CS 4824/ECE 4424: Clustering

Acknowledgement:
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EM algorithm — recap

- EM is a general procedure for learning from partly observed data
- Given observed variables X, unobserved Z ($X=\{F,A,H,N\}$, $Z=\{S\}$)

Begin with arbitrary choice for parameters θ

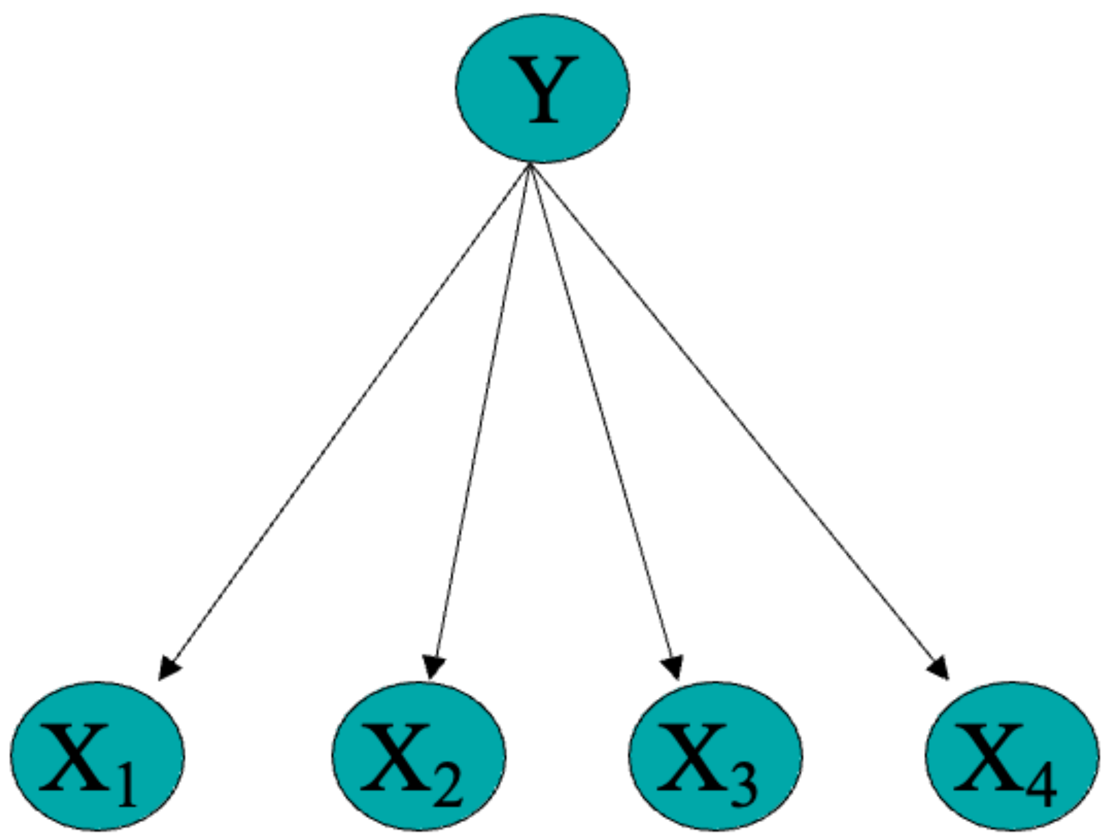
Iterate until convergence:

- E Step: estimate the values of unobserved Z conditioned on X using θ
- M Step: use observed values plus E-step estimates to derive a better θ

- Guaranteed to find local maximum. Each iteration increases

$$E_{P(Z|X,\theta)}[\log P(X,Z|\theta')]$$

What if we have no labeled data at all ?



