Deep Generative Models: Variational Inference

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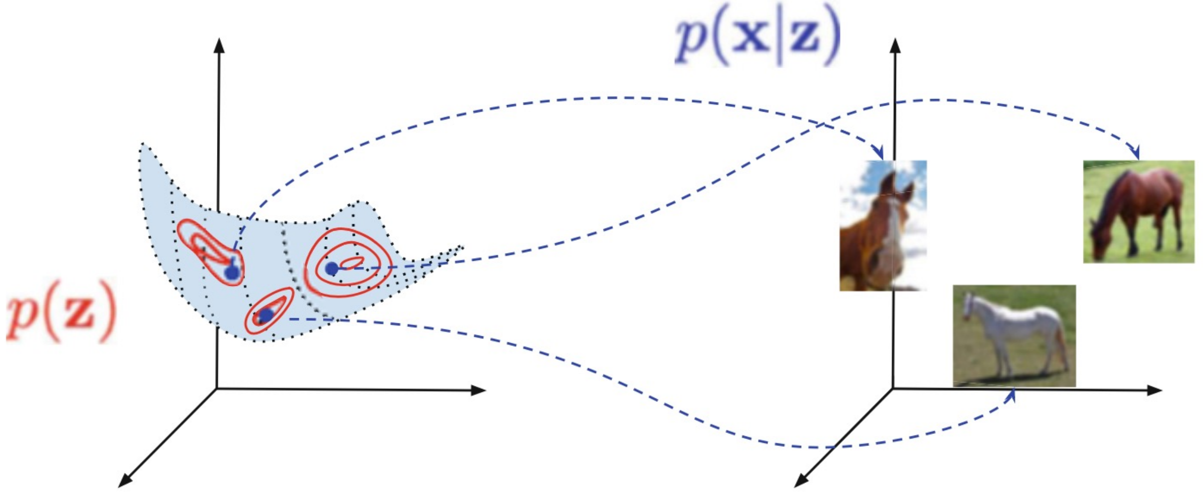
Latent Variable Models

- X = observed variable
- Z = latent variable

- $\mathbf{z} \sim p(\mathbf{z})$
- $\mathbf{x} \sim p(\mathbf{x}|\mathbf{z})$



A latent variable model and a generative process. Note the low-dimensional manifold (here 2D) embedded in the high-dimensional space (here 3D)

- Factorization of the joint model

$$p(\boldsymbol{x}, \boldsymbol{z}) = p(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})$$

- Marginalization of the model

$$p(\boldsymbol{x}) = \int p(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})d\boldsymbol{z}$$

Probabilistic Principal Component Analysis (PPCA)

- Let $\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{z}|\boldsymbol{0}, \boldsymbol{I})$ and $\boldsymbol{\varepsilon} \sim \mathcal{N}(\boldsymbol{\varepsilon}|\boldsymbol{0}, \sigma^2\boldsymbol{I})$ be independent.
- In PPCA, the dependency between $\boldsymbol{x} \in \mathbb{R}^D$ and $\boldsymbol{z} \in \mathbb{R}^d$, $d \ll D$, is defined by a linear Gaussian additive model

$$\boldsymbol{x} = \boldsymbol{W}\boldsymbol{z} + \boldsymbol{b} + \boldsymbol{\varepsilon}$$

- **Theorem.** Let $\boldsymbol{\mu}_N$ and $\boldsymbol{\Sigma}_{\mathrm{N}}$ be, respectively, the ML estimates for the mean and the covariance of the data. Let U_1 be the matrix with the top d eigenvectors of $\boldsymbol{\Sigma}_{\mathrm{N}}$, Λ_1 be the matrix with the corresponding top d eigenvalues, and λ_i be the ith largest eigenvalue of $\boldsymbol{\Sigma}_{\mathrm{N}}$. The ML estimates for the PPCA parameters $(\boldsymbol{b}, \boldsymbol{W}, \sigma)$ is given by

$$\boldsymbol{b} = \boldsymbol{\mu}_N,\ \boldsymbol{W} = U_1(\Lambda_1 - \sigma^2 I)^{1/2} R \ \text{ and } \ \sigma^2 = \frac{1}{D-d}\sum_{i=d+1}^{D} \lambda_i$$

where $R \in \mathbb{R}^{d \times d}$ is an arbitrary orthogonal matrix.

