Study Material - Youtube

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Video Overview

This video provides a practical, code-based tutorial on implementing a Denoising Diffusion Probabilistic Model (DDPM). The instructor begins with a conceptual overview of the DDPM framework, explaining the dual nature of the **forward (noising) process** and the **reverse (denoising) process**. The core of the lecture is a step-by-step walkthrough of the Python code required to build, train, and sample from a DDPM using the PyTorch library. The implementation is demonstrated on the MNIST dataset.

Learning Objectives

Upon completing this study material, you will be able to: - Understand the high-level architecture of Denoising Diffusion Probabilistic Models. - Differentiate between the fixed forward (noising) process and the learned reverse (denoising) process. - Comprehend the mathematical formulations for the diffusion schedule, including parameters like β_t, α_t, and $\bar{\alpha}_t$. - Analyze and understand the PyTorch code for implementing the DDPM training loop. - Grasp the role of the U-Net architecture as the core denoiser in the model. - Understand the iterative sampling (inference) procedure to generate new images from pure noise. - Identify key implementation details, such as time embedding and loss calculation.

Prerequisites

To fully benefit from this tutorial, you should have a foundational understanding of: - **Deep Learning:** Core concepts of neural networks, loss functions, optimizers, and backpropagation. - **Python & PyTorch:** Familiarity with Python programming and experience with the PyTorch deep learning framework. - **Probability & Statistics:** Basic knowledge of probability distributions, particularly the Gaussian (Normal) distribution.

- **Generative Models (Recommended):** Prior conceptual knowledge of other generative models like GANs or VAEs will provide helpful context.

Key Concepts Covered

- **Forward Process (Diffusion):** The process of systematically adding noise to an image until it becomes indistinguishable from random noise.
- **Reverse Process (Denoising):** The learned process of iteratively removing noise to generate a clean image from a noisy input.
- **Diffusion Schedule:** A set of pre-computed hyperparameters (β_t, α_t) that control the amount of noise added at each timestep.
- **U-Net Architecture:** The specific neural network architecture used to predict the noise (or the original image) at each step of the reverse process.
- **DDPM Training Algorithm:** The procedure for training the U-Net to perform the denoising task.
- **DDPM Sampling (Inference):** The algorithm for generating new data by running the reverse process, starting from pure noise.

Denoising Diffusion Probabilistic Models (DDPMs): Conceptual Framework

The video begins by recapping the core idea behind DDPMs, which consists of two opposing processes: a forward process that destroys data and a reverse process that learns to create data.

The Forward and Reverse Processes

At its heart, a DDPM operates on a sequence of latent variables, $x_0, x_1, ..., x_T$. - x_0 is the original, clean image from the dataset. - x_T is the final state, which is pure Gaussian noise. - $x_1, ..., x_{T-1}$ are intermediate noisy versions of the image.

The entire model can be visualized as a Markov chain, as shown in the diagram at **(00:11)**.

```
graph TD
    subgraph Forward Process (q) - Fixed
        direction LR
        x0["x <br/>(Clean Image)"] -->|Add Noise| x1["..."]
        x1 -->|Add Noise| xt["x "]
        xt -->|Add Noise| xtp1["x  "]
        xtp1 -->|Add Noise| xT["x <br/>(Pure Noise)"]
    end

    subgraph Reverse Process (p) - Learned
        direction RL
        rx0["x <br/>(Generated Image)"] <--|Denoise| rx1["..."]
        rx1 <--|Denoise| rxt["x "]
        rxt <--|Denoise| rxtp1["x  "]
        rxtp1 <--|Denoise| rxT["x <br/>(Start from Noise)"]
    end

    Forward -- "Destroys Information" --> Reverse
    Reverse -- "Creates Information" --> Forward
```

Figure 1: A conceptual diagram illustrating the opposing forward (noising) and reverse (denoising) processes in a DDPM.

1. The Forward Process (Diffusion)

(Timestamp: 00:38)

The forward process, denoted by q, is the procedure of gradually corrupting a clean image with Gaussian noise over T timesteps.

