Lecture 17: Clustering

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Announcement

- Quiz due today
- The practice final will be released
- Hw1/Midterm regrading

Clustering

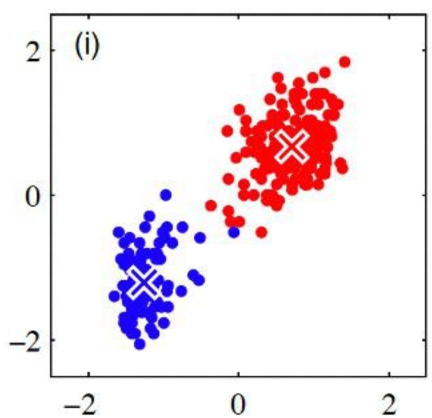
Goal of Clustering

- Given a collection of data points, the goal is to find structure in the data: organize that data into sensible groups.

- Applications
  - Topics in news articles
  - Identify communities within social networks

How to define clusters?

- A set of entities that are “alike”
- May be described as connected regions of a multi-dimensional space



How to define clusters?

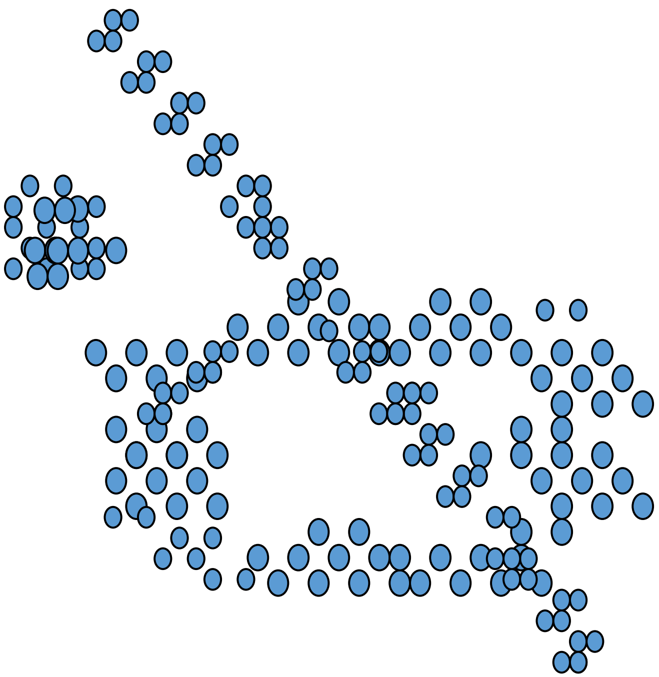







How to define a cluster?

How many clusters do we have?



Today’s lecture

- K-Means

- K-Medoids

- GMM (probabilistic version)

K-Means

Hogwarts (Harry Potter)

- Sorting Hat – cluster kids into four groups based on four underlying prototypes

Godric Gryffindor

Helga Hufflepuff

Rowena Ravenclaw

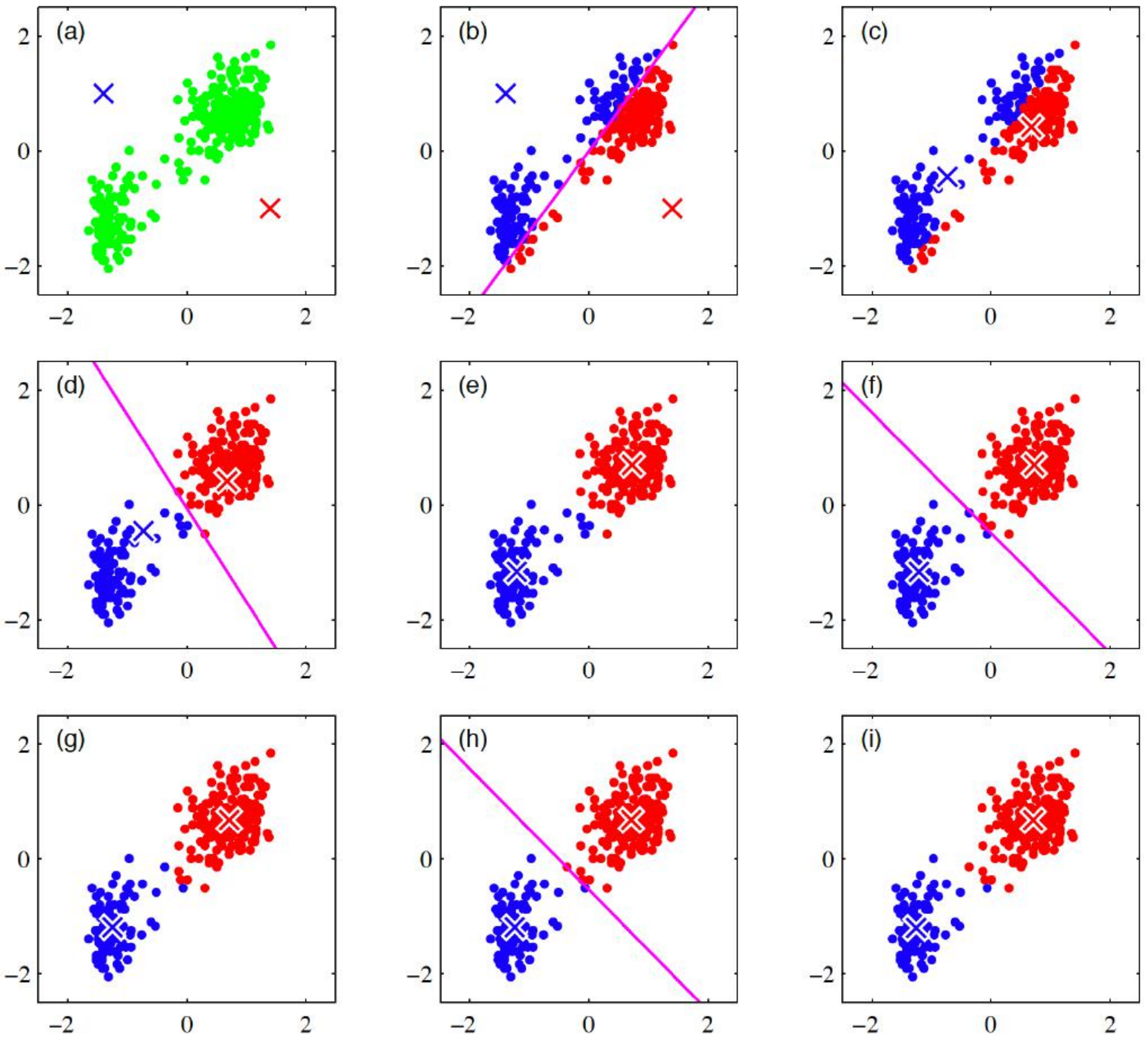
Salazar Slytherin

K-Means Intuition

- Sorting Hat – cluster kids into four groups based on four underlying prototypes

- The prototype of each house is *the average of all kids of the house*
- Algorithm*:*
  Alternatively, updating the prototype & the cluster assignment

Intuition of K-Means



http://shabal.in/visuals/kmeans/6.html

Problem setting

- An optimization problem:
  - Given $D = \{x_n\}_{n=1}^{N}$ and a number K, we want to group data point to K clusters
  - $A(x) \in \{1,2,\dots K\}$: the cluster membership
  - $r_{nk} \in \{0,1\}$ indicates whether $A(x_n) = k$

Problem setting

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  - $r_{nk} \in \{0,1\}$ indicates whether $A(x_n) = k$

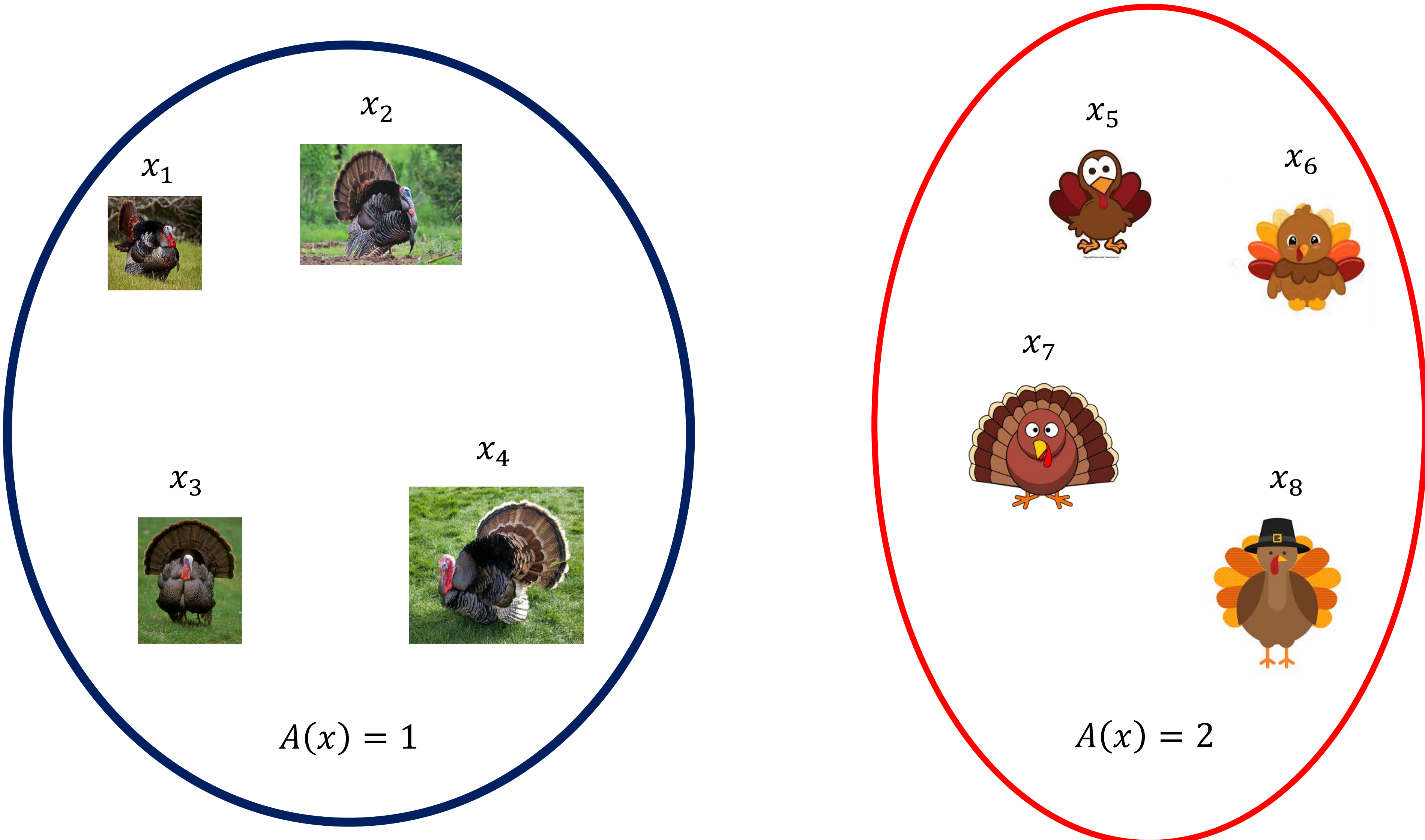
x_1
$A(x_1) = 1$
$r_{11} = 1$
$r_{12} = 0$

