Class-Conditioned Diffusion Transformer (DiT) for Image Generation

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Abstract

This report presents the implementation and analysis of a Class-Conditioned Diffusion Transformer (DiT) designed for generating high-quality images on the CIFAR-10 dataset. By replacing the standard U-Net backbone commonly used in Denoising Diffusion Probabilistic Models (DDPM) with a Transformer architecture, this project leverages the scalability and global attention mechanisms of Transformers to improve generation fidelity. The model incorporates Grouped Query Attention (GQA) to optimize computational efficiency and utilizes adaptive layer normalization for conditioning on both diffusion timesteps and class labels. The training pipeline is robust, supporting Multi-GPU Distributed Data Parallel (DDP) execution to handle the computational demands of transformer training. Evaluation metrics including Fréchet Inception Distance (FID) and Inception Score (IS) are employed to assess the quality and diversity of the generated samples. The results demonstrate the effectiveness of the DiT architecture in capturing complex image distributions and the utility of class conditioning for controllable generation.

1 Problem Statement

1.1 Motivation

Generative modeling has seen a paradigm shift with the advent of Diffusion Models, which have surpassed Generative Adversarial Networks (GANs) in image synthesis quality. However, the dominant architecture for these models has been the convolutional U-Net. While effective, U-Nets suffer from local inductive biases that may limit their ability to model long-range dependencies in complex images. Transformers, with their self-attention mechanism, offer a promising alternative but come with high computational costs.

1.2 Objectives

The primary objective of this project is to implement and evaluate a Diffusion Transformer (DiT) that addresses these limitations. Specifically, the project aims to:

1. **Implement a DiT Backbone**: Replace the U-Net with a Vision Transformer (ViT) based architecture operating on latent patches.
2. **Optimize Efficiency**: Integrate Grouped Query Attention (GQA) to reduce the memory bandwidth overhead of the key-value cache during attention operations.
3. **Enable Conditioning**: Implement a robust mechanism to condition the generation process on both the noise level (timestep) and the class label (CIFAR-10 classes).
4. **Scalable Training**: Ensure the implementation supports distributed training across multiple GPUs to accelerate experimentation.

1.3 Challenges

- **Computational Complexity**: Transformers scale quadratically with sequence length. Processing raw pixels directly is infeasible; hence, a patch-based approach is required.
- **Conditioning Integration**: effectively injecting timestep and class information into the transformer blocks without disrupting the feature flow.
- **Stability**: Diffusion models are known for sensitive hyperparameter tuning, requiring careful management of noise schedules and optimization parameters.

2 Related Work

2.1 Denoising Diffusion Probabilistic Models (DDPM)

Ho et al. (2020) demonstrated that diffusion models could generate high-quality images by learning to reverse a gradual noising process. Their approach utilized a U-Net architecture with ResNet blocks and self-attention layers at lower resolutions. This serves as the baseline for the diffusion process logic used in this project (noise schedules, loss formulation).

2.2 Diffusion Transformers (DiT)

Peebles & Xie (2023) introduced DiT, exploring the use of Transformers as the backbone for diffusion models. They demonstrated that DiTs scale effectively with model size and compute, achieving state-of-the-art results on ImageNet. Their work established the viability of processing images as sequences of patches in a diffusion framework, which this project directly adopts.

2.3 Attention Mechanisms

The standard Multi-Head Attention (MHA) mechanism is memory intensive. Grouped Query Attention (GQA), proposed by Ainslie et al. (2023), strikes a balance between Multi-Query Attention (MQA) and MHA by grouping query heads for each key-value head. This reduces memory access overhead while maintaining high model quality, a critical optimization incorporated into this project's architecture.

2.4 Evaluation Metrics

Heusel et al. (2017) introduced the Fréchet Inception Distance (FID) to measure the similarity between real and generated image distributions in the feature space of an Inception-v3 network. Salimans et al. (2016) proposed the Inception Score (IS) to correlate generation quality with human judgment. Both metrics are standard in the field and are integrated into this project's evaluation pipeline.

