Study Material - Youtube

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Video Overview

This lecture, titled "DDPMs as score-predictors," presents a powerful alternative interpretation of Denoising Diffusion Probabilistic Models (DDPMs). The instructor demonstrates that a DDPM, which is typically trained to predict the noise added during the forward process, can be equivalently viewed as a model that predicts the **score function** of the noisy data distribution. This connection is formally established using **Tweedie's formula**, a classical result from statistics. Understanding DDPMs as score predictors provides a deeper insight into their mechanism and bridges the gap between DDPMs and another important class of generative models known as score-based models. This perspective is particularly valuable for advanced applications like conditional image generation.

Learning Objectives

Upon completing this lecture, students will be able to: - **Define and understand the score function** ($\nabla \log p(x)$) of a probability distribution and its intuitive meaning. - **Comprehend Tweedie's formula** and how it relates the mean of a Gaussian distribution to an observed sample and the score function. - **Apply Tweedie's formula to the DDPM forward process** to establish a direct mathematical link between the added noise (ϵ_t) and the score function. - **Recognize that a DDPM is implicitly learning the score function**, even when its objective is to predict noise. - **Appreciate the equivalence** of various DDPM training objectives, such as predicting the original data, the added noise, or the score function.

Prerequisites

To fully grasp the concepts in this lecture, students should have a solid understanding of: - **Denoising Diffusion Probabilistic Models (DDPMs):** Familiarity with the forward (diffusion) and reverse (denoising) processes. - **Probability and Statistics:** Concepts of Gaussian distributions, conditional probability, expectation, and log-likelihood. - **Multivariable Calculus:** A strong grasp of gradients (∇) and their interpretation. - **Basic Linear Algebra:** Understanding of vectors and matrices, particularly the identity matrix.

Key Concepts Covered

- Score Function
- Tweedie's Formula
- DDPM as a Score Predictor

- Equivalence of DDPM Training Objectives

DDPMs as Score Predictors: A Deep Dive

This section explores an alternative and highly insightful interpretation of what a Denoising Diffusion Probabilistic Model (DDPM) learns. While we have previously seen DDPMs as models that predict the original data (x_0) or the added noise (ϵ_t), we will now demonstrate their equivalence to **score-based models**.

The Score Function and Tweedie's Formula

Intuitive Foundation

At the heart of this new perspective is the **score function**. For any given probability distribution, the score function at a particular point tells us the direction in which the probability density increases most steeply. Imagine a landscape where the height represents probability. The score function is a vector that always points "uphill" towards the nearest peak (mode) of the distribution.

A fundamental result from statistics, **Tweedie's formula**, provides a remarkable connection between this score function and the mean of a Gaussian distribution. It essentially states that if we have a data point sampled from a Gaussian, we can make a better guess about the distribution's mean by starting at our data point and taking a small step in the direction indicated by the score function.

Mathematical Analysis of Tweedie's Formula (00:51)

The instructor introduces Tweedie's formula as a cornerstone for understanding DDPMs as score predictors.

1. Statistical Setup: Let's consider a random variable t drawn from a multivariate Gaussian distribution with mean μ_t and covariance Σ_t. We denote this as:

$$t \sim \mathcal{N}(t; \mu_t, \Sigma_t)$$

The probability density function (PDF) for this distribution is denoted by $p(t)$.

2. The Score Function Definition (02:51): The score function is defined as the gradient of the log-probability density with respect to the random variable t. > **Definition: Score Function** > The score function of a distribution $p(t)$ is given by: >

$$\text{score}(t) = \nabla_t \log p(t)$$

> It's crucial to note that the gradient is taken with respect to the data variable t, not the model parameters.

3. Tweedie's Formula (01:21): Tweedie's formula establishes a relationship between the conditional expectation of the mean μ_t (given an observation t) and the score function at that observation.

