Study Material - Youtube

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Video Overview

This lecture provides a comprehensive review of the optimization framework for latent variable models, focusing on the **Expectation-Maximization (EM) algorithm**. The instructor begins by recapping the core problem of Maximum Likelihood Estimation (MLE) in latent variable models and the use of the **Evidence Lower Bound (ELBO)** as a tractable objective function. The central theme is the joint optimization of model parameters (θ) and a variational distribution (q) that approximates the true latent posterior.

The lecture then introduces the **Gaussian Mixture Model (GMM)** as a canonical example of a latent variable model with discrete latent variables. It details the mathematical formulation of a GMM and explains how the EM algorithm can be applied to learn its parameters. Finally, the lecture highlights the limitations of the standard EM algorithm, particularly its reliance on a computable true posterior, which sets the stage for more advanced techniques like Variational Autoencoders (VAEs) where this posterior is intractable.

Learning Objectives

Upon completing this lecture, students will be able to: - **Recap the ELBO framework** for latent variable model training. - **Understand the joint optimization problem** involving both model parameters (θ) and the variational posterior (q). - **Describe the iterative nature** of the Expectation-Maximization (EM) algorithm. - **Define the E-step and M-step** both conceptually and mathematically. - **Formulate a Gaussian Mixture Model (GMM)** as a latent variable model. - **Apply the EM algorithm framework** to the problem of learning GMM parameters. - **Identify the key limitation** of the standard EM algorithm that motivates the need for more advanced generative models.

Prerequisites

To fully grasp the concepts in this lecture, students should have a solid understanding of: - **Probability Theory**: Joint, conditional, and marginal distributions; Bayes' theorem. - **Calculus**: Differentiation and optimization. - **Latent Variable Models**: The fundamental concept of observed and unobserved variables. - **Maximum Likelihood Estimation (MLE)**: The principle of finding parameters that maximize the likelihood of observed data. - **Jensen's Inequality** and its application in deriving the **Evidence Lower Bound (ELBO)**.

Key Concepts

- Evidence Lower Bound (ELBO)
- Variational Latent Posterior ($q(z|x)$)
- Expectation-Maximization (EM) Algorithm
- E-Step (Expectation Step)
- M-Step (Maximization Step)
- Gaussian Mixture Model (GMM)
- Intractable Posteriors

The ELBO Maximization Framework: A Recap

The Core Optimization Problem

(00:14) The fundamental goal in training a generative latent variable model is to find the optimal parameters θ^* that maximize the log-likelihood of the observed data x. This is the principle of **Maximum Likelihood Estimation (MLE)**.

For a latent variable model, the probability of an observation x is obtained by marginalizing out the latent variable z:

$$p_\theta(x) = \int_z p_\theta(x, z) dz$$

The MLE objective is therefore:

$$\theta^* = \arg\max_\theta \mathbb{E}_{p_x}[\log p_\theta(x)] = \arg\max_\theta \mathbb{E}_{p_x}\left[\log \int_z p_\theta(x, z) dz\right]$$

As established in previous lectures, this objective is often intractable because the logarithm is outside the integral, preventing a closed-form solution.

The Evidence Lower Bound (ELBO) as a Tractable Objective

(00:38) To overcome this intractability, we introduce a variational distribution $q(z|x)$ to approximate the true, but often unknown, posterior $p_\theta(z|x)$. By applying Jensen's Inequality, we derive the **Evidence Lower Bound (ELBO)**, denoted as $J_\theta(q)$, which is a lower bound on the log-likelihood:

$$\log p_\theta(x) \geq \mathbb{E}_{q(z|x)}\left[\log \frac{p_\theta(x, z)}{q(z|x)}\right] = J_\theta(q)$$

Instead of maximizing the intractable log-likelihood, we maximize its tractable lower bound, the ELBO. This transforms the problem into a joint optimization over both the model parameters θ and the variational distribution q.

(01:11) The new optimization problem is:

$$\theta^*, q^* = \arg\max_{\theta, q} J_\theta(q)$$

Expanding the ELBO term, we get:

$$\theta^*, q^* = \arg\max_{\theta, q} \mathbb{E}_{q(z|x)}\left[\log \frac{p_\theta(x, z)}{q(z|x)}\right]$$

This joint optimization is the cornerstone of training many latent variable models, including those discussed in this lecture.

