

data  $x_1, x_2, \dots, x_n$  ;  $x_i \in \mathbb{R}$  ←

mixture models

\* model the probability of observing a data point  $x_i$  as a mixture of  $k$ -pure types

→  $p(x|\theta_j)$  ,  $j=1, \dots, k$

$\theta_j$  ?

Assumption: 'k' is known

$$* \quad \overbrace{p(x)}_{\text{(mixture density)}} = \sum_{j=1}^k \underbrace{\pi_j}_{\text{(pure type density)}} p(x | \theta_j)$$

Now we can see that

$$\begin{aligned} - & 0 \leq \pi_j \leq 1 \\ - & \sum_{j=1}^k \pi_j = 1 \end{aligned} \quad \left. \vphantom{\begin{aligned} - & 0 \leq \pi_j \leq 1 \\ - & \sum_{j=1}^k \pi_j = 1 \end{aligned}} \right\}$$

(mixture proportions)

# Gaussian mixture model

\* Assuming Gaussian pure types, we write

$$\rightarrow p(x) = \sum_{j=1}^k \pi_j N(x | \mu_j, \sigma_j^2) \dots \textcircled{1}$$

$$N(x | \mu_j, \sigma_j^2) = \frac{1}{\sqrt{2\pi} \sigma_j} \exp\left\{-\frac{(x - \mu_j)^2}{2\sigma_j^2}\right\}$$

Unknown parameters of the mixture

\*  $\pi_j$  ;  $0 \leq \pi_j \leq 1$ ,  $\sum_{j=1}^k \pi_j = 1$

\*  $\mu_1, \mu_2, \dots, \mu_k \leftarrow$  mean

\*  $\sigma_1, \sigma_2, \dots, \sigma_k \leftarrow$  variance

An equivalent formulation - "missing data" representation

Dempster et al. (1977) ← Introduced EM algorithm

\* We introduce a binary membership variable

$$z_{ij} \in \{0, 1\}; \quad \underline{\vec{z}_i} \in \{0, 1\}^k, \quad \sum_{j=1}^k z_j = 1$$

for every data point  $x_i$

E.g. if  $x_i$  belongs to cluster  $j$

$$z_{ij} = 1 \text{ and } z_{ij' \neq j} = 0, \quad j' = 1, \dots, k$$

\* We use

$$p(x) = \sum_{\vec{z}} p(x, \vec{z}) = p(x | \vec{z}) p(\vec{z}) \quad \leftarrow$$

- the marginal  $p(\vec{z})$  is modeled as a multinomial

$$\underline{p(z_j = 1) = \pi_j}$$

$$\underline{p(\vec{z})} = \prod_{j=1}^k \pi_j^{z_j} \dots \quad (2)$$

- Assuming normality, we write

$$\underline{p(x | z_j = 1)} = \mathcal{N}(x | \mu_j, \sigma_j^2) \quad \leftarrow$$

$$p(x | \vec{z}) = \prod_{j=1}^k \underbrace{\mathcal{N}(x | \mu_j, \sigma_j^2)}_{\text{membership}} \quad (3)$$

- Combining (2) & (3), we have

$$p(x, z) = \prod_{j=1}^k \left[ \pi_j \mathcal{N}(x | \mu_j, \sigma_j^2) \right]^{z_j}$$

the complete data likelihood

-  $p(x)$  =  $\sum_z p(x, z)$  ←  $z_j \in \{0, 1\}^k$   
 $z_j \in (0, 1)^k$

$$= \sum_z \prod_{j=1}^k \left[ \pi_j \mathcal{N}(x | \mu_j, \sigma_j^2) \right]^{z_j}$$

← other densities

$$= \sum_{j=1}^k \pi_j \mathcal{N}(x | \mu_j, \sigma_j^2)$$

(a Gaussian mixture)

Note: Summation over  $z$  consists of  $k$  terms;

(a) for  $j^{\text{th}}$  term,  $z_j = 1$  and

(b) the product becomes  $\pi_j \mathcal{N}(x | \mu_j, \sigma_j^2)$

for  $j' \neq j^{\text{th}}$  term,  $z_{j'} = 0$

Adv.

