Soft Clustering

Soft Clustering

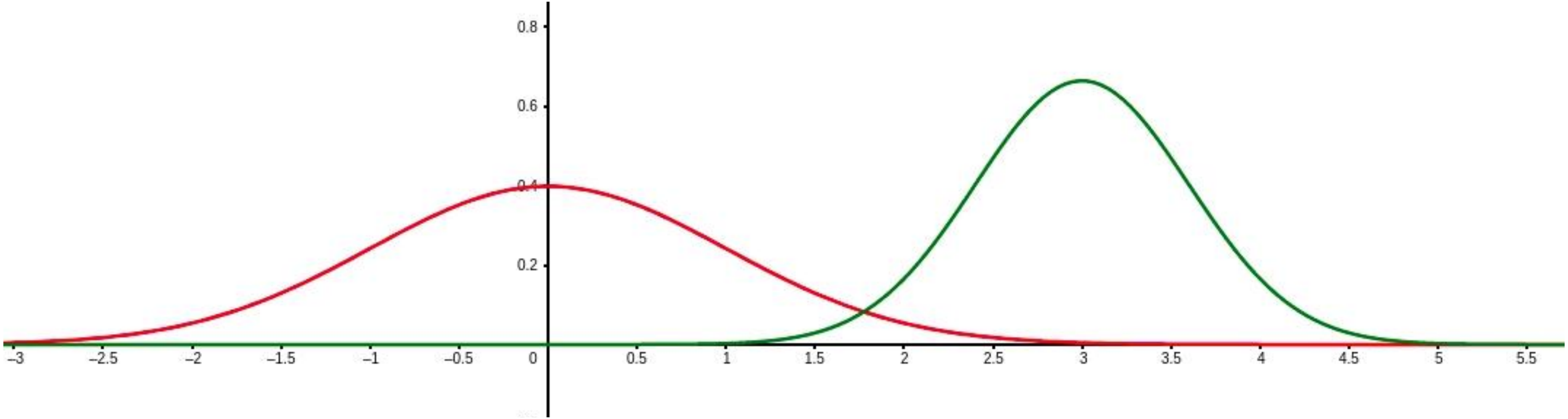
So far, clustering was done using **hard assignments** (1 point -> 1 cluster)

Sometimes this doesn't accurately represent the data: it seems reasonable to have overlapping clusters.

In this case, we can use **soft assignment** to assign points to every cluster with a certain probability.

Soft Clustering - Example

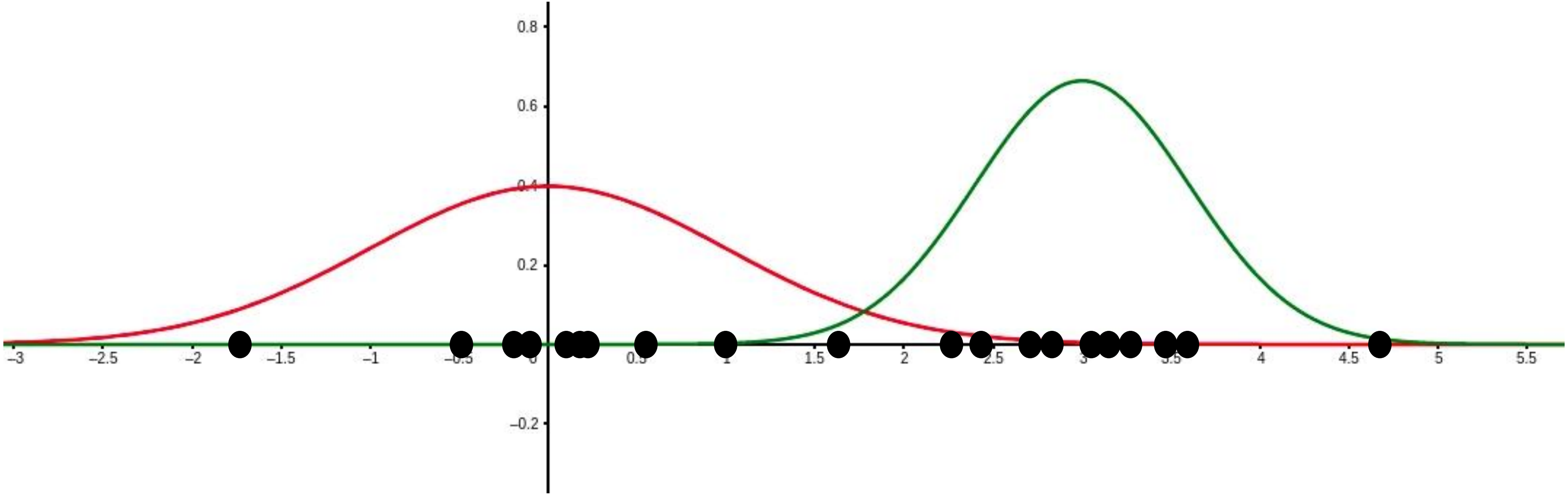
Generate data using $\mathbf{N(\mu_1, \sigma_1)}$ and $\mathbf{N(\mu_2, \sigma_2)}$