What about Latent Variable Models other than PPCA

- We would like to learn the parameters of the model via Maximum Likelihood.
- Since $\boldsymbol{z}$ is latent, we need to marginalize $p_\theta(\boldsymbol{x}) = \int p_\theta(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})d\boldsymbol{z}$, which gives

$$\max_\theta \sum_{i=1}^{N} \log p_\theta(x_i) = \max_\theta \sum_{i=1}^{N} \log \int p_\theta(x_i \mid z)p(z)dz$$

- For PPCA, we could compute $p(\boldsymbol{x})$ in closed form and solve for θ analytically.
- In general, we need many samples of z for each x_i to approximate the integral.

$$\max_\theta \sum_{i=1}^{N} \log \sum_j p_\theta\left(x_i \mid z_j \right)$$

- We address this challenge using **Variational Inference**, which we describe next.

Variational Inference

- **Old ML learning objective**: $\max_\theta \sum_{i=1}^N \log p_\theta(x_i) = \sum_{i=1}^N \log \int p_\theta(x_i \mid z) p(z) dz$
- **Theorem**: the log likelihood can be written as

$$\log p_\theta(x) = \max_{q(\cdot|x): q(\cdot|x) \geq 0, \int q(z|x) dz = 1} \int q(z|x) \log \frac{p_\theta(x,z)}{q(z|x)} dz.$$

and the maximizing distribution is given by $p_\theta(z|x)$

- **New ML learning objective**:

$$\max_\theta \max_{q(\cdot|x_i), \forall i} \sum_{i=1}^N \int q(z|x_i) \log \frac{p_\theta(x_i, z)}{q(z|x_i)} dz$$

- Before going through the derivation, what is the gain here?

Variational Inference

- **New ML learning objective**:

$$\max_{\theta} \max_{q(\cdot|x_i),\forall i} \sum_{i=1}^{N} \int q(z|x_i) \log \frac{p_\theta(x_i, z)}{q(z|x_i)} dz$$

- If $q(z|x)$ is easy to evaluate, we can alternate between optimizing w.r.t. θ with $q(z|x)$ fixed and vice versa, leading to the **Expectation Maximization** algorithm
  - Promise: in many cases we will get closed form solutions in each step

- Else, parameterize $q(\cdot\,|x_i)$ with a NN that takes x_i and outputs a distribution $q_\phi(\cdot\,|x_i)$, where ϕ contains the parameters of the NN, and find (θ, ϕ) via SGD
  - Promise: the output posterior typically has a small variance => Monte Carlo is a good approximation of the integral with respect to z

Variational Inference

- **New ML learning objective**:

$$\max_{\theta} \max_{q(\cdot|x_i),\forall i} \sum_{i=1}^{N} \int q(z|x_i) \log \frac{p_\theta(x_i, z)}{q(z|x_i)} dz$$

- We will use VI for many latent variable models
  - Mixtures of Gaussians (a.k.a. Gaussian Mixture Models) -> EM
  - Probabilistic Principal Component Analysis (PPCA) -> EM
  - Mixtures of PPCA -> EM
  - Variational Auto-Encoders (VAE) -> VI
  - Diffusion models -> VI
  - …

Variational Inference: Derivation

- Proof: Let $q(z|x)$ be the variational distribution. Observe that

$$\log p_\theta(x) = \int q(z|x)\log p_\theta(x)dz = \int q(z|x)\log\frac{p_\theta(x,z)}{p_\theta(z|x)}dz$$

$$= \int q(z|x)\log\frac{p_\theta(x,z)}{q(z|x)}\frac{q(z|x)}{p_\theta(z|x)}dz$$

$$= \underbrace{\boxed{\int q(z|x)\log\frac{p_\theta(x,z)}{q(z|x)}dz}}_{\text{Evidence Lower Bound (ELBO)}} + \underbrace{\boxed{\int q(z|x)\log\frac{q(z|x)}{p_\theta(z|x)}dz}}_{\mathrm{KL}[q(z|x)\,||\,p_\theta(z|x)]}$$

