Unsupervised Learning & Data Clustering

Problem Set-up

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Objective

Objective

Define the set-up
of unsupervised
learning

Learning from Unlabeled Data

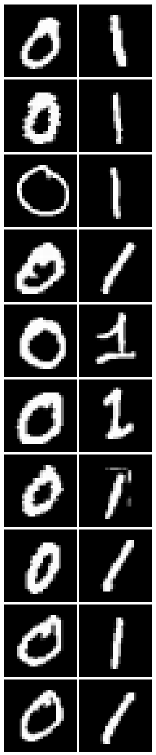
Given a training set of *n* unlabeled samples $\{x^{(i)}\}$

What can we learn from the samples?

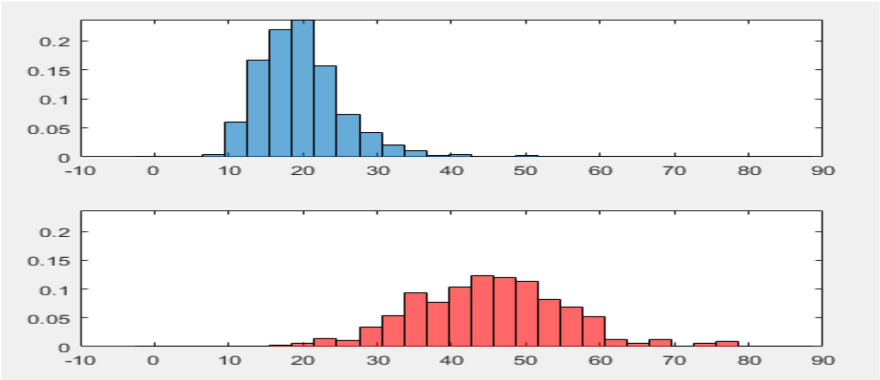
- We could estimate the overall distribution of the data without knowing their label.
- We could figure out the groupings of the samples (if any).
- We could identify some features that may be more important than others.

An Example

Illustrating structures/groupings of unlabeled samples may relate to the (unknown) labels of the samples



→ If we know the labels, we may find the densities of the classes →

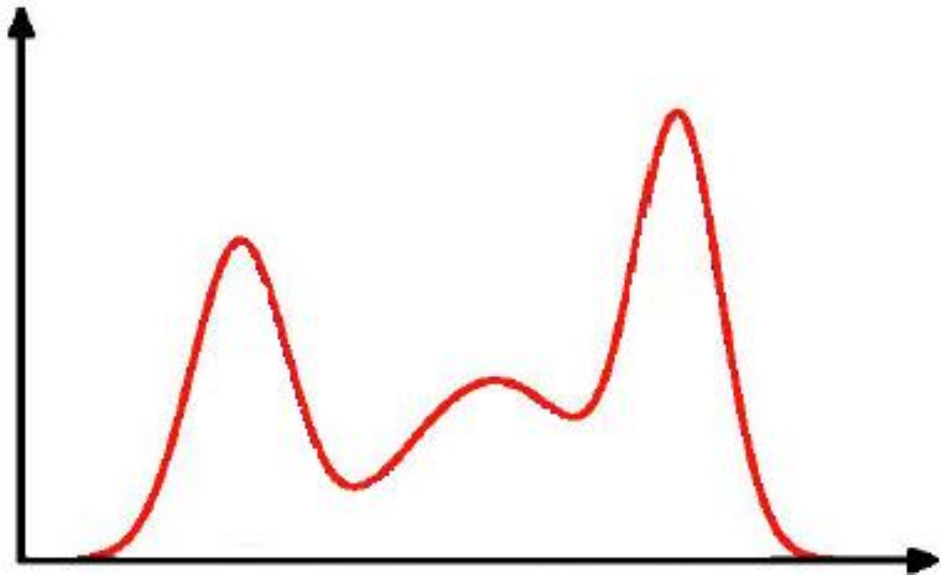


→ What may we see if we have no label for the data samples?

