Study Material - Youtube

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Video Overview

This video lecture provides a detailed tutorial on an alternative interpretation and implementation of Denoising Diffusion Probabilistic Models (DDPMs). Instead of the standard approach of predicting the original clean image x_0, this lecture focuses on reformulating the problem as **predicting the noise** ϵ that was added to the image during the forward diffusion process. The instructor explains the mathematical motivation for this approach and then provides a comprehensive walkthrough of a PyTorch implementation, covering the model architecture (U-Net), training loop, and the image generation (sampling) process.

Learning Objectives

Upon completing this study material, you will be able to:

- Understand the mathematical framework for interpreting DDPMs as a noise regression problem.
- Derive the simplified loss function for noise estimation in DDPMs.
- Analyze and understand a complete PyTorch implementation of a DDPM that predicts noise.
- Explain the role and structure of the U-Net model in this context, including time embeddings.
- Describe the modified training and sampling (inference) loops for a noise-predicting DDPM.
- Identify the key hyperparameters and their impact on the training and generation quality.

Prerequisites

To fully grasp the concepts in this video, you should have a foundational understanding of:

- **Denoising Diffusion Probabilistic Models (DDPMs):** Familiarity with the core concepts of the forward (noising) and reverse (denoising) processes.
- **Deep Learning & PyTorch:** Experience with building and training neural networks using PyTorch, including concepts like `nn.Module`, optimizers, and loss functions.

- **Convolutional Neural Networks (CNNs):** Knowledge of CNN architectures, particularly the U-Net architecture.
- **Probability & Calculus:** Basic understanding of Gaussian distributions, expectation, and gradients.

Key Concepts

- **DDPM as Noise Regression:** The central idea of training the model to predict the noise ϵ added at timestep t, rather than predicting the clean image x_0.
- **Forward Process (Closed-Form):** The equation that defines the noisy image x_t at any timestep t directly from the original image x_0.
- **Simplified Loss Function:** The derivation showing that the DDPM objective can be simplified to a Mean Squared Error (MSE) loss between the actual added noise and the noise predicted by the model.
- **U-Net for Noise Prediction:** Using a U-Net architecture that takes a noisy image x_t and a timestep embedding as input to output a predicted noise map.
- **Sinusoidal Time Embeddings:** A technique to encode the discrete timestep t into a continuous vector representation that can be processed by the neural network.
- **Reverse Diffusion (Sampling):** The iterative process of generating a clean image by starting with pure noise and using the trained model to predict and subtract noise at each step.

DDPM as Regression Over Added Noise

The core of this lecture is an alternative perspective on what a DDPM learns. Instead of training the model to directly predict the original image x_0 from a noisy version x_t, we can train it to predict the noise ϵ that was added to x_0 to create x_t. This reframes the task as a regression problem.

Intuitive Foundation

Imagine you have a clean image (x_0). The DDPM forward process gradually adds Gaussian noise to it over T steps, creating a sequence of increasingly noisy images $x_1, x_2, ..., x_T$. At any step t, the noisy image x_t is just a combination of the original image x_0 and a specific noise sample ϵ.

The standard DDPM tries to reverse this process by learning a function that estimates x_0 from x_t. However, an equally valid approach is to learn a function that estimates the *noise* ϵ from x_t. If we can accurately predict the noise that was added, we can simply subtract it (in a carefully defined way) to recover a cleaner version of the image. This turns out to be a more stable and effective objective for the model to learn.

Mathematical Analysis (00:19)

The mathematical justification for this approach stems from the forward process equation and the DDPM loss function.

Recalling the Forward Process

As established in previous lectures, the forward process can be expressed in a closed form, allowing us to generate a noisy sample x_t for any timestep t directly from the original image x_0.

The equation is:

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

where: - x_0 is the original clean image. - x_t is the noisy image at timestep t. - ϵ is a random noise sample from a standard normal distribution, $\epsilon \sim \mathcal{N}(0, \mathbf{I})$. - $\bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i$, where $\alpha_i = 1 - \beta_i$ are parameters from the noise schedule.

Reformulating for Noise Prediction

(00:20) The instructor shows that we can rearrange the forward process equation to solve for the noise term $\epsilon$. This gives us the ground truth noise that was added to produce $x_t$.

Step-by-step Derivation: 1. Start with the forward process equation:

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

2. Subtract the scaled original image term from both sides:

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

3. Divide by the noise coefficient to isolate $\epsilon$:

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

This equation gives us the actual noise $\epsilon$ that was used to generate $x_t$. Our goal is to train a neural network, $\epsilon_\theta(x_t, t)$, to predict this noise.

