Study Material - Youtube

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Video Overview

This lecture provides a concise yet comprehensive review of the mathematical framework for training latent variable models, culminating in the formulation of the Expectation-Maximization (EM) algorithm. The instructor begins by recapping the derivation of the **Evidence Lower Bound (ELBO)**, which serves as a tractable surrogate for the intractable log-likelihood of the data. The core of the lecture is framing the learning problem as a **joint optimization** of the ELBO with respect to both the model parameters (θ) and a variational distribution (q). This general framework is then illustrated with a classic machine learning example, the **Gaussian Mixture Model (GMM)**, setting the stage for understanding how these foundational concepts are extended to more complex deep generative models.

Learning Objectives

Upon completing this lecture, students will be able to: - **Recall** the derivation of the Evidence Lower Bound (ELBO) from the log-likelihood using Jensen's Inequality. - **Formulate** the joint optimization problem for latent variable models, which involves maximizing the ELBO with respect to both model parameters (θ) and the variational posterior (q). - **Understand** the iterative nature of the Expectation-Maximization (EM) algorithm as a method to solve this joint optimization. - **Define** a Gaussian Mixture Model (GMM) as a specific instance of a latent variable model with discrete latent variables. - **Identify** the key parameters of a GMM that need to be learned from data. - **Recognize** the limitations of the standard EM algorithm when the true posterior is intractable, motivating the need for more advanced techniques like those used in VAEs.

Prerequisites

To fully grasp the concepts in this lecture, students should have a solid understanding of: - **Probability Theory**: Concepts of joint, conditional, and marginal probability distributions, Bayes' theorem, and the definition of expectation. - **Calculus**: Multivariate differentiation and optimization (finding maxima by setting derivatives to zero). - **Machine Learning Fundamentals**: Basic principles of Maximum Likelihood Estimation (MLE) and the concept of latent variables. - **Information Theory**: A basic understanding of Jensen's Inequality is crucial for the ELBO derivation.

Key Concepts Covered in This Video

- Latent Variable Models
- Log-Likelihood Maximization
- Evidence Lower Bound (ELBO)
- Jensen's Inequality
- Variational Inference
- Joint Optimization Problem
- Expectation-Maximization (EM) Algorithm
- Gaussian Mixture Models (GMM)

From Maximum Likelihood to ELBO Maximization

This section recaps the foundational challenge in training latent variable models and how the Evidence Lower Bound (ELBO) provides a tractable solution.

The Challenge of Latent Variable Models

(00:15) The primary goal in many generative models is to perform **Maximum Likelihood Estimation (MLE)**. We want to find the model parameters θ that maximize the likelihood of our observed data X. This is typically done by maximizing the log-likelihood.

For a latent variable model, the probability of an observed data point x, $p_\theta(x)$, is obtained by marginalizing over the unobserved (latent) variable z:

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

The optimization problem is to find the optimal parameters θ^*:

$$\theta^* = \arg\max_\theta \mathbb{E}_{p_x}[\log p_\theta(x)]$$

The core difficulty arises because the log-likelihood function, $L(\theta) = \log p_\theta(x)$, involves a logarithm of an integral (or a sum for discrete latent variables):

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

This expression is often **intractable**, meaning it cannot be computed or optimized analytically. The logarithm prevents us from pushing the integral outside, making direct optimization impossible for most non-trivial models.

Deriving the Evidence Lower Bound (ELBO)

To overcome the intractability of the log-likelihood, we introduce a tractable lower bound. This is achieved through **variational inference**, where we introduce an auxiliary distribution $q(z|x)$ to approximate the true, but unknown, posterior distribution of the latent variables, $p_\theta(z|x)$.

