Study Material - Youtube

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Video Overview

This lecture, "Variational Divergence Minimization," is a segment of the "Mathematical Foundations of Generative AI" series by Prof. Prathosh A P. It provides a rigorous mathematical framework for understanding how generative models can be trained. The core of the lecture is to reframe the problem of minimizing the difference (divergence) between two probability distributions as a tractable optimization problem that can be solved using only samples, which is crucial when the true probability density functions are unknown. The instructor introduces the concept of **f-divergence** as a general measure of distance between distributions and then uses the powerful tool of **Fenchel-Rockafellar duality** (specifically, the convex conjugate) to derive a variational lower bound on this divergence. This transforms the intractable problem into a solvable one based on expectations, which can be approximated using sample averages.

Learning Objectives

Upon completing this lecture, students will be able to: - **Understand the fundamental goal of generative modeling:** To train a model distribution P_θ to match an unknown true data distribution P_x. - **Frame the training process as a divergence minimization problem:** Specifically, minimizing the f-divergence $D_f(P_x \| P_\theta)$. - **Recognize the primary challenge:** The density functions P_x and P_θ are often unknown or intractable, making direct computation of the f-divergence impossible. - **Define and understand the concept of a convex conjugate (Fenchel conjugate)** of a function. - **Follow the derivation of the variational lower bound of the f-divergence** using its dual representation. - **Appreciate how this variational form converts the problem into one of computing expectations**, which can be approximated from samples.

Prerequisites

To fully grasp the concepts in this lecture, students should have a solid understanding of: - **Probability Theory:** Probability distributions, probability density functions (PDFs), and the concept of expectation. - **Calculus:** Integration, differentiation, and basic optimization concepts like supremum. - **Linear Algebra:**

Basic familiarity with vectors and spaces. - **Convex Analysis:** A basic understanding of convex functions is essential. - **Machine Learning:** Familiarity with the basic idea of neural networks as function approximators.

Key Concepts Covered

- Generative Modeling Framework
- f-Divergence (including JS-Divergence and Total Variation Distance as examples)
- The Law of Large Numbers (LOTUS)
- Convex Conjugate (Fenchel Conjugate)
- Fenchel-Rockafellar Duality
- Variational Lower Bound of f-Divergence

The Generative Modeling Problem

The Goal: Learning an Unknown Distribution

(00:27) The fundamental task in generative modeling is to learn a model that can produce new data similar to a given dataset. We start with a dataset D containing n data points:

$$D = \{x_1, x_2, ..., x_n\}$$

We assume these data points are **independent and identically distributed (i.i.d.)** samples drawn from a true, but unknown, data distribution, which we denote as P_x.

> **The Goal of Generative Modeling:** The ultimate objective is to create a model that learns the underlying patterns of P_x so well that it can generate new, synthetic samples that are indistinguishable from the real data. In essence, we want to **learn to sample from** P_x.

The Framework: A Neural Network Generator

(01:08) To achieve this, we design a **generative model**, typically a deep neural network, which we'll call the generator, $g_\theta(z)$.

- **Input:** The generator takes a random vector z as input. This vector is sampled from a simple, well-known distribution, such as a standard normal (Gaussian) distribution, $\mathcal{N}(0, I)$. This input space is often called the **latent space**.
- **Transformation:** The neural network g_θ, parameterized by weights and biases θ, performs a complex, non-linear transformation on the input vector z.
- **Output:** The output of the generator is a synthetic data sample, $\hat{x} = g_\theta(z)$, which lives in the same space as our real data.

The distribution of these generated samples, $\hat{x}$, defines our **model distribution**, which we denote as P_θ. The parameters θ of the neural network control the shape and characteristics of this distribution.

The entire process can be visualized as follows:

```
flowchart TD
    A["Latent Space<br/>Sample z ~ N(0, I)"] --> B["Generator Network<br/>g<sub>&theta;</sub>(z)"];
    B --> C["Data Space<br/>Generated Sample &xcirc; ~ P<sub>&theta;</sub>"];
```

Figure 1: A high-level diagram of the generative modeling process. A simple latent distribution is transformed by a neural network into a complex data distribution.

The Objective: Minimizing f-Divergence

(02:21) To make our model distribution P_θ as close as possible to the true data distribution P_x, we need a way to measure the "distance" or "difference" between them. A powerful and general way to do this is by using **f-divergence**.

The goal is to find the optimal set of parameters θ^* that minimizes this divergence:

$$\theta^* = \arg\min_\theta D_f(P_x \| P_\theta)$$

Here, D_f represents any valid f-divergence, which is defined by a convex function f such that $f(1) = 0$.

The Challenge: Working Without Density Functions

(03:21) The mathematical definition of f-divergence is:

$$D_f(P_x \| P_\theta) = \int P_\theta(x) f\left(\frac{P_x(x)}{P_\theta(x)}\right) dx$$

This formula presents a significant practical challenge:

1. **Unknown True Distribution (P_x):** We do not have an analytical form for the true data distribution $P_x(x)$. We only have access to samples from it (our dataset D).
2. **Intractable Model Distribution (P_θ):** Even for our own model, the density function $P_\theta(x)$ is usually intractable. Because g_θ is a complex, high-dimensional, non-linear function, computing its inverse and the corresponding change of variables to get the density $P_\theta(x)$ is practically impossible.