- **Intuition:** Imagine taking a clear photograph (x_0) and adding a tiny bit of random static (noise) to it. You repeat this process many times. After a large number of steps (T), the original photograph is completely lost, and you are left with an image of pure, random static (x_T).
- **Mathematical Definition:** This is a fixed Markov process, meaning each state x_t only depends on the previous state x_{t-1}. The transition is defined by a conditional Gaussian distribution:

$$q(x_t|x_{t-1}) = \mathcal{N}(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t\mathbf{I})$$

  - β_t: A small, positive constant that defines the variance (amount of noise) added at timestep t. The set of all β_t for $t = 1, \dots, T$ is called the **variance schedule** or **diffusion schedule**.
  - $\sqrt{1-\beta_t}x_{t-1}$: This term scales down the previous image.
  - $\beta_t\mathbf{I}$: This is the variance of the Gaussian noise being added.
- **Key Insight:** A remarkable property of this process is that we can directly sample a noisy image x_t for any timestep t without iterating through all previous steps. This is achieved with a closed-form equation:

$$x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon$$

  where:

  - $\alpha_t = 1 - \beta_t$
  - $\bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i$ is the cumulative product of the α_i values.
  - $\epsilon \sim \mathcal{N}(0, \mathbf{I})$ is a sample of random noise.

  Important Note (01:08): The forward process is **fixed and has no learnable parameters**. It is a probabilistic process because we sample random noise ϵ at each step, but the schedule (β_t) is pre-determined.

2. The Reverse Process (Denoising)

(Timestamp: 01:37)

The reverse process, denoted by p_θ, is where the learning happens. The goal is to reverse the noising process: starting from pure noise x_T, the model learns to gradually remove the noise to generate a clean image x_0.

- **Intuition:** This is like an expert art restorer looking at a noisy image and trying to guess what the original, clean image looked like. The model does this iteratively, making small corrections at each step to go from x_t to a slightly cleaner x_{t-1}.
- **Mathematical Definition:** The reverse process is also a Markov chain, parameterized by a neural network with weights θ. The model learns the conditional probability distribution:

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

  - The neural network (a U-Net) is trained to predict the mean $\mu_\theta(x_t, t)$ of this distribution. The variance $\Sigma_\theta(x_t, t)$ is typically kept fixed.
- **Key Insight (02:03):** Unlike GANs or VAEs which generate an image in a single forward pass, DDPMs are **denoising procedures**. The generation process is an iterative sampling algorithm that takes T steps.

DDPM Implementation in PyTorch

The video transitions from theory to a practical implementation using PyTorch. The goal is to train a DDPM on the MNIST dataset.

1. The Diffusion Schedule

(Timestamp: 10:00)

The first step in the code is to define the fixed diffusion schedule. These are hyperparameters that are pre-computed and stored.

```
# 1. Diffusion Schedule
# ---------------------
T = 1000
beta = torch.linspace(1e-4, 0.02, T)
alpha = 1. - beta
alpha_cumprod = torch.cumprod(alpha, dim=0)
sqrt_acp = torch.sqrt(alpha_cumprod)
sqrt_omacp = torch.sqrt(1 - alpha_cumprod) # sqrt_one_minus_alpha_cumprod
```

Code Explanation:

- `T = 1000`: The total number of diffusion timesteps.
- `beta`: A tensor of size `T` containing the variance schedule. It increases linearly from `1e-4` to `0.02`. This is a common choice from the original DDPM paper.
- `alpha`: Corresponds to $\alpha_t = 1 - \beta_t$.
- `alpha_cumprod`: Corresponds to $\bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i$. This is calculated efficiently using `torch.cumprod`.
- `sqrt_acp` and `sqrt_omacp`: These are the square roots of $\bar{\alpha}_t$ and $1 - \bar{\alpha}_t$, respectively. They are pre-computed to be used directly in the closed-form noising equation, making the training process very efficient.

