ECE 20875
Python for Data Science

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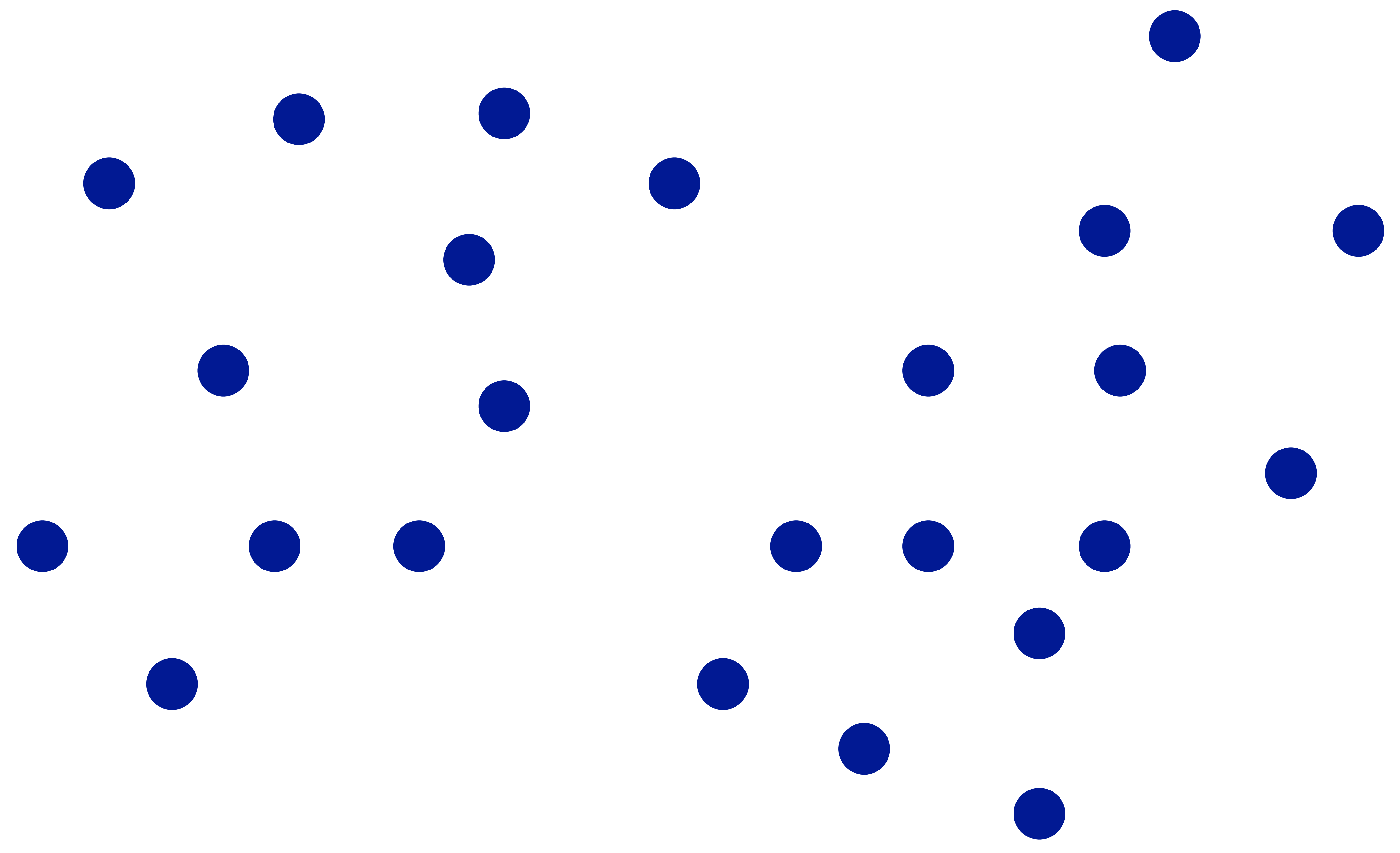
(Adapted from material developed by Profs. Milind Kulkarni, Stanley Chan, Chris Brinton, David Inouye)

clustering

what is clustering?

- Given a set of data points, group them into **clusters**, i.e., subsets of the data set that are "similar"
- What "similar" means depends on what clustering algorithm you use
  - K-means: Points are "near" each other
  - Gaussian mixture models: Points come from same Gaussian distribution
- Basic goal: Identify structure in data *without any labels*
- Lack of labels for the data points makes this **unsupervised learning**
  - We will discuss **supervised learning** more again later (where have we seen it already?)



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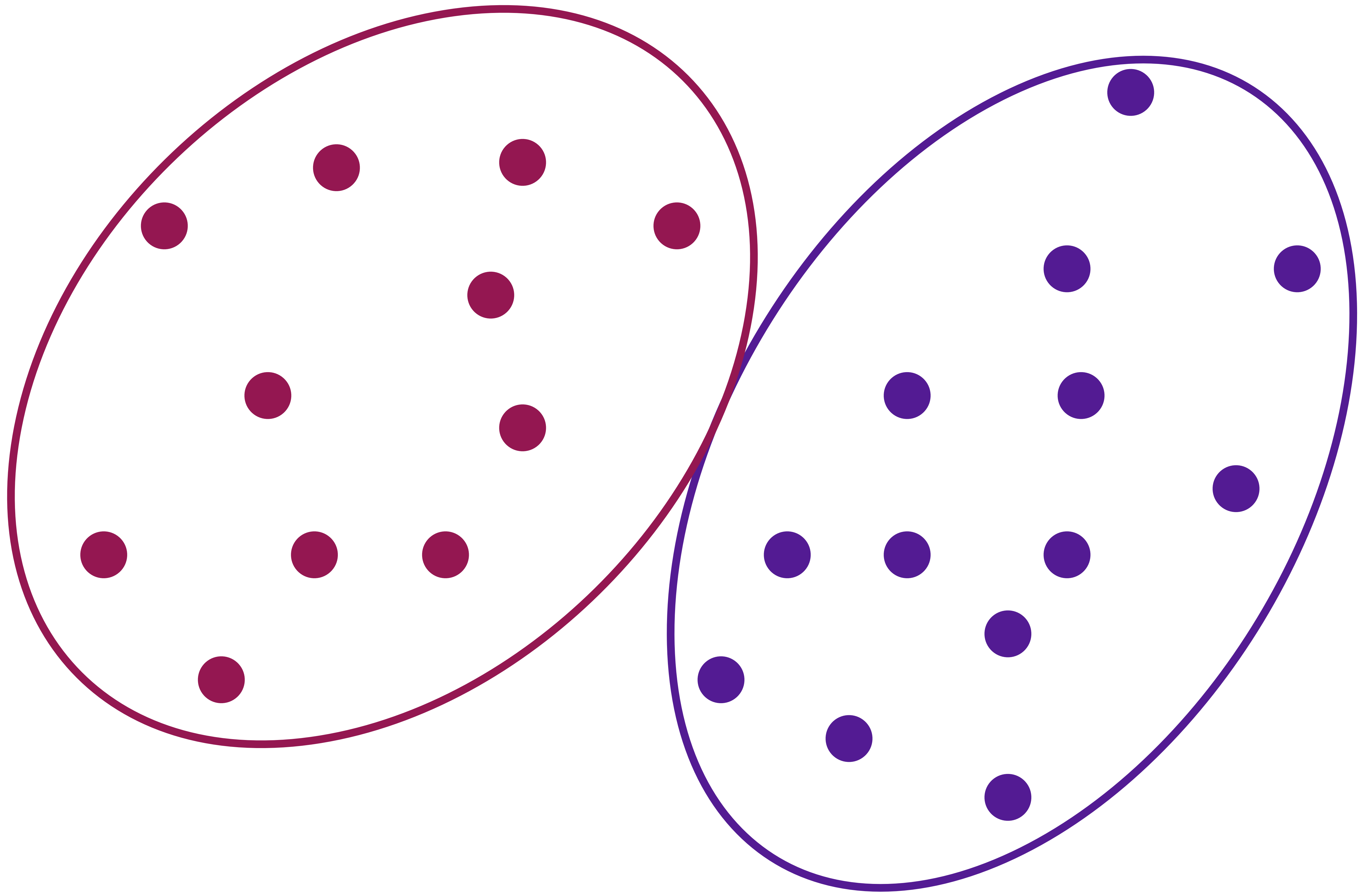


clustering algorithms

- There are probably hundreds of published algorithms for clustering datasets

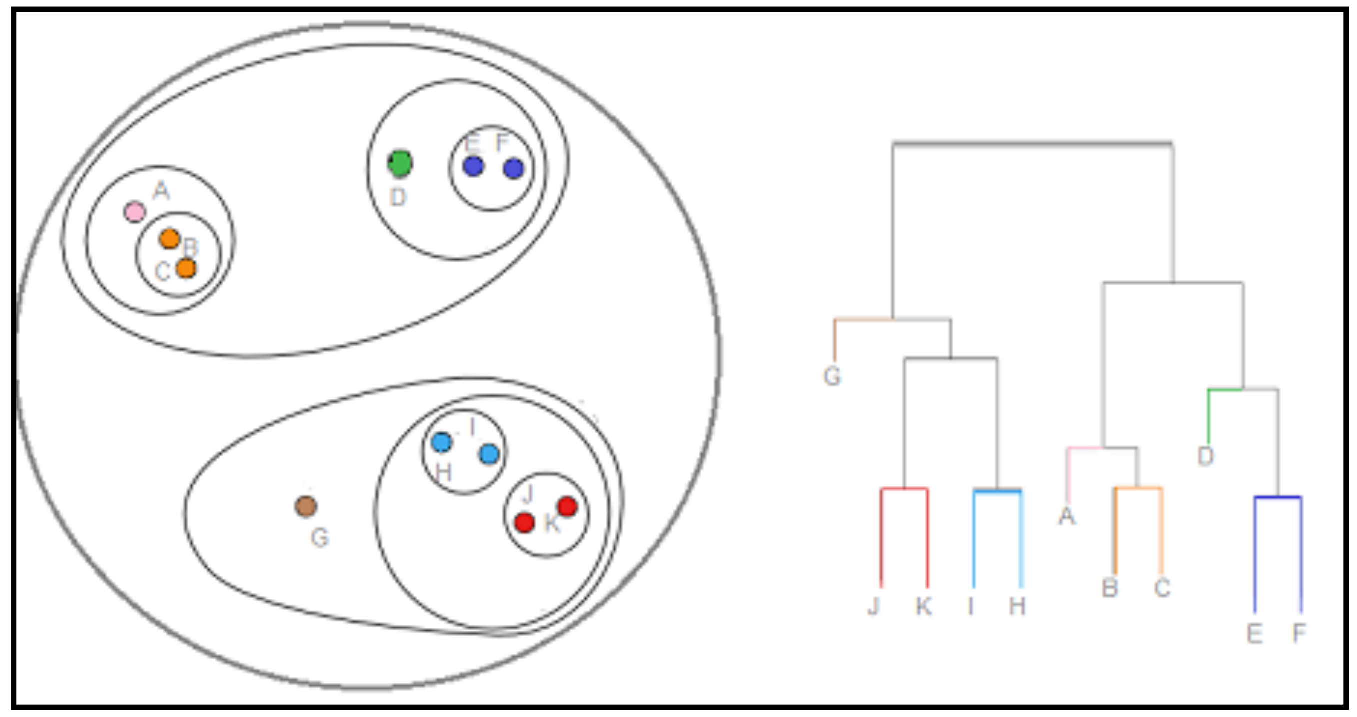
- Clustering algorithms fall into a few general categories:

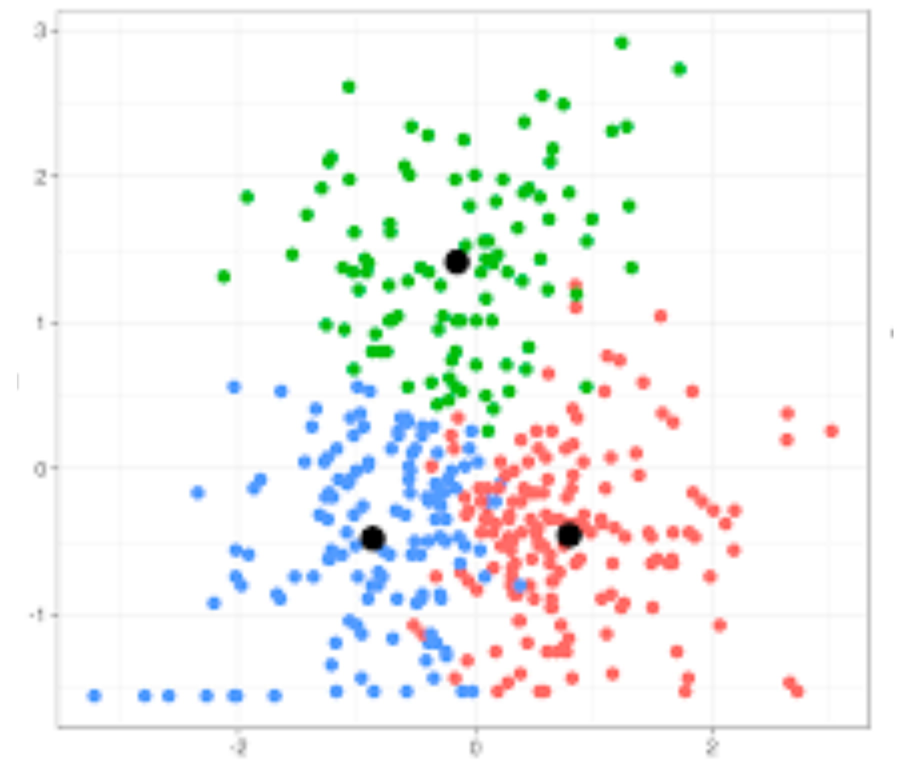
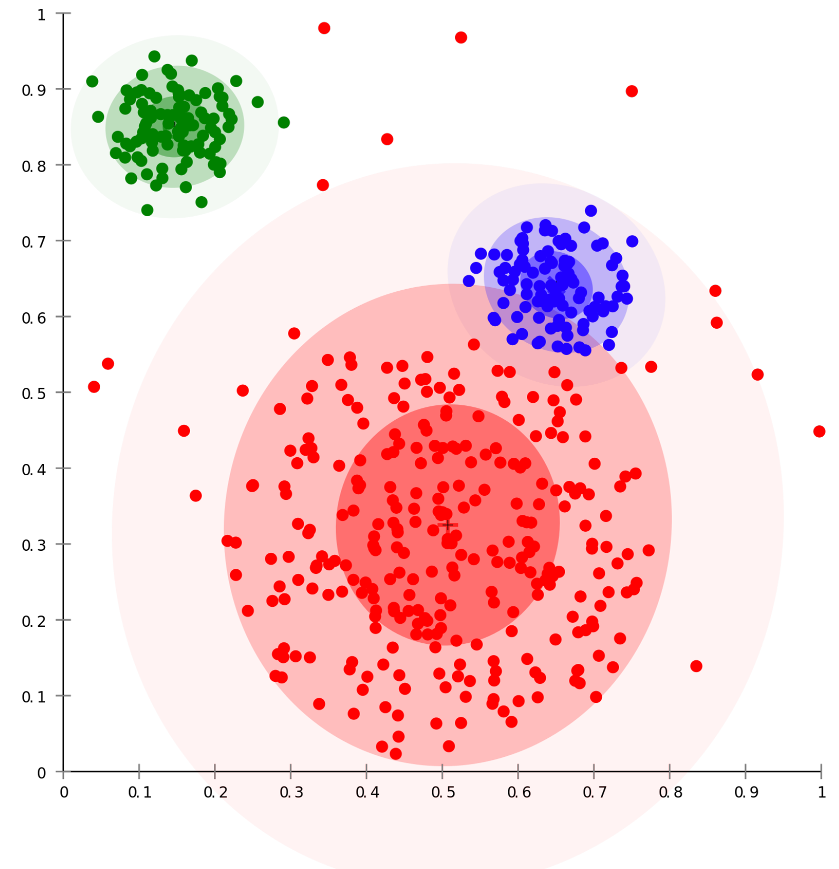
  - **Hierarchical**: Group datapoints together based on how "close" they are to one another

  - **Centroid-based**: Find center points that can be interpreted as cluster centers, and assign each point to one center

  - **Distribution-based**: Datapoints are grouped based on their likelihood of belonging to the same probability distribution

  - **Density-based**: Clusters are defined as areas of higher density in the dataset



two approaches

- We will study two of the most popular clustering methods: K-means and GMMs
  - **K-means**
    - Centroid-based
    - No model required
    - Can only find “simple” structure in data (points that are close together)
  - **Gaussian Mixture Models (GMMs)**
    - Distribution-based
    - Requires having a model in mind
    - Can find interesting structure in data (based on how complex the model is)
- Despite their different flavors, we will also see that both models …
  - require an initial assumption about the number of clusters
  - use **iterative algorithms** to find clusters: Form an initial guess, and refine it

k-means clustering

- Consider a dataset consisting of n points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$, where $\mathbf{x}_j$ is the feature vector representation of observation j (and there is no y_j)

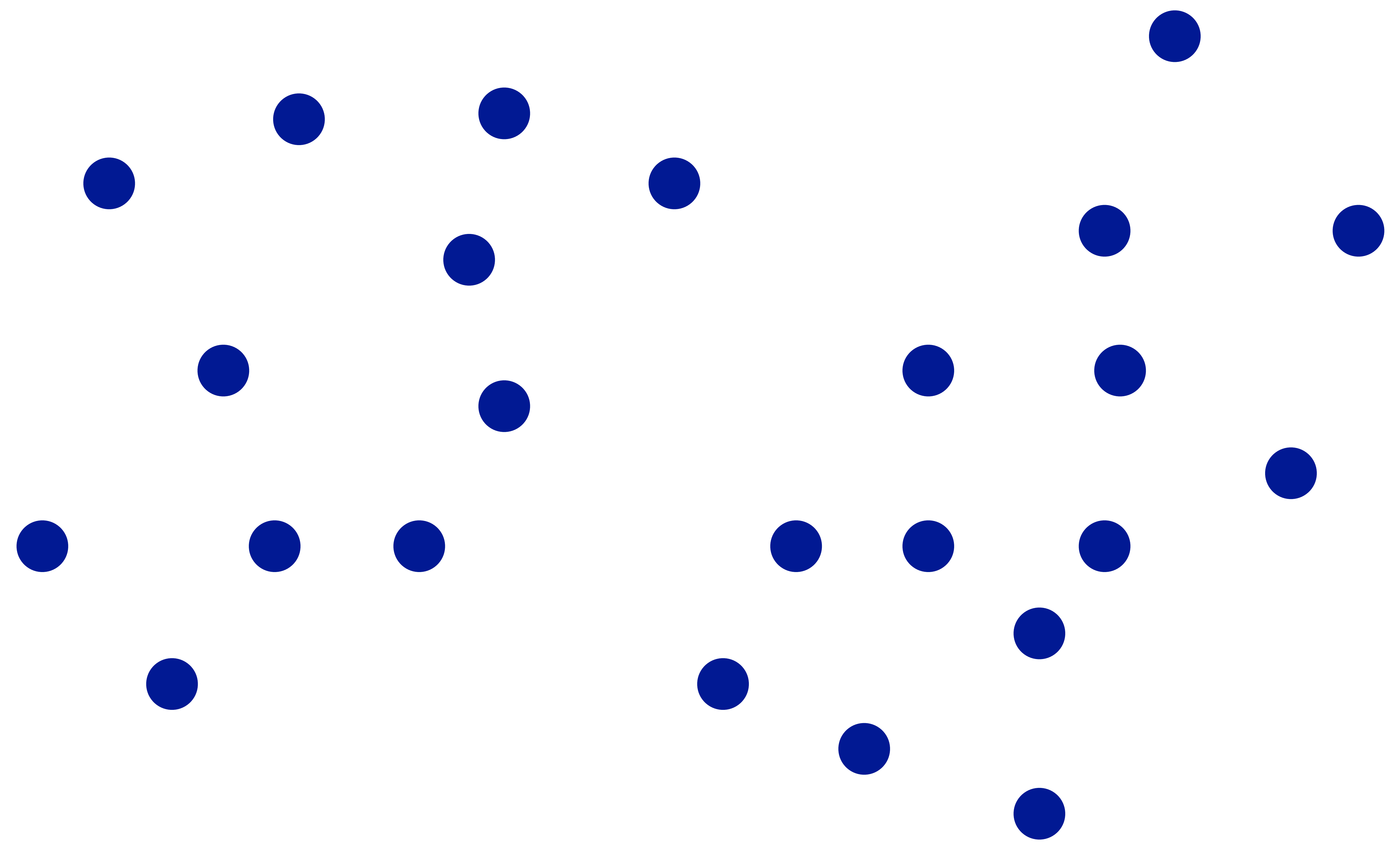
- With ***k*-means**, we seek to divide the dataset into k clusters $S_1, S_2, \ldots, S_k$, where each cluster S_i is defined by a centroid μ_i

  - μ_i is the mean of all the datapoints in S_i

- Formally, we seek to assign each $\mathbf{x}_j$ to a cluster S_i according to the following optimization problem:

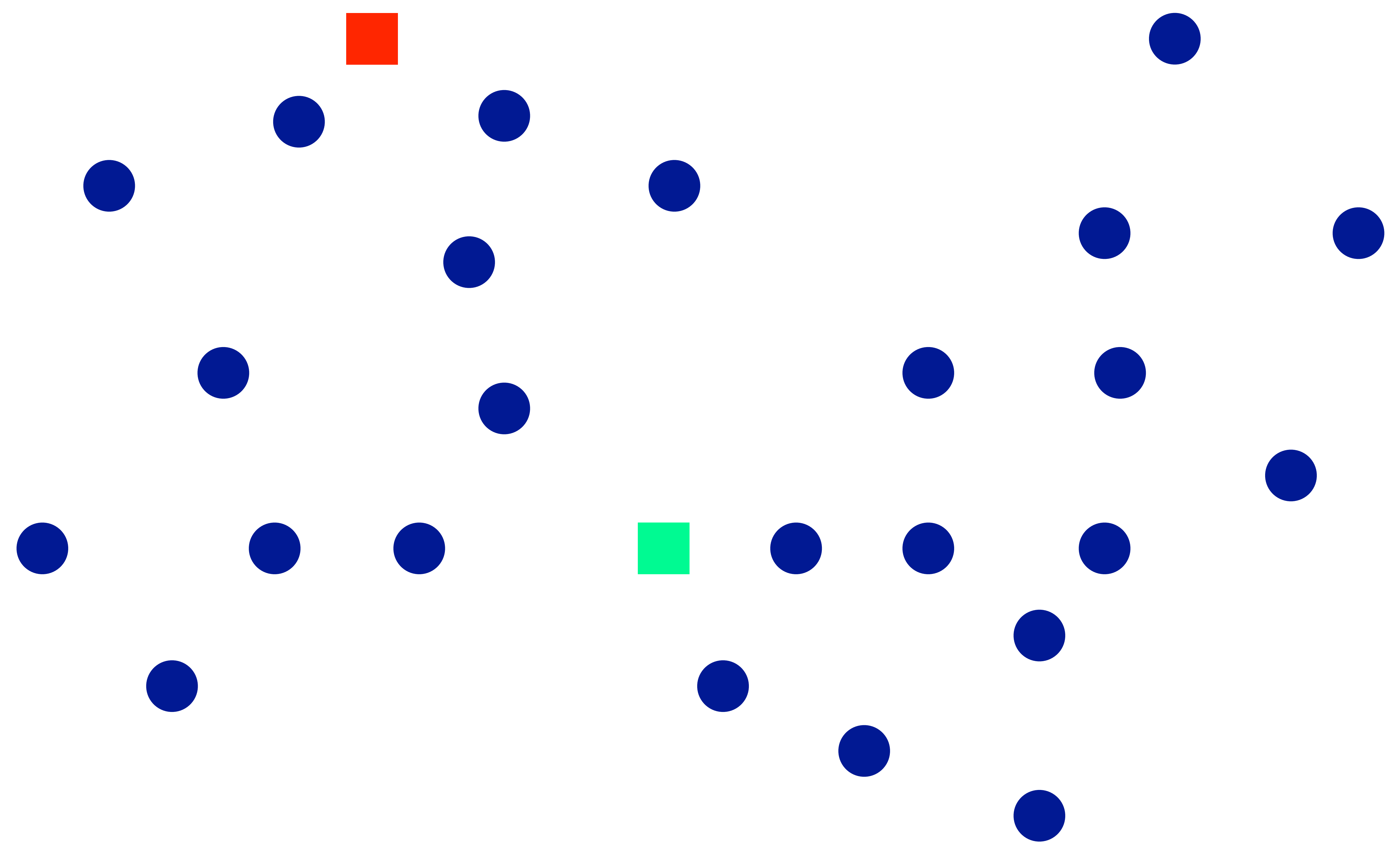
$$\underset{S_1,\ldots,S_k}{\arg\min} \sum_{i=1}^{k} \sum_{\mathbf{x}\in S_i} \|\mathbf{x} - \mu_i\|^2 \longleftarrow$$

