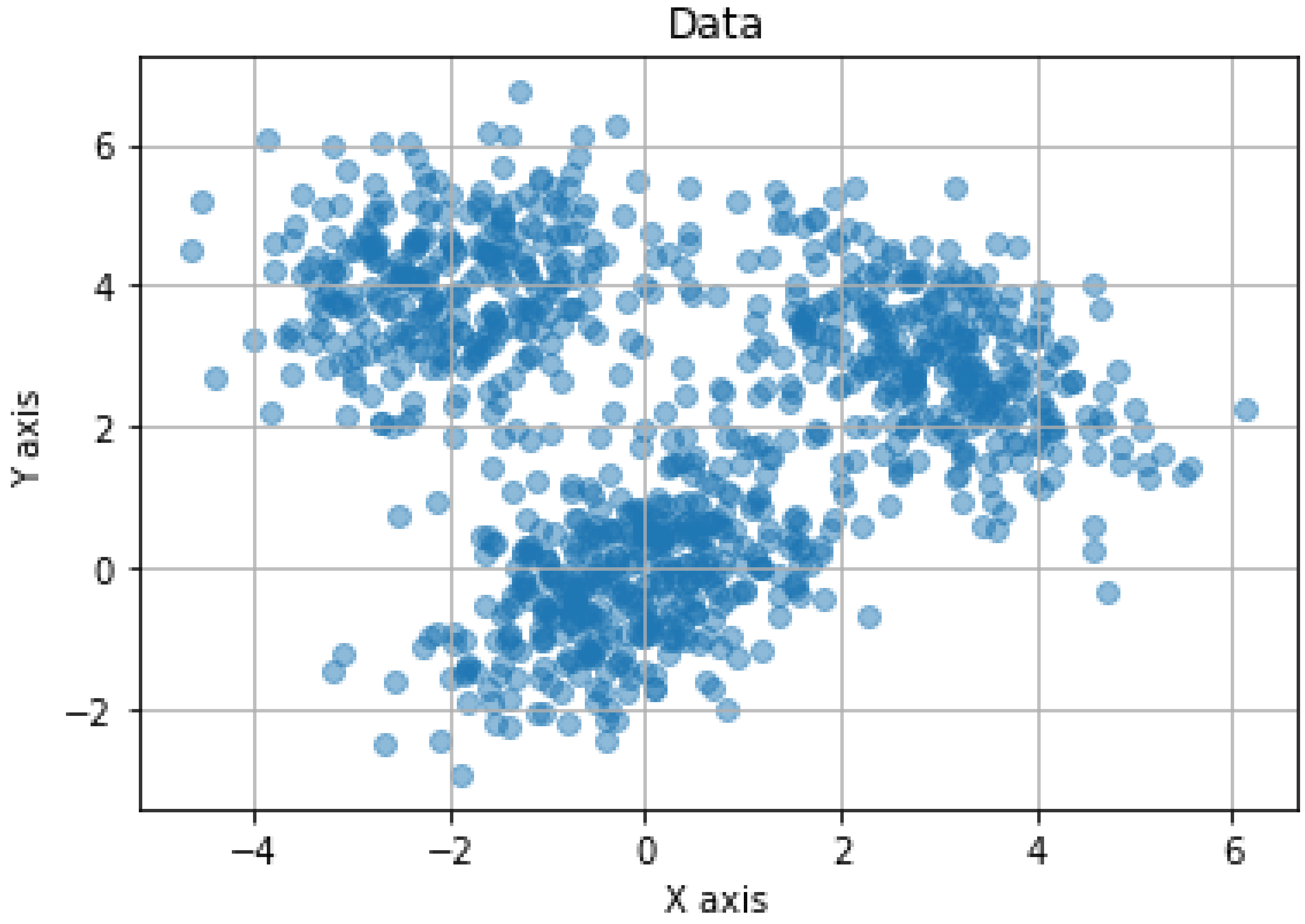
Unsupervised learning

- Input space: $\mathcal{X}$ Images, videos, text, graphs, proteins, programs, etc…
- Output space: None.
- Hypothesis space: $\mathcal{H}$
- Each hypothesis h is a particular way to summarize the data
- Loss function $\ell : \mathcal{H} \times \mathcal{X} \to \mathbb{R}$
- Goal:
  - Discover data structure
  - Often achieved by minimizing the loss

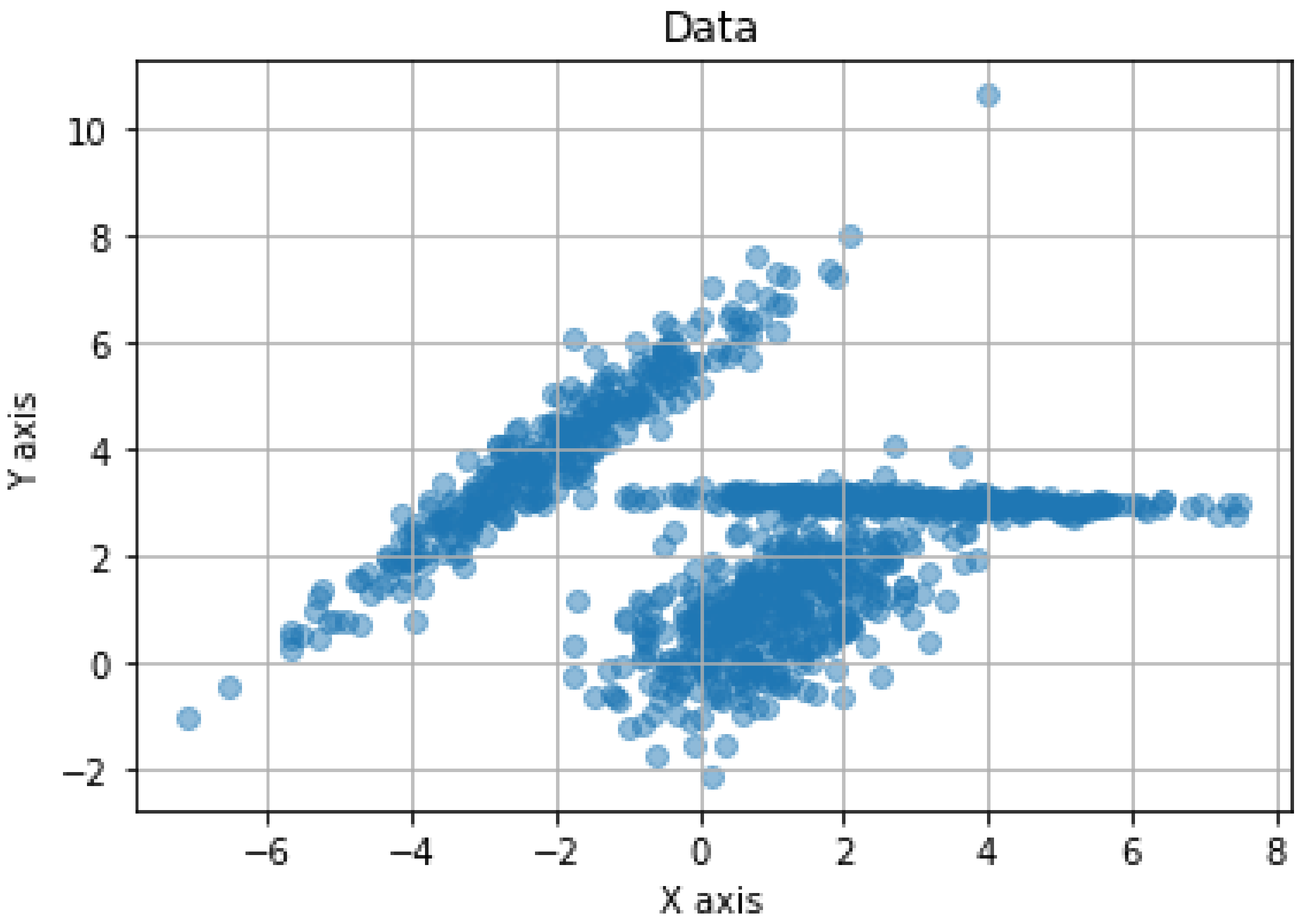
Goal of unsupervised learning is to **learn data structures** without labels

- Discussion: What kind of structures can you see?

What kind of structures can you see?



What kind of structures can you see?



