Outline

1. Review: Clustering and k-means

2. Gaussian mixture models

Review: Clustering and k-means

Supervised versus Unsupervised Learning

Supervised Learning: labeled observations $\{(x_1, y_1), \ldots (x_n, y_n)\}$

- Labels 'teach' algorithm to learn mapping from observations to labels
- Examples: Classification (Logistic Reg., SVMs, Neural Nets, Nearest Neighbors, Decision Trees), Regression (Linear Reg., Neural Nets)

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Unsupervised Learning: unlabeled observations $\{x_1, \ldots, x_n\}$

- Learning algorithm must find latent structure from features alone
- Can be goal in itself (discover hidden patterns, exploratory analysis)
- Can be means to an end (pre-processing for supervised task)
- Examples:
  - Clustering
  - Dimensionality Reduction: Transform an initial feature representation into a more concise representation

Clustering

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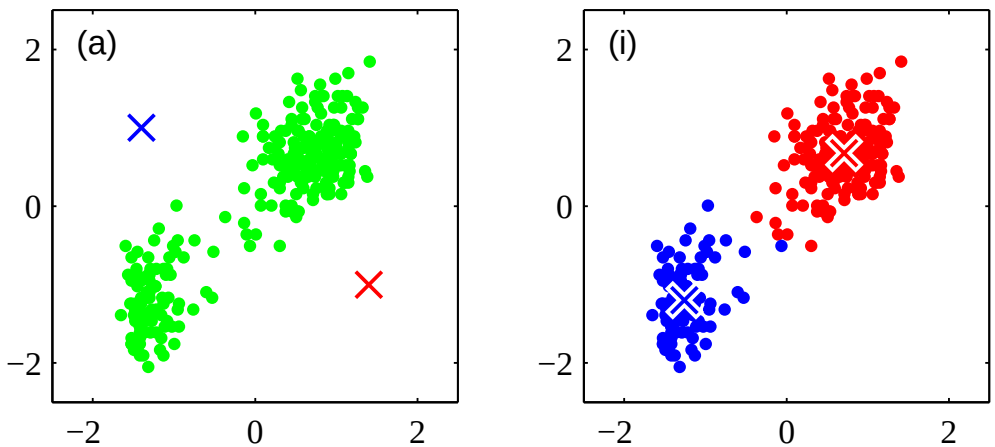
- $\{\boldsymbol{\mu}_k\}_{k=1}^K$: prototypes of clusters

Toy Example Cluster data into two clusters.



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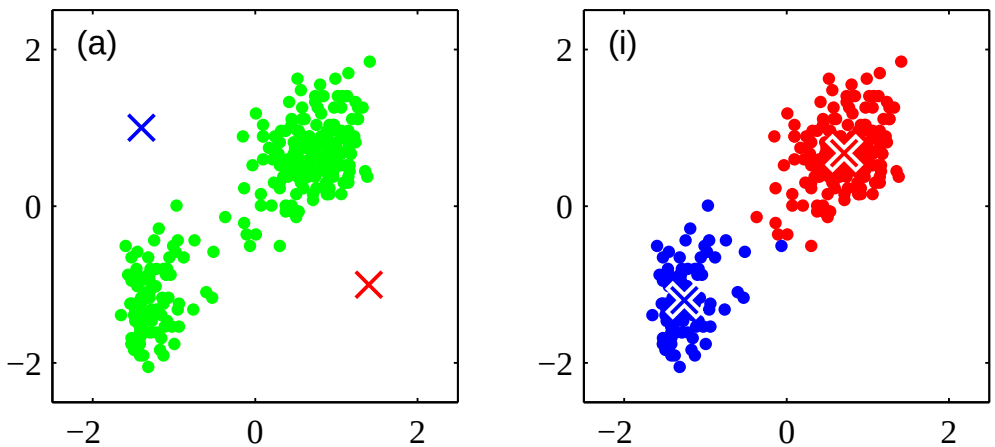

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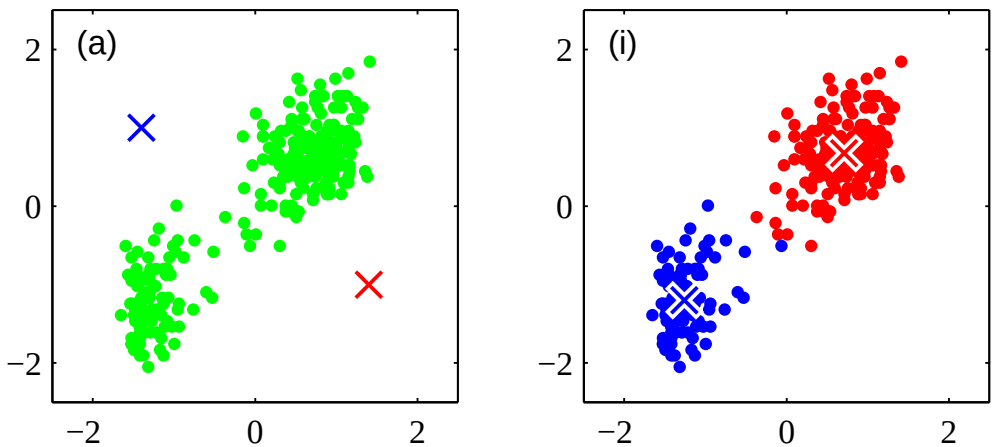

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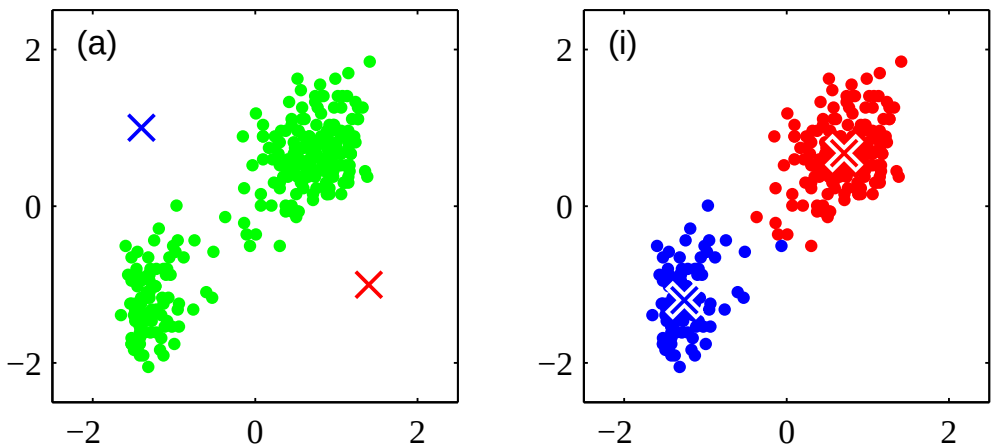


Example Applications

- Identify communities within social networks
- Find topic groups in news stories
- Group similar sequences into gene families

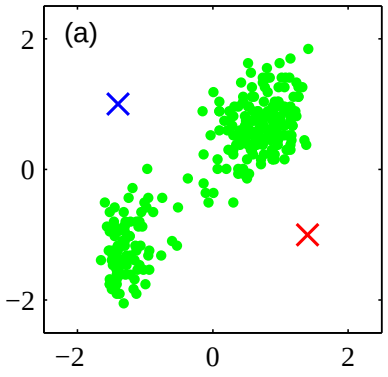
k-means

k-means: an iterative clustering method

High-level idea:

- Initialize: Pick k random points as cluster centers, $\{\mu_1, \ldots, \mu_k\}$
- Alternate:
  1. Assign data points to closest cluster center in $\{\mu_1, \ldots, \mu_k\}$
  2. Change each cluster center to the average of its assigned points
- Stop: When the clusters are stable

k-means example (several iterations)



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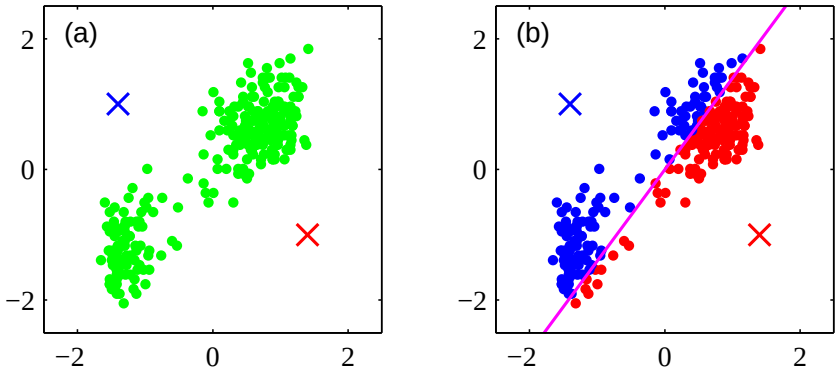

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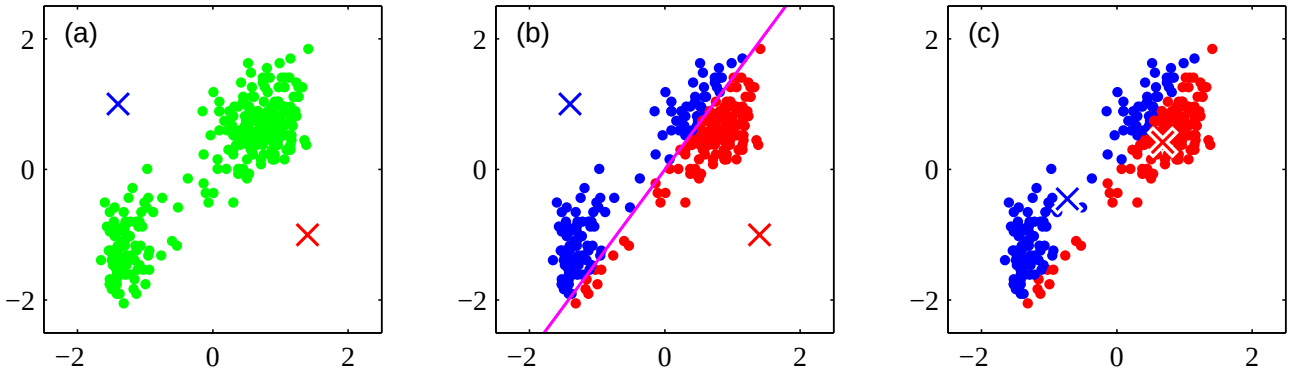