The derivation of the ELBO, as recapped by the instructor (00:38), proceeds as follows:

1. **Start with the log-likelihood** and introduce $q(z|x)$ by multiplying and dividing inside the integral:

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

2. **Recognize the integral as an expectation.** The expression is now the logarithm of an expectation with respect to the distribution $q(z|x)$:

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

3. **Apply Jensen's Inequality.** (01:20) For a concave function like the logarithm, the log of an expectation is greater than or equal to the expectation of the log: $\log \mathbb{E}[Y] \geq \mathbb{E}[\log Y]$. Applying this gives us:

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

4. **Define the ELBO.** This lower bound is known as the **Evidence Lower Bound (ELBO)**, which we denote as $J_\theta(q)$:

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

   Thus, we have the fundamental relationship:

$$L(\theta) \geq J_\theta(q)$$

The following flowchart, inspired by the instructor's recap, illustrates this derivation process.

```
flowchart TD
    A["Start: Log-Likelihood<br/>L( ) = log p(x)"] --> B["Introduce Latent Variable z<br/>L( ) = log   p(
    B --> C["Introduce Variational Posterior q(z|x)<br/>L( ) = log   q(z|x) [p(x,z)/q(z|x)] dz"]
    C --> D["Recognize as Log of Expectation<br/>L( ) = log E_q[p(x,z)/q(z|x)]"]
    D --> E{"Apply Jensen's Inequality<br/>log E[Y]   E[log Y]"}
    E --> F["Obtain Evidence Lower Bound (ELBO)<br/>L( )   E_q[log p(x,z) - log q(z|x)]"]
    F --> G["New Goal: Maximize ELBO<br/>max( ,q) J( ,q)"]
```

This flowchart shows the key steps in deriving the Evidence Lower Bound (ELBO) as a tractable objective function for latent variable models.

The Joint Optimization Problem

(01:51) The ELBO is a function of both the model parameters θ and the variational distribution q. Therefore, our new goal is to **jointly optimize** the ELBO with respect to both:

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

This is the fundamental optimization problem that is solved in any latent variable generative model, including VAEs and Diffusion Models.

The Expectation-Maximization (EM) Algorithm

The joint optimization problem is typically solved with an iterative procedure known as the **Expectation-Maximization (EM) algorithm**. This algorithm breaks the difficult joint optimization into two simpler, alternating steps.

The Iterative EM Procedure

(13:07) The EM algorithm iteratively refines the estimates for θ and q. Let θ_t and q_t be the estimates at iteration t. The algorithm proceeds as follows:

1. **E-Step (Expectation Step):** (14:22) Keep the model parameters θ_t fixed and find the optimal distribution q^*_{t+1} that maximizes the ELBO.

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

   It can be analytically shown that the optimal q that maximizes this bound is the true posterior distribution of the latent variables, conditioned on the data and the current parameters:

   $$q^*_{t+1}(z|x) = p_{\theta_t}(z|x)$$

2. **M-Step (Maximization Step):** (16:24) Keep the distribution q^*_{t+1} fixed and find the new model parameters θ^*_{t+1} that maximize the ELBO.

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

   This step involves maximizing the expected log-likelihood of the complete data (observed and latent), which is typically solved by differentiating the objective with respect to θ and setting the result to zero.

The following diagram illustrates the iterative nature of the EM algorithm.

```
graph TD
    subgraph "EM Iteration (t -> t+1)"
        direction LR
        E_Step["<b>E-Step</b><br/>Fix parameters  _t<br/>Compute optimal q*_{t+1}(z|x) = p_{ _t}(z|x)"]
    end
    Start["Initialize  _0"] --> E_Step
    M_Step --> E_Step
    M_Step --> End("Converged")
```

This diagram shows the alternating E-step and M-step of the EM algorithm, which continues until the parameters converge.

Convergence Guarantee

(18:16) A key property of the EM algorithm is that it guarantees that the log-likelihood will **never decrease** at each iteration:

$$L(\theta_{t+1}) \geq L(\theta_t)$$

While this does not guarantee convergence to the global maximum, it ensures monotonic improvement, typically leading to a good local maximum.

Application: Gaussian Mixture Models (GMM)

(06:55) The instructor uses the Gaussian Mixture Model (GMM) as a concrete example from classical machine learning to illustrate the EM algorithm.

GMM as a Latent Variable Model

A GMM is a probabilistic model that assumes the observed data is generated from a mixture of several Gaussian distributions.