> **Tweedie's Formula:** For a random variable $t \sim \mathcal{N}(t; \mu_t, \Sigma_t)$, the conditional expectation of the mean is:
>
> $$\mathbb{E}[\mu_t | t] = t + \Sigma_t \cdot \nabla_t \log p(t)$$

Intuitive Breakdown of the Formula: - $\mathbb{E}[\mu_t|t]$: This is our best estimate of the true mean μ_t after observing a single sample t. - t: Our starting point is the observed sample. - $\nabla_t \log p(t)$: This is the score function, which provides the direction to move from t to get closer to the mean (the region of highest probability). - Σ_t: The covariance matrix acts as a scaling factor. A larger variance means we should take a larger step, as the distribution is more spread out.

Connecting DDPMs and Score Prediction

We can now apply Tweedie's formula to the forward process of a DDPM to reveal its connection to score prediction.

Step 1: Applying Tweedie's Formula to the DDPM Forward Process (05:02)

Recall the distribution of the noisy image x_t at timestep t, given the original image x_0:

$$q(x_t|x_0) = \mathcal{N}(x_t; \sqrt{\bar{\alpha}_t}x_0, (1-\bar{\alpha}_t)I)$$

Let's map this to the terms in Tweedie's formula: - The random variable is x_t. - The mean is $\mu = \sqrt{\bar{\alpha}_t}x_0$. - The covariance is $\Sigma_t = (1-\bar{\alpha}_t)I$.

Applying Tweedie's formula, we get an expression for the conditional expectation of the mean:

$$\mathbb{E}[\mu|x_t] = x_t + (1-\bar{\alpha}_t)\nabla_{x_t}\log q(x_t)$$

The best estimate for this conditional expectation is the true mean itself. Therefore:

$$\sqrt{\bar{\alpha}_t}x_0 = x_t + (1-\bar{\alpha}_t)\nabla_{x_t}\log q(x_t)$$

Step 2: Deriving the True Score Function (16:47)

We now have two different ways to express x_0: 1. **From Tweedie's Formula (rearranged):**

$$x_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}\left(x_t + (1-\bar{\alpha}_t)\nabla_{x_t}\log q(x_t)\right)$$

2. **From the DDPM Forward Process Definition:**

$$x_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}\left(x_t - \sqrt{1-\bar{\alpha}_t}\epsilon_t\right)$$

By equating these two expressions for x_0 and simplifying, we arrive at a profound result for the true score function:

$$(1-\bar{\alpha}_t)\nabla_{x_t}\log q(x_t) = -\sqrt{1-\bar{\alpha}_t}\epsilon_t$$
$$\nabla_{x_t}\log q(x_t) = -\frac{\epsilon_t}{\sqrt{1-\bar{\alpha}_t}}$$

> **Key Insight:** The true score of the noisy data distribution $q(x_t)$ is simply the **negatively scaled noise** ϵ_t that was added to create x_t.

This means that when we train a neural network $\epsilon_\theta(x_t, t)$ to predict the noise ϵ_t, we are implicitly training it to predict a scaled version of the score function.

Step 3: The DDPM Objective as Score Matching (13:45)

The standard DDPM loss function aims to match the predicted noise with the true noise:

$$L_{noise} \propto ||\epsilon_t - \epsilon_\theta(x_t, t)||_2^2$$

Given our new insight, we can re-interpret this. If we define a score-predicting network $S_\theta(x_t, t)$ such that:

$$S_\theta(x_t, t) \approx \nabla_{x_t}\log q(x_t) = -\frac{\epsilon_t}{\sqrt{1-\bar{\alpha}_t}}$$

This implies that our noise predictor is related to the score predictor by:

$$\epsilon_\theta(x_t, t) \approx -\sqrt{1-\bar{\alpha}_t}S_\theta(x_t, t)$$

Substituting this into the loss function reveals that minimizing the noise prediction error is equivalent to minimizing the score matching error:

$$L_{score} \propto ||\nabla_{x_t} \log q(x_t) - S_\theta(x_t, t)||_2^2$$

This confirms that a DDPM is fundamentally a score-based model.