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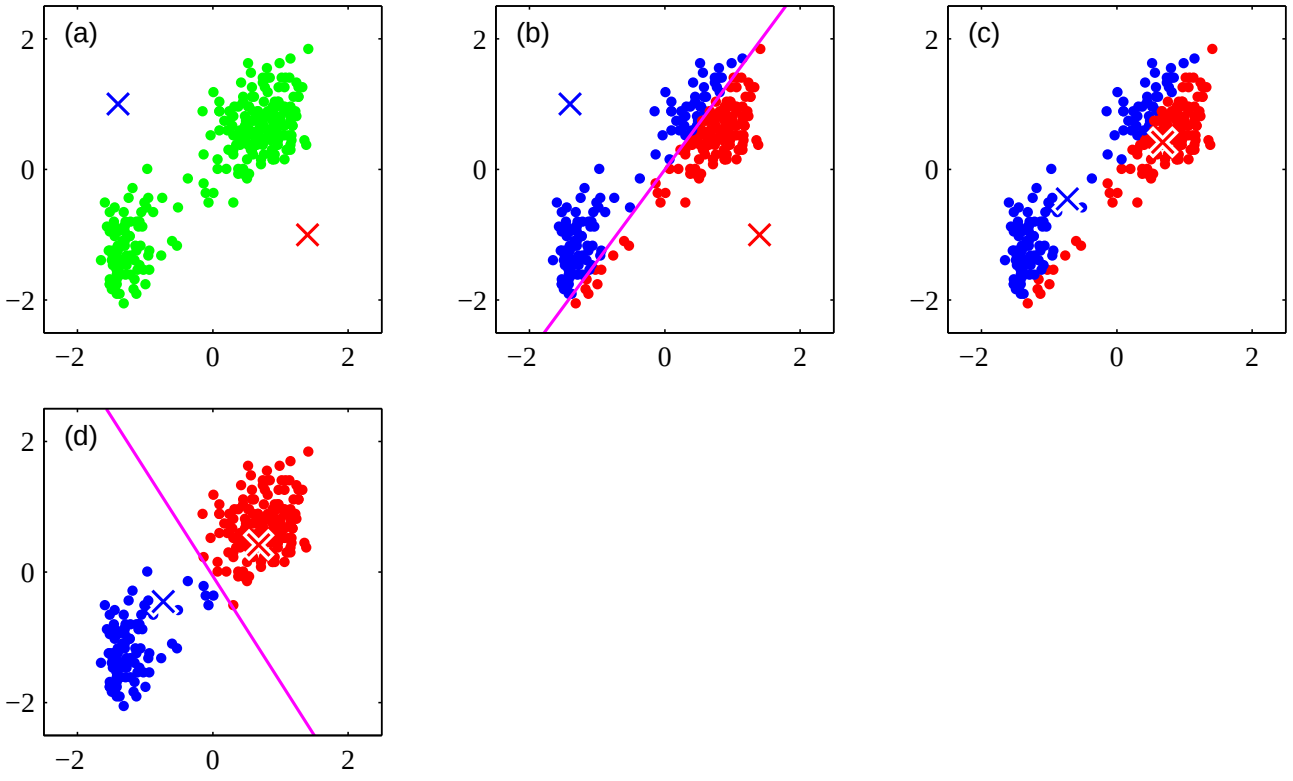

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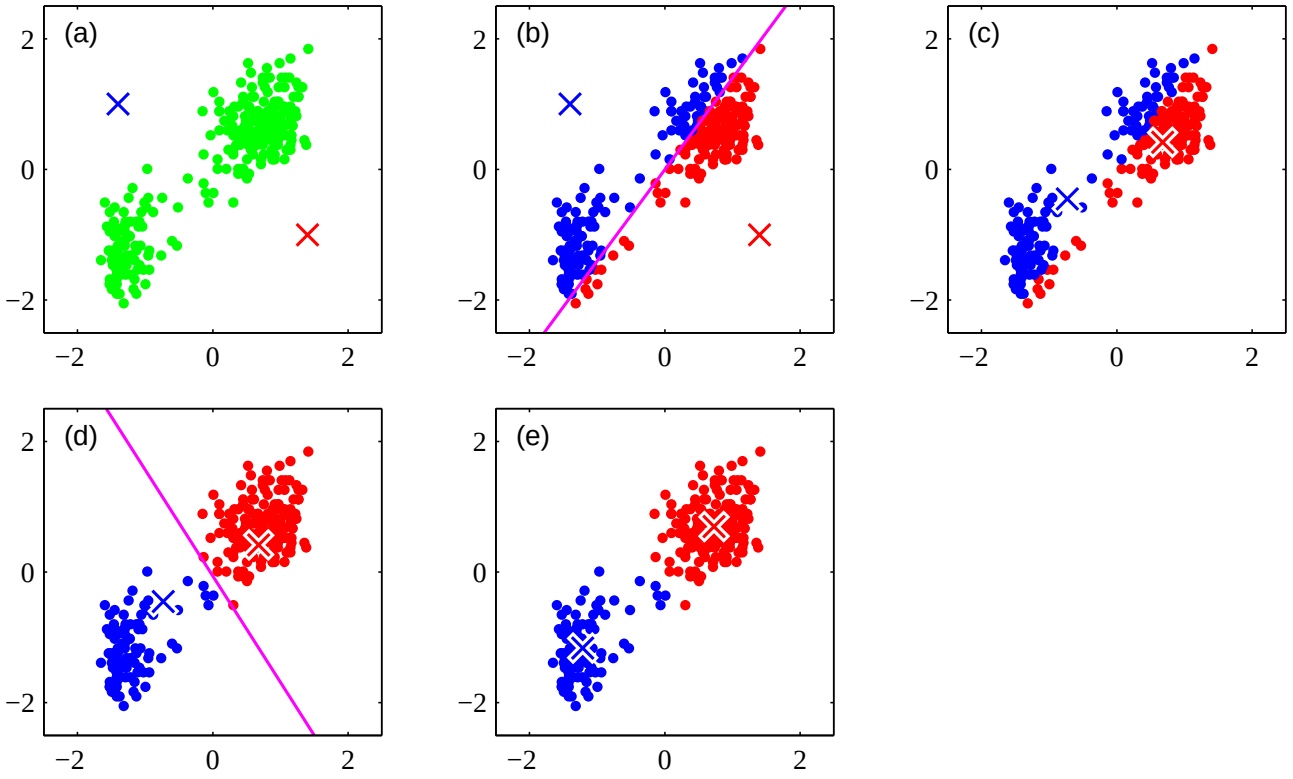

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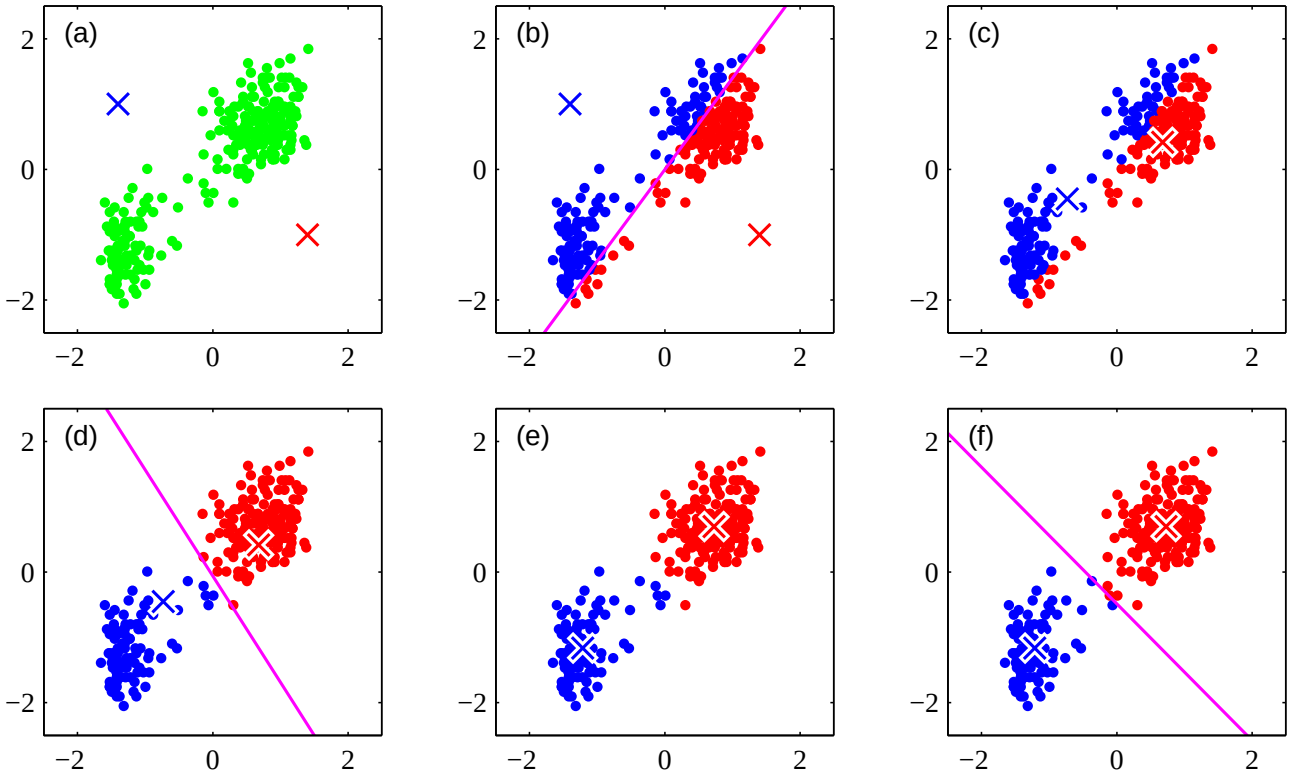