Thus, $\max\limits_{q(\cdot|x)}\int q(z|x)\log\frac{p_\theta(x,z)}{q(z|x)}dz = \max\limits_{q(\cdot|x)}\log p_\theta(x) - \mathrm{KL}[q(z|x)\,||\,p_\theta(z|x)]$

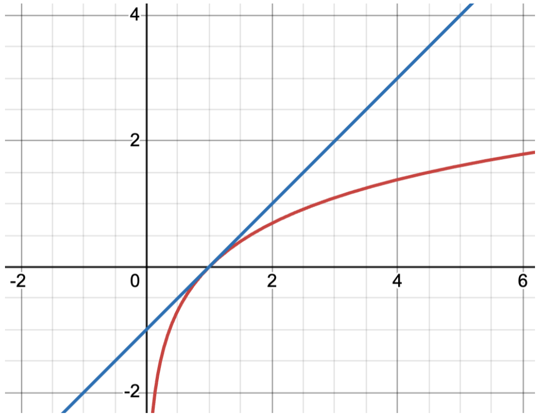
$$= \log p_\theta(x) - \min_{q(\cdot|x)}\mathrm{KL}[q(z|x)\,||\,p_\theta(z|x)] = \log p_\theta(x)$$

- The last step follows because the $KL(q\,||\,p) \geq 0$ and $KL(q\,||\,p) = 0$ iff $p = q$.

Variational Inference: Derivation

- Proposition: $\mathrm{KL}(q \,||\, p) \geq 0$. Further, $\mathrm{KL}(q \,||\, p) = 0$ if and only if $p = q$.

- Lemma: $\log y \leq y - 1$, equality holds if and only if $y = 1$
  - This is by the concavity of $\log(\cdot)$



- Proof of the Proposition: $\mathrm{KL}(q, p) = \int q(x) \log \frac{q(x)}{p(x)} dx$

$$= -\int q(x) \log \frac{p(x)}{q(x)} dx$$

$$\geq -\int q(x) \left(\frac{p(x)}{q(x)} - 1\right) dx \qquad \text{(by the lemma)}$$

$$= -\int p(x) - q(x)\, dx$$

$$= -1 + 1 = 0$$

Deep Generative Models: Expectation Maximization

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Variational Inference

- **Theorem**: the log likelihood criterion can be written in variational form as

$$\max_{\theta} \sum_{i=1}^{N} \log p_\theta(x_i) \equiv \max_{\theta} \max_{q(\cdot|x_i),\forall i} \sum_{i=1}^{N} \int q(z|x_i) \log \frac{p_\theta(x_i, z)}{q(z|x_i)} dz$$

and the maximizing distribution is given by $q^*(z \mid x) = p_\theta(z|x)$

- **Expectation Maximization:** If $q(z|x)$ is easy to evaluate, we can alternate between optimizing w.r.t. θ with $q(z|x)$ fixed and vice versa

- **Variational AutoEncoders:** parameterize $q(\cdot\,|x_i)$ with a NN with parameters ψ that takes x_i and outputs a distribution $q_\psi(\cdot\,|x_i)$, and find (θ, ψ) via SGD

$$\max_{\theta} \max_{\psi} \sum_{i=1}^{N} \int q_\psi(z|x_i) \log \frac{p_\theta(x_i, z)}{q_\psi(z|x_i)} dz$$

Expectation Maximization

$$\max_{\theta} \sum_{i=1}^{N} \log p_\theta(x_i) = \max_{\theta} \max_{q(z|x_i),\forall i} \sum_{i=1}^{N} \int_z q(z|x_i) \log \frac{p_\theta(x_i, z)}{q(z|x_i)} dz$$