We have a joint density  $p(x, z)$  with a hidden variable  $z$  - missing data. It helps

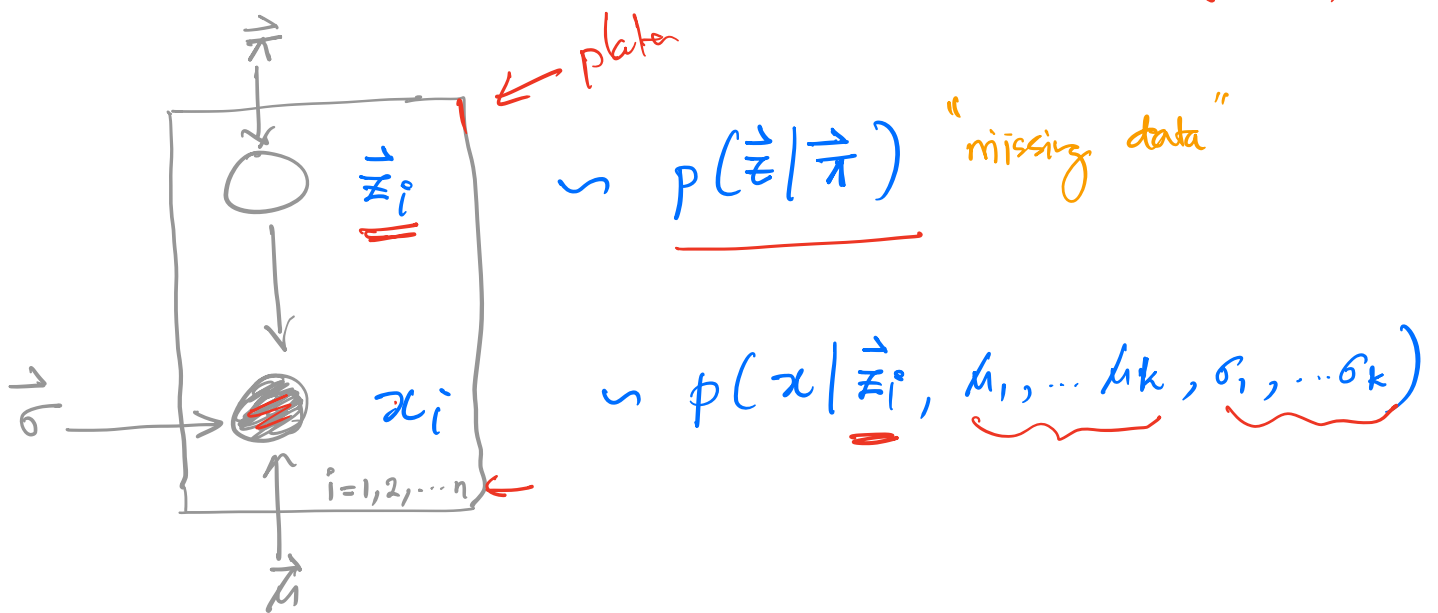
- MLE using EM (Dempster et al. 1977)
- and Bayesian posterior inference