x_2
$A(x_2) = 2$
$r_{21} = 0$
$r_{22} = 1$

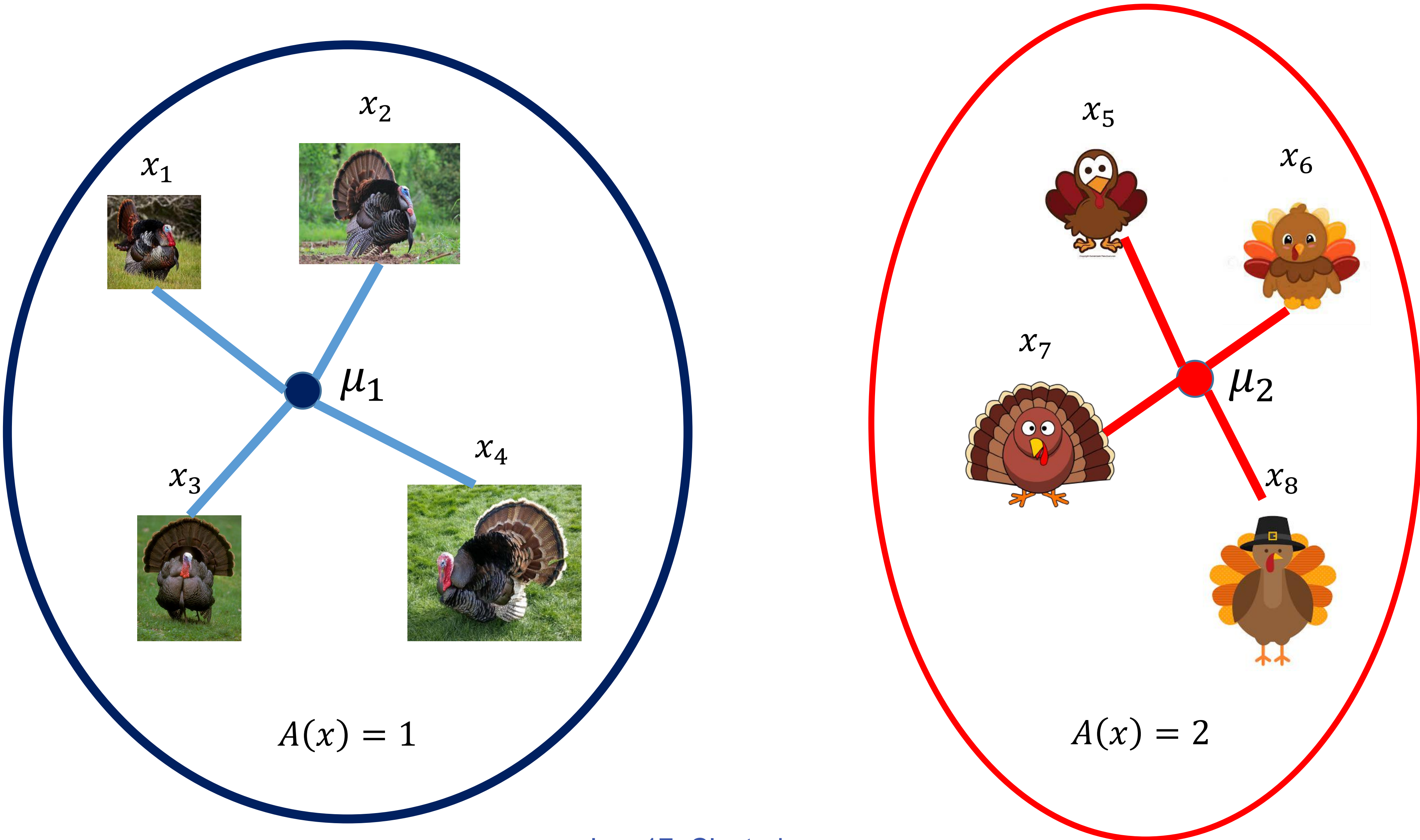
x_3
$A(x_3) = 1$
$r_{31} = 1$
$r_{32} = 0$

K-Means clustering

K-Means clustering

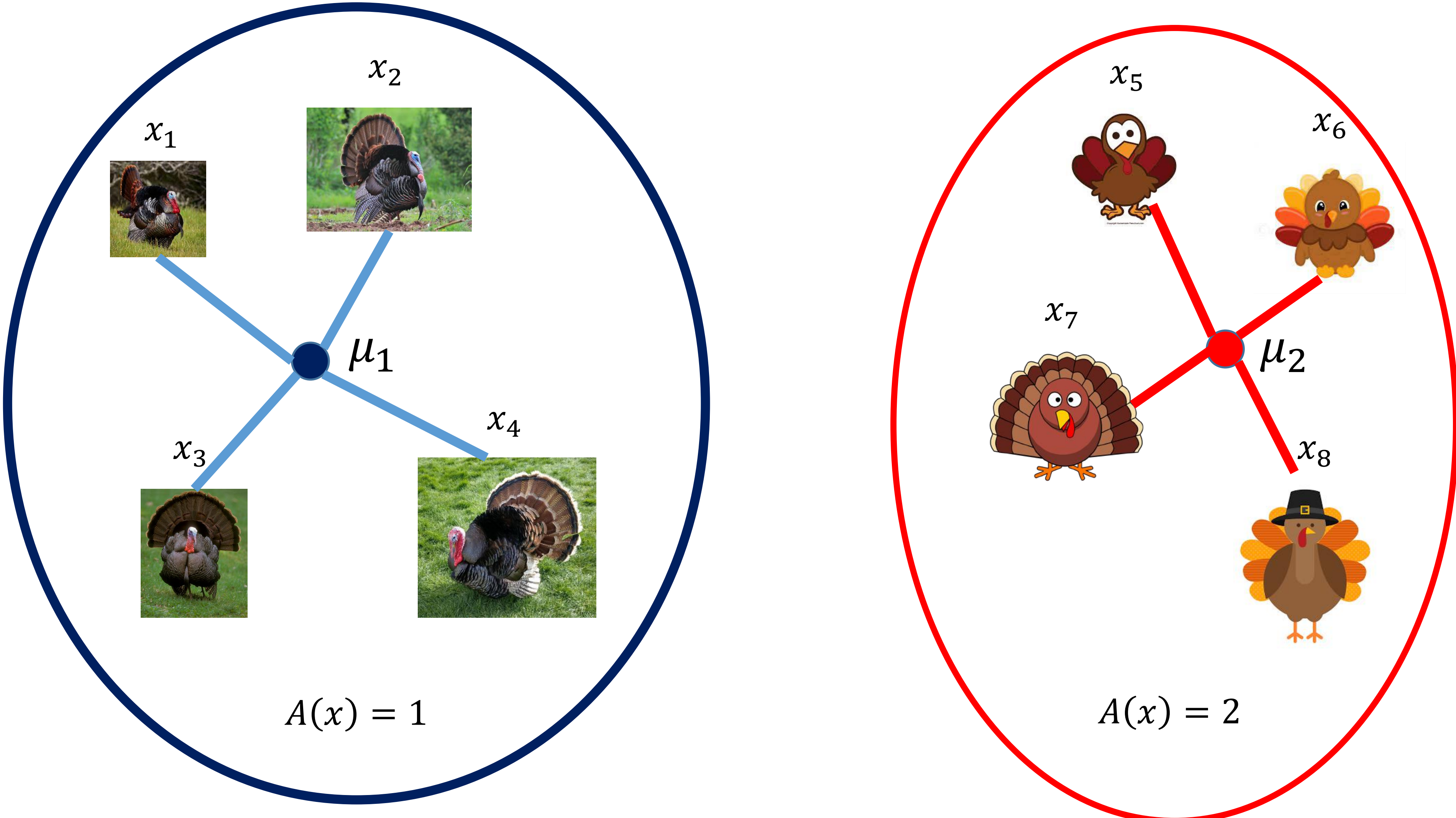


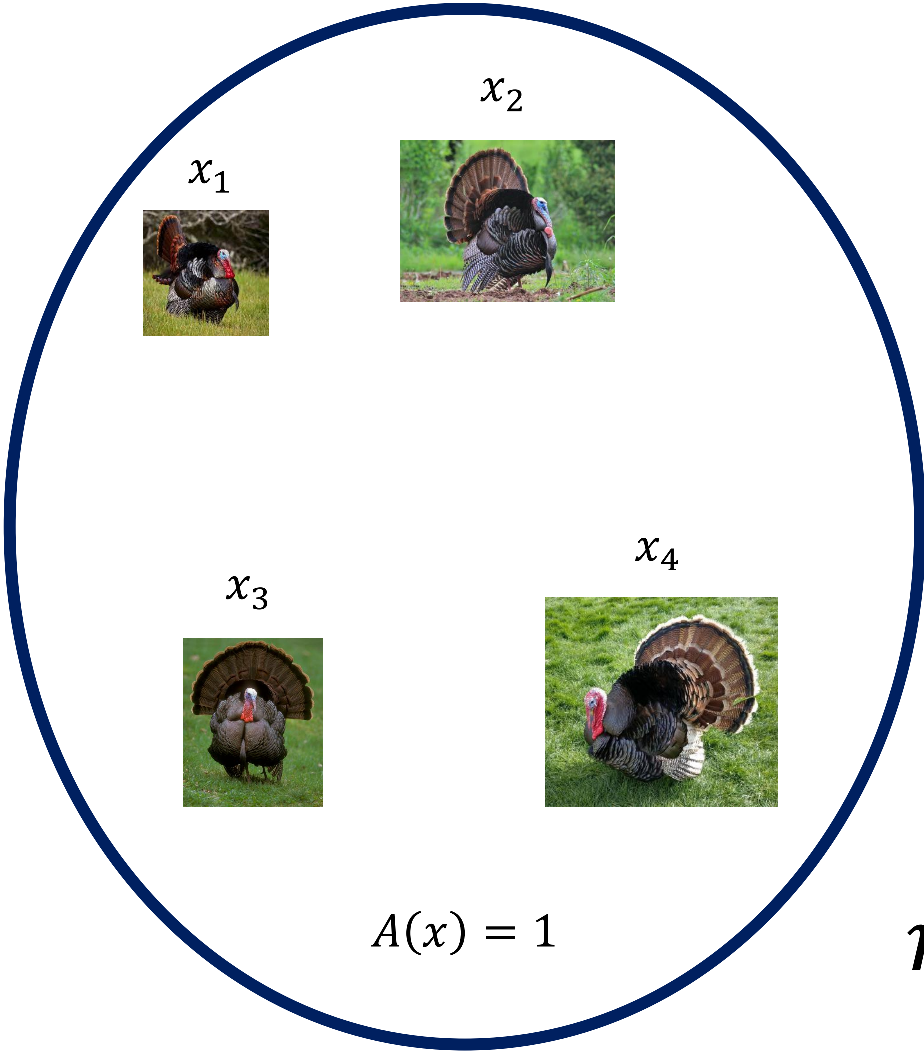
K-Means clustering



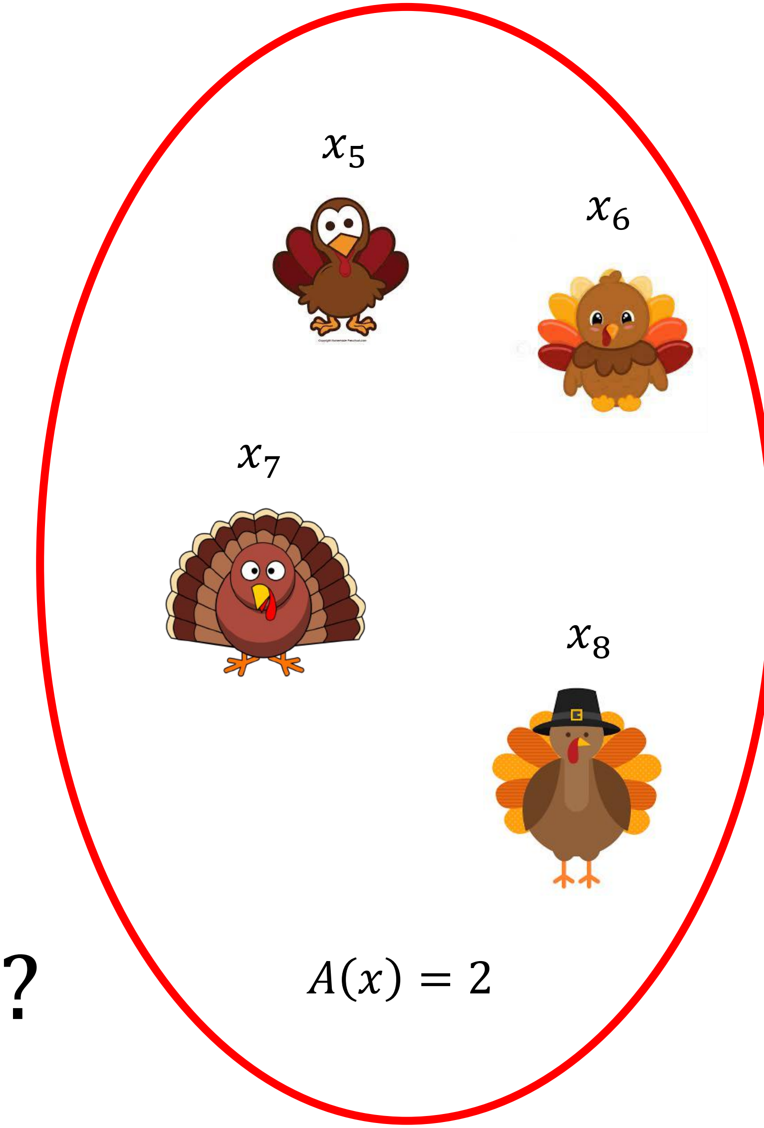
Quantify the clustering quality by $\sum_{n=1}^{4} ||x_n - \mu_1||^2 + \sum_{n=5}^{8} ||x_n - \mu_2||^2$

