Study Material - Youtube

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Video Overview

This lecture, "Variational Divergence Minimization," is part of the "Mathematical Foundations of Generative AI" series. It provides a foundational understanding of how to train generative models when the true data distribution is unknown and only accessible through samples. The core idea is to reframe the problem of minimizing an f-divergence between two distributions into a tractable optimization problem. The instructor introduces the standard generative modeling setup, highlights the challenge of dealing with unknown probability densities, and then masterfully derives a variational lower bound for the f-divergence using the concept of the Fenchel-Legendre conjugate. This derivation forms the theoretical basis for many modern generative models, particularly Generative Adversarial Networks (GANs).

Learning Objectives

Upon completing this lecture, students will be able to: - **Understand the fundamental goal of generative modeling:** To learn a model distribution p_θ that approximates an unknown true data distribution p_x. - **Formulate generative modeling as a divergence minimization problem:** Specifically, minimizing the f-divergence $D_f(p_x||p_\theta)$. - **Identify the primary challenge:** The intractability of computing the divergence directly because the density functions p_x and p_θ are unknown. - **Grasp the concept of the Fenchel-Legendre (convex) conjugate:** Understand its definition and the duality property where the conjugate of a conjugate returns the original function. - **Follow the step-by-step derivation of the variational lower bound for f-divergence:** This is the central mathematical result of the lecture. - **Appreciate how this variational form makes the problem tractable:** By converting the objective into expectations that can be approximated using samples.

Prerequisites

To fully grasp the concepts in this lecture, students should have a solid understanding of: - **Probability and Statistics:** Probability density functions (PDFs), expectation of a random variable, and the Law of Large Numbers. - **Calculus:** Integrals, derivatives, and the concept of a supremum. - **Convex Analysis:** Basic familiarity with convex functions. - **Generative Models (Introductory):** A high-level understanding of what a generative model is and the role of a generator network.

Key Concepts Covered in This Video

- Generative Modeling Framework
- f-Divergence
- The Law of Large Numbers (LLN)
- Convex Conjugate (Fenchel-Legendre Transform)
- Variational Representation of f-Divergence

The Generative Modeling Problem

The Goal: Learning an Unknown Data Distribution

(0:29) The fundamental task in generative modeling is to learn from a given dataset. We assume we have a dataset D consisting of n data points:

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

These data points are assumed to be sampled **independently and identically distributed (i.i.d.)** from a true but unknown underlying data distribution, which we denote as p_x.

> **(0:58) Key Assumption:** The data points x_i are i.i.d. samples from p_x, written as $x_i \sim p_x$. We do not know the analytical formula for $p_x(x)$, but we have access to samples from it (our dataset D).

(1:18) The ultimate goal is to create a model that can generate new samples that look like they came from the original distribution p_x.

The Framework: Generator Networks

To achieve this, we build a generative model. A common approach, as discussed here, is to use a **deep neural network** as a generator, denoted by $g_\theta(z)$.

- **(1:43) The generator g_θ takes a simple noise vector z as input.** This vector is typically sampled from a well-known, simple distribution, such as a standard normal (Gaussian) distribution, $\mathcal{N}(0, I)$.
- **(1:49) The network transforms this noise vector into an output sample $\hat{x} = g_\theta(z)$.** The parameters of this network are denoted by θ.
- **(2:06) The distribution of these generated samples $\hat{x}$ is called the model distribution, $p_\theta(\hat{x})$.** Our goal is to adjust the parameters θ so that p_θ becomes a good approximation of p_x.

This process can be visualized as follows:

