EM Algorithm for Latent Variable Models

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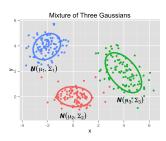
Gaussian Mixture Model: Review

Gaussian Mixture Model Parameters (k Components)

Cluster probabilities: $\pi = (\pi_1, ..., \pi_k)$

Cluster means: $\mu = (\mu_1, ..., \mu_k)$

Cluster covariance matrices: $\Sigma = (\Sigma_1, \dots \Sigma_k)$



GMM: The Joint and the Marginal Likelihood

Generative model description:

$$z \sim \mathsf{Categorical}(\pi_1, \dots, \pi_k)$$
 Cluster assignment $x \mid z \sim \mathcal{N}(\mu_z, \Sigma_z)$ Choose point from cluster distribution

Joint distribution (includes observed x and unobserved z):

$$p(x,z) = p(x | z)p(z)$$

= $\mathcal{N}(x | \mu_z, \Sigma_z) \pi_z$

Marginal distribution (just observed variable x):

$$p(x) = \sum_{z=1}^{k} p(x, z) = \sum_{z=1}^{k} \pi_z \mathcal{N}(x \mid \mu_z, \Sigma_z)$$

Maximum Likelihood for the Gaussian Mixture Model

- Find parameters that give observed data the highest likelihood.
- The model likelihood for $\mathcal{D} = \{x_1, \dots, x_n\}$ is

$$p(\mathcal{D}) = \prod_{i=1}^{n} p(x_i) = \prod_{i=1}^{n} \left[\sum_{z=1}^{k} \pi_z \mathcal{N}(x_i \mid \mu_z, \Sigma_z) \right].$$

The log-likelihood objective function:

$$J(\pi, \mu, \Sigma) = \sum_{i=1}^{n} \log \left[\sum_{z=1}^{k} \pi_{z} \mathcal{N}(x_{i} | \mu_{z}, \Sigma_{z}) \right]$$

• MLE is $\left(\hat{\pi},\hat{\mu},\hat{\Sigma}\right) = \arg\max_{\pi,\mu,\Sigma} J(\pi,\mu,\Sigma)$. EM algorithm to find it...

The EM Algorithm for GMM

Cluster Probabilities and Expected Cluster Sizes

• Probability that observed value x_i comes from cluster c:

$$\gamma_i^c := \mathbb{P}(z_i = c \mid x_i).$$

- The vector $(\gamma_i^1, \dots, \gamma_i^k)$ gives the **soft cluster assignments** for x_i .
- Let n_c be the expected number of points in cluster c:

$$n_{c} = \mathbb{E}\left[\sum_{i} 1(z_{i} = c) \mid x_{1}, \dots, x_{n}\right]$$
$$= \sum_{i} \mathbb{P}(z_{i} = c \mid x_{i})$$
$$= \sum_{i=1}^{n} \gamma_{i}^{c}$$

EM Algorithm for GMM

- **1** Initialize parameters μ , Σ , π .
- (2) "E step". Evaluate the **responsibilities** using current parameters:

$$\gamma_i^j = \mathbb{P}(z_i = j \mid x_i) = \frac{\pi_j \mathcal{N}(x_i \mid \mu_j, \Sigma_j)}{\sum_{c=1}^k \pi_c \mathcal{N}(x_i \mid \mu_c, \Sigma_c)},$$

for i = 1, ..., n and j = 1, ..., k.

(3) "M step". Re-estimate the parameters using responsibilities:

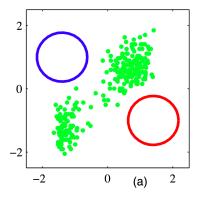
$$\mu_c^{\text{new}} = \frac{1}{n_c} \sum_{i=1}^n \gamma_i^c x_i$$

$$\Sigma_c^{\text{new}} = \frac{1}{n_c} \sum_{i=1}^n \gamma_i^c (x_i - \mu_{\text{MLE}}) (x_i - \mu_{\text{MLE}})^T$$

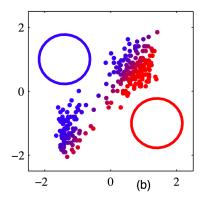
$$\pi_c^{\text{new}} = \frac{n_c}{n_c},$$

Repeat from Step 2, until log-likelihood converges.