Or: we are given the weights of animals. Unknown to us these are weights from two different species. Can we determine the species (group / assignment) from the height?

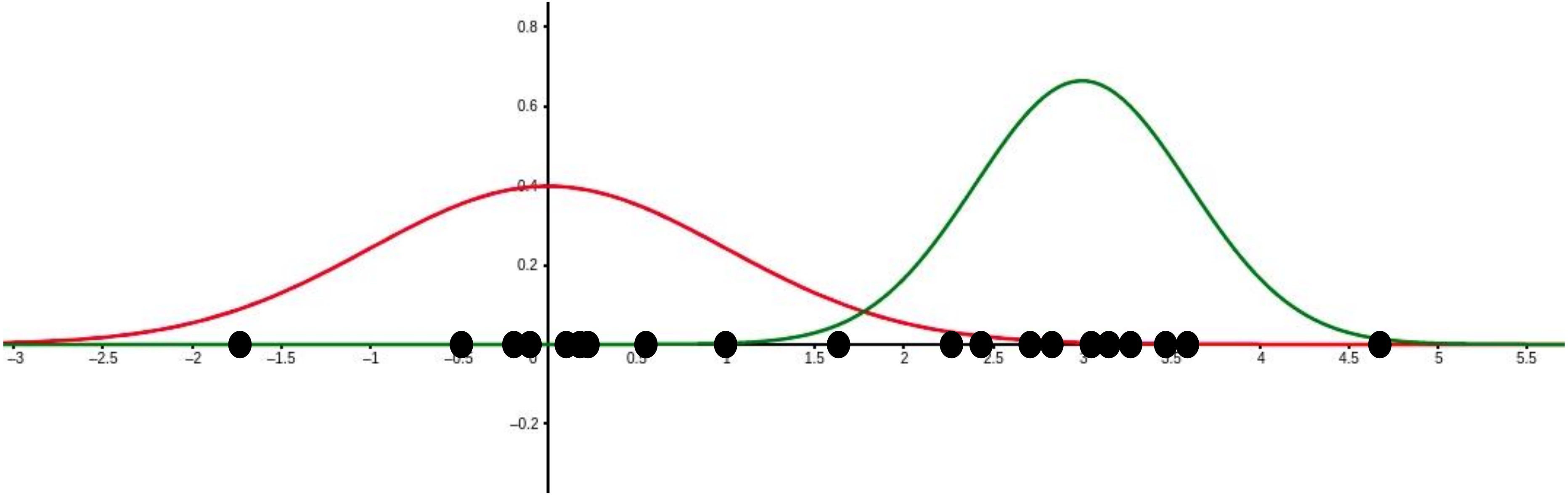
Soft Clustering - Example

Generate data using **N(μ_1, σ_1)** and **N(μ_2, σ_2)**



Soft Clustering - Example

