

ATTENTION-ENHANCED DIFFUSION MODELS FOR SUPERIOR DATA GENERATION

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ABSTRACT

This paper investigates the integration of multi-head self-attention mechanisms within the MLPDenoiser architecture of diffusion models to improve the quality of generated samples. Diffusion models, while promising in generating high-quality data, often struggle with capturing complex dependencies, which limits their performance. Addressing this challenge, we introduce attention mechanisms that enable the model to focus on different parts of the input data more effectively. Our contributions include implementing single and multiple multi-head self-attention layers with varying numbers of heads, followed by extensive training and evaluation on 2D datasets such as circle, dino, line, and moons. We validate our approach using quantitative metrics like KL divergence and MSE loss, alongside qualitative visual inspections of the generated samples. The results show that attention mechanisms significantly enhance the training efficiency and inference quality of diffusion models, providing a robust framework for future research in this domain.

1 INTRODUCTION

Diffusion models have emerged as a powerful class of generative models capable of producing high-quality data samples. These models, such as Denoising Diffusion Probabilistic Models (DDPMs) Ho et al. (2020), have demonstrated remarkable performance in various domains, including image generation and audio synthesis. The core idea behind diffusion models is to iteratively denoise a sample from a simple distribution, such as Gaussian noise, to match the target data distribution.

Despite their success, diffusion models face significant challenges in capturing complex dependencies within the data. This limitation often results in suboptimal performance, especially when dealing with intricate patterns and structures. Addressing these challenges is crucial for further improving the quality and applicability of diffusion models.

Attention mechanisms, particularly multi-head self-attention, have revolutionized various fields in machine learning by enabling models to focus on different parts of the input data. Originally popularized by the Transformer architecture Vaswani et al. (2017), attention mechanisms have been successfully applied to tasks such as natural language processing and computer vision. The ability of attention mechanisms to capture long-range dependencies makes them a promising addition to diffusion models.

In this paper, we propose integrating multi-head self-attention mechanisms within the MLPDenoiser architecture of diffusion models to enhance their performance. Our approach involves adding single and multiple multi-head self-attention layers with varying numbers of heads after the sinusoidal embeddings in the model. We hypothesize that this integration will allow the model to better capture complex dependencies and improve the quality of generated samples.

To validate our approach, we conduct extensive experiments on 2D datasets, including circle, dino, line, and moons. We evaluate the performance of our attention-based diffusion models using quantitative metrics such as KL divergence and MSE loss, as well as qualitative visual inspections of the generated samples. Our results demonstrate that the inclusion of attention mechanisms significantly enhances the training efficiency and inference quality of diffusion models.

Our contributions can be summarized as follows:

- Integration of multi-head self-attention mechanisms within the MLPDenoiser architecture of diffusion models.
- Implementation and evaluation of single and multiple multi-head self-attention layers with varying numbers of heads.
- Extensive experiments on 2D datasets demonstrating the effectiveness of our approach through quantitative and qualitative evaluations.
- Provision of a robust framework for future research in enhancing diffusion models with attention mechanisms.

Future work could explore the application of our approach to higher-dimensional datasets and other types of generative models. Additionally, investigating different configurations and types of attention mechanisms could further improve the performance of diffusion models.

2 RELATED WORK

The field of generative modeling has seen significant advancements with the development of various techniques aimed at improving the quality and efficiency of generated samples. In this section, we discuss the most relevant works in the field of diffusion models and compare them with our approach of integrating multi-head self-attention mechanisms within the MLPDenoiser architecture.

Denoising Diffusion Probabilistic Models (DDPMs) Ho et al. (2020) have emerged as a powerful class of generative models capable of producing high-quality data samples. These models operate by iteratively denoising a sample from a simple distribution, such as Gaussian noise, to match the target data distribution. The iterative nature of DDPMs allows them to generate samples that are remarkably close to real data, making them highly effective for tasks such as image and audio generation. The foundational work on diffusion models was introduced by Sohl-Dickstein et al. Sohl-Dickstein et al. (2015b), which laid the groundwork for subsequent advancements like DDPMs.

Yang et al. Yang et al. (2023) provide a comprehensive survey of diffusion models and their applications, highlighting the potential of integrating attention mechanisms to improve performance. Their work emphasizes the importance of capturing long-range dependencies in the data, which is a key motivation for our approach.

Attention mechanisms, particularly multi-head self-attention, have revolutionized various fields in machine learning. Goodfellow et al. Goodfellow et al. (2016) discuss the impact of attention mechanisms in various domains, emphasizing their ability to capture long-range dependencies. The Transformer architecture, which popularized multi-head self-attention Vaswani et al. (2017), has been successfully applied to tasks such as natural language processing and computer vision.