Another Example

- A density estimated from unlabeled samples may help us to identify densities of different classes

- If we know there are three classes in the data, each having a normal distribution …



A Mixture-Density Model

- **Assume a parametric model like this:**
  - The samples come from C classes.
  - The prior probabilities $P(\omega_j)$ for each class are known, for $j = 1, \ldots, C$.
  - The form of $p(\mathbf{x} \mid \omega_j, \theta_j)$ ($j = 1, \ldots, C$) are known.
  - The C parameter vectors $\theta_1, \theta_2, \ldots, \theta_C$ are unknown.
- **Samples from this distribution are given, but the labels of the training samples are *unknown*.**

A Mixture-Density Model (cont'd)

- What is the PDF of the unlabeled samples?

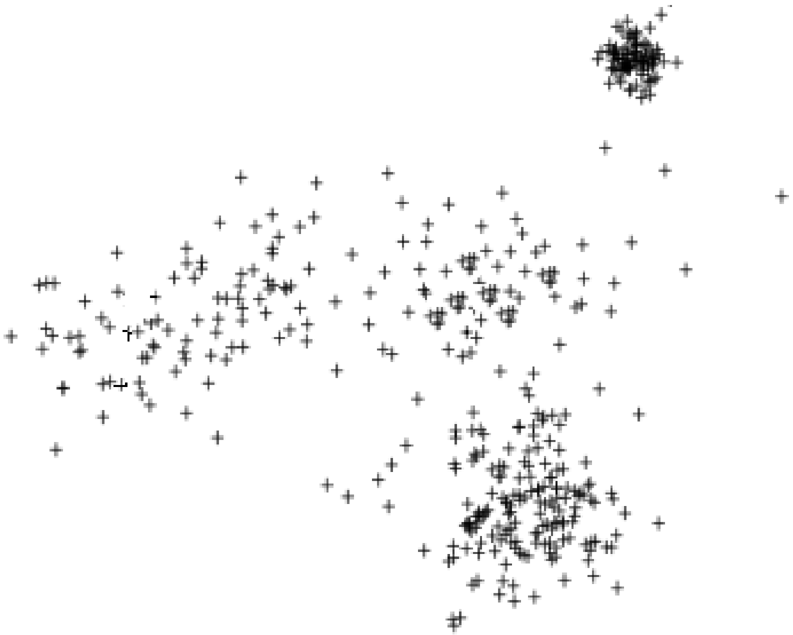
$$p(\mathbf{x} \mid \boldsymbol{\theta}) = \sum_{j=1}^{C} p(\mathbf{x} \mid \omega_j, \boldsymbol{\theta}_j) P(\omega_j)$$

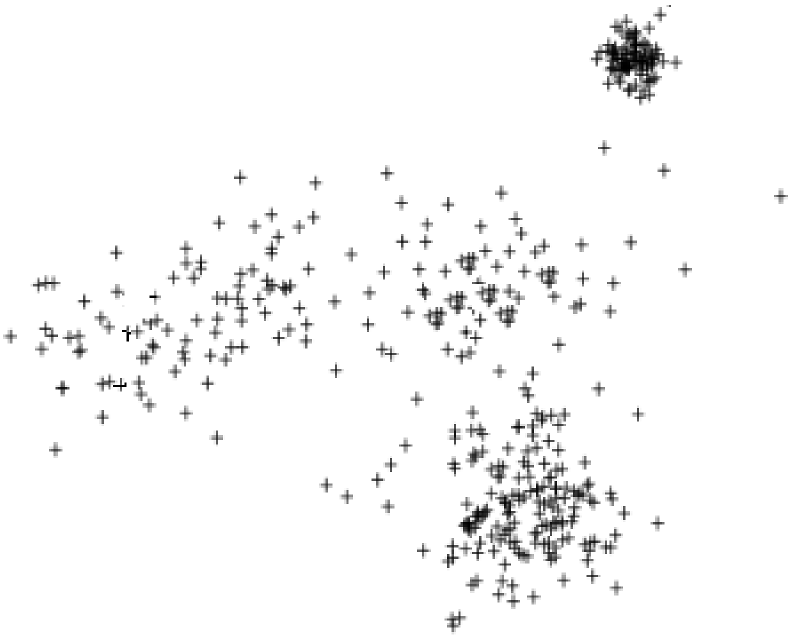
where $\theta = (\theta_1, \theta_2, \ldots, \theta_C)$

- Can we learn θ from unlabeled samples from this mixture density?