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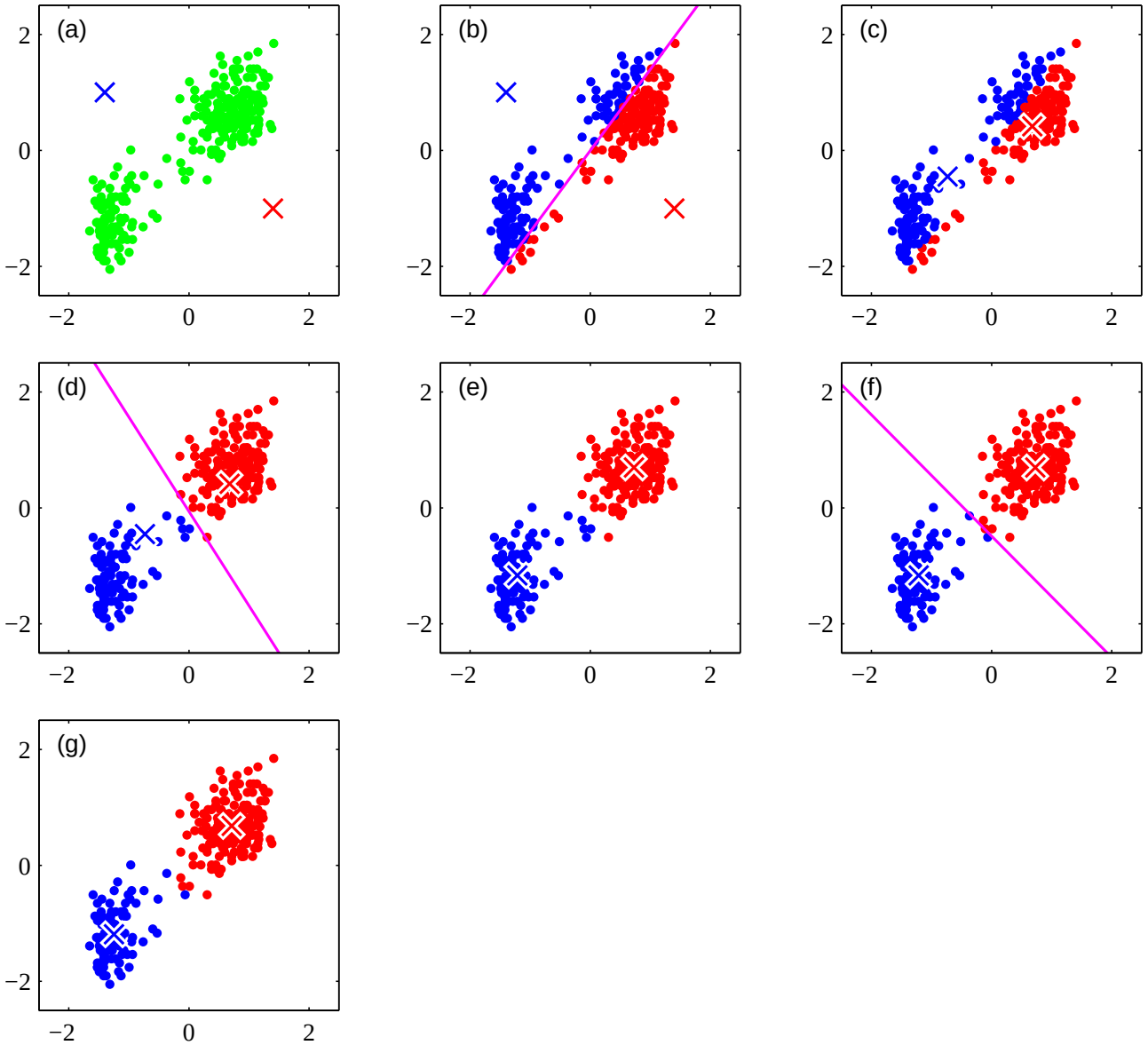

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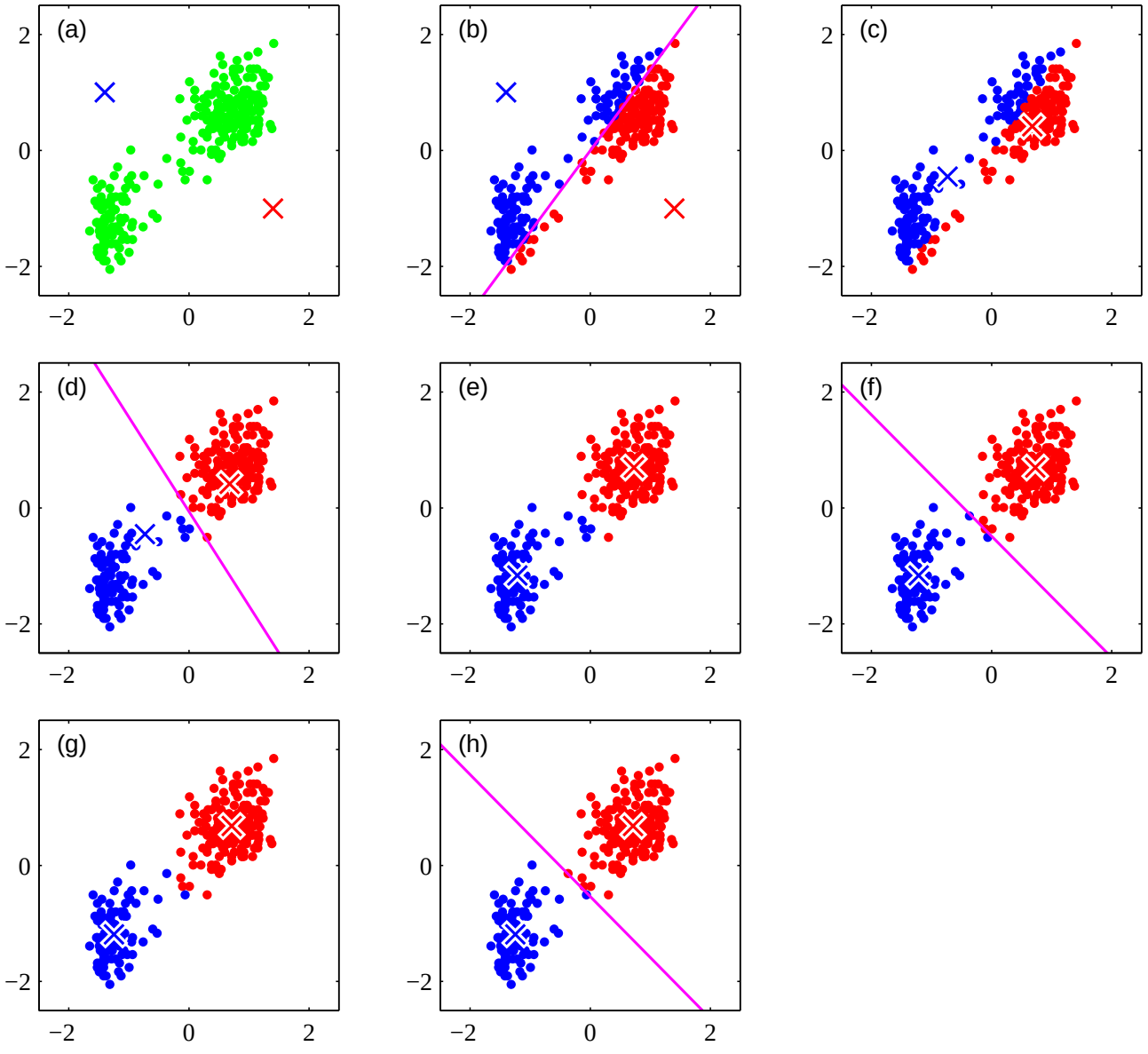

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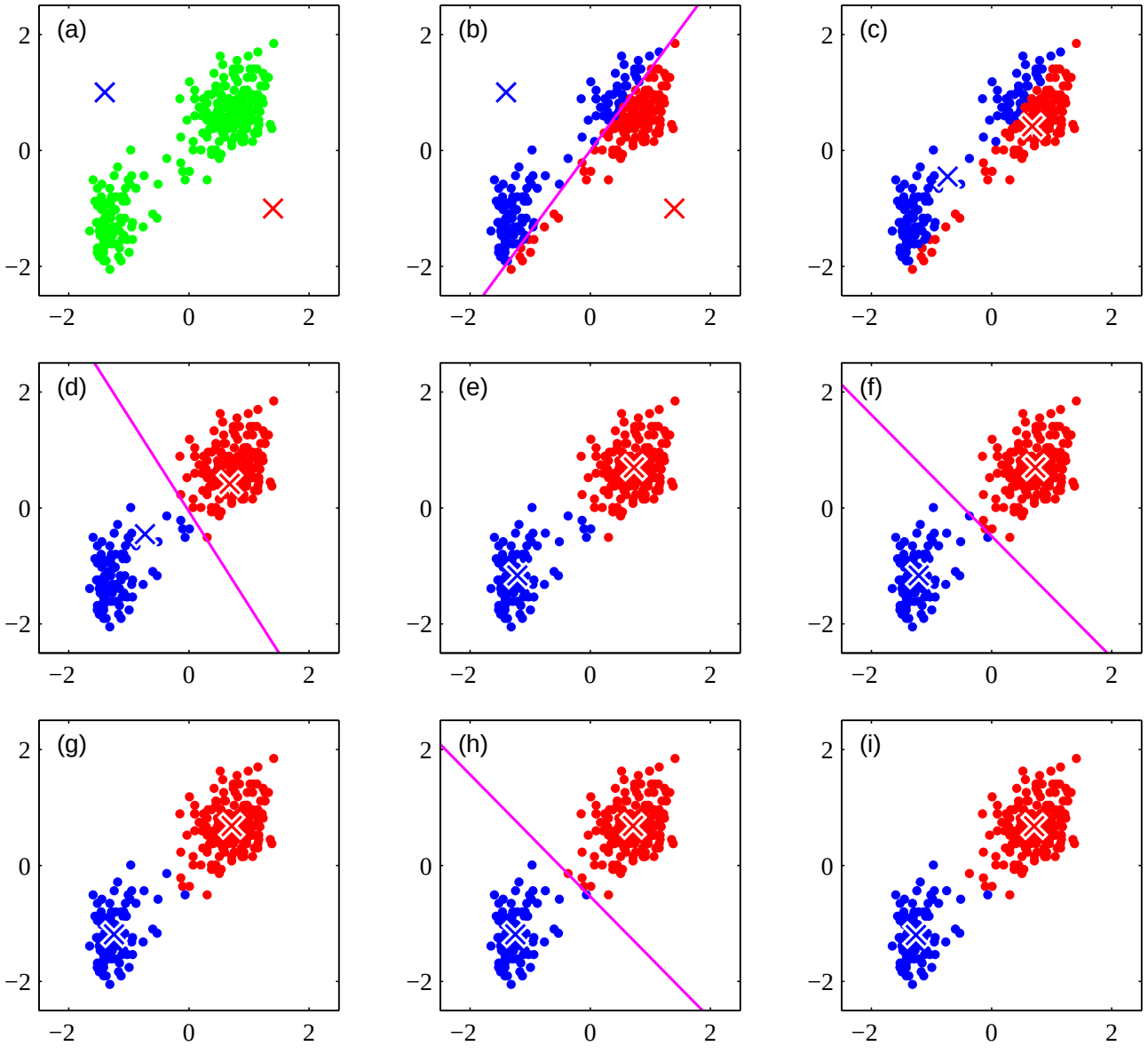

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where $r_{nk} \in \{0, 1\}$ is an indicator variable

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- Canonical example is the 2-norm, i.e., $|| \cdot ||_2^2$, but could be something else!

Algorithm

Minimize distortion Alternative optimization between $\{r_{nk}\}$ and $\{\boldsymbol{\mu}_k\}$

- **Step 0** Initialize $\{\boldsymbol{\mu}_k\}$ to some values
- **Step 1** Fix $\{\boldsymbol{\mu}_k\}$ and minimize over $\{r_{nk}\}$, to get this assignment:

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

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- **Step 3** Return to Step 1 unless stopping criterion is met

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What's the runtime?

