Study Material - Youtube

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Video Overview

This video lecture provides a detailed mathematical derivation of the Expectation-Maximization (EM) algorithm for Gaussian Mixture Models (GMMs). The instructor begins by defining GMMs as a type of latent variable model where the latent variables are discrete. The core of the lecture is a step-by-step derivation of the update rules for the model's parameters—mixing coefficients, means, and covariances—within the EM framework. The lecture is heavily based on the derivations found in Christopher Bishop's "Pattern Recognition and Machine Learning" textbook.

Learning Objectives

Upon completing this lecture, students will be able to: - Define a Gaussian Mixture Model (GMM) and its components. - Understand the role of discrete latent variables in GMMs. - Formulate the log-likelihood function for a GMM. - Comprehend the two main steps of the EM algorithm: the Expectation (E) step and the Maximization (M) step. - Derive the update equations for the means, mixing coefficients, and covariances of the Gaussian components. - Understand the concept of "responsibilities" and their role in the E-step. - Follow the application of Lagrange multipliers for constrained optimization of the mixing coefficients.

Prerequisites

To fully grasp the concepts in this video, students should have a solid understanding of: - **Probability Theory:** Gaussian (Normal) distribution, probability density functions, conditional probability, and Bayes' theorem. - **Calculus:** Multivariate calculus, including partial differentiation and optimization. - **Linear Algebra:** Vectors, matrices, matrix inverse, and transpose. - **Machine Learning Fundamentals:** Basic concepts of latent variable models and the general framework of the Expectation-Maximization (EM) algorithm.

Key Concepts Covered

- Gaussian Mixture Models (GMMs)
- Latent Variables
- Expectation-Maximization (EM) Algorithm
- Log-Likelihood Maximization

- Responsibilities (Posterior Probabilities)
- Constrained Optimization with Lagrange Multipliers

Gaussian Mixture Models (GMMs) - Deep Understanding

Intuitive Foundation and Problem Formulation

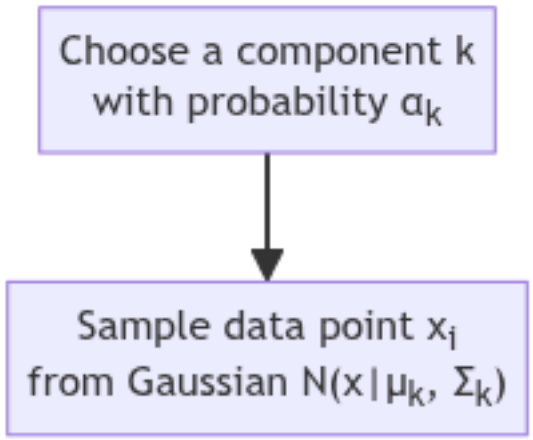
A **Gaussian Mixture Model (GMM)** is a probabilistic model that assumes all the data points are generated from a mixture of a finite number of Gaussian distributions with unknown parameters.

Intuitive Analogy: Imagine you have a collection of height measurements from a large population of adults. This population consists of both males and females. The heights of males might follow one Gaussian (bell-curve) distribution, and the heights of females might follow another, slightly different Gaussian distribution. A GMM would model the overall height distribution as a weighted sum of these two individual Gaussian distributions.

Formal Problem Setup (01:20):

1. **Observed Data:** We have a dataset of observed data points $X = \{x_1, x_2, \dots, x_n\}$, where each $x_i \in \mathbb{R}^d$. We assume these points are drawn independently and identically distributed (i.i.d.) from an underlying data distribution $p(x)$.
2. **Latent Variable:** For each observed data point x_i, we introduce a corresponding **latent variable** z_i. This variable is "hidden" or unobserved. In the context of GMMs, z_i is a discrete random variable that specifies which of the K Gaussian components generated the data point x_i.
    - The latent variable Z can take one of K possible values, representing the K components in the mixture. We can represent this with a 1-of-K encoding, where z is a vector with one element equal to 1 and all others equal to 0.
3. **The Generative Process:** The GMM assumes the following generative process for each data point x_i:
    a. First, a component is chosen by sampling the latent variable z_i from a categorical distribution. The probability of choosing the k-th component is given by the **mixing coefficient** α_k.
    b. Second, once a component k is chosen, the data point x_i is generated by sampling from the corresponding Gaussian distribution $\mathcal{N}(x|\mu_k, \Sigma_k)$.

