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 variable is discrete. The core of the lecture is a step-by-step derivation of the E-step and M-step of the EM algorithm, culminating in the update equations for the model's parameters: the mixing coefficients, means, and covariance matrices. The lecture is highly mathematical and assumes a foundational understanding of calculus, probability, and linear algebra.

Learning Objectives

Upon completing this lecture, a student will be able to: - **Define** a Gaussian Mixture Model (GMM) in its mathematical form. - **Understand** the role of discrete latent variables in GMMs. - **Formulate** the log-likelihood function for a GMM and understand why its direct optimization is challenging. - **Explain** the two main steps of the Expectation-Maximization (EM) algorithm: the E-step and the M-step. - **Derive** the update equations for all GMM parameters (μ_k, Σ_k, and α_k) from first principles. - **Explain** the concept of "responsibilities" and their role in the E-step. - **Apply** Lagrange multipliers to solve the constrained optimization problem for the mixing coefficients.

Prerequisites

To fully grasp the concepts in this video, students should be familiar with: - **Probability Theory:** Basic probability rules, probability density functions (PDFs), conditional probability, and Bayes' theorem. - **Calculus:** Differentiation, partial derivatives, and maximization of functions by setting derivatives to zero. - **Linear Algebra:** Vectors, matrices, and covariance matrices. - **Gaussian (Normal) Distribution:** The mathematical form of the univariate and multivariate Gaussian distributions. - **Machine Learning Concepts:** A basic understanding of latent variable models and the general idea of the EM algorithm is beneficial.

Key Concepts Covered in This Video

- Gaussian Mixture Models (GMMs)
- Latent Variable Models

- Expectation-Maximization (EM) Algorithm
- Log-Likelihood Maximization
- E-Step: Calculating Responsibilities
- M-Step: Re-estimating Parameters
- Constrained Optimization with Lagrange Multipliers

Gaussian Mixture Models (GMMs): A Deep Dive

Introduction and Foundational Concepts (00:11 - 01:24)

The lecture begins by introducing the central topic: **Gaussian Mixture Models (GMMs)**.

> **Instructor's Recommendation (00:36):** The lecturer strongly recommends referring to Chapter 9 of the book "Pattern Recognition and Machine Learning" by Christopher Bishop for a more in-depth treatment of GMMs and the EM algorithm. The derivations and notation used in this lecture are based on this text.

Intuitive Foundation: What is a GMM?

A Gaussian Mixture Model is a powerful probabilistic model used for representing complex data distributions. The core idea is that any complex distribution can be approximated as a **mixture**, or a weighted sum, of several simpler Gaussian (normal) distributions.

Imagine you have a dataset of heights of a large population. This population might consist of several distinct subgroups (e.g., children, adult women, adult men). The height distribution of each subgroup can be modeled by a simple bell-shaped Gaussian curve. The overall height distribution of the entire population, however, would be more complex, likely showing multiple peaks. A GMM can model this complex, multi-peaked distribution by "mixing" the individual Gaussian distributions of the subgroups.

Each Gaussian component in the mixture is defined by its own mean (μ) and covariance (Σ), and the "mixing" is controlled by a set of weights, known as mixing coefficients (α).

Mathematical Formulation of GMMs (01:24 - 04:38)

Problem Setup

We start with a dataset X consisting of n i.i.d. (independently and identically distributed) data points:

$$X = \{x_1, x_2, \dots, x_n\}$$

Each data point x_i is a vector in a d-dimensional space, i.e., $x_i \in \mathbb{R}^d$.

The Latent Variable `Z`

GMMs are a type of **latent variable model**. A latent variable is a hidden or unobserved variable that we introduce to simplify the model's structure.

- In a GMM, we introduce a discrete latent variable Z.
- This variable Z can take one of K possible values, where K is the number of Gaussian components in our mixture.
- The role of Z is to specify which of the K components was responsible for generating a given data point x_i. If $Z = k$, it means that x_i was drawn from the k-th Gaussian component.

The generative process can be visualized as follows:

```
graph TD
    A["Start"] --> B{Choose a component 'k'<br>with probability _k};
```

```
B --> C["Sample data point x_i<br>from Gaussian N( _k, Σ_k)"];
C --> D["Output x_i"];
```

Figure 1: The generative process for a single data point in a Gaussian Mixture Model.

The GMM Probability Density Function

The probability of observing a single data point x_i is obtained by summing (marginalizing) over all possible latent states (i.e., all K components).

The joint probability of observing x_i and it belonging to component k is $p(x_i, z = k)$. Using the product rule of probability:

$$p(x_i, z = k) = p(x_i|z = k)p(z = k)$$

To get the marginal probability of x_i, we sum over all K components:

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

Let's define the terms in this equation: - $p(z = k) = \alpha_k$: This is the **mixing coefficient**, representing the prior probability of choosing the k-th component. It must satisfy $\alpha_k \geq 0$ and $\sum_{k=1}^{K} \alpha_k = 1$. - $p(x_i|z = k) = \mathcal{N}(x_i|\mu_k, \Sigma_k)$: This is the probability of observing x_i given that it came from the k-th component. It is a multivariate Gaussian distribution with mean μ_k and covariance matrix Σ_k.