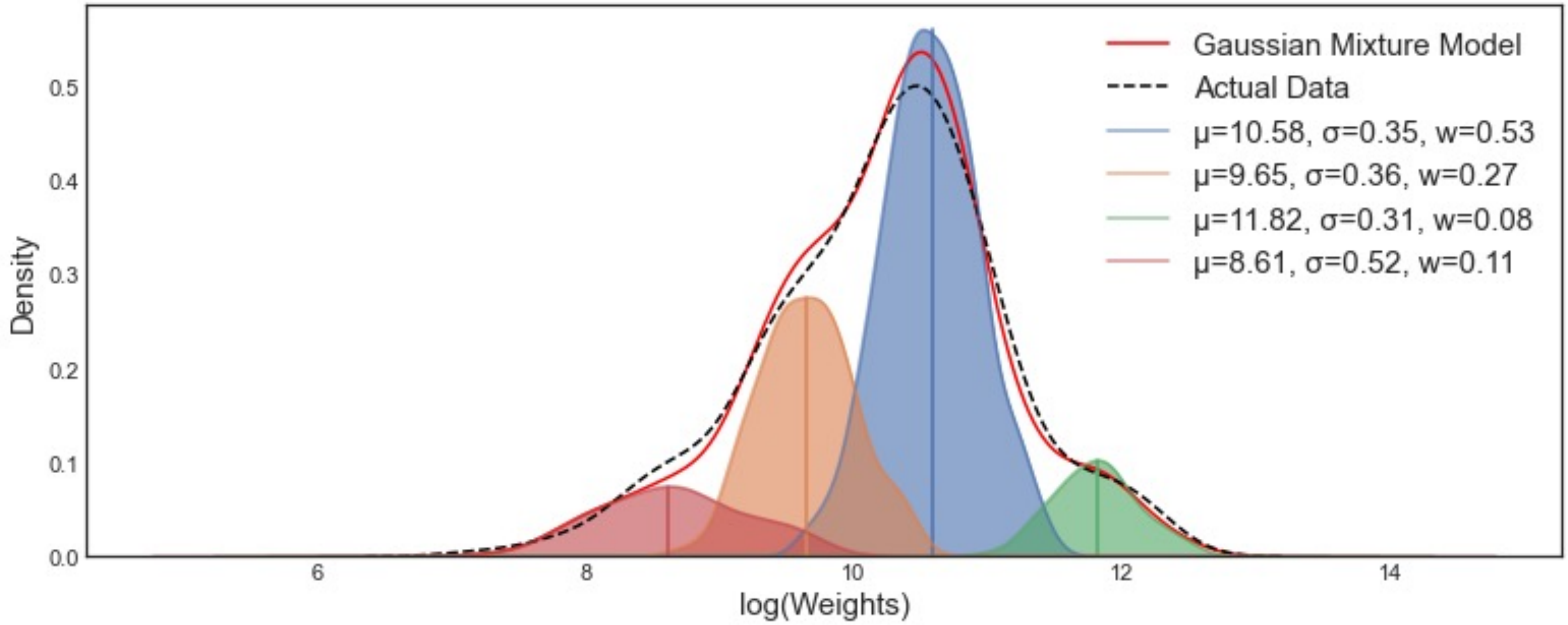
- Expectation Maximization alternates between two steps (k: iteration)

- E-step: $q^k(z|x_i) = p_{\theta_k}(z|x_i)$ maximizing w.r.t. q with θ fixed
- M-step: $\theta^{k+1} = \mathrm{argmax}_\theta \sum_{i=1}^{N} \int_z q^k(z|x_i) \log p_\theta(x_i, z)\, dz$

  maximizing w.r.t. θ with q fixed
- Examples
  - For a mixture of Gaussians, E & M steps are closed-form (next slide)
  - Often E-step can be done by sampling (MCMC) and M-step can be done by optimization (SGD)

E.g.: EM for Gaussian Mixture Model

- **Mixture Model**: $p_\theta(\boldsymbol{x}) = \sum_{j=1}^{n} p(x \mid z=j)p(z=j) = \pi_1 p_{\theta_1}(\boldsymbol{x}) + \pi_2 p_{\theta_2}(\boldsymbol{x}) + \cdots + \pi_n p_{\theta_n}(\boldsymbol{x})$
  - $\pi_j > 0$: prior probability of drawing a point from the j-th model; $\sum_{j=1}^{n} \pi_j = 1$
  - $p_{\theta_j} = \mathcal{N}(\mu_j, \Sigma_j)$. $\theta_i = (\mu_j, \Sigma_j)$: mean and covariance of the j-th Gaussian distribution
  - $\theta = (\theta_1, \ldots, \theta_n, \pi_1, \ldots, \pi_n)$: the parameters of the mixture model