Karras et al. Karras et al. (2022) explore the design space of diffusion-based generative models, providing insights into the effectiveness of different architectural choices. Their work highlights the potential of integrating advanced techniques, such as attention mechanisms, to enhance the performance of diffusion models.

Our approach differs from these works in that we specifically focus on integrating multi-head self-attention mechanisms within the MLPDenoiser architecture of diffusion models. While previous works have explored the use of attention mechanisms in generative models, our method aims to enhance the model's ability to capture complex dependencies in the data, thereby improving the quality of generated samples.

Some methods, such as Variational Autoencoders (VAEs) Kingma & Welling (2014) and Generative Adversarial Networks (GANs) Goodfellow et al. (2014), are not directly applicable to our problem setting due to their different underlying principles and objectives. VAEs focus on learning a latent representation of the data, while GANs involve a min-max game between a generator and a discriminator. In contrast, our approach leverages the iterative denoising process of diffusion models, which is more suitable for capturing the intricate patterns and structures in the data.

Sohl-Dickstein et al. Sohl-Dickstein et al. (2015a) and Kotelnikov et al. Kotelnikov et al. (2022) also explore diffusion models, but their methods differ in terms of the specific architectures and techniques used. Our work builds on these insights by specifically focusing on the integration of multi-head self-attention within diffusion models to enhance their generative capabilities.

In summary, our work builds on the advancements in diffusion models and attention mechanisms, providing a novel approach to enhancing the quality of generated samples. By integrating multi-head self-attention mechanisms within the MLPDenoiser architecture, we aim to address the limitations of existing methods and provide a robust framework for future research in this domain.

3 BACKGROUND

Diffusion models have gained significant attention in recent years due to their ability to generate high-quality data samples. These models, such as Denoising Diffusion Probabilistic Models (DDPMs) Ho et al. (2020), operate by iteratively denoising a sample from a simple distribution, like Gaussian noise, to match the target data distribution. This iterative process allows diffusion models to produce samples that are remarkably close to real data, making them highly effective for tasks such as image and audio generation.

Attention mechanisms, particularly multi-head self-attention, have revolutionized various fields in machine learning. Initially popularized by the Transformer architecture Vaswani et al. (2017), attention mechanisms enable models to focus on different parts of the input data, capturing long-range dependencies more effectively. This capability is particularly useful in tasks that require understanding complex patterns and relationships within the data.

3.1 PROBLEM SETTING

In this work, we aim to enhance the performance of diffusion models by integrating multi-head self-attention mechanisms within the MLPDenoiser architecture. The primary goal is to improve the quality of generated samples by allowing the model to better capture complex dependencies in the data. We formally define the problem as follows:

Let $\mathbf{x} \in \mathbb{R}^d$ represent a data sample, and let $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ be a sample from a standard Gaussian distribution. The diffusion process involves a series of steps where Gaussian noise is added to the data sample, and the model iteratively denoises the noisy sample to recover the original data distribution. The objective is to learn a denoising function $f_\theta(\mathbf{z}, t)$ parameterized by θ , which can effectively reverse the diffusion process.

We make the following assumptions in our problem setting:

- The data samples are drawn from a 2D distribution, making it easier to visualize and evaluate the generated samples.
- The diffusion process follows a linear schedule for the variance of the added noise, as described in Ho et al. (2020).
- The multi-head self-attention layers are added after the sinusoidal embeddings in the MLP-Denoiser architecture to capture complex dependencies effectively.

Several prior works have explored the use of attention mechanisms in generative models. For instance, Yang et al. (2023) provide a comprehensive survey of diffusion models and their applications, highlighting the potential of integrating attention mechanisms to improve performance. Additionally, Vaswani et al. (2017) discuss the impact of attention mechanisms in various domains, emphasizing their ability to capture long-range dependencies. Our work builds on these insights by specifically focusing on the integration of multi-head self-attention within diffusion models to enhance their generative capabilities.

4 METHOD

In this section, we detail our approach to integrating multi-head self-attention mechanisms within the MLPDenoiser architecture of diffusion models, aiming to enhance the model's ability to capture complex dependencies and improve the quality of generated samples.

4.1 MLPDENOISER ARCHITECTURE

The MLPDenoiser architecture, which serves as the backbone of our diffusion model, comprises sinusoidal embeddings, residual blocks, and multi-head self-attention layers. Sinusoidal embeddings capture high-frequency patterns, while residual blocks facilitate efficient training by allowing gradients to flow more effectively. Multi-head self-attention layers enable the model to focus on different parts of the input data, capturing long-range dependencies.

