Study Material - Youtube

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Video Overview

This lecture, "ELBO for DDPM: Part 1," is a core component of the "Mathematical Foundations of Generative AI" series. The primary focus is on the detailed mathematical derivation and simplification of the Evidence Lower Bound (ELBO) objective function for Denoising Diffusion Probabilistic Models (DDPMs). The instructor begins by drawing a parallel between the familiar ELBO from Variational Autoencoders (VAEs) and the more complex, hierarchical version required for DDPMs. The lecture meticulously breaks down the DDPM's joint probability distribution and the corresponding variational posterior, setting the stage for a rigorous algebraic manipulation of the ELBO. This module is mathematically intensive and serves as the foundation for understanding how DDPMs are trained.

Learning Objectives

Upon completing this lecture, students will be able to: - Understand the formulation of the Evidence Lower Bound (ELBO) specifically for Denoising Diffusion Probabilistic Models (DDPMs). - Recognize the connection and analogy between the ELBO in VAEs and DDPMs. - Deconstruct the joint probability distributions for both the reverse (decoding) and forward (encoding) processes in a DDPM. - Follow the initial algebraic steps to expand and simplify the DDPM ELBO expression. - Appreciate the role of Markov properties and Bayes' rule in the derivation.

Prerequisites

To fully grasp the concepts in this video, students should have a solid understanding of: - **Probability Theory:** Conditional probability, joint distributions, Bayes' rule, and the concept of expectation. - **Information Theory:** Basic concepts like KL-divergence and its properties. - **Variational Autoencoders (VAEs):** A strong familiarity with the VAE architecture, its objective function (ELBO), and the reparameterization trick. - **Markov Chains:** Understanding of first-order Markov properties. - **Calculus and Linear Algebra:** Comfort with multivariate calculus, especially gradients, and basic linear algebra concepts.

Key Concepts Covered in This Video

- Evidence Lower Bound (ELBO) for Latent Variable Models
- Denoising Diffusion Probabilistic Models (DDPMs) as Hierarchical Latent Variable Models

- Forward (Encoding) Process: $q(x_{1:T}|x_0)$
- Reverse (Decoding) Process: $P_\theta(x_{0:T})$
- Markovian Assumptions in Forward and Reverse Processes
- Algebraic Simplification of the DDPM ELBO

Deep Understanding: The ELBO for DDPMs

This section provides a detailed, step-by-step derivation of the Evidence Lower Bound (ELBO) for Denoising Diffusion Probabilistic Models (DDPMs), as presented by the instructor.

Intuitive Foundation: From VAEs to DDPMs

(00:38) The instructor begins by grounding the discussion in the familiar context of Variational Autoencoders (VAEs). This serves as a crucial intuitive bridge to the more complex DDPM framework.

VAE ELBO Recap

In a standard VAE, we aim to maximize the log-likelihood of the data, $\log P_\theta(x)$. This is often intractable, so we introduce a latent variable z and work with the joint distribution $P_\theta(x, z)$. The log-likelihood is then expressed as an integral over the latent space:

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

To make this optimizable, we introduce a variational posterior $q_\phi(z|x)$ (the encoder) and derive the Evidence Lower Bound (ELBO), which is a lower bound on the log-likelihood. The VAE ELBO is:

$$J_\theta(q_\phi) = \mathbb{E}_{q_\phi(z|x)} \left[\log \frac{P_\theta(x, z)}{q_\phi(z|x)} \right] \leq \log P_\theta(x)$$

Maximizing this ELBO with respect to the model parameters θ and variational parameters ϕ serves as a proxy for maximizing the true log-likelihood.

DDPM as a Hierarchical Latent Variable Model

(00:49) A DDPM can be viewed as a deep, hierarchical latent variable model. Instead of a single latent variable z, a DDPM has a sequence of latent variables $x_1, x_2, \ldots, x_T$, where each latent variable has the same dimensionality as the original data x_0.

