

Lecture 17: Clustering and density estimation

Professor Ilias Bilonis

Density estimation using Gaussian mixtures

Density estimation

You are given n observations:

$$\mathbf{x}_{1:n} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$$

(inputs, features, ...)

Problem: Assuming the observations are independent, find the probability density $p(\mathbf{x})$.

Mixtures of Gaussians

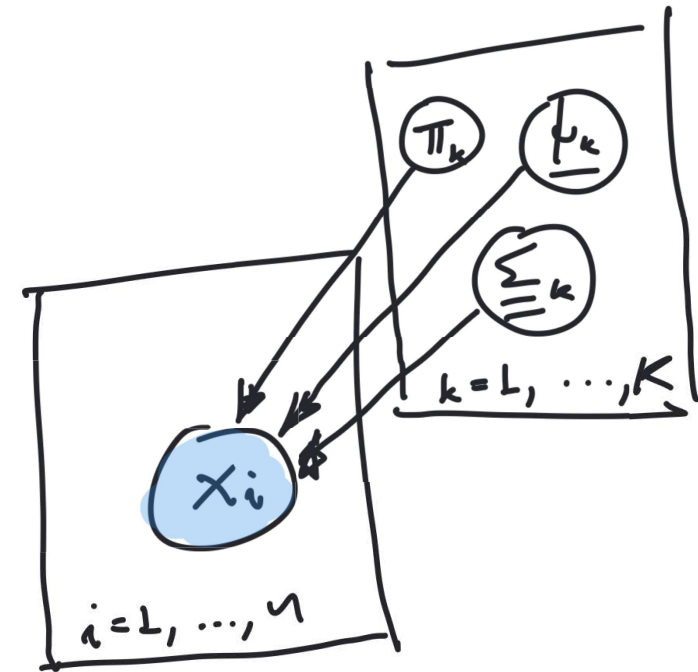
$$P(\underline{x} | \underline{\psi}) = \pi_1 N(\underline{x} | \underline{\mu}_1, \underline{\Sigma}_1) + \pi_2 N(\underline{x} | \underline{\mu}_2, \underline{\Sigma}_2) + \dots + \pi_K N(\underline{x} | \underline{\mu}_K, \underline{\Sigma}_K)$$

Handwritten notes:
 - $\pi, \underline{\mu}, \underline{\Sigma}$ } must find
 - $\underline{\mu}_1, \underline{\Sigma}_1$ } near comp.
 - π_1 } p. of sampling comp 1
 - π_2 } p. of sampling comp 2
 - π_K }

probability of sampling component 1

p. of sampling comp 2

restrictions: $\sum_{i=1}^K \pi_i = 1, \underline{\Sigma}_i$ pos. def.



Training the model

Likelihood:

$$p(x_{1:n} | \underline{\pi}, \underline{\mu}, \underline{\Sigma}) = \prod_{i=1}^n p(\underline{x}_i | \underline{\pi}, \underline{\mu}, \underline{\Sigma})$$

$$= \prod_{i=1}^n \left\{ \sum_{k=1}^K \pi_k N(\underline{x}_i | \underline{\mu}_k, \underline{\Sigma}_k) \right\}$$