# The hierarchical model (induced by the missing data formulation)

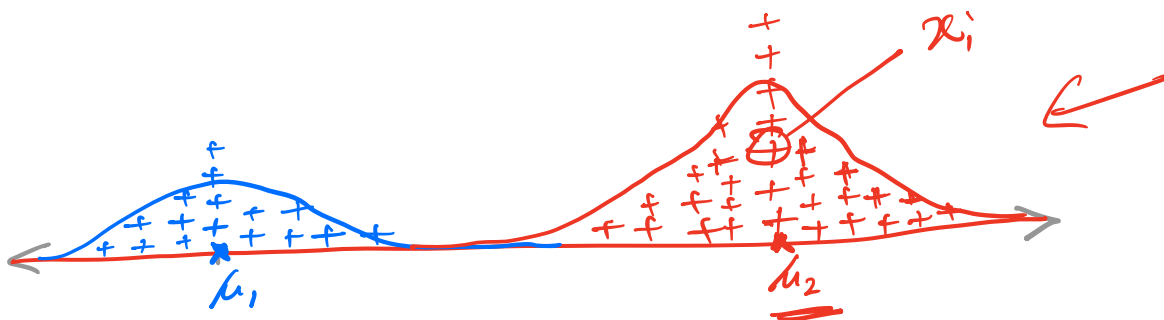
We assume

- there are  $k$  clusters in the data  $\leftarrow$
- $\vec{\pi}, \underbrace{\mu_1, \dots, \mu_k}_{\text{mean}}, \underbrace{\sigma_1, \dots, \sigma_k}_{\text{var}}$  are <sup>known</sup> parameters  $\wedge$
- mixture proportion

For every data point  $x_i, i=1, 2, \dots, n$   $\vec{\pi} \in (0, 1)^k$



Example data generated ( $k=2$ ,  $x_i \in \mathbb{R}$ )

