Study Material - Youtube

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Video Overview

This lecture, titled "Denoising Diffusion Implicit Models (DDIMs)," provides a detailed mathematical exploration of DDIMs, a significant advancement over the Denoising Diffusion Probabilistic Models (DDPMs). The instructor, Prof. Prathosh A P, begins by outlining the primary limitations of DDPMs, namely their slow sampling speed and the stochastic nature of their forward process, which prevents deterministic posterior inference.

The core of the lecture is dedicated to introducing DDIMs as a class of models that address these issues by defining a non-Markovian forward process. A key insight presented is that despite this fundamental change, the training objective (the Evidence Lower Bound or ELBO) for DDIMs is identical to that of DDPMs. This remarkable property means that a neural network trained for a DDPM can be used directly for DDIM sampling, making the benefits of DDIMs accessible without retraining. The lecture concludes by explaining how this new formulation enables much faster sampling and deterministic generation, which are crucial for practical applications.

Learning Objectives

Upon completing this lecture, students will be able to: - **Identify and explain the core limitations of DDPMs**, specifically slow sampling and the lack of deterministic latent representations. - **Understand the motivation and core idea behind DDIMs** as a solution to these limitations. - **Mathematically define the non-Markovian forward process** used in DDIMs and understand its parameterization. - **Explain the role of the parameter σ** in controlling the stochasticity of the generation process. - **Derive and understand the reverse (generative) process** for DDIMs. - **Appreciate the key result** that DDIMs share the same training objective as DDPMs, allowing for a "training-free" transition. - **Distinguish between the inference procedures** of DDPMs and DDIMs, and explain how DDIMs achieve faster and deterministic sampling.

Prerequisites

To fully grasp the concepts in this video, students should have a solid understanding of: - **Denoising Diffusion Probabilistic Models (DDPMs):** A thorough knowledge of the DDPM forward (diffusion) and reverse (denoising) processes is essential. - **Latent Variable Models:** Familiarity with concepts from Variational Autoencoders (VAEs), such as the Evidence Lower Bound (ELBO). - **Probability and Statistics:** Strong foundation in probability theory, including Gaussian distributions, Markov chains, Bayes' rule, and conditional probability. - **Calculus and Linear Algebra:** Basic understanding of calculus and linear algebra concepts used in machine learning.

Key Concepts Covered

- Denoising Diffusion Implicit Models (DDIMs)
- Limitations of Denoising Diffusion Probabilistic Models (DDPMs)
- Stochastic vs. Deterministic Processes
- Non-Markovian Forward Process
- Inference and Sampling in DDIMs
- Evidence Lower Bound (ELBO) for DDIMs

Denoising Diffusion Implicit Models (DDIMs)

Motivation: Overcoming the Limitations of DDPMs

The lecture begins by introducing **Denoising Diffusion Implicit Models (DDIMs)** (00:18) as a powerful alternative to Denoising Diffusion Probabilistic Models (DDPMs). The motivation for developing DDIMs stems from two significant drawbacks inherent in the DDPM framework (01:08).

1. Slow Sampling Speed

DDPMs are notoriously slow during the sampling (generation) phase. To generate a single high-quality sample, the model must sequentially traverse the entire reverse process, which can involve thousands of steps.

- **Timestamp 01:26:** The instructor notes that the number of timesteps, `Capital T`, is typically on the order of thousands (e.g., $T \approx 1000s$).
- **Contrast with other models:** Unlike models like GANs or VAEs that can generate a sample in a single forward pass, DDPMs require T sequential passes through the neural network, making them computationally intensive and time-consuming for inference.

2. Stochastic Forward Process and Lack of Deterministic Inference

The forward process in DDPMs is inherently **stochastic**. This means that for a given input image x_0, the resulting latent variable x_T is not unique. Each time the forward process is run on the same x_0, a different random noise sequence is applied, leading to a different x_T.