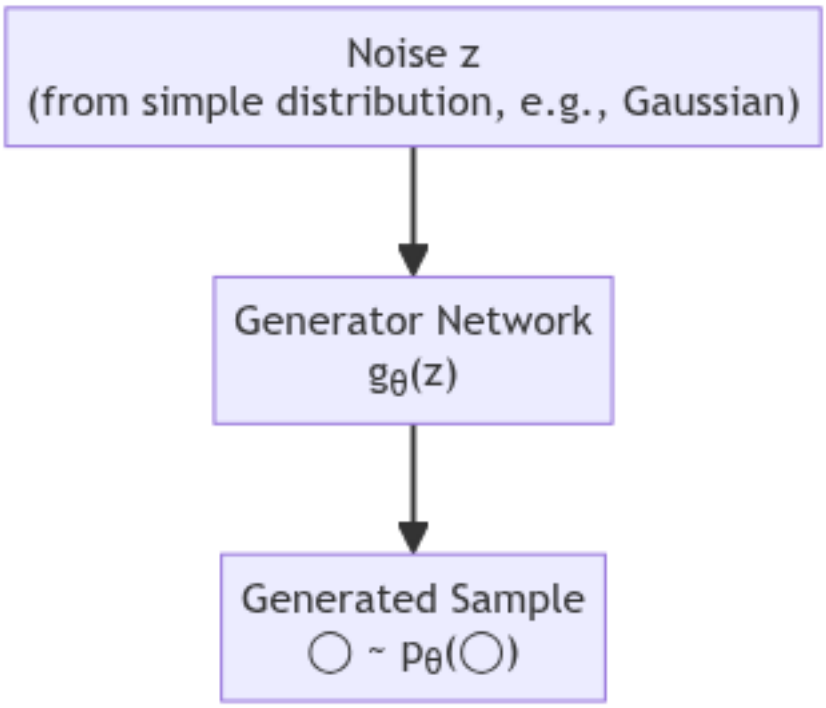


Figure 1: A flowchart illustrating the process of generating a sample using a generator network, as described at 1:30.

The Objective: Minimizing f-Divergence

To make the model distribution p_θ similar to the data distribution p_x, we need a way to measure the "distance" or "divergence" between them. This lecture uses the general family of **f-divergences**.

(3:02) The training objective is to find the optimal set of parameters θ^* that minimizes the f-divergence between the true data distribution and the model distribution:

$$\theta^* = \arg\min_\theta D_f(p_x||p_\theta)$$

This framework is very general and can represent various specific objectives depending on the choice of the function f. For example: - If $f(u) = u \log u$, this becomes the **Kullback-Leibler (KL) divergence**. - If $f(u) = \frac{1}{2}|u-1|$, this becomes the **Total Variation Distance**.

The Challenge of Intractable Densities

(3:21) A major hurdle arises when we try to compute the f-divergence directly. The definition of f-divergence is an integral over the entire data space X:

$$D_f(p_x||p_\theta) = \int_{x \in X} p_\theta(x) f\left(\frac{p_x(x)}{p_\theta(x)}\right) dx$$

This computation is practically impossible for several reasons: 1. **Unknown Densities:** We do not have the analytical expressions for $p_x(x)$ or $p_\theta(x)$. We only have the ability to draw samples from them. 2.

Intractable Integral: Even if we knew the densities, the integral is often over a very high-dimensional space (e.g., for images), making it computationally intractable to solve.

> **(4:24) The Core Problem:** How can we minimize a divergence metric that we cannot directly compute? The solution lies in finding an alternative formulation that relies only on samples, which we do have access to.

Variational Divergence Minimization: The Core Idea

The lecture presents a powerful technique to overcome this challenge by reformulating the f-divergence into a form that can be estimated from samples. This involves two key statistical and mathematical concepts.

From Integrals to Expectations: The Law of Large Numbers

(8:41) The first key idea is to connect integrals to expectations, which can then be approximated by sample averages.

- **Expectation as an Integral:** The expectation of a function $h(x)$ with respect to a probability distribution p_x is defined as:
$$I = \mathbb{E}_{x\sim p_x}[h(x)] = \int_x h(x)p_x(x)dx$$
- **(11:33) The Law of Large Numbers (LLN):** This fundamental theorem of statistics states that the average of a large number of i.i.d. samples of a random variable converges to its expected value. Given n i.i.d. samples $\{x_1, x_2, ..., x_n\}$ from p_x, we can approximate the expectation:
$$\mathbb{E}_{x\sim p_x}[h(x)] \approx \frac{1}{n}\sum_{i=1}^{n} h(x_i)$$
This approximation becomes more accurate as the number of samples n increases. In the limit, it's an equality:
$$\lim_{n\to\infty} \frac{1}{n}\sum_{i=1}^{n} h(x_i) = \mathbb{E}_{x\sim p_x}[h(x)]$$

This gives us a practical way to compute expectations using only samples, without needing to know the underlying density function.