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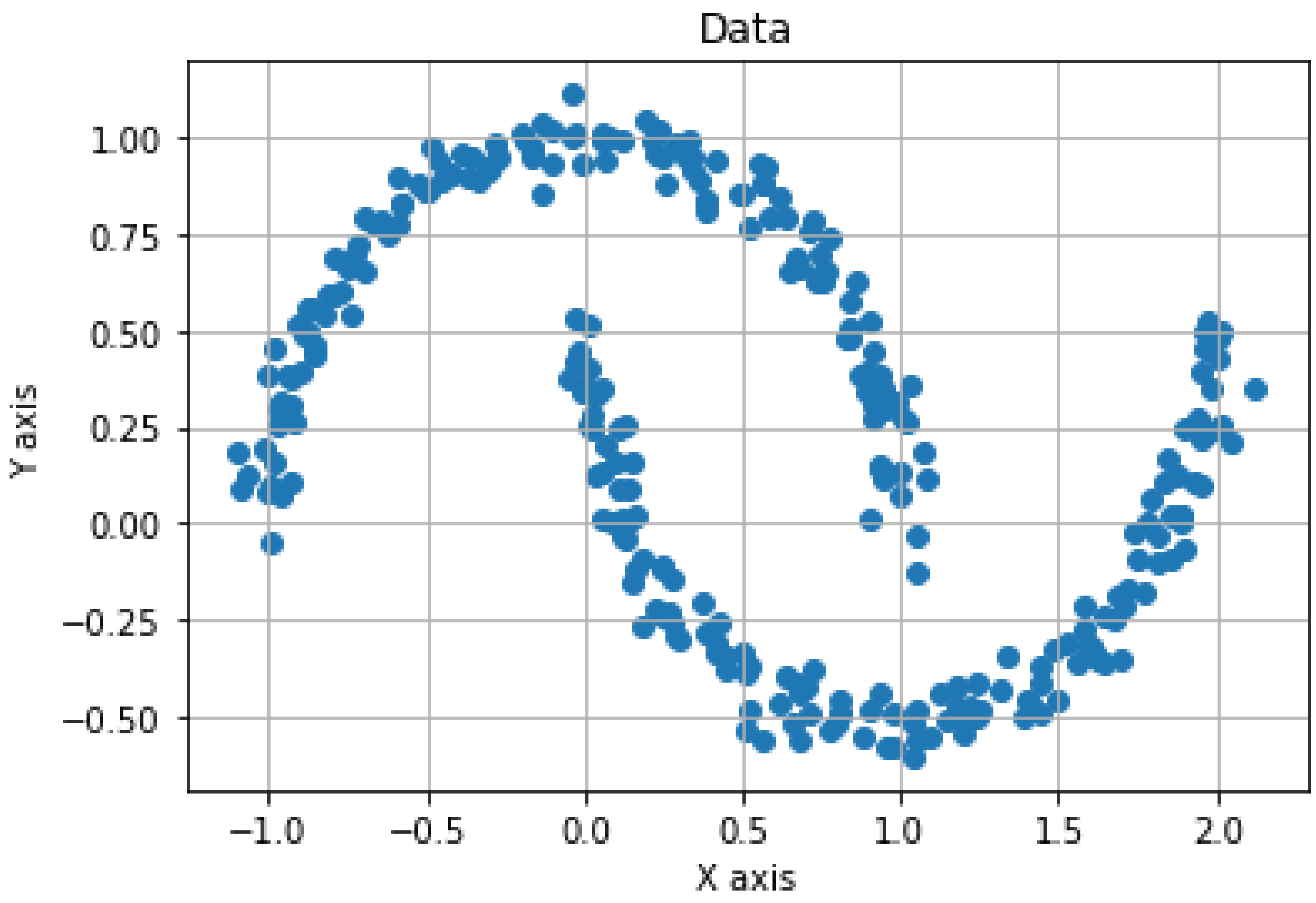

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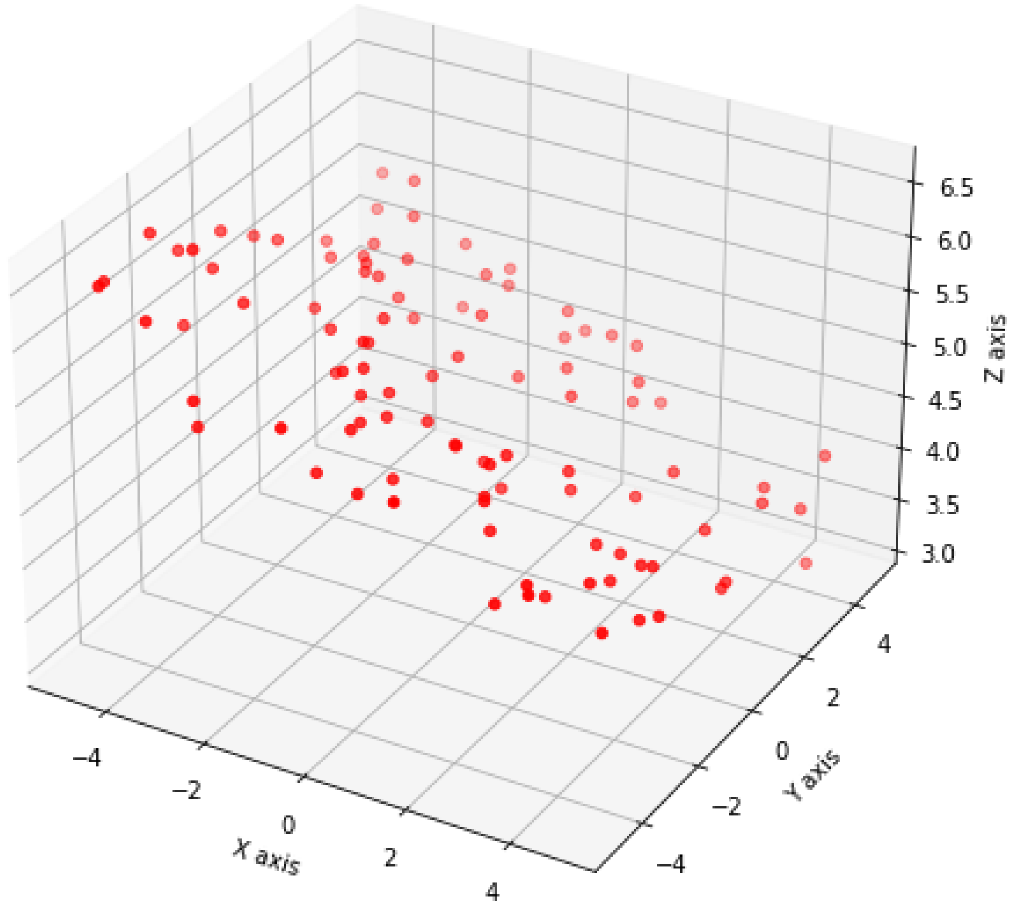

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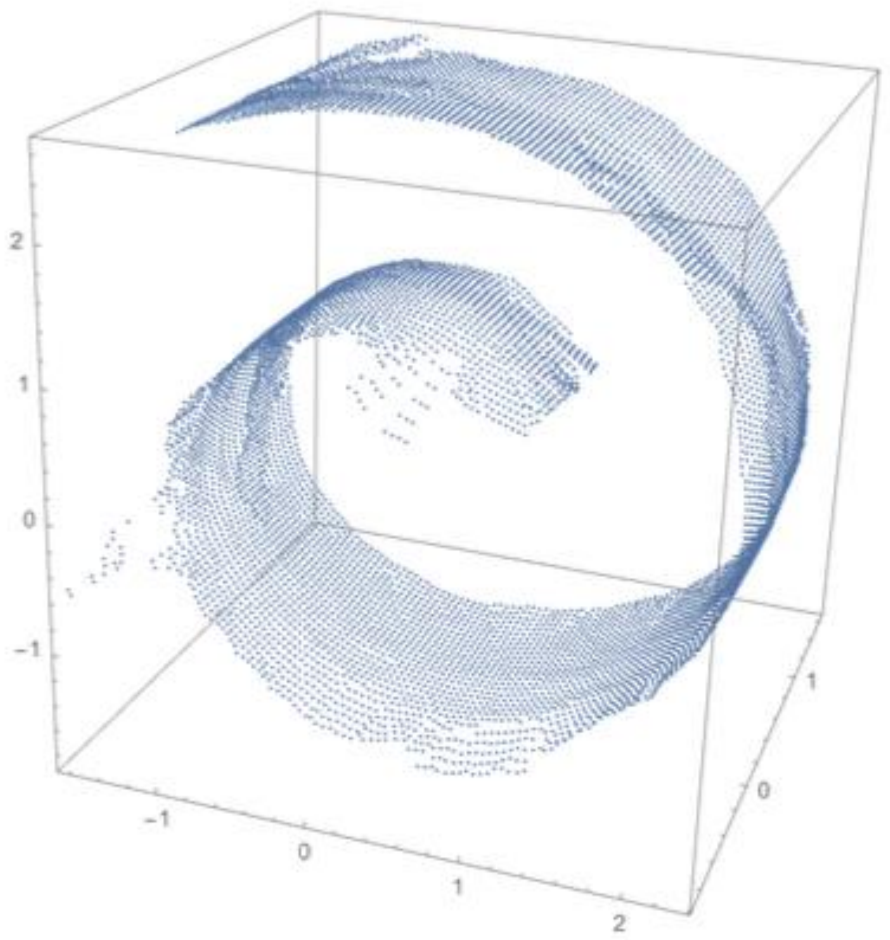
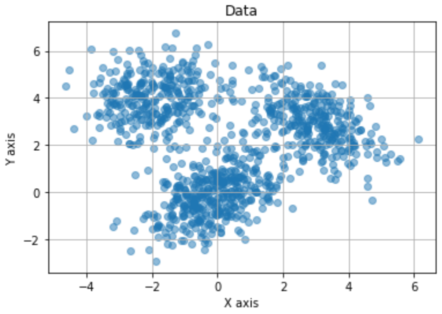
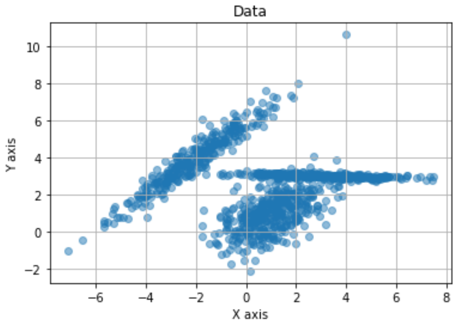
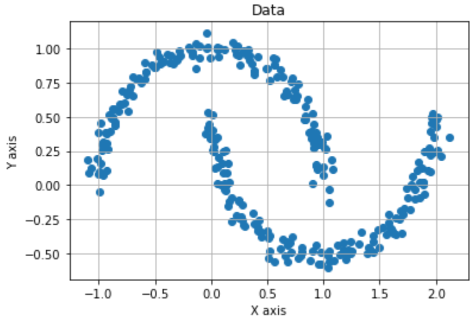