Hard to solve: μ_i depends on S_i, and S_i depends on μ_i!



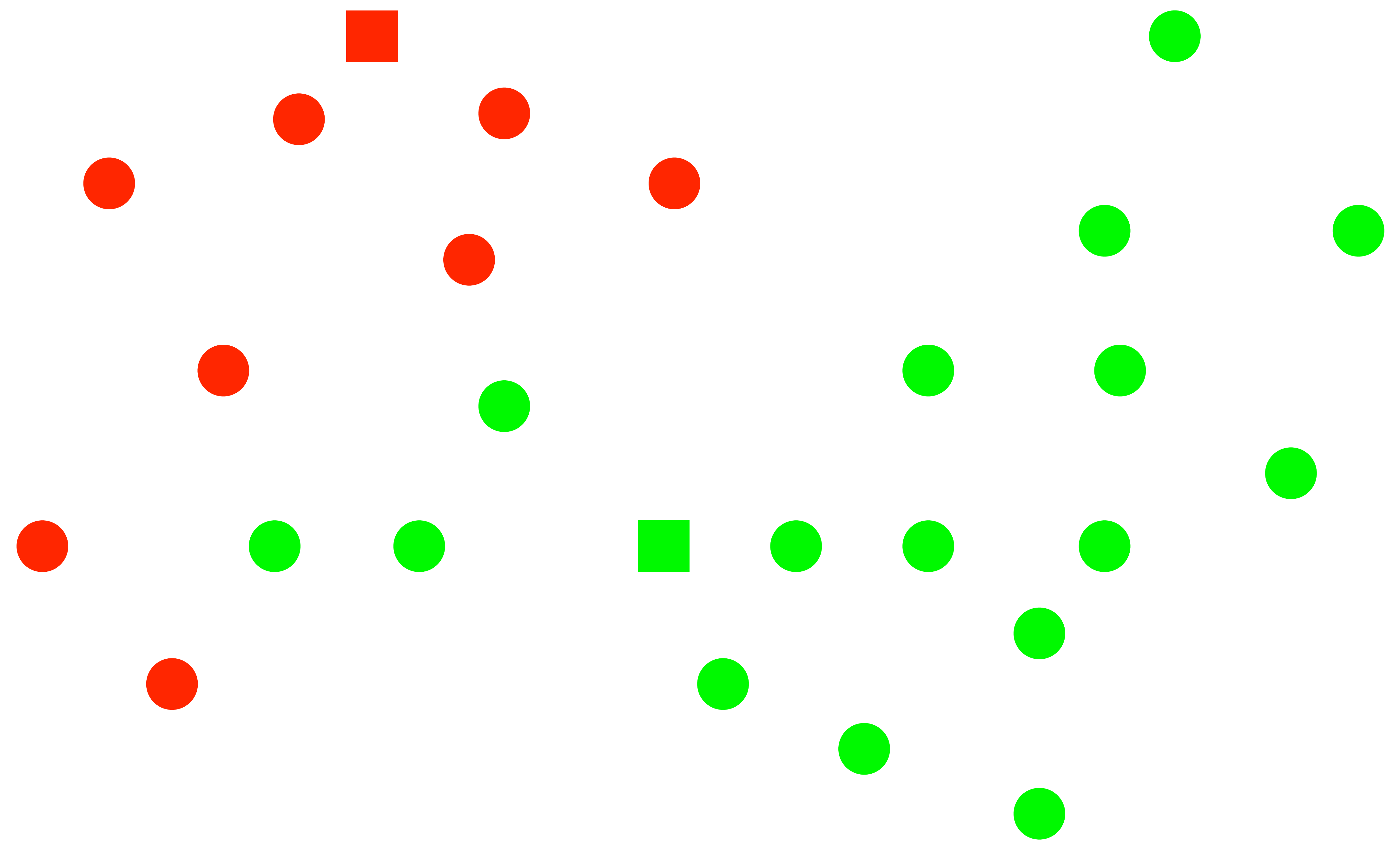
k-means algorithm

- Start out by initializing k "centroids" that define the clusters
    - Could just be random choice



k-means algorithm

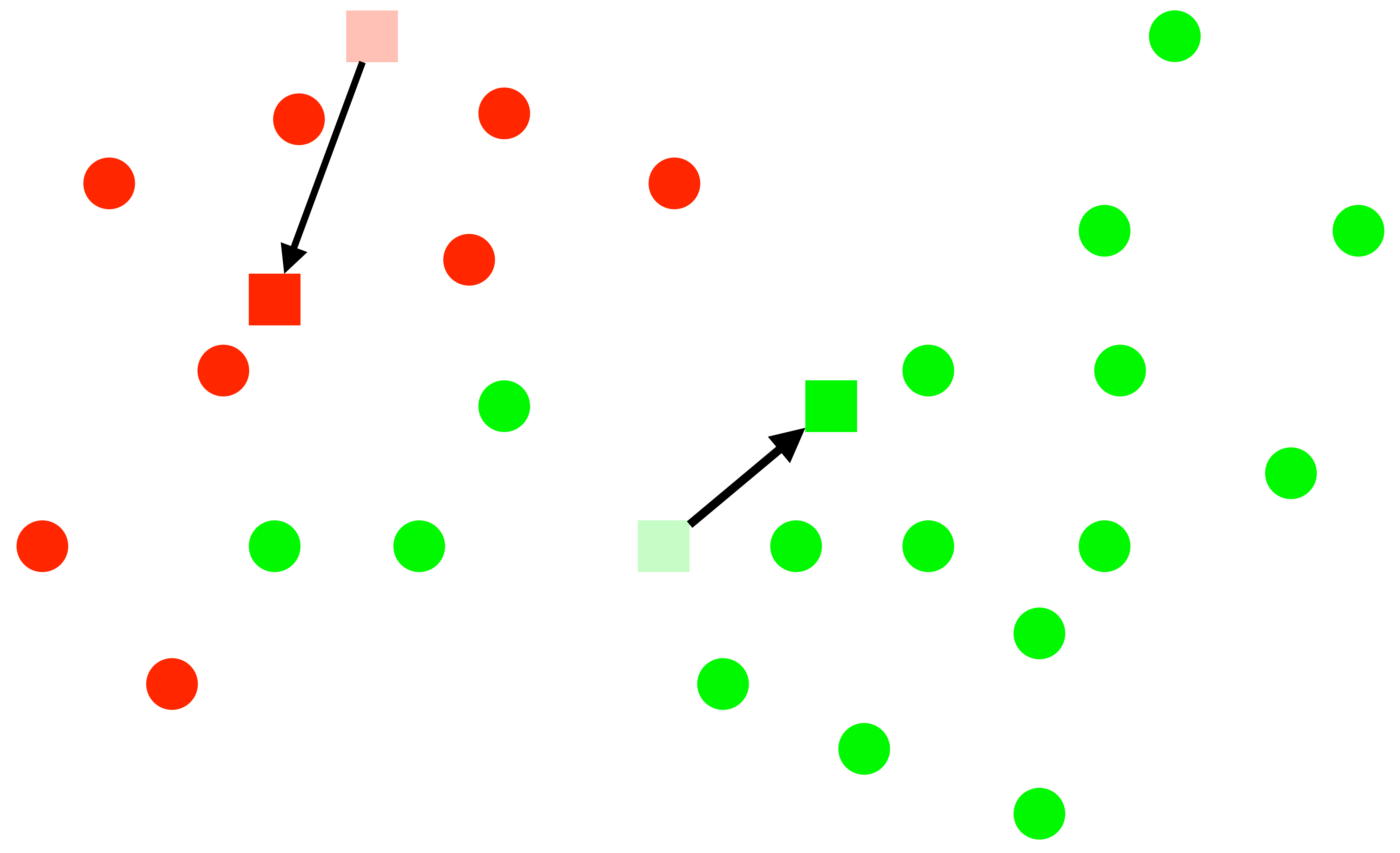
- Start out by initializing k "centroids" that define the clusters
- **Assignment step**: Assign each data point to a cluster
  - Each data point is assigned to the cluster it is closest to
  - According to Euclidean distance, i.e., $\arg\min_i ||\mathbf{x}_j - \mu_i||$



