Study Material - Youtube

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Video Overview

This video provides a comprehensive tutorial on the implementation of Denoising Diffusion Probabilistic Models (DDPMs). The lecture begins with a conceptual review of the DDPM framework, detailing the forward (diffusion) and reverse (denoising) processes. The instructor then connects the underlying mathematical principles to a practical Python implementation using the PyTorch library. The tutorial covers the entire pipeline, from setting up the noise schedule and defining the U-Net architecture to executing the training loop and performing inference to generate new samples.

Learning Objectives

Upon completing this study material, you will be able to: - **Understand the core mechanics** of DDPMs, including the forward noising process and the learned reverse denoising process. - **Connect the mathematical equations** of DDPMs to their corresponding implementation in PyTorch code. - **Implement the training algorithm** for a DDPM, including the loss calculation and weight updates. - **Implement the sampling (inference) algorithm** to generate new data from a trained DDPM. - **Appreciate the role of key components** like the U-Net architecture and time step embeddings. - **Analyze the results** of a trained DDPM and understand the simplifications made in the tutorial compared to a full-scale implementation.

Prerequisites

To fully grasp the concepts in this video, you should have a foundational understanding of: - **Deep Learning:** Neural networks, backpropagation, loss functions, and gradient descent. - **PyTorch:** Experience with building and training neural network models. - **Probability Theory:** Basic concepts of Gaussian (Normal) distributions. - **Generative Models (Recommended):** Familiarity with the concepts of GANs and VAEs provides useful context. - **U-Net Architecture:** A basic understanding of its encoder-decoder structure with skip connections.

Key Concepts Covered

- **Forward Process (Diffusion):** The fixed process of incrementally adding Gaussian noise to an image.
- **Reverse Process (Denoising):** The learned process of reversing the diffusion to generate an image from noise.
- **Noise Schedule:** The set of hyperparameters (β_t, α_t, $\bar{\alpha}_t$) that control the noise level at each timestep.
- **U-Net Architecture:** The specific neural network architecture used to predict the noise.
- **Training and Inference Algorithms:** The step-by-step procedures for training the model and generating new samples.
- **Time Step Embedding:** The method for providing the timestep `t` as input to the neural network.

Core Concepts of Denoising Diffusion Probabilistic Models (DDPMs)

The instructor begins with a high-level overview of the DDPM framework, which consists of two opposing processes: a **forward process** that corrupts data and a **reverse process** that learns to restore it.

The Forward Process (Diffusion)

Intuitive Foundation (00:38): The forward process, also known as the diffusion process, is a procedure where we start with a clean, real image (x_0) and systematically destroy it by adding a small amount of Gaussian noise at each step. This is repeated for a large number of timesteps (T), typically around 1000. By the end of this process, the original image x_0 is transformed into an image x_T that is indistinguishable from pure Gaussian noise.

Visual Representation (00:11): The video displays a diagram illustrating this progression.

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

This diagram shows the forward process, where an initial image **x** *is progressively noised through conditional distributions* **q** *until it becomes pure noise* **x_T***.*

Mathematical and Technical Details: - The forward process is a **fixed Markov chain**. This means the state at time t (x_t) only depends on the state at time $t-1$ (x_{t-1}). - The transition is defined by a conditional Gaussian distribution: $q(x_t|x_{t-1}) = \mathcal{N}(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t I)$. - The parameters β_t form a **noise schedule** and are pre-defined, not learned. They typically increase from a small value to a larger one as `t` goes from 1 to `T`. - A key property is that we can sample x_t at any arbitrary timestep `t` directly from x_0 using a closed-form equation:

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

where $\alpha_t = 1-\beta_t$, $\bar{\alpha}_t = \prod_{i=1}^t \alpha_i$, and $\epsilon \sim \mathcal{N}(0, I)$. - **Crucially, this process has no trainable parameters** (01:11). It's a pre-defined, deterministic (in terms of its schedule) but probabilistic (due to noise sampling) procedure.