Illustrating Mixture-Density Model

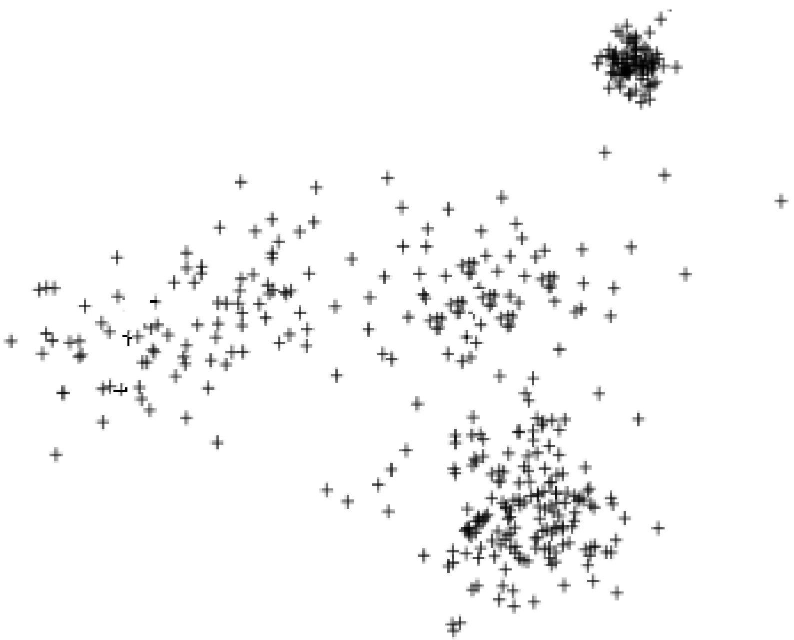
An example: with the assumption of 4 classes

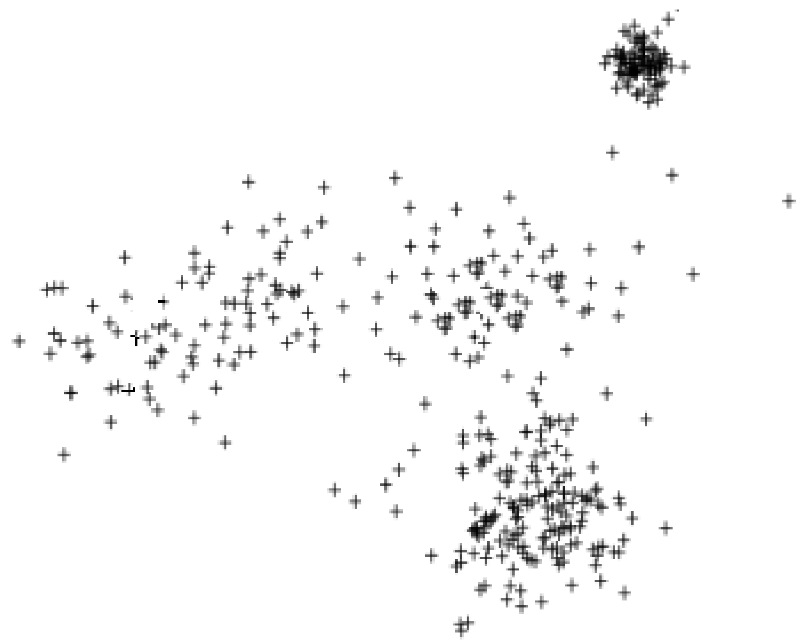




Illustrating Mixture-Density Model

An example: with the assumption of 2 classes





The Question of Identifiability

- **Can we learn a unique θ from a set of unlabeled samples from a mixture density?**
  - For continuous features (with PDFs), the answer is often "Yes".
- **An example in discrete case (with PMF).**
  - Two coins with P(head) being p & q respectively.
  - Randomly pick one and toss it; Record the outcome.
  - With only the outcomes of N tosses, but not knowing which coin was used each time (→ unsupervised), can we figure out p and q?