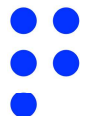
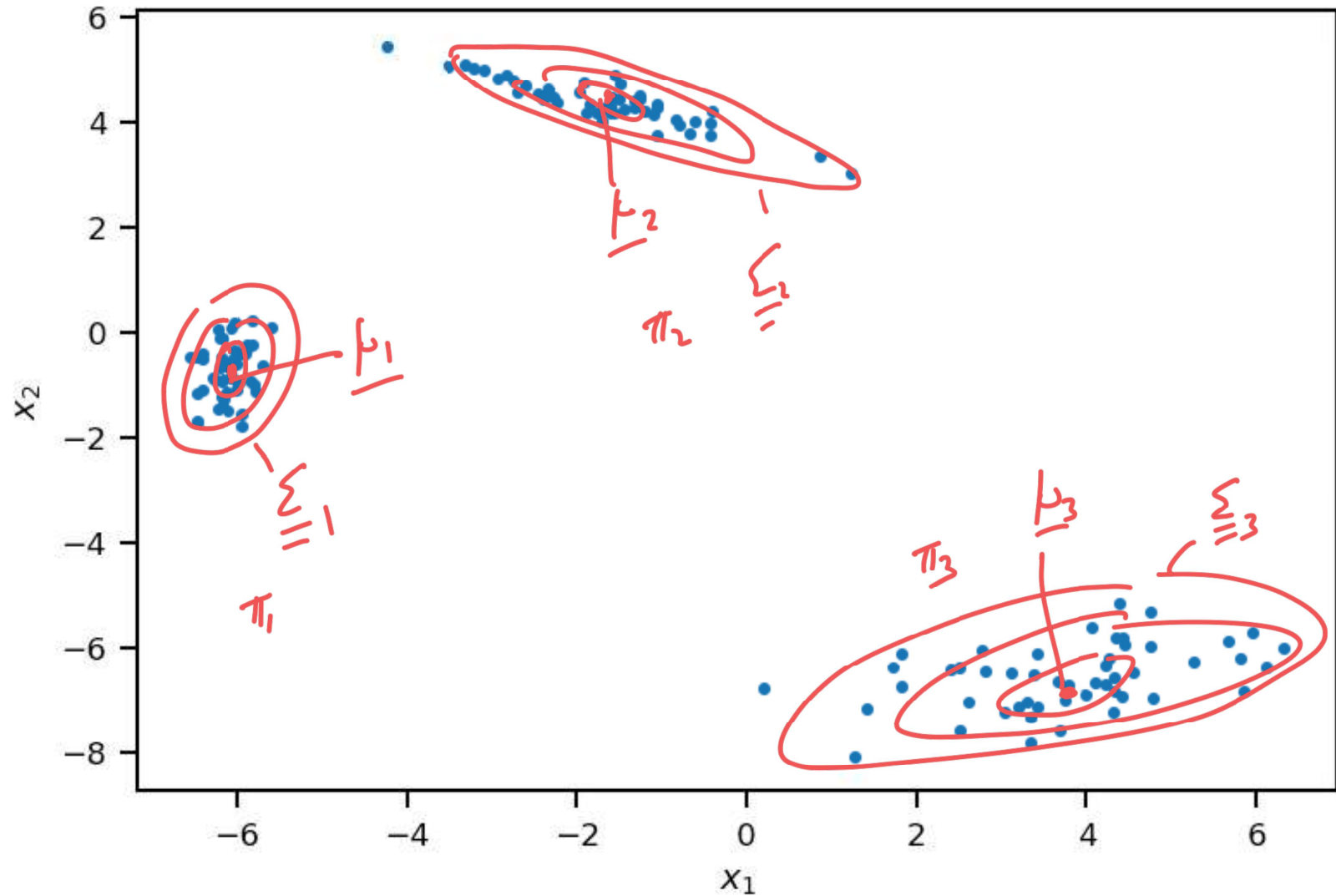
log
rules

$$\max_{\underline{\pi}, \underline{\mu}, \underline{\Sigma}} \log p(x_{1:n} | \underline{\pi}, \underline{\mu}, \underline{\Sigma}) = \sum_{i=1}^n \log(\dots)$$