Two broad categories of unsupervised learning (1) Clustering (2) Dimension reduction

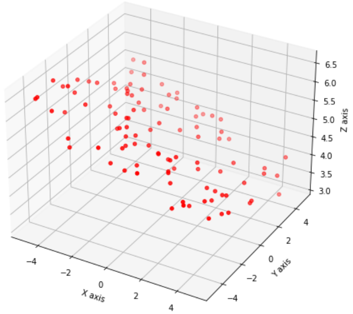
- Clustering:
  - finding a partition of the data that makes sense.

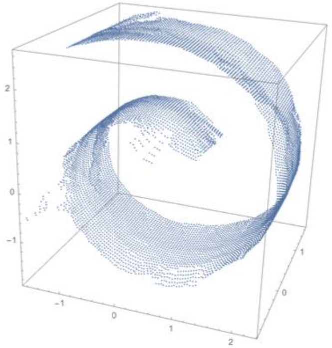




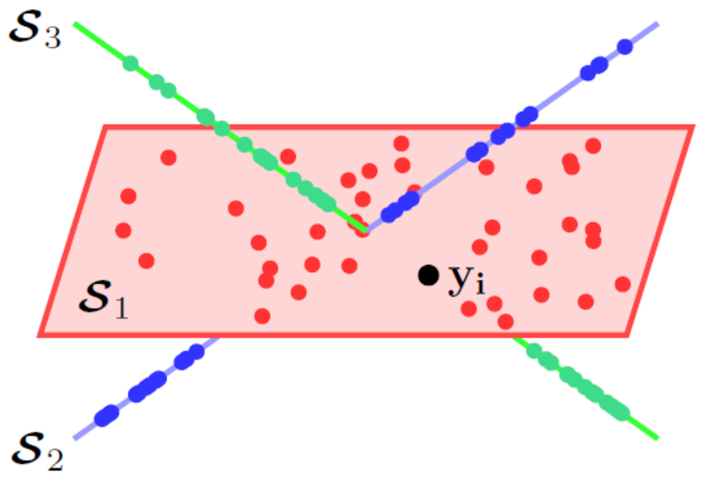


- Dimension reduction:
  - identifying a more compact representation (low-dimension) of data



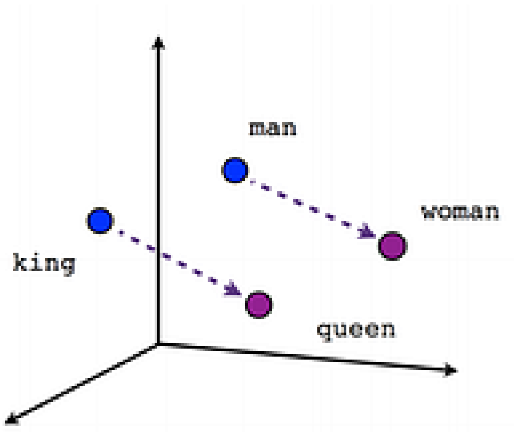


Application: Motion segmentation and subspace clustering

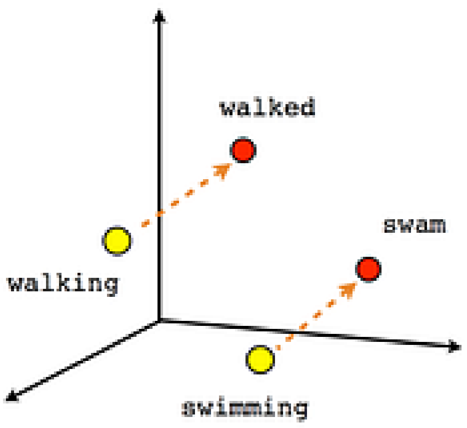


Applications: learn useful vector space representation of language

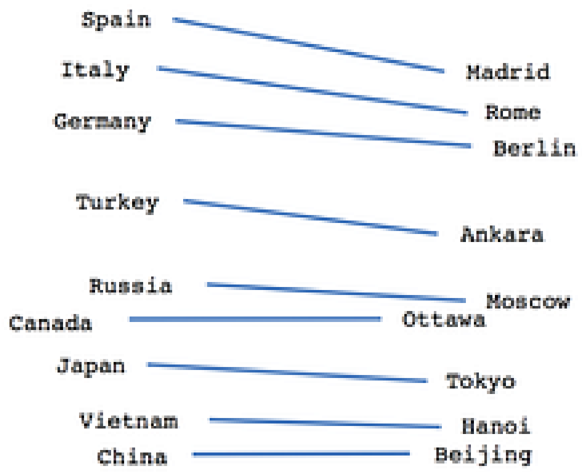
- So you can do algebra on them..