E.g.: EM for Gaussian Mixture Model

- **Mixture Model**: $p_\theta(\boldsymbol{x}) = \sum_{\mathrm{j}=1}^{n} p(x \mid z = j) p(z = j) = \pi_1 p_{\theta_1}(\boldsymbol{x}) + \pi_2 p_{\theta_2}(\boldsymbol{x}) + \cdots + \pi_n p_{\theta_n}(\boldsymbol{x})$
  - $\pi_j > 0$: prior probability of drawing a point from the j-th model; $\sum_{\mathrm{j}=1}^{n} \pi_j = 1$
  - $p_{\theta_j} = \mathcal{N}(\mu_j, \Sigma_\mathrm{j})$. $\theta_i = (\mu_j, \Sigma_\mathrm{j})$: mean and covariance of the j-th Gaussian distribution
  - $\theta = (\theta_1, \ldots, \theta_n, \pi_1, \ldots, \pi_n)$: the parameters of the mixture model

- **Goal**: estimate θ from N i.i.d. samples $x_1, \ldots, x_N$ from p_θ using EM
  - For $i = 1, \ldots N$, let $z_i = j$ if x_i belongs to class j , and let $q_{ij} = q(z_i = j \mid x_i)$

$$\max_\theta \sum_{i=1}^{N} \log p_\theta(x_i) = \max_{\theta} \max_{q_{ij} \geq 0 : \sum_j q_{ij} = 1, \forall i} \sum_{i=1}^{N} \sum_{j=1}^{n} q_{ij} \log \frac{p_\theta(x_i, z_i = j\ )}{q_{ij}}$$

- **E-step**: compute $q_{ij}^k = p_{\theta^k}(\boldsymbol{z}_i = \mathrm{j} \mid \boldsymbol{x}_i) = \dfrac{p_{\theta^k}(\boldsymbol{x}_i | z_i = j) p_{\theta^k}(\boldsymbol{z}_i = j)}{p_{\theta^k}(\boldsymbol{x}_i)} = \dfrac{p_{\theta_j^k}(\boldsymbol{x}_i) \pi_j^k}{\sum_{\mathrm{j}=1}^{n} p_{\theta_j^k}(\boldsymbol{x}_i) \pi_j^k}$

E.g.: EM for Gaussian Mixture Model

- **M-step**: $\theta^{k+1} = \underset{\theta}{\operatorname{argmax}} \sum_{i=1}^{N} \sum_{j=1}^{n} q_{ij}^{k} \log \frac{p_\theta(x_i, z_i = j)}{q_{ij}^{k}} = \underset{\theta}{\operatorname{argmax}} \sum_{i=1}^{N} \sum_{j=1}^{n} q_{ij}^{k} \log p_\theta(x_i, z_i = j)$
  - If we spell out θ and $p_\theta(x_i, z_i = j)$, the above becomes $\underset{\{\theta_j\}_{j=1}^{n}, \{\pi_j\}_{j=1}^{n}}{\operatorname{argmax}} \sum_{i=1}^{N} \sum_{j=1}^{n} q_{ij}^{k} \log\left(\pi_j \cdot p_{\theta_j}(\boldsymbol{x}_\mathrm{i})\right)$
  - For π_j's: $\max_{\{\pi_j\}_{j=1}^{n} : \sum_{\mathrm{j}=1}^{n} \pi_j = 1} \sum_{i=1}^{N} \sum_{j=1}^{n} q_{ij}^{k} \log(\pi_j)$
  - To analyze the solution of a constrained optimization problem, we use the method of Lagrange multipliers:

$$L\left(\{\pi_j\}_j, \lambda\right) = \sum_{i=1}^{N} \sum_{j=1}^{n} q_{ij}^{k} \log(\pi_j) - \lambda\left(\sum_{\mathrm{j}=1}^{n} \pi_j = 1\right)$$