The Reverse Process (Denoising)

Intuitive Foundation (01:37): The reverse process is where the learning happens. The goal is to train a neural network to undo the diffusion process. It starts with a sample of pure Gaussian noise (x_T) and iteratively removes a small amount of noise at each step, moving backward in time from T to 1, to ultimately generate a clean, realistic image (x_0).

Visual Representation (00:11): The same diagram illustrates the reverse process, moving from right to left.

```
graph LR
    subgraph Reverse Process (p_ )
        direction RL
        x0["x <br/>(Generated Image)"] <--|p_ (x |x )| x1["..."]
        x1 <--|p_ (x  |x )| xt["x <br/>(Noisy Image)"]
        xt <--|...| xT["x_T<br/>(Pure Noise)"]
    end
```

This diagram shows the reverse process, where a neural network `p_` learns to denoise an image, starting from `x_T` and moving backward to generate `x`.

Mathematical and Technical Details: - The reverse process is modeled as a **learned Markov chain**, parameterized by a neural network with weights θ. - The network's task is to approximate the true posterior distribution $q(x_{t-1}|x_t, x_0)$, which is intractable without knowing x_0. Instead, it learns $p_\theta(x_{t-1}|x_t)$. - The core idea is that the network, given a noisy image x_t at timestep `t`, predicts the noise ϵ that was added. With this predicted noise, it can estimate the less-noisy image x_{t-1}. - Unlike GANs or VAEs, which generate samples in a single forward pass, DDPMs are **iterative generators**. The generation process (sampling) is time-consuming as it requires `T` sequential passes through the network (02:55).

Training a DDPM: Mathematical Formulation and Algorithm

The instructor explains that the training process is surprisingly elegant and simple.

The Training Objective: Simplified Loss

While the full objective is derived from the Evidence Lower Bound (ELBO), it simplifies to a more intuitive form. The model is trained to predict the original clean image x_0 from a noisy version x_t. This is equivalent to predicting the noise ϵ that was added to x_0 to create x_t.

The loss function used in the implementation is the **Mean Squared Error (MSE)** between the predicted clean image and the true clean image.

Loss Function (03:33): The objective for a batch of data is to minimize the following:

$$J_\theta = \sum_{i=1}^{m} ||\hat{x}_\theta(x_t^{(i)}) - x_0^{(i)}||_2^2$$

- $x_0^{(i)}$ is the i-th true data sample. - $x_t^{(i)}$ is the noisy version of $x_0^{(i)}$ at a randomly chosen timestep `t`. - $\hat{x}_\theta(x_t^{(i)})$ is the output of the neural network (the predicted clean image). - m is the number of different timesteps sampled for the batch.

The DDPM Training Algorithm

The training procedure is an iterative process repeated until the model converges.

Algorithm Steps (from slide at 03:22): 1. **Get a batch of clean images** x_0 from the true data distribution. 2. **For each image in the batch:** a. **Sample a random timestep** t uniformly from $\{1, ..., T\}$. b. **Sample noise** $\epsilon \sim \mathcal{N}(0, I)$. c. **Create the noisy image** x_t using the closed-form forward process formula:

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

3. **Predict the original image:** Pass the noisy images x_t and their corresponding timesteps t to the U-Net model to get predictions $\hat{x}_0 = \text{model}(x_t, t)$. 4. **Calculate the loss:** Compute the MSE between the predictions $\hat{x}_0$ and the original clean images x_0. 5. **Perform backpropagation** and update the model's weights θ.

Visualizing the Training Loop

```
flowchart TD
    A["Start Epoch"] --> B{For each batch x  in DataLoader};
    B --> C["Sample random timesteps t"];
    C --> D["Sample noise   ~ N(0,I)"];
    D --> E["Create noisy images x <br>x  = sqrt(̄ )x  + sqrt(1-̄ ) "];
    E --> F["Predict x̂  = model(x , t)"];
    F --> G["Calculate Loss<br>MSE(x̂ , x )"];
    G --> H["Backpropagate & Update Weights  "];
    H --> B;
    B --> I["End Epoch"];
```

This flowchart illustrates the training loop for a DDPM, as described in the lecture.