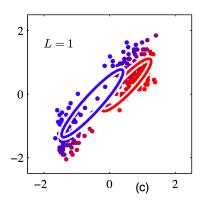
Initialization



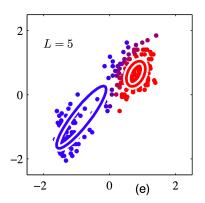
• First soft assignment:



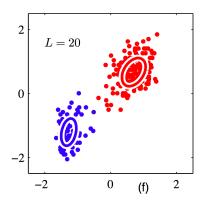
• First soft assignment:



After 5 rounds of EM:



After 20 rounds of EM:



Relation to K-Means

- EM for GMM seems a little like k-means.
- In fact, there is a precise correspondence.
- First, fix each cluster covariance matrix to be $\sigma^2 I$.
- As we take $\sigma^2 \to 0$, the update equations converge to doing *k*-means.
- If you do a quick experiment yourself, you'll find
 - Soft assignments converge to hard assignments.
 - Has to do with the tail behavior (exponential decay) of Gaussian.

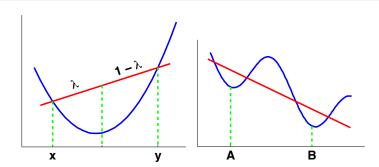
Math Prerequisites

Convex and Concave Functions

Definition

A function $f : \mathbb{R}^n \to \mathbb{R}$ is **convex** if for all $x, y \in \mathbb{R}^n$ and $0 \le \theta \le 1$, we have

$$f(\theta x + (1-\theta)y) \le \theta f(x) + (1-\theta)f(y).$$



Jensen's Inequality

Theorem (Jensen's Inequality)

If $f : R \to R$ is a **convex** function, and x is a random variable, then

$$\mathbb{E}f(x) \geqslant f(\mathbb{E}x).$$

Moreover, if f is **strictly convex**, then equality implies that $x = \mathbb{E}x$ with probability 1 (i.e. x is a constant).

• e.g. $f(x) = x^2$ is convex. So $\mathbb{E}x^2 \geqslant (\mathbb{E}x)^2$. Thus

$$Var x = \mathbb{E} x^2 - (\mathbb{E} x)^2 \geqslant 0.$$

Kullback-Leibler Divergence

- Let p(x) and q(x) be probability mass functions (PMFs) on \mathfrak{X} .
- How can we measure how "different" p and q are?
- The Kullback-Leibler or "KL" Divergence is defined by

$$KL(p||q) = \sum_{x \in \mathcal{X}} p(x) \log \frac{p(x)}{q(x)}.$$

(Assumes
$$q(x) = 0$$
 implies $p(x) = 0$.)

Can also write this as

$$\mathrm{KL}(p\|q) = \mathbb{E}_{x \sim p} \log \frac{p(x)}{q(x)}.$$

Gibbs Inequality $(KL(p||q) \ge 0 \text{ and } KL(p||p) = 0)$

Theorem (Gibbs Inequality)

Let p(x) and q(x) be PMFs on \mathfrak{X} . Then

$$KL(p||q) \geqslant 0$$
,

with equality iff p(x) = q(x) for all $x \in X$.

- KL divergence measures the "distance" between distributions.
- Note:
 - KL divergence not a metric.
 - KL divergence is not symmetric.

Gibbs Inequality: Proof

$$\begin{split} \mathrm{KL}(\rho\|q) &= \mathbb{E}_{\rho}\left[-\log\left(\frac{q(x)}{\rho(x)}\right)\right] \\ &\geqslant -\log\left[\mathbb{E}_{\rho}\left(\frac{q(x)}{\rho(x)}\right)\right] \quad \text{(Jensen's)} \\ &= -\log\left[\sum_{\{x\mid \rho(x)>0\}} p(x)\frac{q(x)}{\rho(x)}\right] \\ &= -\log\left[\sum_{x\in\mathcal{X}} q(x)\right] \\ &= -\log 1 = 0. \end{split}$$

• Since $-\log$ is strictly convex, we have strict equality iff q(x)/p(x) is a constant, which implies q=p .

EM Algorithm for Latent Variable Models

General Latent Variable Model

- Two sets of random variables: z and x.
- z consists of unobserved hidden variables.
- x consists of observed variables.
- Joint probability model parameterized by $\theta \in \Theta$:

$$p(x,z \mid \theta)$$

Notation abuse

Notation $p(x, z \mid \theta)$ suggests a Bayesian setting, in which θ is a r.v. However we are **not** assuming a Bayesian setting. $p(x, z \mid \theta)$ is just easier to read than $p_{\theta}(x, z)$, once θ gets more complicated.