This process can be visualized as follows:



Caption: The generative process for a single data point in a GMM.

Mathematical Formulation of GMMs

The probability distribution of an observed data point x is a weighted sum (a mixture) of K Gaussian distributions.

(02:48) The probability of a single data point x_i is given by marginalizing the joint distribution $p(x_i, z)$ over all possible states of the latent variable z:

$$p(x_i) = \sum_{k=1}^{K} p(z = k)p(x_i|z = k)$$

Here, the parameters of the model, collectively denoted by θ, are: - **Mixing Coefficients (α_k):** The prior probability of selecting the k-th component. These must satisfy: - $0 \leq \alpha_k \leq 1$ - $\sum_{k=1}^{K} \alpha_k = 1$ - **Component Means (μ_k):** The mean vector for each of the K Gaussian distributions. - **Component Covariances (Σ_k):** The covariance matrix for each of the K Gaussian distributions.

Substituting the specific distributions, the GMM is defined as:

$$p(x_i|\theta) = \sum_{k=1}^{K} \alpha_k \mathcal{N}(x_i; \mu_k, \Sigma_k)$$

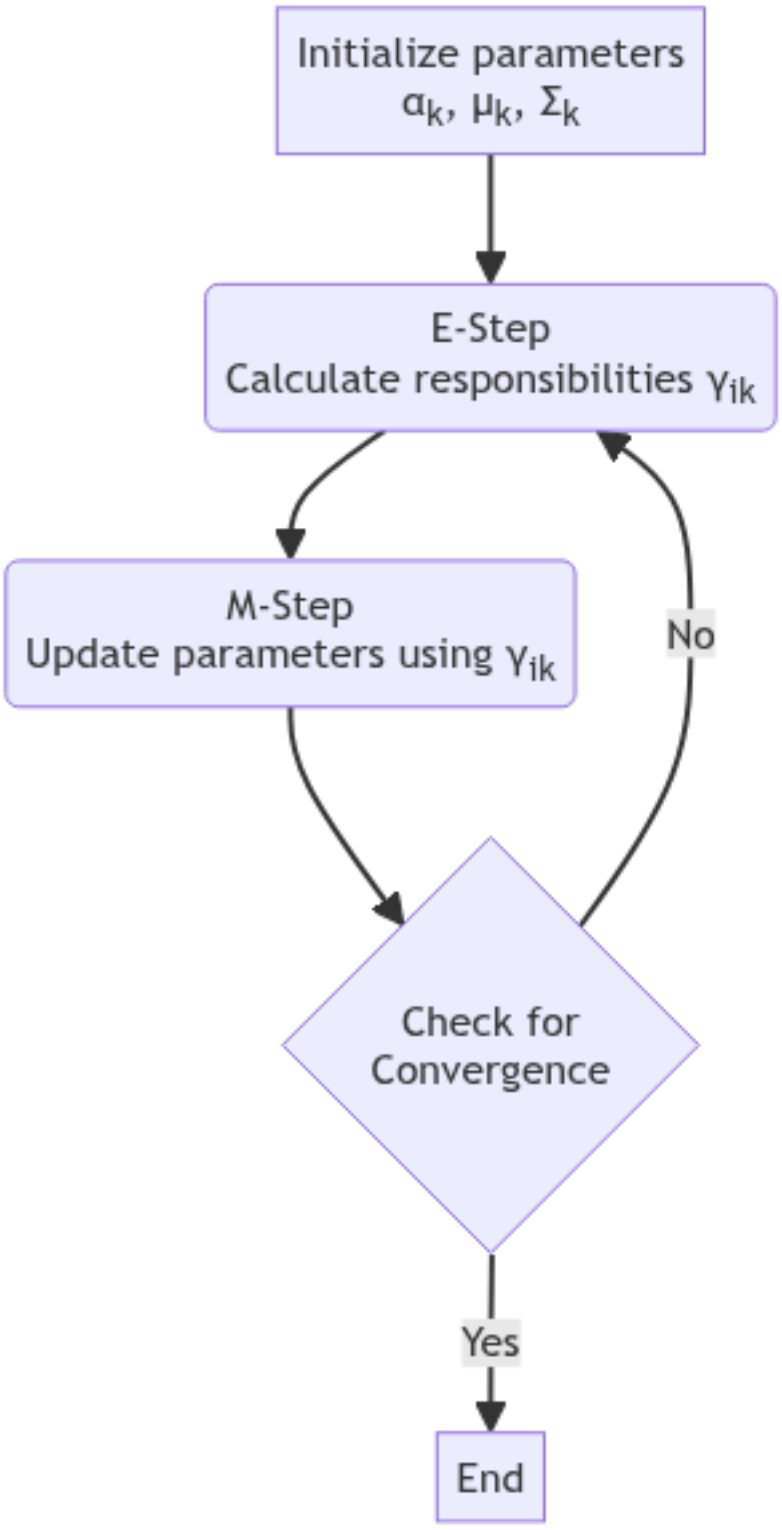
where $\mathcal{N}(x_i; \mu_k, \Sigma_k)$ is the probability density function of the multivariate Gaussian distribution for the k-th component.