The following diagram illustrates this alternative interpretation:

```
flowchart TD
    A["Input<br>x_t, t"] --> B{U-Net<br>S<sub>&theta;</sub>(x<sub>t</sub>, t)};
    B --> C["Predicted Score<br>S<sub>&theta;</sub>(x<sub>t</sub>)"];
    D["True Score<br> <sub>x<sub>t</sub></sub> log p(x<sub>t</sub>)"] --> E{Loss Calculation};
    C --> E;
    E --> F["Minimize<br>|| <sub>x<sub>t</sub></sub> log p(x<sub>t</sub>) - S<sub>&theta;</sub>(x<sub>t<
```

Figure 1: A DDPM viewed as a regressor on the score function. The U-Net takes the noisy data x_t and timestep t to predict the score, which is then compared to the true score to compute the loss.

Key Takeaways from This Video

- **DDPMs are Implicit Score Predictors:** The central message is that training a DDPM to denoise an image (by predicting the noise ϵ_t) is mathematically equivalent to training it to predict the score function ($\nabla_{x_t} \log q(x_t)$) of the noisy data distribution.
- **True Score is Scaled Noise:** For the DDPM forward process, the true score is elegantly shown to be the negatively scaled version of the noise that was added, i.e., $\nabla_{x_t} \log q(x_t) \propto -\epsilon_t$.
- **Equivalence of Objectives:** The lecture highlights that the objectives of predicting noise, predicting the original data x_0, or predicting the score are all mathematically equivalent, differing only by scaling and shifting. This provides flexibility in how DDPMs are formulated and understood.
- **Connection to Score-Based Models:** This interpretation formally connects DDPMs to the broader family of score-based generative models, unifying different approaches to generative modeling.

Self-Assessment for This Video

Test your understanding of the concepts covered in this lecture.

Question 1: In your own words, what is the "score function" of a probability distribution, and what is its geometric interpretation?

Question 2: You are given a data point $t = 5$ sampled from a 1D Gaussian distribution $p(t) = \mathcal{N}(t; \mu, \sigma^2 = 4)$. If the score at this point is $\nabla_t \log p(t) = -0.5$, what is the best estimate for the mean μ according to Tweedie's formula?

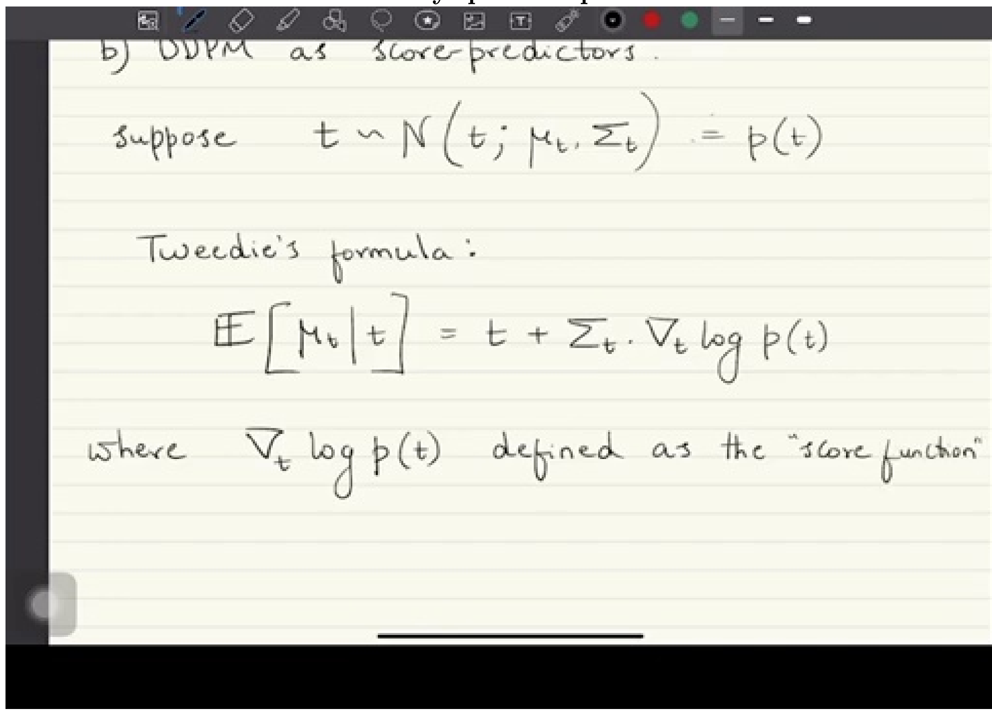
Question 3: Explain the logical steps that connect the DDPM noise prediction objective, $||\epsilon_t - \epsilon_\theta(x_t, t)||_2^2$, to the score matching objective, $||\nabla_{x_t} \log q(x_t) - S_\theta(x_t, t)||_2^2$.