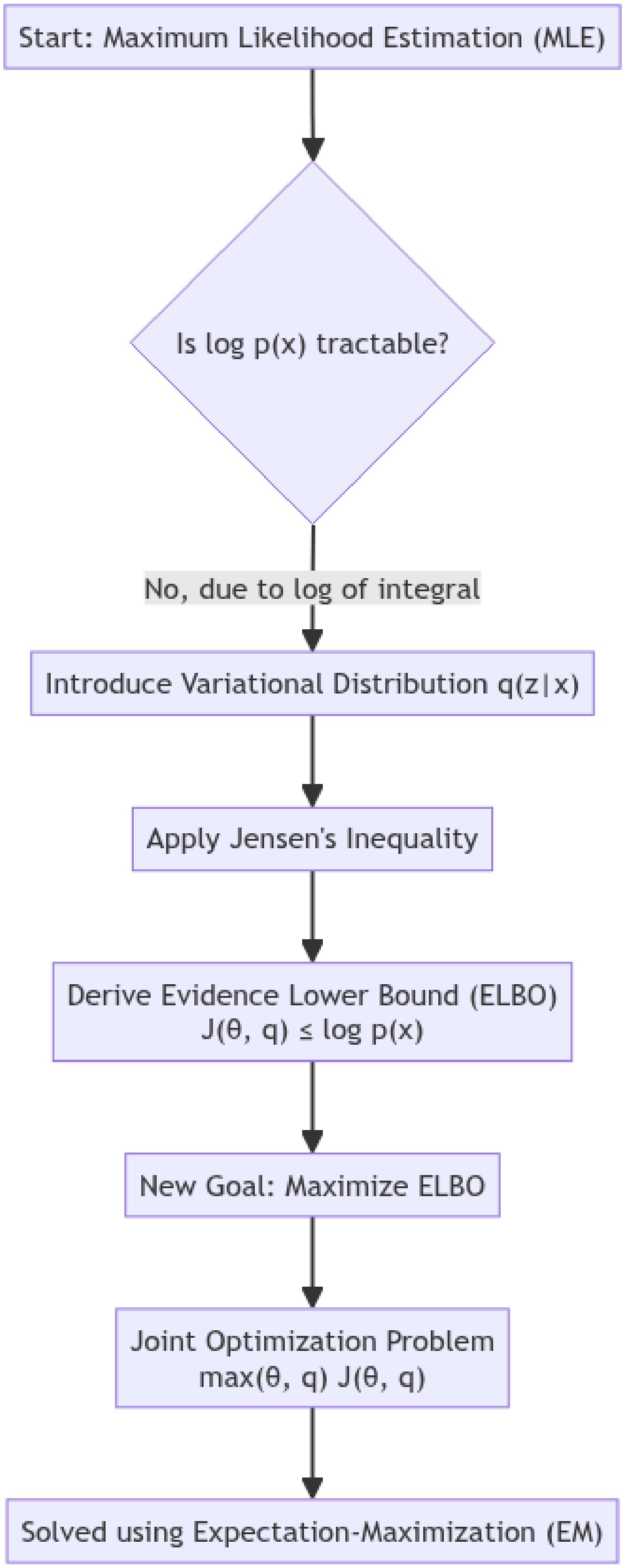

Start: Maximum Likelihood Estimation (MLE)
Is log p(x) tractable?
No, due to log of integral
Introduce Variational Distribution q(z|x)
Apply Jensen's Inequality
Derive Evidence Lower Bound (ELBO)
J(θ, q) ≤ log p(x)
New Goal: Maximize ELBO
Joint Optimization Problem
max(θ, q) J(θ, q)
Solved using Expectation-Maximization (EM)

Figure 1: The logical flow from the intractable MLE problem to the tractable ELBO optimization framework.

The Expectation-Maximization (EM) Algorithm

The Expectation-Maximization (EM) algorithm is a powerful iterative method for solving the joint optimization problem of maximizing the ELBO. It breaks the problem into two alternating steps.

Intuitive Foundation

(13:02) Instead of trying to solve for θ and q simultaneously, which is difficult, the EM algorithm tackles them one at a time in an iterative loop.