Mean square distance

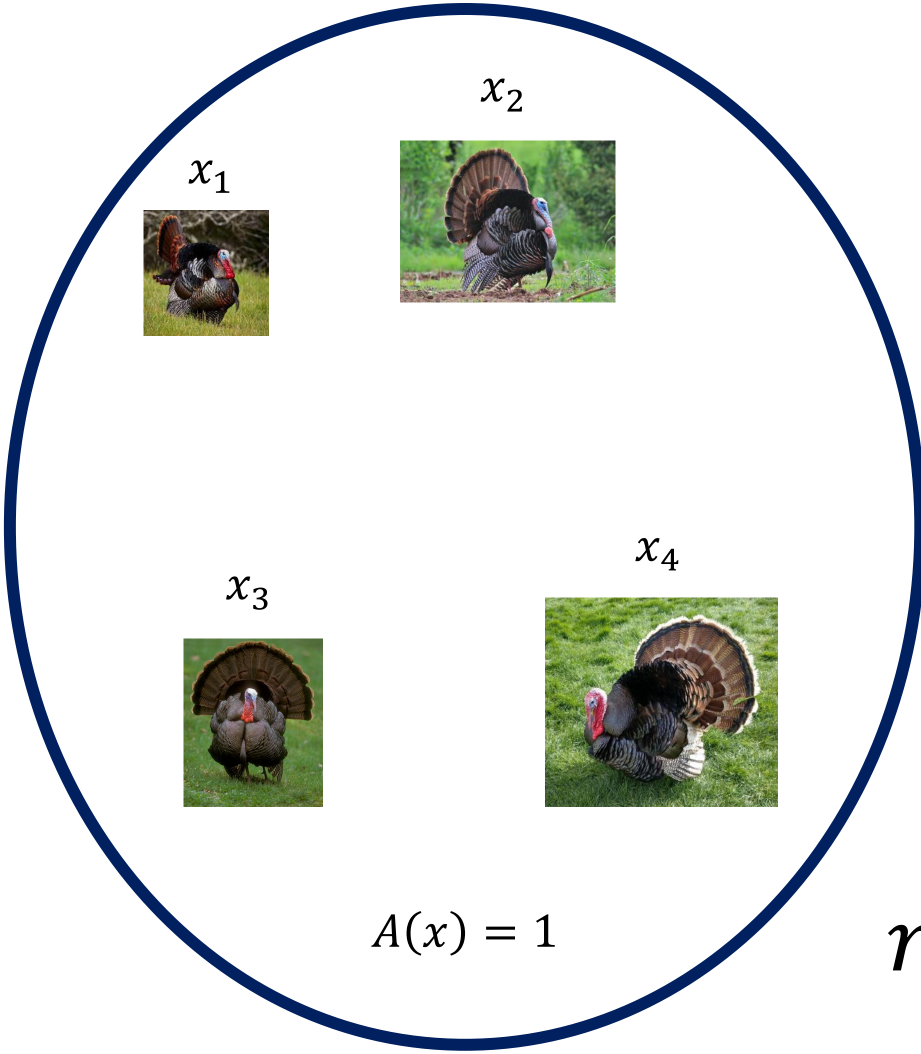




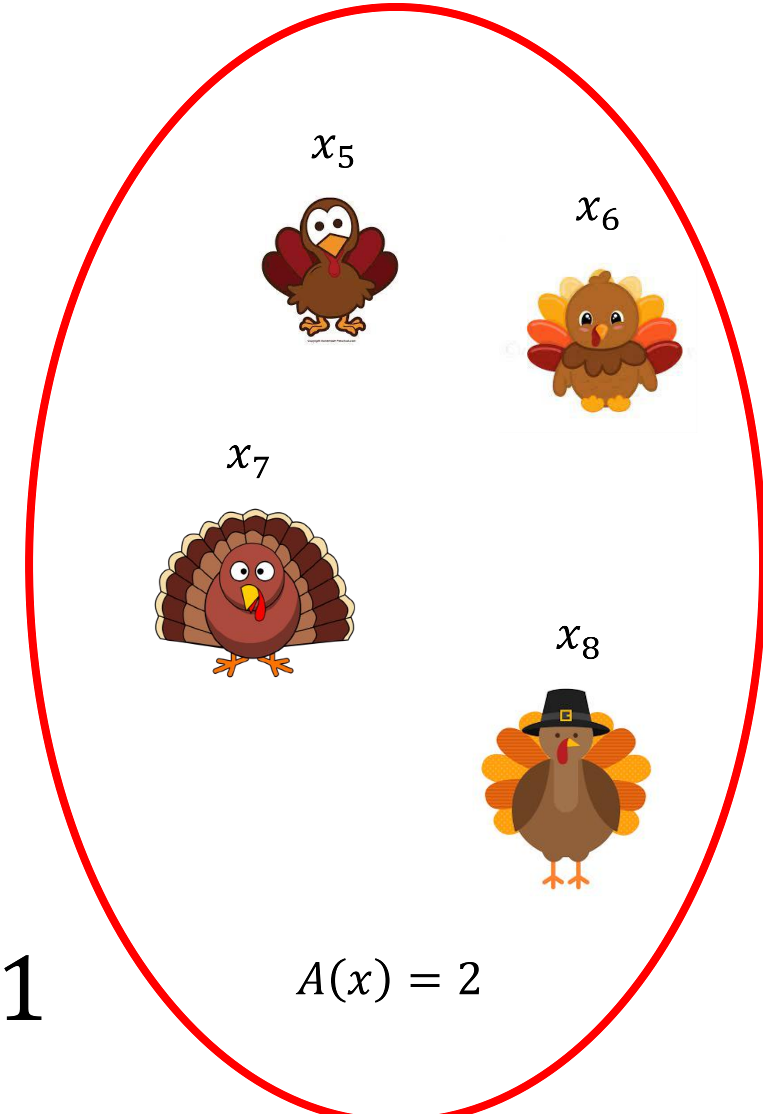
$$r_{31} = ?$$



Quantify the clustering quality by $\sum_{n=1}^{8} \sum_{k=1}^{2} r_{nk} \, ||x_n - \mu_k||^2$



$$r_{31} = 1$$



K-means clustering

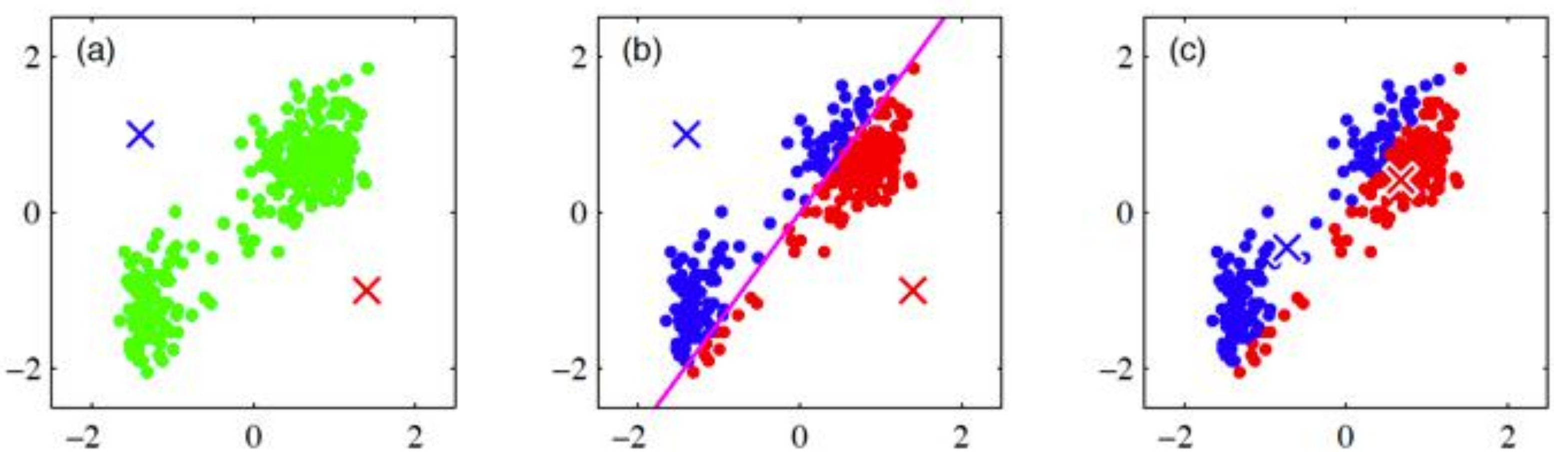
Sum of distances of all the points to their cluster center

- Distortion measure (loss function for clustering)

$$J(\{r_{nk}\}, \{\boldsymbol{\mu}_k\}) = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|_2^2$$

where $r_{nk} \in \{0, 1\}$ is an indicator variable

$$r_{nk} = 1 \quad \text{if and only if} \quad A(\boldsymbol{x}_n) = k$$



K-means objective

$$argmin_{\{r_{nk}\},\{\boldsymbol{\mu}_k\}} J(\{r_{nk}\},\{\boldsymbol{\mu}_k\}) = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|_2^2$$

where $r_{nk} \in \{0,1\}$ is an indicator variable

$$r_{nk} = 1 \quad \text{if and only if} \quad A(\boldsymbol{x}_n) = k$$

- It is a non-convex objective function
- Minimizing the above objective is NP-hard.