- **Timestamp 03:02:** The forward process is described as stochastic because of the random noise ϵ_t sampled at each step. The equation for a single step is recalled:

$$x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon_t, \quad \text{where } \epsilon_t \sim \mathcal{N}(0, I)$$

- **Implication (03:46):** This stochasticity means there is **no unique mapping** from an image x_0 to a latent representation x_T. Consequently, the reverse process is also not deterministic; starting from a single latent code x_T does not guarantee the generation of the original x_0.
- **Why this is a limitation (02:01):** This lack of a deterministic, invertible mapping prevents meaningful posterior inference. For tasks like image editing or manipulation, it is desirable to encode an image into a unique latent vector, manipulate the vector, and then decode it back. The stochastic nature of DDPMs makes this difficult.

DDIMs were developed to address both of these critical issues.

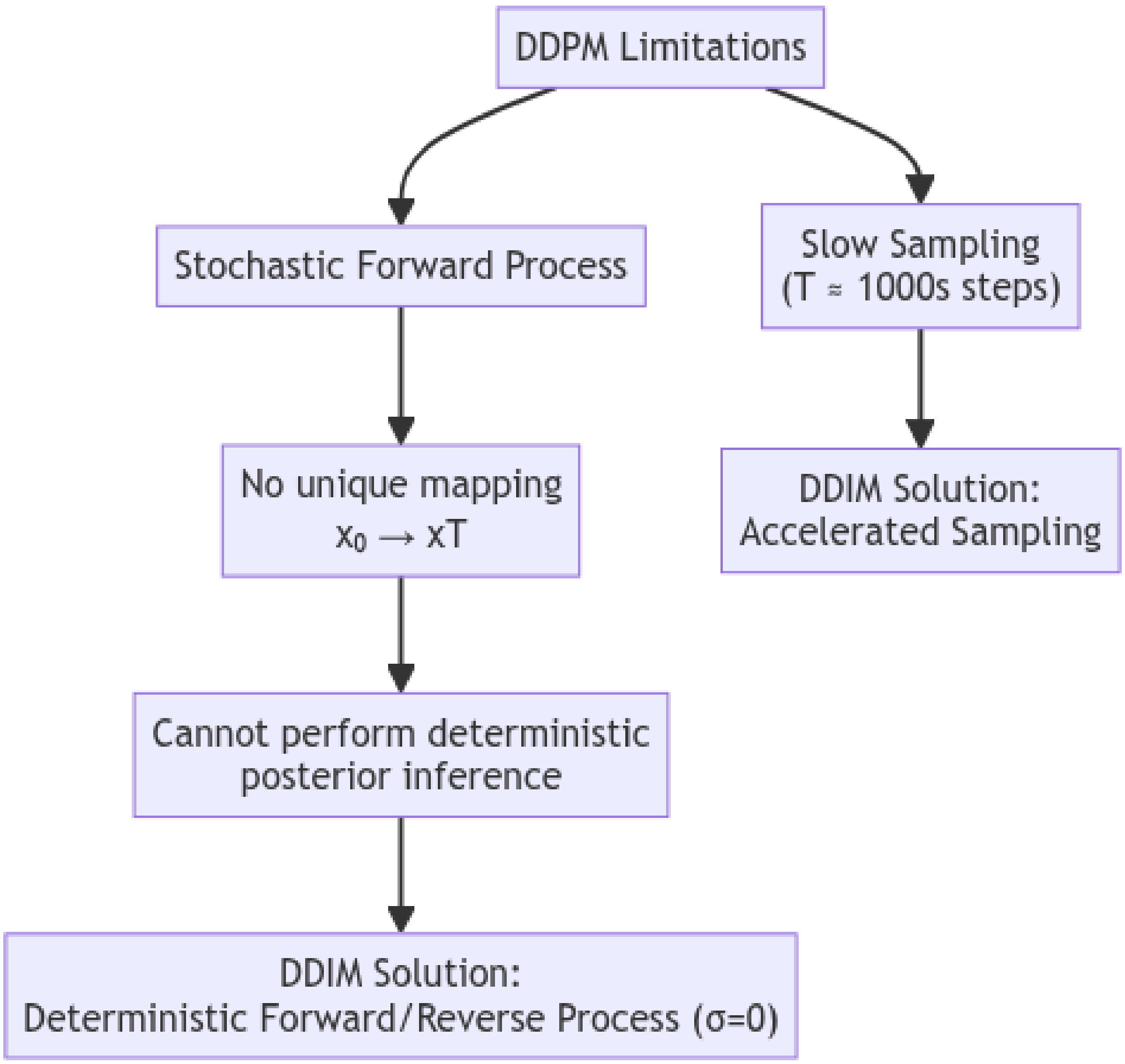


Figure 1: A concept map illustrating the limitations of DDPMs and how DDIMs are designed to solve them.