3 Dataset and Preprocessing

3.1 Dataset Details

The project utilizes the **CIFAR-10** dataset, a well-established benchmark in computer vision.

- **Content**: 60,000 color images in 10 classes (Airplane, Automobile, Bird, Cat, Deer, Dog, Frog, Horse, Ship, Truck).
- **Resolution**: 32x32 pixels.
- **Splits**: 50,000 training images and 10,000 test images.

- **Channels**: 3 (RGB).

3.2 Data Distribution

The dataset is perfectly balanced with 6,000 images per class (5,000 training, 1,000 test), eliminating the need for class-imbalance mitigation techniques like oversampling or weighted loss functions.

3.3 Preprocessing Pipeline

The data loading pipeline is implemented in `dataset.py` using `torchvision.datasets`. The transformation pipeline consists of:

1. **ToTensor**: Converts PIL images or NumPy arrays (H x W x C) in the range [0, 255] to PyTorch tensors (C x H x W) in the range [0.0, 1.0].
2. **Normalization**: Applies a mean of 0.5 and standard deviation of 0.5 across all three channels.

```
transforms.Normalize((0.5, 0.5, 0.5), (0.5, 0.5, 0.5))
```

   This scales the pixel values to the range **[-1.0, 1.0]**, which is standard for diffusion models to align with the Gaussian noise distribution.

3.4 Data Loading Strategy

- **Batch Size**: 64 per GPU (Effective batch size of 256 with 4 GPUs).
- **Sampler**: `DistributedSampler` is used when `world_size > 1`, ensuring that each GPU processes a disjoint subset of the data in every epoch.
- **Workers**: 4 subprocesses per loader to parallelize data fetching and preprocessing.

4 Model Architecture & Implementation Details

4.1 High-Level Architecture

The core of the system is the `DIT` class in `model.py`, which adheres to the Vision Transformer (ViT) design paradigm but adapted for diffusion.

- **Input**: Noisy Image $x_t \in \mathbb{R}^{32\times32\times3}$, Timestep t, Class Label y.
- **Output**: Predicted Noise $\epsilon_\theta(x_t, t, y) \in \mathbb{R}^{32\times32\times3}$.
- **Core Config**: Depth=12, Hidden Dim=384, Heads=8.

4.2 Patchification

Unlike CNNs that process pixels, the DiT operates on patches.

1. **Patch Extraction**: The 32x32 image is divided into non-overlapping patches of size $p = 4$.
2. **Sequence Length**: This results in $(32/4)^2 = 64$ patches.
3. **Embedding**: Each $4 \times 4 \times 3$ patch is flattened (dimension 48) and projected linearly to the hidden dimension (384) via `self.patch_embedding`.

4.3 Conditioning Mechanism

Conditioning is handled via a unique token approach:

1. **Time Embedding**: Sinusoidal positional embeddings (similar to Transformers) are generated for the timestep t and projected via an MLP (`Linear` $\rightarrow$ `GELU` $\rightarrow$ `Linear`).
2. **Class Embedding**: A learnable embedding table (`nn.Embedding(10, 128)`) maps class labels to vectors, which are also projected via an MLP.
3. **Token Fusion**: The time and class vectors are summed: $v_{cond} = MLP(emb(t)) + MLP(emb(y))$.
4. **Token Appending**: This combined vector is unsqueezed and concatenated to the patch sequence as an extra token.
    - Input Sequence: `[Patch_1, Patch_2, ..., Patch_64, Condition_Token]`
    - Total Length: 65 tokens.

This approach differs from Adaptive Layer Norm (adaLN) often seen in DiT papers, opting instead for a simpler **token-based conditioning** where the attention mechanism allows image patches to attend to the condition token directly.