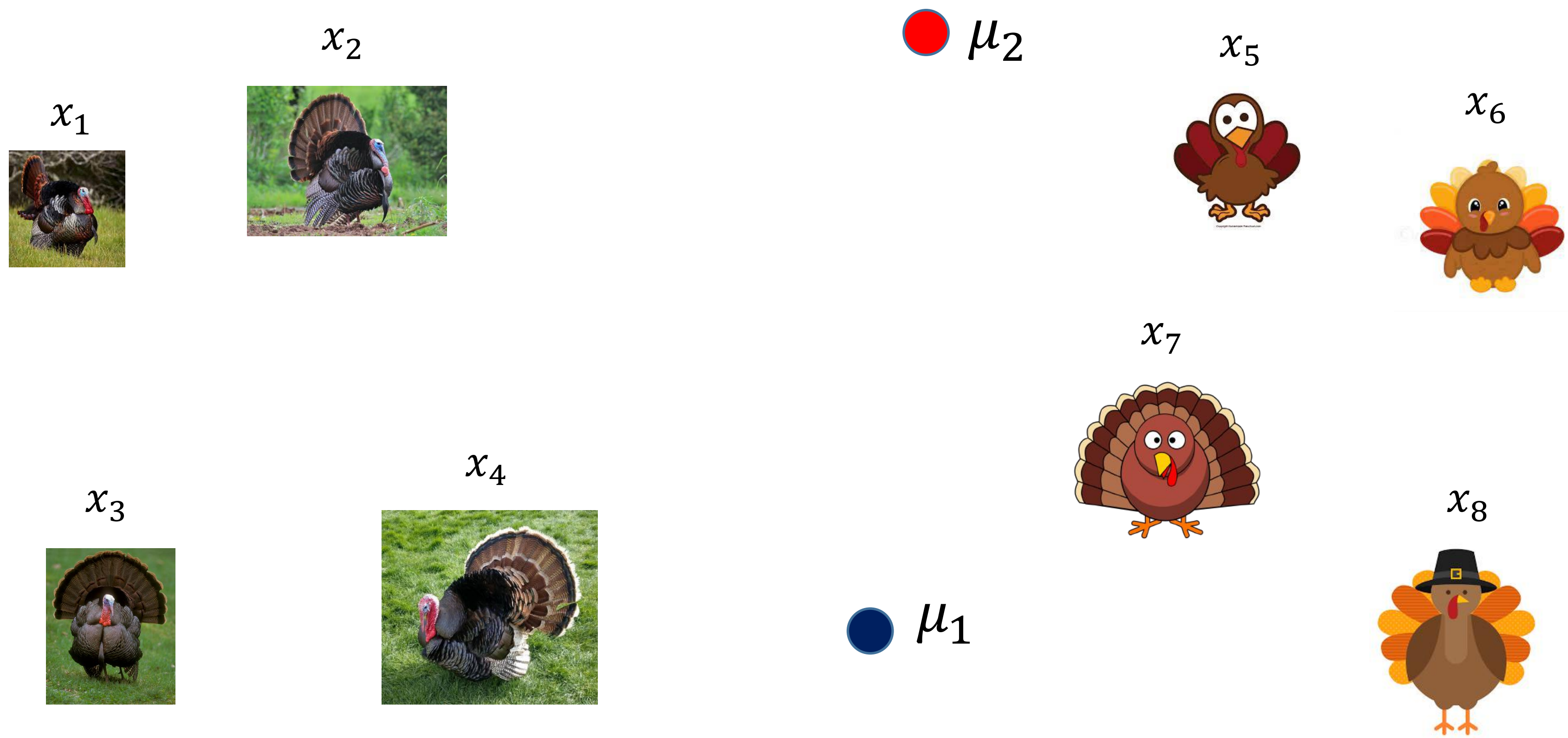
K-means algorithm a.k.a Llyod's algorithm

- A greedy algorithm for minimizing K-means objective – alternative update $\{r_{nk}\}, \{\boldsymbol{\mu}_k\}$
- Step 0: randomly assign the cluster centers $\{\mu_k\}$
- Step 1: Minimize J over $\{r_{nk}\}$ -- reassign cluster member
- Step 2: Minimize J over $\{\mu_k\}$ -- update the cluster centers
- Loop until it converges

$$\boxed{J(\{r_{nk}\}, \{\boldsymbol{\mu}_k\}) = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|_2^2}$$

Step 1: Minimize J over $\{r_{nk}\}$

$$J(\{r_{nk}\}, \{\boldsymbol{\mu}_k\}) = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|_2^2$$

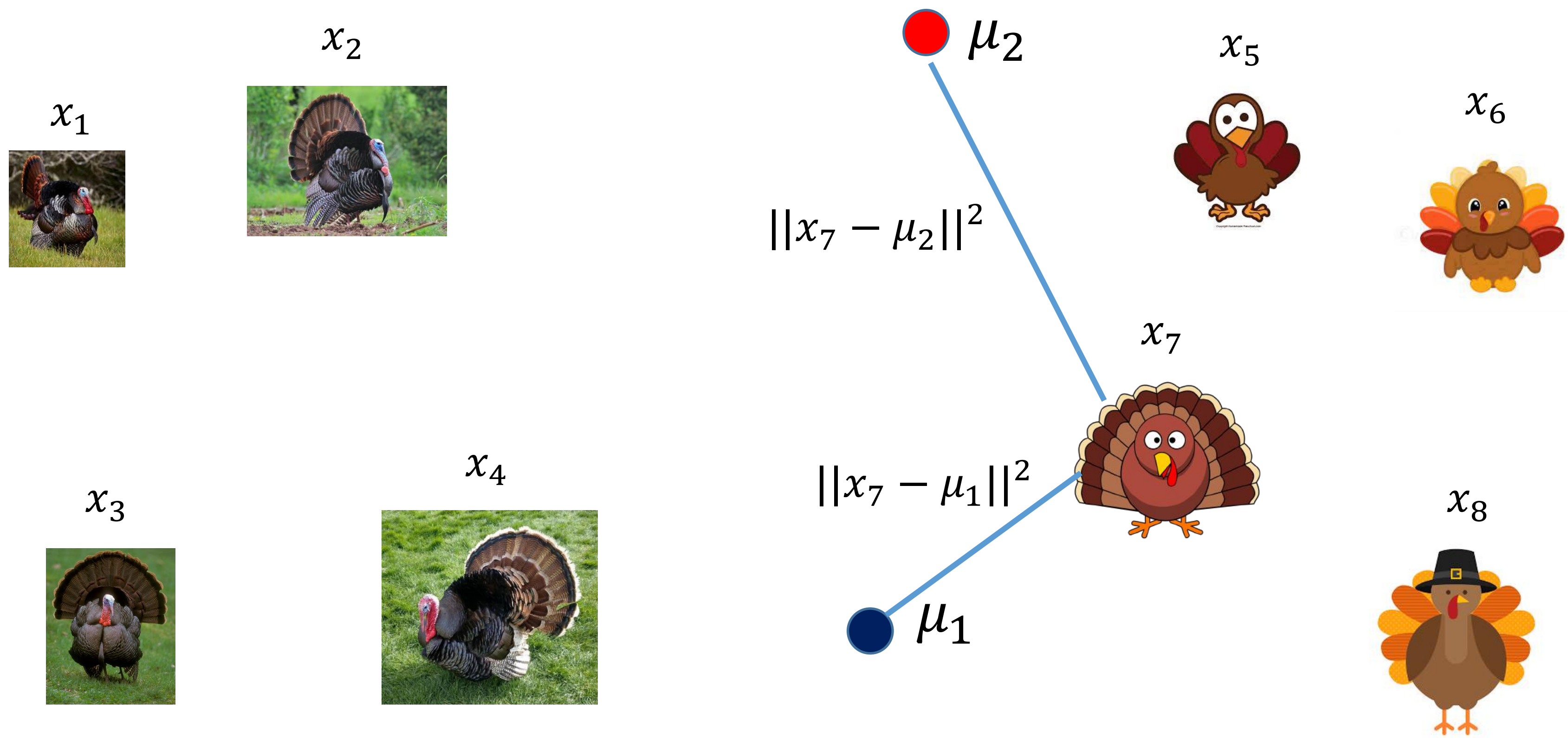


$A(x) = 1$

$A(x) = 2$

Step 1: Minimize J over $\{r_{nk}\}$

$$J(\{r_{nk}\}, \{\boldsymbol{\mu}_k\}) = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|_2^2$$



$A(x) = 1$ $\qquad\qquad$ $A(x) = 2$

K-means algorithm
a.k.a Llyod's algorithm

- A greedy algorithm for minimizing K-means objective – alternative update $\{r_{nk}\}, \{\boldsymbol{\mu}_k\}$
- Step 0: randomly assign the cluster centers $\{\mu_k\}$
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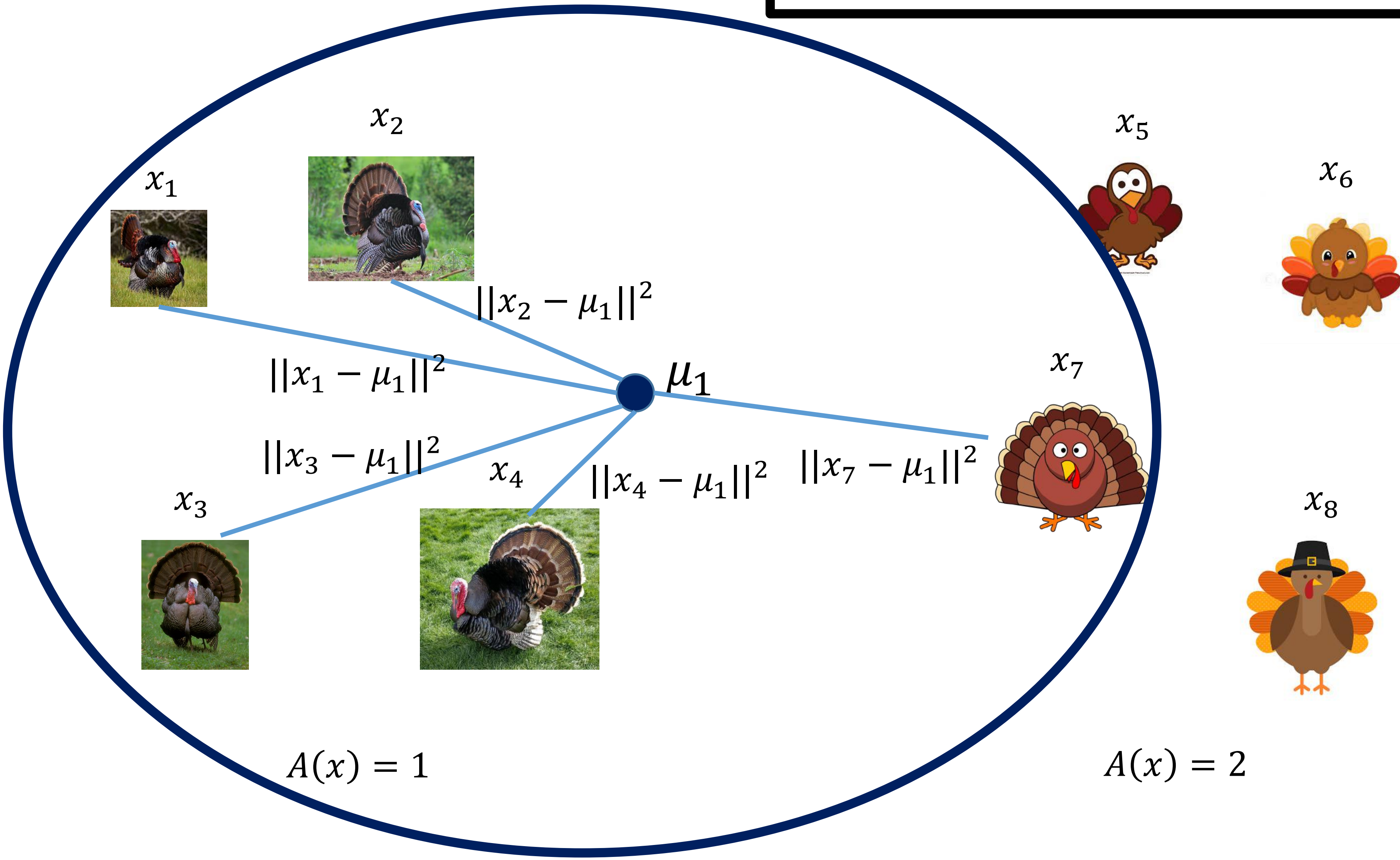
$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\boldsymbol{x}_n - \boldsymbol{\mu}_j\|_2^2 \\ 0 & \text{otherwise} \end{cases}$$

- Step 2: Minimize J over $\{\mu_k\}$ -- update the cluster centers
- Loop until it converges

Step 2: Minimize J over $\{\mu_k\}$

$$J(\{r_{nk}\}, \{\boldsymbol{\mu}_k\}) = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|_2^2$$



K-means algorithm
a.k.a Llyod's algorithm

- Step 0: randomly assign the cluster centers $\{\mu_k\}$
- Step 1: Minimize J over $\{r_{nk}\}$ -- Assign every point to the closest cluster center