Question 4: Why is the insight that "true score = negatively scaled noise" so important for understanding DDPMs?

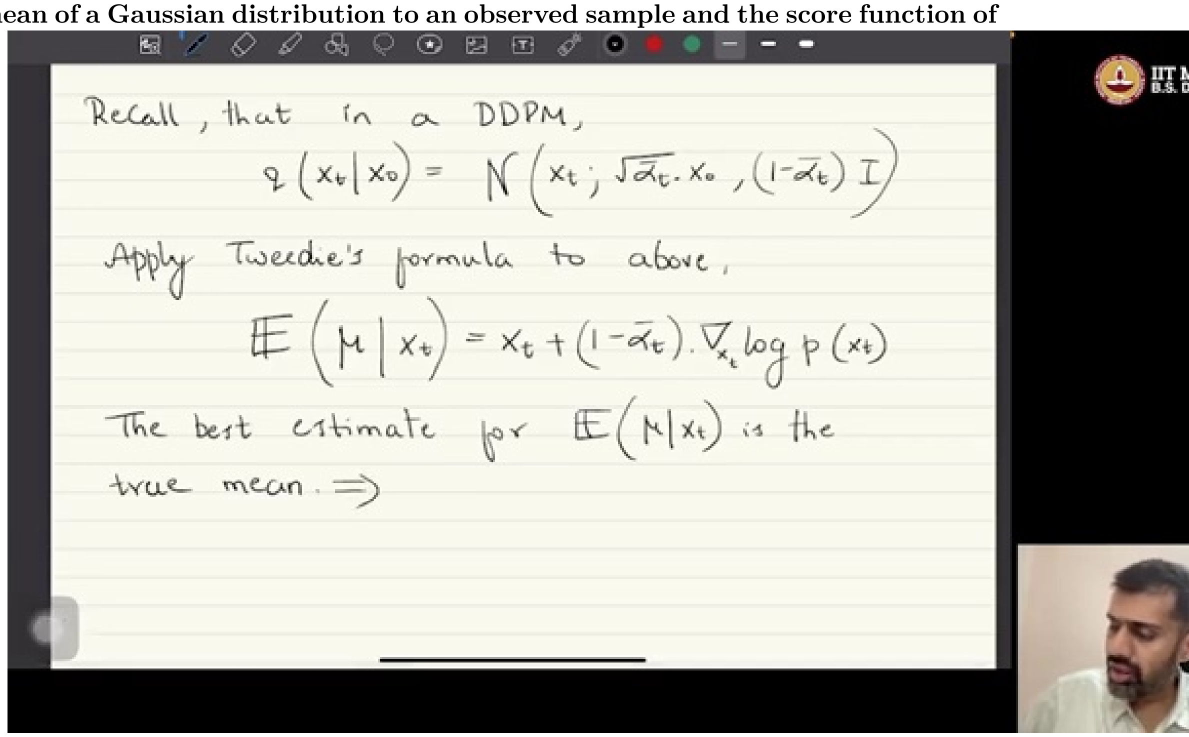
Question 5: If a DDPM is trained to predict the score function $S_\theta(x_t, t)$, how can you recover the predicted noise $\epsilon_\theta(x_t, t)$ from it?

