Advanced Machine Learning

Lecture 6: Mixture models fitting

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Content

Mixture Models Fitting

- Data-to-knowledge
  - Statistical model fitting $\rightarrow$ model learning
  - Feature extraction: behavior, shapes...
  - Data characterisation $\rightarrow$ Complex modelling
- Complex estimation problems, e.g. many parameters, non parametric estimation...
- Clustering / Classification: Modes $\simeq$ clusters / classes
- Dealing with missing (latent) data: unknown labels can be generalized to unobserved data...

How to fit a mixture model to data? Inference/ Learning

Today’s Lecture

1. The Gaussian Mixture Model
    1. Two component case
    2. Generalization

2. EM algorithm

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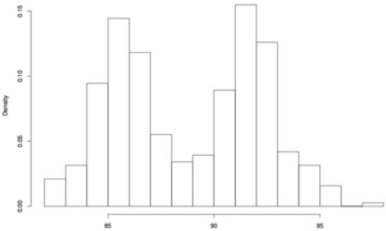
Gaussian Mixture Model

Example

Sizes of small animals coming from two different regions

Length	82	83	84	85	86	87	88	89
Observations	5	3	12	36	55	45	21	13

Length	90	91	92	93	94	95	96	98
Observations	15	34	59	48	16	12	6	1



Corresponding histogram

Whiteboard

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Gaussian Mixture Model: two component case

In our previous example...

There seems to be two separate underlying regimes, so we model X as a mixture of two normal distributions:

$$
\begin{aligned}
Y_1 &\sim \mathcal{N}(\mu_1, \sigma_1^2) \\
Y_2 &\sim \mathcal{N}(\mu_2, \sigma_2^2) \\
X &= Z\,Y_1 + (1 - Z)\,Y_2
\end{aligned}
$$

where $Z \sim \mathcal{B}(1, p)$

- $P(Z = 1) = p$ and $P(Z = 0) = 1 - p$.
- The data *follows the first distribution / belongs to the first cluster* with a probability p.

$\rightarrow$ Generative representation: generate $Z \in \{0, 1\}$ with probability p, and then depending on the outcome, deliver either Y_1 or Y_2.

Gaussian Mixture Model : two components

- Generative model $P(z,x) = P(z)P(x|z)$
- The pdf over x is defined by marginalizing (summing out z)

$$f_X(x) = \sum_{k=1}^{2} P(Z=k)P(x|Z=k)$$

Denote $\phi_\theta(x)$ the Gaussian PDF with parameters $\theta = (\mu, \sigma^2)$:

$\rightarrow$ PDF for X:

$$f_X(x) = p\,\phi_{\theta_1}(x) + (1-p)\,\phi_{\theta_2}(x)$$

$\rightarrow$ log-likelihood for n observations $(X_1, \ldots, X_n)$

$$\ell(\theta; \mathbf{x}) = \sum_{i=1}^{n} \log\left(p\,\phi_{\theta_1}(x_i) + (1-p)\,\phi_{\theta_2}(x_i)\right)$$

How to estimate the unknown parameters p, θ_1, θ_2? MLE...

Gaussian Mixture Model: MLE

Maximizing $\ell(\theta; \mathbf{x})$ is difficult...

- $\theta = (p, \theta_1, \theta_2)$, 5 unknown parameters in the simplest case...
- The sum inside the log couples all the parameters of all the component Gaussian distributions of the mixture

Idea: consider unobserved latent variables $(Z_1, \ldots, Z_n)$ where Z_i is the latent class of X_i $\rightarrow$ Computing MLEs becomes trivial...

$$\ell(\theta; \mathbf{x}, \mathbf{z}) = \sum_{i=1}^{n} \left(z_i \log(\phi_{\theta_1}(x_i)) + (1 - z_i) \log(\phi_{\theta_2}(x_i))\right) + \sum_{i=1}^{n} \left(z_i \log(p) + (1 - z_i) \log(1 - p)\right)$$

where $\mathbf{x} = (x_1, \ldots, x_n)$ and $\mathbf{z} = (z_1, \ldots, z_n)$.

Gaussian Mixture Model: MLE

Maximizing $\ell(\theta; \mathbf{x})$ is difficult...