1. **E-Step (Expectation):** Assume the current model parameters θ are correct. Based on this assumption, calculate the most likely distribution for the latent variables, $q(z|x)$. This is like "filling in" the missing information (the latent variables) based on our current best guess of the model.
2. **M-Step (Maximization):** Now, assume the latent variable distribution $q(z|x)$ calculated in the E-step is correct. Update the model parameters θ to maximize the likelihood of the data *and* these "filled-in" latent variables.

This two-step process is repeated until the parameters converge.

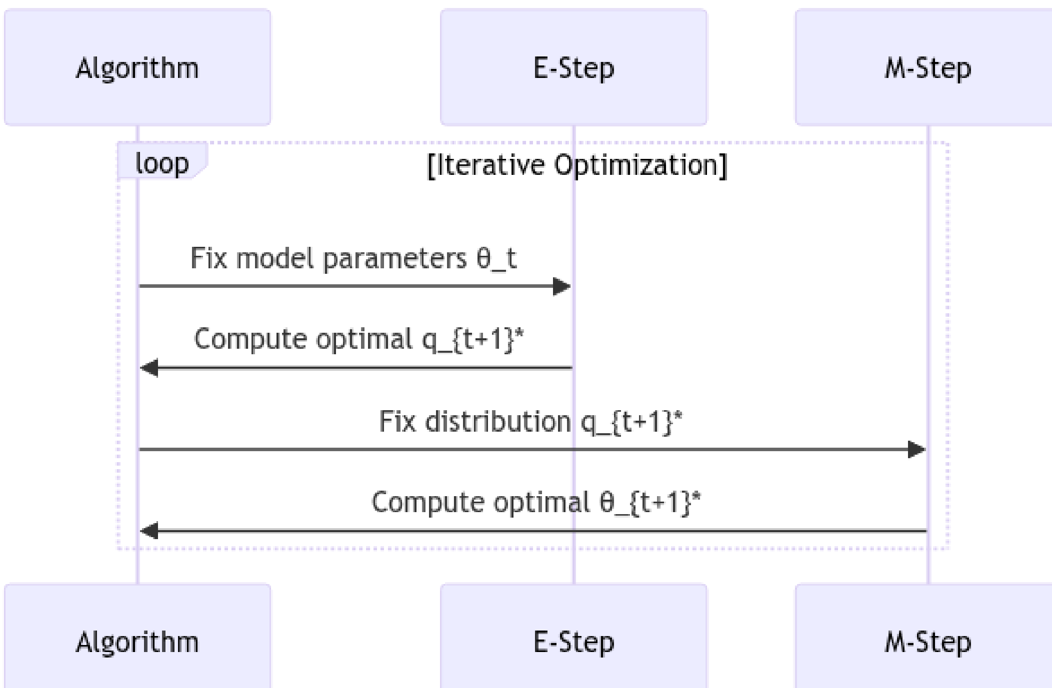


Figure 2: The iterative process of the EM algorithm, alternating between the E-step and M-step.

Mathematical Formulation of EM

Let θ_t and q_t be the estimates at iteration t.

E-Step: Optimizing for q

(14:50) In the E-step, we fix the model parameters to their current estimate, θ_t, and find the variational distribution q that maximizes the ELBO.

$$q_{t+1}^* = \arg\max_q J_{\theta_t}(q)$$

It can be analytically shown that the ELBO is maximized when the KL divergence between $q(z|x)$ and the true posterior $p_{\theta_t}(z|x)$ is zero. This occurs when q is exactly equal to the true posterior.

> **Key Result of the E-Step:** The optimal variational distribution q^* is the true posterior of the latent variables given the data and the current model parameters.
>
> $$q_{t+1}^*(z|x) = p_{\theta_t}(z|x)$$

M-Step: Optimizing for θ

(16:23) In the M-step, we fix the variational distribution to the one we found in the E-step, q_{t+1}^*, and update the model parameters θ to maximize the ELBO.

$$\theta_{t+1}^* = \arg\max_\theta J_\theta(q_{t+1}^*)$$

Let's expand the ELBO expression for this step:

$$J_\theta(q_{t+1}^*) = \mathbb{E}_{q_{t+1}^*(z|x)}[\log p_\theta(x,z)] - \mathbb{E}_{q_{t_1}^*(z|x)}[\log q_{t+1}^*(z|x)]$$

Since the second term does not depend on θ, maximizing the ELBO is equivalent to maximizing only the first term.