The Expectation-Maximization (EM) Algorithm for GMMs

The goal is to find the parameters $\theta = \{\alpha_k, \mu_k, \Sigma_k\}_{k=1}^{K}$ that maximize the likelihood of the observed data. The log-likelihood of the entire dataset X is:

$$\log p(X|\theta) = \sum_{i=1}^{n} \log p(x_i|\theta) = \sum_{i=1}^{n} \log \left(\sum_{k=1}^{K} \alpha_k \mathcal{N}(x_i; \mu_k, \Sigma_k) \right)$$

Directly maximizing this function is difficult because the logarithm cannot be pushed inside the summation. The EM algorithm provides an iterative approach to solve this problem. It consists of two repeating steps: the E-step and the M-step.



Caption: The iterative flow of the Expectation-Maximization (EM) algorithm for GMMs.

The E-Step: Calculating Responsibilities

(04:40) In the **Expectation (E) step**, we use the current set of parameters θ^{old} to calculate the posterior probability of the latent variable for each data point. This posterior is called the **responsibility** of component k for data point x_i.

Intuition: The responsibility γ_{ik} answers the question: "Given the data point x_i and our current model, what is the probability that it was generated by the k-th Gaussian component?"

Using Bayes' theorem, the responsibility γ_{ik} is calculated as:

$$\gamma_{ik} = p(z = k|x_i; \theta^{\text{old}}) = \frac{p(z = k)p(x_i|z = k)}{\sum_{j=1}^{K} p(z = j)p(x_i|z = j)}$$

Substituting the GMM components, we get the formula for the E-step:

$$\gamma_{ik} = \frac{\alpha_k^{\text{old}} \mathcal{N}(x_i; \mu_k^{\text{old}}, \Sigma_k^{\text{old}})}{\sum_{j=1}^{K} \alpha_j^{\text{old}} \mathcal{N}(x_i; \mu_j^{\text{old}}, \Sigma_j^{\text{old}})}$$

This calculation is performed for every data point i and every component k.

The M-Step: Parameter Re-estimation

In the **Maximization (M) step**, we use the responsibilities γ_{ik} calculated in the E-step to update the model parameters θ. We find the new parameters θ^{new} that maximize the expected complete-data log-likelihood.