Substituting these into the equation, we get the final form of the GMM probability density function (PDF) for a single data point x_i:

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

Here, $\theta = \{\alpha_k, \mu_k, \Sigma_k\}_{k=1}^{K}$ represents the set of all parameters for the model.

The Expectation-Maximization (EM) Algorithm for GMMs

Our goal is to find the parameters θ that best fit our data X. We achieve this by maximizing the **log-likelihood** of the data.

The Log-Likelihood Function

The likelihood of the entire dataset is the product of the probabilities of each data point, assuming they are i.i.d.:

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

The log-likelihood, denoted as $\ln p(X|\theta)$, is:

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

> **Why is this difficult?** (06:41) The direct maximization of this function is computationally intractable. The presence of the logarithm outside the summation couples all the parameters of the mixture model. Differentiating this expression and setting it to zero does not lead to a closed-form solution.

To solve this, we use the **Expectation-Maximization (EM) algorithm**, an iterative method for finding maximum likelihood estimates in models with latent variables.

The EM Algorithm Flow

The EM algorithm alternates between two steps: an Expectation (E) step and a Maximization (M) step.

```
flowchart TD
    A["Step 1: Initialize parameters<br> _k, Σ_k,  _k"] --> B["Loop until convergence"];
    B --> C["<b>E-Step</b><br>Calculate responsibilities  _ik<br>using current parameters"];
    C --> D["<b>M-Step</b><br>Re-estimate parameters  _k, Σ_k,  _k<br>using the responsibilities"];
    D --> E{"Check for convergence<br>(e.g., log-likelihood change is small)"};
    E -->|No| C;
    E -->|Yes| F["End"];
```

Figure 2: The iterative process of the EM algorithm for training GMMs.

E-Step: Evaluating Responsibilities (04:38 - 06:18)

Intuition: In the E-step, we use our current set of parameters $(\mu_k, \Sigma_k, \alpha_k)$ to calculate the posterior probability of the latent variable Z. This posterior, known as the **responsibility**, tells us how much each Gaussian component k is "responsible" for generating each data point x_i.

The responsibility of component k for data point x_i is denoted by γ_{ik} (or $\gamma(z_{ik})$ in Bishop's notation) and is calculated using Bayes' theorem:

$$\gamma_{ik} = p(z = k|x_i, \theta) = \frac{p(x_i|z = k)p(z = k)}{p(x_i)}$$

Substituting the GMM expressions:

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

We compute this value for every data point i and every component k.

M-Step: Re-estimating the Parameters (06:18 - 24:44)

Intuition: In the M-step, we use the responsibilities calculated in the E-step to update the model parameters. We treat the responsibilities as "soft assignments" of data points to components and re-estimate the parameters to maximize the expected log-likelihood.

1. Re-estimating the Means (μ_k) The new mean for each component k, μ_k^{new}, is a weighted average of all data points, where the weights are the responsibilities.

First, we define the "effective number of points" assigned to component k:

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

The update rule for the mean is:

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

This is derived by differentiating the expected complete-data log-likelihood with respect to μ_k and setting it to zero.

2. Re-estimating the Covariances (Σ_k) Similarly, the new covariance matrix for each component k, Σ_k^{new}, is a weighted covariance calculation:

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

Note that we use the newly computed mean μ_k^{new} in this calculation.

3. Re-estimating the Mixing Coefficients (α_k) The update for the mixing coefficients α_k is a constrained optimization problem, as we must ensure that $\sum_{k=1}^{K} \alpha_k = 1$. We use a **Lagrange multiplier** λ to enforce this constraint.

The objective function (Lagrangian) to maximize is (12:21):

$$L = \ln p(X|\theta) + \lambda \left(\sum_{k=1}^{K} \alpha_k - 1 \right)$$

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

We differentiate L with respect to a specific mixing coefficient α_j and set the result to zero (14:40):

$$\frac{\partial L}{\partial \alpha_j} = \sum_{i=1}^{n} \frac{\mathcal{N}(x_i|\mu_j, \Sigma_j)}{\sum_{k=1}^{K} \alpha_k \mathcal{N}(x_i|\mu_k, \Sigma_k)} + \lambda = 0$$

Multiplying the equation by α_j gives:

$$\sum_{i=1}^{n} \frac{\alpha_j \mathcal{N}(x_i|\mu_j, \Sigma_j)}{\sum_{k=1}^{K} \alpha_k \mathcal{N}(x_i|\mu_k, \Sigma_k)} + \lambda \alpha_j = 0$$

The fractional term is exactly the responsibility γ_{ij}. So, we have:

$$\sum_{i=1}^{n} \gamma_{ij} + \lambda \alpha_j = 0 \implies N_j + \lambda \alpha_j = 0$$

To find λ, we sum this equation over all components $j = 1, \ldots, K$:

$$\sum_{j=1}^{K} N_j + \sum_{j=1}^{K} \lambda \alpha_j = 0$$

$$n + \lambda(1) = 0 \implies \lambda = -n$$

Here, $\sum N_j = \sum_j \sum_i \gamma_{ij} = \sum_i \sum_j \gamma_{ij} = \sum_i 1 = n$, and $\sum \alpha_j = 1$.