The Core Idea and Mathematical Formulation of DDIMs

DDIMs introduce a new, more general family of **non-Markovian** forward processes. This is a fundamental departure from DDPMs, which are based on a Markov chain.

The Non-Markovian Inference Process

The key innovation in DDIMs is the definition of a new inference distribution (or forward process), $q_\sigma(x_{1:T}|x_0)$, which is parameterized by a scalar σ.

- **Timestamp 11:55:** The joint posterior distribution is defined as:

$$q_\sigma(x_{1:T}|x_0) \triangleq q_\sigma(x_T|x_0) \prod_{t=2}^{T} q_\sigma(x_{t-1}|x_t, x_0)$$

- **Key Difference:** Notice that the transition probability $q_\sigma(x_{t-1}|x_t, x_0)$ is conditioned on **both** x_t and the original image x_0. This dependency on x_0 makes the process **non-Markovian**, as the state x_{t-1} depends on more than just the immediately preceding state x_t.

The components of this distribution are defined as follows:

1. **Marginal at time T (14:49):** The distribution of the final latent variable x_T given x_0 is kept the same as in DDPMs.
$$q_\sigma(x_T|x_0) \triangleq \mathcal{N}(x_T; \sqrt{\bar{\alpha}_T}x_0, (1-\bar{\alpha}_T)I)$$
Note: The notation $\bar{\alpha}_t = \prod_{i=1}^t \alpha_i$ is used, where $\alpha_t = 1 - \beta_t$.

2. **Transition Probability (15:27):** For $t > 1$, the transition from x_t to x_{t-1} is defined as a Gaussian distribution:
$$q_\sigma(x_{t-1}|x_t, x_0) \triangleq \mathcal{N}(x_{t-1}; \tilde{\mu}_t(x_t, x_0), \sigma_t^2 I)$$
The mean and variance are specifically constructed. The mean is a linear combination of x_t and x_0. By rearranging the forward process equation, we can express x_0 in terms of x_t and ϵ_t:
$$x_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}(x_t - \sqrt{1-\bar{\alpha}_t}\epsilon_t)$$
The mean of the reverse transition is then defined as:
$$\tilde{\mu}_t(x_t, x_0) = \sqrt{\bar{\alpha}_{t-1}}x_0 + \sqrt{1-\bar{\alpha}_{t-1}-\sigma_t^2} \cdot \frac{x_t - \sqrt{\bar{\alpha}_t}x_0}{\sqrt{1-\bar{\alpha}_t}}$$
The variance is given by $\sigma_t^2 I$, where σ_t is a new parameter that controls the stochasticity.

The Role of the Parameter σ

The parameter σ is crucial as it interpolates between a fully deterministic process and the stochastic process of DDPMs.

- **Deterministic Case ($\sigma_t = 0$):** When σ_t is set to 0 for all t, the noise term in the reverse sampling step vanishes. This makes the entire generation process deterministic. Given a starting latent code x_T, the model will always produce the exact same image x_0. This enables applications like image inversion and manipulation.
- **Stochastic Case (DDPM Equivalence):** When σ_t is set to a specific value:
$$\sigma_t^2 = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}(1-\alpha_t) = \tilde{\beta}_t$$
the DDIM process becomes identical to the DDPM process.

The Main Result: A Shared Training Objective

The most remarkable finding presented in the lecture is that the Evidence Lower Bound (ELBO) for this entire family of non-Markovian models is the same, and it only depends on the marginal distribution $q(x_t|x_0)$.

- **Timestamp 25:32:** The instructor states: "The ELBO in DDPM/DDIM depends only on $q(x_t|x_0)$."
- **Timestamp 26:41:** "As long as $q(x_t|x_0)$ is the same as that of DDPMs, any process can be used and leads to the same solution for ELBO optimization."