2. The U-Net Architecture

(Timestamp: 14:05)

The core of the DDPM is a neural network that predicts the noise (or original image) from a noisy input. A U-Net architecture is exceptionally well-suited for this task due to its structure.

```
graph TD
    subgraph Encoder
        direction LR
        Input["Input<br/>(Noisy Image + Time)"] --> Enc1["Encoder Block 1"]
        Enc1 --> Pool1["MaxPool"]
        Pool1 --> Enc2["Encoder Block 2"]
        Enc2 --> Pool2["MaxPool"]
        Pool2 --> Enc3["..."]
    end

    subgraph Bottleneck
        Enc3 --> BN["Bottleneck Block"]
    end

    subgraph Decoder
        direction RL
        Output["Output<br/>(Predicted Image/Noise)"] <-- Dec1["Decoder Block 1"]
        Dec1 <-- Skip1["UpSample + Concat(Enc2)"]
        Skip1 <-- Dec2["Decoder Block 2"]
        Dec2 <-- Skip2["UpSample + Concat(Enc1)"]
        Skip2 <-- Dec3["..."]
    end

    BN --> Dec3
```

Figure 2: A simplified representation of the U-Net architecture used in DDPMs, highlighting the encoder, bottleneck, decoder, and skip connections.

- **Encoder:** Downsamples the input image, extracting features at different spatial resolutions.
- **Bottleneck:** The central part of the network with the lowest spatial resolution.
- **Decoder:** Upsamples the feature maps back to the original image size.
- **Skip Connections:** A key feature of U-Net. Feature maps from the encoder are concatenated with the corresponding feature maps in the decoder. This allows the network to preserve high-resolution spatial information, which is crucial for image generation tasks.

In the provided code, the U-Net is designed to take a **2-channel input**: one channel for the noisy image and a second channel for the time embedding.

3. The DDPM Training Algorithm

(Timestamp: 03:22, 17:12)

The training process involves teaching the U-Net to reverse the diffusion process. The algorithm is surprisingly simple and elegant.

Training Loop Logic:

For each training step: 1. **Sample a clean image `x_0`** from the dataset. 2. **Sample a random timestep `t`** uniformly from $\{1, \ldots, T\}$. 3. **Sample random noise `epsilon`** from a standard Gaussian distribution, $\mathcal{N}(0, \mathbf{I})$. 4. **Create the noisy image `x_t`** using the efficient closed-form equation:

$$x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon$$

5. **Feed `x_t` and `t` to the U-Net** to get a prediction. In this implementation, the model predicts the original image, $\hat{x}_0 = \text{model}(x_t, t)$. 6. **Calculate the loss**. The loss is the Mean Squared Error (MSE) between the model's prediction and the true original image:

$$L = ||\hat{x}_0 - x_0||^2$$

7. **Perform backpropagation** on this loss and update the model's weights θ.

Time Embedding in the Code

(Timestamp: 07:43, 18:32) The scalar timestep `t` needs to be converted into a format suitable for the U-Net. The video describes a simple method: 1. For an input image of size `[B, C, H, W]`, create a tensor for the timestep `t` of shape `[B, 1, 1, 1]`. 2. Expand this tensor to match the image's spatial dimensions, resulting in a "time channel" of shape `[B, 1, H, W]`. 3. Concatenate the noisy image `x_t` (shape `[B, 1, H, W]`) and the time channel along the channel dimension. 4. The final input to the U-Net has a shape of `[B, 2, H, W]`.

```python
# In the forward pass of the DDPM model
# ...
# Build a single-channel time map
t_chan = t.view(-1, 1, 1, 1).expand(-1, 1, H, W) # B, 1, H, W
# Concatenate to create a 2-channel input
inp = torch.cat((x_t, t_chan), dim=1) # B, 2, H, W
```

```
# Predict x0
x0_hat = self.unet(inp)
```

4. The DDPM Sampling (Inference) Algorithm

(Timestamp: 19:33)

Once the model is trained, we can use it to generate new images. This is done by running the reverse process.