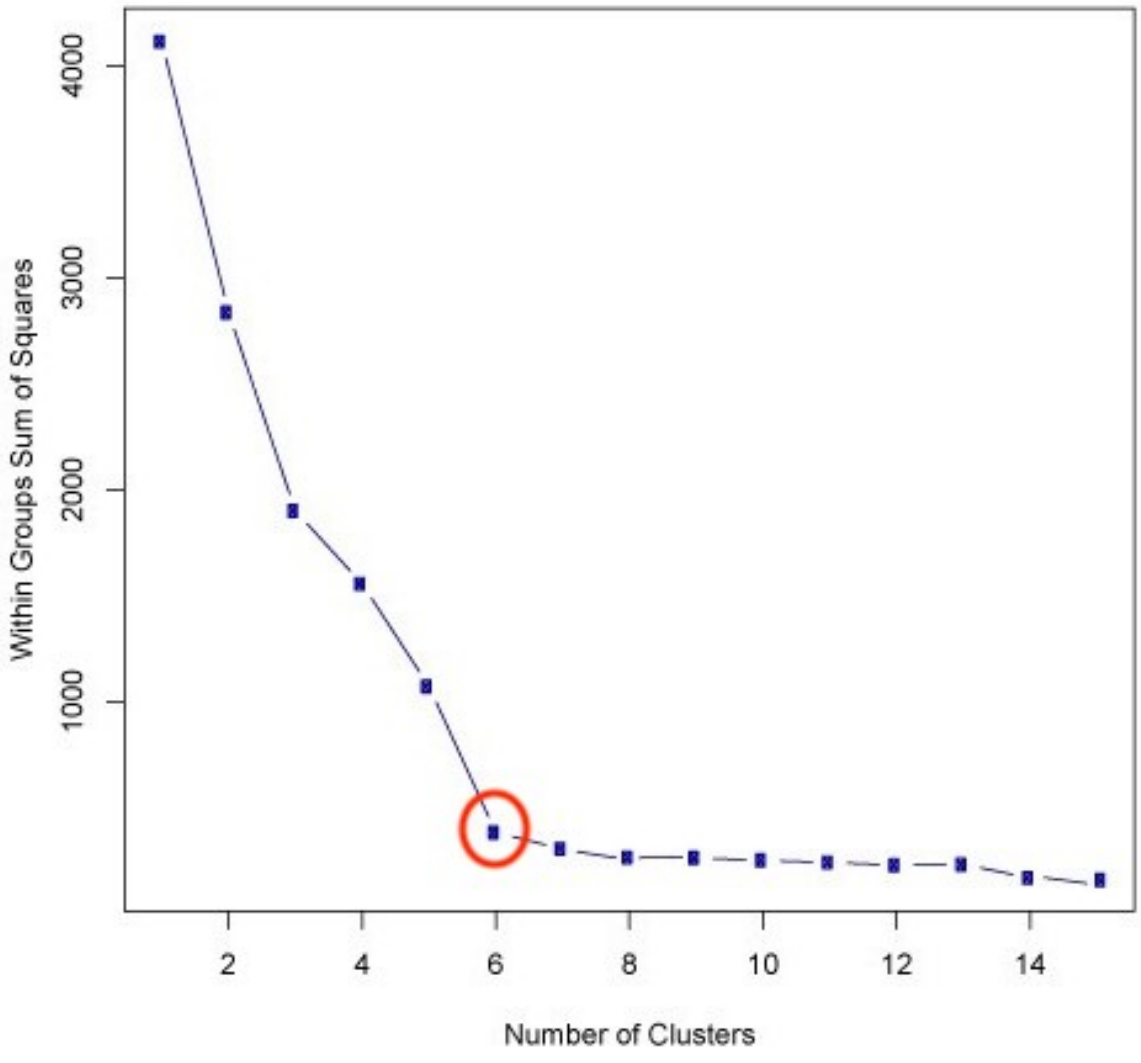
- **Running time per iteration**:
  - Assume: n data points, each with d features, and k clusters
  - Assign data points to closest cluster: $O(ndk)$
  - Re-compute cluster centers: $O(ndk)$
- **Thus, total runtime is**: $O(ndki)$, where i is the number of iterations

Practical Issues with k-means

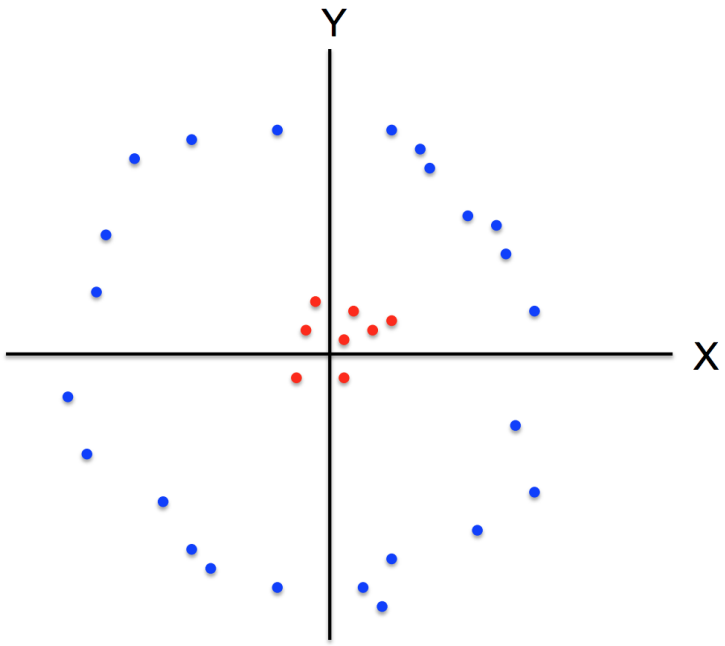
- How to select k?
  - Prior knowledge
  - Heuristics (e.g., elbow method)
- How to select distance measure?
  - Often requires some knowledge of problem
  - Some examples: Euclidean distance (for images), Hamming distance (distance between two strings), shared key words (for websites)
- How to initialize cluster centers?
  - The final clustering can depend significantly on the initial points you pick!

Elbow method

Key idea: select a small value of k that minimizes within-cluster distances



How to get k-means to work on this data?



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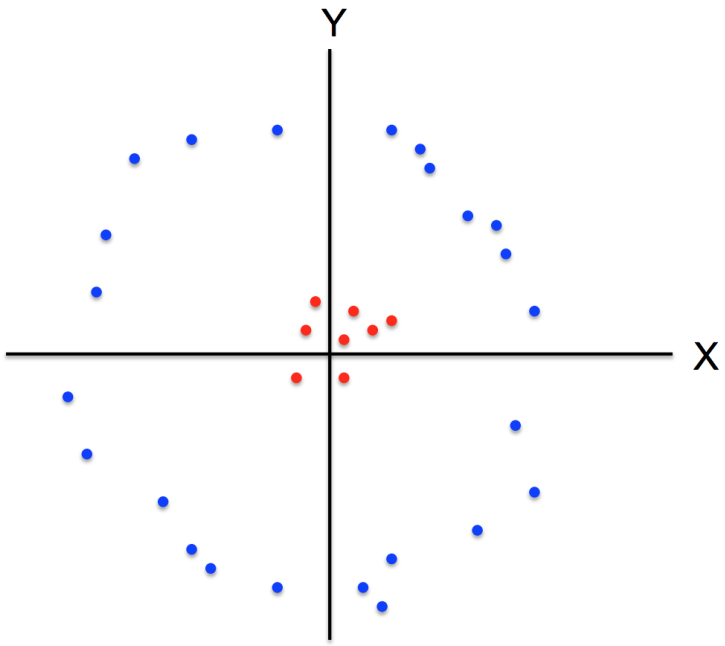
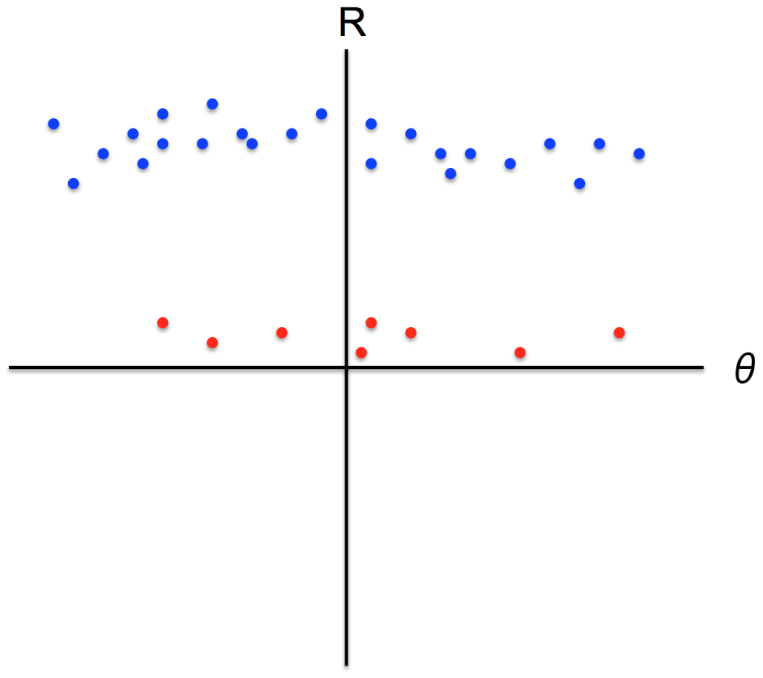


Should look at the distance of the data points from the origin $\sqrt{x_n^2 + y_n^2}$

Distance measure

Changing features (distance measure) can help



If the cluster i mean is $(\mu_{i,x}, \mu_{i,y})$, the distance of (x_n, y_n) from it can be defined as $|\sqrt{\mu_{i,x}^2 + \mu_{i,y}^2} - \sqrt{x_n^2 + y_n^2}|$

k-means++

Key idea: Run k-means, but with a better initialization

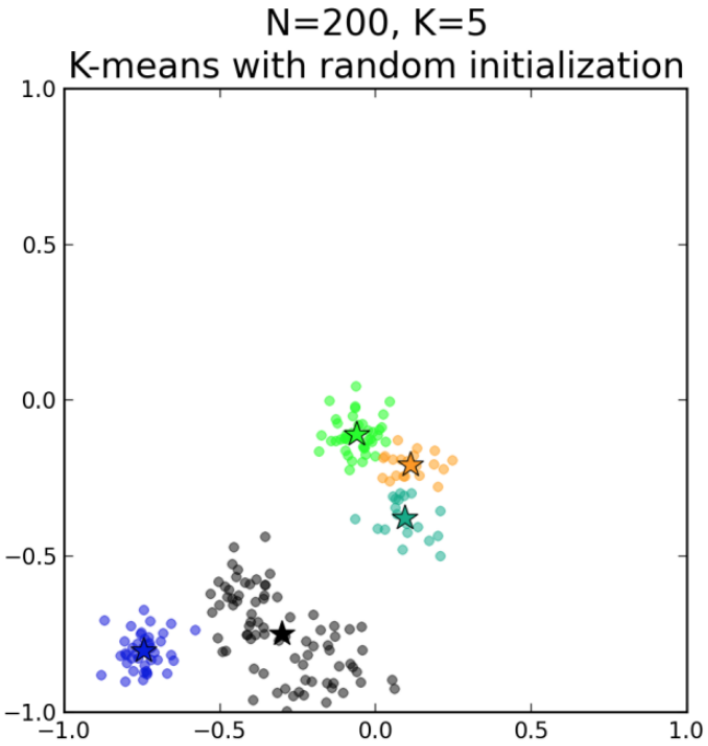
- Choose center μ_1 at random
- For $j = 2, \ldots, k$
  - Choose μ_j among $x_1, \ldots, x_n$ with probability:
  - $P(\mu_j = x_i) \propto min_{j' < j} ||x_i - \mu_{j'}||^2$

Initialization helps to get good coverage of the space

Theorem: k-means++ always obtains a $O(logk)$ approximation to the optimal solution in expectation.