k-means algorithm

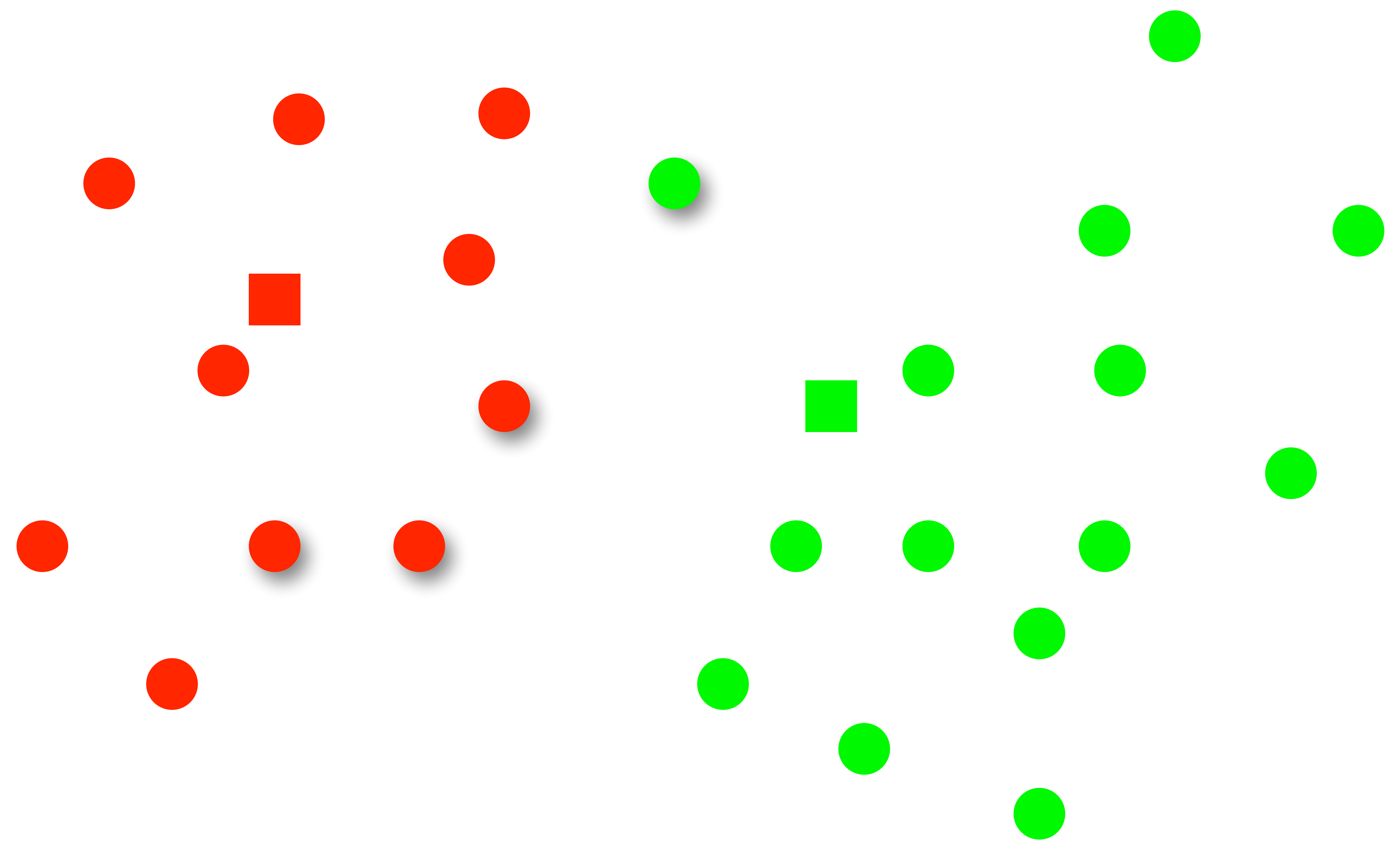
- Start out by initializing k "centroids" that define the clusters
- **Assignment step**: Assign each data point to a cluster
- **Update step**: Move each centroid to the "middle" of its cluster
    - Compute the average position of the data points
    - Compute mean according to

$$\mu_i = \frac{1}{|S_i|} \sum_{\mathbf{x} \in S_i} \mathbf{x}$$



k-means algorithm

- Start out by initializing k "centroids" that define the clusters
- **Assignment step**: Assign each data point to a cluster
- **Update step**: Move each centroid to the "middle" of its cluster
- Repeat assignment step with new centroid locations



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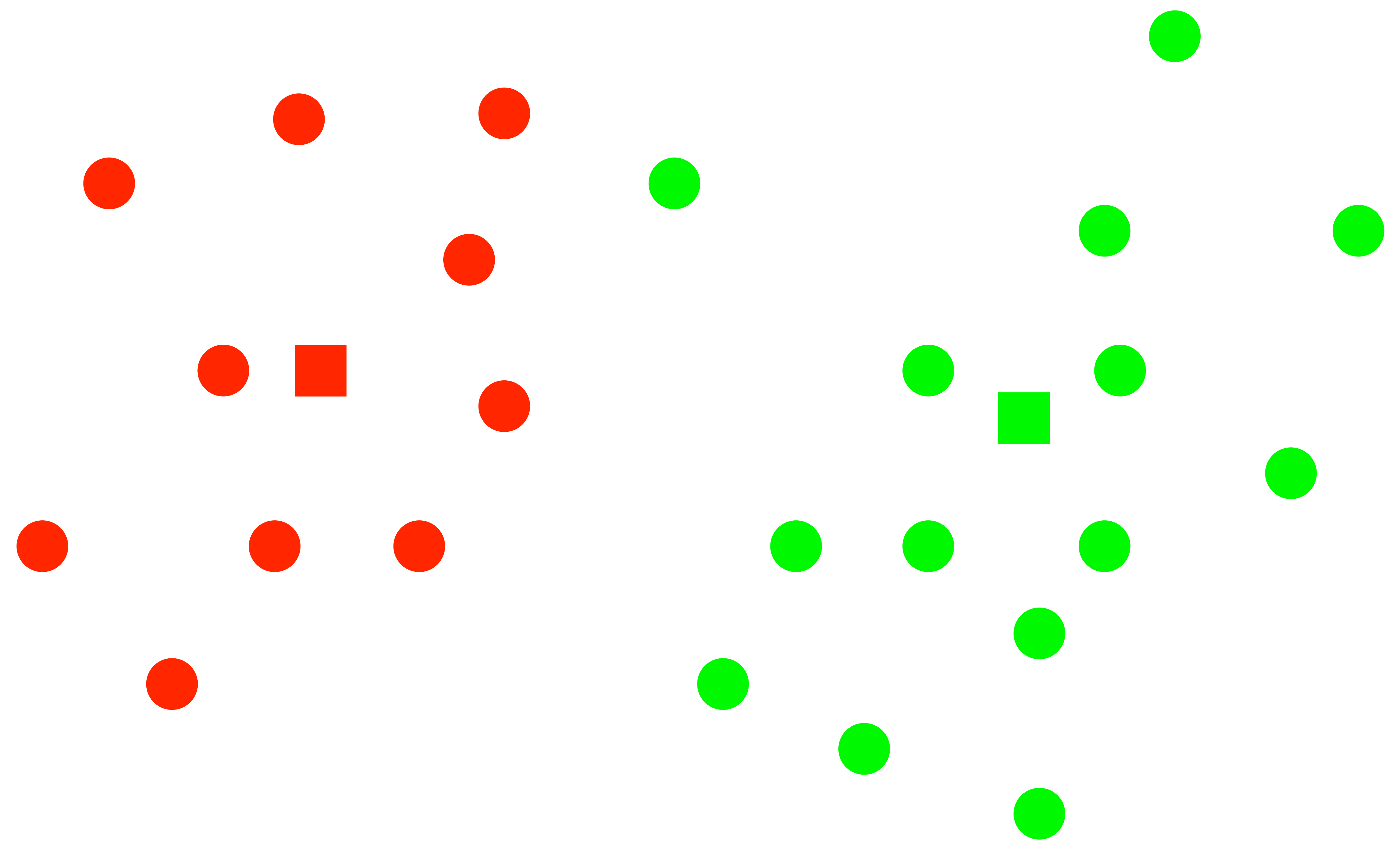
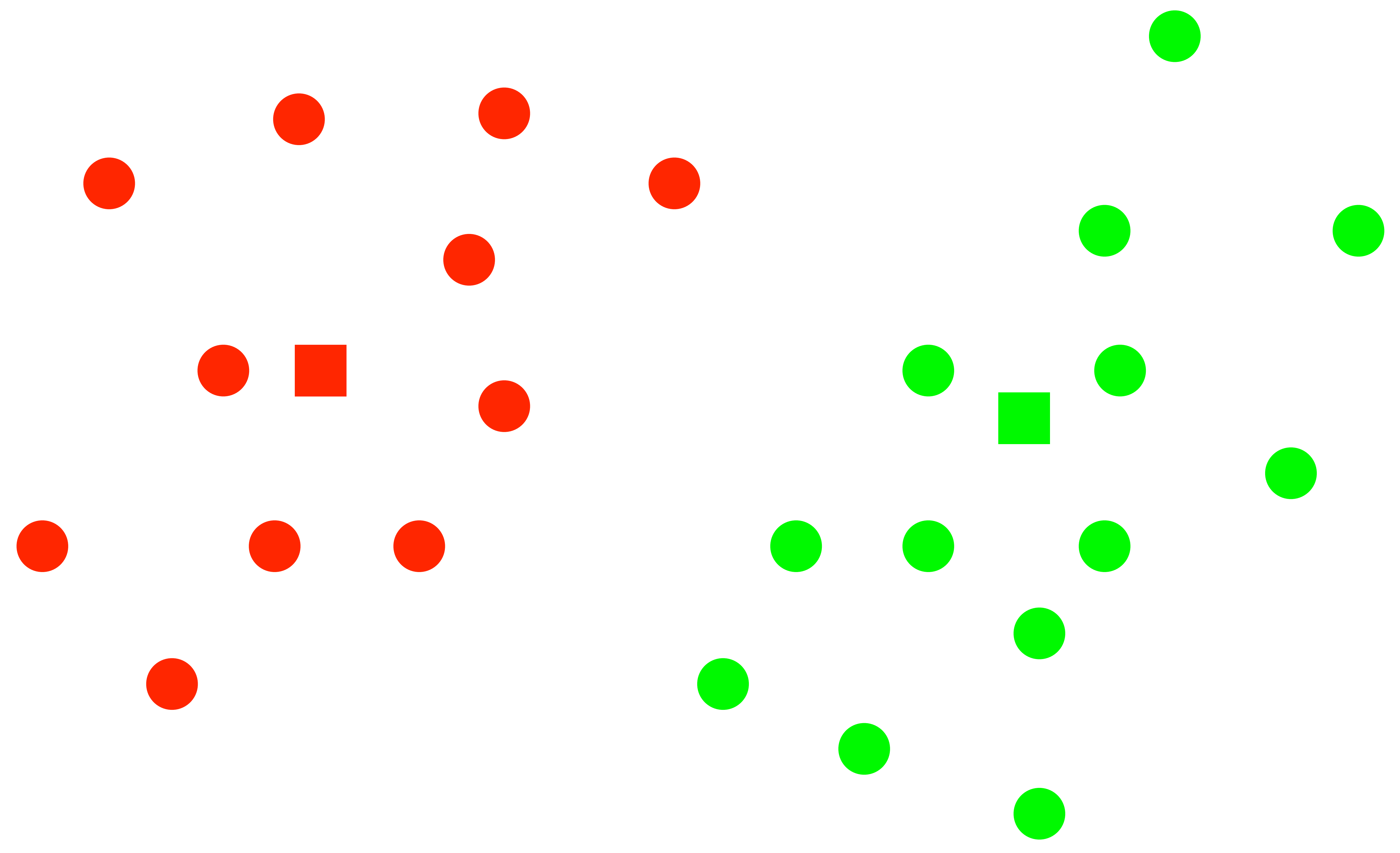
- Repeat assignment step with new centroid locations
- Repeat update step with new clusters



k-means algorithm summary

- Start out by initializing k "centroids" that define the clusters
- **Assignment step**: Assign each data point to a cluster
- **Update step**: Move each centroid to the "middle" of its cluster
- Repeat assignment, update, assignment, update, … until convergence