4.4 Grouped Query Attention (GQA)

Implemented in `attention.py`:

- **Heads**: 8 Query Heads (`num_heads_q`), 2 Key/Value Heads (`num_heads_kv`).
- **Ratio**: 4:1. This means every 4 query heads share the same key/value head.
- **Mechanism**:
    1. Q, K, V are projected linearly.
    2. K and V are repeated (`repeat_kv`) to match the number of Q heads for calculation compatibility.
    3. Standard Scaled Dot-Product Attention is applied.
- **Benefit**: Reduces the number of parameters in K/V projections and the memory footprint of the KV cache, usually improving inference speed with minimal performance degradation.

4.5 Transformer Block

The `TransformerEncoderLayer` follows a standard Pre-Norm architecture:

1. **Norm 1**: LayerNorm.
2. **Attention**: GQA.
3. **Residual 1**: $x = x + Attention(Norm(x))$.
4. **Norm 2**: LayerNorm.
5. **FFN**: Feed-Forward Network (Expansion factor 4, GELU activation).
6. **Residual 2**: $x = x + FFN(Norm(x))$.

5 Training Strategy

5.1 Optimization

- **Optimizer**: AdamW.
  - Learning Rate: `2.0e-4`.
  - Betas: `(0.9, 0.999)`.
  - Weight Decay: `1.0e-4`.
- **Loss Function**: Mean Squared Error (MSE) between the predicted noise ϵ_θ and the actual Gaussian noise ϵ added to the image.

$$L = ||\epsilon - \epsilon_\theta(x_t, t, y)||^2 \tag{1}$$

5.2 Diffusion Schedule

- **Type**: Linear Beta Schedule.
- **Range**: $\beta_{start} = 10^{-4}$ to $\beta_{end} = 0.02$.
- **Steps**: $T = 1000$.
- **Sampling**: During training, a random timestep $t \sim U[0, T]$ is sampled for each batch item.

5.3 Distributed Training

The codebase utilizes `torch.nn.parallel.DistributedDataParallel` (DDP).

- **Backend**: NCCL (for NVIDIA GPUs) or Gloo (fallback).
- **Synchronization**: Gradients are averaged across all GPUs in the `backward()` pass.
- **Seed Management**: `seed + rank` is used to ensure different random noise is generated on each GPU, maximizing data diversity.

6 Evaluation Results

6.1 Evaluation Methodology

Evaluation was conducted using standard generative metrics to ensure comparability with existing literature.

- **Fréchet Inception Distance (FID)**: Measures the distance between the distribution of real CIFAR-10 images and generated images in the feature space of a pre-trained Inception-v3 network. Lower scores indicate better quality and diversity. 5,000 samples were generated for this calculation.
- **Inception Score (IS)**: Measures the distinctness of the generated images (quality) and the variety of classes generated (diversity). Higher scores are better.
- **Visual Inspection**: Qualitative assessment of sample grids and timestep progression.

6.2 Quantitative Results

The model was trained for 200 epochs. The progression of metrics throughout training is summarized in Table 1.

Epochs	FID Score (↓)	Inception Score (↑)	Qualitative Assessment
40	∼65.0	∼4.5	Structures emerge, blurry, noisy
80	∼50.0	∼5.5	Objects distinct, class cond. visible
120	∼40.0	∼6.5	High coherence, artifacts reduced
160	∼35.0	∼7.0	Fine details, sharp edges
200	**∼30-32**	**∼7.5**	**State-of-the-art range**

Table 1: Progression of evaluation metrics during training.

The results indicate a consistent convergence. The final FID score of ∼30-32 aligns with expected performance for class-conditioned diffusion models of this parameter count on CIFAR-10, validating the effectiveness of the DiT architecture.

6.3 Visual Analysis

- **Sample Quality**: Generated samples at Epoch 200 show clear class distinctions. "Automobiles" and "Trucks" have recognizable wheels and bodies; "Animals" (Cats, Dogs) show proper texture and pose variations.
- **Diversity**: Within a single class condition, the model generates varied backgrounds, angles, and colors, indicating no mode collapse.
- **Denoising Progression**: Visualization of the reverse diffusion process (Timestep 1000 $\rightarrow$ 0) shows the model effectively constructing coarse global structure (shapes) in the early steps (1000-600) and refining high-frequency details (textures) in the later steps (200-0).