Y	X1	X2	X3	X4
?	0	0	1	1
?	0	1	0	0
?	0	0	1	0
?	0	1	1	0
?	0	1	0	1

un
~~semi-~~supervised learning

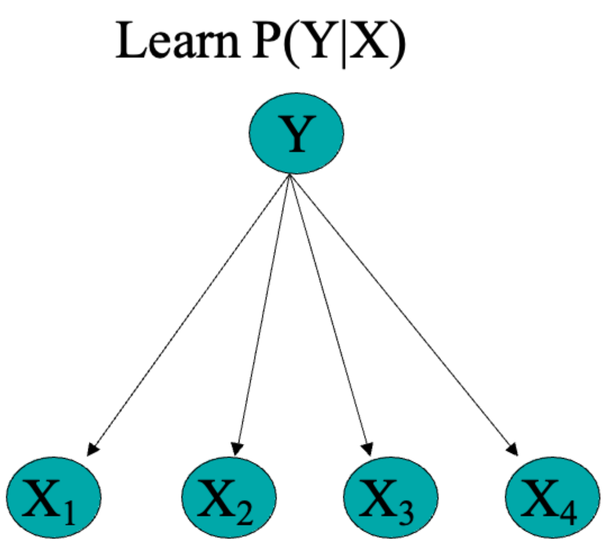
Unsupervised clustering

Just extreme case of EM with zero labeled examples…

From partially unlabeled data to no labeled data at all…

Y	X1	X2	X3	X4
1	0	0	1	1
0	0	1	0	0
0	0	0	1	0
?	0	1	1	0
?	0	1	0	1

semi-supervised learning



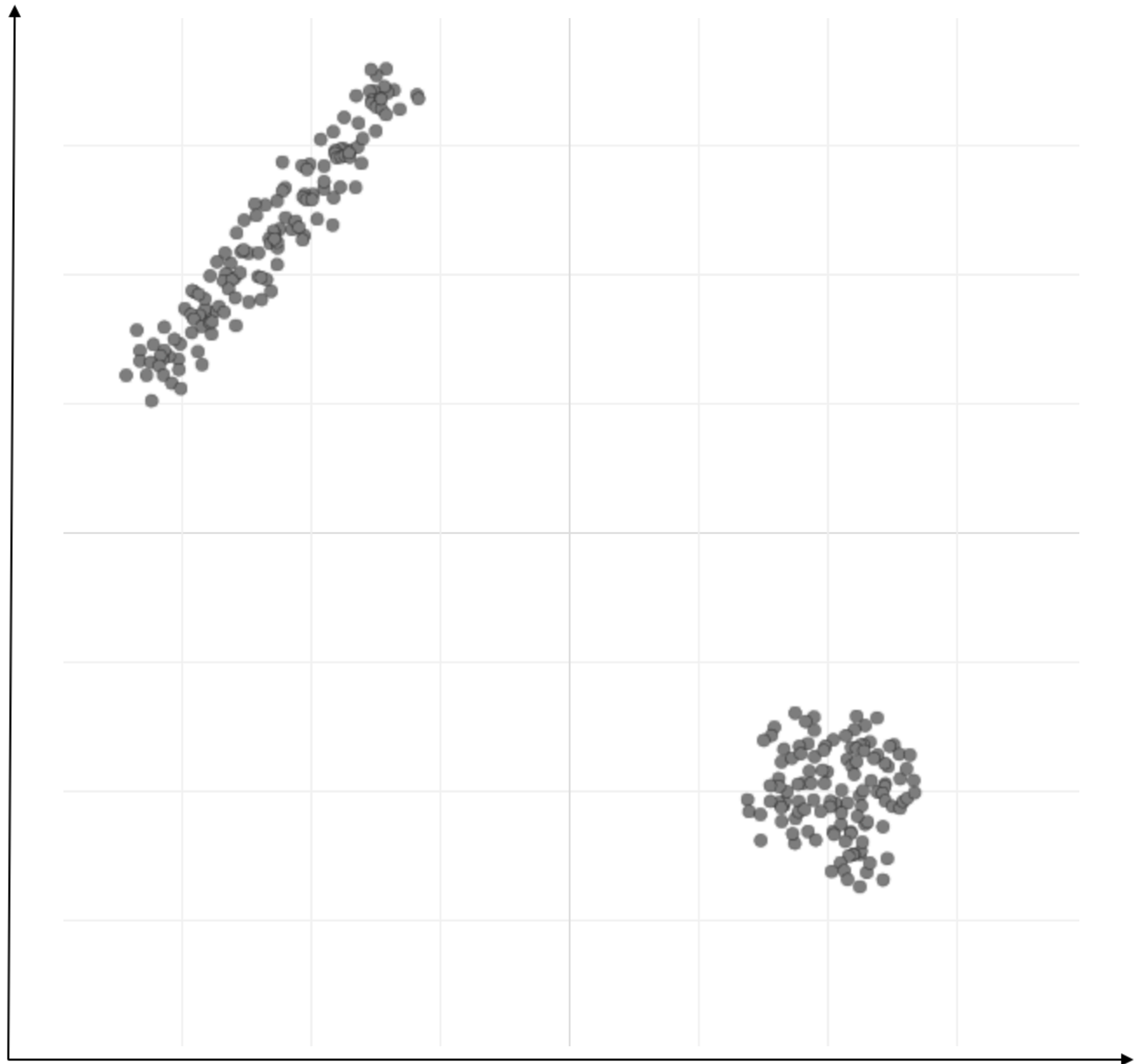
Y	X1	X2	X3	X4
?	0	0	1	1
?	0	1	0	0
?	0	0	1	0
?	0	1	1	0
?	0	1	0	1