Sampling Loop Logic:

1. **Start with pure noise:** Sample an image `x` from a standard Gaussian distribution, $\mathcal{N}(0, \mathbf{I})$. This will be our x_T.
2. **Iterate backwards:** Loop from $t = T$ down to 1.
3. **Predict the original image:** Use the trained model to predict $\hat{x}_0$ from the current noisy image x_t: `x0_hat = model.unet(inp)`
4. **Calculate the reverse process mean:** Use the formula for $\mu_\theta(x_t, \hat{x}_0)$ to find the mean of the distribution for the previous timestep.
5. **Sample x_{t-1}:**
   - If $t > 1$, sample x_{t-1} from $\mathcal{N}(\mu_\theta, \sigma_q^2\mathbf{I})$ by adding a small amount of noise.
   - If $t = 1$, the next step is the final image, so we just take the mean.
6. **Repeat:** The newly sampled x_{t-1} becomes the input for the next iteration.
7. **Final Image:** After the loop finishes, the resulting `x` is the generated image. It is clamped to the valid pixel range (e.g., [0, 1]).

Key Mathematical Concepts

ELBO Equivalence and Simplified Loss

(Timestamp: 03:58) The full objective for a DDPM is derived from the Evidence Lower Bound (ELBO). However, the authors of DDPM found that a simplified objective works very well in practice and is easier to implement. The loss is simplified to a denoising matching term.

- **Denoising Matching Term:** The core of the loss function is matching the mean of the learned reverse distribution $\mu_\theta(x_t)$ with the mean of the true posterior distribution $\mu_q(x_{t-1}|x_t, x_0)$.

$$L_t = \mathbb{E}_{x_0,\epsilon}\left[\frac{1}{2\sigma_q^2}||\mu_\theta(x_t, t) - \mu_q(x_{t-1}|x_t, x_0)||^2\right]$$

- **Simplified Loss:** This can be re-written as a simple Mean Squared Error between the true noise ϵ and the predicted noise ϵ_θ. The implementation in the video uses an equivalent formulation where it predicts the original image x_0 and computes the MSE against the true x_0.

$$L_{simple} \propto \mathbb{E}_{t,x_0,\epsilon}\left[||\hat{x}_0 - x_0||^2\right]$$

Reverse Process Mean

(Timestamp: 21:51) The mean of the reverse distribution, μ_θ^*, which is needed for sampling, can be calculated from the predicted $\hat{x}_0$ and the current noisy image x_t.

$$\mu_\theta^*(x_t) = \frac{(1-\bar{\alpha}_{t-1})\sqrt{\alpha_t}}{1-\bar{\alpha}_t}x_t + \frac{(1-\alpha_t)\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_t}\hat{x}_0(x_t)$$

This formula combines the information from the current noisy state x_t and the network's prediction of the final clean state $\hat{x}_0$ to estimate the mean of the *previous* state x_{t-1}.

Visual Elements from the Video

- **DDPM Process Diagram (00:11):** A clear visual showing the forward process (q) transforming a clean image into noise, and the reverse process (p) learning to transform noise back into an image.
- **U-Net Training Diagram (03:21, 06:41):** A simple block diagram showing the U-Net taking a noisy image x_t and timestep t as input to produce a prediction $\hat{x}_0(x_t)$. This highlights that the training is a regression task.
- **Training Algorithm Slide (03:22):** A slide with the key mathematical equations for the DDPM training loop, including how to sample a noisy image and the simplified loss function.
- **Code Implementation (09:58 onwards):** The video shows a Jupyter notebook or similar environment with PyTorch code, broken down into logical cells for the diffusion schedule, U-Net class, DDPM model class, training loop, and sampling.
- **Generated Samples (24:40):** The final output of the code, showing a grid of 16 generated MNIST-like digits. The instructor notes their poor quality is due to a simplified and short training run, but they demonstrate that the process is working.