Complete and Incomplete Data

- An observation of x is called an incomplete data set.
- An observation (x, z) is called a **complete data set**.
 - We never have a complete data set for latent variable models.
 - But it's a useful construct.
- Suppose we have an incomplete data set $\mathcal{D} = (x_1, \dots, x_n)$.
- To simplify notation, take x to represent the entire dataset

$$x=(x_1,\ldots,x_n)$$
,

and Z to represent the corresponding unobserved variables

$$z = (z_1, \ldots, z_n)$$
.

The EM Algorithm Key Idea

Marginal log-likelihood is hard to optimize:

$$\max_{\theta} \log \left\{ \sum_{z} p(x, z \mid \theta) \right\}$$

Assume that complete data log-likelihood would be easy to optimize:

$$\max_{\theta} \log p(x, z \mid \theta)$$

- What if we had a **distribution** q(z) for the latent variables z?
- Then maximize the expected complete data log-likelihood:

$$\max_{\theta} \sum_{z} q(z) \log p(x, z \mid \theta)$$

EM assumes this maximization is feasible.

Lower Bound for Likelihood

• Let q(z) be any PMF on \mathbb{Z} , the support of Z:

$$\log p(x \mid \theta) = \log \left[\sum_{z} p(x, z \mid \theta) \right]$$

$$= \log \left[\sum_{z} q(z) \left(\frac{p(x, z \mid \theta)}{q(z)} \right) \right] \quad \text{(log of an expectation)}$$

$$\geq \sum_{z} q(z) \log \left(\frac{p(x, z \mid \theta)}{q(z)} \right) \quad \text{(expectation of log)}$$

$$=: \mathcal{L}(q, \theta).$$

• The inequality is by Jensen's, by concavity of the log.

This is the key step for "variational methods".

Lower Bound and Expected Complete Log-Likelihood

• Consider maximizing the lower bound $\mathcal{L}(q, \theta)$:

$$\mathcal{L}(q,\theta) = \sum_{z} q(z) \log \left(\frac{p(x,z \mid \theta)}{q(z)} \right)$$

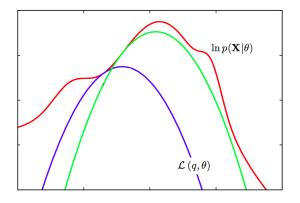
$$= \sum_{z} q(z) \log p(x,z \mid \theta) - \sum_{z} q(z) \log q(z)$$

$$\mathbb{E}[\text{complete data log-likelihood}] \quad \text{no } \theta \text{ here}$$

• Maximizing $\mathcal{L}(q, \theta)$ equivalent to maximizing $\mathbb{E}[\text{complete data log-likelihood}].$

A Family of Lower Bounds

- Each q gives a different lower bound: $\log p(x \mid \theta) \geqslant \mathcal{L}(q, \theta)$
- Two lower bounds, as functions of θ :



From Bishop's Pattern recognition and machine learning, Figure 9.14.

EM: Big Picture Idea

• The following inequality holds for all θ and q:

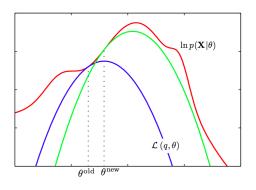
$$\log p(x \mid \theta) \geqslant \mathcal{L}(q, \theta).$$

- We want to find θ that maximizes $\log p(x \mid \theta)$.
- $\log p(x \mid \theta)$ is hard to maximize directly.
- Two step version of the EM algorithm:
 - **1** We vary q and θ , searching for the biggest $\mathcal{L}(q,\theta)$ we can find.
 - ② Final result is $\hat{\theta}$ corresponding to the largest $\mathcal{L}(q, \theta)$ we found.
- Often this is a local maximum of the likelihood.
- One question left: How to choose the sequence of q's and θ 's we try?

EM: Coordinate Ascent on Lower Bound

- Choose sequence of q's and θ 's by "coordinate ascent".
- EM Algorithm (high level):
 - **1** Choose initial θ^{old} .
 - 2 Let $q^* = \arg\max_{q} \mathcal{L}(q, \theta^{\text{old}})$
 - 3 Let $\theta^{\text{new}} = \arg \max_{\theta} \mathcal{L}(q^*, \theta^{\text{old}})$.
 - 4 Go to step 2, until converged.
- Will show: $p(x \mid \theta^{new}) \ge p(x \mid \theta^{old})$
- ullet Get sequence of θ 's with monotonically increasing likelihood.