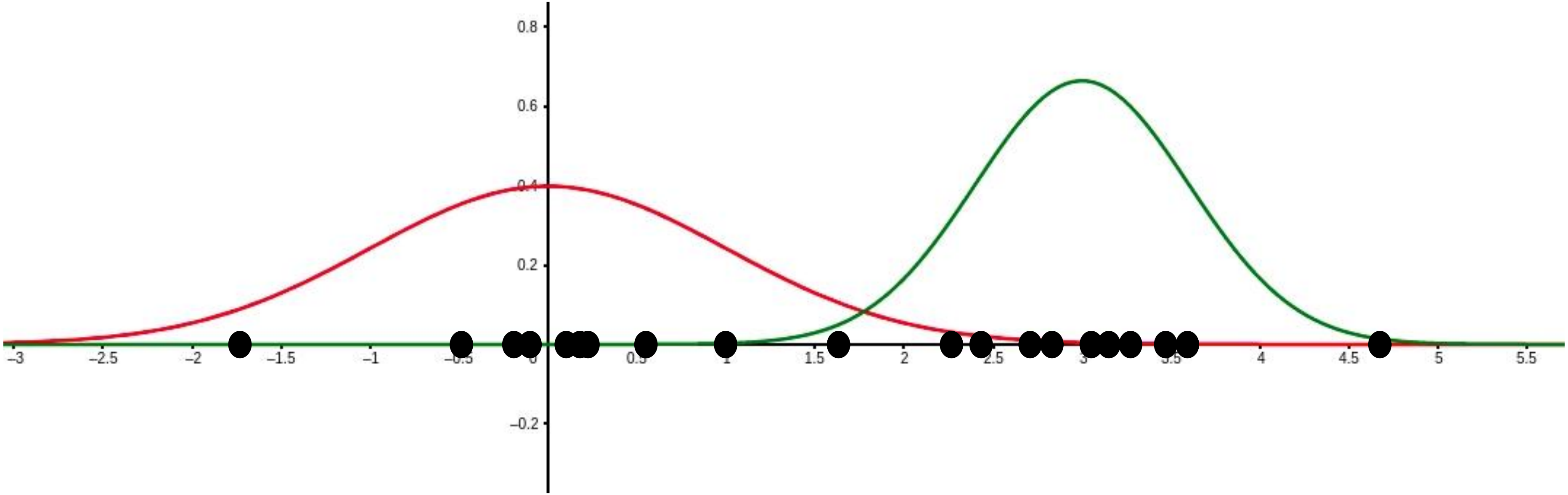
Generate data using **N(μ_1, σ_1)** and **N(μ_2, σ_2)**



Any of these points could technically have been generated from either curve.

Soft Clustering - Example

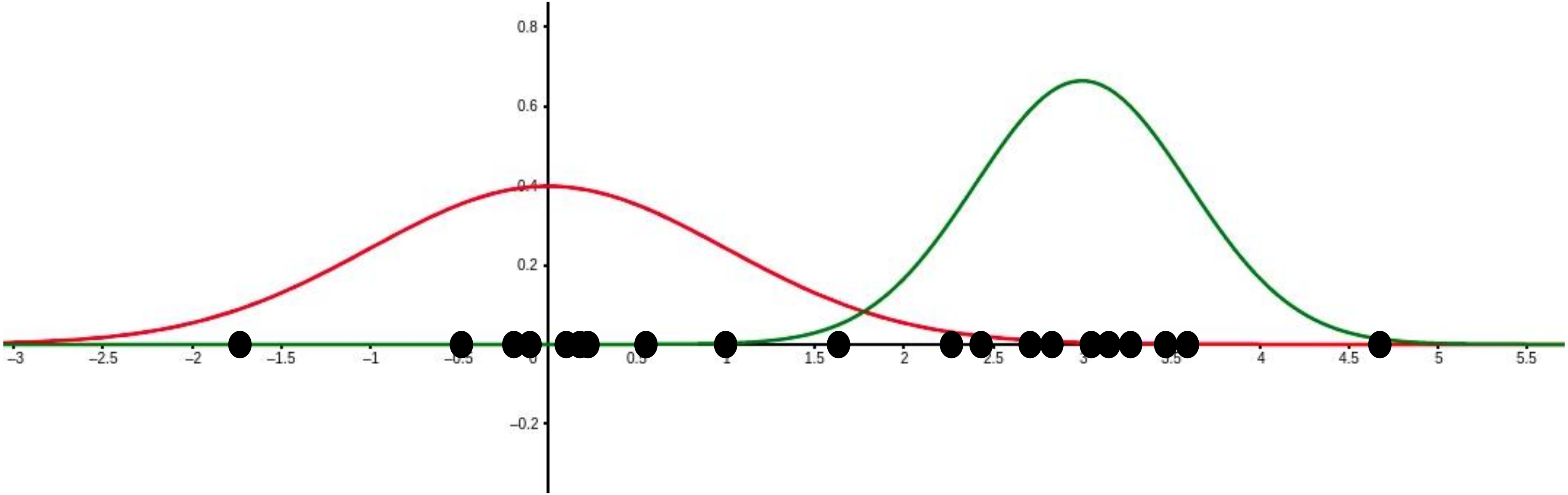
Generate data using **N(μ_1, σ_1)** and **N(μ_2, σ_2)**