Substituting $\lambda = -n$ back into $N_j + \lambda \alpha_j = 0$, we get $N_j - n\alpha_j = 0$. This gives the update rule for α_j:

$$\alpha_j^{new} = \frac{N_j}{n} = \frac{\sum_{i=1}^{n} \gamma_{ij}}{n}$$

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

Key Mathematical Concepts

1. GMM Probability Density Function

The probability of a data point x_i is a weighted sum of K Gaussian densities.

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

2. Log-Likelihood Function

The function to be maximized to find the optimal parameters θ.

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

3. E-Step: Responsibility Update

The responsibility of component k for data point x_i.

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

4. M-Step: Parameter Updates

- **Mean Update:**
$$\mu_k^{new} = \frac{1}{N_k} \sum_{i=1}^{n} \gamma_{ik} x_i$$
- **Covariance Update:**
$$\Sigma_k^{new} = \frac{1}{N_k} \sum_{i=1}^{n} \gamma_{ik} (x_i - \mu_k^{new})(x_i - \mu_k^{new})^T$$
- **Mixing Coefficient Update:**
$$\alpha_k^{new} = \frac{N_k}{n}$$

  where $N_k = \sum_{i=1}^{n} \gamma_{ik}$ and n is the total number of data points.

Visual Elements from the Video

The lecture is presented on a digital whiteboard. The key visual elements are the handwritten mathematical derivations.

- **(01:48)** The instructor writes down the formula for the dataset $X = \{x_1, \ldots, x_n\}$ and the assumption that each $x_i \in \mathbb{R}^d$.
- **(02:18)** The definition of the latent variable Z as a discrete random variable is introduced.
- **(02:46)** The marginal probability $p_\theta(x_i)$ is written as a sum over the joint probability $p_\theta(x_i, z)$.
- **(04:08)** The final form of the GMM PDF is written, showing the mixture of weighted Gaussians.
- **(04:50)** The posterior probability $p(z = k|x_i)$, which is the responsibility γ_{ik}, is derived using Bayes' rule.
- **(06:41)** The log-likelihood function is written out, highlighting the difficulty of optimization due to the log-sum form.
- **(12:21)** The Lagrangian for the constrained optimization of α_k is formulated.
- **(14:40 - 18:00)** A detailed, step-by-step derivation of the update rule for α_j is shown.

- **(22:35 - 24:28)** The update rules for μ_j and Σ_j are presented.
- **(25:11)** The complete EM algorithm for GMMs is summarized in four clear steps.

Self-Assessment for This Video

1. **Conceptual Understanding:**
   - What is the primary motivation for using a Gaussian Mixture Model instead of a single Gaussian distribution?
   - Explain the role of the latent variable Z in the GMM framework. Why is it considered "latent"?
   - What is the intuitive meaning of a "responsibility" (γ_{ik})? How does it represent a "soft assignment"?
2. **Mathematical Derivation:**
   - Write down the complete log-likelihood function for a GMM. Explain why taking the derivative and setting it to zero is not a feasible approach for optimization.
   - Starting from Bayes' theorem, derive the formula for the responsibility γ_{ik}.
   - Using the Lagrangian $L = \ln p(X|\theta) + \lambda(\sum_k \alpha_k - 1)$, derive the M-step update rule for the mixing coefficients α_j. Show all steps, including how you find the value of λ.
3. **Algorithmic Understanding:**
   - Outline the four main steps of the EM algorithm for GMMs.
   - In the M-step, why must we use the *newly computed* mean μ_k^{new} when calculating the *new* covariance Σ_k^{new}?
   - What are some possible criteria for checking if the EM algorithm has converged?

Key Takeaways from This Video

- **GMMs Model Complexity:** GMMs are flexible models that can represent complex, multi-modal data distributions by combining multiple simple Gaussian components.
- **Latent Variables Simplify Modeling:** The introduction of a discrete latent variable Z simplifies the conceptual and mathematical framework, allowing us to think of the model as a generative process.
- **EM is Essential for GMMs:** Direct maximization of the GMM log-likelihood is intractable. The Expectation-Maximization (EM) algorithm provides an elegant and effective iterative solution.
- **E-Step is Inference:** The E-step is an inference step where we compute the expected values of the latent variables (the responsibilities) given the data and current parameters.
- **M-Step is Optimization:** The M-step is an optimization step where we update the model parameters to maximize the likelihood, using the responsibilities as weights. The updates for the mean, covariance, and mixing coefficients are intuitive weighted averages.