EM: Coordinate Ascent on Lower Bound



- Start at θ^{old} .
- ② Find q giving best lower bound at $\theta^{\text{old}} \Longrightarrow \mathcal{L}(q,\theta)$.

From Bishop's Pattern recognition and machine learning, Figure 9.14.

The Lower Bound

Let's investigate the lower bound:

$$\begin{split} \mathcal{L}(q,\theta) &= \sum_{z} q(z) \log \left(\frac{p(x,z \mid \theta)}{q(z)} \right) \\ &= \sum_{z} q(z) \log \left(\frac{p(z \mid x,\theta) p(x \mid \theta)}{q(z)} \right) \\ &= \sum_{z} q(z) \log \left(\frac{p(z \mid x,\theta)}{q(z)} \right) + \sum_{z} q(z) \log p(x \mid \theta) \\ &= -\mathrm{KL}[q(z), p(z \mid x,\theta)] + \log p(x \mid \theta) \end{split}$$

• Amazing! We get back an equality for the marginal likelihood:

$$\log p(x \mid \theta) = \mathcal{L}(q, \theta) + \text{KL}[q(z), p(z \mid x, \theta)]$$

The Best Lower Bound

Find q maximizing

$$\mathcal{L}(q, \theta^{\mathsf{old}}) = -\mathrm{KL}[q(z), p(z \mid x, \theta^{\mathsf{old}})] + \underbrace{\log p(x \mid \theta^{\mathsf{old}})}_{\mathsf{no} \ q \ \mathsf{here}}$$

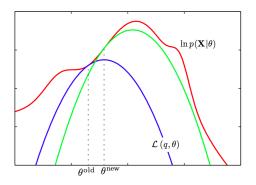
- Recall $KL(p||q) \ge 0$, and KL(p||p) = 0.
- Best q is $q^*(z) = p(z \mid x, \theta^{\text{old}})$. Proof:

$$\mathcal{L}(q^*, \theta^{\text{old}}) = -\underbrace{\text{KL}[p(z \mid x, \theta^{\text{old}}), p(z \mid x, \theta^{\text{old}})]}_{=0} + \log p(x \mid \theta^{\text{old}})$$

Summary:

$$\begin{array}{lll} \log p(x \mid \theta^{\mathrm{old}}) & = & \mathcal{L}(q^*, \theta^{\mathrm{old}}) & (\mathsf{tangent} \ \mathsf{at} \ \theta^{\mathrm{old}}). \\ \log p(x \mid \theta) & \geqslant & \mathcal{L}(q^*, \theta) & \forall \theta \end{array}$$

Tight lower bound for any chosen θ



Fix any θ' and take $q'(z) = p(z \mid x, \theta')$. Then

- **1** log $p(x | \theta)$ ≥ $\mathcal{L}(q', \theta) \forall \theta$. [Global lower bound].
- ② $\log p(x \mid \theta') = \mathcal{L}(q', \theta')$. [Lower bound is **tight** at θ' .]

From Bishop's Pattern recognition and machine learning, Figure 9.14.

General EM Algorithm

- Choose initial θ^{old} .
- Expectation Step
 - Let $q^*(z) = p(z \mid x, \theta^{\text{old}})$. $[q^* \text{ gives best lower bound at } \theta^{\text{old}}]$
 - Let

$$J(\theta) := \mathcal{L}(q^*, \theta) = \sum_{z} q^*(z) \log \left(\frac{p(x, z \mid \theta)}{q^*(z)} \right)$$

- Note that $J(\theta)$ is an **expectation** w.r.t. $z \sim q^*(z)$.
- Maximization Step

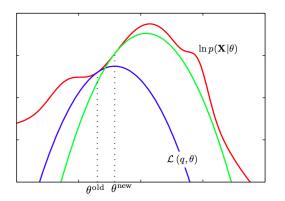
$$\theta^{\text{new}} = \underset{\theta}{\text{arg max}} J(\theta).$$

[Equivalent to maximizing expected complete log-likelihood.]

Go to step 2, until converged.

