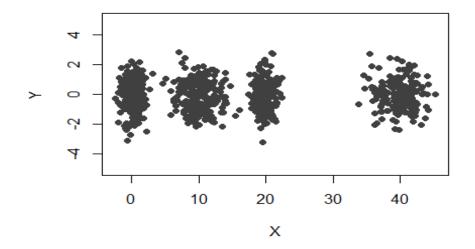
# Lecture 7: Clustering

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## What does Clustering do

- Let's start with the Gaussian mixture model (GMM), that has been one of the most popular clustering model.
- GMM assumes that the data come from not just one distribution but a few.



### Formulation of GMM

- Suppose that there are M distributions mixed together.
- For each data point  $x_n$ , the probability that it comes from the m<sup>th</sup> distribution is denoted as  $\pi_m$ , while  $\sum_{m=1}^M \pi_m = 1$ .
- In GMM, the m<sup>th</sup> distribution is  $N(\mu_m, \Sigma_m)$ .
- The task is to learn the unknown parameters  $\{\mu_m, \Sigma_m, m=1\}$

# Log-likelihood function of GMM

The complete log-likelihood function is:

$$l(\mathbf{\Theta}) = \log \prod_{n=1}^{N} p(\mathbf{x}_{n} | z_{nm} = 1; \mathbf{\Theta}),$$

$$= \log \prod_{n=1}^{N} p(\mathbf{x}_{n}, z_{nm} | \mathbf{\Theta}),$$

$$= \log \prod_{n=1}^{N} \prod_{m=1}^{M} [p(\mathbf{x}_{n} | z_{nm} = 1, \mathbf{\Theta}) p(z_{nm} = 1)]^{z_{nm}},$$

$$= \sum_{n=1}^{N} \sum_{m=1}^{M} [z_{nm} \log p(\mathbf{x}_{n} | z_{nm} = 1, \mathbf{\Theta}) + z_{nm} \log \pi_{m}].$$

# Log-likelihood function of GMM (cont'd)

Meanwhile, we can derive that

$$p(\mathbf{x}_n|z_{nm}=1;\mathbf{\Theta})=(2\pi)^{-p/2}|\mathbf{\Sigma}_m|^{-1/2}\exp\left\{-\frac{1}{2}(\mathbf{x}_n-\mathbf{\Phi})^{-p/2}|\mathbf{\Sigma}_m|^{-1/2}\right\}$$

### A two-step iterative procedure

To optimize for  $\Theta$ , we need to overcome the challenge that  $z_{nm}$ s are latent and unknown. Here, an intuitive proposal could be:

• Even we don't know  $z_{nm}$ , but we can estimate it if we have known  $\Theta$ . For instance, it is easy to know that

$$p(z_{nm}=1|\mathbf{X},\mathbf{\Theta}) = \frac{p(x_n|z_{nm}=1,\mathbf{\Theta})\pi_m}{\sum_{k=1}^{M} p(x_n|z_{nk}=1,\mathbf{\Theta})\pi_k}.$$

Thus, given  $\Theta$ , the best estimate of  $z_{nm}$  could be the expectation of  $z_{nm}$  as

$$\langle z_{nm} \rangle_{p(z_{nm}|\mathbf{X},\mathbf{\Theta})} = 1 \cdot p(z_{nm} = 1|\mathbf{X},\mathbf{\Theta}) + 0 \cdot p(z_{nm} = 0|\mathbf{X},\mathbf{\Theta}) = \frac{\sum_{k=1}^{M} p(x_{n}|z_{nk}=1,\mathbf{\Theta})\pi_{k}}{\sum_{k=1}^{M} p(x_{n}|z_{nk}=1,\mathbf{\Theta})\pi_{k}}.$$

• We can fill in  $l(\Theta)$  with the estimated  $z_{nm}$  and optimize it to update  $\Theta$ . Feed this updated back to Step 1 and repeat the iterations, until all the parameters in the iterations don't change significantly.

# The EM-algorithm

This two-step iterative procedure is known as the EM algorithm.

- The E-step: Derive the posterior distribution of  $\mathbf{Z}$  as  $p(\mathbf{Z}|\mathbf{X}, \mathbf{\Theta})$ . Calculate the expectation of  $l(\mathbf{\Theta})$  according to this distribution, i.e., denoted as  $\langle l(\mathbf{\Theta}) \rangle_{p(\mathbf{Z}|\mathbf{X},\mathbf{\Theta})}$ .
- The M-step: obtain  $\Theta$  by maximizing  $\langle l(\Theta) \rangle_{p(\mathbf{Z}|\mathbf{X},\Theta)}$ .

The power of the EM algorithm is that it guarantees (under mild conditions) that the objective function won't decrease along the iterations.

#### R lab

- Download the markdown code from course website
- Conduct the experiments
- Interpret the results
- Repeat the analysis on other datasets