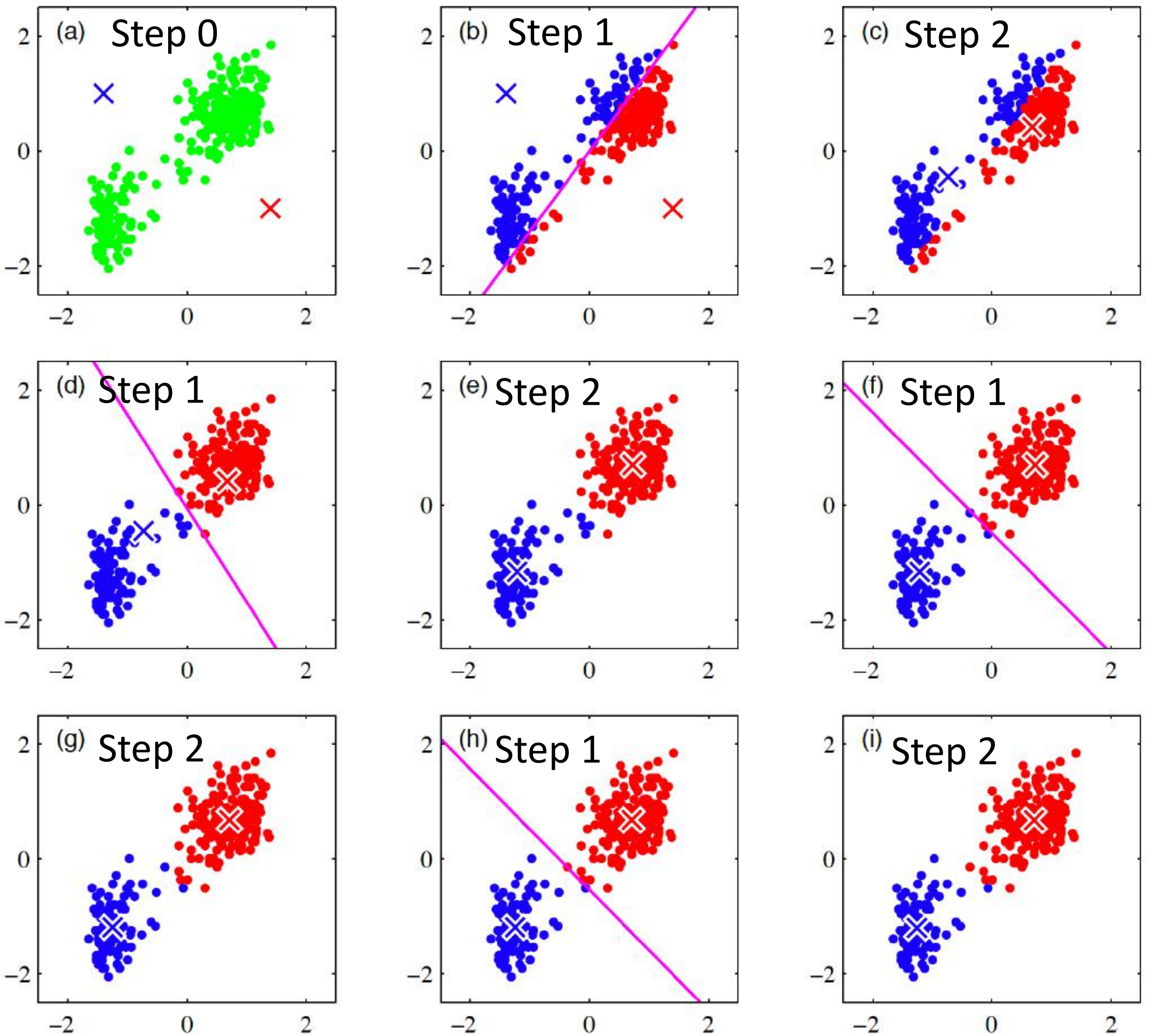
$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\boldsymbol{x}_n - \boldsymbol{\mu}_j\|_2^2 \\ 0 & \text{otherwise} \end{cases}$$

- Step 2: Minimize J over $\{\mu_k\}$ -- update the cluster centers

$$\boldsymbol{\mu}_k = \frac{\sum_n r_{nk}\boldsymbol{x}_n}{\sum_n r_{nk}}$$

- Loop until it converges

Example



(a) Step 0
(b) Step 1
(c) Step 2
(d) Step 1
(e) Step 2
(f) Step 1
(g) Step 2
(h) Step 1
(i) Step 2

Remarks

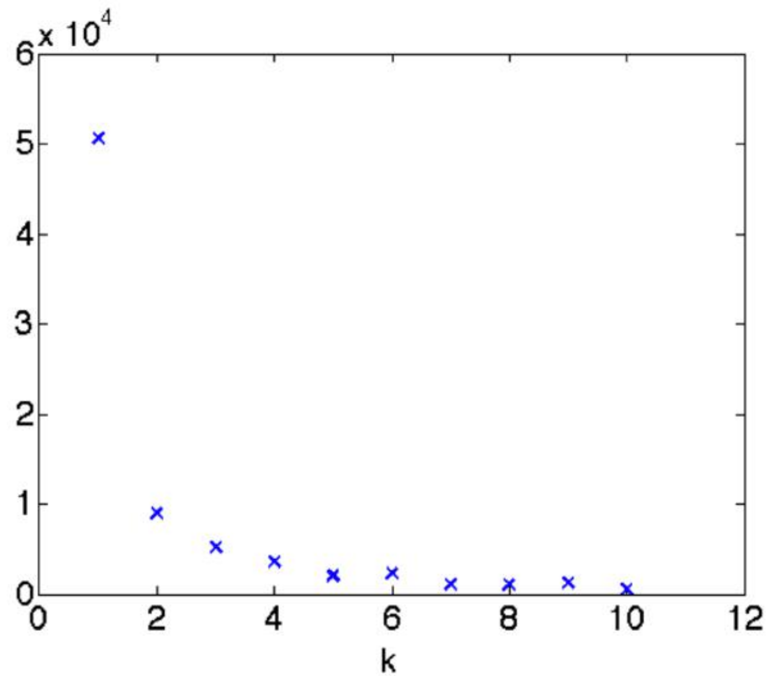
- Prototype μ_k is the mean of data points assigned to the cluster k, hence `K-means'
- μ_k may not in the training set
- Need to pre-define K
  - There are some other approaches for the case k is unknown – not cover in class
- The procedure reduces J in both Step 1 and Step 2 and thus makes improvements or stay the same on each iteration

Properties of the K-means algorithm

- Does the K-means algorithm converge
  - Yes
- How long does it take to converge?
  - In the worst case, exponential in the number of data points
  - In practice, usually quick
- How good is its solution?
  - Local minimum (depends on the initialization)

Choosing K

- Increasing K will always decrease the optimal value of the K-means objective
  - It doesn't mean a better clustering
  - Analogous to overfitting in supervised learning.



K-means can be sensitive to the outlier

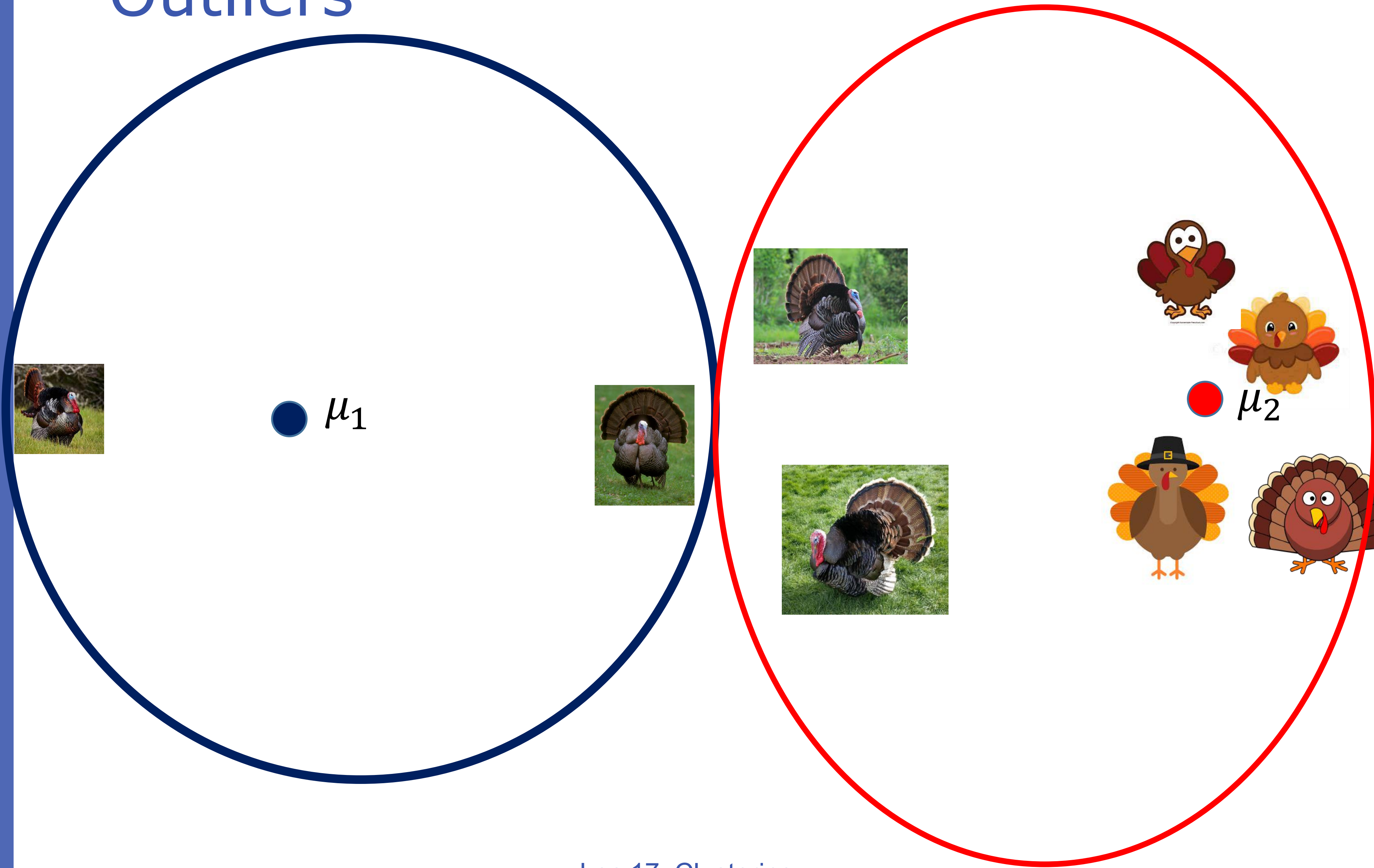
- One data point can make the center shift

K-Medoids

K-medoids

- K-means is sensitive to outliers.
- In some applications we want the prototypes to be one of the points.
- Leads to K-medoids.