   The Core Problem: How can we minimize a quantity that we cannot compute? We need a method that relies only on our ability to draw samples from both distributions, not on their explicit density functions.

Variational Divergence Minimization: The Core Idea

The solution lies in transforming the f-divergence into a different form—one that can be estimated using samples. This is achieved through a powerful mathematical concept known as **Fenchel-Rockafellar duality**.

From Integrals to Expectations: The Law of Large Numbers

(07:35) The bridge between intractable integrals and a practical, sample-based approach is the **Law of Large Numbers (LLN)**. Specifically, the Law of the Unconscious Statistician (LOTUS) tells us that the expectation of a function $h(x)$ under a distribution P_x is:

$$\mathbb{E}_{x \sim P_x}[h(x)] = \int h(x) P_x(x) dx$$

The LLN states that we can approximate this expectation using a sample average:

$$\mathbb{E}_{x \sim P_x}[h(x)] \approx \frac{1}{N} \sum_{i=1}^{N} h(x_i), \quad \text{where } x_i \sim \text{i.i.d. from } P_x$$

This approximation becomes more accurate as the number of samples N increases.

Our strategy is to rewrite the f-divergence in a form that involves expectations, so we can use this sample-based approximation.

The Fenchel-Rockafellar Duality

Convex Conjugate: Intuition and Definition

(19:25) The key tool for this transformation is the **convex conjugate** (or Fenchel conjugate) of a function. For any convex function $f(u)$, its conjugate $f^*(t)$ is defined as:

$$f^*(t) = \sup_{u \in \text{dom}(f)} \{ut - f(u)\}$$

- **Intuition:** The term $ut - f(u)$ can be seen as the vertical distance (gap) between the line $y = ut$ and the function $f(u)$. The conjugate $f^*(t)$ finds the maximum possible gap for a given slope t by varying the point u.
- **Pointwise Supremum:** This is a pointwise definition. For every value of t, we solve an optimization problem over u to find the value of $f^*(t)$.

Key Properties of the Conjugate

(26:56) The convex conjugate has two crucial properties for our derivation:

1. **Convexity:** The conjugate function $f^*(t)$ is always convex, regardless of whether the original function f was strictly convex.
2. **Duality (Fenchel-Moreau Theorem):** The conjugate of the conjugate is the original function. This is a powerful duality relationship.

$$f(u) = (f^*)^*(u) = \sup_{t \in \text{dom}(f^*)} \{tu - f^*(t)\}$$

This second property allows us to express any convex function $f(u)$ as a supremum over a simpler, linear-in-u expression.

Deriving the Variational Lower Bound for f-Divergence

(28:52) We can now derive the variational form of the f-divergence.

1. **Start with the f-divergence definition:**

$$D_f(P_x \| P_\theta) = \int P_\theta(x) f\left(\frac{P_x(x)}{P_\theta(x)}\right) dx$$

2. **Substitute the dual form of $f(u)$:** We replace $f(u)$ with its conjugate representation, where $u = \frac{P_x(x)}{P_\theta(x)}$.

$$D_f(P_x \| P_\theta) = \int P_\theta(x) \left[\sup_t \left\{ t \cdot \frac{P_x(x)}{P_\theta(x)} - f^*(t) \right\}\right] dx$$

3. **Introduce a Function Space:** The optimal t in the supremum depends on the value of u, which in turn depends on x. Therefore, the supremum is not over a single scalar t, but over a class of functions $T(x)$. This gives us a variational form.

$$D_f(P_x \| P_\theta) = \sup_{T \in \mathcal{T}} \int P_\theta(x) \left\{ T(x) \frac{P_x(x)}{P_\theta(x)} - f^*(T(x)) \right\} dx$$

Here, $\mathcal{T}$ is the space of all possible functions from the data domain $\mathcal{X}$ to the domain of f^*.

4. **Separate the Integral:** We can split the integral into two parts.

$$D_f(P_x \| P_\theta) = \sup_{T \in \mathcal{T}} \left(\int P_\theta(x) T(x) \frac{P_x(x)}{P_\theta(x)} dx - \int P_\theta(x) f^*(T(x)) dx \right)$$

5. **Simplify and Express as Expectations:** The $P_\theta(x)$ terms in the first integral cancel out. We can now recognize both integrals as expectations.

$$D_f(P_x \| P_\theta) = \sup_{T \in \mathcal{T}} \left(\int T(x) P_x(x) dx - \int f^*(T(x)) P_\theta(x) dx \right)$$

This leads to the final variational representation:

$$D_f(P_x \| P_\theta) = \sup_{T \in \mathcal{T}} \left\{ \mathbb{E}_{x \sim P_x}[T(x)] - \mathbb{E}_{x \sim P_\theta}[f^*(T(x))] \right\}$$

The Breakthrough: This final expression is a significant achievement. We have transformed the f-divergence, which required knowing the density functions, into an optimization problem over a function $T(x)$ that only involves expectations. These expectations can be approximated using samples from P_x (our real data) and P_θ (our generator's output).