> **Key Result of the M-Step:** The parameter update is found by maximizing the expectation of the complete-data log-likelihood, where the expectation is taken with respect to the posterior from the E-step.
>
> $$\theta_{t+1}^* = \arg\max_\theta \mathbb{E}_{q_{t+1}^*(z|x)}[\log p_\theta(x,z)]$$

(18:16) It can be proven that this iterative procedure is guaranteed to never decrease the log-likelihood function, i.e., $l(\theta_{t+1}) \geq l(\theta_t)$.

Case Study: Expectation-Maximization for Gaussian Mixture Models (GMM)

(06:55) A Gaussian Mixture Model (GMM) is a classic latent variable model used for clustering. It assumes that the observed data is generated from a mixture of several Gaussian distributions.

GMM Definition

- **Latent Variable** z: A discrete variable, $z \in \{1, 2, \dots, M\}$, indicating which of the M Gaussian components generated a data point.
- **Model Parameters** θ: The set of all parameters for the mixture:
  - **Mixture Weights** α_j: The prior probability of selecting component j, $p(z = j) = \alpha_j$. These must satisfy $0 \leq \alpha_j \leq 1$ and $\sum_{j=1}^M \alpha_j = 1$.
  - **Component Means** μ_j: The mean of the j-th Gaussian component.
  - **Component Covariances** Σ_j: The covariance matrix of the j-th Gaussian component. The full parameter set is $\theta = \{\alpha_j, \mu_j, \Sigma_j\}_{j=1}^M$.

- **Generative Process**: The probability of observing a data point x is a weighted sum of the probabilities from each Gaussian component:

$$p_\theta(x) = \sum_{j=1}^{M} p_\theta(z=j) \cdot p_\theta(x|z=j) = \sum_{j=1}^{M} \alpha_j \mathcal{N}(x; \mu_j, \Sigma_j)$$

Applying the EM Algorithm to GMM

(18:52) We can use the EM algorithm to find the parameters θ of the GMM.

E-Step for GMM

The goal is to compute $q^*_{t+1}(z=j|x) = p_{\theta_t}(z=j|x)$. Using Bayes' rule, we can compute this posterior probability, often called the **responsibility**, for each component j and data point x.

$$q^*_{t+1}(z=j|x) = \frac{p_{\theta_t}(x|z=j)p_{\theta_t}(z=j)}{\sum_{k=1}^{M} p_{\theta_t}(x|z=k)p_{\theta_t}(z=k)} = \frac{\alpha_j^t \mathcal{N}(x; \mu_j^t, \Sigma_j^t)}{\sum_{k=1}^{M} \alpha_k^t \mathcal{N}(x; \mu_k^t, \Sigma_k^t)}$$

This step calculates, for each data point, the probability that it was generated by each of the Gaussian components, given the current parameter estimates.

M-Step for GMM

(22:53) The M-step updates the parameters θ by maximizing the expected complete-data log-likelihood. For GMMs, this leads to intuitive, closed-form update rules (derived by differentiating the objective and setting to zero).

- **Update for Means** μ_j: The new mean for a component is the weighted average of all data points, where the weights are the responsibilities calculated in the E-step.
- **Update for Covariances** Σ_j: The new covariance is the weighted covariance of the data points around the new mean.
- **Update for Mixture Weights** α_j: The new mixture weight for a component is the average responsibility of that component over all data points.

The Critical Limitation of Standard EM

(27:26) The EM algorithm, as described, is highly effective for models like GMMs. Its success hinges on one critical condition: **the ability to analytically compute the true posterior of the latent variables,** $p_\theta(z|x)$.

In a GMM, this is possible because the denominator in Bayes' rule, $p_\theta(x)$, is a simple sum that can be easily computed.

However, for more complex **deep generative models** (like VAEs and Diffusion Models), the relationship between z and x is defined by a complex, non-linear function (a neural network). In these cases, the marginal likelihood $p_\theta(x) = \int p_\theta(x, z)dz$ becomes intractable to compute.

> **The Central Challenge:** If $p_\theta(x)$ is intractable, we cannot compute the true posterior $p_\theta(z|x)$. This means the E-step of the standard EM algorithm fails.

(28:22) This leads to the fundamental question that motivates modern generative models: **How do we learn a latent variable model for cases where the posterior $p_\theta(z|x)$ is unknown or intractable?**

The answer lies in approximating this posterior, which is the core idea behind Variational Autoencoders (VAEs), a topic for a future lecture.