Running k-means after this initialization can only improve on the result

k-means++


N=200, K=5
K-means with random initialization
1.0
0.5
0.0
−0.5
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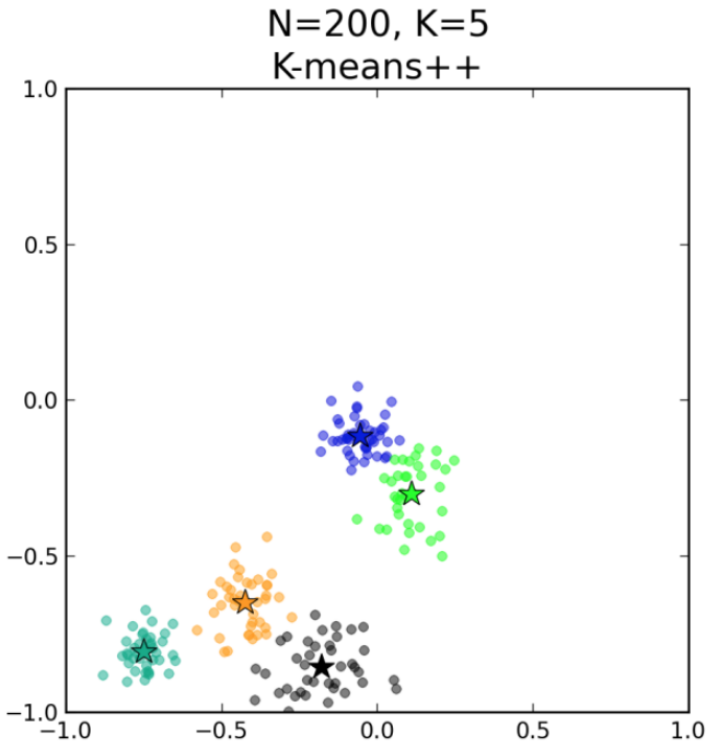
1.0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Connection to k-Nearest Neighbors

- Nearest Neighbors is a supervised learning method
  - Each training point $\mathbf{x}_n$ has a corresponding given label y_n
  - Objective: Assign label to a new $\mathbf{x}$ by looking at the labels of its k nearest points
- Clustering is an unsupervised learning method
  - We are given training points $\mathbf{x}_n$ without labels
  - Objective: Divide them into k groups to understand patterns in the data

Clustering can make Nearest Neighbors more efficient

- A drawback of nearest neighbors is that we have to remember the training data
- Clustering can help compress the training data into a small number of representative points

Algorithm to Improve Nearest Neighbors

- For all training data points $\mathbf{x}_n$ with label $y_n = c$, for C classes $c = 1, \ldots C$, cluster the $\mathbf{x}_n$ into R groups.
- Store these R cluster means for each of the C classes
- For a test data point $\mathbf{x}$, find the k nearest neighbors among the RC cluster means and assign their majority label to $\mathbf{x}$

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Gaussian mixture models

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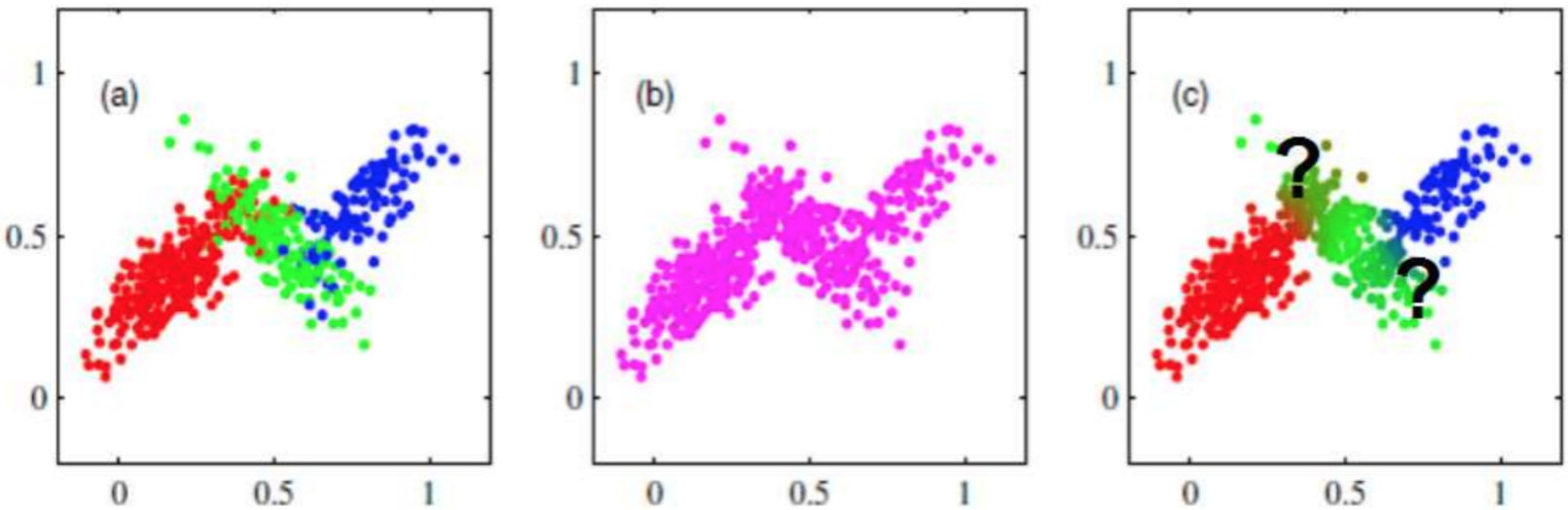
Data points are assigned *deterministically* to one (and only one) cluster

Potential issues with k-means ...

Data points are assigned *deterministically* to one (and only one) cluster

In reality, clusters may overlap, and it may be better to identify the *probability* that a point belongs to each cluster



Also, distances are measured in a homogeneous manner.

Probabilistic interpretation of clustering?

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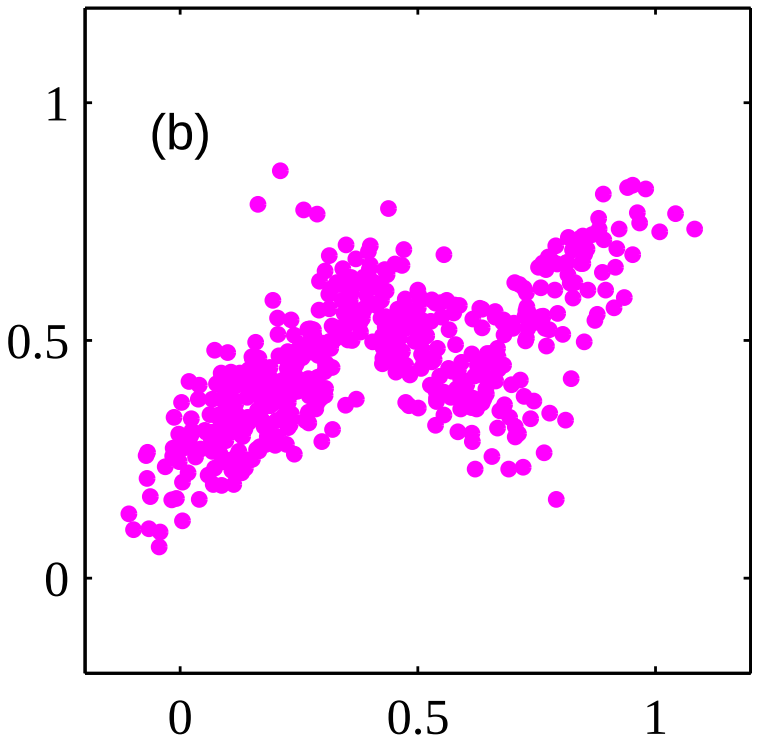

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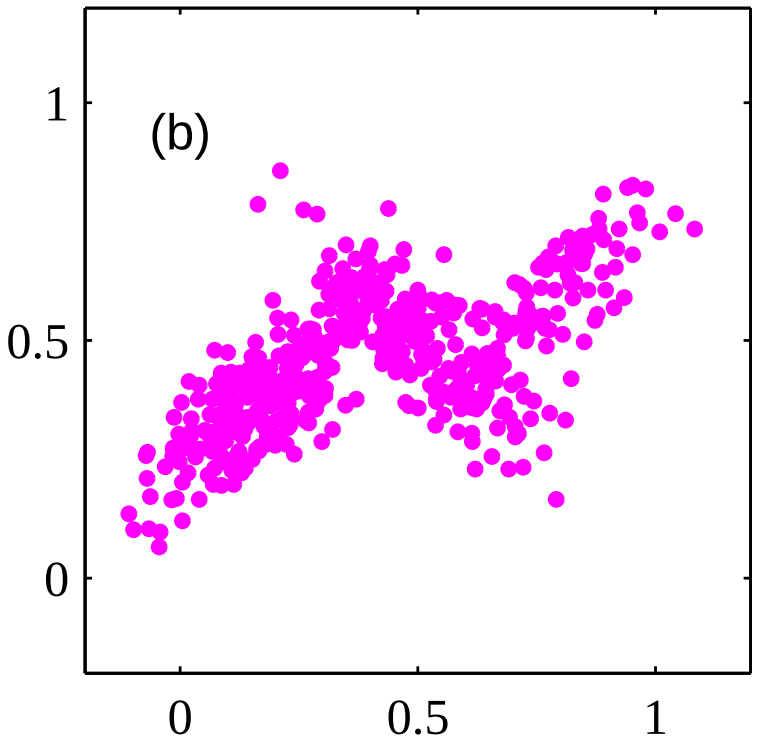

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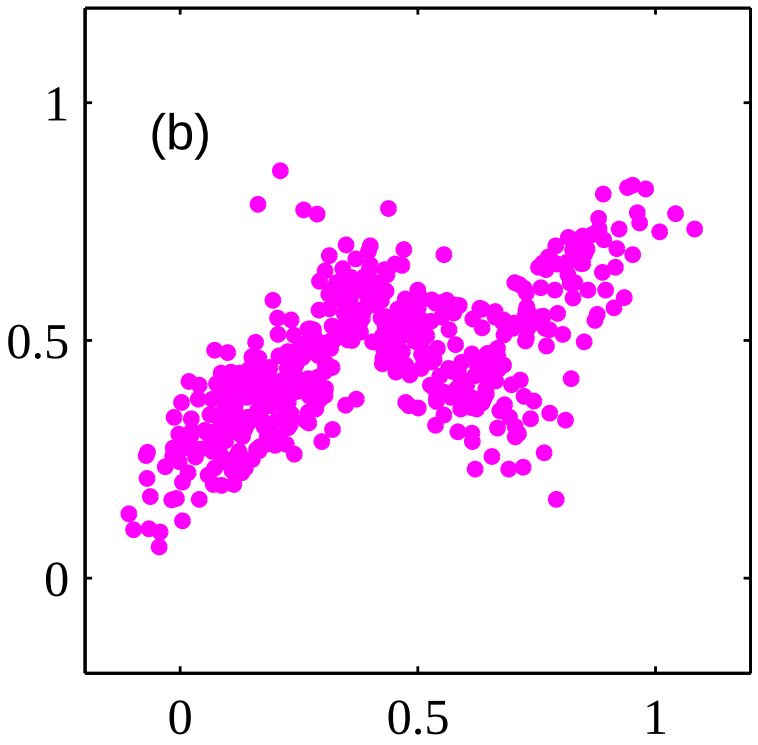