The Fenchel-Legendre Duality: A New Representation for f-Divergence

The second key idea is to use a property of convex functions known as the **Fenchel-Legendre transform**, or **convex conjugate**, to rewrite $f(u)$.

- **(19:31) Definition of the Convex Conjugate:** For any convex function $f(u)$, its conjugate, denoted $f^*(t)$, is defined as:
$$f^*(t) = \sup_{u\in \text{dom}(f)} \{ut - f(u)\}$$
Here, sup denotes the supremum (the least upper bound), which for well-behaved functions is equivalent to the maximum. The optimization is over all possible values of u in the domain of f.
- **(27:23) Duality Property:** A crucial property is that the conjugate of the conjugate is the original function. This is known as Fenchel-Moreau theorem.
$$f(u) = (f^*)^*(u) = \sup_{t\in \text{dom}(f^*)} \{tu - f^*(t)\}$$

Deriving the Variational Lower Bound

We can now combine these ideas to derive a tractable form for the f-divergence.

1. **(29:08) Start with the definition of f-divergence:**

$$D_f(p_x||p_\theta) = \int_x p_\theta(x) f\left(\frac{p_x(x)}{p_\theta(x)}\right) dx$$

2. **(29:43) Apply the duality property to** $f(u)$, where $u = \frac{p_x(x)}{p_\theta(x)}$:

$$f\left(\frac{p_x(x)}{p_\theta(x)}\right) = \sup_{t \in \text{dom}(f^*)} \left\{ t \cdot \frac{p_x(x)}{p_\theta(x)} - f^*(t) \right\}$$

3. **(30:26) Substitute this back into the divergence integral:**

$$D_f(p_x||p_\theta) = \int_x p_\theta(x) \left[\sup_{t \in \text{dom}(f^*)} \left\{ t \cdot \frac{p_x(x)}{p_\theta(x)} - f^*(t) \right\} \right] dx$$

4. **(31:49) Introduce a function** $T(x)$**:** The optimal value of t in the supremum depends on the value of x. Therefore, we can replace the scalar variable t with a function $T(x)$. The search for the supremum is now over a space of functions $\mathcal{T}$. This gives the **variational representation**:

$$D_f(p_x||p_\theta) = \sup_{T \in \mathcal{T}} \int_x p_\theta(x) \left\{ T(x) \frac{p_x(x)}{p_\theta(x)} - f^*(T(x)) \right\} dx$$

5. **(33:47) Rearrange and express as expectations:**

$$D_f(p_x||p_\theta) = \sup_{T \in \mathcal{T}} \left\{ \int_x T(x) p_x(x) dx - \int_x p_\theta(x) f^*(T(x)) dx \right\}$$

   This can be written entirely in terms of expectations:

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

   (37:51) Important Insight: This final expression is a major breakthrough. It represents the f-divergence as a maximization problem over a class of functions $T(x)$. Crucially, the objective inside the maximization only involves expectations, which we can approximate using samples from p_x (our data) and p_θ (our generator). This forms a lower bound on the true divergence, often called the **variational lower bound**.

The process can be summarized with the following diagram:

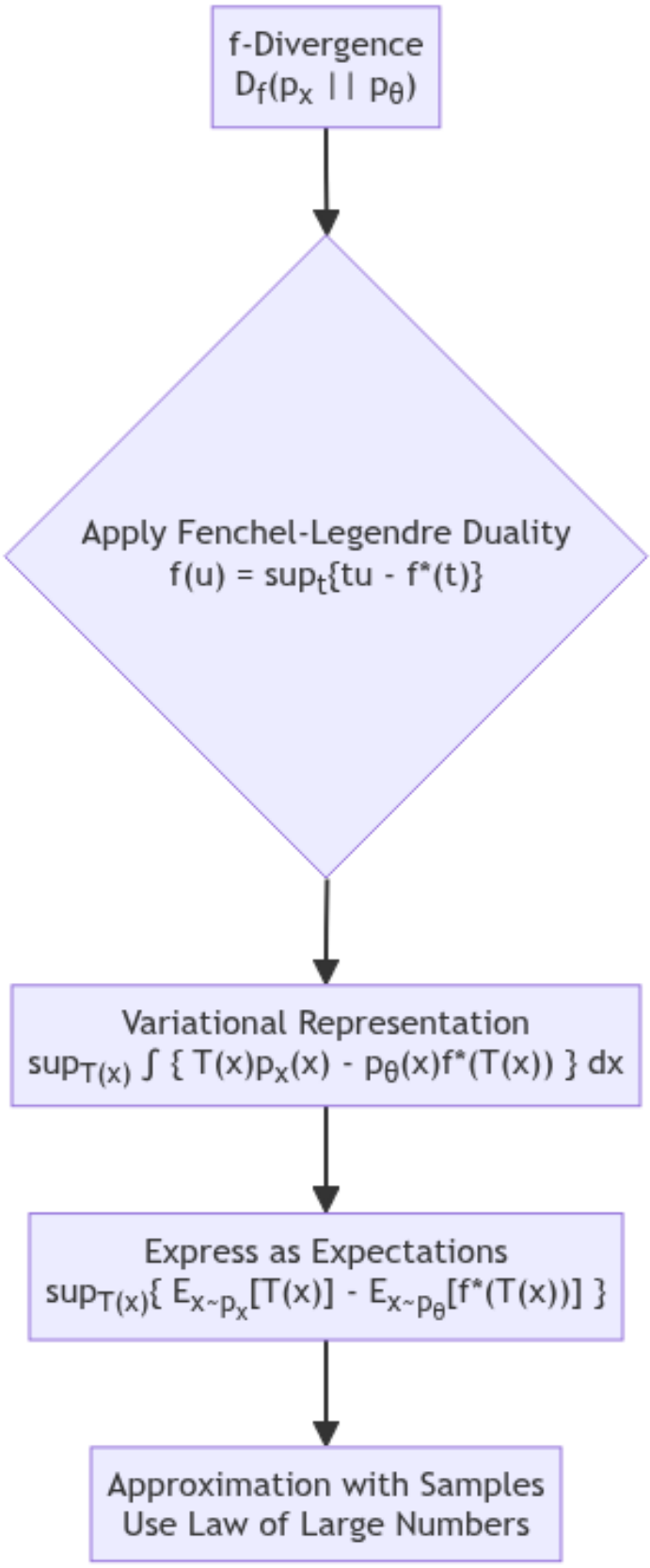

f-Divergence
$D_f(p_x \mid\mid p_\theta)$
Apply Fenchel-Legendre Duality
$f(u) = \sup_t\{tu - f^*(t)\}$
Variational Representation
$\sup_{T(x)} \int \{ T(x)p_x(x) - p_\theta(x)f^*(T(x)) \} dx$
Express as Expectations
$\sup_{T(x)}\{ E_{x\sim p_x}[T(x)] - E_{x\sim p_\theta}[f^*(T(x))] \}$
Approximation with Samples
Use Law of Large Numbers

Figure 2: The conceptual flow from the intractable f-divergence definition to a tractable, sample-based approximation.

Key Mathematical Concepts

Generative Model Objective

The goal is to find parameters θ^* that minimize the f-divergence between the true data distribution p_x and the model distribution p_θ.

$$\theta^* = \arg\min_\theta D_f(p_x||p_\theta)$$

Variational Lower Bound on f-Divergence

(41:22) The central result of the lecture is the variational representation of f-divergence, which provides a lower bound that can be optimized in practice.

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

- $T(x)$ is a function (often called the critic or discriminator) that we optimize. - f^* is the convex conjugate of the function f that defines the specific f-divergence. - The expectations can be approximated using mini-batches of real data ($x \sim p_x$) and generated data ($\hat{x} \sim p_\theta$).