Self-Assessment for This Video

1. **Explain in your own words why we optimize the ELBO instead of the log-likelihood directly in latent variable models.** *Answer: Maximizing the log-likelihood* $\log p_\theta(x)$ *directly is often intractable because it involves taking the logarithm of an integral over the latent variables,* $\log \int p_\theta(x, z)dz$. *The ELBO is a tractable lower bound on this quantity, which we can optimize instead. Maximizing the ELBO simultaneously pushes up the true log-likelihood and minimizes the KL divergence between our approximate posterior* $q(z|x)$ *and the true posterior* $p_\theta(z|x)$.

2. **What are the two alternating steps of the EM algorithm, and what is the goal of each step?** *Answer: The two steps are the Expectation (E-step) and Maximization (M-step). The goal of the E-step is to find the best possible approximation* $q(z|x)$ *for the latent posterior, given the current model parameters* θ_t. *The goal of the M-step is to find the best model parameters* θ_{t+1} *that maximize the expected complete-data log-likelihood, given the latent posterior distribution q found in the E-step.*

3. **In the context of the EM algorithm, what is the optimal choice for the variational distribution** $q^*(z|x)$ **in the E-step?** *Answer: The optimal choice for* $q^*(z|x)$ *is the true posterior distribution of the latent variables,* $p_\theta(z|x)$, *calculated using the current model parameters.*

4. **What is a Gaussian Mixture Model (GMM)? Identify its parameters.** *Answer: A GMM is a probabilistic model that represents a dataset as a mixture of several Gaussian distributions. Its parameters (*θ*) are the mixture weights (*α_j*), the means of each Gaussian component (*μ_j*), and the covariance matrices of each component (*Σ_j*).*

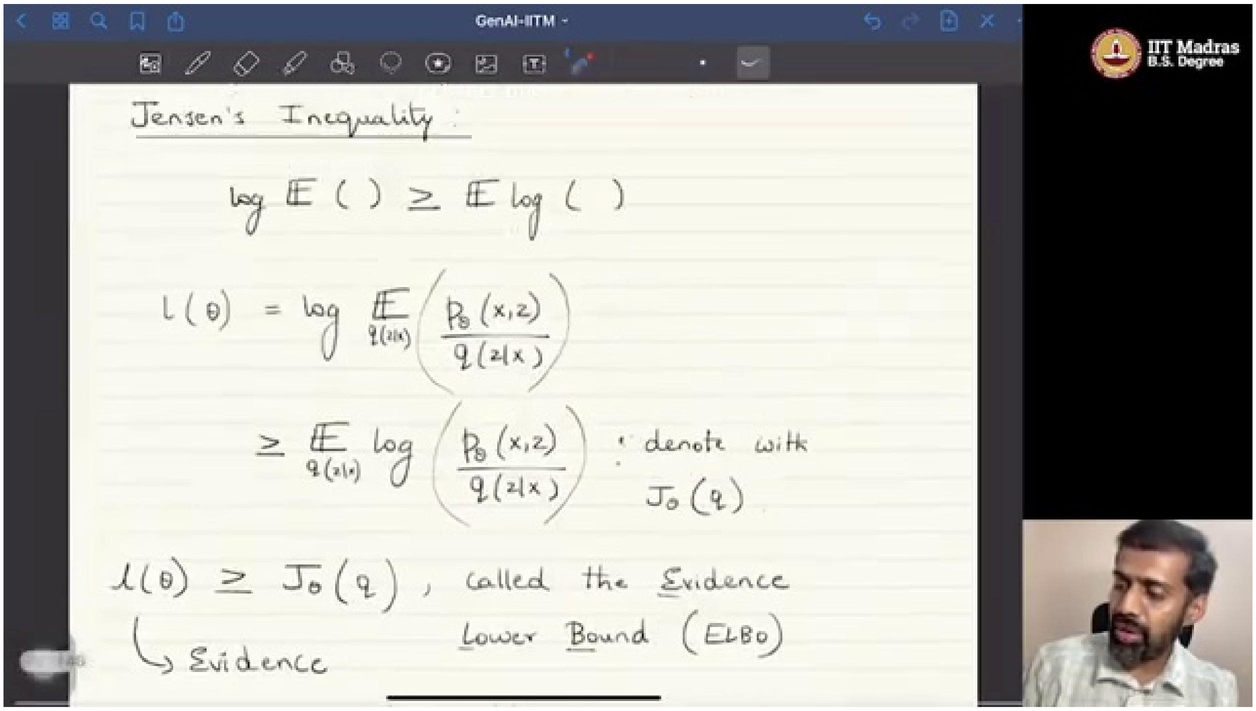
5. **Why does the standard EM algorithm fail for many deep generative models like VAEs?** *Answer: The standard EM algorithm requires computing the true posterior* $p_\theta(z|x)$ *in the E-step. For deep generative models, the likelihood function* $p_\theta(x|z)$ *is defined by a complex neural network, making the marginal likelihood* $p_\theta(x)$ *(the denominator in Bayes' rule) intractable to compute. Without* $p_\theta(x)$, *we cannot compute the true posterior, and the E-step fails.*