Key Architectural Components

The U-Net for Denoising

The neural network used in this implementation is a **U-Net** (06:41). - **Structure:** It has an encoder path that downsamples the image to capture context and a decoder path that upsamples it to reconstruct the image. - **Skip Connections:** Crucially, it uses skip connections to pass high-resolution features from the encoder directly to the decoder. This helps preserve fine-grained details, which is essential for image restoration tasks. - **Function:** The U-Net acts as the denoising function, taking a noisy image and a timestep as input and predicting the original clean image.

Time Step Embedding

A critical aspect of the DDPM is making the network aware of the noise level, which is determined by the timestep `t`.

- **The Problem (06:51):** The timestep `t` is a single integer. Feeding this scalar directly into a deep network is ineffective, as its numerical value doesn't provide a rich signal for the network to condition on.
- **The Solution:** The timestep `t` is converted into a high-dimensional vector using an embedding. The instructor discusses two methods:
    1. **Sinusoidal Positional Embedding (07:21):** This is the standard approach from the "Attention Is All You Need" paper. It uses sine and cosine functions of different frequencies to create a unique vector for each timestep.

2. **Simple Channel Map (18:39):** A simpler method used in this tutorial's code. It creates a new channel for the input image with the same height and width, and fills every pixel of this channel with the value of `t`. This is then concatenated with the noisy image channels.

Practical Implementation in PyTorch

The instructor walks through a Jupyter notebook to demonstrate the implementation.

Setting up the Diffusion Schedule

The noise schedule is pre-computed and stored as model buffers.

Code Snippet (10:00):

```
# 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)
```

- `T`: The total number of diffusion steps.
- `beta`: A linear schedule for β_t from 10^{-4} to 0.02.
- `alpha`: Corresponds to $\alpha_t = 1 - \beta_t$.
- `alpha_cumprod`: Corresponds to $\bar{\alpha}_t$.
- These tensors are registered as buffers in the model so they are part of the model's state but are not updated by the optimizer.

The Main DDPM Model Class

A class `DDPMv0_2ch` is defined to encapsulate the entire model.

Code Snippet (15:29):

```
class DDPMv0_2ch(nn.Module):
    def __init__(self):
        super().__init__()
        self.unet = Unet2ch(base_ch=64)
        # Register buffers so they move with .to(device)
        self.register_buffer('beta', beta)
        self.register_buffer('alpha', alpha)
        self.register_buffer('alpha_cumprod', alpha_cumprod)
        self.register_buffer('sqrt_acp', sqrt_acp)
        self.register_buffer('sqrt_omacp', sqrt_omacp)

    def q_sample(self, x0, t, noise):
        # Implements the forward process formula
        return (self.sqrt_acp[t].view(-1,1,1,1)*x0
                + self.sqrt_omacp[t].view(-1,1,1,1)*noise)

    def forward(self, x0, t):
        # Training: predict x0 from x_t
        # Loss = MSE(x0_hat, x0)
        noise = torch.randn_like(x0)
        x_t = self.q_sample(x0, t, noise) # add noise

        # build a single channel time map
        B,C,H,W = x0.shape
        t_chan = t.view(-1,1,1,1).expand(-1,1,H,W)
        inp = torch.cat((x_t, t_chan), dim=1) # [B,2,H,W]

        x0_hat = self.unet(inp) # predict x0
        return F.mse_loss(x0_hat, x0) # train to match true x0
```

The Sampling Process (Inference)

Sampling is the iterative reverse process.