Update for the Means, μ_k

(18:26) To find the new mean μ_k^{new}, we differentiate the log-likelihood with respect to μ_k and set the derivative to zero. This yields the following update rule:

$$\mu_k^{\text{new}} = \frac{\sum_{i=1}^{n} \gamma_{ik} x_i}{\sum_{i=1}^{n} \gamma_{ik}}$$

Let's define N_k as the *effective number of points* assigned to component k:

$$N_k = \sum_{i=1}^{n} \gamma_{ik}$$

The update rule for the mean becomes a weighted average of all data points, where the weights are the responsibilities:

$$\mu_k^{\text{new}} = \frac{1}{N_k} \sum_{i=1}^{n} \gamma_{ik} x_i$$

Update for the Covariances, Σ_k

(23:27) Similarly, by differentiating the log-likelihood with respect to Σ_k, we obtain the update rule for the covariance matrix. It is a weighted covariance, where each data point's contribution is weighted by its responsibility for that component.

$$\Sigma_k^{\text{new}} = \frac{1}{N_k} \sum_{i=1}^{n} \gamma_{ik} (x_i - \mu_k^{\text{new}})(x_i - \mu_k^{\text{new}})^T$$

Update for the Mixing Coefficients, α_k

(11:23) The update for the mixing coefficients α_k requires **constrained optimization** because of the constraint that $\sum_{k=1}^{K} \alpha_k = 1$. We use a **Lagrange multiplier** λ to incorporate this constraint. The Lagrangian function is:

$$L = \sum_{i=1}^{n} \log \left(\sum_{k=1}^{K} \alpha_k \mathcal{N}(x_i; \mu_k, \Sigma_k) \right) + \lambda \left(\sum_{k=1}^{K} \alpha_k - 1 \right)$$

By differentiating L with respect to α_k and setting it to zero, we arrive at the update rule:

$$\alpha_k^{\text{new}} = \frac{N_k}{n}$$

Intuition: The new mixing coefficient for a component is simply the average responsibility that the component takes over all data points.

The Complete EM Algorithm for GMMs

(24:45) The full algorithm is as follows:

1. **Initialization:**
   - Initialize the means μ_k, covariances Σ_k, and mixing coefficients α_k for $k = 1, \ldots, K$. This can be done randomly or using an algorithm like K-Means.
   - Compute the initial log-likelihood of the model.
2. **E-Step (Expectation):**
   - Using the current parameters, evaluate the responsibilities for each data point i and each component k:
   $$\gamma_{ik} = \frac{\alpha_k \mathcal{N}(x_i; \mu_k, \Sigma_k)}{\sum_{j=1}^{K} \alpha_j \mathcal{N}(x_i; \mu_j, \Sigma_j)}$$
3. **M-Step (Maximization):**
   - Re-estimate the parameters using the calculated responsibilities:
     - $N_k = \sum_{i=1}^{n} \gamma_{ik}$
     - $\mu_k^{\text{new}} = \frac{1}{N_k} \sum_{i=1}^{n} \gamma_{ik} x_i$
     - $\Sigma_k^{\text{new}} = \frac{1}{N_k} \sum_{i=1}^{n} \gamma_{ik} (x_i - \mu_k^{\text{new}})(x_i - \mu_k^{\text{new}})^T$
     - $\alpha_k^{\text{new}} = \frac{N_k}{n}$
4. **Convergence Check:**
   - Evaluate the new log-likelihood:
   $$\log p(X|\theta^{\text{new}}) = \sum_{i=1}^{n} \log \left(\sum_{k=1}^{K} \alpha_k^{\text{new}} \mathcal{N}(x_i; \mu_k^{\text{new}}, \Sigma_k^{\text{new}}) \right)$$
   - If the log-likelihood value has not changed significantly or a maximum number of iterations has been reached, stop. Otherwise, set $\theta^{\text{old}} = \theta^{\text{new}}$ and return to Step 2.