Self-Assessment for This Video

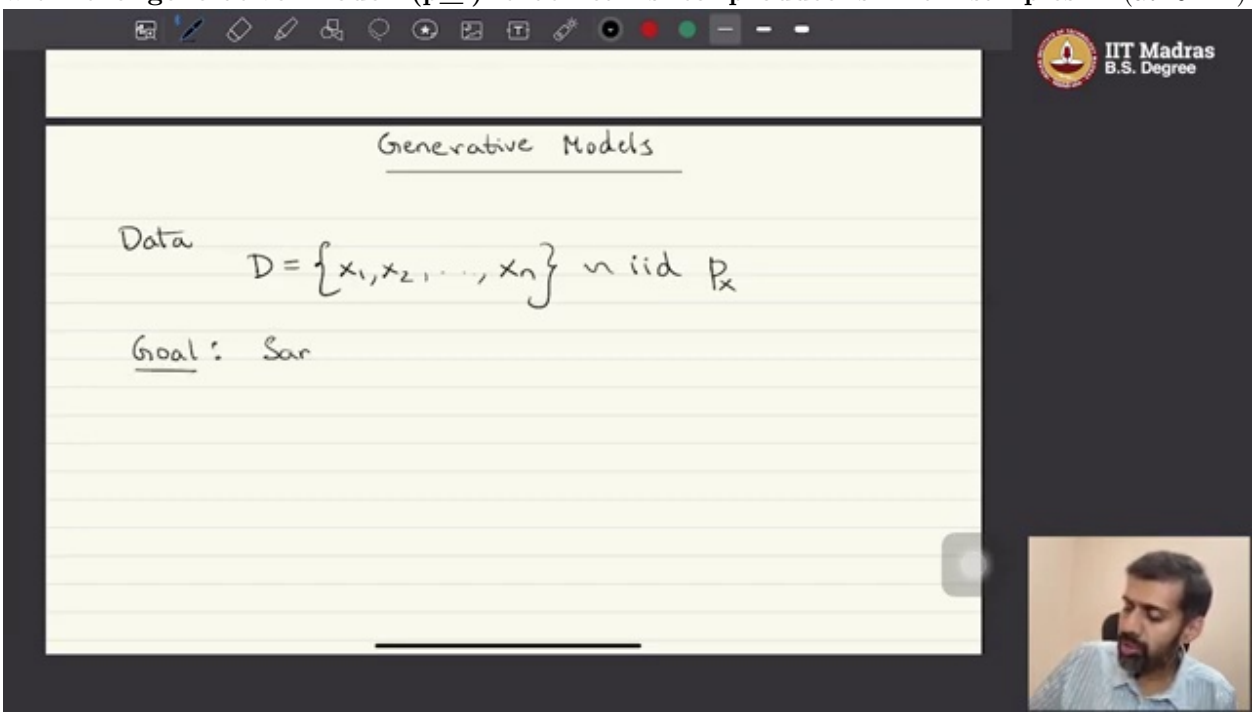
1. **Conceptual Question:** What is the fundamental challenge in training generative models by directly minimizing a statistical divergence like KL or f-divergence?
2. **Mathematical Derivation:** Starting from the definition of the convex conjugate $f^*(t)$, prove the duality property $f(u) = \sup_t\{tu - f^*(t)\}$.
3. **Problem Solving:** Given the KL-divergence where $f(u) = u\log u$, find its convex conjugate $f^*(t)$.
4. **Application:** Using the result from question 3, write down the variational lower bound for the KL-divergence $D_{KL}(p_x||p_\theta)$.
5. **Explanation:** Explain in your own words why the optimization variable in the variational formulation must be a function $T(x)$ rather than a scalar t.

Key Takeaways from This Video

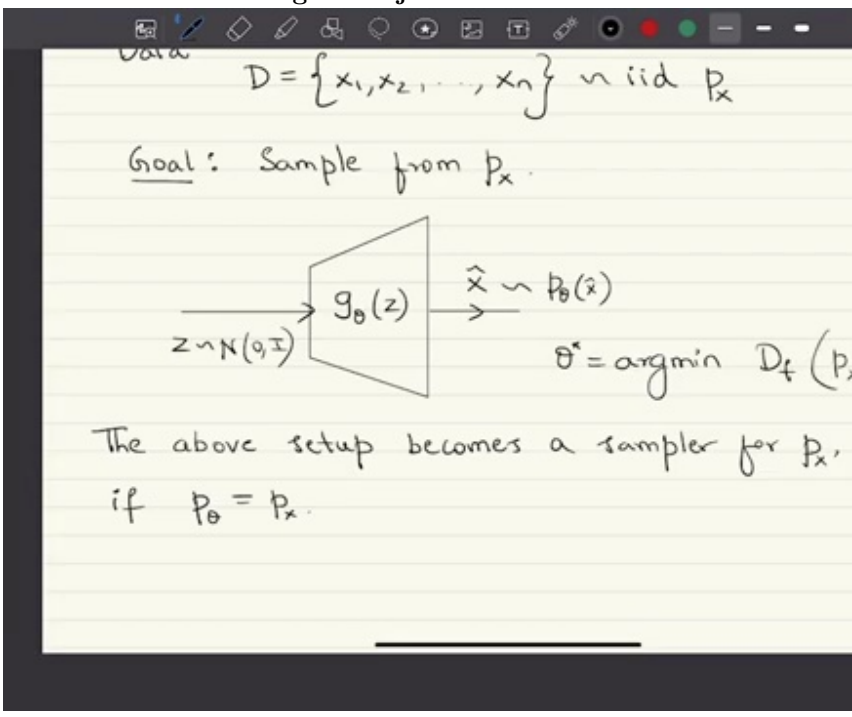
- **Generative Modeling as Divergence Minimization:** The core of training generative models is to make the model's output distribution as close as possible to the real data's distribution, a task framed as minimizing a divergence.
- **The Intractability of Direct Optimization:** We cannot compute divergences directly because we lack analytical formulas for the distributions and are working in high-dimensional spaces. We only have samples.
- **The Power of Variational Formulation:** By using the Fenchel-Legendre duality, we can transform the intractable divergence calculation into a tractable optimization problem. This new objective is a lower bound on the actual divergence.
- **From Theory to Practice:** This variational objective is expressed in terms of expectations, which can be estimated using sample averages. This provides a practical algorithm for training generative models using only samples from the real and generated distributions, laying the groundwork for methods like GANs.