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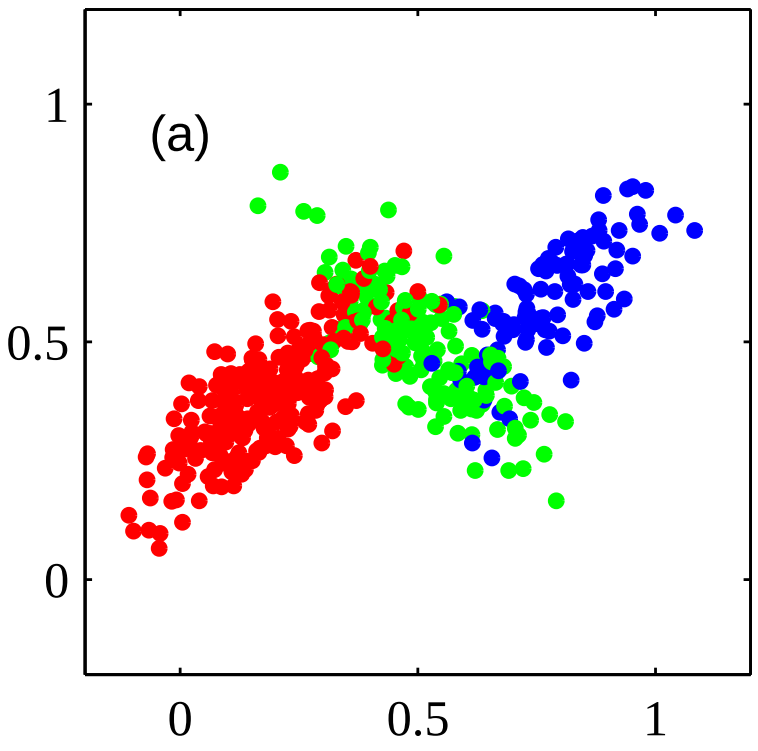
- E.g., the data is not a Gaussian b/c we have 3 distinct concentrated regions

Gaussian mixture models: intuition



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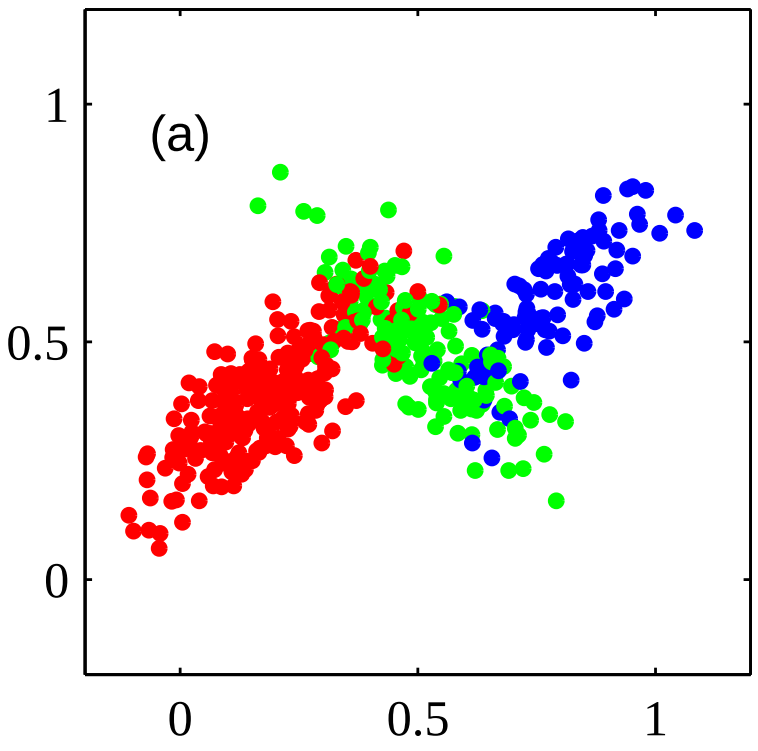

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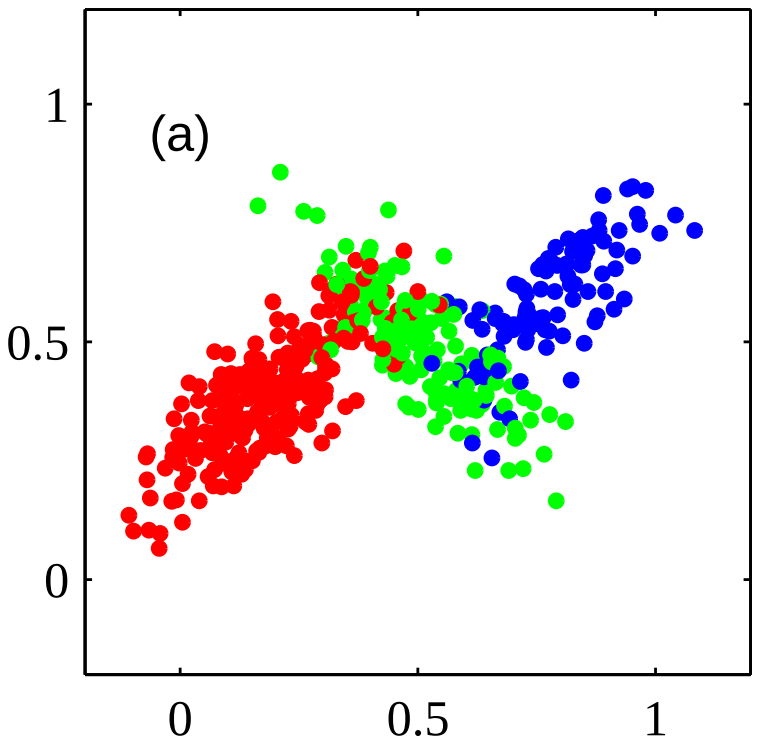

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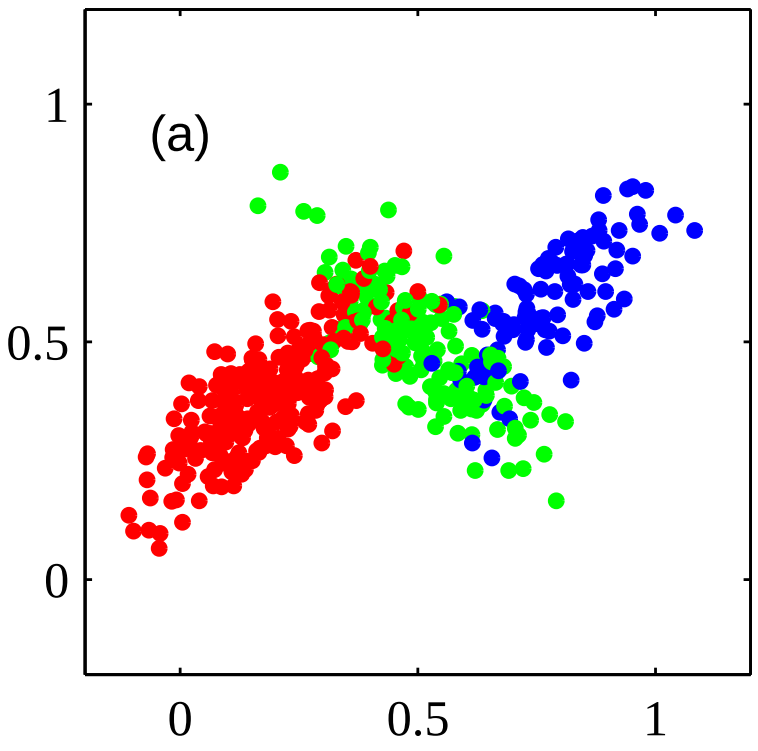

- Key idea: Model *each* region with a distinct distribution
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- *However*, we don't know *cluster assignments* (label), *parameters* of Gaussians, or *mixture components*!

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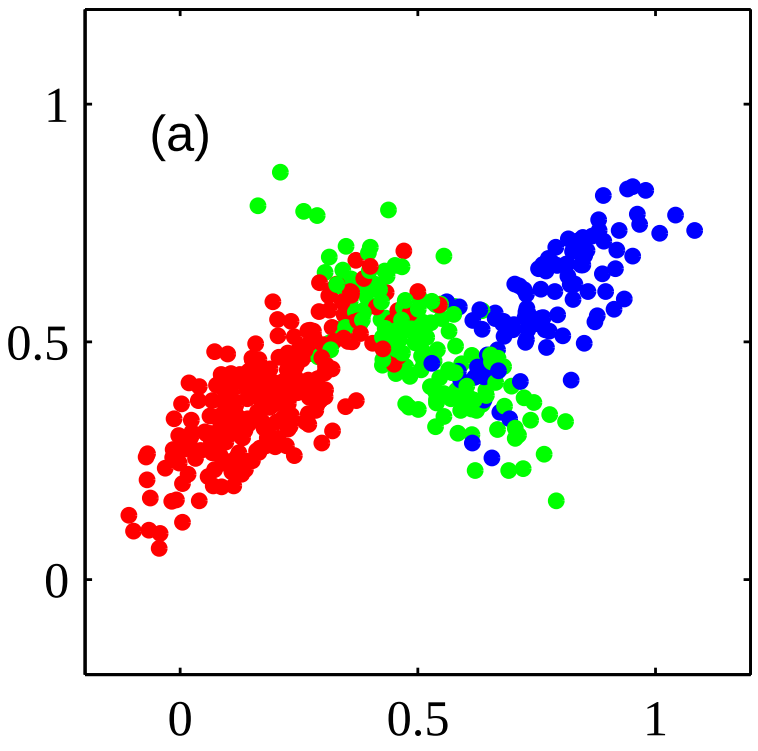
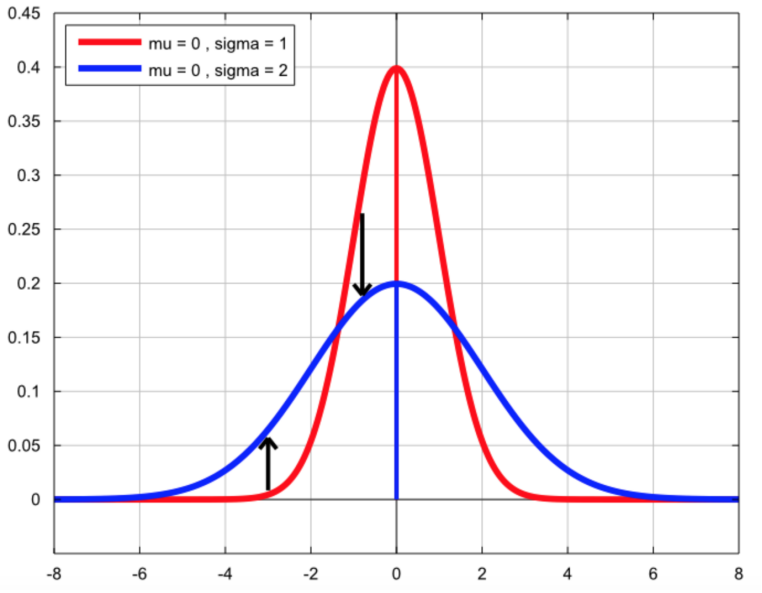