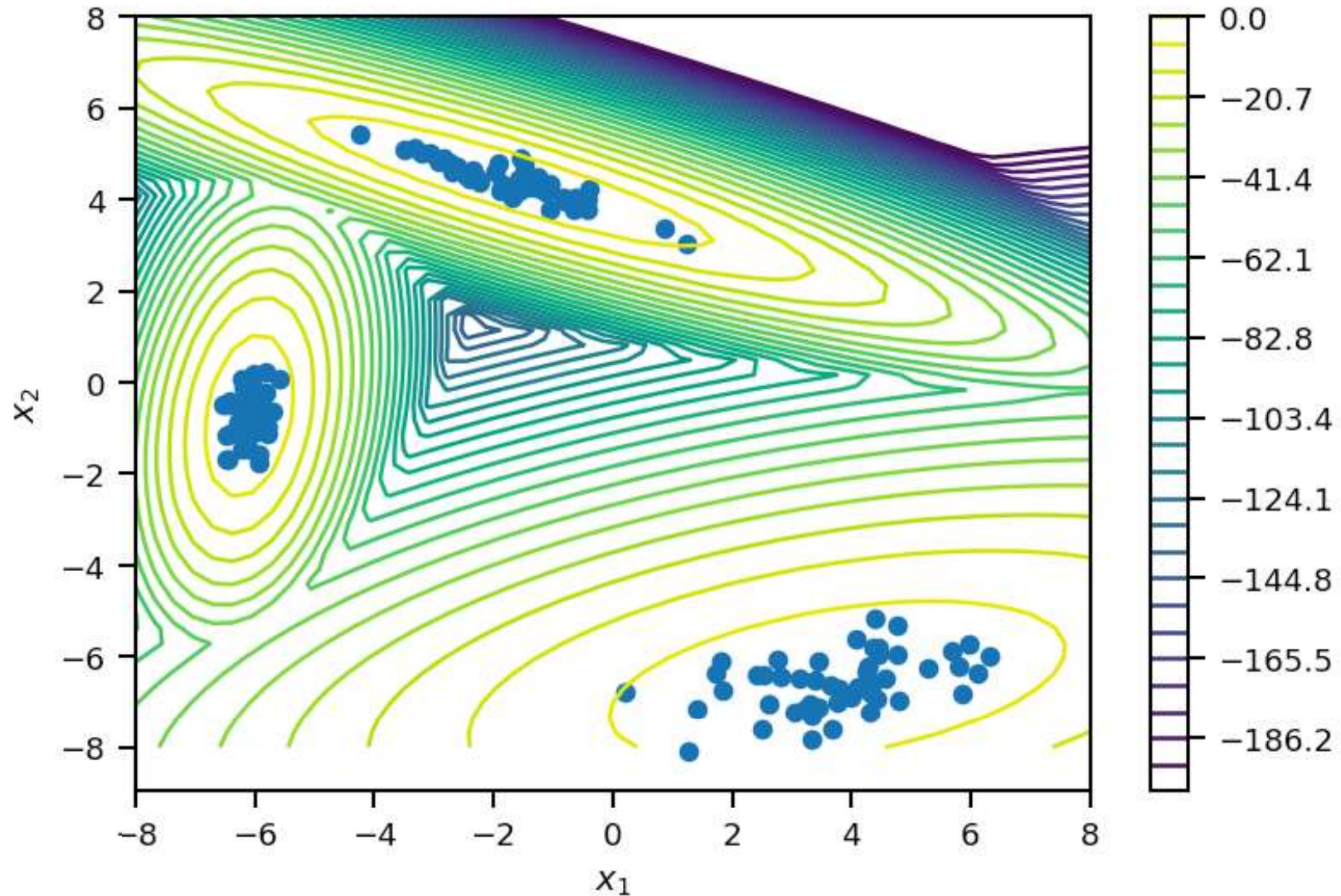
Expectation-Maximization

Bishop 2006.