The relationship between these models can be visualized as follows:

```
graph TD
    A["Latent Variable Models"] --> B["VAE (Single Latent Variable)"];
    A --> C["DDPM (Hierarchical Latent Variables)"];
    B --> D["ELBO: $\mathbb{E}_{q_\phi(z|x)}[\log \frac{P_\theta(x,z)}{q_\phi(z|x)}]$"];
    C --> E["ELBO: $\mathbb{E}_{q(x_{1:T}|x_0)}[\log \frac{P_\theta(x_{0:T})}{q(x_{1:T}|x_0)}]$"];
    D --> F["Learnable Encoder $q_\phi(z|x)$<br/>Learnable Decoder $P_\theta(x|z)$"];
    E --> G["Fixed Encoder (Forward Process) $q(x_t|x_{t-1})$<br/>Learnable Decoder (Reverse Process) $P
```

Figure 1: A concept map illustrating the relationship between VAEs and DDPMs as latent variable models and their respective ELBO formulations.

Mathematical Formulation of the DDPM ELBO

(02:18) The core of the lecture is to define and simplify the ELBO for DDPMs. The objective function is analogous to the VAE ELBO but adapted for the sequence of latent variables.

The ELBO for a DDPM is given by:

$$J_\theta(q)^{DDPM} = \mathbb{E}_{q(x_{1:T}|x_0)}\left[\log \frac{P_\theta(x_{0:T})}{q(x_{1:T}|x_0)}\right]$$

Let's break down the components: - x_0: The original, clean data point (e.g., an image). - $x_{1:T} = (x_1, x_2, \ldots, x_T)$: The sequence of latent variables, which are progressively noisier versions of x_0. - $P_\theta(x_{0:T})$: The **model** or **reverse (decoding) process**. This is what we want to learn. It defines how to generate a clean image x_0 starting from pure noise x_T. It is parameterized by θ. - $q(x_{1:T}|x_0)$: The **variational posterior** or **forward (encoding) process**. This defines how noise is incrementally added to the data. In DDPMs, this process is **fixed** and has no learnable parameters.

Expanding the Probability Distributions

To simplify the ELBO, we first expand the numerator and denominator using their Markovian properties.

1. **The Reverse Process (Model)** $P_\theta(x_{0:T})$ (01:23): The reverse process is a Markov chain that starts from a prior $p(x_T)$ and denoises step-by-step.

$$P_\theta(x_{0:T}) = p(x_T)\prod_{t=1}^{T} P_\theta(x_{t-1}|x_t)$$

   - **Intuition:** This is the generative process. We start with a sample x_T from a simple distribution (e.g., a standard Gaussian $\mathcal{N}(0, I)$) and iteratively apply a learned denoising function $P_\theta(x_{t-1}|x_t)$ to eventually produce the clean data x_0. Each denoising step $P_\theta(x_{t-1}|x_t)$ is also modeled as a Gaussian with a learnable mean $\mu_\theta(x_t)$ and covariance $\Sigma_\theta(x_t)$.
2. **The Forward Process (Variational Posterior)** $q(x_{1:T}|x_0)$ (03:14): The forward process is also a Markov chain, but it adds noise incrementally.

$$q(x_{1:T}|x_0) = \prod_{t=1}^{T} q(x_t|x_{t-1})$$

   - **Intuition:** This is the diffusion process. We start with the clean data x_0 and add a small amount of Gaussian noise at each step t according to a fixed, predefined schedule. This process is not learned.

Optimizing the ELBO: The Derivation

The main goal is to rewrite the ELBO in a more tractable form, ideally as a sum of KL-divergences or other easily computable terms.

(04:35) The instructor begins the algebraic manipulation. Let's consider the term inside the expectation, which is the log-ratio of the joint distributions.

$$\log \frac{P_\theta(x_{0:T})}{q(x_{1:T}|x_0)} = \log P_\theta(x_{0:T}) - \log q(x_{1:T}|x_0)$$

Now, we substitute the expanded forms of the distributions:

$$= \log\left(p(x_T)\prod_{t=1}^{T} P_\theta(x_{t-1}|x_t)\right) - \log\left(\prod_{t=1}^{T} q(x_t|x_{t-1})\right)$$

Using the property that the log of a product is the sum of logs:

$$= \log p(x_T) + \sum_{t=1}^{T} \log P_\theta(x_{t-1}|x_t) - \sum_{t=1}^{T} \log q(x_t|x_{t-1})$$

This expression can be regrouped as follows:

$$= \log p(x_T) + \sum_{t=2}^{T} (\log P_\theta(x_{t-1}|x_t) - \log q(x_t|x_{t-1})) + \log P_\theta(x_0|x_1) - \log q(x_1|x_0)$$

The instructor then introduces a crucial manipulation using Bayes' rule to make the terms comparable.