Key Mathematical Concepts

- **GMM Probability Density Function:**

$$p(x_i|\theta) = \sum_{k=1}^{K} \alpha_k \mathcal{N}(x_i; \mu_k, \Sigma_k)$$

- **Log-Likelihood Function:**

$$\log p(X|\theta) = \sum_{i=1}^{n} \log \left(\sum_{k=1}^{K} \alpha_k \mathcal{N}(x_i; \mu_k, \Sigma_k) \right)$$

- **Responsibility (E-Step):**

$$\gamma_{ik} = \frac{\alpha_k \mathcal{N}(x_i; \mu_k, \Sigma_k)}{\sum_{j=1}^{K} \alpha_j \mathcal{N}(x_i; \mu_j, \Sigma_j)}$$

- **Parameter Updates (M-Step):**
  - Mean: $\mu_k^{\text{new}} = \frac{1}{N_k} \sum_{i=1}^{n} \gamma_{ik} x_i$
  - Covariance: $\Sigma_k^{\text{new}} = \frac{1}{N_k} \sum_{i=1}^{n} \gamma_{ik} (x_i - \mu_k^{\text{new}})(x_i - \mu_k^{\text{new}})^T$
  - Mixing Coefficient: $\alpha_k^{\text{new}} = \frac{N_k}{n}$, where $N_k = \sum_{i=1}^{n} \gamma_{ik}$

Self-Assessment for This Video

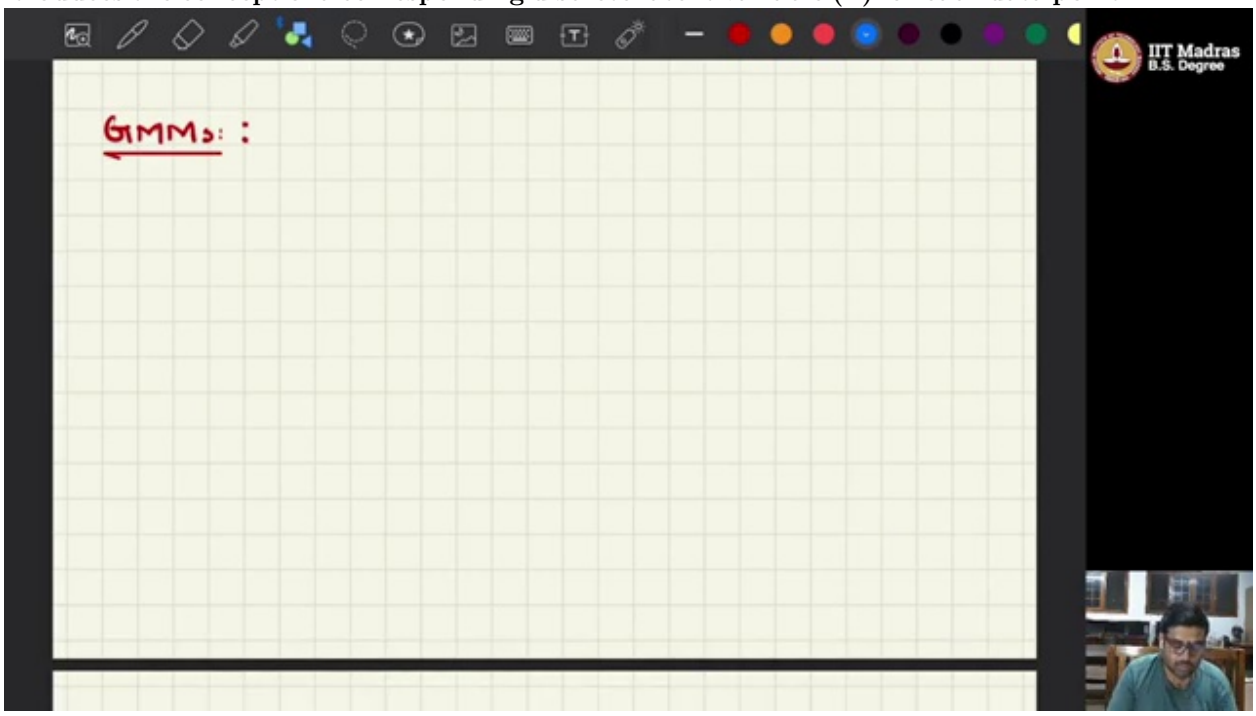
1. **Conceptual Understanding:**
   - In your own words, what is a Gaussian Mixture Model and what does it represent?
   - What is the role of the latent variable z in a GMM? Why is it considered "latent"?
   - Explain the intuition behind the E-step and M-step of the EM algorithm for GMMs. What does each step try to achieve?
   - What is a "responsibility" in the context of GMMs, and what does its value signify?
2. **Mathematical Derivations:**
   - Write down the complete log-likelihood function for a dataset X given a GMM with K components. Explain why it is difficult to optimize directly.
   - Derive the update rule for the mean of the k-th component, μ_k, starting from the log-likelihood function.
   - Why is a Lagrange multiplier needed to derive the update rule for the mixing coefficients α_k? Walk through the derivation.
3. **Application and Algorithm:**
   - Outline the complete, iterative EM algorithm for GMMs, listing the four main stages.
   - What is the convergence criterion for the EM algorithm? What happens at each iteration to the log-likelihood value?
   - If you were to implement this algorithm, how would you initialize the parameters? Discuss one possible strategy.