For each point we can compute the probability of it being generated from either curve

Soft Clustering - Example

Generate data using $\mathbf{N(\mu_1, \sigma_1)}$ and $\mathbf{N(\mu_2, \sigma_2)}$



We can create soft assignments based on these probabilities.

Mixture Model

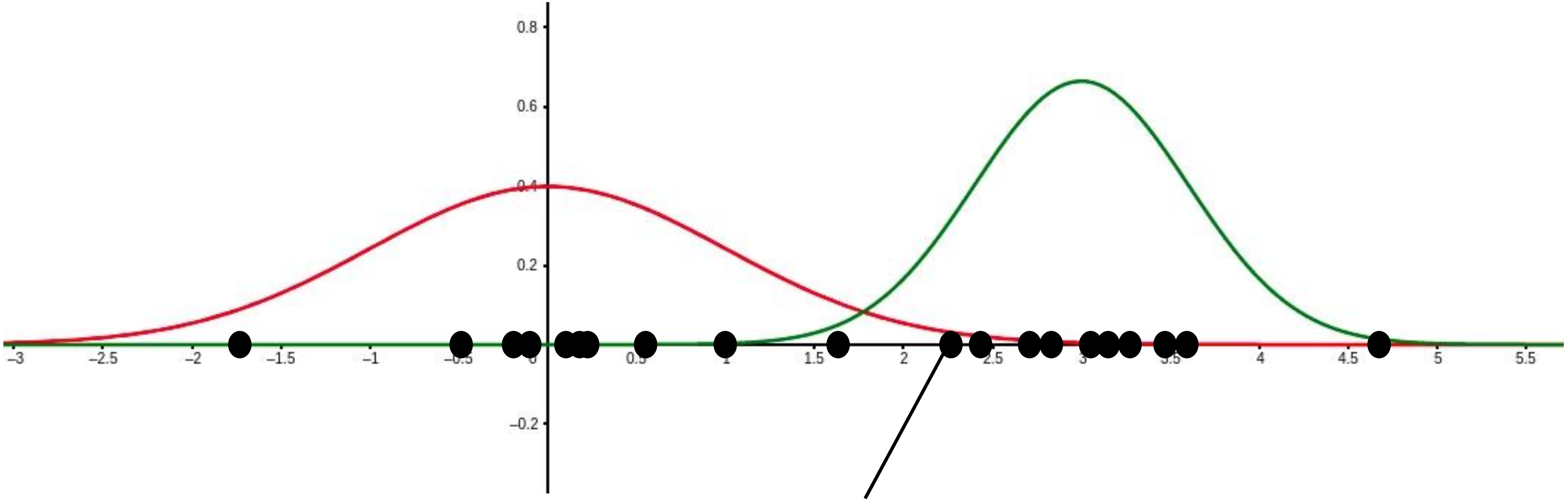
X comes from a mixture model with k mixture components if the probability distribution of X is:

$$P(X=x) = \sum_{j=1}^{k} P(C_j) P(X=x|C_j)$$

Mixture proportion
Represents the probability of belonging to C_j

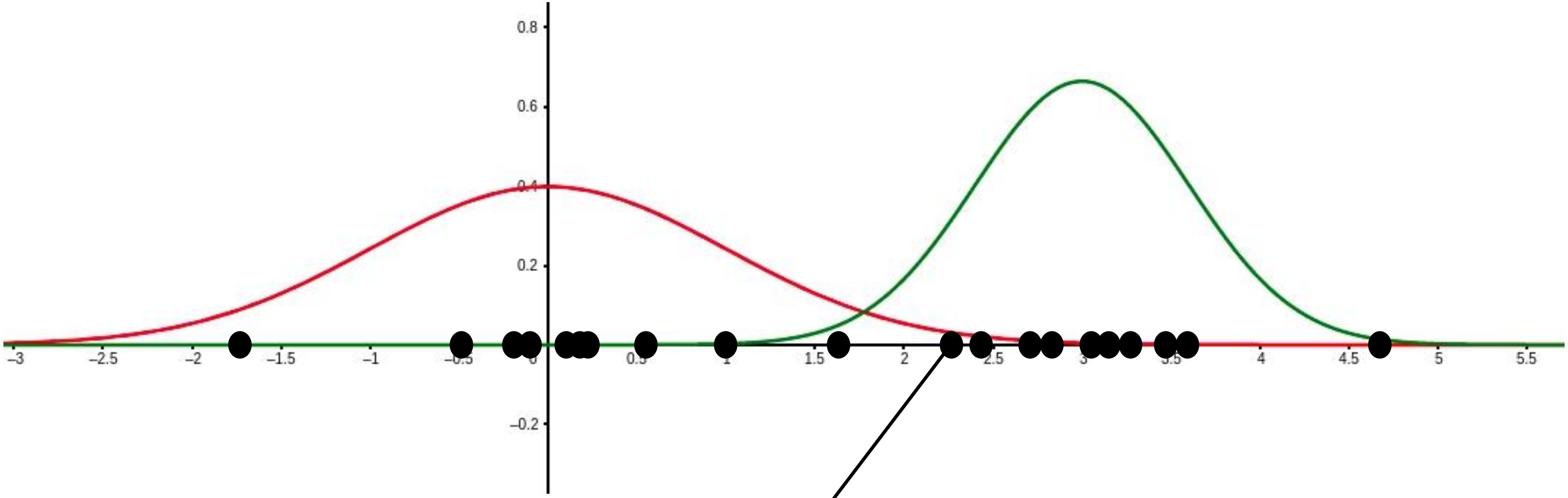
Probability of seeing x when sampling from C_j

Example



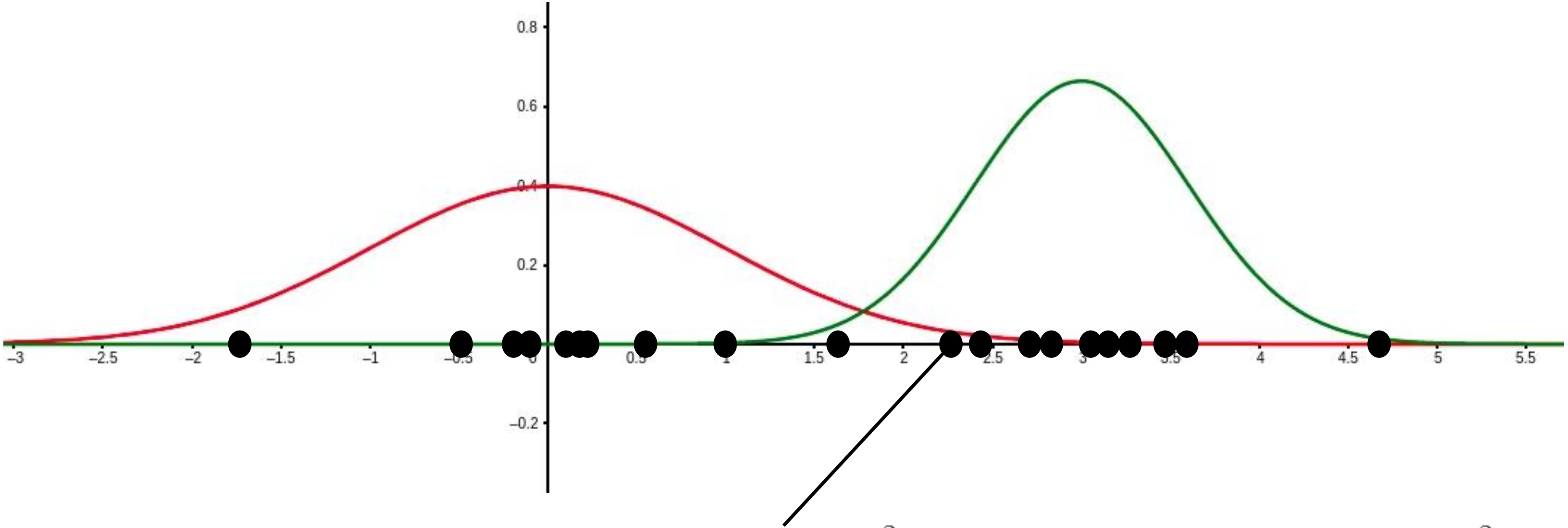
What is the probability distribution here?