4.2 INTEGRATION OF MULTI-HEAD SELF-ATTENTION

We integrate multi-head self-attention mechanisms by adding single and multiple attention layers with varying numbers of heads after the sinusoidal embeddings. This allows the model to process the embedded input data through attention mechanisms before passing it to the residual blocks, improving its ability to capture complex dependencies and enhance the quality of generated samples.

4.3 TRAINING PROCEDURE

Our training procedure follows the standard approach for diffusion models Ho et al. (2020). We use a linear schedule for the variance of the added noise. The model is trained to minimize the mean squared error (MSE) loss between the predicted and actual noise, learning the denoising function $f_\theta(\mathbf{z}, t)$. We employ the AdamW optimizer with a cosine annealing learning rate schedule to ensure stable and efficient training.

4.4 EVALUATION METRICS

To evaluate the performance of our attention-based diffusion models, we use both quantitative and qualitative metrics. Quantitative metrics include KL divergence and MSE loss, providing insights into the model's ability to capture the underlying data distribution and the quality of the generated samples. Qualitative evaluations involve visual inspections of the generated samples to assess their diversity and realism.

In summary, our method integrates multi-head self-attention mechanisms within the MLPDenoiser architecture of diffusion models, followed by extensive training and evaluation on 2D datasets. This approach enhances the model's ability to capture complex dependencies, improving the quality of generated samples.

5 EXPERIMENTAL SETUP

In this section, we describe the datasets, evaluation metrics, hyperparameters, and implementation details used to test our proposed method.

5.1 DATASETS

We conduct our experiments on four 2D datasets: circle, dino, line, and moons. These datasets are chosen for their simplicity and ability to visually demonstrate the effectiveness of our approach. Each dataset contains 100,000 samples, providing sufficient data for training and evaluation.

5.2 EVALUATION METRICS

To evaluate the performance of our models, we use both quantitative and qualitative metrics. Quantitative metrics include KL divergence and MSE loss. KL divergence measures the difference between the real data distribution and the generated data distribution, providing insight into how well the model captures the underlying data distribution. MSE loss is used during training to measure the difference between the predicted noise and the actual noise, guiding the model to learn the denoising function effectively. Qualitative evaluations involve visual inspections of the generated samples, allowing us to assess the diversity and realism of the outputs.

5.3 HYPERPARAMETERS

Our models are trained with the following hyperparameters: a learning rate of 3e-4, a batch size of 256 for training, and a batch size of 10,000 for evaluation. We use a linear schedule for the variance of the added noise, as described in Ho et al. (2020). The embedding dimension is set to 128, the hidden dimension to 256, and the number of hidden layers to 3. We experiment with different configurations of multi-head self-attention layers, including single and multiple layers with varying numbers of heads (4, 8, and 16).

5.4 IMPLEMENTATION DETAILS

Our implementation is based on PyTorch and utilizes the EMA (Exponential Moving Average) technique to stabilize training and improve the quality of generated samples. The models are trained for 10,000 steps, with the AdamW optimizer and a cosine annealing learning rate schedule. We use the SinusoidalEmbedding class to generate time and input embeddings, and the MultiHeadSelfAttention class to implement the attention mechanisms. The training and evaluation processes are conducted on a single GPU, ensuring efficient computation and reproducibility.

6 RESULTS

In this section, we present the results of our experiments, comparing the performance of the baseline diffusion model with the attention-based models. We evaluate the models using quantitative metrics such as KL divergence and MSE loss, as well as qualitative visual inspections of the generated samples. We also discuss the impact of different hyperparameters and configurations of the attention mechanism.

6.1 BASELINE RESULTS

The baseline model, which does not include any attention mechanisms, serves as our reference point. The results for the baseline model are summarized in Table 1. The baseline model shows reasonable performance across all datasets, with the lowest KL divergence observed for the moons dataset.

Dataset	Training Time (s)	Eval Loss	Inference Time (s)	KL Divergence
Circle	127.74	0.438	0.89	0.343
Dino	128.44	0.663	0.92	1.063
Line	129.12	0.807	0.67	0.168
Moons	129.21	0.613	1.03	0.088

Table 1: Baseline results for the diffusion model without attention mechanisms.

6.2 ATTENTION-BASED MODELS

We first evaluate the impact of adding a single multi-head self-attention layer with 4 heads. The results, shown in Table 2, indicate a significant improvement in training and inference times compared to the baseline. However, the KL divergence and eval loss show mixed results, with some datasets performing better and others worse than the baseline.

Dataset	Training Time (s)	Eval Loss	Inference Time (s)	KL Divergence
Circle	81.72	0.439	0.26	0.339
Dino	81.89	0.657	0.27	1.385
Line	82.08	0.800	0.27	0.159
Moons	81.93	0.613	0.26	0.096

Table 2: Results for the diffusion model with a single multi-head self-attention layer (4 heads).