unsupervised learning

Clustering

- Given set of data points, without class labels, group them
- Unsupervised learning
- Which news items are similar? (or which customers, faces, web pages, …)
- Many practical applications…

Clustering



Mixture Distributions

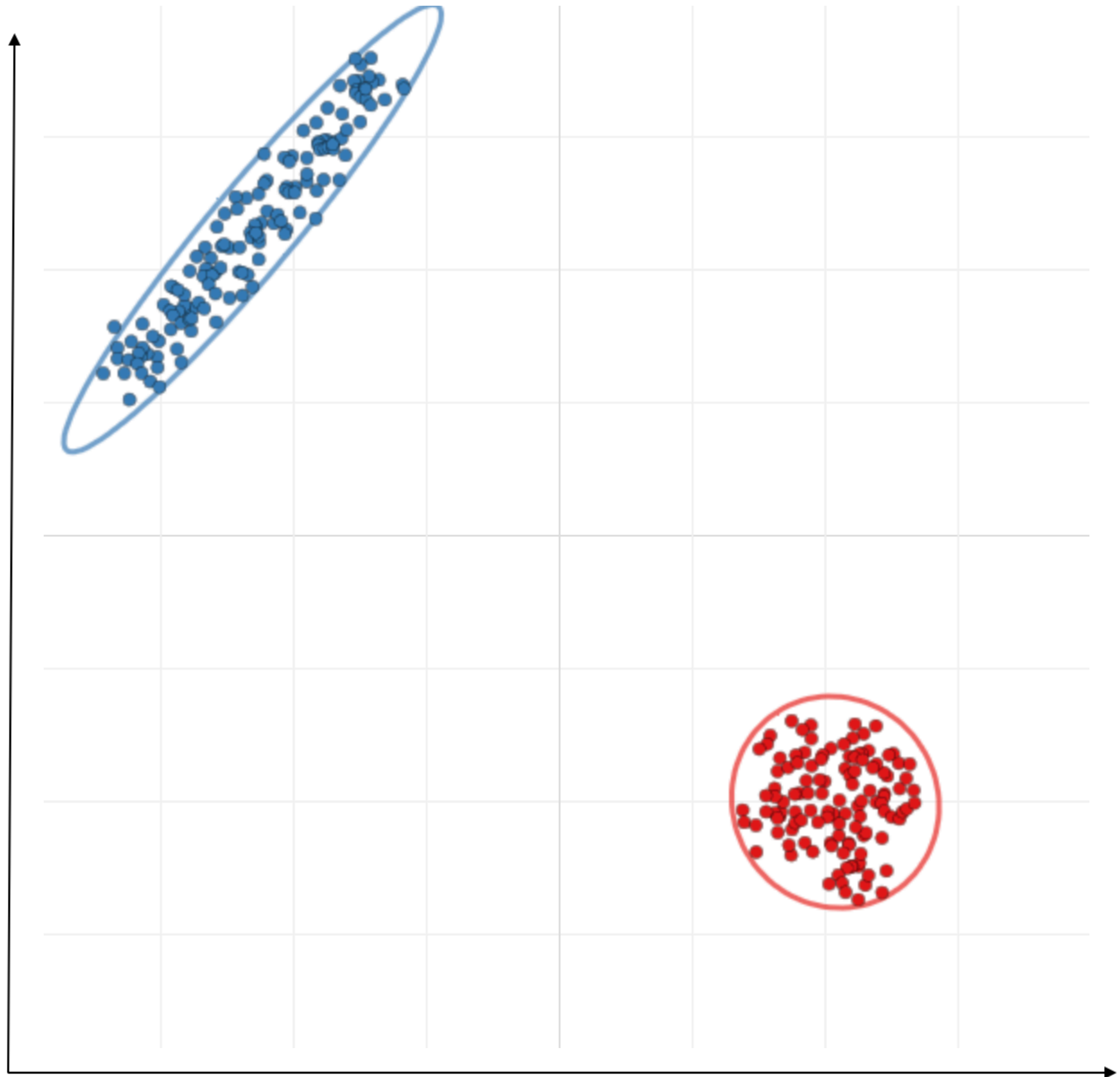
- Model joint distribution $P(X_1 \ldots X_n)$ as mixture of multiple distributions