Male-Female



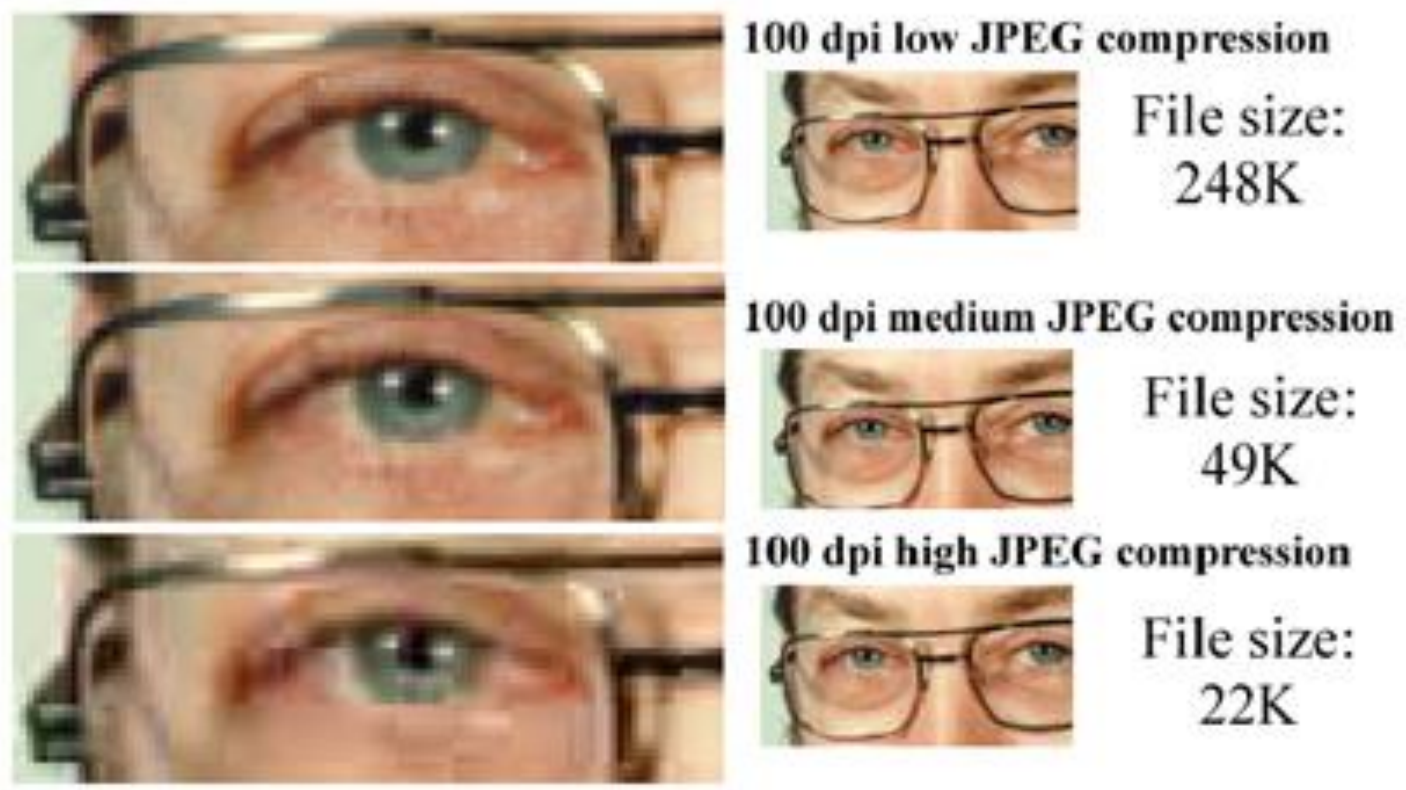
Verb tense



Country-Capital

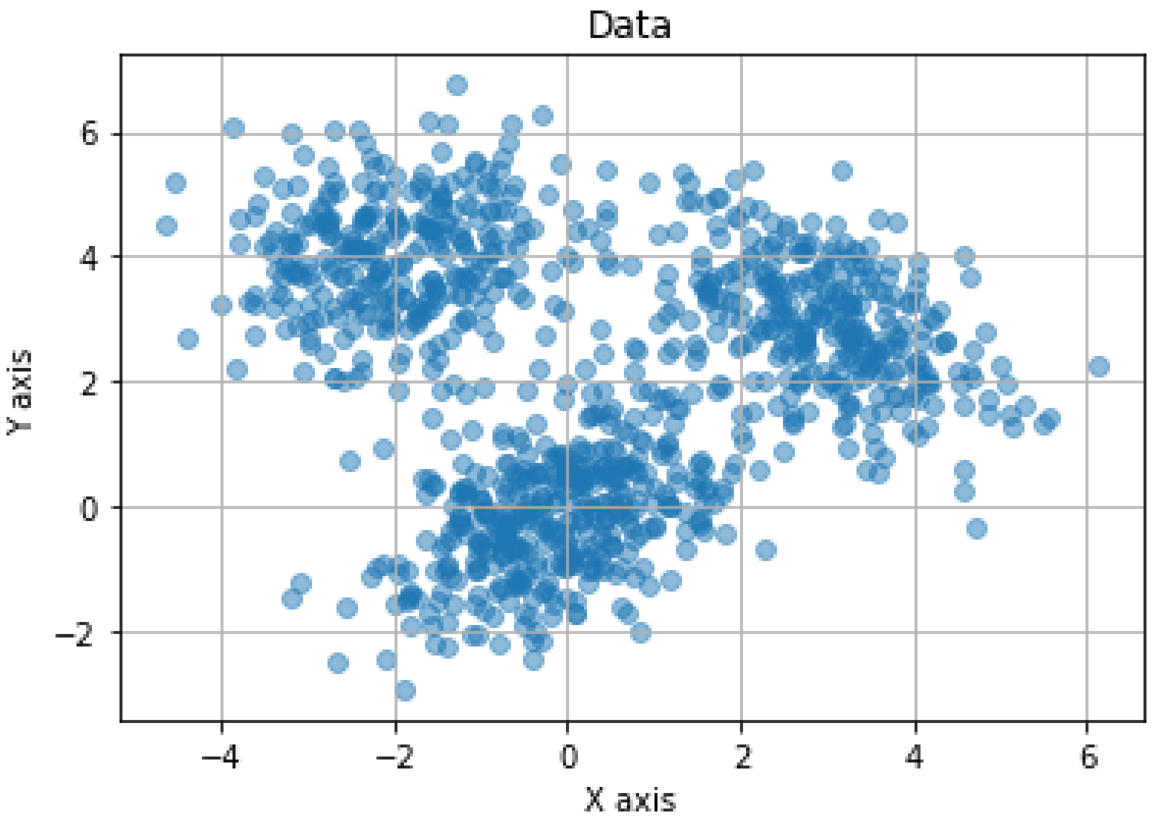
Source: https://towardsdatascience.com/creating-word-embeddings-coding-the-word2vec-algorithm-in-python-using-deep-learning-b337d0ba17a8

Application: Image / video compression



Source: http://preservationtutorial.library.cornell.edu/intro/intro-07.html

How do you learn the structure you see?



- Come up with a loss function to minimize?
- Come up a probabilistic model that generates the data?

The problem of k-means clustering

$$\arg\min_{\mathbf{S}} \sum_{i=1}^{k} \sum_{\mathbf{x} \in S_i} \|\mathbf{x} - \boldsymbol{\mu}_i\|^2$$

- Where $\mathbf{S} = \{S_1, S_2, \ldots, S_k\}$ is a partition of the datase $(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n)$,
- And $\boldsymbol{\mu}_i = \frac{1}{|S_i|} \sum_{\mathbf{x} \in S_i} \mathbf{x},$ is called a cluster center (centroid) of S_i

The above optimization problem is equivalent to the following loss minimization

$$\min_{\mu_1, \ldots, \mu_k \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} \min_{j \in [k]} \|x_i - \mu_j\|^2$$

- Once we find the **centroids**, finding the partition of the data is easy.
- If we have the partition, finding the corresponding centroids is also easy.
- **Idea:** Alternating minimizing the centroids and cluster assignments.

K-means clustering with Lloyd's algorithm

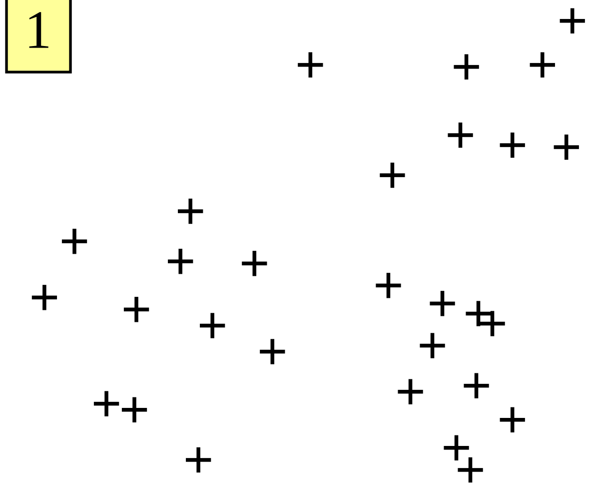
K is a hyperparameter

Algorithm KMeans(D, K) – K-means clustering using Euclidean distance Dis_2.

Input : data $D \subseteq \mathbb{R}^d$; number of clusters $K \in \mathbb{N}$.
Output : K cluster means $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K \in \mathbb{R}^d$.

randomly initialise K vectors $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K \in \mathbb{R}^d$;
repeat
  assign each $\mathbf{x} \in D$ to $\arg\min_j \mathrm{Dis}_2(\mathbf{x}, \boldsymbol{\mu}_j)$; ⟵ *1-Nearest neighbor assignment*
  for $j = 1$ to K **do**
    $D_j \leftarrow \{\mathbf{x} \in D | \mathbf{x}$ assigned to cluster $j\}$; ⟵ *Partition defined by assignment*
    $\boldsymbol{\mu}_j = \frac{1}{|D_j|} \sum_{\mathbf{x} \in D_j} \mathbf{x}$; ⟵ *Re-compute the cluster mean*
  end
until no change in $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$;
return $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$;

1



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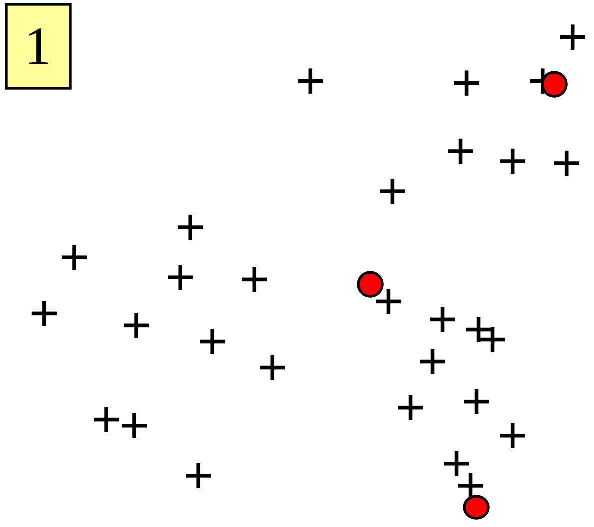

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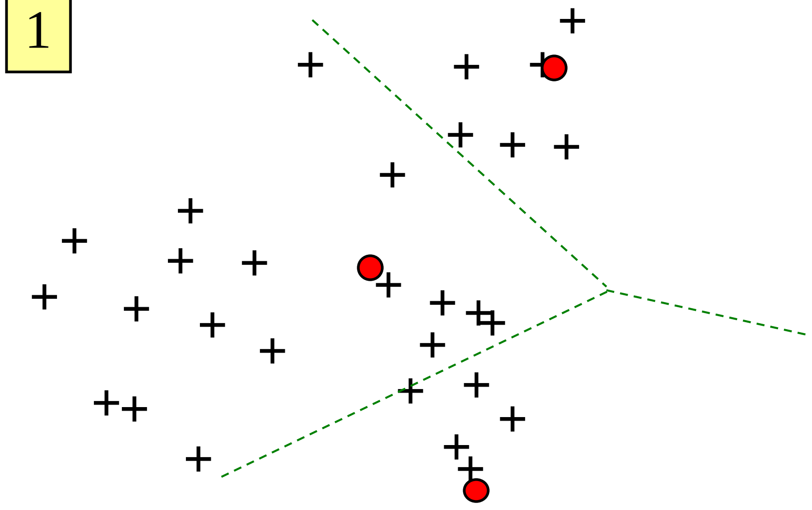