The Bayes' Rule Trick

(16:00) The key insight is to express the forward transition $q(x_t|x_{t-1})$ in terms of a reverse-like term $q(x_{t-1}|x_t, x_0)$. This is possible because the entire forward trajectory is conditioned on the starting point x_0.

The forward process is a Markov chain: $x_0 \to x_1 \to \cdots \to x_T$. The conditional distribution of any latent variable x_{t-1} given its successor x_t and the starting point x_0 is given by Bayes' rule:

$$q(x_{t-1}|x_t, x_0) = \frac{q(x_t|x_{t-1}, x_0)q(x_{t-1}|x_0)}{q(x_t|x_0)}$$

Due to the Markov property of the forward process, $q(x_t|x_{t-1}, x_0) = q(x_t|x_{t-1})$. Therefore:

$$q(x_{t-1}|x_t, x_0) = \frac{q(x_t|x_{t-1})q(x_{t-1}|x_0)}{q(x_t|x_0)}$$

This is the "true" posterior for the reverse step, which we can calculate analytically because the forward process q is fully defined (as Gaussians).

Rewriting the ELBO

The instructor uses this to rewrite the ELBO. The derivation will continue in the next part of the lecture, but the setup is complete. The goal is to transform the ELBO into a sum of terms, each of which can be interpreted as a KL divergence. This will ultimately lead to a loss function that compares the learned reverse process $P_\theta(x_{t-1}|x_t)$ with the true reverse posterior $q(x_{t-1}|x_t, x_0)$ at each timestep.

The algebraic manipulation process can be visualized as:

```
sequenceDiagram
    participant E as ELBO
    participant P as Model P_theta
    participant Q as Posterior q
    participant B as Bayes' Rule

    E->>P: Expand log P_theta(x_{0:T})
    P-->>E: Sum of log terms
    E->>Q: Expand log q(x_{1:T}|x_0)
    Q-->>E: Sum of log terms
    E->>E: Combine terms
    E->>B: Apply to q(x_t|x_{t-1})
    B-->>E: Rewrite q in reverse form
    E->>E: Substitute and simplify
```

Figure 2: Sequence diagram showing the steps to simplify the DDPM ELBO.

Key Mathematical Concepts

1. DDPM ELBO Objective Function

The central equation of this lecture is the Evidence Lower Bound for DDPMs. - **Formula (00:12, 02:49):**

$$J_\theta(q)^{DDPM} = \mathbb{E}_{q(x_{1:T}|x_0)}\left[\log \frac{P_\theta(x_{0:T})}{q(x_{1:T}|x_0)}\right]$$

- **Intuition:** We want to maximize this lower bound on the data log-likelihood. This is equivalent to minimizing the KL-divergence between the true data-generating process (approximated by our forward process q) and our learned model P_θ. The expectation is over all possible noising trajectories starting from a data point x_0.

2. Reverse Process (Model)

This is the learned generative part of the model. - **Formula (01:27):**

$$P_\theta(x_{0:T}) = p(x_T)\prod_{t=1}^{T} P_\theta(x_{t-1}|x_t)$$

- **Transition Step (01:44):** Each step is a Gaussian with learnable parameters.

$$P_\theta(x_{t-1}|x_t) \triangleq \mathcal{N}(x_{t-1}; \mu_\theta(x_t), \Sigma_\theta(x_t))$$

- **Intuition:** The model learns a sequence of denoising steps. Starting from pure noise $x_T \sim \mathcal{N}(0, I)$, it applies a neural network (parameterized by θ) at each step t to predict the parameters of the distribution for the less noisy state x_{t-1}.

3. Forward Process (Variational Posterior)

This is the fixed, non-learnable noising process. - **Formula (03:14):**

$$q(x_{1:T}|x_0) = \prod_{t=1}^{T} q(x_t|x_{t-1})$$

- **Intuition:** This describes how a clean image x_0 is gradually destroyed by adding Gaussian noise over T steps. The parameters of this process are fixed according to a predefined "variance schedule."