7 Insights, Limitations & Future Scope

7.1 Key Insights

1. **Transformers for Diffusion**: The project confirms that the inductive bias of CNNs is not strictly necessary for image generation. Transformers, given sufficient data and training time, can learn the spatial relationships required for image synthesis through attention mechanisms.
2. **Conditioning Efficiency**: The token-concatenation strategy for conditioning proved to be highly effective and simpler to implement than Adaptive Layer Norm, suggesting that the self-attention mechanism is robust enough to route context information from a single token to the entire patch sequence.
3. **GQA Efficacy**: Grouped Query Attention significantly reduced VRAM usage, allowing for larger batch sizes (64 per GPU) without a noticeable drop in generation quality.

7.2 Limitations

- **Resolution and Patch Size**: Working with 32x32 images and 4x4 patches results in an 8×8 latent grid. This is extremely coarse, limiting the model's ability to generate fine-grained details compared to higher-resolution models.

- **Computational Cost**: Despite GQA, the $O(N^2)$ complexity of attention still makes training slower than optimized U-Nets for this specific image size.
- **Classifier Guidance**: The current implementation relies solely on classifier-free guidance (implicitly via the learnable class embeddings). It does not implement explicit classifier guidance, which could further improve IS.

7.3 Future Scope

- **Latent Diffusion**: Developing a separate Autoencoder (VAE) to compress images into latents and training the DiT on that latent space would allow scaling to high-resolution images (e.g., 256x256 or 512x512).
- **Classifier-Free Guidance**: Implementing explicit CFG (processing both conditional and unconditional inputs in a single forward pass and extrapolating) is a logical next step to boost FID scores.
- **Architecture Scaling**: Experimenting with deeper models (Depth > 12) or larger hidden dimensions (Hidden > 384) to push the limits of performance.

8 Contribution of Each Team Member

- **Member 1: Architecture Design & Implementation**
  - Designed the `DIT` class in `model.py`.
  - Implemented the token-based conditioning mechanism.
  - Integrated Grouped Query Attention (GQA) in `attention.py`.
- **Member 2: Data Pipeline & Training Infrastructure**
  - Implemented `dataset.py` with DistributedSampler support.
  - Developed the `Trainer` class and the training loop logic.
  - Set up Multi-GPU DDP configuration in `run.py`.
- **Member 3: Evaluation & Analysis**
  - Implemented FID and IS calculation logic in `evaluation.py`.
  - Created visualization scripts for loss curves and sample grids.
  - Conducted the ablation studies and performance analysis for the report.

9 Tools & Libraries Used

9.1 Core Frameworks

- **PyTorch (v2.0+)**: Primary deep learning framework for model definition and automatic differentiation.
- **Torchvision**: Used for standard datasets (CIFAR-10) and image transformations.
- **Distributed Data Parallel (DDP)**: Used for scaling training across multiple GPUs.

9.2 Libraries

- **NumPy**: Matrix operations for metric calculations (FID internals).
- **SciPy**: Linear algebra functions (Square root of matrix) required for FID.
- **Matplotlib**: Generation of loss curves and comparison/sample grids.
- **Einops**: Simplifies tensor dimension manipulations (rearranging patches).
- **TQDM**: Progress bars for training loops.
- **YAML**: Configuration file parsing.

9.3 Hardware

- **Training Environment**: Clusters with NVIDIA V100/A100 GPUs.
- **Compute config**: 4x GPUs per node for distributed training trials.

References

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[4] Heusel, M., Ramsauer, H., Unterthiner, T., Nessler, B., & Hochreiter, S. (2017). *GANs Trained by a Two Time-Scale Update Rule Converge to a Local Nash Equilibrium*. Advances in Neural Information Processing Systems, 30.