Unsupervised Learning

Gaussian Mixture Models and the EM Algorithm

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Objective

Objective

Define the Gaussian Mixture Model

Objective

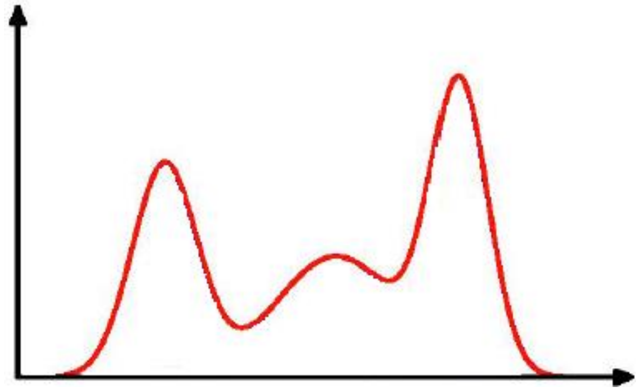
Illustrate the Expectation-Maximization Algorithm

The Gaussian Mixture Models

- **The mixture model:**

$$p(\mathbf{x} \mid \boldsymbol{\theta}) = \sum_{j=1}^{C} \underline{p(\mathbf{x} \mid \omega_j, \boldsymbol{\theta}_j)} P(\omega_j)$$

- **GMM: each component density is a Gaussian distribution.**
  - Can be a good approximation to many real data distributions.



If We Do Have Labels…

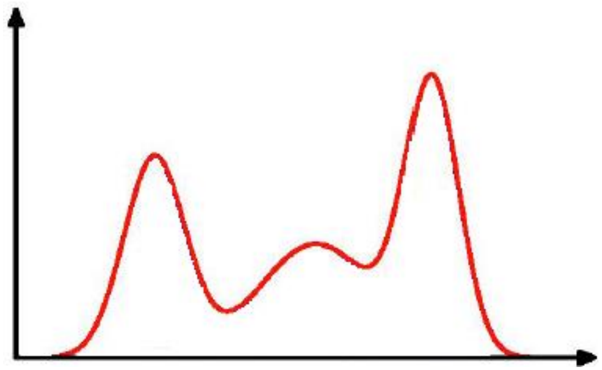
$$p(\mathbf{x} \mid \boldsymbol{\theta}) = \sum_{j=1}^{C} \underline{p(\mathbf{x} \mid \omega_j, \boldsymbol{\theta}_j)} P(\omega_j)$$

- This becomes supervised learning for each component (class).

- It is more difficult without labels.

Unsupervised Case

- Consider an iterative method using the *maximum likelihood estimation* concept.
- Consider a 3-component 1-d example.



- What are the parameters in this case?
- We might have some initial (imprecise) guesses for the parameter, e.g., vs the *k-means algorithm*.
  - *How to improve the initial guesses?*

Unsupervised Case (cont'd)

Iterate on t

Given parameter estimates at iteration t-1

An example of Expectation-Maximization Algorithm.

Step 1. For a sample j, compute its probability of being from class *k*

$$P[y_j = k \mid x_j, \theta^{(t-1)}] \propto P_k^{(t-1)} p(x_j \mid \mu_k^{(t-1)}, \sigma_k^{(t-1)}), \ \forall k = 1, 2, 3$$

Step 2. Update the estimates of the parameters

$$\mu_k^{(t)} = \frac{\sum_j x_j P[y_j = k \mid x_j, \theta^{(t-1)}]}{\sum_j P[y_j = k \mid x_j, \theta^{(t-1)}]}$$

$$P_k^{(t)} = \frac{\sum_j P[y_j = k \mid x_j, \theta^{(t-1)}]}{\text{total \# of samples}}$$

Unsupervised Learning

The k-Means Algorithm

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Objective

Objective

Discuss the basics of data clustering

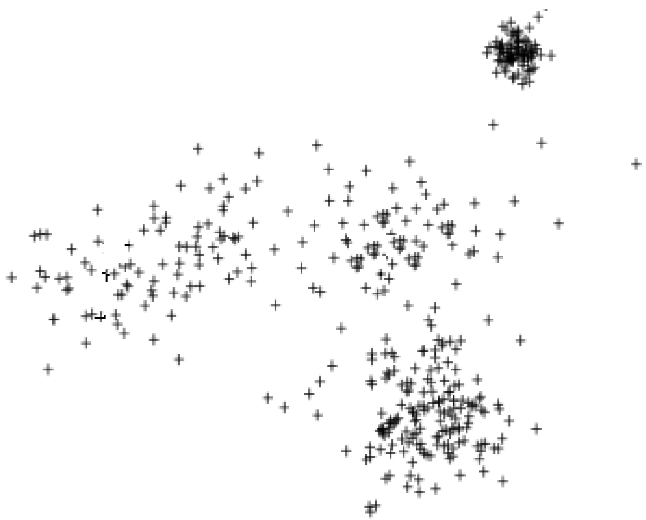
Objective

Illustrate the k-Means Algorithm

Finding the Clusters/Groupings of the Samples

A few basic questions to answer

- How to represent the clusters?
  - ➔ We will use the centroid to represent a cluster.
- Which cluster a sample should be assigned to (e.g., membership)?
  - ➔ We will use the similarity to the centroid to determine the membership.
- What similarity measure to use?
  - E.g., Euclidean distance