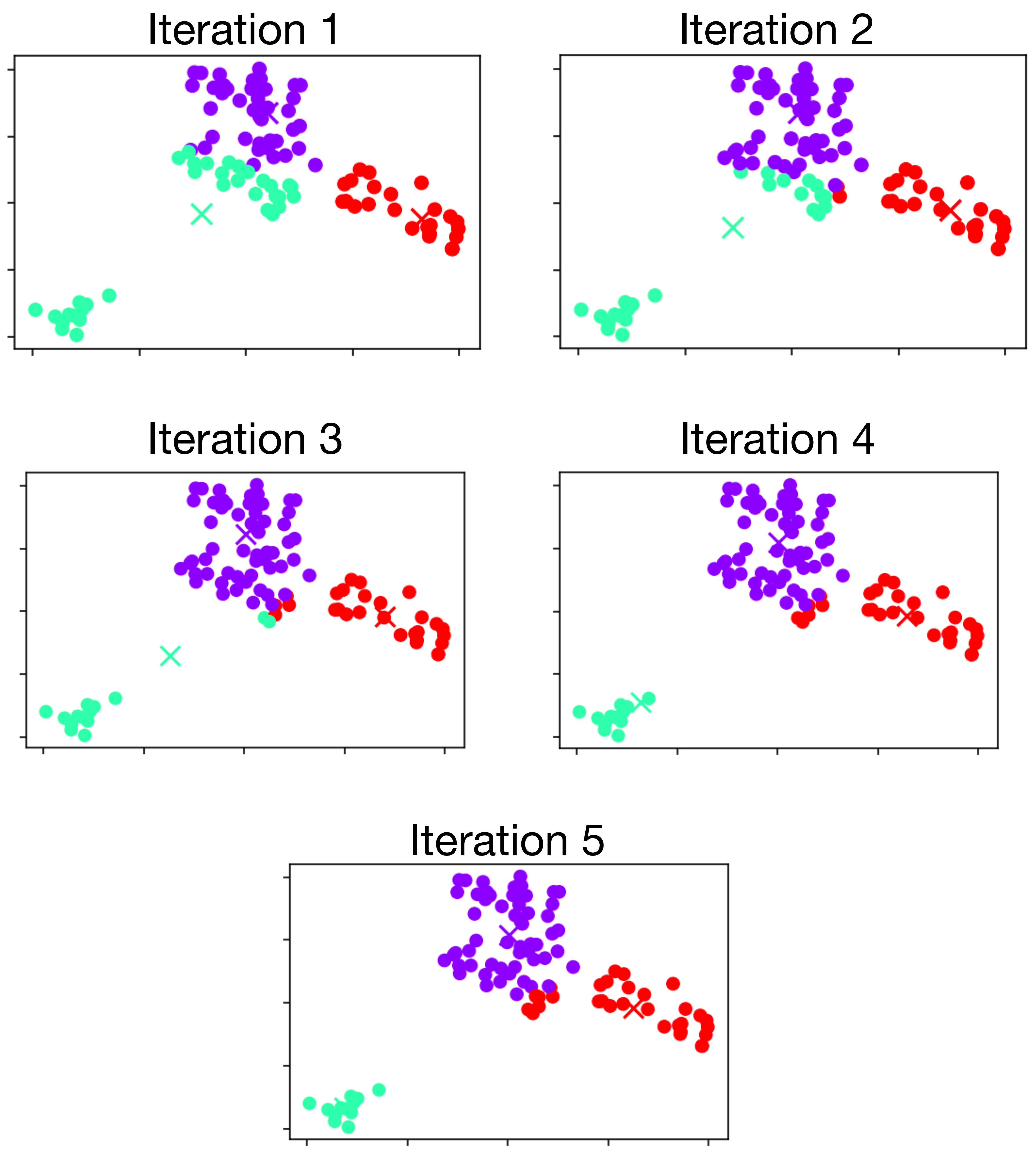
implementation and considerations

- In Python: `KMeans` class from `sklearn.cluster` (https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html)

```
kmeans = KMeans(n_clusters, n_init,
random_state, …)   #kmeans object

kmeans.fit(X)   #fit kmeans to X

kmeans.labels_  #Cluster assignments of X

kmeans.cluster_centers_  #Cluster centers
```

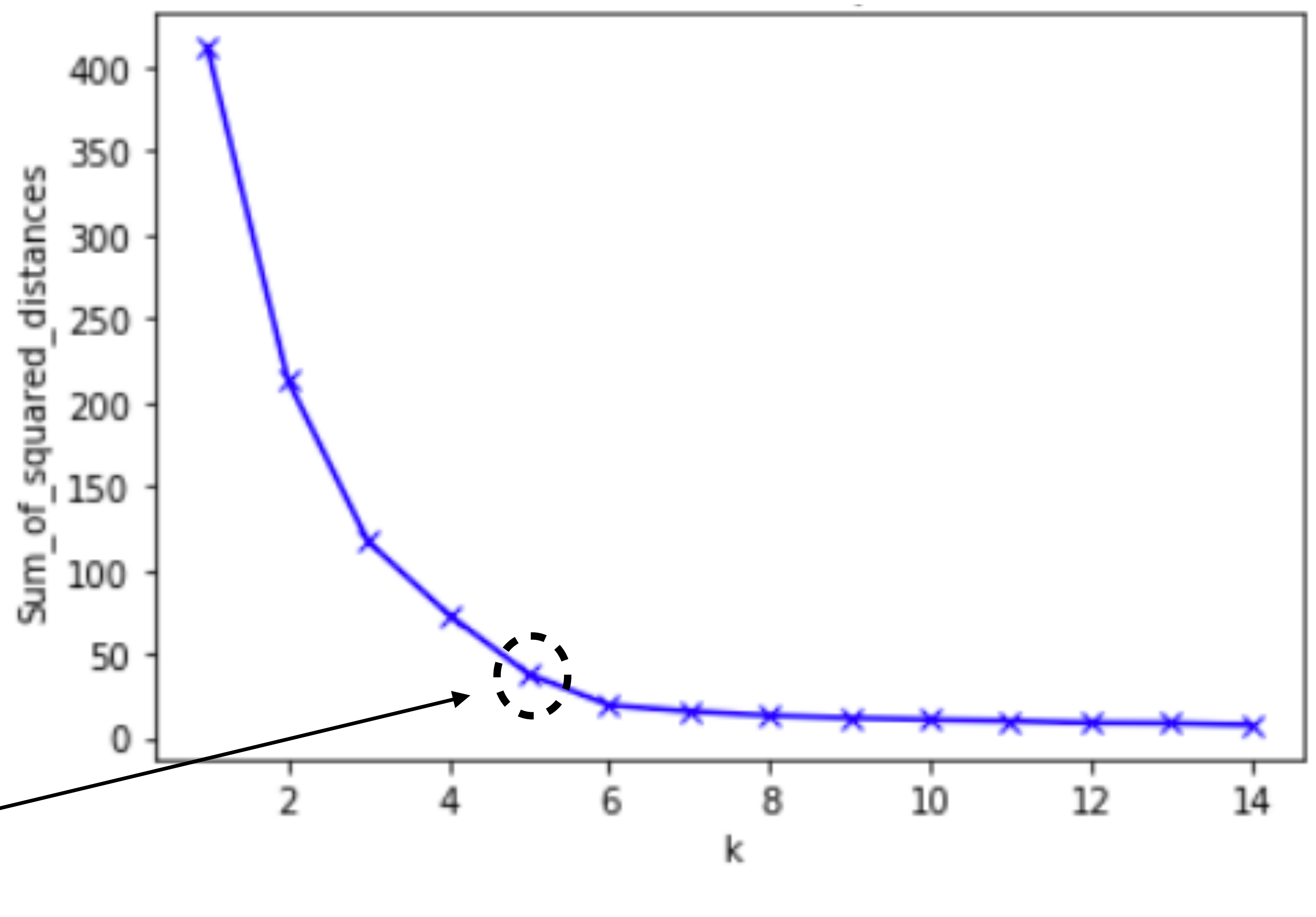
- A simpler approach than GMMs (which we will see next): No need for an *a priori* model

- But is less sophisticated than GMMs: Clusters that *k*-means finds have limitations



choosing k

- How do we know how many centroids to start with?
- One possibility: Can pick a k and see how far points in a cluster are from their centroid
    - If there are too few centroids, average distance is high
- As seen on the right, as k increases, the distance drops
    - But drop "slows down" after a while
    - **Knee** or **elbow method**: Look for the "knee" of the curve
- Can also use cross validation!
    - Too many clusters: New data points are not well represented by the clusters



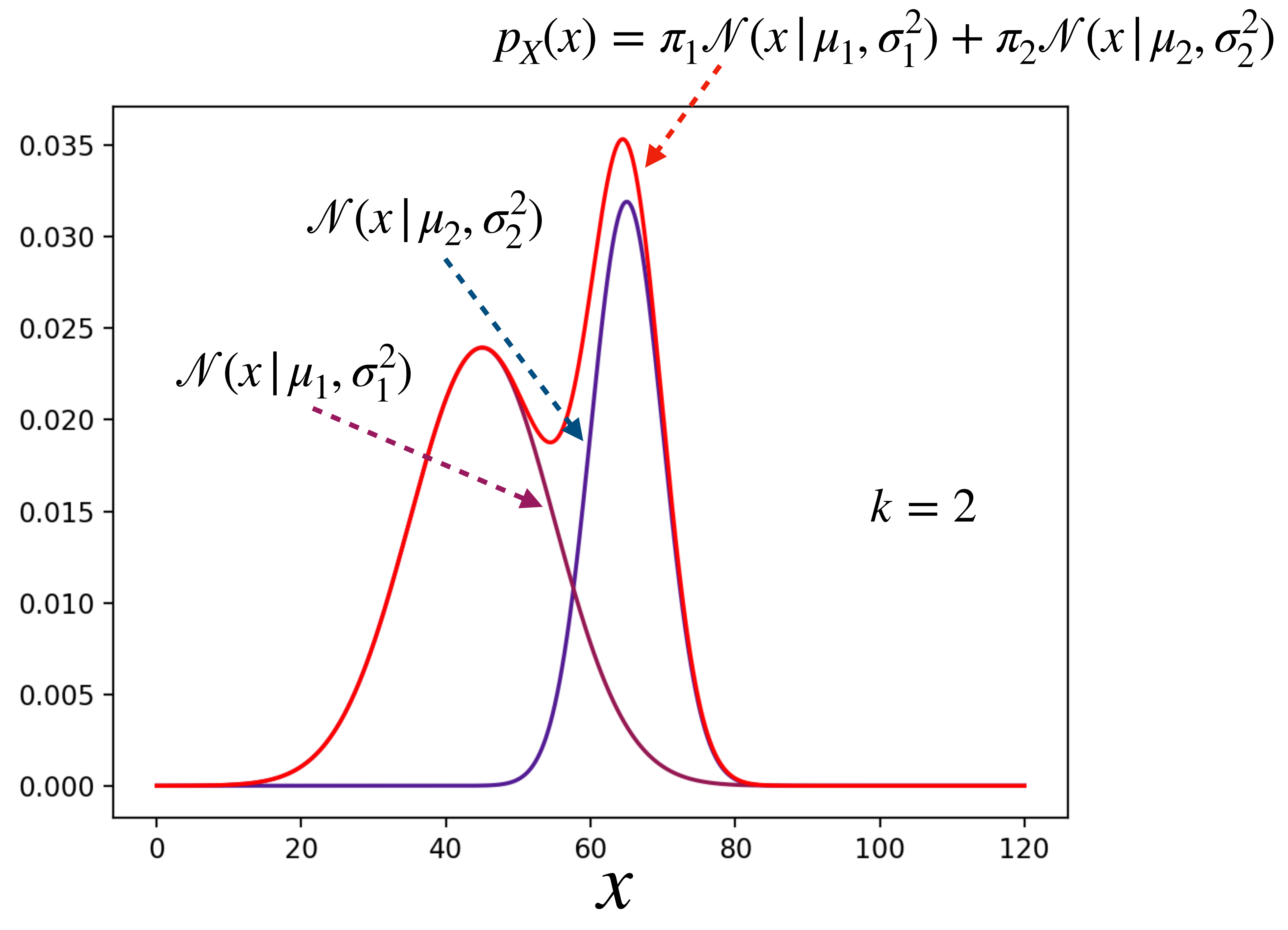
gaussian mixture models

- A **Gaussian mixture model (GMM)** with k components (clusters) is a probability distribution that is a weighted sum of k Gaussians:

$$p_X(x) = \sum_{i=1}^{k} \pi_i \mathcal{N}(x \mid \mu_i, \sigma_i^2)$$

- μ_i : mean of ith Gaussian
- σ_i^2 : variance of ith Gaussian
- π_i : weight of ith Gaussian