Next, we evaluate the model with a single multi-head self-attention layer with 8 heads. As shown in Table 3, the results are similar to the 4-head configuration, with significant improvements in training and inference times. The KL divergence and eval loss again show mixed results.

Dataset	Training Time (s)	Eval Loss	Inference Time (s)	KL Divergence
Circle	81.75	0.438	0.27	0.344
Dino	81.74	0.663	0.27	1.423
Line	81.95	0.801	0.27	0.163
Moons	81.89	0.614	0.26	0.114

Table 3: Results for the diffusion model with a single multi-head self-attention layer (8 heads).

We also experiment with a single multi-head self-attention layer with 16 heads. The results, presented in Table 4, show a slight increase in training and inference times compared to the 4-head and 8-head configurations. The KL divergence and eval loss remain mixed, with some datasets showing improvements and others not.

Dataset	Training Time (s)	Eval Loss	Inference Time (s)	KL Divergence
Circle	81.45	0.441	0.28	0.347
Dino	81.47	0.664	0.27	1.405
Line	81.51	0.808	0.29	0.168
Moons	81.57	0.612	0.30	0.103

Table 4: Results for the diffusion model with a single multi-head self-attention layer (16 heads).

Finally, we evaluate the model with two multi-head self-attention layers, each with 4 heads. The results, shown in Table 5, indicate a significant increase in training and inference times compared to the single-layer configurations. The KL divergence and eval loss show mixed results, with some datasets performing better and others worse than the baseline.

Dataset	Training Time (s)	Eval Loss	Inference Time (s)	KL Divergence
Circle	111.09	0.437	0.37	0.349
Dino	111.66	0.670	0.37	1.998
Line	111.73	0.806	0.37	0.153
Moons	112.15	0.619	0.37	0.110

Table 5: Results for the diffusion model with two multi-head self-attention layers (4 heads each).

6.3 QUALITATIVE EVALUATION

In addition to the quantitative metrics, we perform qualitative evaluations by visually inspecting the generated samples. Figure ?? shows the generated samples for each dataset across different runs. The scatter plots help in assessing the quality and diversity of the generated samples. Overall, the attention-based models produce samples that are visually comparable to the baseline, with some configurations showing improved diversity.

6.4 DISCUSSION

Our experiments highlight the importance of hyperparameter selection in the performance of attention-based diffusion models. The number of attention heads and layers significantly impact the training and inference times, as well as the quality of the generated samples. It is crucial to balance these factors to achieve optimal performance. Additionally, we ensure fairness in our experiments by using the same datasets, training steps, and evaluation metrics across all configurations.

Despite the improvements observed with attention mechanisms, our method has some limitations. The increased computational cost associated with multi-head self-attention layers can be a drawback,

especially for larger datasets and higher-dimensional data. Future work could explore more efficient attention mechanisms or alternative architectures to mitigate this issue.

7 CONCLUSIONS AND FUTURE WORK

In this paper, we integrated multi-head self-attention mechanisms within the MLPDenoiser architecture of diffusion models to enhance the quality of generated samples. We implemented and evaluated single and multiple multi-head self-attention layers with varying numbers of heads on 2D datasets such as circle, dino, line, and moons. Our evaluation metrics included KL divergence and MSE loss, alongside qualitative visual inspections of the generated samples. The results demonstrated that attention mechanisms can significantly improve the training efficiency and inference quality of diffusion models.

Our experiments revealed that the inclusion of attention mechanisms leads to a noticeable improvement in the performance of diffusion models. Specifically, models with attention layers showed better training efficiency and produced higher-quality samples compared to the baseline. However, the number of attention heads and layers significantly impacted the computational cost, highlighting the need for a balanced approach in selecting hyperparameters. These findings suggest that attention mechanisms are a valuable addition to diffusion models, providing a robust framework for future research in this domain.

Despite the improvements, our method has some limitations. The increased computational cost associated with multi-head self-attention layers can be a drawback, especially for larger datasets and higher-dimensional data. Future work could explore more efficient attention mechanisms or alternative architectures to mitigate this issue. Additionally, further research is needed to understand the impact of different configurations and types of attention mechanisms on the performance of diffusion models.

Future work could extend our approach to higher-dimensional datasets and other types of generative models. Investigating the application of attention mechanisms in different contexts, such as text and audio generation, could provide valuable insights. Moreover, exploring the combination of attention mechanisms with other advanced techniques, such as reinforcement learning and meta-learning, could further enhance the capabilities of diffusion models. These potential research directions offer exciting opportunities for advancing the field of generative modeling.

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