- Use discrete-valued random var Z to indicate which distribution is being use for each random draw

$$P(X_1 \ldots X_n) = \sum_i P(Z=i) \;\; P(X_1 \ldots X_n | Z)$$

- Mixture of *Gaussians*:
  - Assume each data point $X=<X_1, \ldots X_n>$ is generated by one of several Gaussians, as follows:
    - randomly choose Gaussian *i*, according to *P(Z=i)*
    - randomly generate a data point $<x_1, x_2 \ldots x_n>$ according to the parameters of the Gaussian distributions corresponding to *i*

Mixture of Gaussians



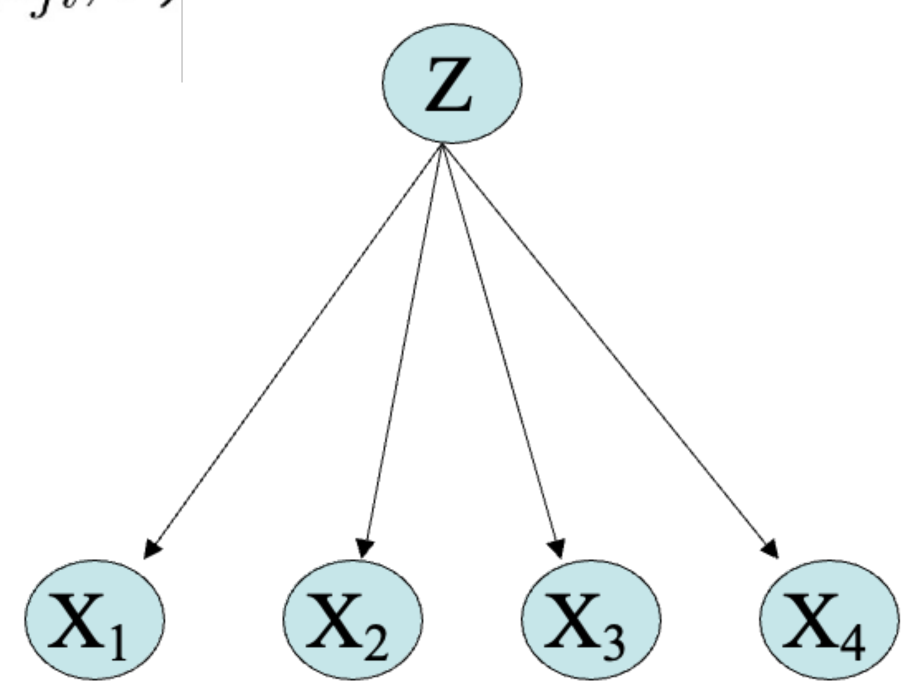
EM for Mixture of Gaussian Clustering

- Let's simplify to make this easier:
  - Assume $X=<X_1 \ldots X_n>$, and the X_i are conditionally independent given Z. $P(X|Z=j)=\prod_i N(X_i|\mu_{ji},\sigma_{ji})$
  - Assume only 2 clusters (values of Z), and $\forall i, j, \sigma_{ji}=\sigma$

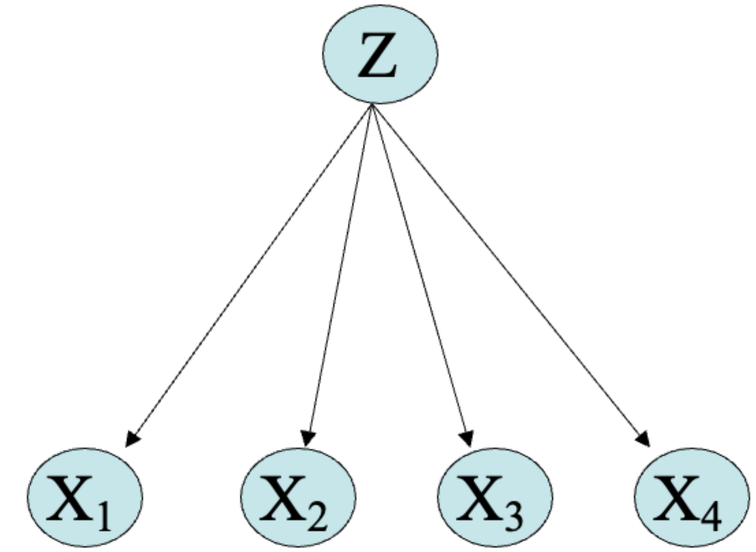
$$P(\mathbf{X})=\sum_{j=1}^{2} P(Z=j|\pi)\prod_i N(x_i|\mu_{ji},\sigma)$$

  - Assume σ known, $\pi_1 \ldots \pi_K, \mu_{1i} \ldots \mu_{Ki}$

- Observed: $X=<X_1 \ldots X_n>$
- Unobserved: Z



EM

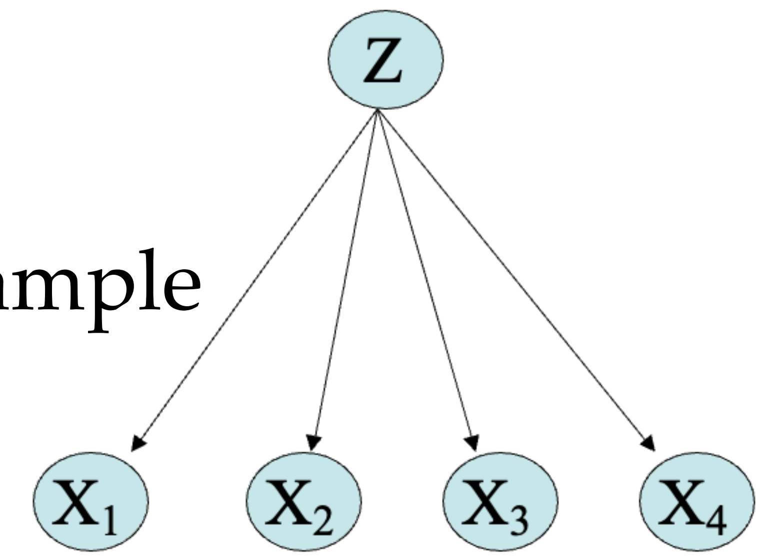


- Given observed variables X, unobserved Z,
  - define $Q(\theta'|\theta) = E_{Z|X,\theta}[\log P(X, Z|\theta')]$ where $\theta = \langle \pi, \mu_{ji} \rangle$