The Final Optimization Objective

(31:49) The derived variational form gives us a practical way to minimize the f-divergence. Our original goal was:

$$\min_\theta D_f(P_x \| P_\theta)$$

Using the variational representation, this becomes a minimax problem:

$$\min_\theta \max_{T \in \mathcal{T}} \left\{ \mathbb{E}_{x \sim P_x}[T(x)] - \mathbb{E}_{x \sim P_\theta}[f^*(T(x))] \right\}$$

Here, the function $T(x)$ is often called the **discriminator** or **critic** in the context of Generative Adversarial Networks (GANs). It is another neural network that we train simultaneously with the generator g_θ.

The optimization proceeds as follows: 1. **Inner Loop (Maximization):** For a fixed generator g_θ, we find the best function $T(x)$ that maximizes the lower bound. 2. **Outer Loop (Minimization):** We then update the generator's parameters θ to minimize the value of this maximized bound.

This adversarial, two-player game is the foundation of many modern generative models.

Key Mathematical Concepts

f-Divergence Examples

- **JS-Divergence:** (00:11)
$$f(u) = \frac{1}{2} \left(u \log u - (u+1) \log \left(\frac{u+1}{2} \right) \right)$$
- **Total Variation Distance:** (00:13)
$$f(u) = \frac{1}{2} |u - 1|$$

Generative Model Objective

- **Goal:** Minimize the divergence between the true data distribution P_x and the model distribution P_θ.

$$\theta^* = \arg\min_\theta D_f(P_x \| P_\theta)$$

Convex Conjugate (Fenchel Conjugate)

- **Definition:** (20:50) For a convex function $f(u)$, its conjugate $f^*(t)$ is:

$$f^*(t) = \sup_{u \in \text{dom}(f)} \{ut - f(u)\}$$

- **Duality:** (27:13) The original function can be recovered from its conjugate:

$$f(u) = \sup_{t \in \text{dom}(f^*)} \{tu - f^*(t)\}$$

Variational Lower Bound of f-Divergence

- **The final, crucial result:** (31:49)

$$D_f(P_x \| P_\theta) \geq \sup_{T(x) \in \mathcal{T}} \left\{ \mathbb{E}_{x \sim P_x}[T(x)] - \mathbb{E}_{x \sim P_\theta}[f^*(T(x))] \right\}$$

  This provides a lower bound on the divergence that can be estimated from samples.

Visual Elements from the Video

- **Generative Model Diagram (01:30):** The instructor draws a simple block diagram illustrating the flow of the generative model. A latent variable z from a simple distribution is fed into the generator network g_θ to produce a sample $\hat{x}$ from the complex model distribution P_θ.

```
graph TD
    subgraph Generative Model
        Z["z ~ N(0, I)"] --> G["g<sub>&theta;</sub>(z)<br/>Generator Network"];
        G --> X_hat["&xcirc; ~ P<sub>&theta;</sub>(x)"];
    end
```

Figure 2: Diagram illustrating the generative model architecture as shown in the lecture.

- **Convex Function and Tangent Lines (22:05):** The instructor draws a parabola to represent a convex function $f(u)$ and illustrates how the term $ut - f(u)$ in the conjugate definition represents the gap between a line with slope t and the function itself. This visual helps build intuition for the supremum operation.

Self-Assessment for This Video

1. **Conceptual Questions:**
   - What is the primary goal of a generative model in the context of probability distributions?
   - Why is it generally impossible to directly calculate the f-divergence between a model distribution P_θ and the true data distribution P_x?
   - Explain the intuitive meaning of the convex conjugate $f^*(t)$. What does the supremum operation achieve?

- What is the "variational" aspect of the derived lower bound for f-divergence? Why do we optimize over a space of functions $T(x)$ instead of a scalar t?

2. **Mathematical Problems:**
   - Given the Law of Large Numbers, write down the sample-based approximation for the variational lower bound of the f-divergence.
   - The f-divergence for the forward KL-divergence is given by $f(u) = u \log u$. Find its convex conjugate, $f^*(t)$.
   - Using your result from the previous question, write down the variational lower bound for the KL-divergence $D_{KL}(P_x \| P_\theta)$.

Key Takeaways from This Video

- **Generative modeling is divergence minimization.** Training a generative model is equivalent to finding model parameters θ that minimize the f-divergence between the model distribution P_θ and the true data distribution P_x.
- **Direct optimization is intractable.** We cannot compute the f-divergence directly because we lack analytical forms for the probability density functions.
- **Fenchel-Rockafellar duality is the key.** By using the convex conjugate, we can derive a variational lower bound for the f-divergence.
- **The problem is transformed into expectation computation.** The variational form involves expectations with respect to P_x and P_θ, which can be approximated using samples from the real dataset and the generator network.
- **This sets the stage for adversarial training.** The final objective is a minimax problem, which forms the theoretical basis for training algorithms like Generative Adversarial Networks (GANs).