- **Latent Variable** z: (07:31) For a GMM with M components, the latent variable z is discrete and indicates which of the M Gaussians generated a data point x.

$$z \in \{1, 2, \dots, M\}$$

- **Model Parameters** θ: (10:25) The parameters of a GMM are:
  - **Mixing Coefficients** α_j: The prior probability of selecting component j, where $p_\theta(z = j) = \alpha_j$. These must satisfy $\alpha_j \geq 0$ and $\sum_{j=1}^{M} \alpha_j = 1$.
  - **Component Means** μ_j: The mean of each Gaussian component, $\mu_j \in \mathbb{R}^d$.
  - **Component Covariances** Σ_j: The covariance matrix of each Gaussian component, $\Sigma_j \in \mathbb{R}^{d\times d}$. The full set of parameters is $\theta = \{\alpha_j, \mu_j, \Sigma_j\}_{j=1}^{M}$.
- **Likelihood Function**: The likelihood of a data point x is a weighted sum of the Gaussian densities:

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

EM Algorithm for GMM

(18:53) For a GMM, the steps of the EM algorithm have a clear, analytical form.

- **E-Step**: (19:06) This step corresponds to computing the posterior probability of the latent variable z given the data x and the current parameters θ_t. This is often called the "responsibility" that component j takes for data point x.

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

- **M-Step**: (22:53) This step involves updating the parameters θ to maximize the ELBO, using the responsibilities computed in the E-step. This leads to closed-form update rules for α_j, μ_j, and Σ_j.

Limitations and The Path to Deep Generative Models

(26:00) The instructor concludes by highlighting a critical limitation of the standard EM algorithm, which motivates the development of more powerful generative models.

- **The Intractability Problem Revisited**: The EM algorithm is only feasible if the posterior distribution $p_\theta(z|x)$ can be computed. This is true for GMMs but is **not true** for more complex models where $p_\theta(x)$ is defined by an intricate function, such as a deep neural network. In such cases, the denominator $p_\theta(x) = \int p_\theta(x, z)dz$ is intractable, making the posterior $p_\theta(z|x) = \frac{p_\theta(x,z)}{p_\theta(x)}$ also intractable.
- **The Core Question for Modern Generative Models**: (28:05) > How do we learn a latent variable model for cases where the posterior $p_\theta(z|x)$ is unknown or intractable?

This question is the central challenge that models like **Variational Autoencoders (VAEs)** and **Diffusion Models** are designed to solve. They use neural networks to approximate these intractable distributions, extending the fundamental principles of ELBO and EM into the deep learning era.

Self-Assessment for This Video

1. **Explain** why the log-likelihood function $L(\theta) = \log \int p_\theta(x, z)dz$ is generally intractable for latent variable models.

2. **Derive** the Evidence Lower Bound (ELBO) from the log-likelihood, clearly stating where and why Jensen's Inequality is applied.
3. The ELBO is a function of which two quantities? Write down the final joint optimization problem that we aim to solve.
4. Describe the two alternating steps of the Expectation-Maximization (EM) algorithm. What is being optimized in each step, and what is held constant?
5. In the context of a GMM, what does the latent variable z represent? What are the three types of parameters that constitute θ?
6. What is the key condition that must be met for the standard EM algorithm to be applicable? Why does this condition fail for complex models like VAEs?

Key Takeaways from This Video

- **ELBO is a Tractable Proxy**: Direct optimization of log-likelihood in latent variable models is often impossible. The ELBO provides a computable lower bound that we can maximize instead.
- **Learning is Joint Optimization**: Training a latent variable model requires finding the best model parameters (θ) and the best approximation for the posterior (q) simultaneously.
- **EM is an Iterative Solution**: The EM algorithm provides an elegant, iterative way to perform this joint optimization by alternating between updating the posterior approximation (E-step) and updating the model parameters (M-step).
- **GMM is a Foundational Example**: Gaussian Mixture Models are a classic, analytically tractable case where the EM algorithm can be applied directly.
- **Intractable Posteriors Motivate Deep Generative Models**: The inability to compute the true posterior $p_\theta(z|x)$ in complex models is the primary reason for the development of advanced methods like VAEs, which use neural networks to learn an approximation.