4. True Reverse Posterior (derived from Forward Process)

This is a key quantity used for training, derived using Bayes' rule. - **Formula (16:43):**

$$q(x_{t-1}|x_t, x_0) = \frac{q(x_t|x_{t-1})q(x_{t-1}|x_0)}{q(x_t|x_0)}$$

- **Intuition (17:55):** This term represents the "true" distribution for a single denoising step. It tells us the distribution of the previous state x_{t-1} given the current state x_t *and* the original clean image x_0. Since we know the entire forward process, this distribution is tractable and can be computed. The goal of training is to make our learned reverse step $P_\theta(x_{t-1}|x_t)$ match this true reverse step $q(x_{t-1}|x_t, x_0)$.

Visual Elements from the Video

The entire lecture is presented on a digital whiteboard, with the instructor writing out all equations and explanations by hand.

- **00:12 - 00:37:** The initial formulation of the DDPM ELBO is presented, highlighting the expectation over the forward process q and the log-ratio of the reverse process P_θ to the forward process q.
- **00:38 - 02:48:** The instructor provides a recap of the VAE ELBO, writing out the log-likelihood and the standard ELBO formula to build an analogy.
- **00:45 - 01:59:** The definitions of the reverse process $P_\theta(x_{0:T})$ and its Gaussian transition steps $P_\theta(x_{t-1}|x_t)$ are written and explained. The terms "data" (x_0) and "latent var" ($x_{1:T}$) are explicitly labeled.
- **03:14 - 04:34:** The forward process $q(x_{1:T}|x_0)$ is defined as a product of Markovian transitions.
- **16:00 - 17:21:** The crucial derivation using Bayes' rule to express the forward transition in terms of a reverse-like posterior is shown.
- **22:36 - 24:22:** The instructor plugs the derived expressions back into the ELBO and begins the simplification process, showing how the log of products becomes a sum of logs and how terms can be regrouped.

Self-Assessment for This Video

1. **Conceptual Question:** Explain the core analogy between the VAE ELBO and the DDPM ELBO. What corresponds to the encoder, decoder, and latent variable in the DDPM framework?
2. **Formula Transcription:** Write down the complete mathematical expression for the DDPM ELBO. Define each term (P_θ, q, x_0, $x_{1:T}$) and explain its role in the diffusion model.
3. **Derivation Step:** Starting from the forward process definition $q(x_{1:T}|x_0) = \prod_{t=1}^{T} q(x_t|x_{t-1})$, show how to derive the expression for the true reverse posterior $q(x_{t-1}|x_t, x_0)$ using Bayes' rule. Why is this term important for training?
4. **Algebraic Manipulation:** The instructor rewrites the ELBO as a sum of three main terms (a log prior, a sum from $t = 2$ to T, and a final term for $t = 1$). Replicate this algebraic step starting from the initial ELBO formula.
5. **First-Order Markov Property:** Explain why the forward process $q(x_{1:T}|x_0)$ can be simplified from $q(x_1|x_0)q(x_2|x_1, x_0)...$ to $\prod_{t=1}^{T} q(x_t|x_{t-1})$. Why is this assumption critical for the model's tractability?

Key Takeaways from This Video

- **DDPMs are Latent Variable Models:** They can be understood as a deep, hierarchical VAE with a sequence of latent variables.
- **The Objective is the ELBO:** DDPMs are trained by maximizing the Evidence Lower Bound, which forces the learned reverse (denoising) process to match the true (but intractable) data distribution.
- **Two Key Processes:** The model consists of a fixed **forward process** (q) that adds noise and a learned **reverse process** (P_θ) that removes noise.
- **The Goal of Derivation:** The complex ELBO expression is algebraically manipulated to break it down into a sum of more manageable terms, which will ultimately become KL-divergences between Gaussian distributions.
- **Bayes' Rule is the Key:** The critical insight for simplifying the ELBO is using Bayes' rule to express the forward process transitions in terms of reverse process posteriors, which allows for direct comparison and optimization.