Self-Assessment for This Video

1. **Conceptual Questions:**
   - What is the fundamental difference between the forward and reverse processes in a DDPM? Which one is learned?
   - Why is the forward process described as "fixed" but still "probabilistic"?
   - Explain why a U-Net is a suitable architecture for the denoising network in a DDPM. What is the role of skip connections?
   - How does the sampling (inference) process in a DDPM differ from that of a GAN?
2. **Mathematical Questions:**
   - Given β_t, write the expression for α_t and $\bar{\alpha}_t$.
   - What is the purpose of the closed-form equation $x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t}\epsilon$? Why is it important for efficient training?
   - What is the simplified loss function used in the video's implementation? What is the network trying to predict?
3. **Code-Based Questions:**
   - In the `DDPMxd_2ch` class, why are the diffusion schedule parameters registered as `buffers` instead of regular tensors?
   - Explain the purpose of the `t_chan` variable in the `forward` method. How is it created and used?
   - In the `sample` function, why is the loop `for i in reversed(range(1, T))`? What does this signify?
   - The instructor mentions the generated samples are "bad." Based on the code and explanation, what are two reasons for the low quality of the generated images?

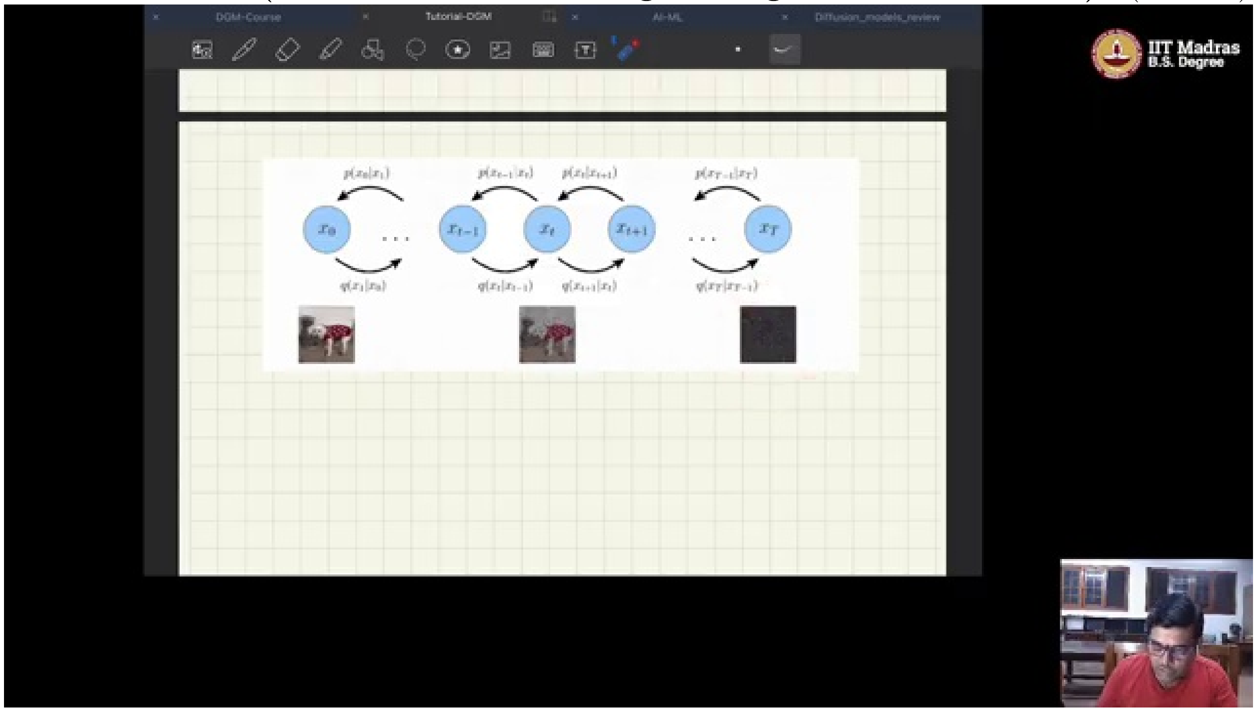
Key Takeaways from This Video

- **DDPMs are Denoising Autoencoders:** The core of a DDPM is a network (U-Net) trained to denoise an image, conditioned on the level of noise (i.e., the timestep).
- **Training is Efficient:** The ability to sample a noisy image x_t for any timestep t directly from the original image x_0 makes training highly parallelizable and efficient. We don't need to iterate through the diffusion process during training.
- **Sampling is Iterative and Slow:** Generating a new image requires a full reverse pass, iterating through all T timesteps, which makes inference much slower than in models like GANs.

