Study Material - Youtube

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Video Overview

This lecture introduces **Denoising Diffusion Implicit Models (DDIMs)**, a significant advancement over the previously discussed Denoising Diffusion Probabilistic Models (DDPMs). The instructor, Prof. Prathosh A P, explains the core motivations behind the development of DDIMs by first outlining the key limitations of DDPMs. The lecture then delves into the mathematical formulation of DDIMs, highlighting how they generalize DDPMs by introducing a non-Markovian forward process. A crucial insight presented is that despite this new formulation, DDIMs share the same training objective as DDPMs, which means a pre-trained DDPM model can be used for DDIM inference. This leads to the primary benefits of DDIMs: significantly faster sampling and the ability to perform deterministic, invertible mappings between the data and latent spaces.

Learning Objectives

Upon completing this lecture, students will be able to: - **Identify and explain the two primary limitations of DDPMs**: slow sampling speed and the stochastic, non-invertible nature of the forward process. - **Understand the core motivation for DDIMs** as a solution to these limitations. - **Describe the key difference between DDPM and DDIM forward processes**, specifically the transition from a Markovian to a non-Markovian process. - **Analyze the mathematical formulation of the DDIM inference distribution**, parameterized by a new scalar variable σ. - **Grasp the fundamental result** that the Evidence Lower Bound (ELBO) objective function is the same for both DDPMs and the entire family of DDIMs. - **Understand the practical implications of this shared objective**: a single trained DDPM model can be used to perform inference with any DDIM process. - **Explain how DDIMs enable accelerated sampling** and deterministic posterior inference.

Prerequisites

To fully understand the concepts in this lecture, students should have a solid grasp of: - **Denoising Diffusion Probabilistic Models (DDPMs):** A thorough understanding of the DDPM forward (diffusion) and reverse (denoising) processes is essential. - **Latent Variable Models:** Familiarity with concepts like Variational Autoencoders (VAEs), the Evidence Lower Bound (ELBO), posterior distributions, and inference. - **Probability and Statistics:** Strong knowledge of Gaussian distributions, conditional probability, Bayes' rule, and the properties of stochastic processes, including Markov chains. - **Calculus and Linear Algebra:** Basic understanding of derivatives, integrals, and vector/matrix operations.

Key Concepts Covered

- Denoising Diffusion Implicit Models (DDIMs)
- Limitations of DDPMs
- Non-Markovian Forward Process
- Deterministic vs. Stochastic Sampling
- Family of Inference Distributions
- Shared Evidence Lower Bound (ELBO)
- Accelerated Generation

Denoising Diffusion Implicit Models (DDIMs)

Motivation: Overcoming the Limitations of DDPMs

(01:07) The lecture begins by introducing Denoising Diffusion Implicit Models (DDIMs) as a powerful alternative to DDPMs. DDIMs were developed to address two significant drawbacks inherent in the DDPM framework.

Limitation 1: Slow Sampling

(01:18) A major practical issue with DDPMs is their **slow sampling speed**. - **The Problem:** To generate a single sample (e.g., an image), a DDPM must sequentially traverse the entire reverse process, starting from pure noise x_T and stepping down to the final data point x_0. - **Computational Cost:** The number of timesteps, T, is typically very large, often in the order of thousands ($T \approx 1000s$). This means that generating one image requires thousands of sequential forward passes through the neural network, making the process computationally intensive and time-consuming, especially compared to models like GANs which can generate samples in a single pass.

> **Key Takeaway:** The iterative, step-by-step nature of the DDPM reverse process, with a large number of steps T, is the bottleneck for fast sample generation.

Limitation 2: Stochastic and Non-Invertible Forward Process

(02:01) The second, more subtle limitation is that the DDPM forward process is **stochastic** and therefore **not uniquely invertible**.

- **Intuitive Explanation:** In many machine learning applications, particularly those involving data manipulation (like image editing), it is highly desirable to have a unique and deterministic mapping from a data point to its latent representation. This allows for consistent analysis and modification in the latent space.
- **The DDPM Forward Process:** The forward process in a DDPM, which maps a data point x_0 to a noisy version x_t, is defined as:

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

  The presence of the random noise term ϵ_t makes this process stochastic.
- **The Consequence (3:03):** If you take the same input image x_0 and run the forward process multiple times, you will get a different noisy latent vector x_T each time due to the freshly sampled noise ϵ_t. This means there is **no single, unique latent representation** for a given input. This lack of a deterministic mapping makes it difficult to perform tasks that rely on encoding an image into a consistent latent code for manipulation.

```
graph LR
    subgraph DDPM Forward Process (Stochastic)
        X0["Input Image (x )"] --> F1["Forward Process (t=1)"]
```

```
    X0 --> F2["Forward Process (t=2)"]
    X0 --> F3["Forward Process (t=...)"]
    F1 --> Z1["Latent Code 1 (x_T)"]
    F2 --> Z2["Latent Code 2 (x_T)"]
    F3 --> Z3["Latent Code 3 (x_T)"]
end
style Z1 fill:#f9f,stroke:#333,stroke-width:2px
style Z2 fill:#f9f,stroke:#333,stroke-width:2px
style Z3 fill:#f9f,stroke:#333,stroke-width:2px
```

Figure 1: This diagram illustrates the stochastic nature of the DDPM forward process. A single input x_0 can map to multiple different latent codes x_T due to the random noise added at each step.

The Core Idea of DDIMs: A Non-Markovian Approach

(17:00) DDIMs address these limitations by defining a new, more general **non-Markovian forward process**.

- **DDPM's Markovian Assumption:** The DDPM forward process is a Markov chain, where x_t depends only on x_{t-1}.
- **DDIM's Non-Markovian Process:** The DDIM forward process breaks this assumption. The distribution of the latent variable at the previous step, x_{t-1}, is conditioned not only on the current latent variable x_t but also on the initial data point x_0.

  $$q_\sigma(x_{t-1}|x_t, x_0)$$

  This explicit dependency on x_0 makes the process non-Markovian, as the state at $t-1$ now depends on a state far in the past ($t = 0$). This seemingly small change has profound consequences.

Mathematical Formulation of DDIMs

Defining a New Family of Forward Processes

(11:15) The central innovation of DDIM is the introduction of a family of inference distributions, parameterized by a scalar $\sigma \geq 0$.

The joint inference distribution (the forward process) is defined as:

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

Where the conditional transition probability is defined as a Gaussian:

$$q_\sigma(x_{t-1}|x_t, x_0) \triangleq \mathcal{N}\left(x_{t-1}; \tilde{\mu}_\sigma(x_t, x_0), \sigma_t^2 I\right)$$

The parameters of this Gaussian are: - **Mean:** $\tilde{\mu}_\sigma(x_t, x_0) = \sqrt{\bar{\alpha}_{t-1}}x_0 + \sqrt{1 - \bar{\alpha}_{t-1} - \sigma_t^2} \cdot \frac{x_t - \sqrt{\bar{\alpha}_t}x_0}{\sqrt{1-\bar{\alpha}_t}}$ - **Variance:** $\sigma_t^2 I$

Here, σ_t is a new hyperparameter that controls the stochasticity of the process.

The Key Insight: A Shared Training Objective

(22:43) The most remarkable result of the DDIM paper is that despite this new, complex-looking forward process, the **training objective remains identical to that of DDPMs**.

- **Invariant Marginal Distribution:** The authors prove that the marginal distribution of the latent variable x_t given the input x_0 is independent of the new parameter σ. It is exactly the same as in DDPMs:

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

- **Identical ELBO:** The Evidence Lower Bound (ELBO) for diffusion models depends only on these marginals, $q(x_t|x_0)$. Since these marginals are the same for DDPMs and all DDIMs (for any valid choice of σ), the ELBO is also the same.

  The Main Result (36:43): Training a standard DDPM model is **implicitly training an entire family of non-Markovian models (DDIMs)**. The same learned neural network, ϵ_θ, can be used for any model in this family. The only thing that changes is the inference (sampling) procedure.

This is a profound insight. It means we can take an off-the-shelf, pre-trained DDPM and use it with the DDIM sampling procedure to gain its benefits without any retraining.

The DDIM Reverse Process and Inference

Deriving the Reverse (Generative) Step

(31:37) The generative or reverse process, $p_\theta(x_{t-1}|x_t)$, is designed to approximate the true posterior, $q_\sigma(x_{t-1}|x_t, x_0)$. The key is to substitute the unknown x_0 with its predicted value, $\hat{x}_0$, which is derived from the neural network's noise prediction $\epsilon_\theta(x_t, t)$.

1. **Predict the "denoised" image** x_0:

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

   This term represents the model's best guess for the original image, given the noisy image x_t.

2. **Predict the direction to** x_{t-1}: The term $\frac{x_t - \sqrt{\bar{\alpha}_t}x_0}{\sqrt{1-\bar{\alpha}_t}}$ in the mean of q_σ is an estimate of the noise ϵ. We replace it with the network's prediction $\epsilon_\theta(x_t, t)$.