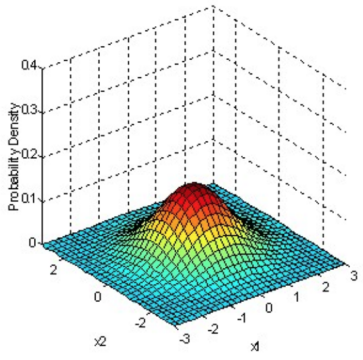
- Key idea: Model *each* region with a distinct distribution
- Can use Gaussians — Gaussian mixture models (GMMs)
- *However*, we don't know *cluster assignments* (label), *parameters* of Gaussians, or *mixture components*!
- Must learn from *unlabeled* data $\mathcal{D} = \{\boldsymbol{x}_n\}_{n=1}^N$

Recall: Gaussian (Normal) distributions

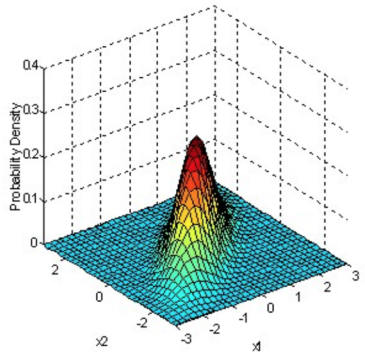
$$\boldsymbol{x} \sim N(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-d/2}|\Sigma|^{-1/2} \exp\left\{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right\}$$



$\boldsymbol{\mu} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \boldsymbol{\Sigma} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$



$\boldsymbol{\mu} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \boldsymbol{\Sigma} = \begin{pmatrix} 1 & 0.8 \\ 0.8 & 1 \end{pmatrix}$



Gaussian Mixture Models: Formal Definition

GMM has the following density function for $\boldsymbol{x}$

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

- K: number of Gaussians — they are called mixture components
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$$\forall\ k,\ \omega_k > 0, \quad \text{and} \quad \sum_k \omega_k = 1$$

These properties ensure that $p(\boldsymbol{x})$ is a probability density function

GMM as the marginal distribution of a joint distribution

Consider the following joint distribution

$$p(\boldsymbol{x}, z) = p(z)p(\boldsymbol{x}|z)$$

where z is a discrete random variable taking values between 1 and K.

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Then, the marginal distribution of $\boldsymbol{x}$ is

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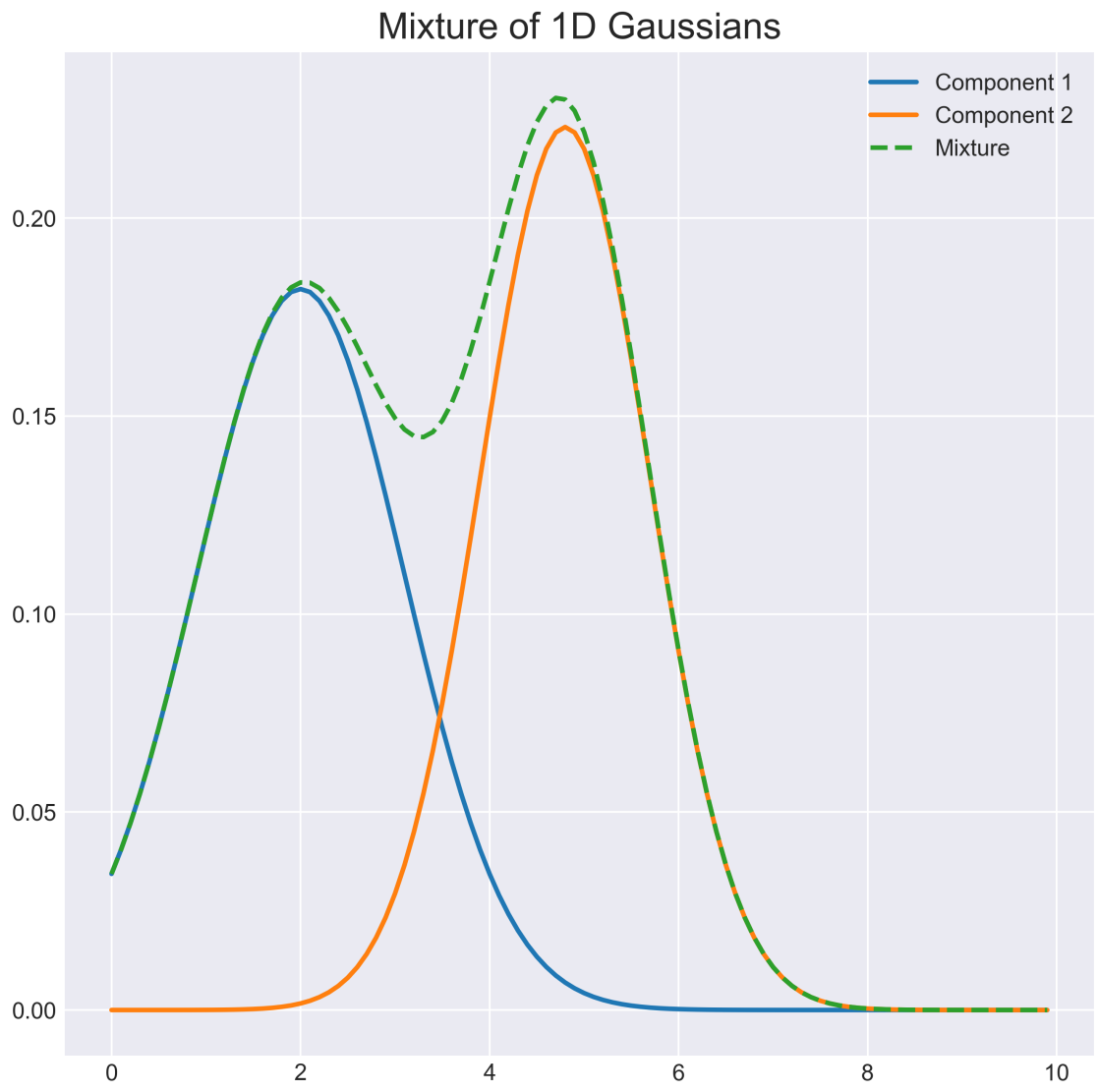
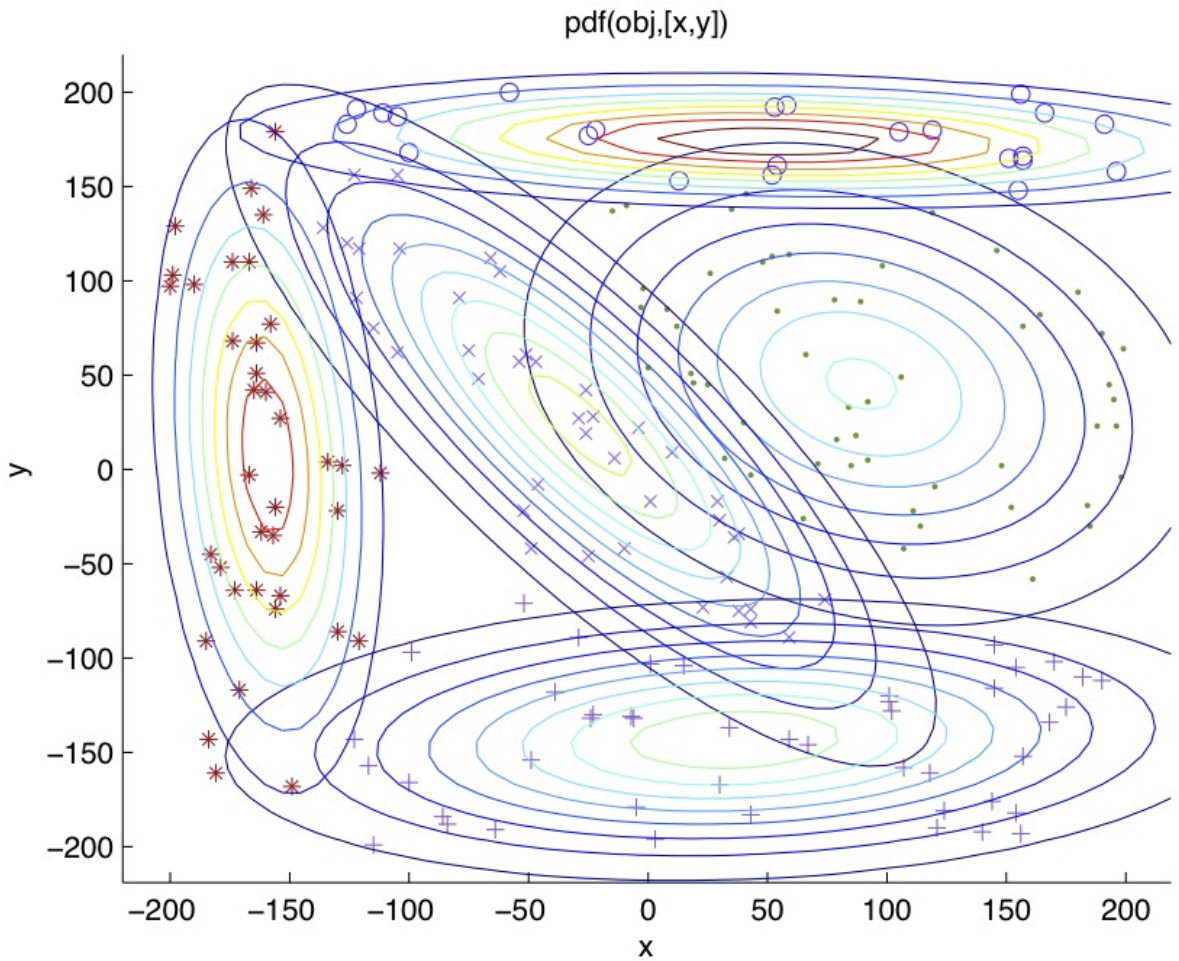
Namely, the Gaussian mixture model