More on Similarity Measures

- **If we use Euclidean distance as the measure:**
  - It is invariant to translations & rotations of the feature space.
  - But not to more general transformations.
- **E.g., if one feature is scaled.**

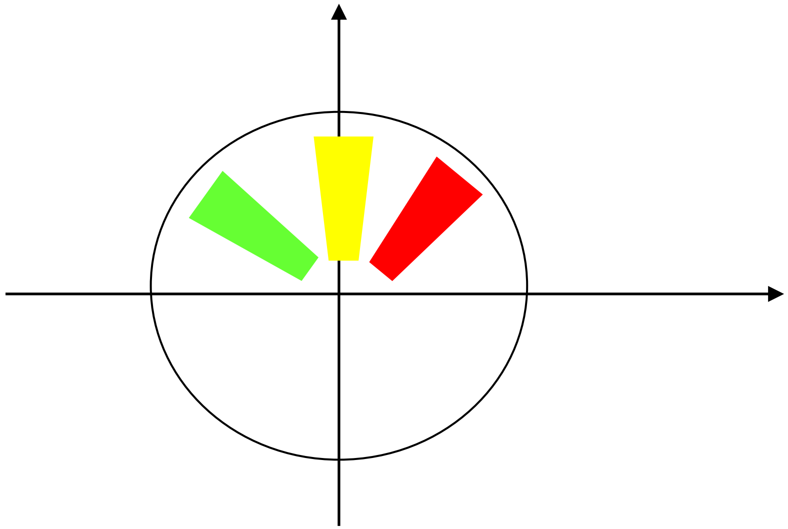
More on Similarity Measures (cont'd)

- Other types of similarity measures

$$s(\mathbf{x}, \mathbf{x}') = \frac{\mathbf{x}^t \mathbf{x}'}{\|\mathbf{x}\| \|\mathbf{x}'\|}$$

- E.g., cosine similarity

- E.g., distance on a graph, like shortest path.



Clustering as Optimization

The sum-of-squared-error criterion/cost

- Let D_i be the subset of samples from class i.
- Let n_i be the number of samples in D_i, and $\mathbf{m}_i$ the mean of those samples

$$\mathbf{m}_i = \frac{1}{n_i} \sum_{\mathbf{x} \in D_i} \mathbf{x}$$

- The sum of squared error is:

$$J_e = \sum_{i=1}^{C} \sum_{\mathbf{x} \in D_i} \left\| \mathbf{x} - \mathbf{m}_i \right\|^2$$

➔ Well-separated, compact data “clouds” tend to give small errors when the clusters coincide with the clouds.

Clustering as Optimization (cont'd)

$$J_e = \sum_{i=1}^{C} \sum_{\mathbf{x} \in D_i} \left\| \mathbf{x} - \mathbf{m}_i \right\|^2$$

- **An optimization problem to solve for finding a "good" clustering: to find the partition of the data that minimizes J_e**

- If the membership of a sample is determined by the distance to the means $\mathbf{m}_i$
  - Then the task is to find the optimal set of $\{m_i\}$
  - The problem is NP-hard.

k-Means Clustering

- **Input: Given n data samples**

- **Goal: Partition them into *k* clusters/sets D_i, with respective center/mean vectors $\mu_1, \mu_2, \ldots, \mu_k$, so as to minimize**

$$\sum_{i=1}^{k} \sum_{\mathbf{x} \in D_i} \|\mathbf{x} - \boldsymbol{\mu}_i\|^2$$

- **Comparing with the mixture models:**
  - Here we do “hard” assignment of the membership to a sample (simply based on its distance to the cluster center).

The Basic k-Means Algorithm

Given: n samples, a number k.