Example



$$P(X=x) = P(C_1)P(X=x|C_1) + P(C_2)P(X=x|C_2)$$

Example



$$P(X=x) = P(C_1)\frac{1}{\sigma_1\sqrt{2\pi}}e^{-\frac{1}{2}\left(\frac{x-\mu_1}{\sigma_1}\right)^2} + P(C_2)\frac{1}{\sigma_2\sqrt{2\pi}}e^{-\frac{1}{2}\left(\frac{x-\mu_2}{\sigma_2}\right)^2}$$

Gaussian Mixture Model

A Gaussian Mixture Model (GMM) is a mixture model where

$$P(X = x | C_i) \sim N(\mu, \sigma)$$

GMM Clustering

Goal: Find the GMM that maximizes the probability of seeing the data we have.

Finding the GMM means finding the parameters that uniquely characterize it. What are these parameters?

$\mathbf{P(C_i)}$ & $\boldsymbol{\mu_i}$ & $\boldsymbol{\sigma_i}$ for all **k** components.

GMM Clustering

Goal:

$$\theta^* = \arg\max_{\theta} \prod_{i=1}^{n} \sum_{j=1}^{k} P(C_j)P(X_i \mid C_j)$$

Joint probability distribution of our data

Assuming our data are independent

GMM Clustering

How do we find the critical points of this function?

Notice: taking the log-transform does not change the critical points

Define:

$$\begin{aligned} l(\theta) &= \log(L(\theta)) \\ &= \sum_{i=1}^{n} \log(\sum_{j=1}^{k} P(C_j)P(X_i \mid C_j)) \end{aligned}$$

GMM Clustering

For $\boldsymbol{\mu} = [\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_k]^T$ and $\boldsymbol{\Sigma} = [\boldsymbol{\Sigma}_1, \ldots, \boldsymbol{\Sigma}_k]^T$

We can solve

$$\frac{d}{d\Sigma} l(\theta) = 0 \qquad \frac{d}{d\mu} l(\theta) = 0$$

GMM Clustering

To get

$$\hat{\mu}_j = \frac{\sum_{i=1}^{n} P(C_j|X_i)X_i}{\sum_{i=1}^{n} P(C_j|X_i)}$$

$$\hat{\Sigma}_j = \frac{\sum_{i=1}^{n} P(C_j|X_i)(X_i - \hat{\mu}_j)^T(X_i - \hat{\mu}_j)}{\sum_{i=1}^{n} P(C_j|X_i)}$$

$$\hat{P}(C_j) = \frac{1}{n}\sum_{i=1}^{n} P(C_j|X_i)$$

GMM Clustering

Do we have everything we need to solve this?

Still need **$P(C_j \mid X_i)$** (i.e. the probability that X_i was drawn from C_j)

GMM Clustering

$$P(C_j|X_i) = \frac{P(X_i|C_j)}{P(X_i)}P(C_j)$$

$$= \frac{P(X_i|C_j)P(C_j)}{\sum_{j=1}^{k} P(C_j)P(X_i|C_j)}$$

Looks like a loop! Seems we need $P(C_j)$ to get $P(C_j \mid X_i)$ and $P(C_j \mid X_i)$ to get $P(C_j)$

Expectation Maximization Algorithm

1. Start with random **θ**
2. Compute **$P(C_j \mid X_l)$** for all **X_i** by using **θ**
3. Compute / Update **θ** from **$P(C_j \mid X_l)$**
4. Repeat 2 & 3 until convergence

Demo