- Iterate until convergence:
  - E Step:
    - Calculate P(Z(n)|X(n),θ) for each example X(n).
    - Use this to construct $Q(\theta'|\theta)$
  - M Step:
    - Replace current θ by

$$\theta \leftarrow \arg\max_{\theta'} Q(\theta'|\theta)$$

EM — E Step



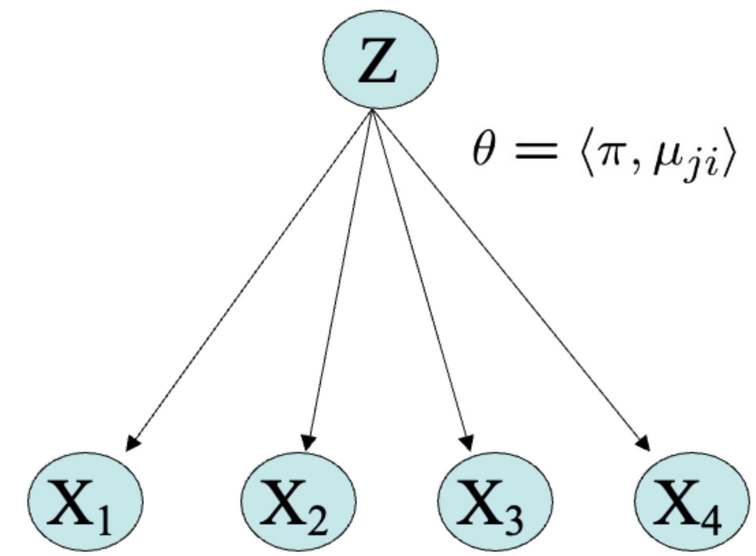
- Calculate P(Z(n)|X(n),θ) for each observed example X(n)=<x_1(n), x_2(n), … x_T(n)>

$$P(z(n)=k|x(n),\theta)=\frac{P(x(n)|z(n)=k,\theta)\quad P(z(n)=k|\theta)}{\sum_{j=0}^{1} p(x(n)|z(n)=j,\theta)\ P(z(n)=j|\theta)}$$

$$P(z(n)=k|x(n),\theta)=\frac{[\prod_i P(x_i(n)|z(n)=k,\theta)]\quad P(z(n)=k|\theta)}{\sum_{j=0}^{1} \prod_i P(x_i(n)|z(n)=j,\theta)\ P(z(n)=j|\theta)}$$

$$\boxed{P(z(n)=k|x(n),\theta)=\frac{[\prod_i N(x_i(n)|\mu_{k,i},\sigma)]\quad (\pi^k(1-\pi)^{(1-k)})}{\sum_{j=0}^{1}[\prod_i N(x_i(n)|\mu_{j,i},\sigma)]\quad (\pi^j(1-\pi)^{(1-j)})}}$$