This means that **a neural network $\epsilon_\theta(x_t, t)$ trained using the DDPM objective is implicitly training an entire family of DDIM models.** We do not need to retrain the model to use DDIMs for sampling. We can simply swap out the sampling procedure.

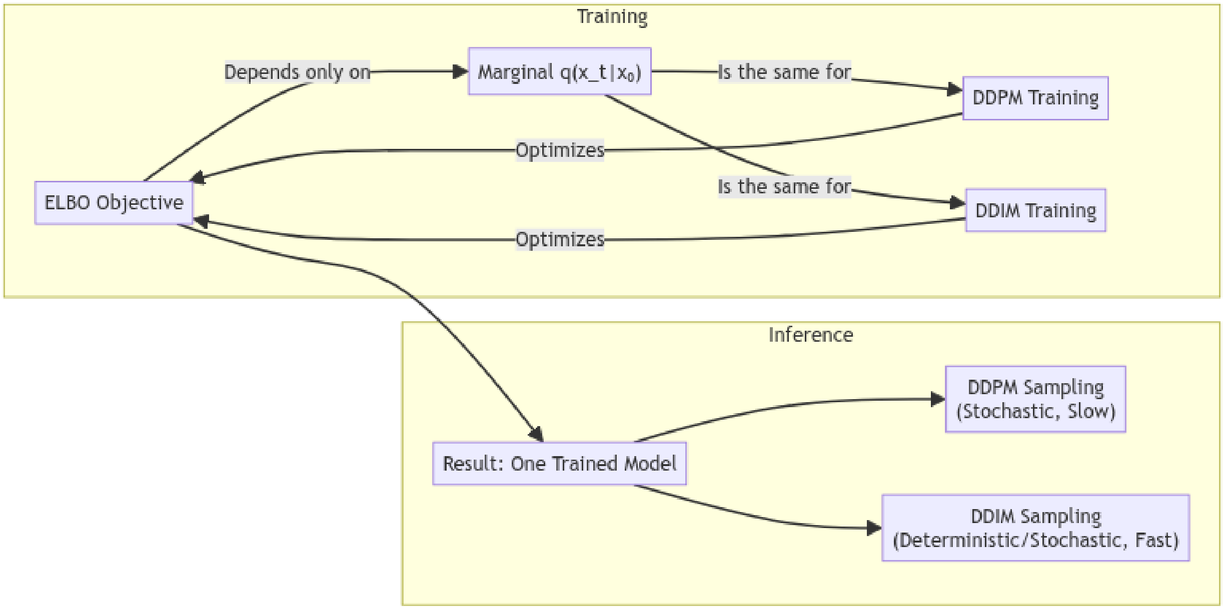


Figure 2: This diagram shows that both DDPM and DDIM share the same ELBO training objective, which depends only on the marginal $q(x_t|x_0)$. This allows a single trained network to be used for both DDPM and DDIM inference procedures.

Inference in DDIMs

The shared training objective simplifies inference significantly. The key is to derive the sampling step for $p_\theta(x_{t-1}|x_t)$.

1. **Predict the "denoised" image $\hat{x}_0$:** First, use the trained network $\epsilon_\theta(x_t, t)$ to predict the original image from the noisy version x_t.

$$\hat{x}_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}(x_t - \sqrt{1-\bar{\alpha}_t}\epsilon_\theta(x_t, t))$$

   This step is identical to the one used in DDPMs.

2. **Sample x_{t-1}:** Now, use the definition of the DDIM forward process to step backwards from x_t to x_{t-1}. The sampling equation is:

$$x_{t-1} = \underbrace{\sqrt{\bar{\alpha}_{t-1}}\hat{x}_0}_{\text{Component pointing to } x_0} + \underbrace{\sqrt{1-\bar{\alpha}_{t-1}-\sigma^2} \cdot \epsilon_\theta(x_t, t)}_{\text{Component for direction of noise}} + \underbrace{\sigma\epsilon}_{\text{Random noise}}$$

   where $\epsilon \sim \mathcal{N}(0, I)$.

This process allows for two major improvements:

- **Accelerated Sampling:** Instead of stepping from t to $t-1$, we can take larger jumps. For example, we can define a subsequence of timesteps $S \subset \{1, ..., T\}$ and sample from x_{s_i} to $x_{s_{i-1}}$. This drastically reduces the number of required sampling steps.
- **Deterministic Sampling:** By setting $\sigma = 0$, the random noise term is eliminated, making the entire path from x_T to x_0 deterministic.