Key Takeaways from This Video

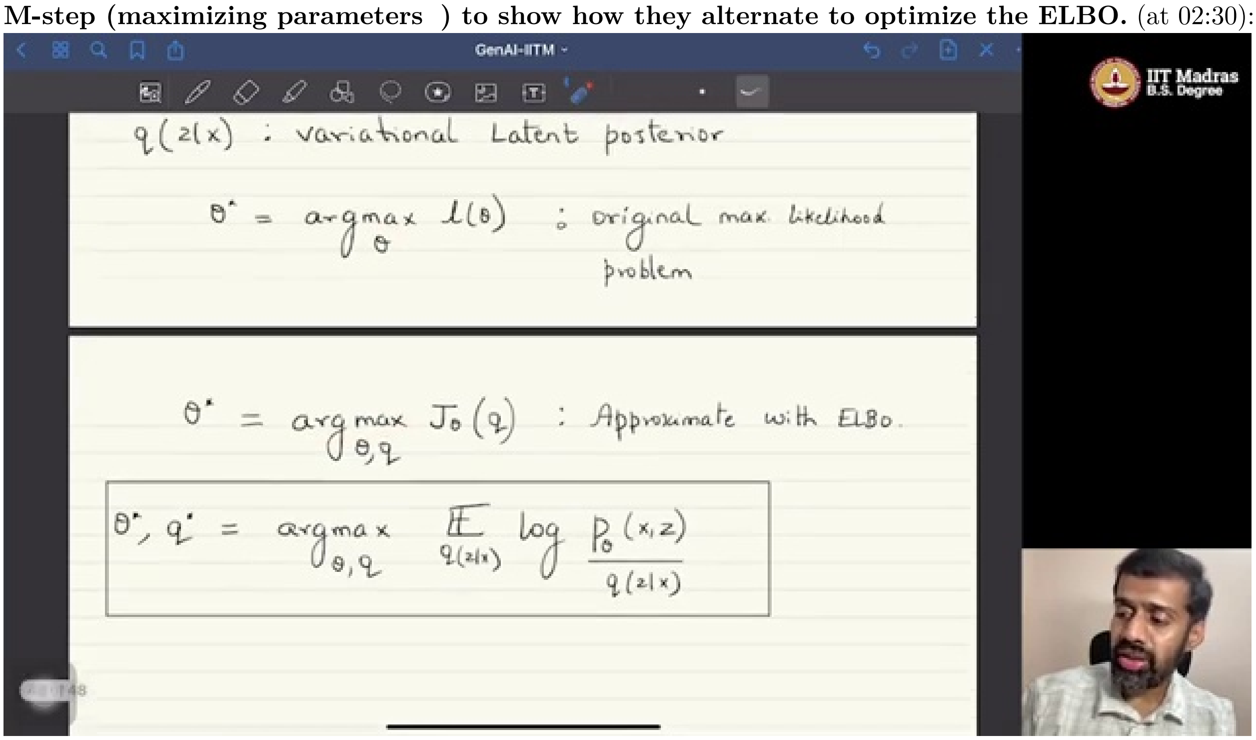
- Training latent variable models involves a joint optimization of the ELBO with respect to model parameters θ and a variational posterior q.
- The Expectation-Maximization (EM) algorithm is an iterative procedure that solves this by alternating between an E-step (updating q) and an M-step (updating θ).
- The optimal E-step sets q to be the true latent posterior $p_\theta(z|x)$.
- The M-step updates θ to maximize the expected complete-data log-likelihood.
- This framework is directly applicable to models like GMMs where the posterior is computable.
- For complex models where the posterior is intractable, the standard EM algorithm is not feasible, necessitating the advanced techniques used in deep generative models.