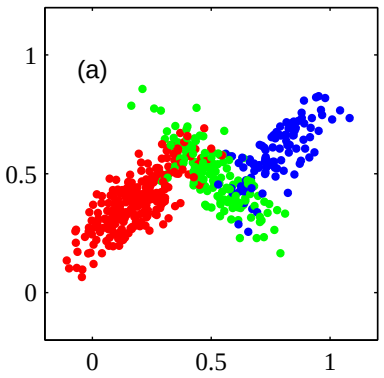
Gaussian mixtures in 1D



Gaussian mixture model for clustering



GMMs: example



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

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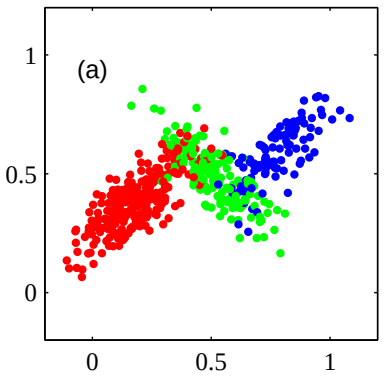

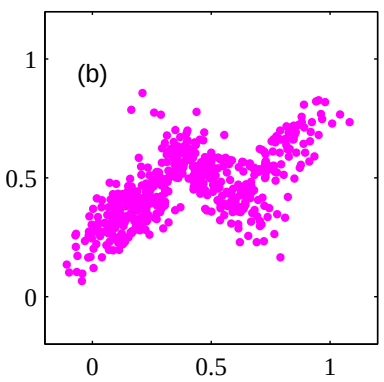

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The marginal distribution is thus

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

Parameter estimation for Gaussian mixture models

The parameters in GMMs are

Parameter estimation for Gaussian mixture models

The parameters in GMMs are $\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$

Let's first consider the simple/unrealistic case where *we have labels z*

Define $\mathcal{D}' = \{\boldsymbol{x}_n, z_n\}_{n=1}^N$, $\mathcal{D} = \{\boldsymbol{x}_n\}_{n=1}^N$

- $\mathcal{D}'$ is the complete data
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Given $\mathcal{D}'$, the maximum likelihood estimation of the $\boldsymbol{\theta}$ is given by

$$\boldsymbol{\theta} = \arg\max \log \mathcal{D}' = \sum_n \log p(\boldsymbol{x}_n, z_n)$$

Parameter estimation for GMMs: complete data

The complete likelihood is decomposable

$$\sum_n \log p(\boldsymbol{x}_n, z_n) = \sum_n \log p(z_n) p(\boldsymbol{x}_n | z_n) = \sum_k \sum_{n:z_n=k} \log p(z_n) p(\boldsymbol{x}_n | z_n)$$

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Note: in the complete setting the r_{nk} are binary, but later we will 'relax' these variables and allow them to take on fractional values

Parameter estimation for GMMs: complete data

From our previous discussion, we have

$$\sum_n \log p(\boldsymbol{x}_n, z_n) = \sum_k \sum_n r_{nk} \left[\log \omega_k + \log N(\boldsymbol{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\right]$$

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The term inside the braces depends on k-th component's parameters. It is now easy to show that (left as an exercise) the MLE is:

$$\omega_k = \frac{\sum_n r_{nk}}{\sum_k \sum_n r_{nk}}, \quad \boldsymbol{\mu}_k = \frac{1}{\sum_n r_{nk}} \sum_n r_{nk} \boldsymbol{x}_n$$

$$\boldsymbol{\Sigma}_k = \frac{1}{\sum_n r_{nk}} \sum_n r_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top$$

What's the intuition?

Intuition

Since r_{nk} is binary, the previous solution is nothing but:

- ω_k: fraction of total data points whose cluster label z_n is k
  - note that $\sum_k \sum_n r_{nk} = N$
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We use the knowledge of true cluster labels z_n (which imply the r_{nk}) to estimate $\boldsymbol{\theta}$.

What do we do when we *do not* know z_n (incomplete data)

Parameter estimation for GMMs: Incomplete data

GMM Parameters

$$\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^{K}$$

Incomplete Data

Our data contains observed and unobserved data, and hence is incomplete

- Observed: $\mathcal{D} = \{\boldsymbol{x}_n\}$
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$$= \arg\max \sum_n \log \sum_{\boldsymbol{z}_n} p(\boldsymbol{x}_n, \boldsymbol{z}_n|\boldsymbol{\theta})$$

The objective function $\ell(\boldsymbol{\theta})$ is called the *incomplete* log-likelihood.

Parameter estimation for GMMs: incomplete data

When z_n is not given, we can guess it via the posterior probability (recall: Bayes' rule!)

$$p(z_n = k|\boldsymbol{x}_n) = \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{p(\boldsymbol{x}_n)} = \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{\sum_{k'=1}^{K} p(\boldsymbol{x}_n|z_n = k')p(z_n = k')}$$
$$= \frac{N(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \times \omega_k}{\sum_{k'=1}^{K} N(\boldsymbol{x}_n|\boldsymbol{\mu}_{k'}, \boldsymbol{\Sigma}_{k'}) \times \omega_{k'}}$$

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To compute the posterior probability, we need to know the parameters $\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^{K}$

Idea: Let's pretend we know these parameters so we can compute the posterior probability.

How is that going to help us?

Estimation with soft r_{nk}

We define $r_{nk} = p(z_n = k|\boldsymbol{x}_n)$

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If we solve for the MLE of $\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$ given soft r_{nk}s, we get the same expressions as before!

$$\omega_k = \frac{\sum_n r_{nk}}{\sum_k \sum_n r_{nk}}, \quad \boldsymbol{\mu}_k = \frac{1}{\sum_n r_{nk}} \sum_n r_{nk} \boldsymbol{x}_n$$

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But remember, we're 'cheating' by using $\boldsymbol{\theta}$ to compute r_{nk}!

Iterative procedure

Alternate between estimating r_{nk} and computing parameters

- Step 0: initialize $\boldsymbol{\theta}$ with some values (random or otherwise)
- Step 1: set $r_{nk} = p(z_n = k|\boldsymbol{x}_n)$ for current $\boldsymbol{\theta}$ using Bayes Rule
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At the end convert r_{nk} back to binary by setting the largest r_{nk} for point x_n to 1 and others to 0.

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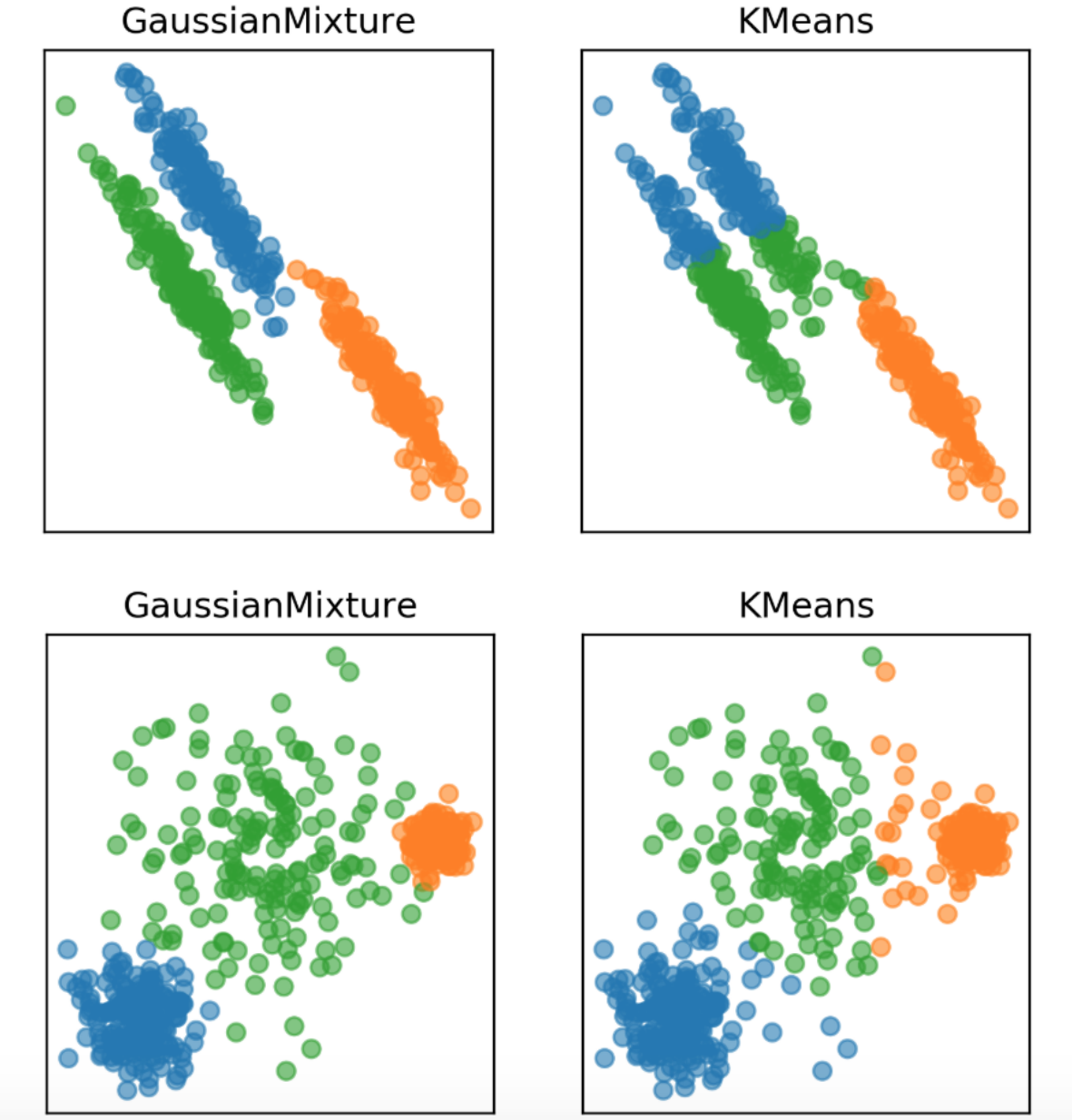
Connection with K-means?

- GMMs provide probabilistic interpretation for K-means
- K-means is "hard" GMM or GMMs is "soft" K-means
- Posterior r_{nk} provides a probabilistic assignment for $\boldsymbol{x}_n$ to cluster k

GMMs vs. k-means



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Pros/Cons

- k-means is a simpler, more straightforward method, but might not be as accurate because of deterministic clustering
- GMMs can be more accurate, as they model more information (soft clustering, variance), but can be more expensive to compute
- Both methods have a similar set of practical issues (having to select k, the distance, and the initialization)

What you should know . . .

- How GMMs differ from k-means (and why we care)

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- The difference between complete, incomplete data/likelihood
- How to learn the parameters in a GMM

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- I am teaching 18-667: Algorithms for Large-scale ML in Spring 2021. Please consider registering if you are interested! The class with cover the latest research papers in:
  - Distributed SGD
  - Federated learning optimization algorithms
  - Communication-efficient strategies such as local-update SGD and gradient compression

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