EM Monotonically Increases Likelihood

EM Gives Monotonically Increasing Likelihood: By Picture



EM Gives Monotonically Increasing Likelihood: By Math

- Start at θ^{old} .
- ② Choose $q^*(z) = \arg\max_q \mathcal{L}(q, \theta^{\text{old}})$. We've shown

$$\log p(x \mid \theta^{\text{old}}) = \mathcal{L}(q^*, \theta^{\text{old}})$$

 $\textbf{3} \ \, \mathsf{Choose} \,\, \theta^{\mathsf{new}} = \mathrm{arg} \, \mathsf{max}_{\theta} \, \mathcal{L}(q^*, \theta^{\mathsf{old}}). \,\, \mathsf{So} \,\,$

$$\mathcal{L}(q^*, \theta^{\mathsf{new}}) \geqslant \mathcal{L}(q^*, \theta^{\mathsf{old}}).$$

Putting it together, we get

$$\begin{array}{ll} \log p(x \,|\: \theta^{\mathsf{new}}) & \geqslant & \mathcal{L}(q^*, \theta^{\mathsf{new}}) & \mathcal{L} \text{ is a lower bound} \\ & \geqslant & \mathcal{L}(q^*, \theta^{\mathsf{old}}) & \text{By definition of } \theta^{\mathsf{new}} \\ & = & \log p(x \,|\: \theta^{\mathsf{old}}) & \text{Bound is tight at } \theta^{\mathsf{old}}. \end{array}$$

Suppose We Maximize the Lower Bound...

• Suppose we have found a global maximum of $\mathcal{L}(q, \theta)$:

$$L(q^*, \theta^*) \geqslant L(q, \theta) \forall q, \theta,$$

where of course

$$q^*(z) = p(z \mid x, \theta^*).$$

- Claim: θ^* is a global maximum of $\log p(x \mid \theta^*)$.
- Proof: For any θ' , we showed that for $q'(z) = p(z \mid x, \theta')$ we have

$$\log p(x \mid \theta') = \mathcal{L}(q', \theta') + \text{KL}[q', p(z \mid x, \theta')]$$

$$= \mathcal{L}(q', \theta')$$

$$\leq \mathcal{L}(q^*, \theta^*)$$

$$= \log p(x \mid \theta^*)$$

Convergence of EM

- Let θ_n be value of EM algorithm after n steps.
- Define "transition function" $M(\cdot)$ such that $\theta_{n+1} = M(\theta_n)$.
- Suppose log-likelihood function $\ell(\theta) = \log p(x \mid \theta)$ is differentiable.
- Let S be the set of stationary points of $\ell(\theta)$. (i.e. $\nabla_{\theta}\ell(\theta) = 0$)

Theorem

Under mild regularity conditions^a, for any starting point θ_0 ,

- $\lim_{n\to\infty}\theta_n=\theta^*$ for some stationary point $\theta^*\in S$ and
- θ^* is a fixed point of the EM algorithm, i.e. $M(\theta^*) = \theta^*$. Moreover,
- $\ell(\theta_n)$ strictly increases to $\ell(\theta^*)$ as $n \to \infty$, unless $\theta_n \equiv \theta^*$.

http://www3.stat.sinica.edu.tw/statistica/oldpdf/a15n316.pdf

^aFor details, see "Parameter Convergence for EM and MM Algorithms" by Florin Vaida in *Statistica Sinica* (2005).

Variations on EM

EM Gives Us Two New Problems

• The "E" Step: Computing

$$J(\theta) := \mathcal{L}(q^*, \theta) = \sum_{z} q^*(z) \log \left(\frac{p(x, z \mid \theta)}{q^*(z)} \right)$$

• The "M" Step: Computing

$$\theta^{\mathsf{new}} = \underset{\alpha}{\mathsf{arg}} \max_{\alpha} J(\theta).$$

• Either of these can be too hard to do in practice.

Generalized EM (GEM)

- Addresses the problem of a difficult "M" step.
- Rather than finding

$$\theta^{\text{new}} = \underset{\theta}{\text{arg max}} J(\theta),$$

find any θ^{new} for which

$$J(\theta^{\text{new}}) > J(\theta^{\text{old}}).$$

- Can use a standard nonlinear optimization strategy
 - e.g. take a gradient step on J.
- We still get monotonically increasing likelihood.