Visual References

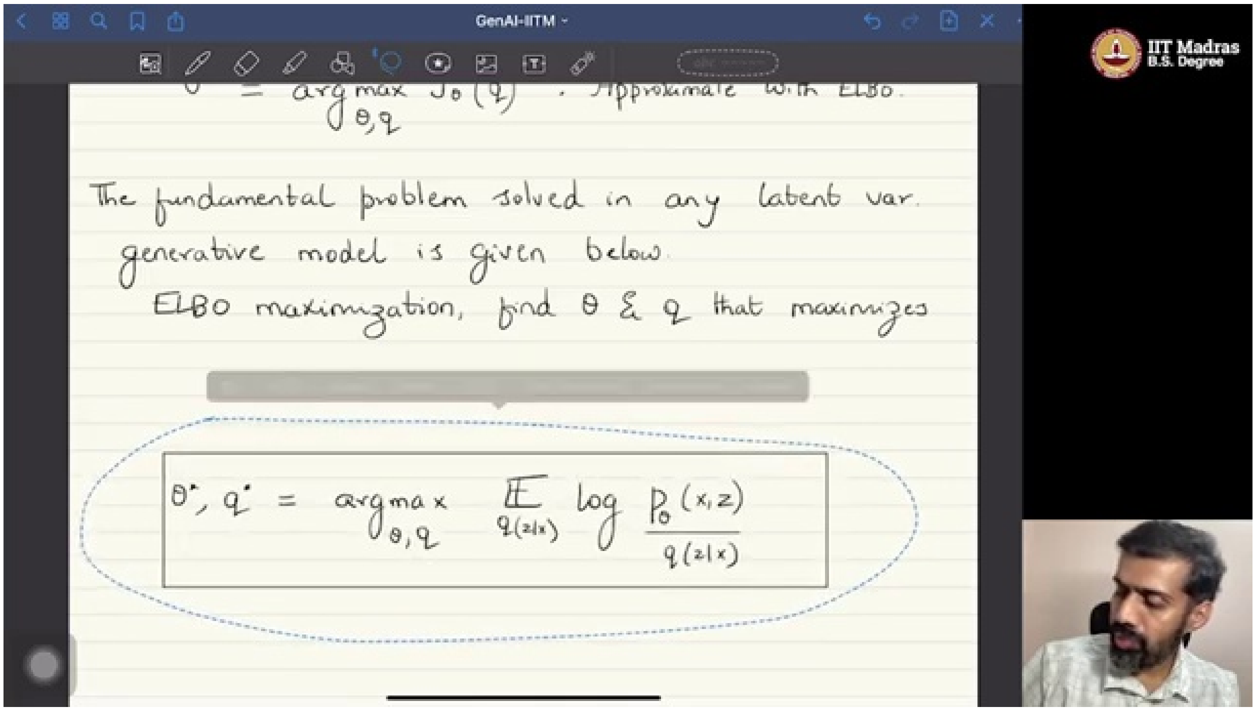
Introduction to the core optimization problem. This slide shows the Maximum Likelihood Estimation (MLE) objective and the integral equation for the marginal probability p(x), which sets up the need for the Evidence Lower Bound (ELBO). (at 00:14):



A conceptual diagram illustrating the iterative nature of the Expectation-Maximization (EM) algorithm. It would visually separate the E-step (computing expectations/updating q) and the M-step (maximizing parameters) to show how they alternate to optimize the ELBO. (at 02:30):



The specific update equations for the Expectation-Maximization algorithm applied to Gaussian Mixture Models (GMMs). This slide would show the formulas for the 'responsibilities' in the E-step and the updates for the means ( ), covariances (Σ), and mixture weights ( ) in the M-step. (at



06:00):

A summary slide listing the key takeaways of the lecture. This would likely recap the ELBO framework, the E-step/M-step definitions, the GMM case study, and crucially, the limitation of the standard EM algorithm (requiring a computable true posterior). (at 09:15):