3. **Construct the reverse step**: Plugging these into the definition of $q_\sigma(x_{t-1}|x_t, x_0)$ gives the DDIM sampling step:

$$x_{t-1} = \underbrace{\sqrt{\bar{\alpha}_{t-1}}\hat{x}_0(x_t, t)}_{\text{Predicted } x_0 \text{ component}} + \underbrace{\sqrt{1-\bar{\alpha}_{t-1}-\sigma_t^2} \cdot \epsilon_\theta(x_t, t)}_{\text{Direction to } x_{t-1}} + \underbrace{\sigma_t \epsilon}_{\text{Random Noise}}$$

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

The Role of the Parameter σ: From Stochastic to Deterministic

The hyperparameter σ_t controls the trade-off between a DDPM-like stochastic process and a new deterministic one.

- **Case 1: Recovering DDPM (σ_t is non-zero)** If we set $\sigma_t^2 = \tilde{\beta}_t = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}(1-\beta_t)$, the DDIM sampling step becomes identical to the DDPM sampling step. The process is **stochastic**.

- **Case 2: Deterministic DDIM ($\sigma_t = 0$)** (42:02) If we set $\sigma_t = 0$ for all t, the random noise term $\sigma_t\epsilon$ vanishes. The update rule becomes fully **deterministic**:

$$x_{t-1} = \sqrt{\bar{\alpha}_{t-1}}\hat{x}_0(x_t, t) + \sqrt{1-\bar{\alpha}_{t-1}} \cdot \epsilon_\theta(x_t, t)$$

  In this case, given a starting noise vector x_T, the entire generation trajectory is fixed. This is why DDIMs are called "Implicit Models," as they define an implicit, deterministic function from the latent space to the data space.

Practical Advantages of DDIMs

The DDIM formulation directly solves the two main limitations of DDPMs.

1. **Accelerated Sampling:** Because the process can be made deterministic, we are no longer required to use all T steps. We can define a new, shorter trajectory of timesteps (e.g., 50 steps instead of 1000) and jump between them. This dramatically speeds up the generation process, making it competitive with GANs in terms of sampling time.
2. **Deterministic Mapping and Invertibility:** With $\sigma = 0$, the mapping from x_T to x_0 is deterministic. More importantly, the process is invertible. We can take a real image x_0 and use the DDIM equations to find its unique corresponding latent code x_T. This enables a wide range of applications, such as image interpolation and manipulation, that were not feasible with the stochastic DDPM forward process.

```
flowchart TD
    subgraph DDPM Sampling (Slow & Stochastic)
        X_T["Start: Noise (x_T)"] --> S_T["Step T"]
        S_T --> S_T_minus_1["Step T-1"]
        S_T_minus_1 -->    ["... (1000 steps) ..."]
            --> S_1["Step 1"]
        S_1 --> X_0["Output: Image (x_0)"]
    end

    subgraph DDIM Sampling (Fast & Deterministic,  =0)
        Y_T["Start: Noise (x_T)"] --> D_T["Step T"]
        D_T --> D_T_minus_k["Step T-k (Skip)"]
        D_T_minus_k -->    2["... (e.g., 50 steps) ..."]
           2 --> D_1["Step 1"]
        D_1 --> Y_0["Output: Image (x_0)"]
    end

    style S_T fill:#ffc,stroke:#333
    style D_T fill:#cff,stroke:#333
```

Figure 2: A comparison of the sampling processes. DDPM requires a large number of sequential steps. DDIM, in its deterministic form, can skip steps, leading to much faster generation.

Self-Assessment

1. **Explain in your own words the two main limitations of DDPMs that motivated the creation of DDIMs.**
2. **What is the key difference between the forward process of a DDPM and a DDIM? Why is this difference significant?**
3. **What is the role of the parameter σ in the DDIM framework? What happens when $\sigma = 0$?**
4. **A researcher has already spent weeks training a large DDPM on a massive dataset. They now want to use DDIM for faster sampling. Do they need to retrain their model? Explain why or why not, referencing the ELBO.**
5. **Consider the DDIM reverse step equation. Identify the three main components of the equation and explain the intuitive role of each in generating x_{t-1} from x_t.**

Key Takeaways

- **DDIMs are a generalization of DDPMs** that use a non-Markovian forward process.
- They were designed to overcome DDPM's **slow sampling speed** and **stochastic, non-invertible nature**.
- The most critical finding is that **DDIMs share the same training objective (ELBO) as DDPMs**. This allows a single trained model to be used for both frameworks.
- By setting the hyperparameter $\sigma = 0$, DDIMs become **deterministic**, which enables:
  1. **Accelerated Sampling:** Generating high-quality images in far fewer steps (e.g., 50 vs. 1000).
  2. **Deterministic Invertibility:** Creating a unique mapping from a data point to a latent code, which is crucial for applications like image editing and interpolation.