- $\theta = (p, \theta_1, \theta_2)$, 5 unknown parameters in the simplest case...
- The sum inside the log couples all the parameters of all the component Gaussian distributions of the mixture $\rightarrow$ **Unseparable!**

Idea: consider unobserved latent variables $(Z_1, \ldots, Z_n)$ where Z_i is the latent class of X_i $\rightarrow$ Computing MLEs becomes trivial...

$$\ell(\theta; \mathbf{x}, \mathbf{z}) = \sum_{i=1}^{n} \left(z_i \log(\phi_{\theta_1}(x_i)) + (1 - z_i) \log(\phi_{\theta_2}(x_i))\right) + \sum_{i=1}^{n} \left(z_i \log(p) + (1 - z_i) \log(1 - p)\right)$$

where $\mathbf{x} = (x_1, \ldots, x_n)$ and $\mathbf{z} = (z_1, \ldots, z_n)$. $\rightarrow$ **Separable!**

But Z is unknown in practice...

Gaussian Mixture Model : posterior inference

- Let's consider that the parameters are known
- A GMM with known parameters defines a joint distribution over (X_i, Z_i) $\rightarrow$ probabilistic/posterior inference

We infer the posterior over Z using Bayes' rule (*e.g., k=1*):

$$
\begin{aligned}
P(Z_i = 1|x_i) &= \frac{P(Z_i = 1)P(X_i|Z_i = 1)}{P(X_i)} \\
&= \frac{p_1\phi_{\theta_1}(x_i)}{p\phi_{\theta_1}(x_i) + (1-p)\phi_{\theta_2}(x_i)}
\end{aligned}
$$

Responsibility γ_i

The expected value of Z_i conditional to the observed data and known parameters

$$\gamma_i^k(\theta) = E[Z_i|\theta, \mathbf{x}] = P(Z_i = k|\theta, \mathbf{x})$$

Gaussian Mixture Model : EM algorithm

- Chicken and egg problem
- Use an iterative approach : alternately fix the parameters/the latent variables

Algorithm: Expectation-Maximization (EM)

- Random initialization of $\theta^{(0)}$
- Repeat until CV for $t = 0, 1, \ldots$
  (a) **E-Step:** Compute the responsibilities
  $$\hat{\gamma}_i = \frac{\hat{p}\,\phi_{\hat{\theta}_1}(x_i)}{\hat{p}\,\phi_{\hat{\theta}_1}(x_i) + (1-\hat{p})\,\phi_{\hat{\theta}_2}(x_i)}, \text{ for } i = 1, \ldots, n$$
  (b) **M-Step:** Compute the parameters...
  $$\hat{\mu}_1 = \frac{\sum_i \hat{\gamma}_i x_i}{\sum_i \hat{\gamma}_i}, \hat{\sigma}_1^2 = \frac{\sum_i \hat{\gamma}_i (x_i - \hat{\mu}_1)^2}{\sum_i \hat{\gamma}_i}, \ldots \text{ and } \hat{p} = \sum_i \hat{\gamma}_i / n.$$

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Mixture Model

Goal: Model the statistical behaviour of several populations, groups or classes...

- different objects x_i in an image containing N pixels
- population of animals: x_i corresponds to the size of the i^{th} animal, classes correspond to age/sex/origin (young, old, female, male)...

- n observations of i.i.d. random variables/vectors $(X_1, \ldots, X_n)$
- K different clusters containing n_k observations with $n = \sum_{k=1}^{K} n_k$
- p_k the probability of belonging to the k^{th} class and f_k the PDF of r.v. in this class.

PDF of a mixture

$$f(x) = \sum_{k=1}^{K} p_k \times f_k(x)$$

Gaussian Mixture Model: GMM

Gaussian Mixture Model

$$f(x) = \sum_{k=1}^{K} p_k \times \frac{1}{\sqrt{2\pi\sigma_k^2}} \exp\left(-\frac{(x-\mu_k)^2}{2\sigma_k^2}\right)$$

with $\sum_{k=1}^{K} p_k = 1$ and $\forall k \in \{1, \ldots, K\}, \mu_k \in \mathbb{R}, \sigma_k \in \mathbb{R}_+^*$.