EM — M Step



- First consider update for π

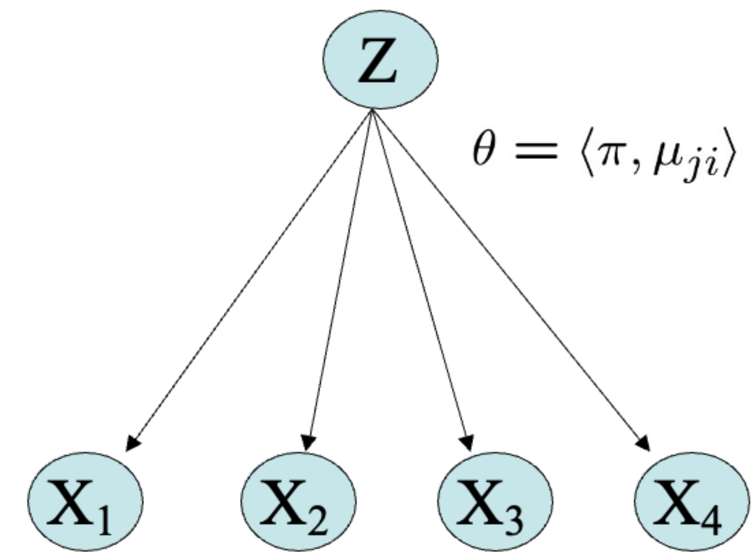
$$Q(\theta'|\theta) = E_{Z|X,\theta}[\log P(X,Z|\theta')] = E[\log P(X|Z,\theta') + \log P(Z|\theta')]$$

$$\pi \leftarrow \arg\max_{\pi'} E_{Z|X,\theta}[\log P(Z|\pi')]$$

$$E_{Z|X,\theta}\left[\log P(Z|\pi')\right] =$$

$$\frac{\partial E_{Z|X,\theta}[\log P(Z|\pi')]}{\partial \pi'} =$$

EM — M Step



- First consider update for π

$$Q(\theta'|\theta) = E_{Z|X,\theta}[\log P(X,Z|\theta')] = E[\log P(X|Z,\theta') + \log P(Z|\theta')]$$

$$\pi \leftarrow \arg\max_{\pi'} E_{Z|X,\theta}[\log P(Z|\pi')]$$

$$E_{Z|X,\theta}\left[\log P(Z|\pi')\right] = E_{Z|X,\theta}\left[\log\left(\pi'^{\sum_n z(n)}(1-\pi')^{\sum_n (1-z(n))}\right)\right]$$

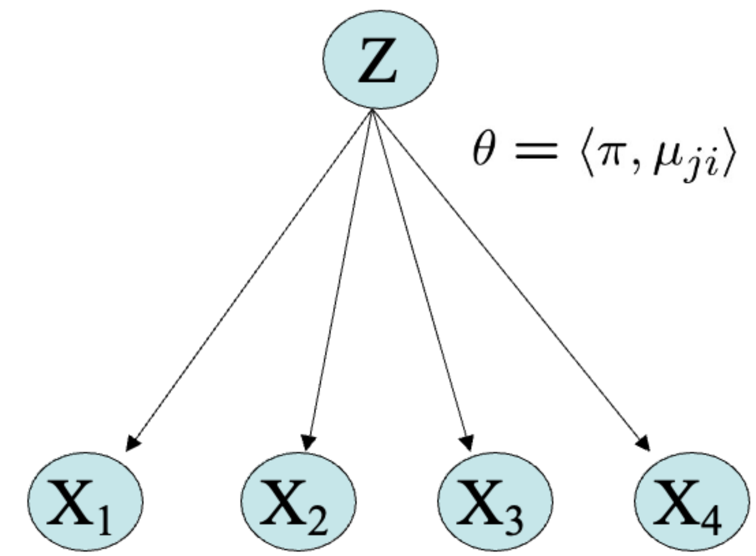
$$= E_{Z|X,\theta}\left[\left(\sum_n z(n)\right)\log \pi' + \left(\sum_n (1-z(n))\right)\log(1-\pi')\right]$$

$$= \left(\sum_n E_{Z|X,\theta}[z(n)]\right)\log \pi' + \left(\sum_n E_{Z|X,\theta}[(1-z(n))]\right)\log(1-\pi')$$

$$\frac{\partial E_{Z|X,\theta}[\log P(Z|\pi')]}{\partial \pi'} = \left(\sum_n E_{Z|X,\theta}[z(n)]\right)\frac{1}{\pi'} + \left(\sum_n E_{Z|X,\theta}[(1-z(n))]\right)\frac{(-1)}{1-\pi'}$$

$$\boxed{\pi \leftarrow \frac{\sum_{n=1}^N E[z(n)]}{\left(\sum_{n=1}^N E[z(n)]\right) + \left(\sum_{n=1}^N (1 - E[z(n)])\right)} = \frac{1}{N}\sum_{n=1}^N E[z(n)]}$$