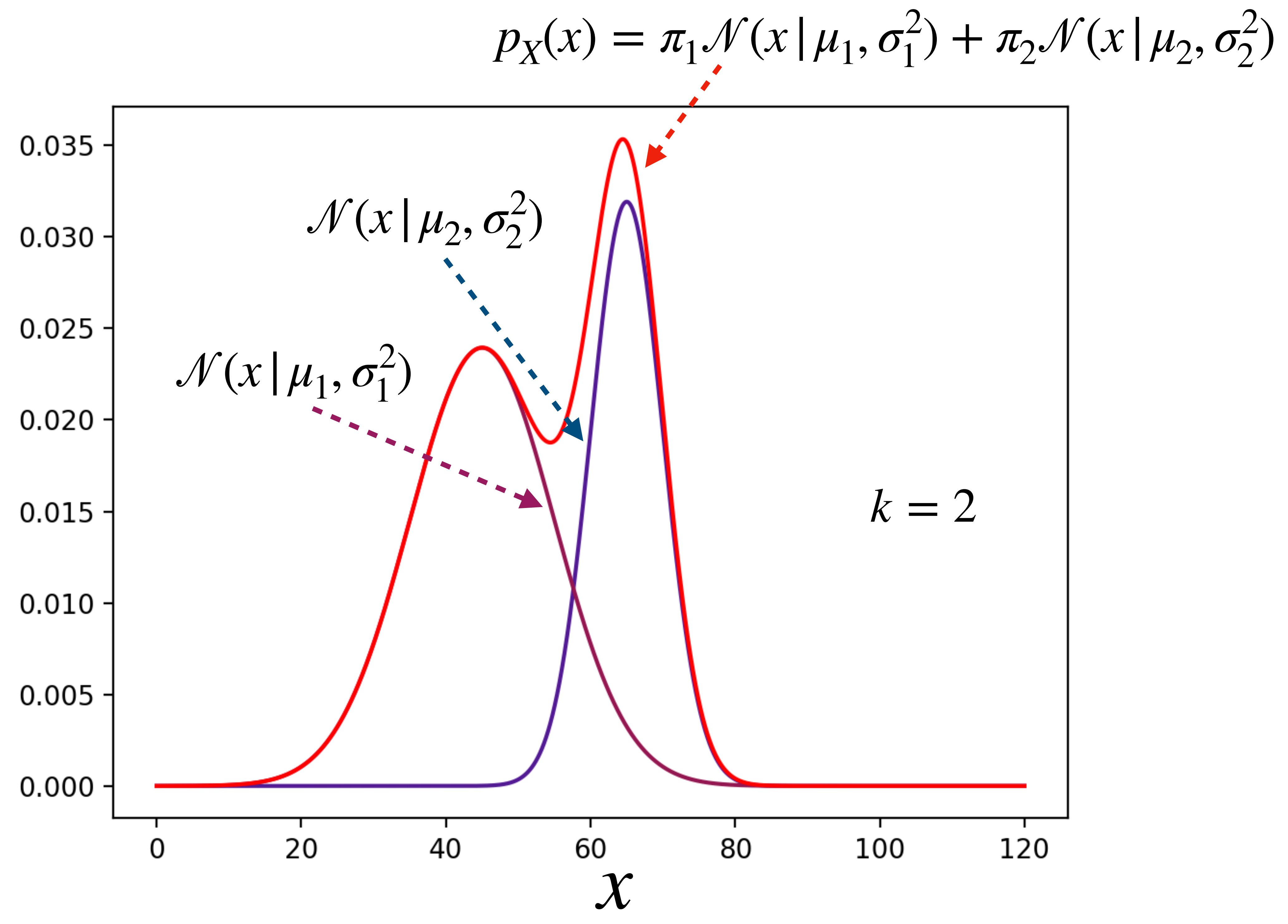
Note: $\pi_i \geq 0, \ \sum_i \pi_i = 1$ (why?)



gaussian mixture models

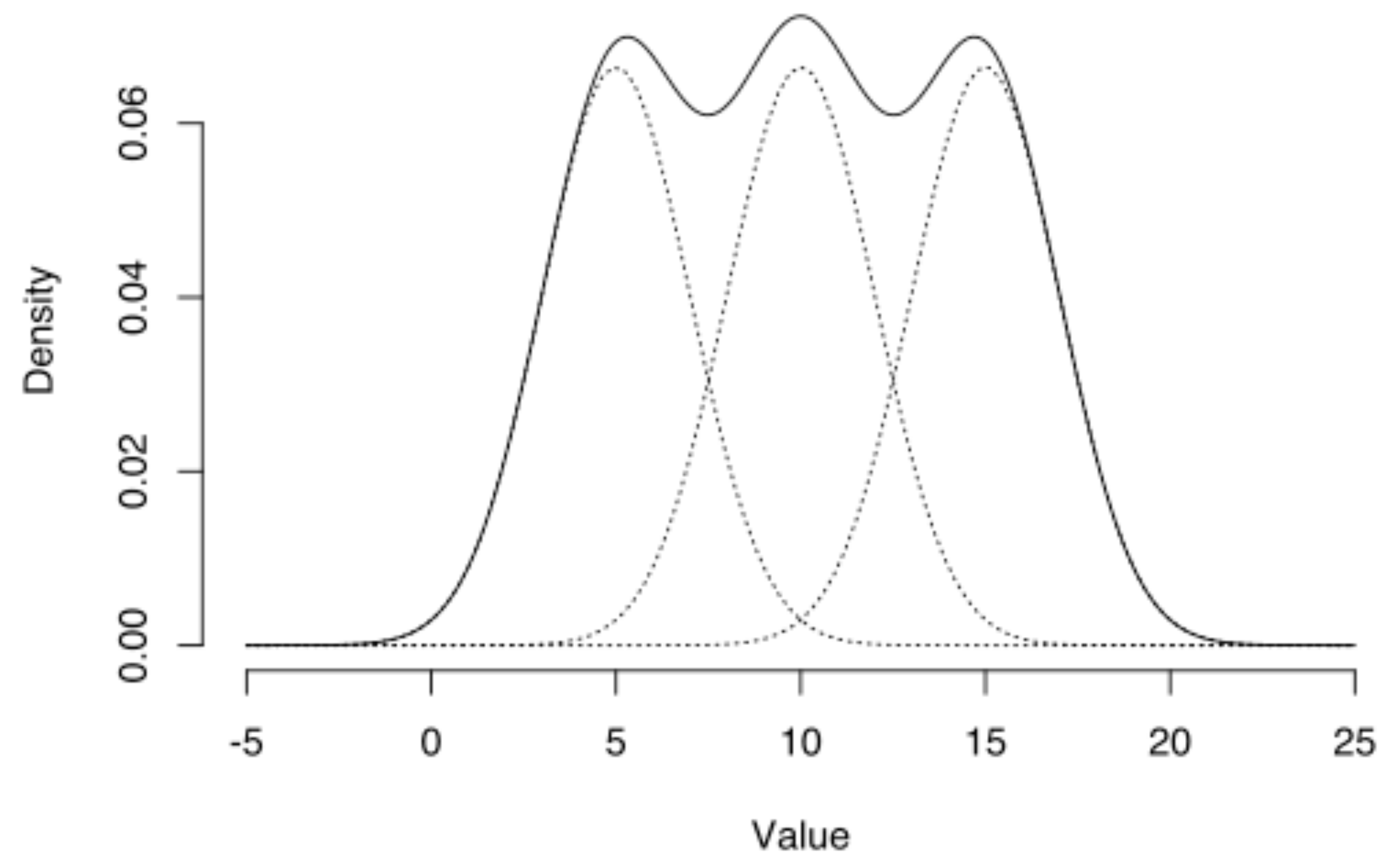
- Using GMMs for clustering:
  - Given N data points $x_1, \ldots, x_N$, how do we determine what the parameters of the k Gaussians are that best fit the data?
  - The parameters are the π_i, μ_i, σ_i
- Intuition:
  - Move the Gaussians around until their sum best fits the red curve (i.e., the dataset)

$$p_X(x) = \sum_{i=1}^{k} \pi_i \mathcal{N}(x \mid \mu_i, \sigma_i^2)$$



expectation maximization

- Like with KMeans, we will use an iterative approach to fit the parameters
- **Expectation maximization** is an iterative approach to finding the parameters of a statistical model, where the model depends on unobserved, **latent variables**
    - Here, our latent variables are cluster labels (i.e., which of the *k* Gaussians each point belongs to)
- Start with a random guess for the Gaussian parameters
- Compute **expectation** (E-step)
    - Given the current parameters, what is the likelihood that each point comes from a particular Gaussian?
- Perform **maximization** (M-step)
    - Given these new likelihoods (which are essentially weights), update the means, (co)variances, and weights of the Gaussians using weighted averages



E step

- For each data point x_j, compute the likelihood that the data point comes from Gaussian *i*’s random variable G_i:

$$\gamma_{ij} = P(G_i \mid x_j) = \frac{P(x_j \mid G_i)P(G_i)}{P(x_j)} \longleftarrow \textbf{Bayes' Theorem}$$

- $P(x_j \mid G_i)$ is the (conditional) probability of observing x_j from G_i
- $P(G_i)$ is the (unconditional) probability of observing the Gaussian G_i
- $P(x_j)$ is the (unconditional) probability of observing x_j (from any Gaussian)

E step

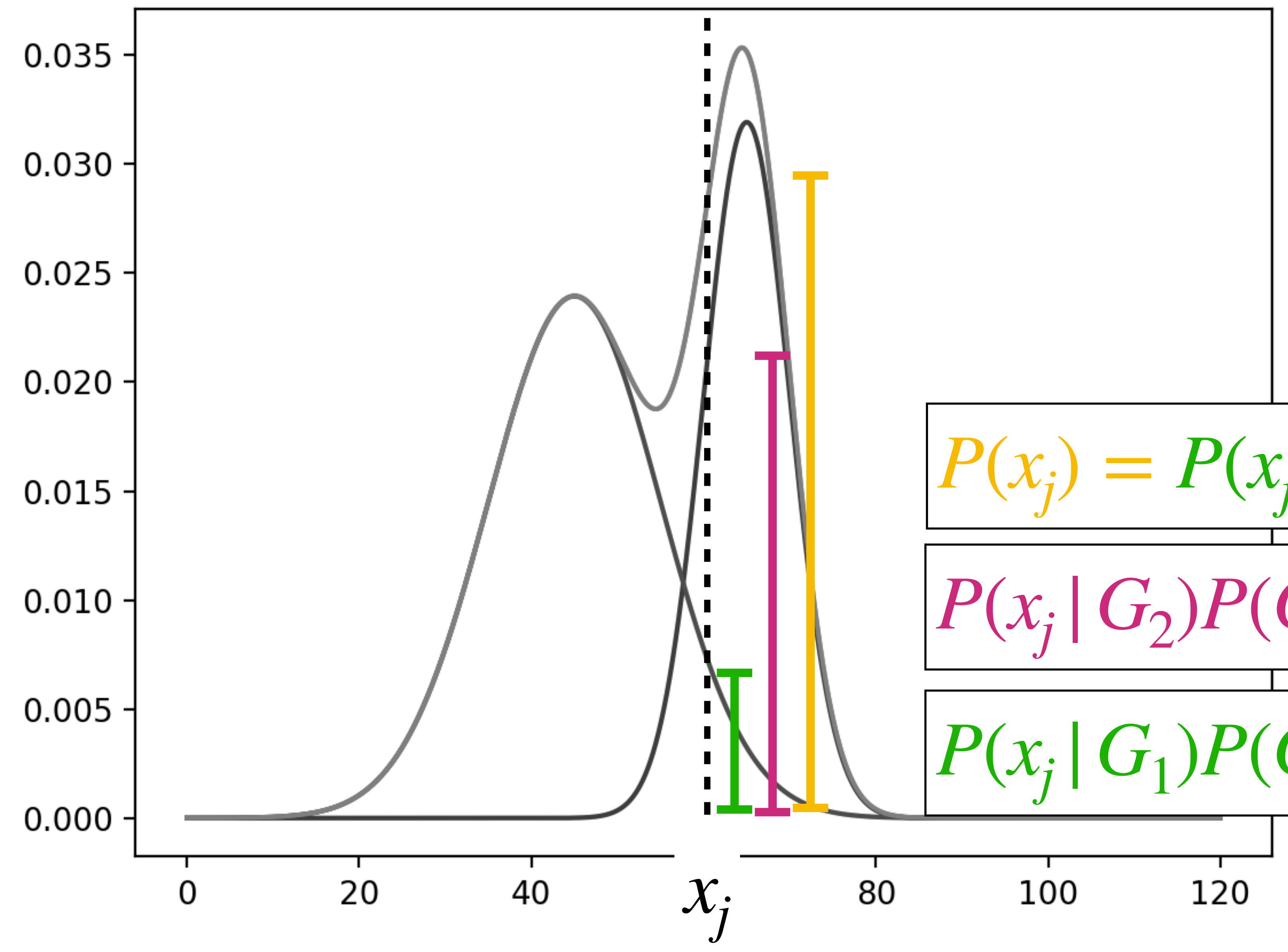
- For each data point x_j, compute the likelihood that the data point comes from Gaussian *i*'s random variable G_i:

$$\gamma_{ij} = P(G_i \mid x_j) = \frac{\boxed{P(x_j \mid G_i)}\boxed{P(G_i)}}{\boxed{P(x_j)}}$$