Challenges

- Many unknown parameters $\theta = (p_k, \mu_k, \sigma_k)_{k=1,\ldots,K}$
- What about K ? Known, unknown ?

But useful for modelling a wide range of distributions!

GMMs: Examples

(a) $\frac{1}{5}\mathcal{N}(0,1) + \frac{1}{5}\mathcal{N}(1/2,(2/3)^2) + \frac{3}{5}\mathcal{N}(13/15,(5/9)^2)$,

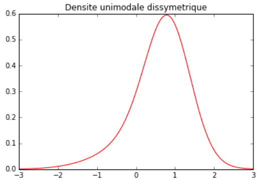
(b) $\sum_{k=0}^{7} \mathcal{N}(3((2/3)^k - 1),(2/3)^{2k})$

(c) $\frac{1}{2}\mathcal{N}(-1,(2/3)^2) + \frac{1}{2}\mathcal{N}(1,(2/3)^2)$

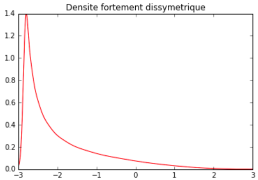
(d) $\frac{3}{4}\mathcal{N}(0,1) + \frac{1}{4}\mathcal{N}(3/2,(1/3)^2)$

(e) $\frac{9}{2}0\mathcal{N}(-6/5,(3/5)^2) + \frac{9}{2}0\mathcal{N}(6/5,(3/5)^2) + \frac{1}{1}0\mathcal{N}(0,(1/4)^2)$

(f) $\frac{1}{2}\mathcal{N}(0,1) + \sum_{k=-2}^{2} \frac{2^{1-k}}{31}\mathcal{N}(k+1/2,(2^{-k}/10)^2)$

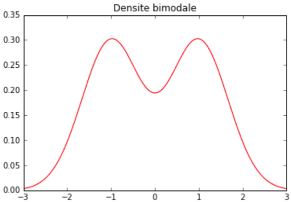


(a) Asymmetric unimodal PDF

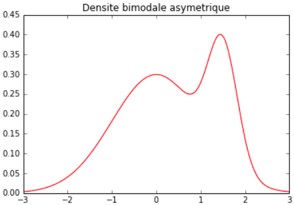


(b) Strongly asymmetric unimodal PDF

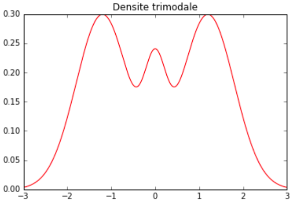
GMMs: Examples



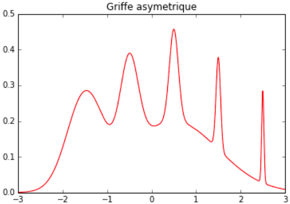
(c) Bimodal PDF



(d) Asymmetric bimodal PDF



(e) Tri-modal PDF



(f) More complex PDF

GMM: simulation

In order to simulate the mixture $f(x) = \sum_{k=1}^{K} p_k \times \frac{1}{\sqrt{2\pi\sigma_k^2}} \exp\left(-\frac{(x-\mu_k)^2}{2\sigma_k^2}\right)$, one needs to introduce a latent variable Z (or missing data) corresponding to the class of the variable X.

Now, the complete data $T = (X, Z)$ is defined by:

- Z follows a discrete distribution $(p_1, \dots, p_K)$ on $\{1, \dots, K\}$ such that $\forall k$, one has (Multinomial distribution)

$$P(Z = k) = p_k, \text{ with } \sum_k p_k = 1$$

- $\forall k \in \{1, \dots, K\}$, conditionally to $\{Z = k\}$, X has a PDF f_k:

$$\mathcal{L}(x|Z = k) = f_k(x)$$

$\rightarrow$ Goal: estimation of $\theta = (p_k, \mu_k, \sigma_k)_{k=1,\dots,K}$

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Reminders: Bayesian probabilities/statistics

For two events (or r. v. ...), one has:

- Conditional probabilities

$$P(A|B) = \frac{P(A \cap B)}{P(B)}$$

- Bayes rule

$$P(B|A) = \frac{P(A|B)\,P(B)}{P(A)}$$

- if $B_1, \ldots, B_n$ is a partition of Ω, i.e. $\bigcup_{i=1}^{n} B_i = \Omega$ and $\forall i \neq j, B_i \cap B_j = \emptyset$, then

$$P(A) = \sum_{i=1}^{n} P(A \cap B_i)$$

EM algorithm

Let us start by considering Z known

- we observe $(x_i, z_i)_{i=1,\ldots,n}$ instead of (only) $(x_i)_{i=1,\ldots,n}$
- this is the maximum-likelihood step $\rightarrow$ again trivial!