Key Takeaways from This Video

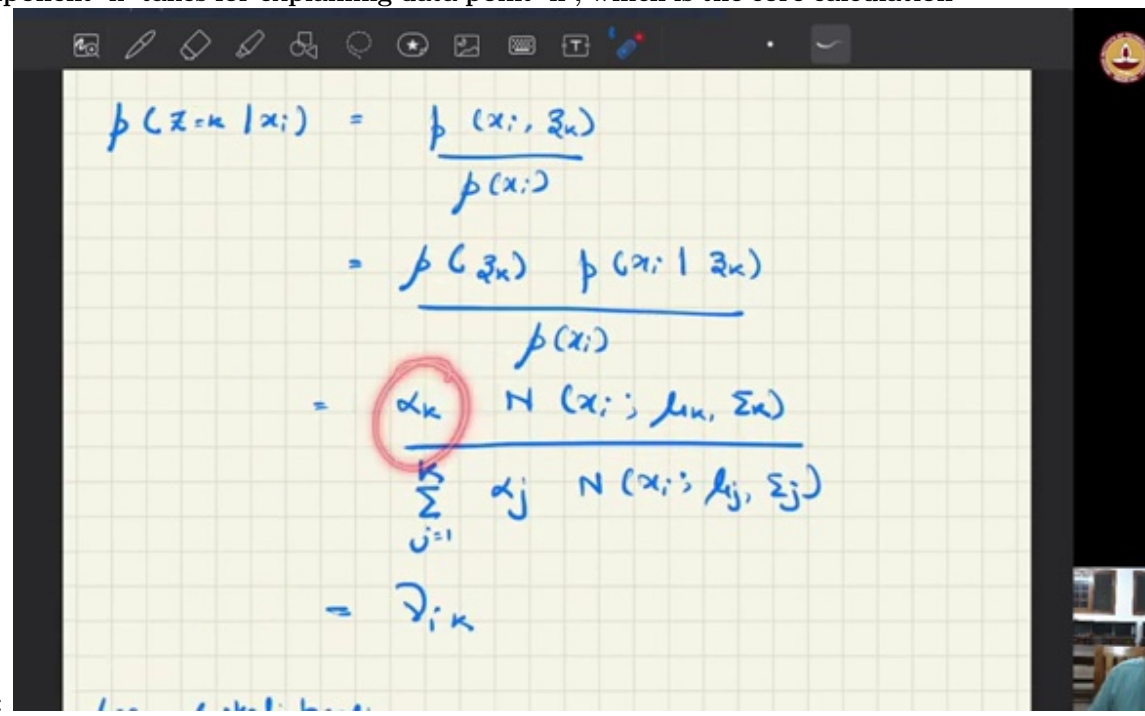
- **GMMs are powerful density estimators:** They can approximate any continuous density by using a sufficient number of Gaussian components.
- **EM is the standard algorithm for GMMs:** It provides an elegant and effective iterative solution to the otherwise intractable problem of maximizing the log-likelihood.
- **The E-step is a "soft" assignment:** Instead of assigning each data point to a single cluster (like in K-Means), the E-step calculates the probability (responsibility) of it belonging to each cluster.
- **The M-step is a weighted maximum likelihood estimate:** The parameters for each component are updated using all data points, but weighted by their respective responsibilities.
- **The math is foundational:** The derivations shown, especially the use of Bayes' rule and Lagrange multipliers, are fundamental techniques in machine learning for optimizing probabilistic models.