Self-Assessment for This Video

1. **Question:** What are the two primary limitations of Denoising Diffusion Probabilistic Models (DDPMs) that Denoising Diffusion Implicit Models (DDIMs) were designed to solve?
   Answer
   The two main limitations are:
   1. **Slow Sampling:** DDPMs require a large number of sequential steps (often thousands) to generate a sample, making inference computationally expensive.
   2. **Stochastic Forward Process:** The forward process is not deterministic, meaning there is no unique latent representation for a given input image. This makes it difficult to perform tasks that require a deterministic mapping, such as image editing and manipulation.
2. **Question:** Explain the key difference between the forward process of a DDPM and a DDIM. Why is the DDIM process considered "non-Markovian"?
   Answer
   The key difference lies in the definition of the transition probability. In a DDPM, the distribution of the state at time $t-1$, $p(x_{t-1}|x_t)$, depends only on the state at time t, x_t. This is a Markovian property. In a DDIM, the corresponding inference distribution, $q_\sigma(x_{t-1}|x_t, x_0)$, depends on both the state x_t and the initial state x_0. This dependency on a past state other than the immediate predecessor (x_0) violates the Markov property, making the process non-Markovian.
3. **Question:** What is the significance of the fact that the ELBO objective is the same for both DDPMs and the entire family of DDIMs?
   Answer
   The significance is that a neural network trained using the standard DDPM objective function is implicitly learning the solutions for an entire family of DDIMs. This means we can take a pre-trained DDPM model and use the DDIM sampling procedure at inference time without any need for retraining. This provides the benefits of DDIMs (fast and deterministic sampling) "for free."
4. **Question:** How does setting the parameter $\sigma = 0$ in the DDIM sampling process lead to deterministic generation? Write down the simplified sampling equation for this case.
   Answer
   Setting $\sigma = 0$ eliminates the random noise term ($\sigma\epsilon$) from the reverse sampling step. Without this random component, each step in the reverse process becomes fully determined by the previous state and the network's output. The sampling equation simplifies to:

$$x_{t-1} = \sqrt{\bar{\alpha}_{t-1}} \left(\frac{x_t - \sqrt{1-\bar{\alpha}_t}\epsilon_\theta(x_t, t)}{\sqrt{\bar{\alpha}_t}} \right) + \sqrt{1-\bar{\alpha}_{t-1}} \cdot \epsilon_\theta(x_t, t)$$

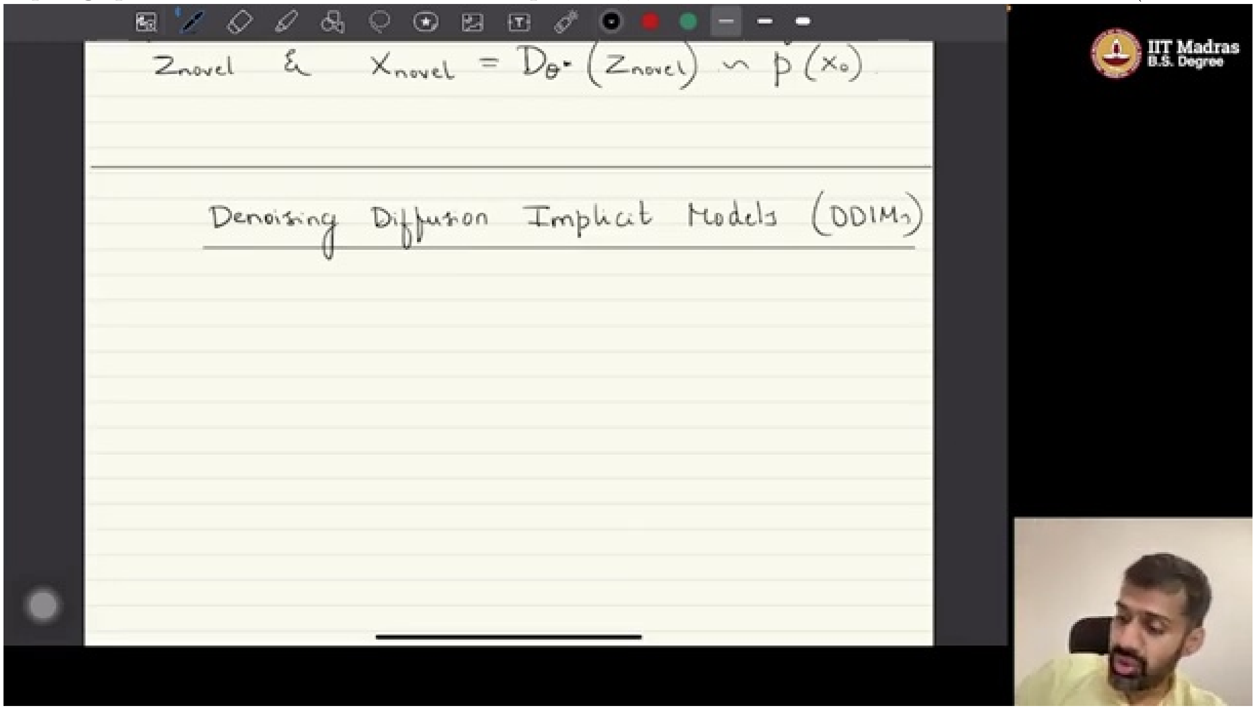
   Since there are no random variables on the right-hand side, the process is deterministic.