<u>Begin</u>

initialize μ_1, μ_2, …, μ_k (randomly selected)

<u>do</u> classify n samples according to nearest μ_i

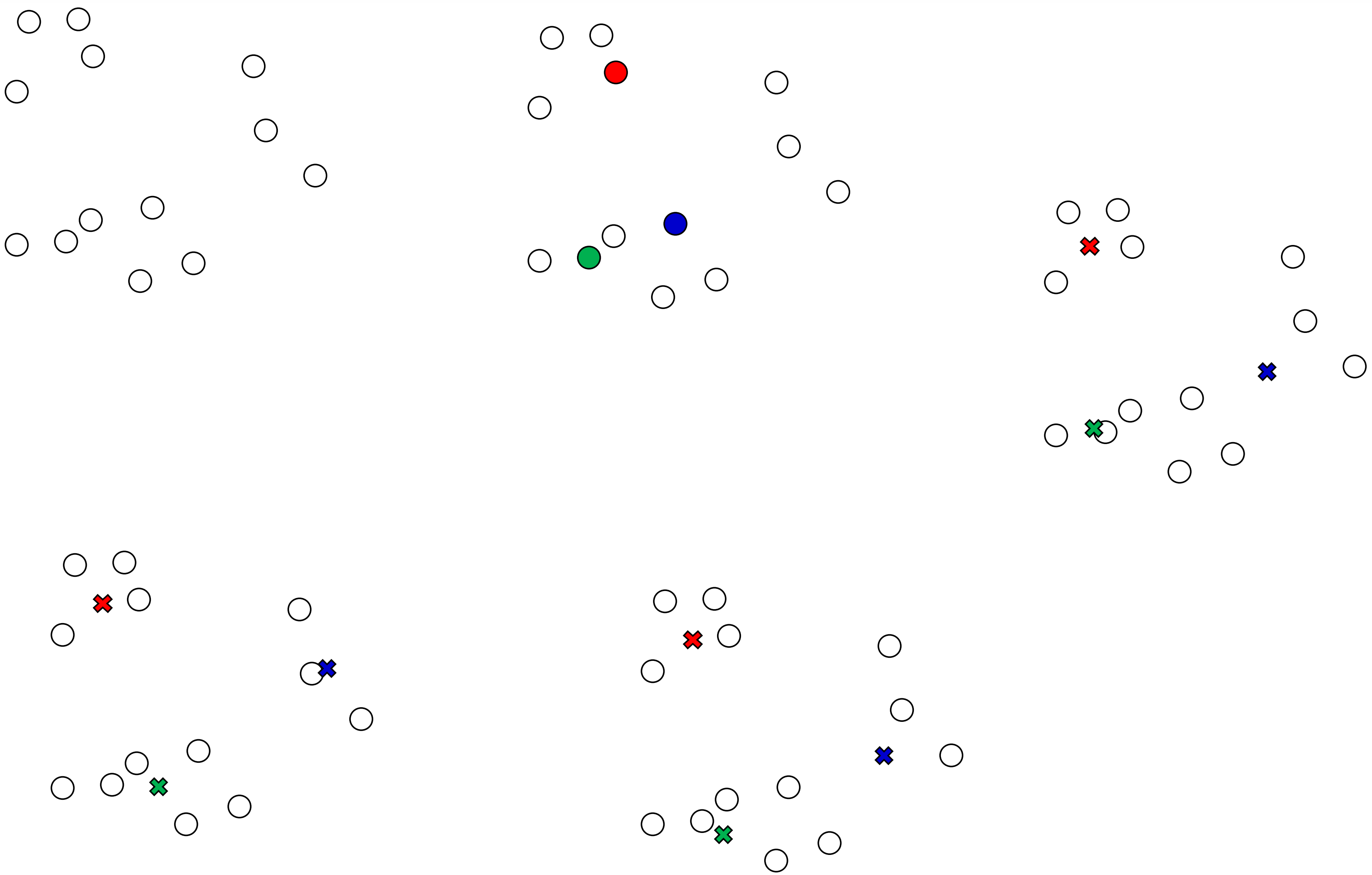
recompute μ_i

<u>until</u> no change in μ_i

<u>return</u> μ_1, μ_2, …, μ_k

<u>End</u>

Illustrating the Algorithm



Unsupervised Learning
Analyzing the k-Means Algorithm

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Objective