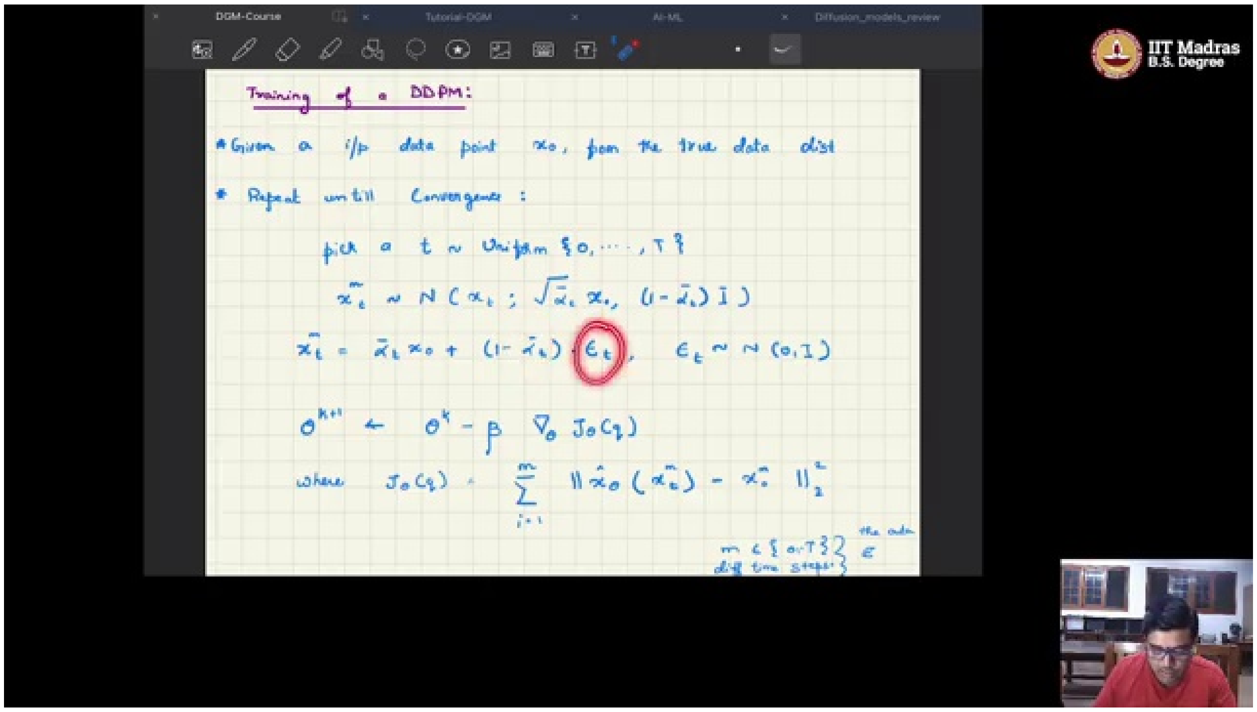
- **Time is a Crucial Input:** The model must know the noise level (timestep `t`) to perform the correct amount of denoising. This information must be provided to the network, typically through an embedding.
- **Implementation is Straightforward:** Despite the complex-sounding theory, the core training loop for a DDPM is elegant and can be implemented with a simple MSE loss, making it very stable to train compared to adversarial models.