Weight of this Gaussian

Compute straight from Gaussian

Estimate from overall distribution (normalizes so probabilities sum to 1)



$$\boxed{P(x_j) = P(x_j \mid G_1)P(G_1) + P(x_j \mid G_2)P(G_2)}$$

$$\boxed{P(x_j \mid G_2)P(G_2)}$$

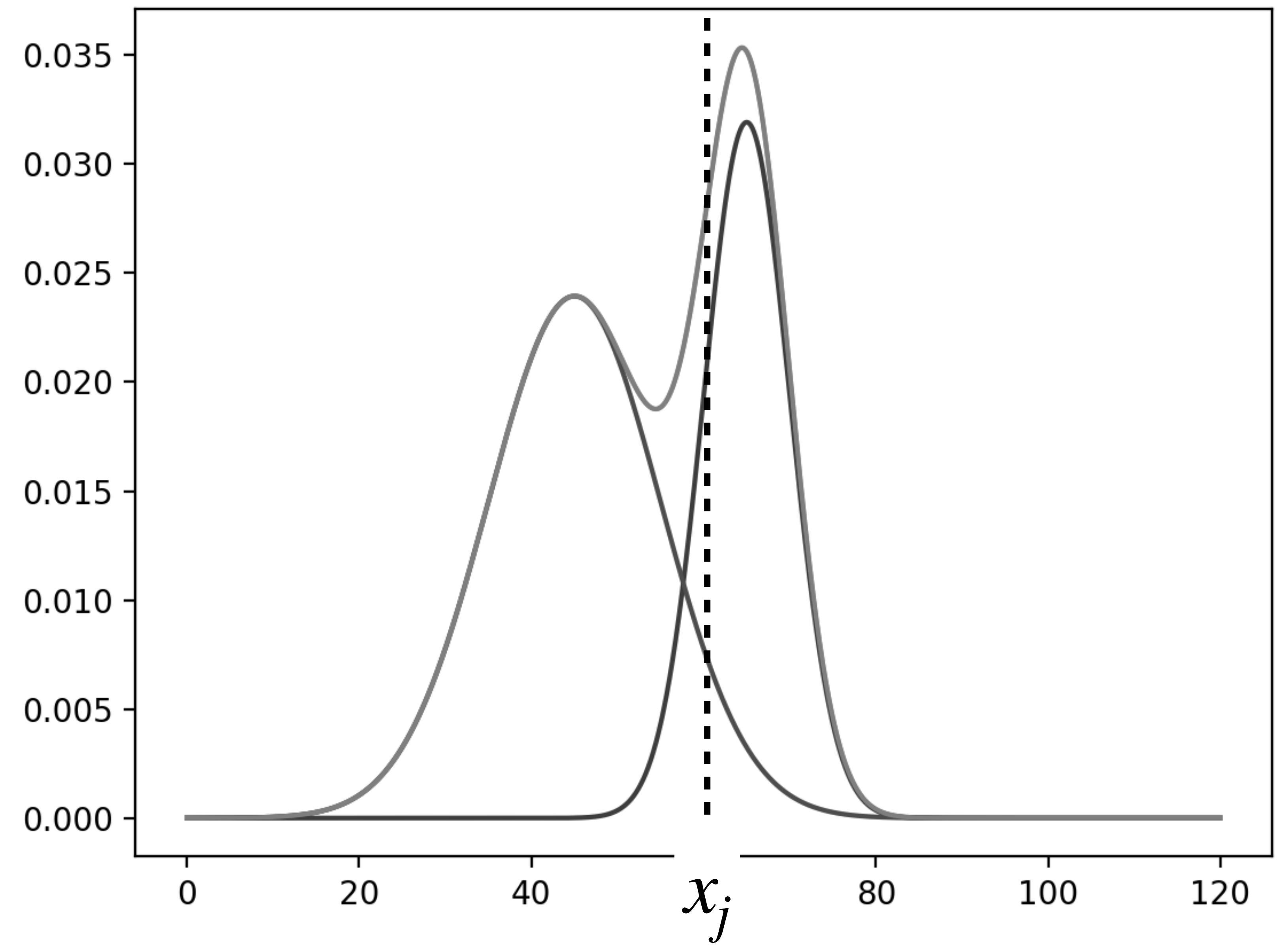
$$\boxed{P(x_j \mid G_1)P(G_1)}$$

E step

- For each data point x_j, compute the likelihood that the data point comes from Gaussian *i*'s random variable G_i:

$$\gamma_{ij} = P(G_i \mid x_j) = \frac{P(x_j \mid G_i)P(G_i)}{P(x_j)}$$

$$= \frac{\pi_i \mathcal{N}(x_j \mid \mu_i, \sigma_i^2)}{\sum_{g=1}^{k} \pi_g \mathcal{N}(x_j \mid \mu_g, \sigma_g^2)}$$



M step

- Now that we have the likelihoods for each datapoint (how likely each is to come from each Gaussian), we *re-estimate* the parameters of each Gaussian i using those weights:

$$N_i = \sum_{j=1}^{N} \gamma_{ij} \qquad \pi_i' = \frac{N_i}{N} \qquad \mu_i' = \frac{\sum_{j=1}^{N} \gamma_{ij} x_j}{N_i} \qquad \sigma_i'^2 = \frac{\sum_{j=1}^{N} \gamma_{ij} (x_j - \mu_i')^2}{N_i}$$

- These expressions are the **maximum likelihood estimators** for Gaussian distributions

  - Derived by setting the derivative of $\log \prod_j p_X(x_j)$ to 0 for each parameter

M step

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Total likelihood of points in this Gaussian

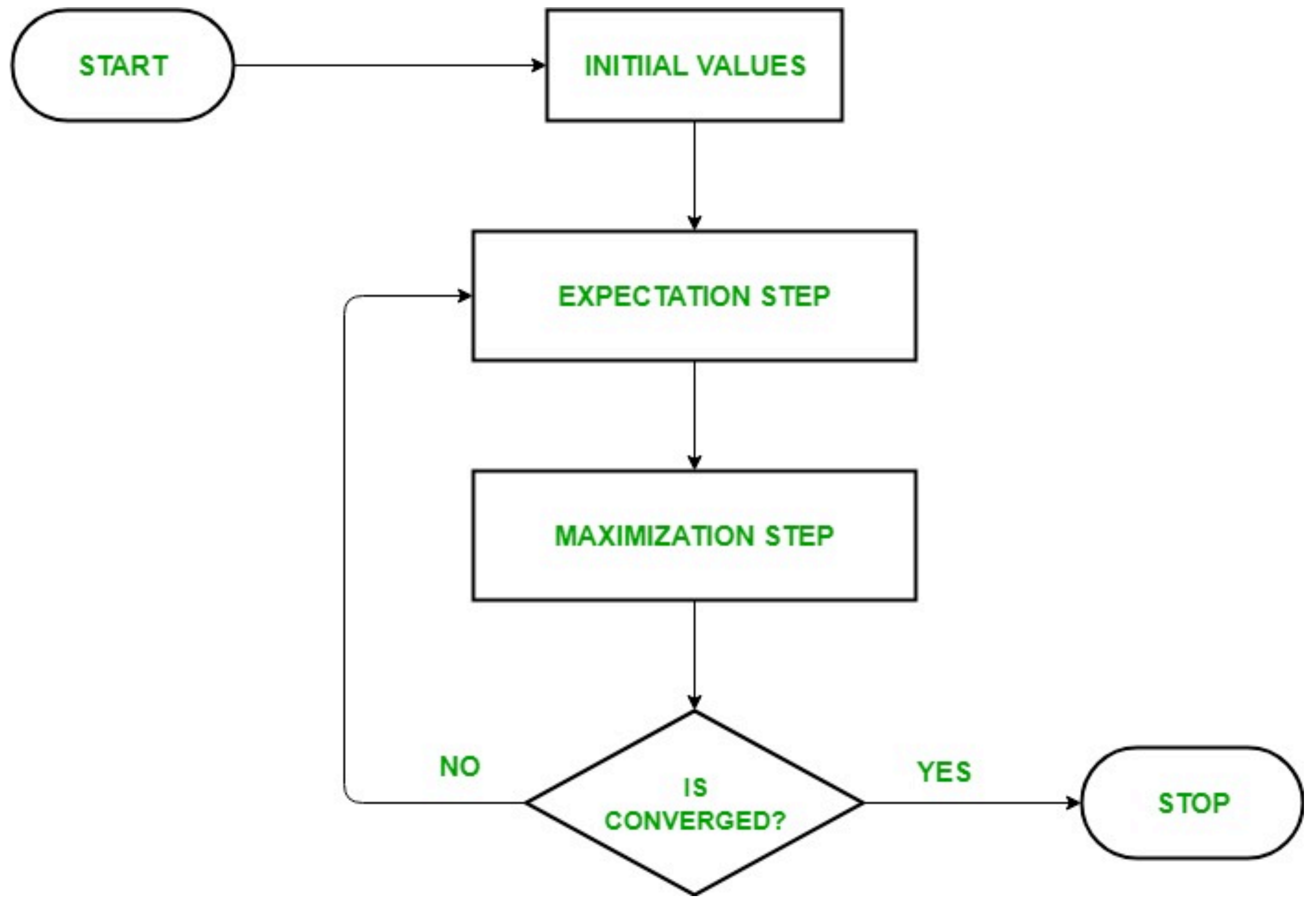
Proportion of points that come from this Gaussian

Weighted mean of this Gaussian

Weighted variance of this Gaussian. Note that this uses the *updated* mean!

learning GMMs

- Repeat E and M steps until convergence
- Note that *what* you converge to can be sensitive to the initial estimates (like KMeans)
- When you are done, you have multiple Gaussians defined that “fit” the data you have
- This is a useful starting point for building Naïve Bayes classifiers!
    - We will discuss this later
- In Python: `GaussianMixture` class from `sklearn.mixture` (https://scikit-learn.org/stable/modules/generated/sklearn.mixture.GaussianMixture.html)



determining convergence

- We continue alternating between E and M steps, but how do we know when the algorithm has converged?