Visual References

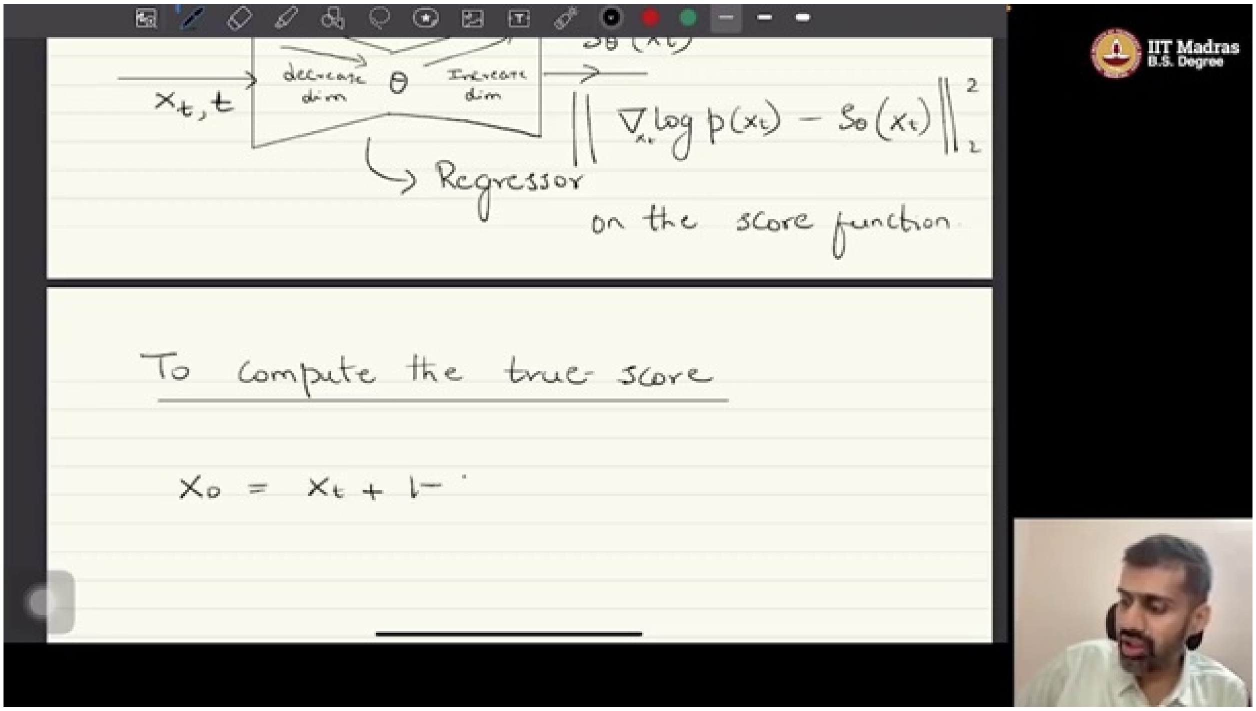
A diagram illustrating the score function (log p(x)) as vectors on a probability density landscape. This visual explains the intuition that the score function always points 'uphill' towards areas of higher probability. (at 03:15):



The formal mathematical statement of Tweedie's formula. This slide presents the key equation that connects the mean of a Gaussian distribution to an observed sample and the score function of the prior. (at 07:30):



The final step of the derivation applying Tweedie's formula to the DDPM forward process. This screenshot shows the crucial equation establishing the direct relationship between the added noise (_t) and the score function of the noisy data distribution (_xt log q(x_t)). (at 15:45):



A summary slide or concept map that visually demonstrates the equivalence of different DDPM training objectives. It shows how predicting the noise, predicting the original data (x_0), and predicting the score function are all mathematically linked and valid approaches. (at 22:10):