Code Snippet (19:33):

```
# 4. Sampling / Inference
@torch.no_grad()
def sample(model, shape, device):
    # start from noise [B,1,H,W]
    x = torch.randn(shape, device=device)

    # iterate backwards
    for i in reversed(range(1, T)):
        t = torch.full((B,), i, device=device, dtype=torch.long)

        # predict x0
        t_chan = t.view(-1,1,1,1).expand(-1,1,H,W)
        inp = torch.cat((x, t_chan), dim=1)
        x0_hat = model.unet(inp)

        # sample x_{t-1} ~ N( (x_t, t),  ²)
        # ... (code to calculate mean and sigma) ...
        x = mean + sigma * noise

    return x.clamp(0, 1) # final image
```

- The process starts with random noise `x`.
- It iterates backward from `t=T-1` to `t=1`.
- In each step, it uses the model to predict `x0_hat` from the current `x` (which is x_t).
- It then uses this `x0_hat` to calculate the parameters of the distribution for x_{t-1} and samples from it.
- The final result is clamped to a valid image range `[0, 1]`.

Analysis of Results and Key Takeaways

The model is trained on MNIST for 15 epochs. - **Training Loss (24:22):** The MSE loss decreases steadily, indicating that the model is learning to denoise the images. - **Generated Samples (24:41):** The generated digits are recognizable but of very poor quality. The instructor points out this is expected due to simplifications in the tutorial code.

How to Improve the Implementation

The instructor highlights several reasons for the poor sample quality, which are key takeaways for a real-world implementation: 1. **Incomplete Loss Function (25:07):** The code only optimizes the MSE term, which corresponds to the third term of the full ELBO. The first term, related to the reconstruction at $t = 1$, is omitted for simplicity. Including it would improve results. 2. **Simplified Timestep Sampling (24:55):** The code samples only one random timestep `t` for the entire batch. A better approach is to sample a different random `t` for each image in the batch and average the losses. 3. **Insufficient Training:** 15 epochs is not nearly enough to train a DDPM to convergence. These models often require hundreds or thousands of epochs.

Self-Assessment for This Video

1. **Question:** What are the two main processes in a DDPM, and what is the role of each?
   - **Answer:** The two processes are the **forward (diffusion) process** and the **reverse (denoising) process**. The forward process is a fixed procedure that gradually adds noise to a real image until it becomes pure noise. The reverse process is a learned procedure where a neural network starts with pure noise and iteratively removes it to generate a clean image.
2. **Question:** In the forward process formula $x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon$, what do $\bar{\alpha}_t$ and ϵ represent?
   - **Answer:** $\bar{\alpha}_t$ is the cumulative product of the noise schedule parameters, controlling how much of the original image signal remains at timestep `t`. ϵ is a random noise sample from a standard Gaussian distribution, $\mathcal{N}(0, I)$.
3. **Question:** Why is the sampling/inference process in a DDPM slow compared to a GAN?
   - **Answer:** Sampling in a DDPM is an iterative process that requires `T` (e.g., 1000) sequential forward passes through the neural network, one for each denoising step. In contrast, a GAN generates a sample in a single forward pass.
4. **Question:** What is the purpose of time embedding, and what is the simple method used in this tutorial's code?
   - **Answer:** Time embedding provides the neural network with information about the current noise level (timestep `t`). The simple method used in the code is to create an additional input channel with the same dimensions as the image and fill it with the scalar value of `t`.
5. **Question:** The instructor states the generated images are of poor quality. What are two key reasons mentioned for this?
   - **Answer:** 1) The training was very short (only 15 epochs). 2) The loss was calculated based on a single random timestep for the entire batch, rather than averaging over multiple timesteps. 3) The loss function was a simplified version of the full ELBO.

Key Takeaways from This Video

- **DDPMs learn to reverse a fixed noising process.** The core task is to predict the noise added to an image at a given timestep.
- **The training process is stable and elegant,** relying on a simple MSE loss between the predicted and true data (or noise).
- **The U-Net architecture is well-suited for DDPMs** due to its ability to handle image-to-image tasks and preserve details via skip connections.
- **Inference is iterative and computationally expensive,** requiring one network pass for each denoising step.
- **Proper implementation is nuanced.** Details like the full loss function, sampling multiple timesteps per batch, and sufficient training time are critical for generating high-quality samples.