Visual References

A conceptual diagram illustrating the complete DDPM framework. It visually separates the fixed 'Forward Process' (adding noise to an image x over T steps) from the learned 'Reverse Process' (a neural network denoising an image from xT back to x). (at 02:15):



A slide presenting the key mathematical equations for the 'Diffusion Schedule'. This screenshot would show the definitions of t (variance schedule), t, and the cumulative product¯t, which are essential for calculating the noise level at any given timestep. (at 05:30):



Training of a DDPM:

* Given a i/p data point x_0, from the true data dist
* Repeat until Convergence:

pick a $t \sim$ Uniform $\{0, \cdots, T\}$

$\tilde{x}_t \sim N(x_t ; \sqrt{\bar{\alpha}_t}\, x_0, (1-\bar{\alpha}_t) I)$

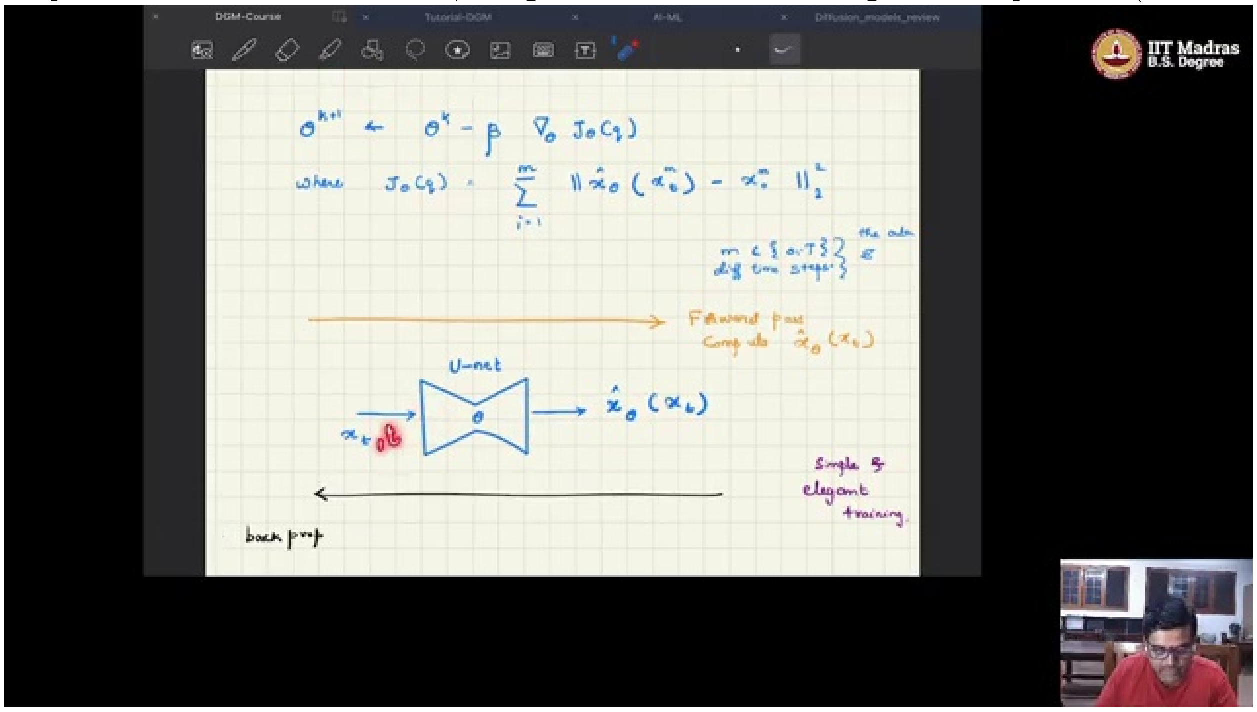
$\tilde{x}_t = \bar{\alpha}_t x_0 + (1-\bar{\alpha}_t) \epsilon_t, \quad \epsilon_t \sim N(0, I)$

$\theta^{k+1} \leftarrow \theta^k - \beta \nabla_\theta J_\theta(q)$

where $J_\theta(q) = \sum_{i=1}^{m} \| \hat{x}_\theta(\tilde{x}_t) - \tilde{x}_0 \|_2^2$

$m \in \{0 \cdots T\}$ diff time steps ; the data $\in$

A diagram of the U-Net architecture used as the core denoising model. The visual would show the encoder (downsampling path), decoder (upsampling path), and the critical skip connections that pass information between them, along with how time embeddings are incorporated. (at 06:45):