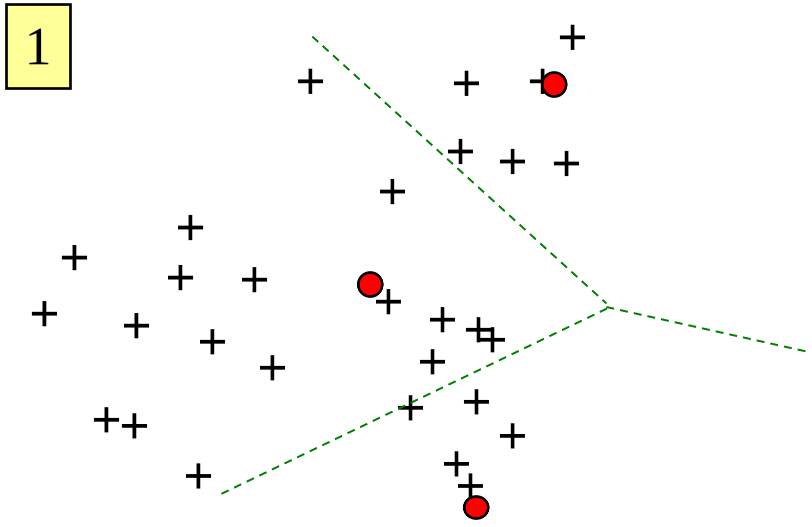
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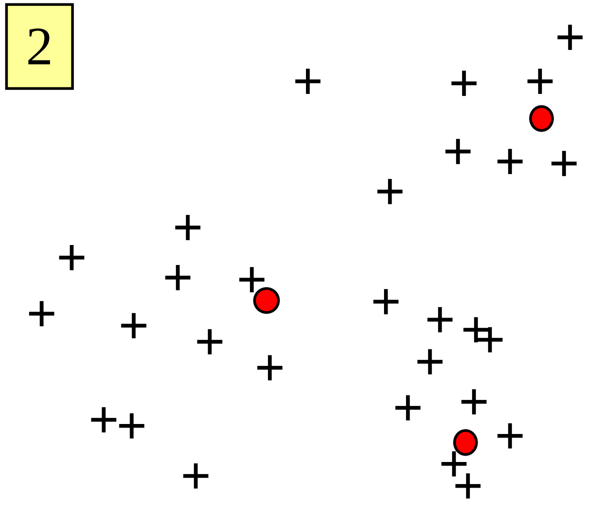
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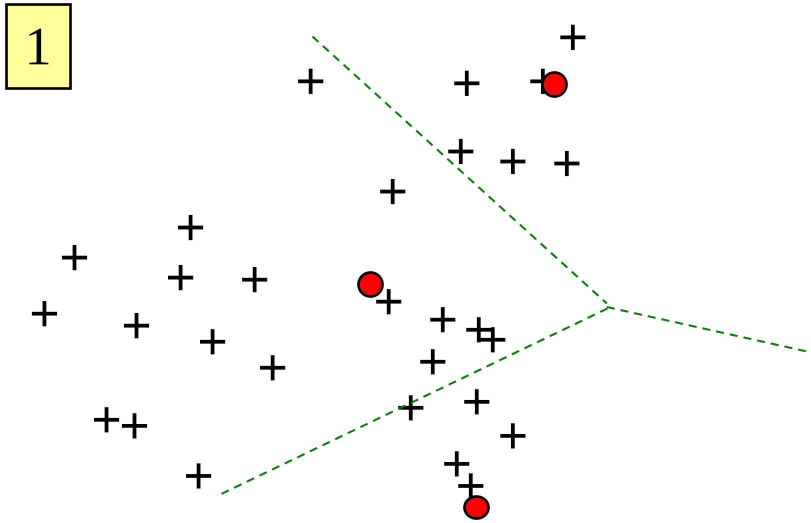
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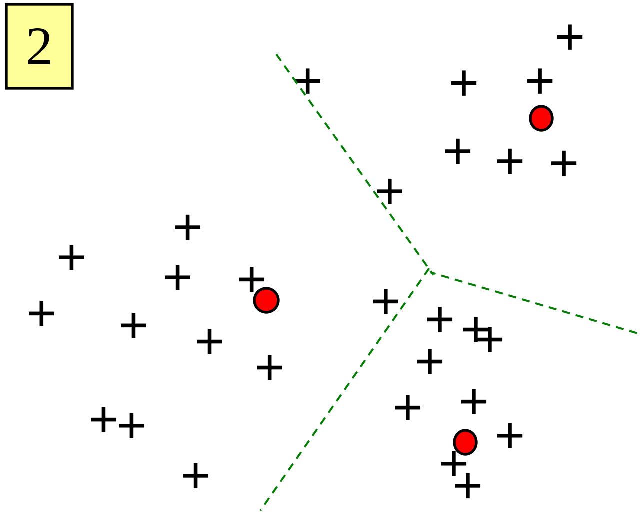