EM — M Step



- Now consider update for μ_{ji}

$$Q(\theta'|\theta) = E_{Z|X,\theta}[\log P(X,Z|\theta')] = E[\log P(X|Z,\theta') + \log P(Z|\theta')]$$

$$\mu_{ji} \leftarrow \arg\max_{\mu'_{ji}} E_{Z|X,\theta}[\log P(X|Z,\theta')]$$

$$\ldots \quad \ldots \quad \ldots$$

$$\boxed{\mu_{ji} \leftarrow \frac{\sum_{n=1}^{N} P(z(n)=j|x(n),\theta) \quad x_i(n)}{\sum_{n=1}^{N} P(z(n)=j|x(n),\theta)}}$$

Compare above to MLE if Z were observable:

$$\mu_{ji} \leftarrow \frac{\sum_{n=1}^{N} \delta(z(n)=j) \quad x_i(n)}{\sum_{n=1}^{N} \delta(z(n)=j)}$$

EM — putting it together

- Given observed variables X, unobserved Z,
  - define $Q(\theta'|\theta) = E_{Z|X,\theta}[\log P(X, Z|\theta')]$ where $\theta = \langle \pi, \mu_{ji} \rangle$

- Iterate until convergence:
  - E Step:
    - For each observed example X(n), calculate P(Z(n)|X(n),θ)

$$P(z(n) = k \mid x(n), \theta) = \frac{[\prod_i N(x_i(n)|\mu_{k,i}, \sigma)] \quad (\pi^k (1-\pi)^{(1-k)})}{\sum_{j=0}^{1} [\prod_i N(x_i(n)|\mu_{j,i}, \sigma)] \quad (\pi^j (1-\pi)^{(1-j)}))}$$

  - M Step:
    - Update current θ by $\theta \leftarrow \arg\max_{\theta'} Q(\theta'|\theta)$

$$\pi \leftarrow \frac{1}{N} \sum_{n=1}^{N} E[z(n)] \qquad \mu_{ji} \leftarrow \frac{\sum_{n=1}^{N} P(z(n) = j|x(n), \theta) \quad x_i(n)}{\sum_{n=1}^{N} P(z(n) = j|x(n), \theta)}$$

Demo Time 🙂

https://lukapopijac.github.io/gaussian-mixture-model/

What you should know

- For learning from partly observed data
- Instead of MLE: $\theta \leftarrow \arg\max_{\theta} \log P(X, Z|\theta)$
- EM estimates: $\theta \leftarrow \arg\max_{\theta} E_{Z|X,\theta}[\log P(X, Z|\theta)]$
  - where X is observed part of the data, and Z is (partly) unobserved
- EM for training Bayes Nets
- Can also develop MAP version instead of EM
  - Write out expression for $E_{Z|X,\theta}[\log P(X, Z|\theta)]$
  - E step: for each training example X^k, calculate $P(Z^k | X^k, \theta)$
  - M step: choose new to maximize $E_{Z|X,\theta}[\log P(X, Z|\theta)]$

Bayes Net—summary

- Representation
  - Bayes Net represent joint distributions as a DAG + conditional distributions
  - Let's us calibrate conditional independence assumptions
- Inference
  - NP-hard in general
  - For some graph, closed form inference possible
  - Approximate methods exists too, e.g., Monte Carlo methods,…
- Learning
  - Easy for known graph, fully observed data (MLE, MAP etc.)
  - EM for partly observed data
  - Can handle the extreme case of completely unlabeled data