Key Takeaways from This Video

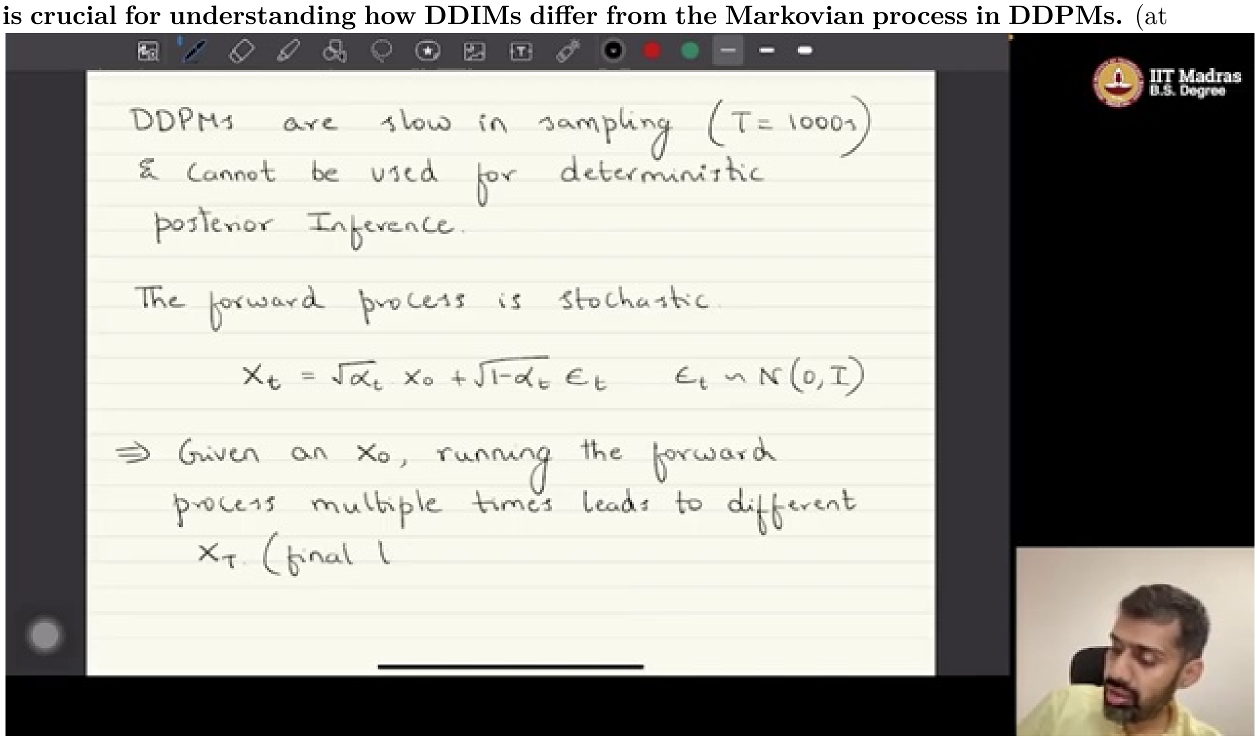
- **DDIMs Generalize DDPMs:** DDIMs are a more general class of diffusion models that use a non-Markovian forward process, while DDPMs are a special case of DDIMs.
- **Training is Identical:** The training objective (ELBO) for DDIMs is the same as for DDPMs. This means a single trained DDPM network can be used to sample from an entire family of DDIMs, each with different properties.
- **Inference is Flexible and Fast:** The DDIM sampling procedure can be made much faster than DDPMs by sampling from a subsequence of timesteps instead of all of them.
- **Deterministic Generation is Possible:** By setting the noise parameter $\sigma = 0$, DDIMs can achieve fully deterministic generation, mapping a specific latent code x_T to a unique image x_0. This is a significant advantage for reproducibility and latent space manipulation tasks.