Objective

Discuss the weaknesses of the k-means algorithm

Objective

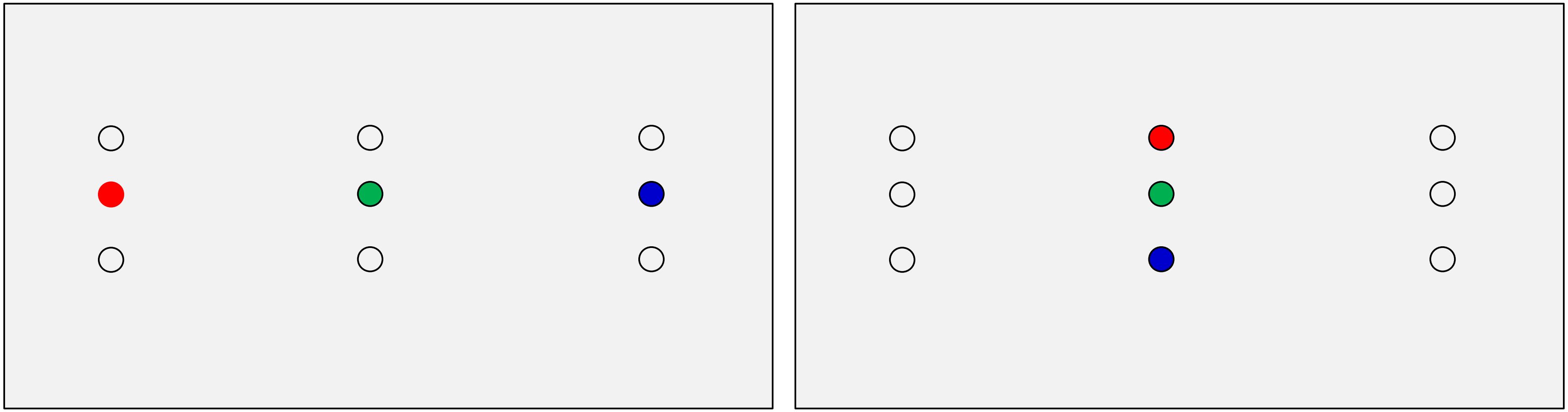
Discuss a few common techniques for potential improvement

Properties of the k-Means Algorithm

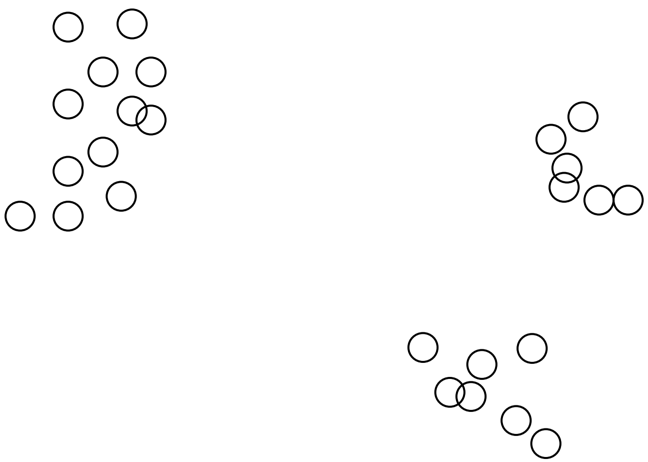
- The algorithm will converge when the cluster centers no longer change.

- But the results may not be an optimal solution.