ML estimates of θ: K classes

Let the observations be $(x_i, z_i)_{i=1,\ldots,n}$, then $\forall k \in \{1, \ldots, K\}$, one has

$$\hat{p}_k = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{z_i=k} \tag{1}$$

$$\hat{\mu}_k = \frac{1}{n\,\hat{p}_k}\sum_{i|z_i=k} x_i \tag{2}$$

$$\hat{\sigma}_k^2 = \frac{1}{n\,\hat{p}_k}\sum_{i|z_i=k} (x_i - \hat{\mu}_k)^2 \tag{3}$$

EM algorithm

However one only observes $(x_1, \ldots, x_n)$ and again...

Maximizing $\ell(x_1, ..., x_n; \theta)$ is difficult

$$\ell_{obs}(x_1, \ldots, x_n; \theta) = \sum_{i=1}^{n} \log \left(\sum_{k=1}^{K} p_k \times f_k(x_i) \right)$$

where $\theta = (p_k, \mu_k, \sigma_k)_{k=1,\ldots,K}$

BUT

EM algorithm

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BUT one can make assumptions on the unobserved $(Z_1, \dots, Z_n)$

EM algorithm

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where $\theta = (p_k, \mu_k, \sigma_k)_{k=1,...,K}$

BUT one can make assumptions on the unobserved $(Z_1, \ldots, Z_n)$

For $\theta \in \Theta, x \in \mathbb{R}$ and $k \in \{1, \ldots, K\}$, one has

$$P_\theta (Z = k | X = x) = \frac{p_k \times f_k(x)}{\sum_{l=1}^{K} p_l \times f_l(x)} \tag{4}$$

$\rightarrow$ Intuition: thanks to some θ_{old}, one can assign a z_i to each x_i (4) and thanks to (1-3), one can compute a θ_{new}...

Whiteboard

General EM algorithm : variants

k-means

Hard assignment: Assign a class to each x_i according to

$$z_i = \arg\max_k P_{\theta_{old}}(Z = k | X_i = x_i)$$

SEM

Randomly assign a class to each x_i according to the distribution

$$P_{\theta_{old}}(Z = .|X_i = x_i)$$

More flexible!

N-SEM

Randomly assign N classes to each x_i

EM: Limit of N-SEM when $N \to \infty$ Very flexible and robust!

k-means

$\rightarrow$ One has to make very strong assumptions:

$$p_1 = \ldots = p_K = \frac{1}{K} \text{ and } \sigma_1 = \ldots = \sigma_K$$

$$\forall \theta, \forall x \in \mathbb{R} \quad \arg\max_k P_\theta \left(Z = k | X = x\right) = \arg\min_k |x - \mu_k|$$

k-means

- Randomly initialize $(z_1, \ldots, z_K)$
- Repeat until CV:
  - for $k \in \{1, \ldots, K\}$, $\mu_k = \frac{1}{n} \sum_{i=1}^{n} x_i \, \mathbb{1}_{z_i = k}$
  - for $i \in \{1, \ldots, n\}$, $z_i = \arg\min_k |x - \mu_k|$

Advantages / Drawbacks ...

Stochastic EM

→ General idea: Stochastic version of the k-means algorithm...