Outliers

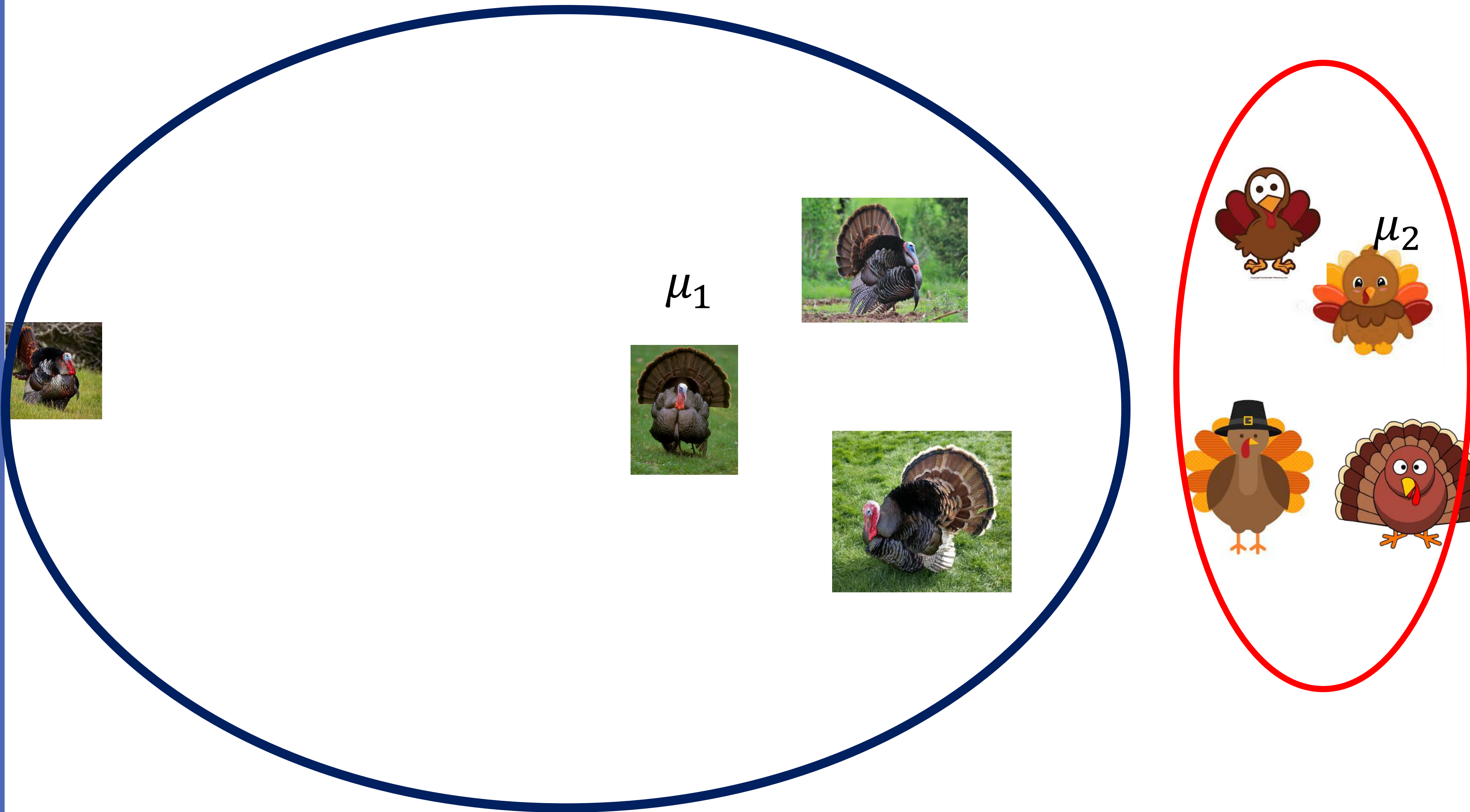


Intuition@ Hogwarts

- Sorting Hat – cluster students into four groups based on four underlying prototypes

- The prototype of each house is the most represented student of the house
  - Alternatively, updating the prototype & the student assignment

K-medoids



K-medoids algorithm

- Step 0: randomly selecting K points as the cluster centers $\{\mu_k\}$
- Step 1: Minimize J over $\{r_{nk}\}$ -- Assign every point to the closest cluster center

$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\boldsymbol{x}_n - \boldsymbol{\mu}_j\|_2^2 \\ 0 & \text{otherwise} \end{cases}$$

- Step 2: Update the cluster centers– the porotype for a cluster is the data that is closest to all other data points in the cluster

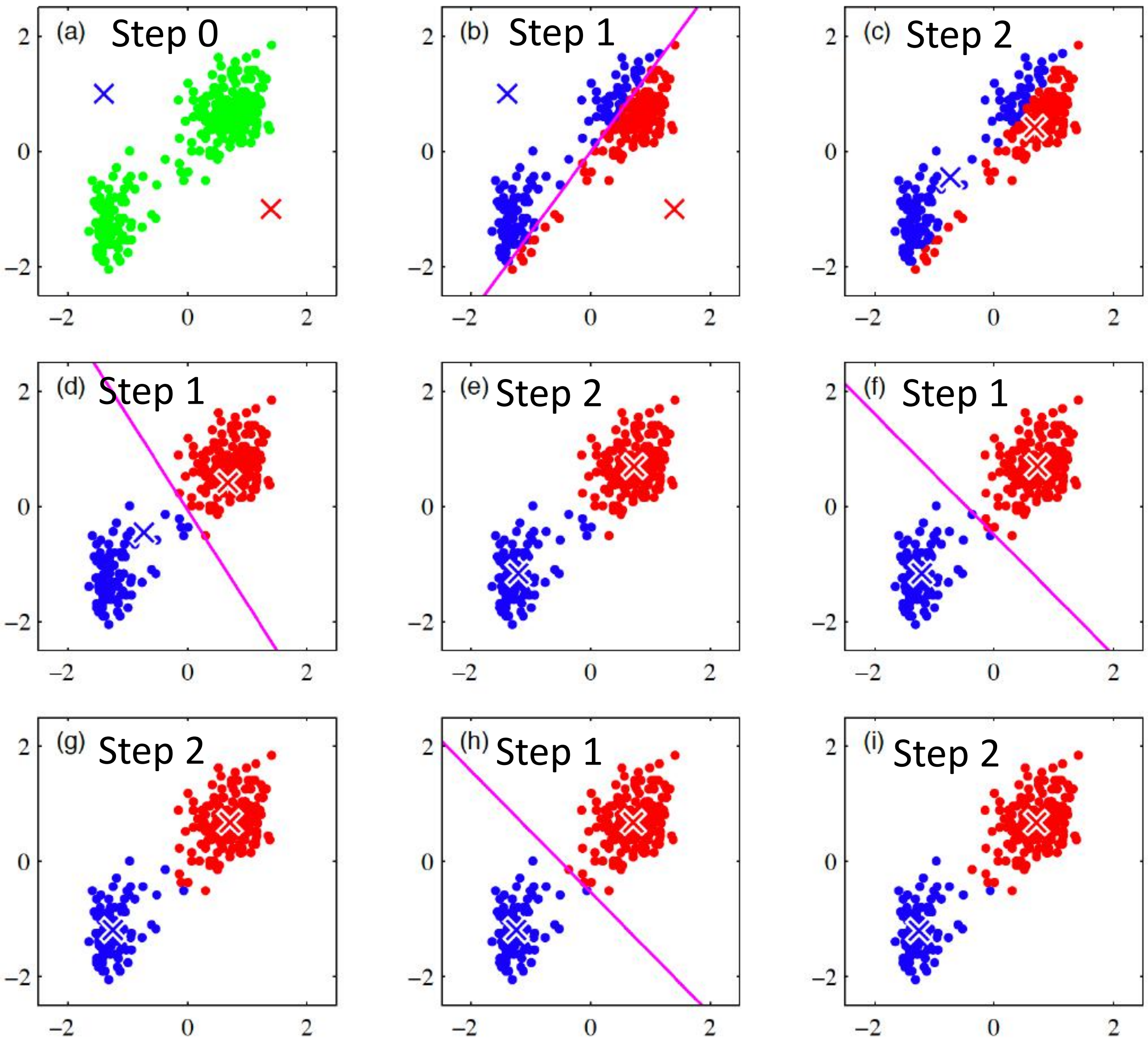
$$k* = \arg\min_{m: r_{mk}=1} \sum_n r_{nk} \|\boldsymbol{x}_n - \boldsymbol{x}_m\|_2^2$$

$$\boldsymbol{\mu}_k = \boldsymbol{x}_{k*}$$

- Loop until it converges

Gaussian Mixture Models

K-Means



(a) Step 0
(b) Step 1
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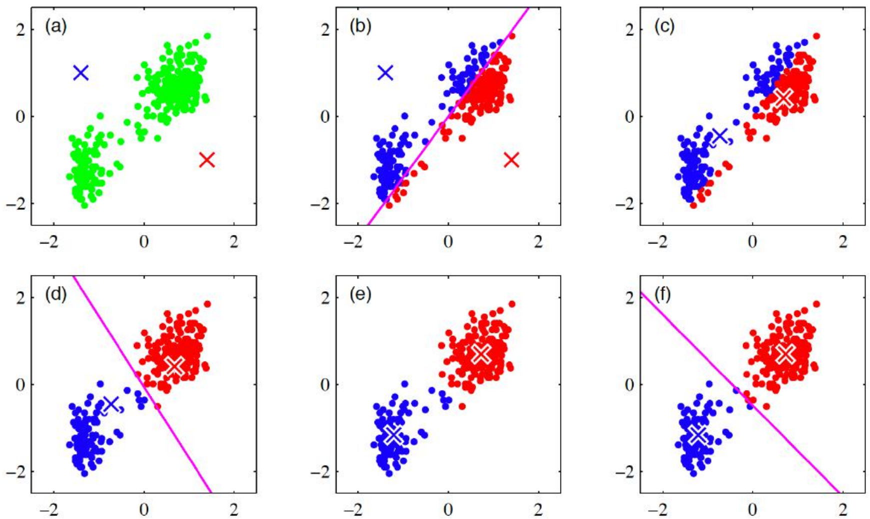
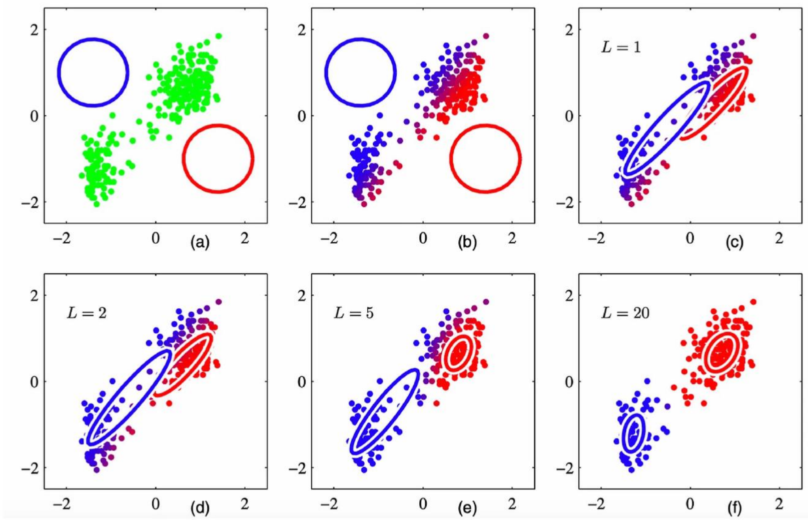
(i) Step 2

Similar to K-means

- Alternatively:
  1) assign points to clusters
  2) update cluster centers/variances…