  - We will use the log likelihood of the data given parameters:

$$\texttt{logl} = \log \prod_{j=1}^{N} p_X(x_j) = \sum_{j=1}^{N} \log p_X(x_j) = \sum_{j=1}^{N} \log \sum_{i=1}^{k} \pi_i \mathcal{N}(x_j \,|\, \mu_i, \sigma_i^2)$$

  - When the log-likelihood stops changing significantly, we can stop EM

  - Formally, we can stop once the change in `logl` is below a certain tolerance `tol`, e.g., `tol = 1`

numerical example

Consider a (very, very small) dataset of five points $x_1 = 12.14$, $x_2 = 4.55$, $x_3 = 2.57$, $x_4 = 12.19$, $x_5 = 12.78$. Find the GMM for this dataset with $k = 2$ clusters.

Assume an initialization of $\mu_1 = 2.57$, $\mu_2 = 7.68$ (i.e., chosen randomly), $\sigma_1 = 1$, $\sigma_2 = 1$, $\pi_1 = 0.5$, and $\pi_2 = 0.5$. Also assume `tol = 1`.

iteration 1

Iteration 1, E-step result:

$\gamma = [\gamma_{ij}] = [[0,\ 0.95,\ 1,\ 0,\ 0],\ [1,\ 0.05,\ 0,\ 1,\ 1]]$

log-likelihood after Iteration 1:

$\mathtt{logl} = -9.251$

Calculation for $\gamma_{:,2}$:

$$\tilde{\gamma}_{1,2} = P(G_1)P(x_2 \mid G_1) = 0.5\mathcal{N}(4.55 \mid 2.57,1) = 0.0281$$
$$\tilde{\gamma}_{2,2} = P(G_2)P(x_2 \mid G_2) = 0.5\mathcal{N}(4.55 \mid 7.68,1) = 0.00149$$
$$\gamma_{:,2} = \left[\frac{\tilde{\gamma}_{1,2}}{\tilde{\gamma}_{1,2} + \tilde{\gamma}_{2,2}}, \frac{\tilde{\gamma}_{2,2}}{\tilde{\gamma}_{1,2} + \tilde{\gamma}_{2,2}}\right] = [0.95,0.05]$$

Iteration 1, M-step result:

$\pi = [\pi_i] = [0.39,0.61], \quad \mu = [\mu_i] = [3.53,12.24], \quad \sigma^2 = [\sigma_i^2] = [0.987,1.12]$

Calculation for π:

$$N_1 = \gamma_{1,1} + \gamma_{1,2} + \gamma_{1,3} + \gamma_{1,4} + \gamma_{1,5} = 0 + 0.95 + 1 + 0 + 0 = 1.95$$
$$N_2 = \gamma_{2,1} + \gamma_{2,2} + \gamma_{2,3} + \gamma_{2,4} + \gamma_{2,5} = 1 + 0.05 + 0 + 1 + 1 = 3.05$$
$$\pi_: = \left[N_1/(N_1 + N_2), N_2/(N_1 + N_2)\right] = [0.39,0.61]$$

Calculation for μ_1:

$$\mu_1 = (1/N_1)\sum_{j=1}^{N} \gamma_{1,j} x_j = (1/1.95)((0.95)x_2 + (1.0)x_3) = (1/1.95)((0.95)4.55 + (1.0)2.57) = 3.53$$

final result

Subsequent iterations are handled the same way. After three iterations, we have the final model, which has these parameters:

$$\gamma \approx [[0,1,1,0,0],[1,0,0,1,1]]$$

$$\pi \approx [0.4,0.6]$$

$$\mu \approx [3.56,12.37]$$

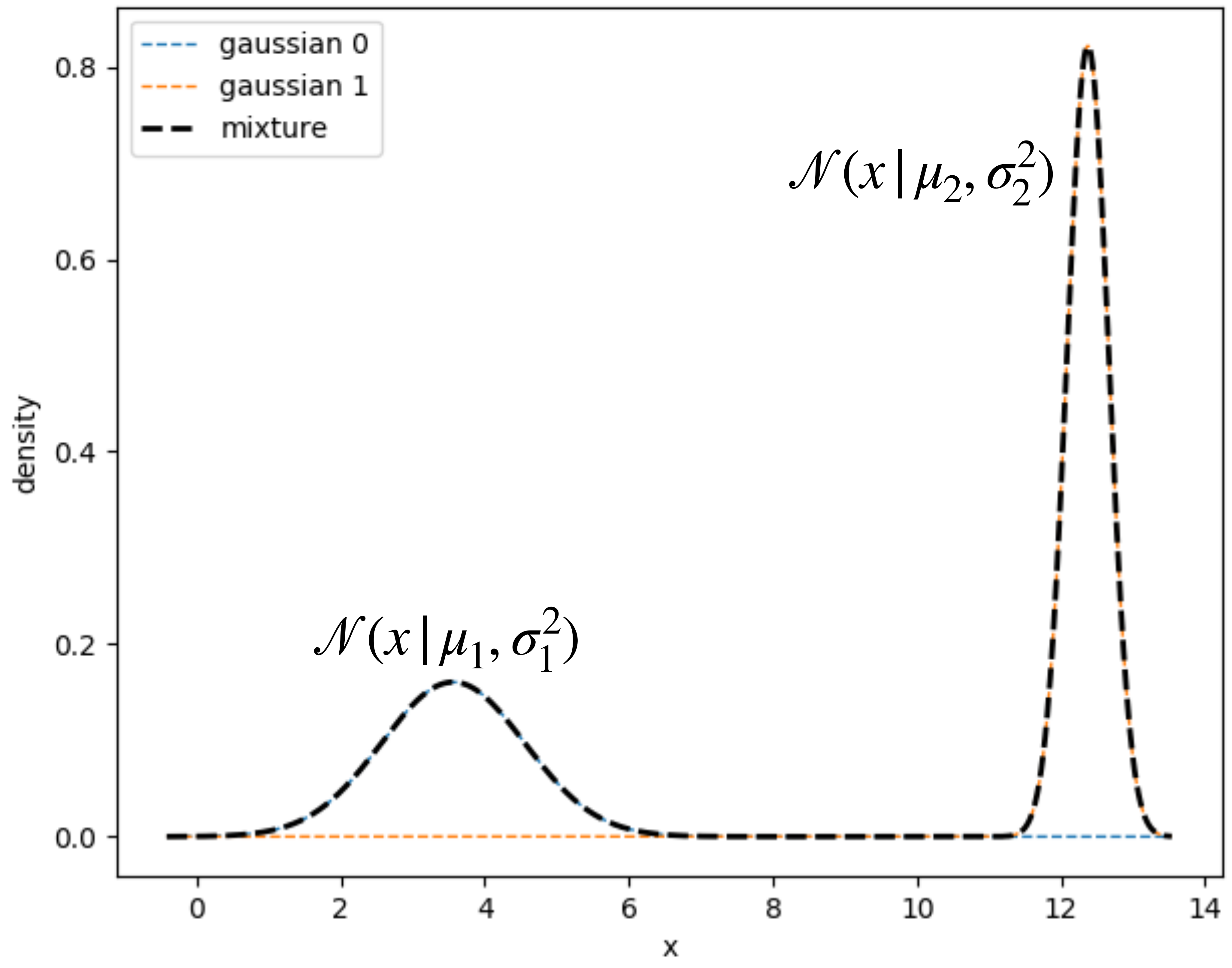
$$\sigma^2 \approx [0.99,0.08]$$

$$\texttt{logl} \approx -6.75$$

And the model is:

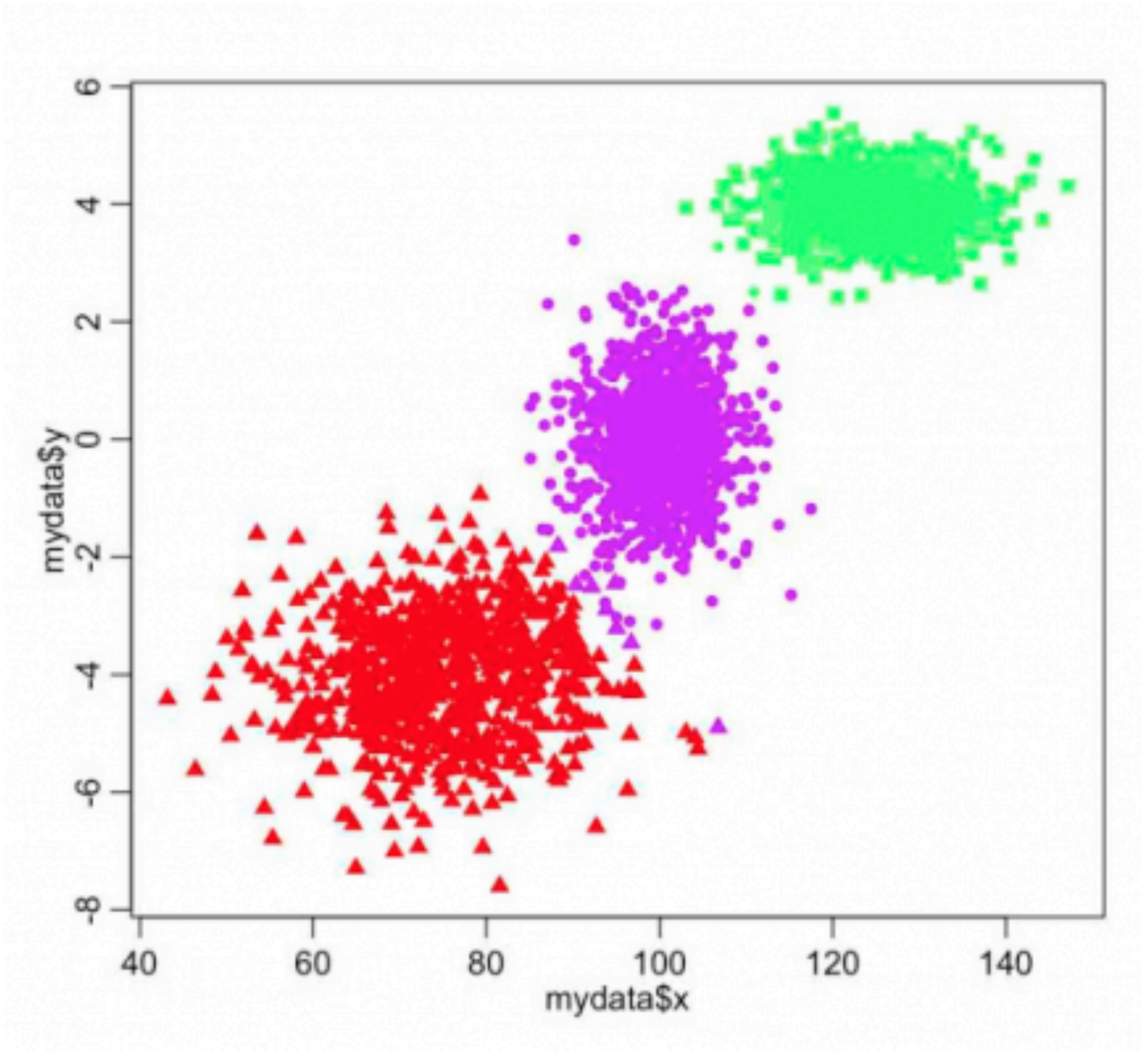
$$p_X(x) = 0.4\mathcal{N}(x \mid 3.56,\ 0.99) + 0.6\mathcal{N}(x \mid 12.37,\ 0.08)$$

The result is plotted in the graph on the right.



parametric vs. non-parametric

- K-means vs. GMM is an instance of a distinction that shows up over and over when we build models:
  - A **parametric** approach starts with some assumptions about the underlying data (what kinds of distribution they have, for example)
  - A **non-parametric** approach makes no assumptions about the underlying data
- K-means is *non-parametric*: Do not assume that the data has any particular distribution (even though we do have one parameter, *k*)
- GMM is *parametric*: Approach assumes something about the structure of the data (that the clusters are normally distributed)
- What about other modeling techniques we've looked at?
  - **Regression?**


mydata$y
mydata$x