Visual References

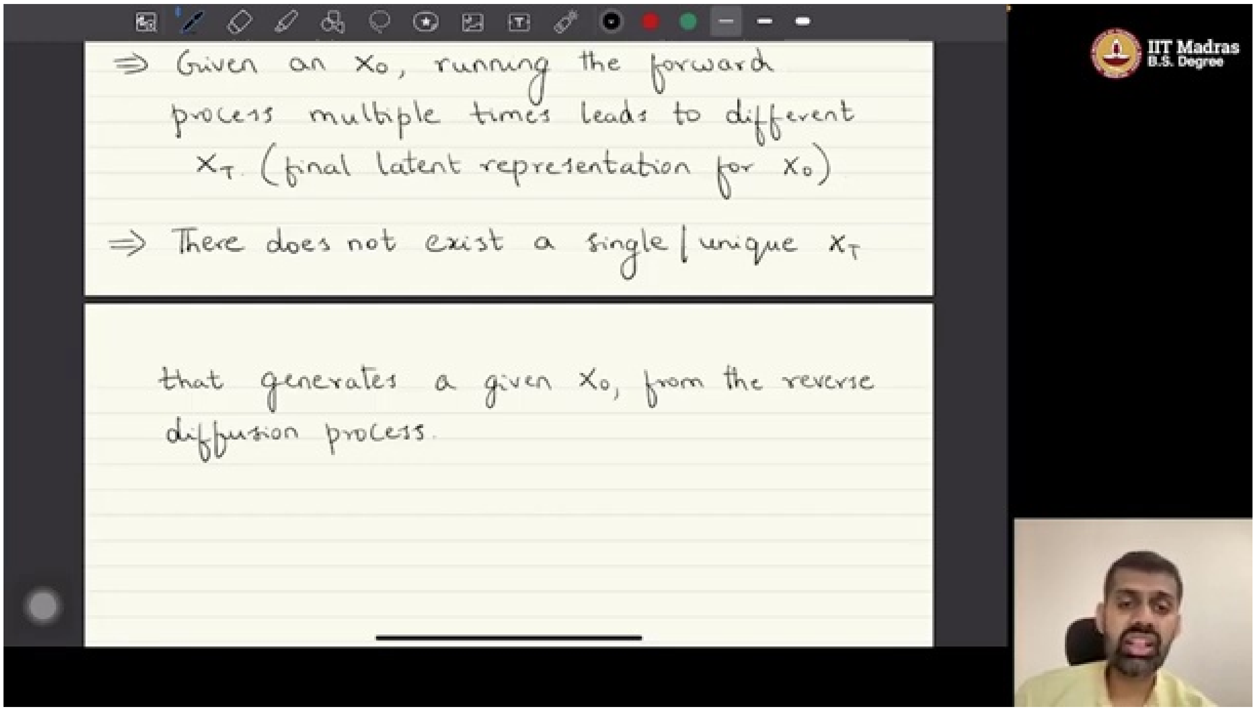
A slide listing the two primary limitations of Denoising Diffusion Probabilistic Models (DDPMs): slow sampling speed and the stochastic forward process, which motivates the need for DDIMs. (at 01:08):