EM and More General Variational Methods

- Suppose "E" step is difficult:
 - Hard to take expectation w.r.t. $q^*(z) = p(z \mid x, \theta^{\text{old}})$.
- Solution: Restrict to distributions Q that are easy to work with.
- Lower bound now looser:

$$q^* = \arg\min_{q \in \mathcal{Q}} \mathrm{KL}[q(z), p(z \mid x, \theta^{\mathrm{old}})]$$

EM in Bayesian Setting

- Suppose we have a prior $p(\theta)$.
- Want to find MAP estimate: $\hat{\theta}_{MAP} = \arg \max_{\theta} p(\theta \mid x)$:

$$p(\theta \mid x) = p(x \mid \theta)p(\theta)/p(x)$$

$$\log p(\theta \mid x) = \log p(x \mid \theta) + \log p(\theta) - \log p(x)$$

.

• Still can use our lower bound on $\log p(x, \theta)$.

$$J(\theta) := \mathcal{L}(q^*, \theta) = \sum_{z} q^*(z) \log \left(\frac{p(x, z \mid \theta)}{q^*(z)} \right)$$

Maximization step becomes

$$\theta^{\text{new}} = \underset{\alpha}{\operatorname{arg\,max}} [J(\theta) + \log p(\theta)]$$

• Homework: Convince yourself our lower bound is still tight at θ .

Homework: Gaussian Mixture Model (Hints)

Homework: Gaussian Mixture Model (Hints)

Homework: Derive EM for GMM from General EM Algorithm

- Subsequent slides may help set things up.
- Key skills:
 - MLE for multivariate Gaussian distributions.
 - Lagrange multipliers

Gaussian Mixture Model (k Components)

GMM Parameters

Cluster probabilities:
$$\pi = (\pi_1, ..., \pi_k)$$

Cluster means:
$$\mu = (\mu_1, ..., \mu_k)$$

Cluster covariance matrices:
$$\Sigma = (\Sigma_1, \dots \Sigma_k)$$

- Let $\theta = (\pi, \mu, \Sigma)$.
- Marginal log-likelihood

$$\log p(x \mid \theta) = \log \left\{ \sum_{z=1}^{k} \pi_z \mathcal{N}(x \mid \mu_z, \Sigma_z) \right\}$$

$q^*(z)$ are "Soft Assignments"

- Suppose we observe n points: $X = (x_1, ..., x_n) \in \mathbb{R}^{n \times d}$.
- Let $z_1, \ldots, z_n \in \{1, \ldots, k\}$ be corresponding hidden variables.
- Optimal distribution q* is:

$$q^*(z) = p(z \mid x, \theta).$$

• Convenient to define the conditional distribution for z_i given x_i as

$$\gamma_i^j := p(z = j \mid x_i)
= \frac{\pi_j \mathcal{N}(x_i \mid \mu_j, \Sigma_j)}{\sum_{c=1}^k \pi_c \mathcal{N}(x_i \mid \mu_c, \Sigma_c)}$$

Expectation Step

• The complete log-likelihood is

$$\log p(x, z \mid \theta) = \sum_{i=1}^{n} \log [\pi_z \mathcal{N}(x_i \mid \mu_z, \Sigma_z)]$$

$$= \sum_{i=1}^{n} \left(\log \pi_z + \underbrace{\log \mathcal{N}(x_i \mid \mu_z, \Sigma_z)}_{\text{simplifies nicely}} \right)$$

Take the expected complete log-likelihood w.r.t. q*:

$$J(\theta) = \sum_{z} q^{*}(z) \log p(x, z \mid \theta)$$
$$= \sum_{i=1}^{n} \sum_{j=1}^{k} \gamma_{i}^{j} [\log \pi_{j} + \log \mathcal{N}(x_{i} \mid \mu_{j}, \Sigma_{j})]$$

Maximization Step

• Find θ^* maximizing $J(\theta)$:

$$\begin{array}{lll} \boldsymbol{\mu}_{c}^{\text{new}} & = & \frac{1}{n_{c}} \sum_{i=1}^{n} \boldsymbol{\gamma}_{i}^{c} \boldsymbol{x}_{i} \\ \\ \boldsymbol{\Sigma}_{c}^{\text{new}} & = & \frac{1}{n_{c}} \sum_{i=1}^{n} \boldsymbol{\gamma}_{i}^{c} \left(\boldsymbol{x}_{i} - \boldsymbol{\mu}_{\text{MLE}} \right) \left(\boldsymbol{x}_{i} - \boldsymbol{\mu}_{\text{MLE}} \right)^{T} \\ \\ \boldsymbol{\pi}_{c}^{\text{new}} & = & \frac{n_{c}}{n}, \end{array}$$

for each $c = 1, \ldots, k$.