The Simplified Loss Function

The original DDPM paper showed that the variational lower bound (ELBO) loss can be simplified. When we parameterize the model to predict noise, the loss function becomes a simple Mean Squared Error (MSE) between the true noise and the predicted noise.

$$L_{simple} = \mathbb{E}_{t, x_0, \epsilon} \left[||\epsilon - \epsilon_\theta(x_t, t)||^2 \right]$$

where $x_t$ is calculated using the forward process formula. This loss function is highly intuitive: it directly penalizes the model if its predicted noise ϵ_θ differs from the actual noise $\epsilon$ that was added.

The instructor notes that this is proportional to the consistency term in the ELBO, which is the KL divergence between the true posterior and the learned reverse process. By simplifying it this way, we get a very direct and stable training objective.

The following flowchart illustrates the conceptual flow of training a noise-predicting DDPM.

```
flowchart TD
    A["Start with a clean image batch<br/>$x_0$"] --> B{"Sample random timesteps<br/>$t \sim U(1, T)$"}
    B --> C["Sample noise from $\mathcal{N}(0, I)$<br/>$\epsilon$"];
    C --> D["Create noisy images using forward process<br/>$x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 -
    D --> E["Input $x_t$ and $t$ into U-Net<br/>$\epsilon_\theta(x_t, t)$"];
    E --> F{"Calculate Loss<br/>$||\epsilon - \epsilon_\theta(x_t, t)||^2$"};
    F --> G["Backpropagate and update<br/>model weights $\theta$"];
    G --> A;
```

Figure 1: The training loop for a DDPM configured for noise estimation. The model's goal is to predict the noise $\epsilon$ that was used to corrupt the original image $x_0$.

Practical Implementation in PyTorch

The lecture then transitions to a detailed code walkthrough of a Jupyter notebook (`ITM_DGM_DDPM_Noise_Estimate.ipynb`) that implements this noise estimation strategy.

Code Structure and Hyperparameters (02:35)

The implementation uses PyTorch and is structured with helper functions, a U-Net model class, and a main training loop.

Key Hyperparameters: - `IMG_SIZE`: 32 (Images are resized to 32x32) - `BATCH_SIZE`: 128 - `EPOCHS`: 25 - `LR`: 0.001 (Learning Rate) - `TIMESTEPS`: 600 (Total number of diffusion steps)

Diffusion Schedule Constants

(03:06) Before training, a set of constants derived from the noise schedule (β_t) are pre-computed. This is an efficiency optimization to avoid recalculating them in every step of the training loop.

```
# Prepare Diffusion Schedule Constants
betas = linear_beta_schedule(timesteps=TIMESTEPS)
alphas = 1. - betas
alphas_cumprod = torch.cumprod(alphas, axis=0)
alphas_cumprod_prev = F.pad(alphas_cumprod[:-1], (1, 0), value=1.0)
sqrt_recip_alphas = torch.sqrt(1.0 / alphas)

# Constants needed for forward process
sqrt_alphas_cumprod = torch.sqrt(alphas_cumprod)
sqrt_one_minus_alphas_cumprod = torch.sqrt(1. - alphas_cumprod)

# Constants needed for the reverse process (sampling)
posterior_variance = betas * (1. - alphas_cumprod_prev) / (1. - alphas_cumprod)
```

- `betas`: A linear schedule of noise variances from a small value to a larger one.
- `alphas`: $1 - \beta_t$.
- `alphas_cumprod` ($\bar{\alpha}_t$): The cumulative product of alphas, essential for the closed-form forward process.
- `sqrt_...`: Pre-computed square roots of these values, which appear directly in the forward and reverse process equations.

U-Net Model Architecture (`SimpleUnet`) (05:51)

The core of the model is a U-Net, which is particularly effective for image-to-image tasks like this. Its job is to take a noisy image and a timestep and predict the noise present in the image.

Key Components:

1. **Sinusoidal Positional Embeddings (06:40):** Timesteps are scalars (e.g., 1, 2, … 600), but neural networks work best with high-dimensional vector inputs. This module converts the timestep `t` into a fixed-size vector embedding using sine and cosine functions of different frequencies, similar to the Transformer architecture. This allows the model to understand "how far" into the diffusion process it is.

2. **Downsampling Path (`self.downs`):** A series of blocks that progressively reduce the spatial dimensions of the feature maps (e.g., 32x32 -> 16x16 -> 8x8) while increasing the number of channels (e.g., 64 -> 128 -> 256). Each block typically consists of convolutions, normalization, and activation functions.

3. **Upsampling Path (`self.ups`):** A symmetric series of blocks that increase the spatial dimensions and decrease the channel count, eventually returning to the original image size.

4. **Skip Connections:** Feature maps from the downsampling path are concatenated with the corresponding feature maps in the upsampling path. This is crucial for preserving high-resolution details and allows the model to combine low-level and high-level features.

5. **Time Embedding Integration:** The time embedding vector is processed by a small MLP and then added to the feature maps at each block of the U-Net. This conditions the entire network on the current timestep `t`.