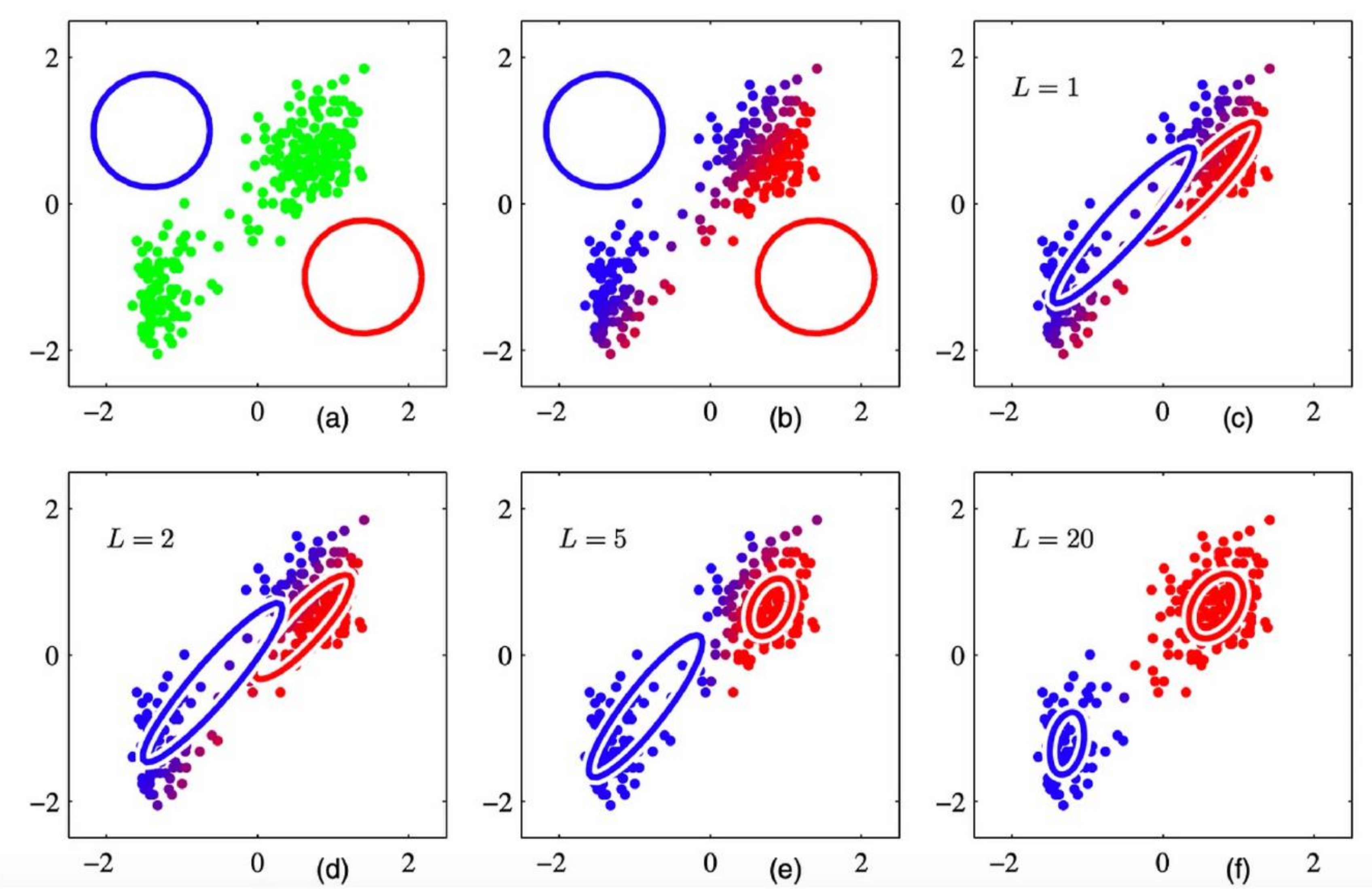


K-Means



GMM

GMM

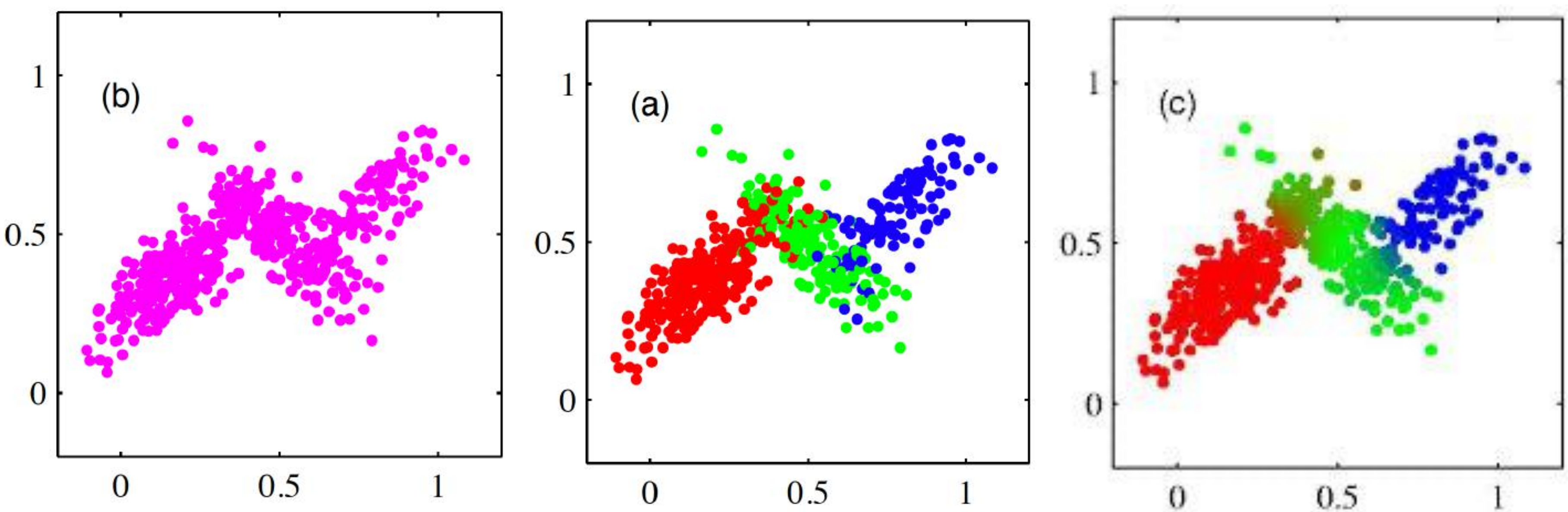


Soft cluster

- Assignment based on the conditional probability $P(A(x_n)|x_n)$

Hard cluster assignment

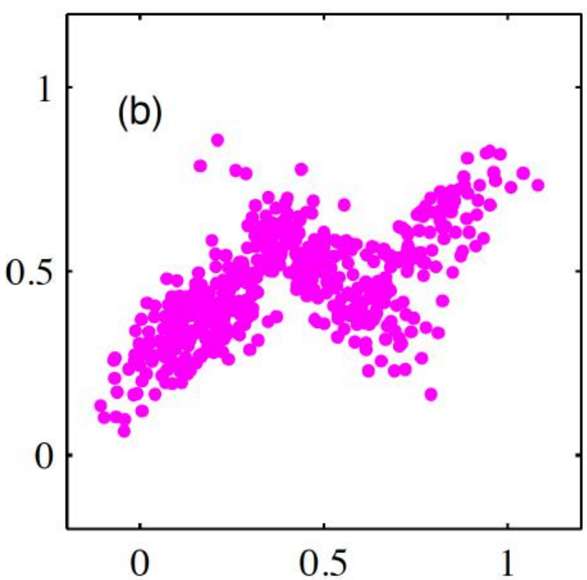
Soft cluster assignment



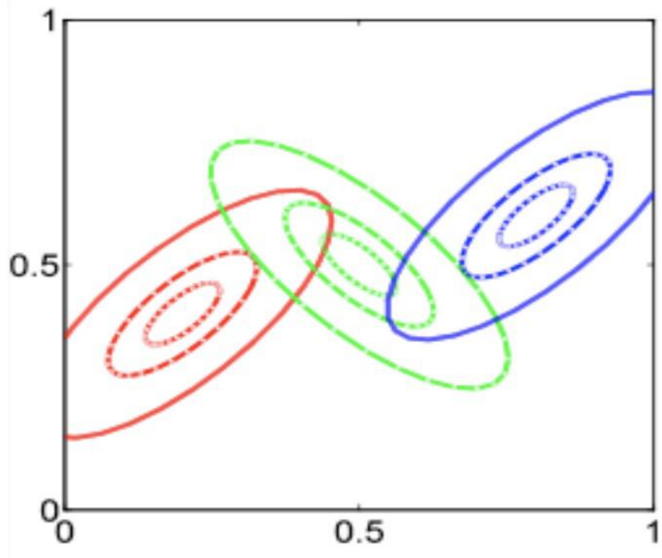
Gaussian mixture models

- Assume the probability density function for x as

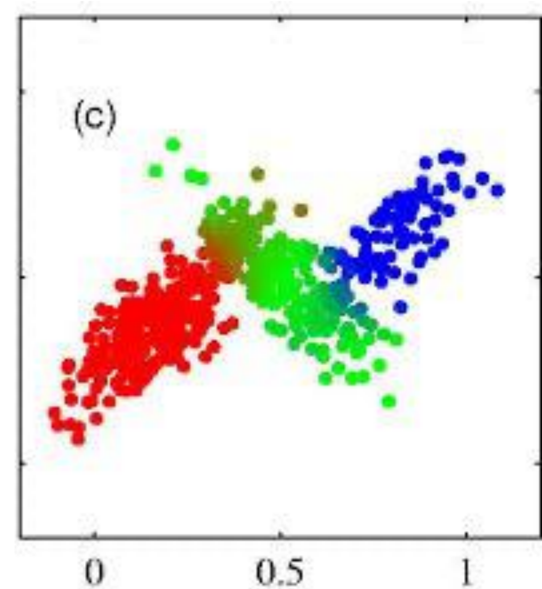
$$p(\boldsymbol{x}) = \sum_{k=1}^{K} \omega_k N(\boldsymbol{x} | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$