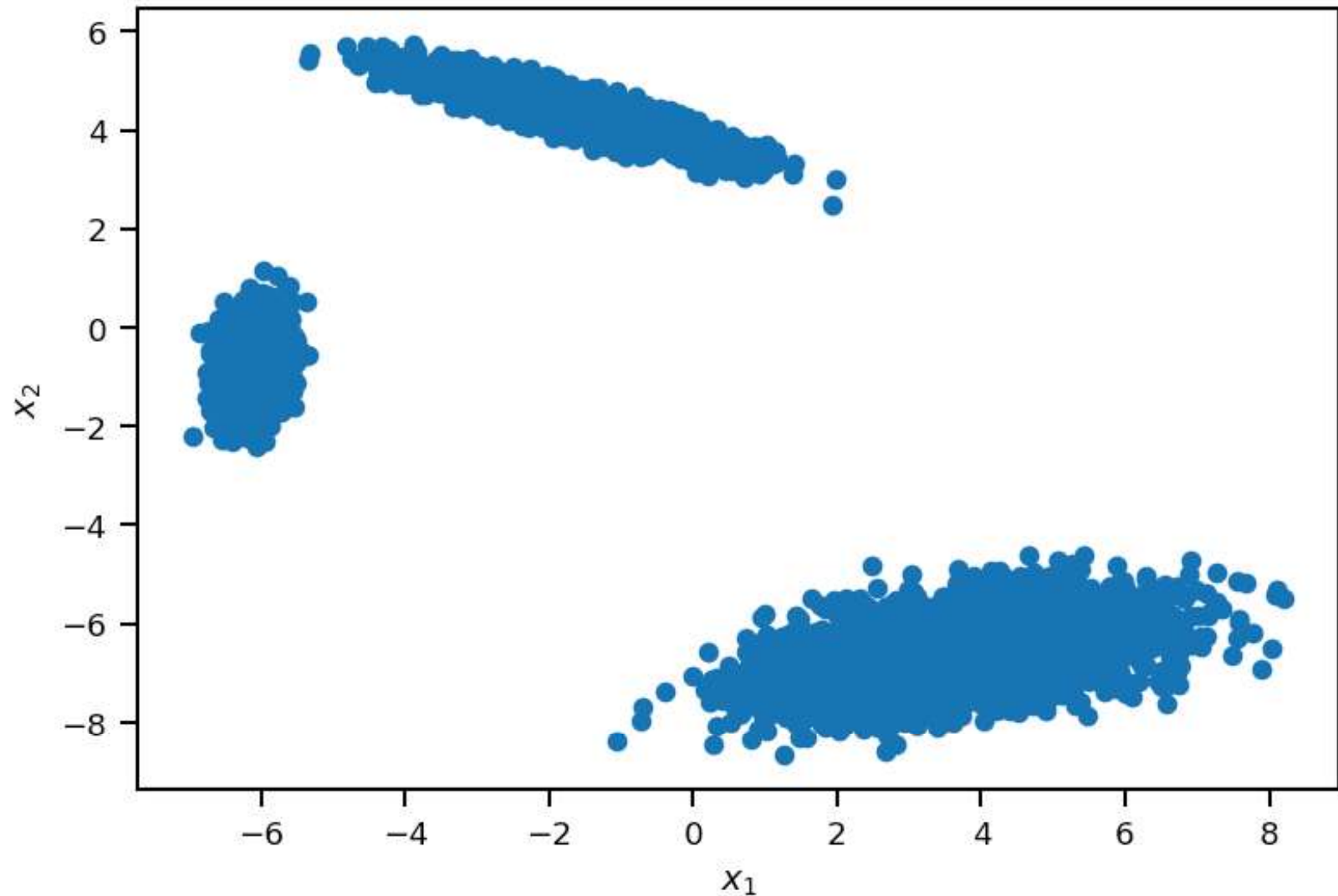
Example



Log probability density: Density estimation with mixtures



You can sample from the density



You can use the model to do clustering

$$p(\underline{x} \text{ belongs to } k^{\text{th}} \text{ comp.} \mid \underline{\pi}, \underline{\Sigma}, \underline{\mu}) \propto \pi_k \cdot \mathcal{N}(\underline{x} \mid \underline{\mu}_k, \underline{\Sigma}_k)$$

$$\frac{\pi_k \mathcal{N}(\underline{x} \mid \underline{\mu}_k, \underline{\Sigma}_k)}{\sum_{k'=1}^K \pi_{k'} \mathcal{N}(\underline{x} \mid \underline{\mu}_{k'}, \underline{\Sigma}_{k'})}$$

to make a hard-assignment to a cluster, take the $\underset{k}{\operatorname{argmax}}(\cdot)$