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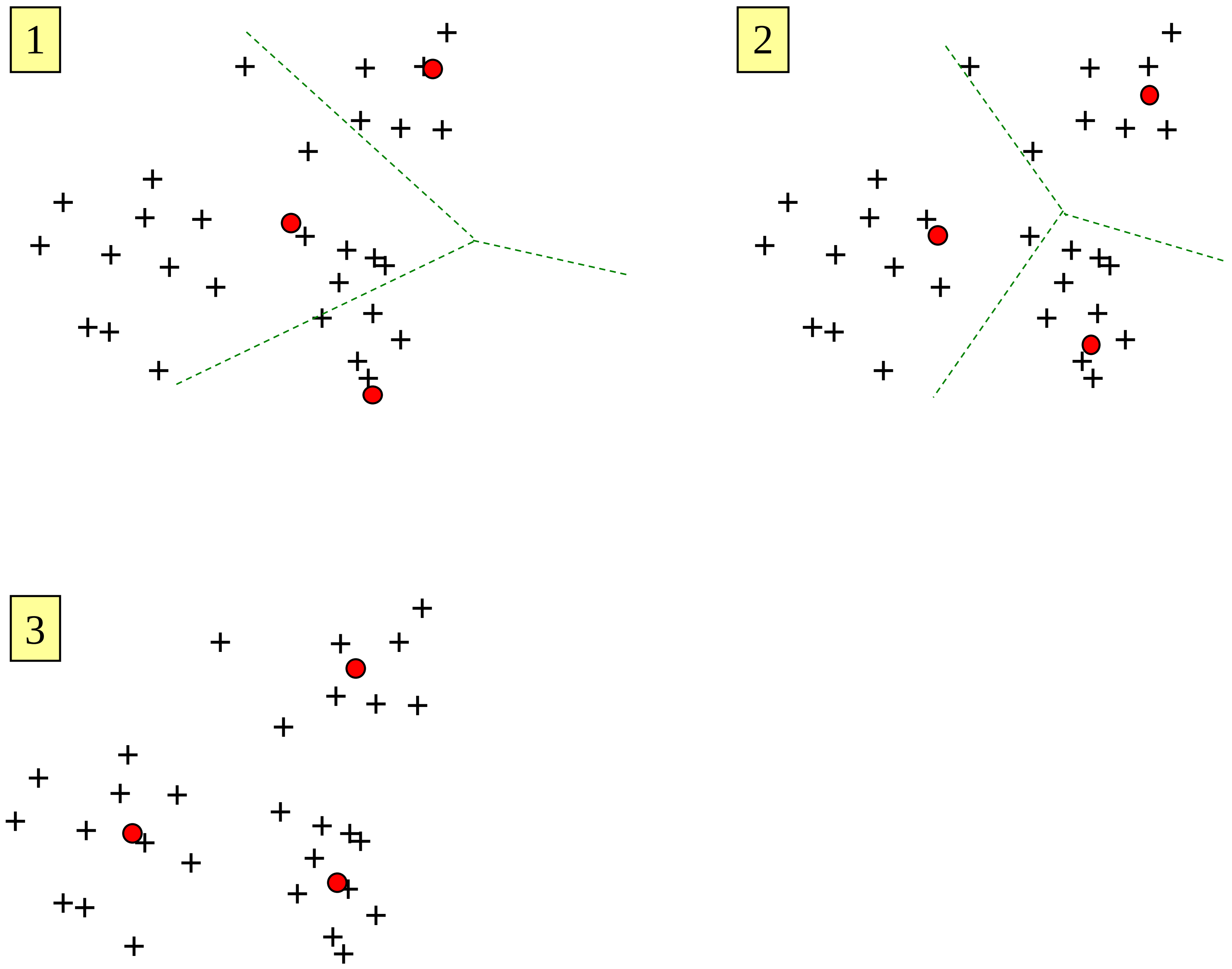
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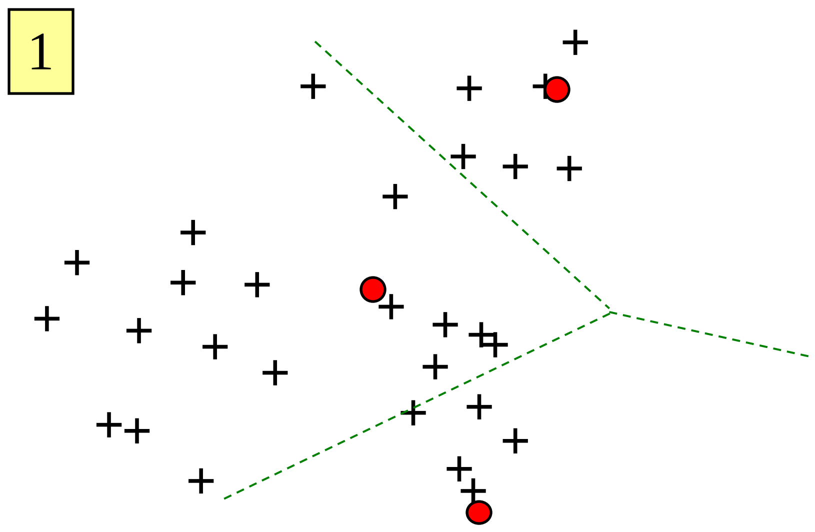
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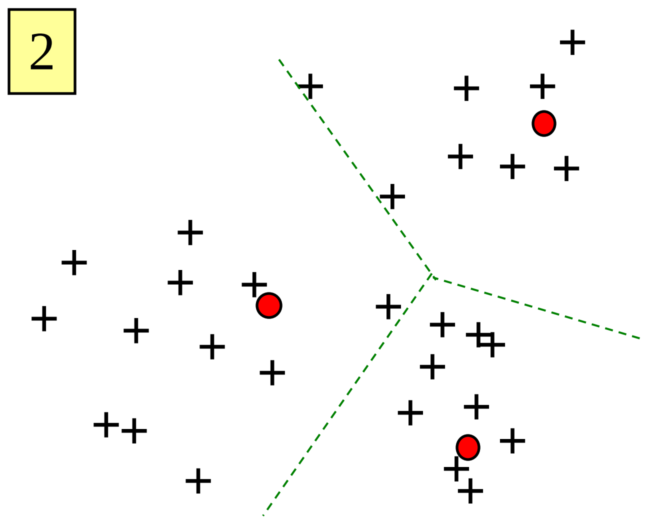
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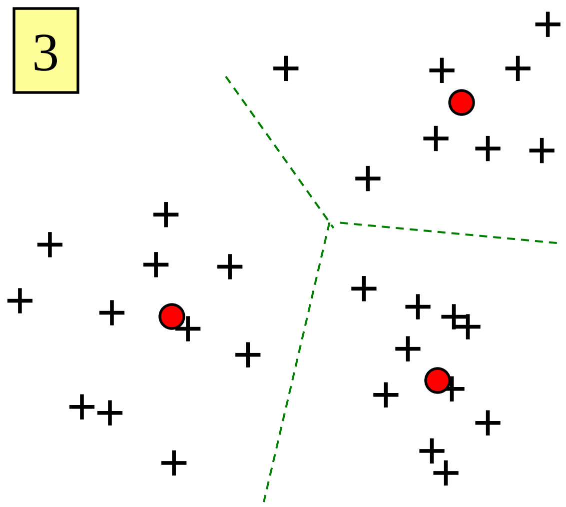