Visual References

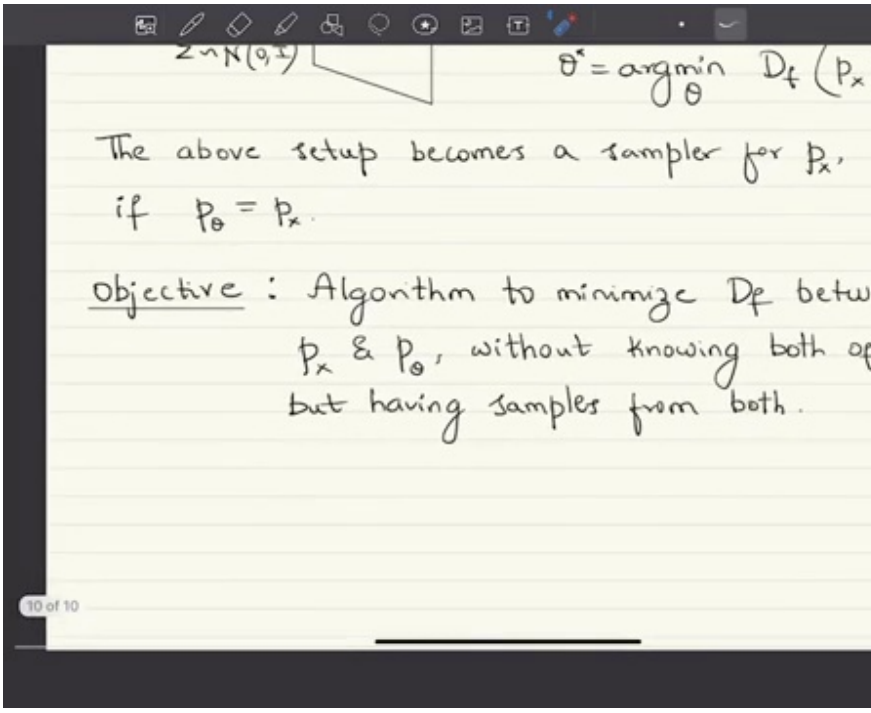
A core conceptual diagram illustrating the generative modeling problem. It visually contrasts the unknown true data distribution (p_x) from which we have samples, with the generative model (p_) that learns to produce similar samples. (at 01:21):



The formal mathematical definition of f-divergence is presented as an integral. This equation, D_f(p || q) = q(x) f(p(x)/q(x)) dx, is fundamental to understanding the objective function that generative models aim to minimize. (at 03:15):



Introduction of the Fenchel-Legendre conjugate (f*). *The screenshot shows the key equation* f*(t) = sup(tu - f(u)), which is the essential mathematical tool used to transform the intractable diver-



gence problem into a solvable one. (at 05:45):

The final and most important result of the lecture: the variational lower bound for f-divergence. This equation shows how the intractable divergence is lower-bounded by a tractable expression involving expectations, which can be estimated from samples. (at 08:15):