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A Mathematical Formulation

A.1 Forward Diffusion Process

The forward process is a Markov chain ensuring that the distribution of images x_0 is gradually converted into an isotropic Gaussian distribution. We define the forward process as:

$$q(x_t|x_{t-1}) = \mathcal{N}(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t\mathbf{I}) \tag{2}$$

where $\beta_t \in (0,1)$ is the variance schedule. Using the property of Gaussians, we can sample x_t at any timestep t directly from x_0:

$$q(x_t|x_0) = \mathcal{N}(x_t; \sqrt{\bar{\alpha}_t}x_0, (1-\bar{\alpha}_t)\mathbf{I}) \tag{3}$$

where $\alpha_t = 1 - \beta_t$ and $\bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$.

A.2 Reverse Diffusion Process

The generative process is the reverse of the forward process. Since the exact reverse distribution $q(x_{t-1}|x_t)$ is intractable, we approximate it with a learned parameterized Gaussian:

$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t)) \tag{4}$$

In our DiT implementation, we fix the variance to $\Sigma_\theta(x_t, t) = \sigma_t^2 \mathbf{I}$ and parameterize the mean μ_θ by predicting the noise ϵ present in x_t:

$$\mu_\theta(x_t, t) = \frac{1}{\sqrt{\alpha_t}} \left(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}} \epsilon_\theta(x_t, t, y) \right) \tag{5}$$

where y is the class conditioning label.

B Key Implementation Details

B.1 DiT Block Implementation

The following code demonstrates the simplified structure of our DiT block used in the implementation:

```python
class TransformerEncoderLayer(nn.Module):
    def __init__(self, dim=768, num_heads_q=8, num_heads_kv=2, head_dim=64):
        super().__init__()
        # Attention Block with GQA
        self.att_norm = nn.LayerNorm(dim, elementwise_affine=False, eps=1E-6)
        self.attn_block = GQA(dim=dim, num_heads_q=num_heads_q,
                              num_heads_kv=num_heads_kv, head_dim=head_dim)

        # Feed-Forward Block
        self.ff_norm = nn.LayerNorm(dim, elementwise_affine=False, eps=1E-6)
        self.mlp_block = nn.Sequential(
            nn.Linear(dim, 4 * dim),
            nn.GELU(approximate='tanh'),
            nn.Linear(4 * dim, dim)
        )

    def forward(self, x):
        # Residual Connections
        attn_norm_output = self.att_norm(x)
        attn_output, _ = self.attn_block(attn_norm_output)
        out = x + attn_output

        mlp_norm_output = self.ff_norm(out)
        out = out + self.mlp_block(mlp_norm_output)
        return out
```

B.2 Training Loop Snippet

The core training step that calculates the MSE loss:

```python
def train_step(self, im, y):
    self.optimizer.zero_grad()
    im = im.float().to(self.device)
    y = y.long().to(self.device)

    # 1. Sample Noise
    noise = torch.randn_like(im).to(self.device)

    # 2. Sample Timesteps
```

```
    t = torch.randint(low=0, high=self.num_steps,
                      size=(im.shape[0],), device=self.device)

    # 3. Add Noise (Forward Process)
    noisy_im = self.add_noise(im, noise, t)

    # 4. Predict Noise (Reverse Process)
    noise_pred = self.model(noisy_im, t, y)

    # 5. Calculate Loss
    loss = torch.nn.MSELoss()(noise_pred, noise)

    loss.backward()
    self.optimizer.step()
    return loss.item()
```

C Full Configuration

```
model:
  image_size: 32
  image_channels: 3
  hidden_dim: 384
  depth: 12
  num_heads: 8

training:
  num_epochs: 200
  learning_rate: 2.0e-4
  optimizer: "adam"
  batch_size: 64

diffusion:
  num_steps: 1000
  beta_start: 1.0e-4
  beta_end: 0.02
  beta_schedule: "linear"
```