Visual References

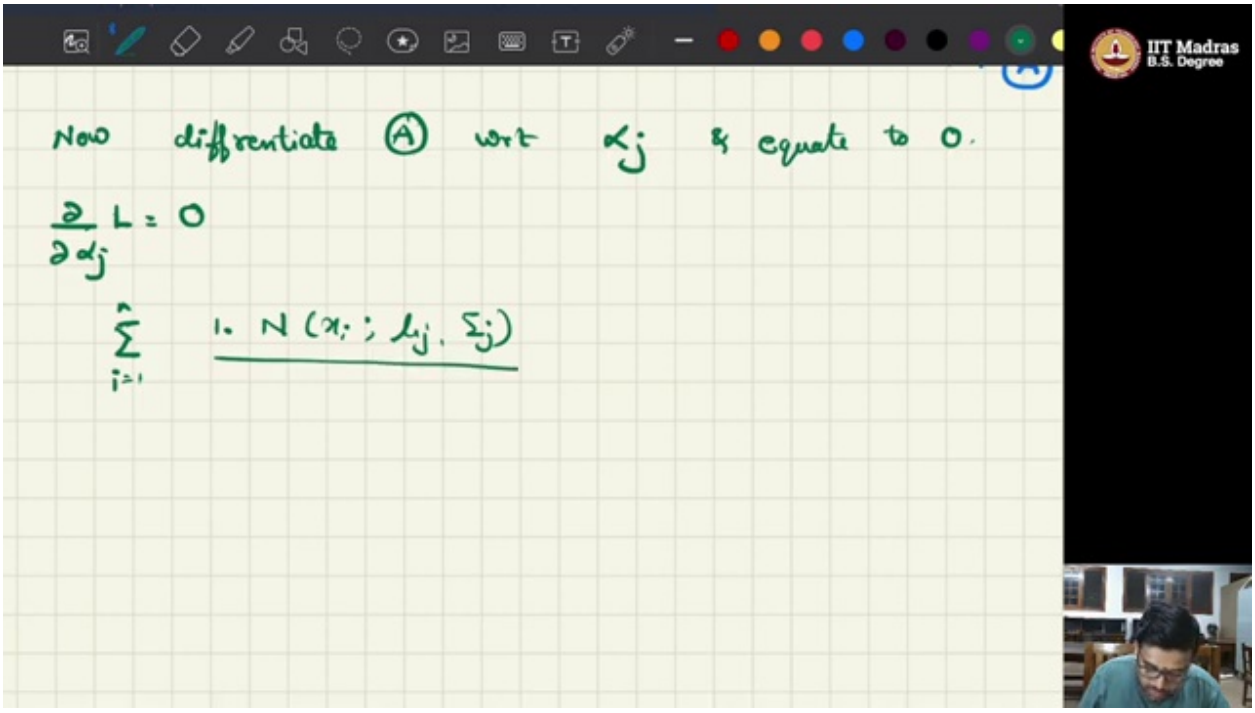
A slide showing the formal problem setup for GMMs. It visually defines the observed data points (X) and introduces the concept of a corresponding discrete latent variable (Z) for each data point. (at 01:20):



The introduction of 'responsibilities' ( ). This screenshot would show the equation defining the responsibility that component 'k' takes for explaining data point 'n', which is the core calculation of the E-step. (at 09:15):



A summary of the M-step update equations. This visual would show the final derived formulas for updating the means (_k) and covariances (Σ_k) of the Gaussian components based on the responsibilities calculated in the E-step. (at 15:30):



The derivation for the mixing coefficients (_k) using a Lagrange multiplier. This screenshot shows the application of constrained optimization, a key mathematical step for ensuring the mixing coefficients sum to one. (at 19:00):