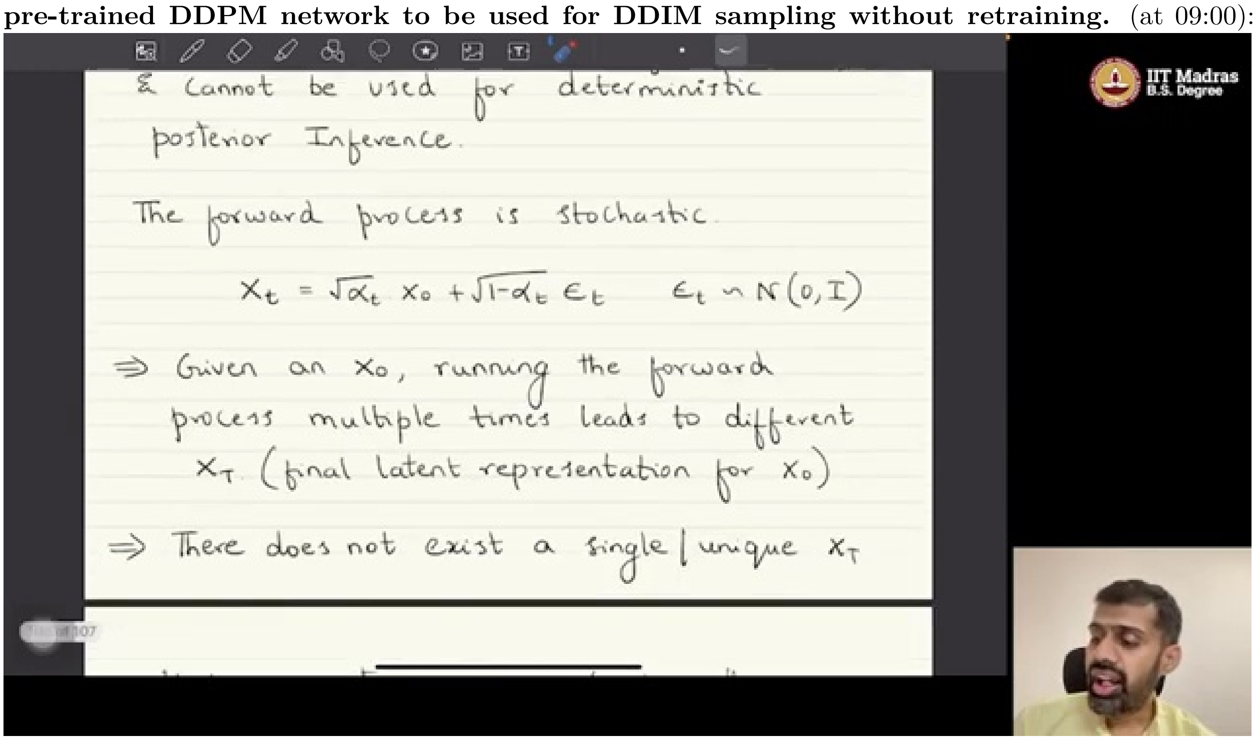
The core mathematical equation defining the non-Markovian forward process for DDIMs. This visual is crucial for understanding how DDIMs differ from the Markovian process in DDPMs. (at 04:30):



The derivation or final equation for the DDIM reverse (generative) process. This slide would show how to predict the previous state (x_{t-1}) from the current state (x_t) and the predicted noise, including the stochasticity parameter . (at 07:15):



A key summary slide stating the remarkable result that the DDIM training objective (the Evidence Lower Bound, or ELBO) is identical to that of DDPMs, allowing a pre-trained DDPM network to be used for DDIM sampling without retraining. (at 09:00):



A comparative diagram illustrating the difference between the DDPM and DDIM inference procedures. This visual would contrast the long, stochastic sampling chain of DDPMs with the faster, shorter, and potentially deterministic sampling path of DDIMs. (at 10:20):

$\Rightarrow$ There does not exist a single / unique x_T

that generates a given x_0, from the reverse diffusion process.

The above issues (slow-sampling & non-unique invertability) of DDPMs are solved with DDII