  - $\frac{\partial L}{\partial \lambda} = 0 \Leftrightarrow \sum_{\mathrm{j}=1}^{n} \pi_j = 1$
  - $\forall j$: $\frac{\partial L}{\partial \pi_j} = 0 \Leftrightarrow \sum_{i=1}^{N} q_{ij}^{k} \frac{1}{\pi_j} - \lambda = 0$
  - The solution is $\lambda = \sum_{\mathrm{i}=1}^{N} \sum_{\mathrm{j}=1}^{n} q_{ij}^{k}$, $\pi_j = \frac{\sum_{\mathrm{i}=1}^{N} q_{ij}^{k}}{\sum_{\mathrm{i}=1}^{N} \sum_{\mathrm{j}=1}^{n} q_{ij}^{k}} =: \pi_j^{k+1}$

E.g.: EM for Gaussian Mixture Model

- **M-step**: $\theta^{k+1} = \underset{\theta}{\operatorname{argmax}} \sum_{i=1}^{N} \sum_{j=1}^{n} q_{ij}^{k} \log \frac{p_\theta(x_i, z_i = j)}{q_{ij}^{k}} = \underset{\theta}{\operatorname{argmax}} \sum_{i=1}^{N} \sum_{j=1}^{n} q_{ij}^{k} \log p_\theta(x_i, z_i = j)$
  - If we spell out θ and $p_\theta(x_i, z_i = j)$, the above becomes $\underset{\{\theta_j\}_{j=1}^{n}, \{\pi_j\}_{j=1}^{n}}{\operatorname{argmax}} \sum_{i=1}^{N} \sum_{j=1}^{n} q_{ij}^{k} \log\left(\pi_j \cdot p_{\theta_j}(\boldsymbol{x}_\mathrm{i})\right)$
  - For θ_j's: $\max_{\mu_j, \Sigma_\mathrm{j}} \boxed{\sum_{\mathrm{i}=1}^{N} q_{ij}^{k} \left(-\frac{1}{2}(\boldsymbol{x}_i - \boldsymbol{\mu}_j)^\top \Sigma_j^{-1} (\boldsymbol{x}_i - \boldsymbol{\mu}_j) - \frac{1}{2} \operatorname{logdet}(\Sigma_j)\right)} =: \boldsymbol{\mathcal{L}}(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$
  - $\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}_j} = \sum_{i=1}^{N} q_{ij}^{k} \Sigma_j^{-1} (\boldsymbol{x}_i - \boldsymbol{\mu}_j) = \Sigma_j^{-1}\left(\sum_{i=1}^{N} q_{ij}^{k} \boldsymbol{x}_i - \left(\sum_{i=1}^{N} q_{ij}^{k}\right) \boldsymbol{\mu}_j\right).$
  - Setting it to 0 $\Rightarrow \boldsymbol{\mu}_j = \frac{\sum_{\mathrm{i}=1}^{N} q_{ij}^{k} \boldsymbol{x}_i}{\sum_{\mathrm{i}=1}^{N} q_{ij}^{k}} =: \boldsymbol{\mu}_j^{k+1}$
  - $\boldsymbol{\mathcal{L}}(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j) = -\frac{1}{2} \operatorname{tr}\left(\Sigma_j^{-1} \sum_{i=1}^{N} q_{ij}^{k} (x_i - \mu_j)(x_i - \mu_j)^\top\right) - \frac{1}{2}\left(\sum_{i=1}^{N} q_{ij}^{k}\right) \operatorname{logdet} \Sigma_j$
  - Reusing our derivation in MLE for Gaussian: $\Sigma_j = \frac{\sum_{i=1}^{N} q_{ij}^{k} \left(\boldsymbol{x}_i - \boldsymbol{\mu}_j^{k+1}\right)\left(\boldsymbol{x}_i - \boldsymbol{\mu}_j^{k+1}\right)^\top}{\sum_{i=1}^{N} q_{ij}^{k}} =: \Sigma_j^{k+1}$