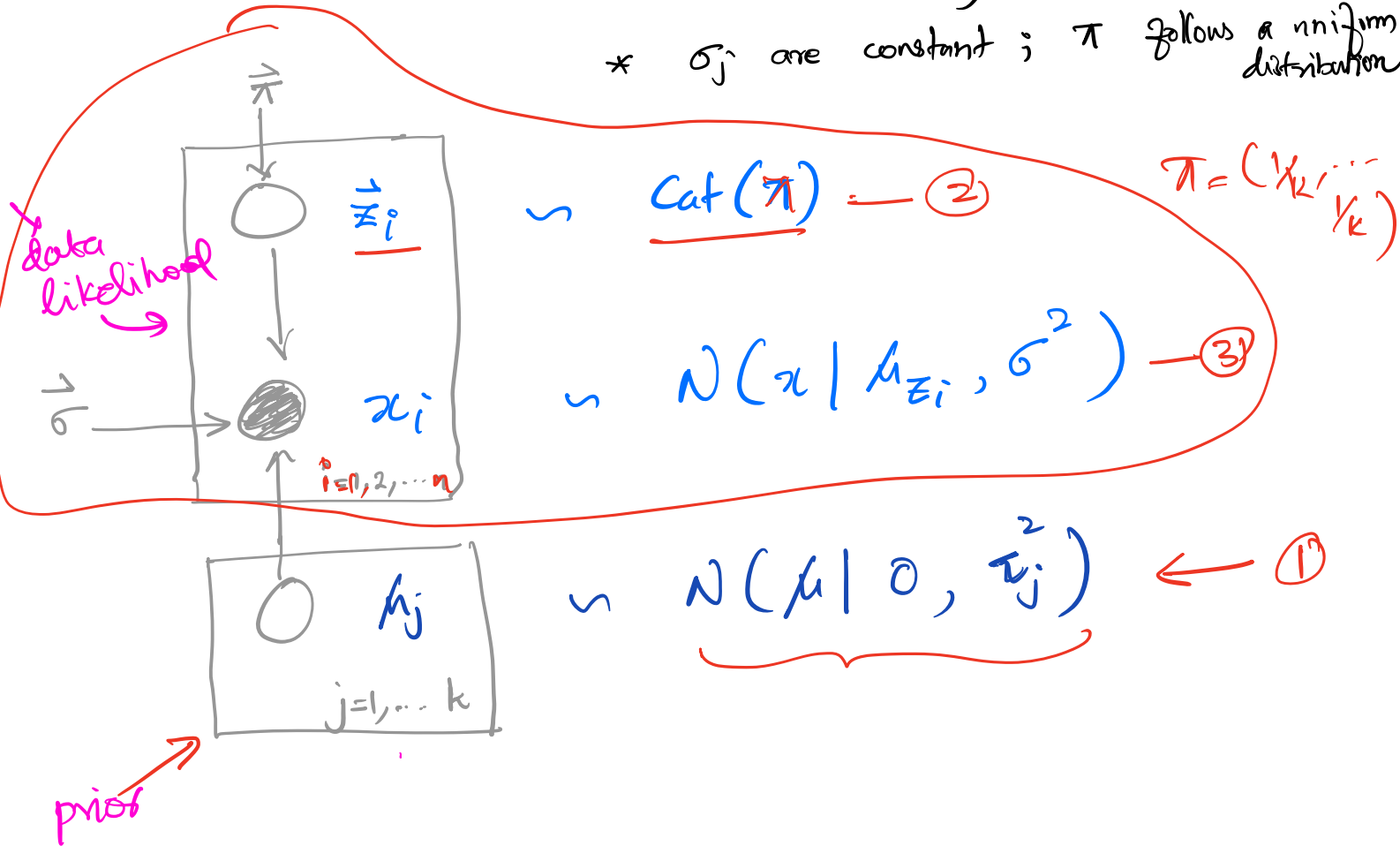


# Bayesian formulation

We assume that the parameters, for example,  $\pi, \mu, \sigma$  are random and distributed according to some prior

To keep it simple, we assume

- \*  $\mu_j$  are normally distributed ✓
- \*  $\sigma_j$  are constant;  $\pi$  follows a uniform distribution





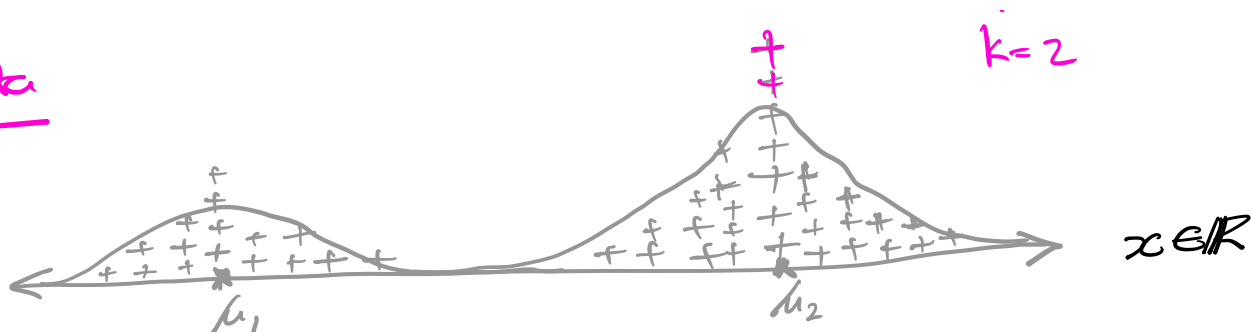
Posterior a distribution over hidden variables

-  $z$  — missing data

-  $\mu$  — prior

given observed data —  $p(z, \mu | x)$

our data



$p(z, \mu | x)$  is intractable

for a given choice of prior, and the likelihood

$$- \prod_{i=1}^n \sum_{j=1}^k \pi_j \mathcal{N}(x_i | \mu_j, \sigma_j^2), \leftarrow x_i$$

the posterior is a mixture with  $k^n$  terms

# Gibbs Sampler

\* we have a posterior density  $p(z, \mu | x)$

\* Our interests: the characteristics of a marginal

$$\underline{p(z)} = \int_{\mu} p(z, \mu | x)$$

- intractable

\* Gibbs sampler allows to sample

-  $z_1, z_2, \dots, z_M \sim p(z)$  [without requiring  $p(z)$ ]

- Once we have a large sample, to calculate the mean of  $p(z)$  we can use the sample mean

- Gibbs sampler generates a sample from  $p(z)$

by sampling from

$$(1) p(z | \mu) \leftarrow z \sim$$

$$p(z | \mu) \leftarrow \text{Multinomial}$$

$$(2) p(\mu | z)$$

$$\mu \sim p(\mu | z) \leftarrow \text{Normal sample}$$

iteratively