SEM

- Randomly initialize $(z_1, \ldots, z_K)$
- Repeat until CV:
  (a) Compute (MLE)

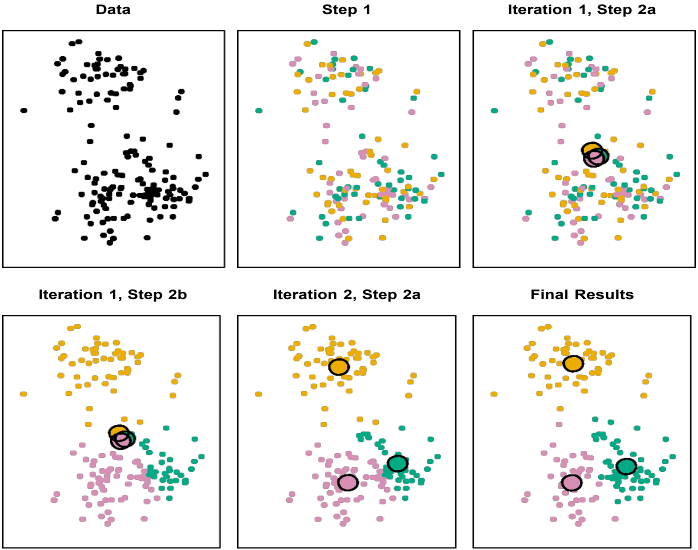
$$\hat{\theta} = \arg\max_{\theta} \ell_{obs}[(x_1, z_1), \ldots, (x_n, z_n); \theta]$$

  (b) for $i \in \{1, \ldots, n\}$, randomly choose z_i according to

$$P_{\hat{\theta}}(Z = .|X_i = x_i)$$

  given by Eq. (4).

Stochastic EM



Stochastic EM - N trials

N-SEM (1)

- Replicate the observations N times: $(x_1, \ldots, x_n) \to \left(x_i^{(j)}\right)_{1 \leq i \leq n, 1 \leq j \leq N}$
- Apply SEM algo to this new dataset.

N-SEM (2)

- Randomly initialize N classes $z_i^1, \ldots, z_i^N \in \{1, \ldots, K\}, \forall i$
- Repeat until CV
  (a) Compute (MLE)
  $$\hat{\theta} = \arg\max_{\theta} \ell_{obs}\left((x_i, z_i^1)_{i=1,\ldots,n} \cup \ldots \cup (x_i, z_i^N)_{i=1,\ldots,n}; \theta\right)$$
  (b) for $i \in \{1, \ldots, n\}$, randomly choose $z_i^1, \ldots, z_i^N$ (independently!) according to
  $$P_{\hat{\theta}}\left(Z = .|X_i = x_i\right)$$
  given by Eq. (4).

EM algorithm

→ General idea: N-SEM when $N \to +\infty$ ...

Given $(x_i)_{1\leq i\leq n}$ and associated classes for N trials $(z_i^k)_{1\leq i\leq n, 1\leq k\leq K}$:

$$\forall\theta, \ell_{obs}\left(\left(x_i, z_i^1\right)_{i=1,\ldots,n} \cup \ldots \cup \left(x_i, z_i^N\right)_{i=1,\ldots,n}; \theta\right) = \sum_{j=1}^N \ell_{obs}\left(\left(x_i, z_i^j\right)_{i=1,\ldots,n}; \theta\right)$$

Theorem [Part I]

Given the observations $(x_i)_{1\leq i\leq n}$ and $\theta_{old} \in \Theta$.

(a) Let $Z_1, ..., Z_n$ independent r.v. such that $Z_i \sim \mathcal{L}_{\theta_{old}}(Z|X = x_i)$. One has $\forall\theta = (p_k, \mu_k, \sigma_k)_{1\leq k\leq K} \in \Theta$,

$$E[\ell\left(\left(x_i, z_i\right)_{i=1,\ldots,n}; \theta\right)] = \sum_{i=1}^n \sum_{k=1}^K P_{\theta_{old}}(Z = k|X = x_i) \log\left(p_k \times f_k(x_i)\right)$$

where $P_{\theta_{old}}(Z = .|X = x_i)$ given by Eq. (4).

EM algorithm

Theorem [Part II] Given the observations $(x_i)_{1\le i\le n}$ and $\theta_{old} \in \Theta$,

(b) One has that $\arg\max_\theta E[\ell\left((x_i, z_i)_{i=1,\dots,n}\,; \theta\right)]$ is given by:

- Class probabilities: $\forall k = 1, \dots, K$,

$$p_k^{argmax} = \frac{1}{n}\sum_{i=1}^{n} P_{\theta_{old}}\left(Z = k | X = x_i\right)$$

- Class means: $\forall k = 1, \dots, K$,

$$\mu_k^{argmax} = \frac{1}{n\, p_k^{argmax}}\sum_{i=1}^{n} P_{\theta_{old}}\left(Z = k | X = x_i\right)\, x_i$$

- Class variances: $\forall k = 1, \dots, K$,

$$(\sigma_k^{argmax})^2 = \frac{1}{n\, p_k^{argmax}}\sum_{i=1}^{n} P_{\theta_{old}}\left(Z = k | X = x_i\right)\, (x_i - \mu_k^{argmax})^2$$

Expectation-Maximization algorithm

$\rightarrow$ So far, our theoretical algorithm looks like...