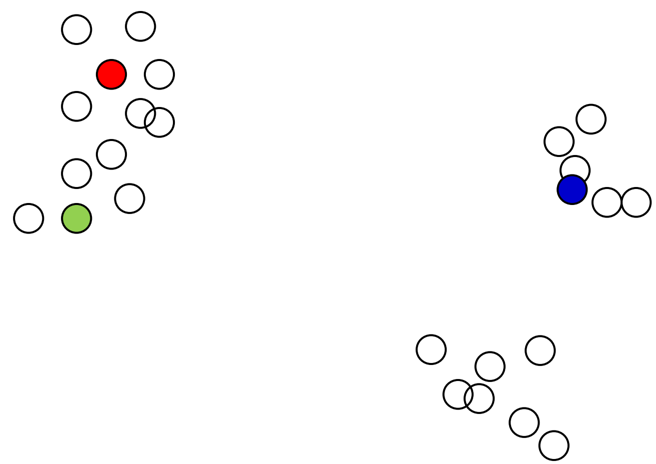
➔ **Sensitivity to initialization**



Another Example



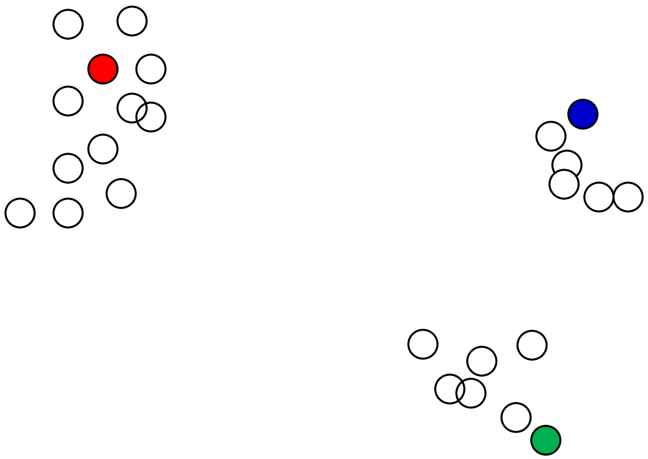
- The natural grouping seems to be so well defined.
- For k=3, what will be the clusters?



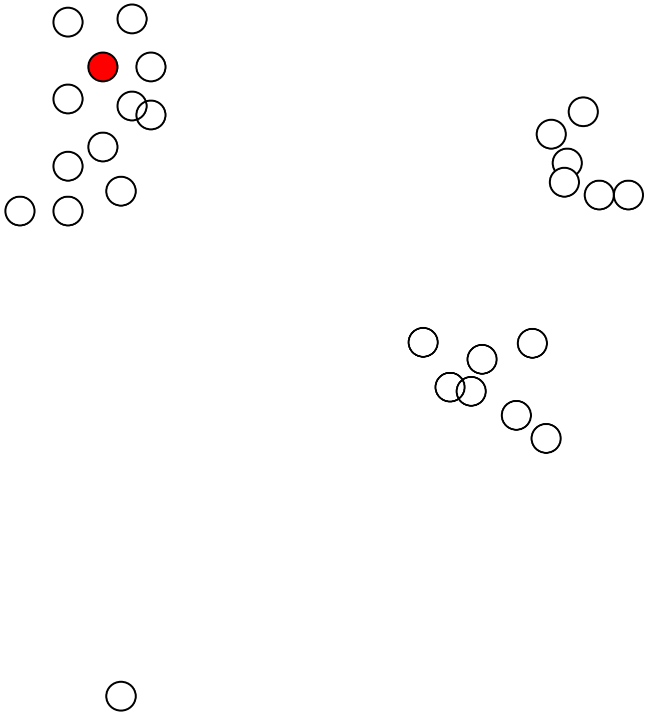
What can we do to improve?

A Few Common “Tricks”

- Choosing the point furthest from the previous centers.
  - Drawback: might be sensitive to “outlies”.



- Multiple runs with different initial centers.



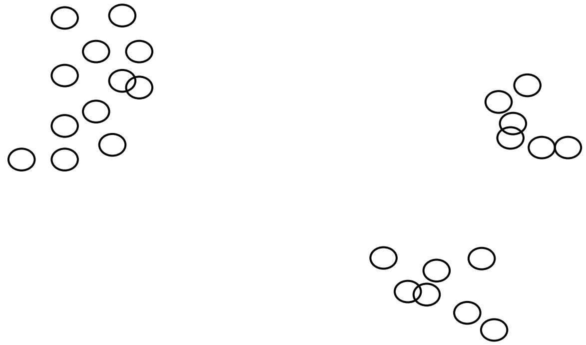
Other Variants of Basic k-Means

k-Means++:

- New centers are chosen with probabilities (as a function of distance to closest prior centers).
- Kind of between “random” and “furthest point” techniques.

Hierarchical approaches

- Agglomerative vs divisive.



The Question of Choosing k

Two trivial extremes

- If k=1, the error is the variance of the samples.
- If k=n, the error can become 0.

What is a proper 1<k<n for capturing the structure of the samples?

Some tricks

- Trick 1: Will the cost function drop dramatically at some point?
- Trick 2: Cross-validation (on, e.g., a classification task)