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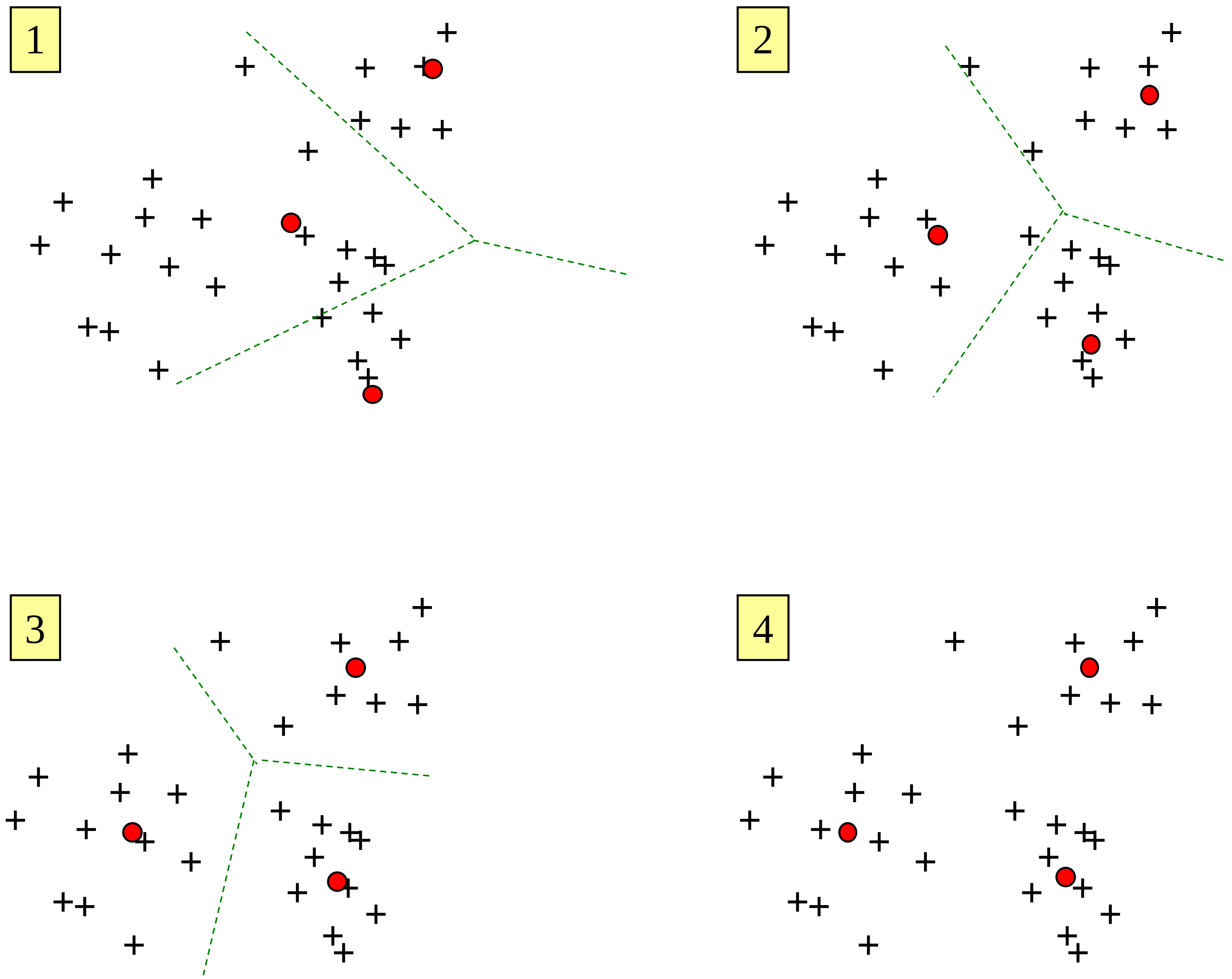
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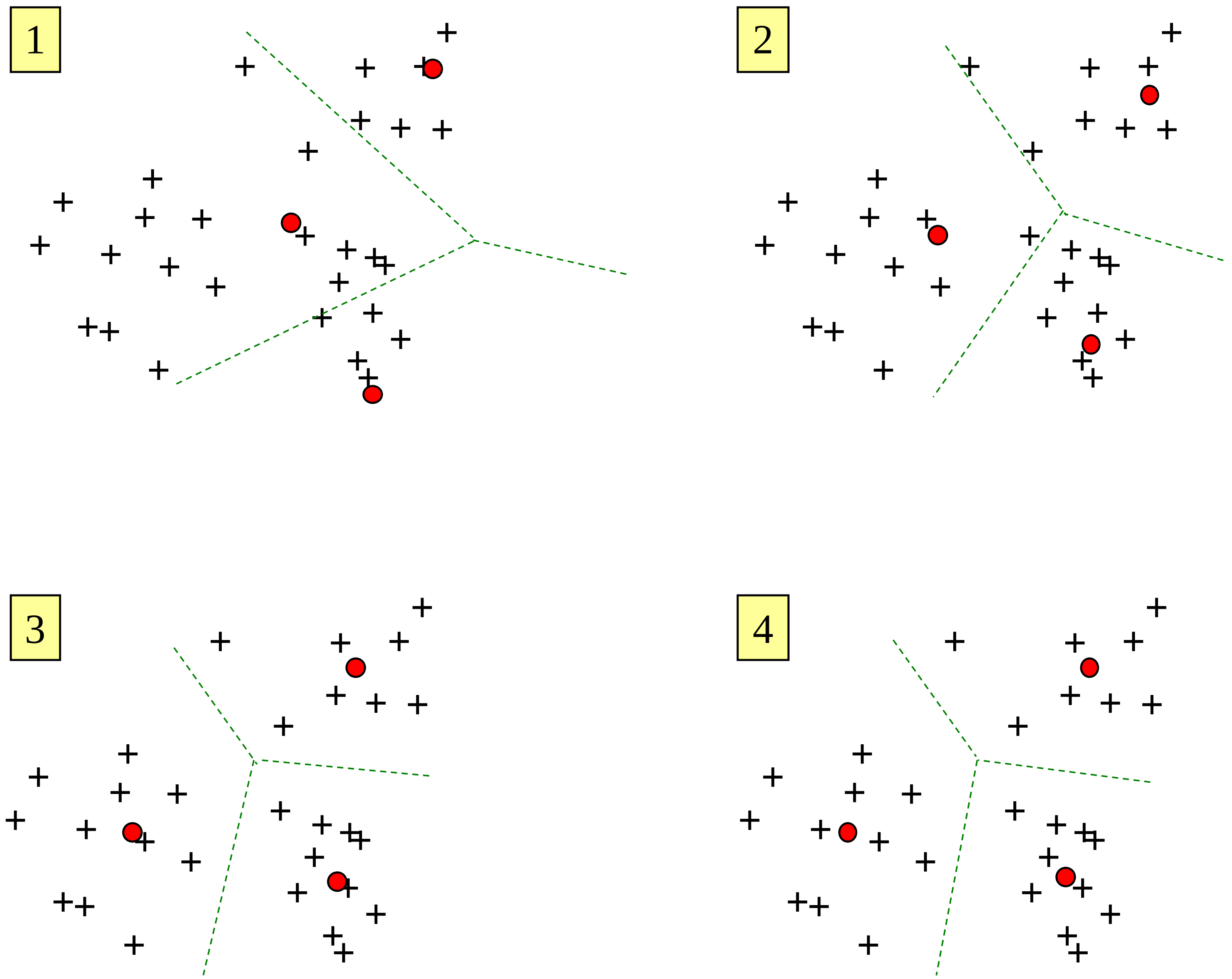
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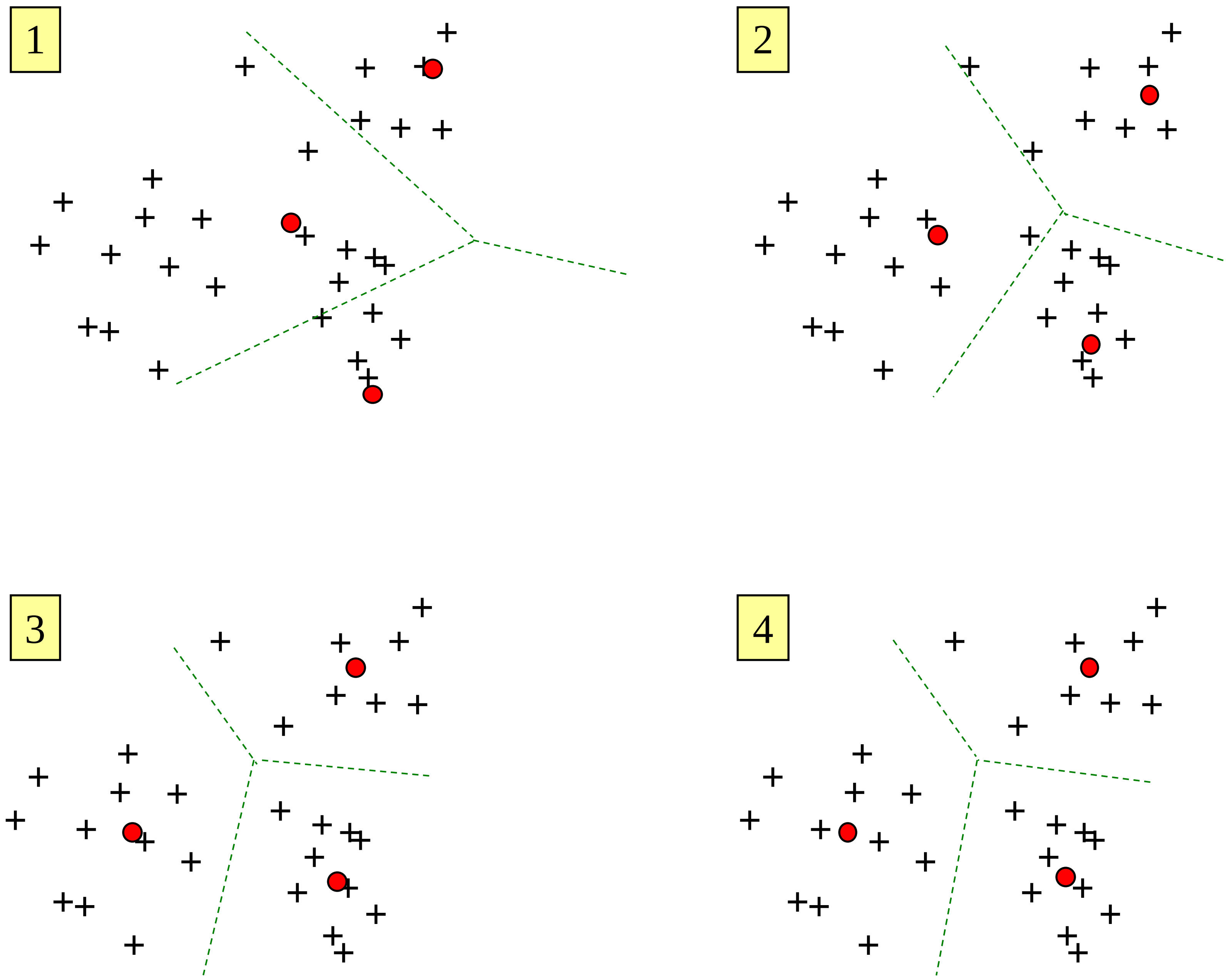
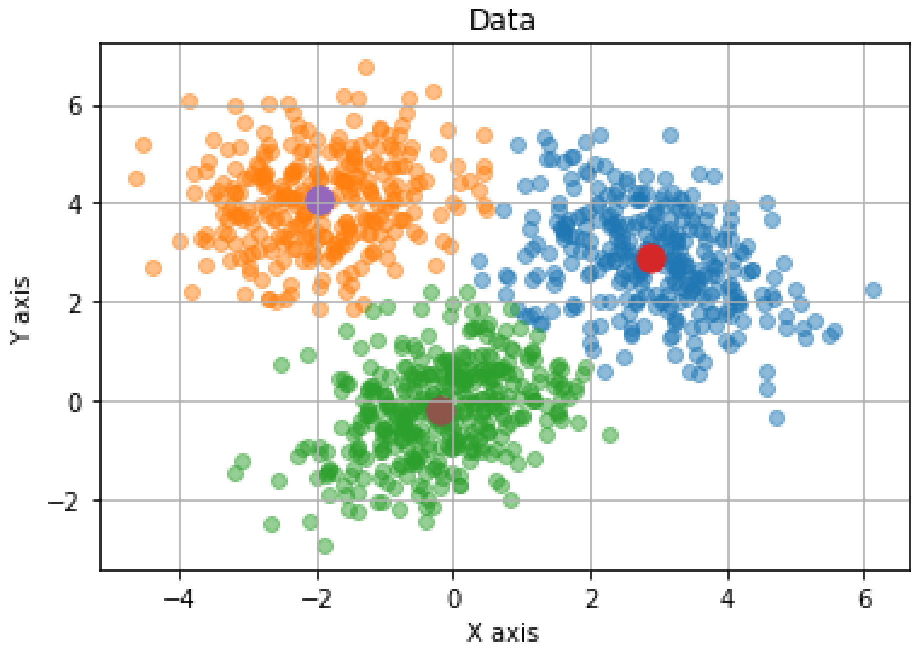
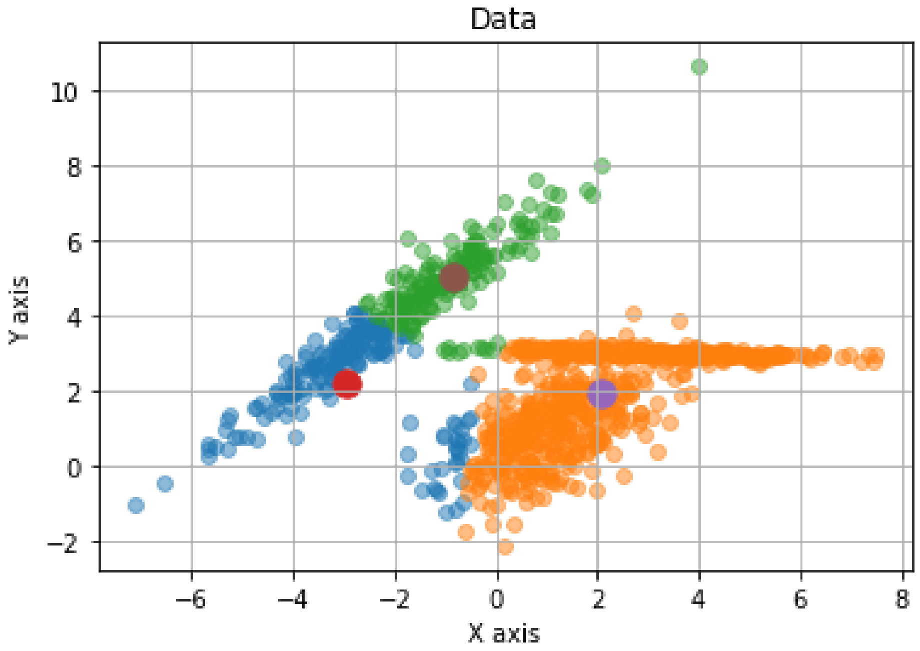