Model by 3 Guassians



Soft cluster assignment

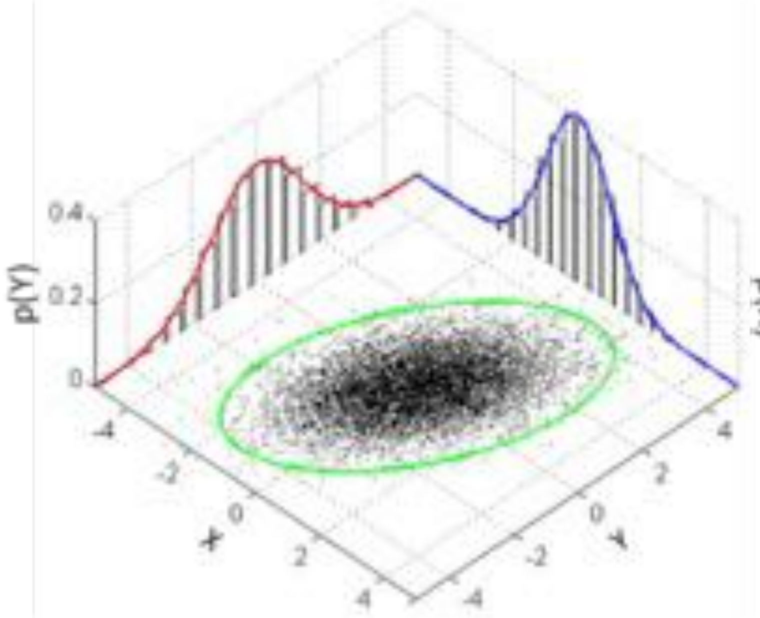


Multivariate Gaussian

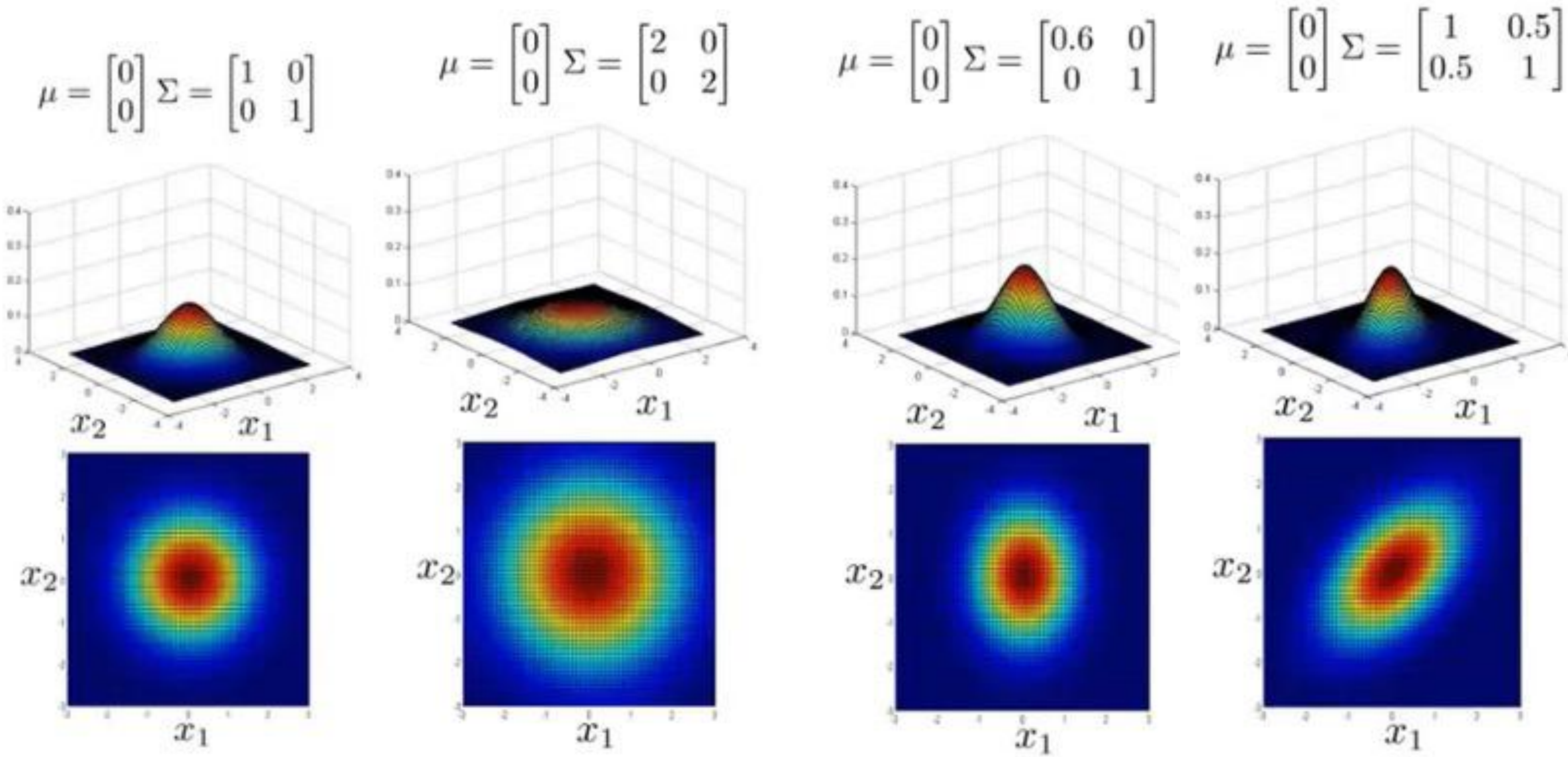
- Mean $\boldsymbol{\mu} \in \mathbf{R}^k$

- Variance $\boldsymbol{\Sigma} \in \mathbf{R}^{k \times k}$

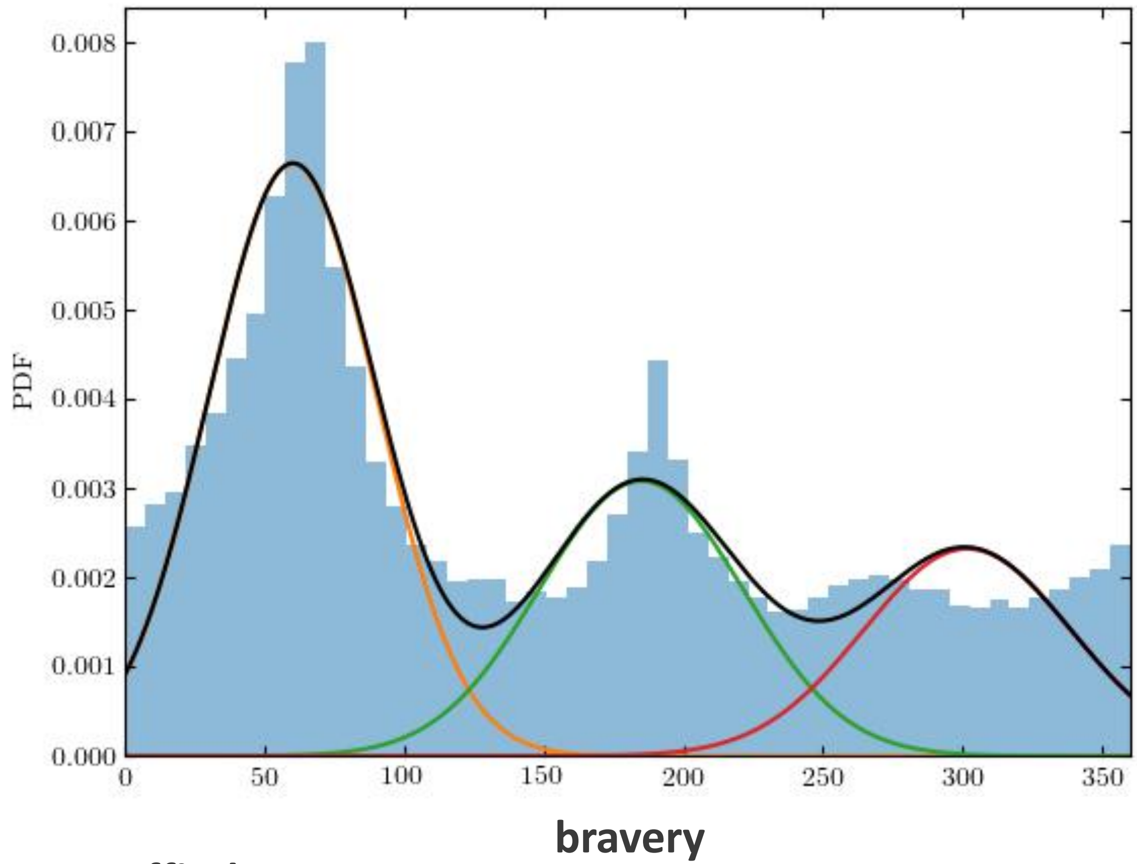
- PDF:



$$(2\pi)^{-\frac{k}{2}} \det(\boldsymbol{\Sigma})^{-\frac{1}{2}} \exp(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\mathsf{T}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}))$$


$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Sigma = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$
$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Sigma = \begin{bmatrix} 0.6 & 0 \\ 0 & 1 \end{bmatrix}$
$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Sigma = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}$
x_2
x_1

Model Four Houses of Hogwarts

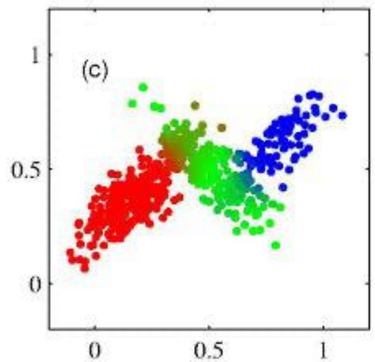


Distribution for students in **Gryffindor**

Distribution for students in **Slytherin**

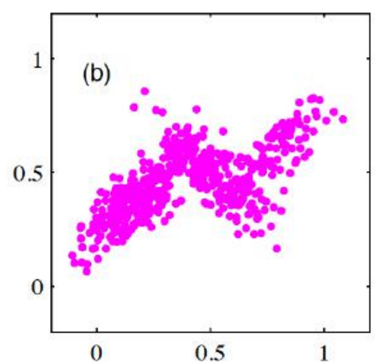
Distribution for students in **Ravenclaw**

Why Mixed Gaussian?



The conditional distribution between $\boldsymbol{x}$ and z (representing color) are

$$p(\boldsymbol{x}|z = red) = N(\boldsymbol{x}|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$$
$$p(\boldsymbol{x}|z = blue) = N(\boldsymbol{x}|\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)$$
$$p(\boldsymbol{x}|z = green) = N(\boldsymbol{x}|\boldsymbol{\mu}_3, \boldsymbol{\Sigma}_3)$$

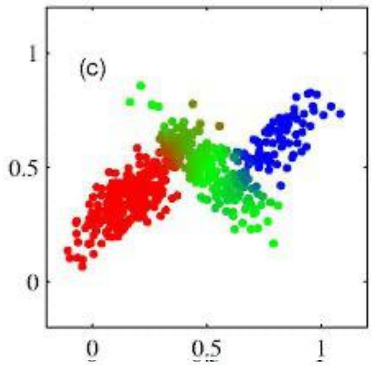


The marginal distribution is thus

$$p(\boldsymbol{x}) = p(red)N(\boldsymbol{x}|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + p(blue)N(\boldsymbol{x}|\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) + p(green)N(\boldsymbol{x}|\boldsymbol{\mu}_3, \boldsymbol{\Sigma}_3)$$

ω_k

Bayes Rule – Posterior distrbution



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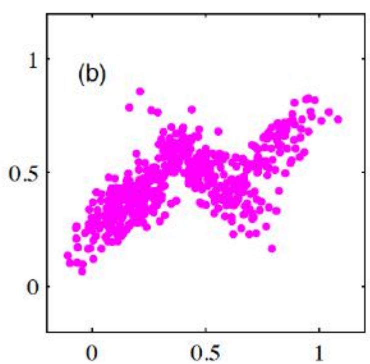

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$$\boxed{p(z_n = k|\boldsymbol{x}_n) = \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{p(\boldsymbol{x}_n)} = \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{\sum_{k'=1}^{K} p(\boldsymbol{x}_n|z_n = k')p(z_n = k')}}$$

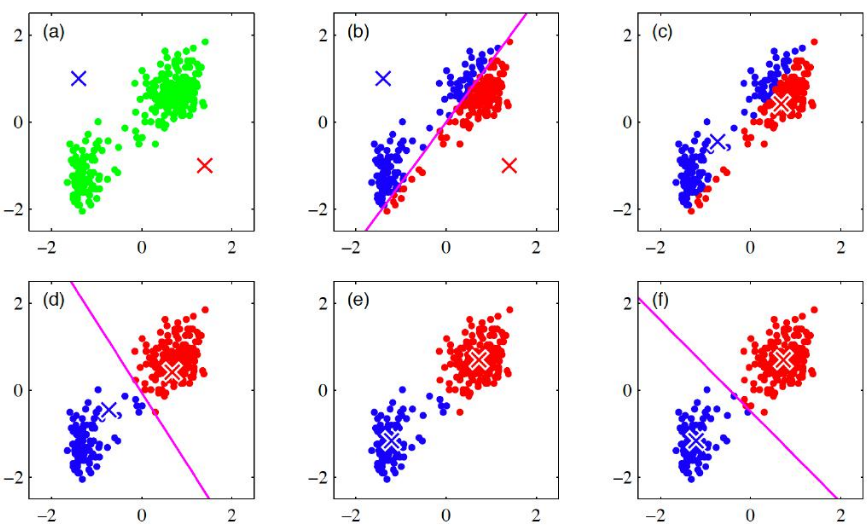
Similar to K-means

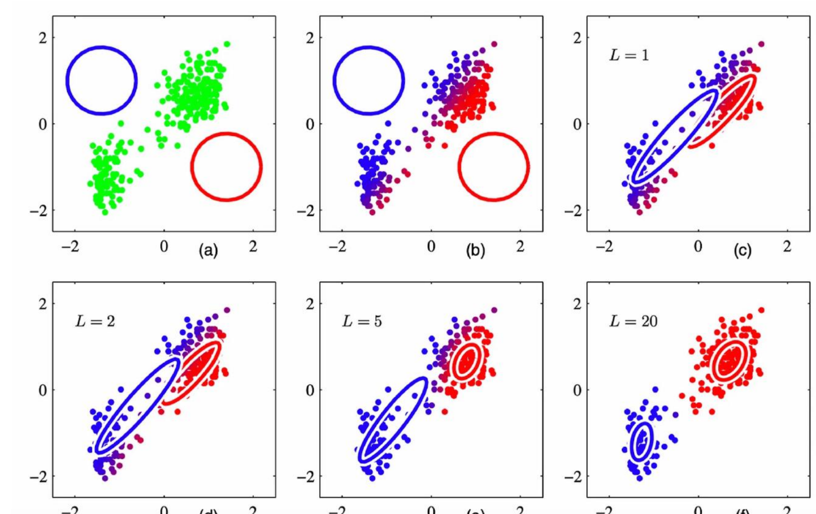
❖ Alternatively:

1) soft assign points to clusters based on

$$p(z_n = k|\boldsymbol{x}_n) = \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{p(\boldsymbol{x}_n)} = \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{\sum_{k'=1}^{K} p(\boldsymbol{x}_n|z_n = k')p(z_n = k')}$$

2) update cluster centers/variances…





Similar to K-means

- Alternatively:
  1) assign points to clusters
  2) update cluster centers/variances based on the weighted mean/variance