Training Loop Breakdown (13:14)

The training loop iterates through the dataset for a specified number of epochs. For each batch of images:

1. **Get Clean Images:** A batch of clean images `x0` is loaded.
2. **Sample Timesteps:** A random timestep `t` is sampled for *each image* in the batch. This ensures the model sees examples from all stages of the diffusion process.
3. **Create Noisy Images (Forward Process):** The `forward_diffusion_sample` function is called. It takes `x0` and `t`, and using the pre-computed constants, it generates the noisy image `xt` and also returns the ground truth noise `noise_target` that was added. `python     # Create noisy images x_t and get the added noise (our target)     xt, noise_target = forward_diffusion_sample(x0, t, sqrt_alphas_cumprod, sqrt_one_minus_alphas_cumprod)`
4. **Predict Noise:** The noisy image `xt` and its corresponding timestep `t` are passed to the U-Net model to get the `predicted_noise`. `python     # Predict the noise using the U-Net model predicted_noise = model(xt, t)`
5. **Calculate Loss:** The MSE loss is computed between the model's prediction and the actual noise. `python     # Calculate the loss between the model's prediction and the actual noise loss = criterion(noise_target, predicted_noise)`
6. **Backpropagation:** Standard backpropagation and optimizer steps are performed to update the model's weights.

Image Generation (Sampling) (17:33)

Once the model is trained, it can be used to generate new images. This is done by simulating the reverse diffusion process.

```
sequenceDiagram
    participant N as Noise
    participant L as Loop
    participant M as Model
    participant I as Image

    N->>L: Start with pure random noise $x_T$
    loop For t from T down to 1
        L->>M: Predict noise $\epsilon_\theta(x_t, t)$
        M-->>L: Return predicted noise
        L->>L: Calculate mean $\mu_\theta(x_t, t)$
        L->>I: Sample $x_{t-1} \sim \mathcal{N}(\mu_\theta, \sigma_t^2 I)$
        I-->>L: Update image to $x_{t-1}$
    end
    L->>I: Final denoised image $x_0$
```

Figure 2: The reverse diffusion process for generating an image. The loop iteratively denoises the image using the model's noise predictions.

Steps in Code: 1. Start with a tensor of pure Gaussian noise, `img`, of the desired image size. 2. Loop backwards through the timesteps (from `T-1` down to `0`). 3. In each step `t`, call a `sample_timestep` function which: a. Uses the model to predict the noise: `predicted_noise = model(x, t)`. b. Calculates the mean of the reverse distribution using the formula:

$$\text{model\_mean} = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(x_t, t)\right)$$

c. If $t > 0$, add scaled random noise for stochasticity. If $t = 0$, no noise is added. d. Returns the less-noisy image for the next step, $x_{t-1}$. 4. The final output of the loop is the generated image.

The generated MNIST digits (18:47) are recognizable but have a noisy, textured background. The instructor notes this is an area for improvement, possibly by training for more epochs or tuning hyperparameters.

Self-Assessment for This Video

1. **Conceptual Questions:**
   - Why is it sometimes preferable to predict the noise ϵ instead of the clean image x_0 in a DDPM?
   - Explain the purpose of sinusoidal positional embeddings for the timestep. Why not just feed the integer `t` directly to the network?
   - In the U-Net architecture, what is the role of skip connections during the upsampling path?
2. **Mathematical Questions:**
   - Starting from the forward process equation $x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon$, derive the expression for the loss function L_{simple}.
   - What is the formula for the mean of the reverse distribution, $\mu_\theta(x_t, t)$, when the model predicts noise ϵ_θ?
3. **Application Exercises:**
   - The final generated images have a noisy background (18:47). Suggest two specific changes to the hyperparameters in the provided code that might improve the image quality and reduce this background noise.
   - Modify the `sample_timestep` function in the code to remove the stochastic element (i.e., make the sampling deterministic). What line(s) would you change or remove?
   - How would you modify the `SimpleUnet` class to handle 3-channel color images (e.g., from the CIFAR-10 dataset) instead of 1-channel grayscale images?

Key Takeaways from This Video

- **Flexibility of DDPMs:** DDPMs can be effectively trained by having the model predict the added noise, which simplifies the loss to a standard MSE regression objective.
- **Importance of Pre-computation:** Pre-calculating diffusion schedule constants (`alphas`, `betas`, etc.) is a crucial optimization for efficient training.
- **U-Net is a Powerful Backbone:** The U-Net architecture, with its skip connections and ability to integrate conditional information like time embeddings, is highly suitable for the noise prediction task.
- **Training vs. Sampling:** The training process involves a single-step forward diffusion to create a (noisy image, noise) pair for the loss calculation. The sampling process is an iterative, multi-step reverse diffusion that uses the trained model repeatedly.
- **Implementation Details Matter:** The quality of generated samples is sensitive to hyperparameters like the number of training epochs, learning rate, and the total number of diffusion timesteps. The generated images in the tutorial show that even with a correct implementation, further tuning is often required for high-fidelity results.