EM: Theory

- Randomly initialization of θ_0
- Repeat until CV for $t = 0, 1, \ldots$
  (a) **E-Step:** Compute

$$L_t(\theta) = E\left[\ell\left(\left(X_i, Z_i^t\right)_{i=1,\ldots,n}; \theta\right)\right] \; \left(Q(\theta, \theta_t) = E\left(l(\theta; \mathbf{t}) | \mathbf{x}, \theta_t\right)\right)$$

  where $Z_1^t, \ldots, Z_n^t$ are i.i.d. with $Z_i^t \sim \mathcal{L}_{\theta_t}(Z | X = x_i)$

  (b) **M-Step:** Maximize $L_t(\theta)$ to obtain $\theta_{t+1} = \arg\max_\theta L_t(\theta)$

- **E** for *Expectation*
- **M** for *Maximization*

Whiteboard

Whiteboard

A different view - *Maximization-Maximization*

- Consider the function $F(\theta, \mathbf{P}) = E_{\mathbf{P}}[l_0(\theta; \mathbf{t})] - E_{\mathbf{P}}[\log(\mathbf{P}(\mathbf{z}))]$
- $\mathbf{P}$ can be any distribution for the *latent* variables $\mathbf{z}$.
- Note that F evaluated at $\mathbf{P}(\mathbf{z}) = P(\mathbf{z}|\mathbf{x}, \theta)$ is the log-likelihood of the observed data.
- EM algo can be viewed as a joint maximization method for F over θ and $\mathbf{P}(\mathbf{z})$. Maximizer over $\mathbf{P}(\mathbf{z})$ for fixed θ can be shown to be $\mathbf{P}(\mathbf{z}) = P(\mathbf{z}|\mathbf{x}, \theta)$. (dist. computed at the E-step).
- M-step: Maximize $F(\theta, \mathbf{P})$ over θ for fixed $\mathbf{P}(\mathbf{z})$, $\iff$ maximizing $E_{\mathbf{P}}[l_0(\theta; \mathbf{t})|\mathbf{x}, \theta^*]$ (2nd term do not depend on θ).

Since $F(\theta, \mathbf{P})$ and the obs. data log-likelihood agree when $\mathbf{P}(\mathbf{z}) = P(\mathbf{z}|\mathbf{x}, \theta)$, maximization of the former accomplishes maximization of the latter.

EM algorithm: In practice

EM Algorithm

- Randomly initialization of θ_0
- Repeat until CV for $t = 0, 1, \ldots$
  (a) **E-Step:** Compute the matrix $(1 \leq i \leq n, 1 \leq k \leq K)$
  $$[P_{\theta_t}(Z = k | X = x_i)] = \left[\frac{p_k^t \times f_{k,t}(x_i)}{\sum_{l=1}^{K} p_l^t \times f_{l,t}(x_i)} \right]$$
  (b) **M-Step:** Compute θ_{t+1}, for all $k = 1, \ldots, K$,
  $$\hat{p}_k^{t+1} = \frac{1}{n} \sum_{i=1}^{n} P_{\theta_t}(Z = k | X = x_i), \tag{5}$$
  $$\hat{\mu}_k^{t+1} = \frac{1}{n\, \hat{p}_k^{t+1}} \sum_{i=1}^{n} x_i P_{\theta_t}(Z = k | X = x_i) \tag{6}$$
  $$\left(\hat{\sigma}_k^{t+1}\right)^2 = \frac{1}{n\, \hat{p}_k^{t+1}} \sum_{i=1}^{n} P_{\theta_t}(Z = k | X = x_i) \left(x_i - \hat{\mu}_k^{t+1}\right)^2 \tag{7}$$

EM example