No change – finished!

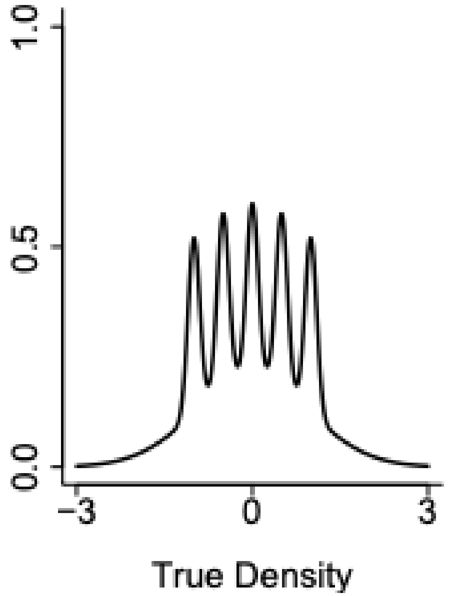
K-means on our previous examples

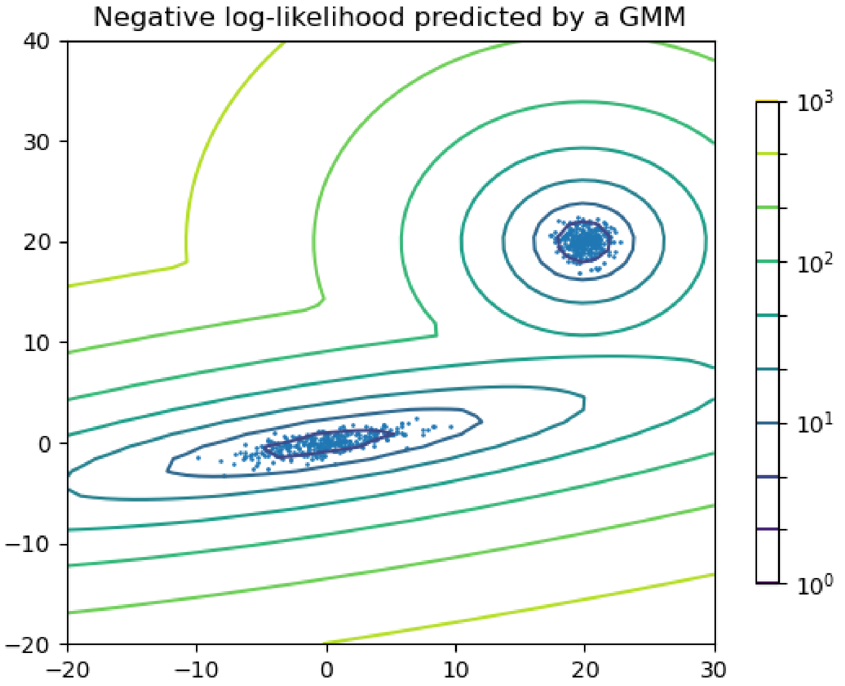




Gaussian mixture models

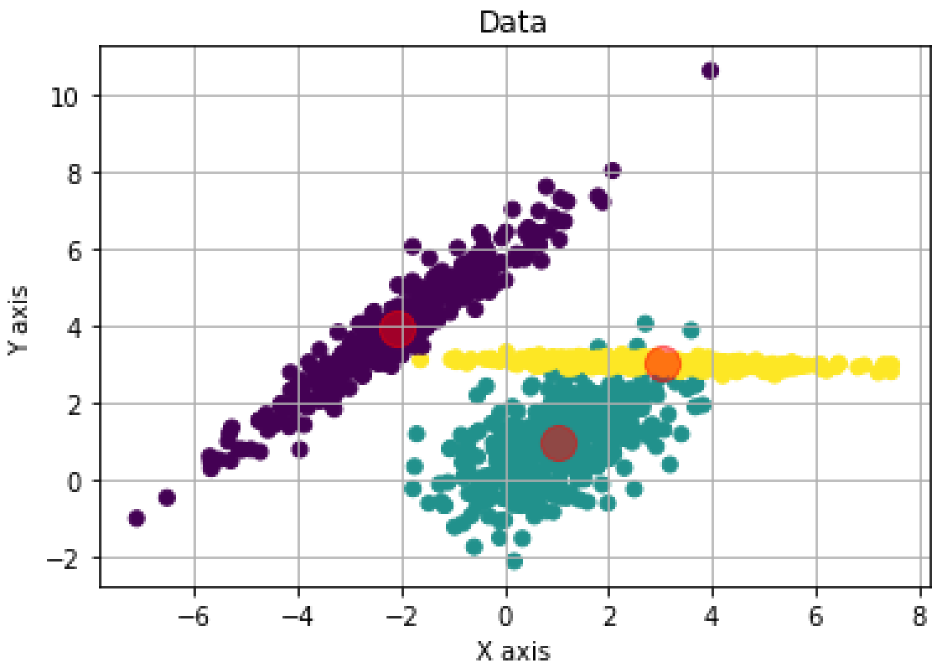
- Assume the data is generated from a mixture of Gaussian distribution

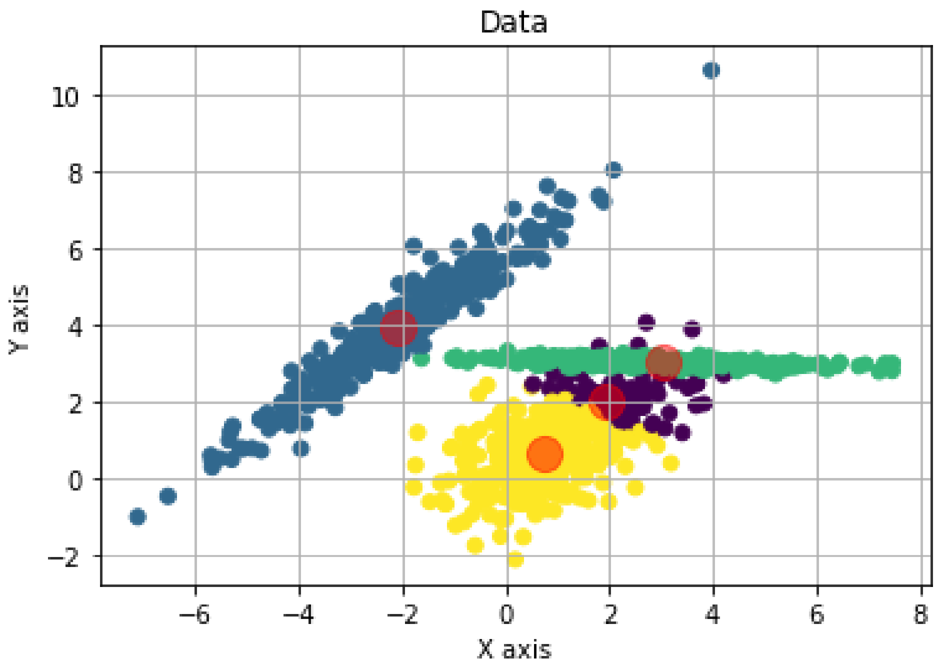




- Data generating process

Fitting mixture of Gaussian model





- Assign **soft** labels to each data point.
- Algorithms for fitting Gaussian mixture models?
  - Expectation-Maximization (not covered in this course… but also alternating making updates)

Summary: Unsupervised Learning

- K-means algorithm
  - Assign hard labels to data points
  - How does it work?
    - Alternating makes updates
    - Which distance function to use?
    - How many cluster centers (centroids) to choose?
    - How to initialize the centroids?

- Gaussian mixture models
  - Assign soft labels to data points
  - A probabilistic model for clustering