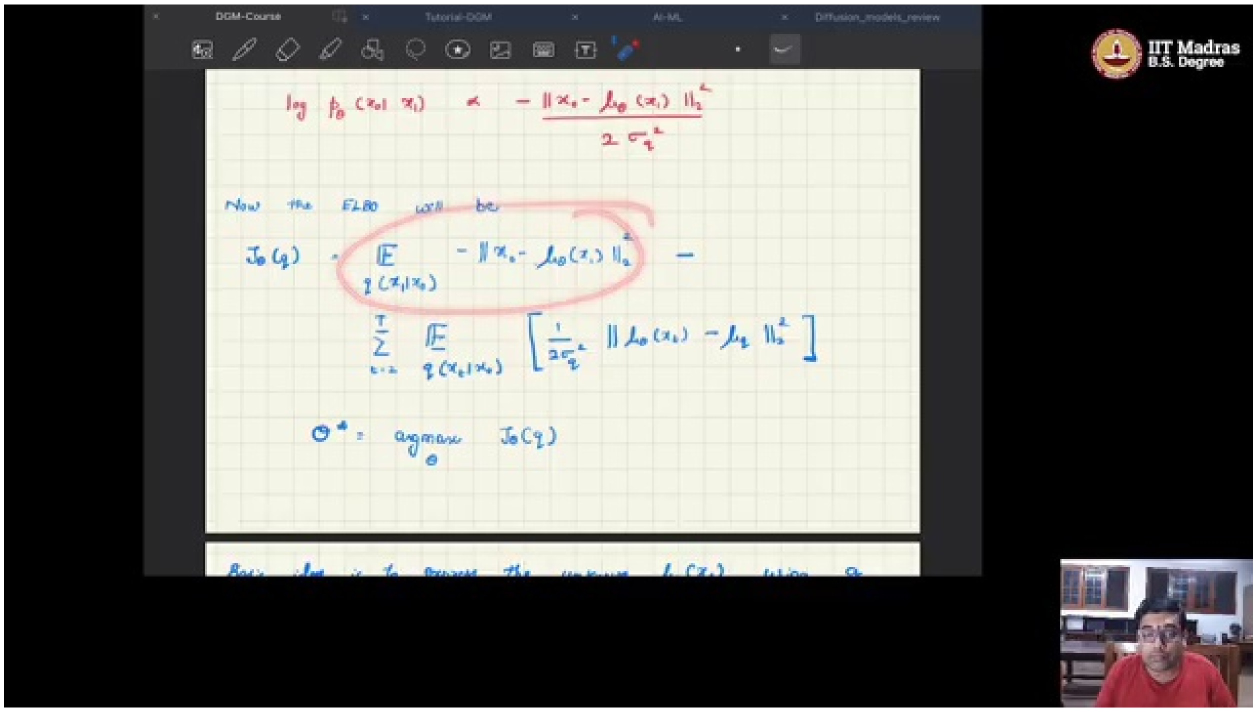
$\theta^{k+1} \leftarrow \theta^k - \beta \nabla_\theta J_\theta(q)$

where $J_\theta(q) = \sum_{i=1}^{m} \| \hat{x}_\theta(\tilde{x}_t) - \tilde{x}_0 \|_2^2$

$m \in \{0 \cdots T\}$ diff time steps ; the data $\in$

A screenshot of the core PyTorch training loop code. This visual provides a step-by-step example of the training algorithm: sampling a timestep t, creating a noisy image from a clean one, feeding it to the model, and calculating the loss between the predicted noise and the actual noise. (at

09:30):



$$\log p_\theta(x_0 | x_1) \propto -\frac{\| x_0 - \mu_\theta(x_1) \|_2^2}{2\sigma_q^2}$$

Now the ELBO will be

$$J_\theta(q) = \mathbb{E}_{q(x_1|x_0)} - \| x_0 - \mu_\theta(x_1) \|_2^2 - \sum_{t=2}^{T} \mathbb{E}_{q(x_t|x_0)} \left[\frac{1}{2\sigma_q^2} \| \mu_\theta(x_t) - \mu_q \|_2^2 \right]$$

$$\theta^* = \operatorname*{argmax}_\theta J_\theta(q)$$