Assignment 2 Report
CS-726: Advanced Machine Learning

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1 Denoising Diffusion Probabilistic Models

1.1 Architecture

The implemented Denoising Diffusion Probabilistic Model (DDPM) architecture consists of several key components:

1.1.1 Time Embedding

We use sinusoidal position embeddings to encode timestep information:

- The `SinusoidalPositionEmbeddings` module transforms scalar timesteps into 16 dimensional embeddings
- This creates a unique representation for each timestep that preserves the notion of time progression
- The embedding uses a combination of sine and cosine functions at different frequencies, allowing the model to distinguish between timesteps

1.1.2 Network Architecture

The model consists of:

- An input linear layer that maps the concatenation of data and time embeddings to a hidden dimension (128 units)
- A series of 5 `DiffusionBlocks`, each containing a linear layer of 128 units followed by a ReLU activation
- An output linear layer that maps back to the data dimensionality

Rather than using convolutional layers as in image-based diffusion models, we use fully connected layers which is appropriate for dataset without temporal or spatial structure. The time embedding ensures the model can adapt its behavior based on the specific noise level at each timestep.

1.2 Results

For NLL caluclation, the temperature is set to 0.1. For EMD calculation, the number of subsamples is set to 250 and the number of iterations is set to 5.

For all training runs, the hyperparameters used are as follows:

- **Epochs**: 100

- **Batch Size**: 64
- **Learning Rate**: 1e-3

1.2.1 Varying Timesteps

Here, lbeta = 0.0001 and ubeta = 0.02.

Dataset	**Metric**	**Timesteps**					
		10	**50**	**100**	**150**	**200**	**500**
Moons	EMD	39.99	28.95	**27.40**	29.64	30.55	44.90
	NLL	1.02	0.96	0.94	**0.93**	0.94	0.95
Circles	EMD	34.60	**31.48**	33.24	34.41	38.62	42.04
	NLL	1.05	0.99	1.00	**0.98**	1.01	1.03
Blobs	EMD	88.78	43.69	20.08	18.36	**17.17**	19.83
	NLL	0.34	0.12	0.04	0.03	**0.01**	0.04
Manycircles	EMD	33.65	**26.41**	27.77	27.98	30.98	30.34
	NLL	0.66	**0.54**	**0.54**	**0.54**	**0.54**	0.58
Helix	EMD	56.00	59.33	57.15	**56.13**	58.87	60.49
	NLL	1.55	1.53	1.52	1.52	1.53	**1.51**

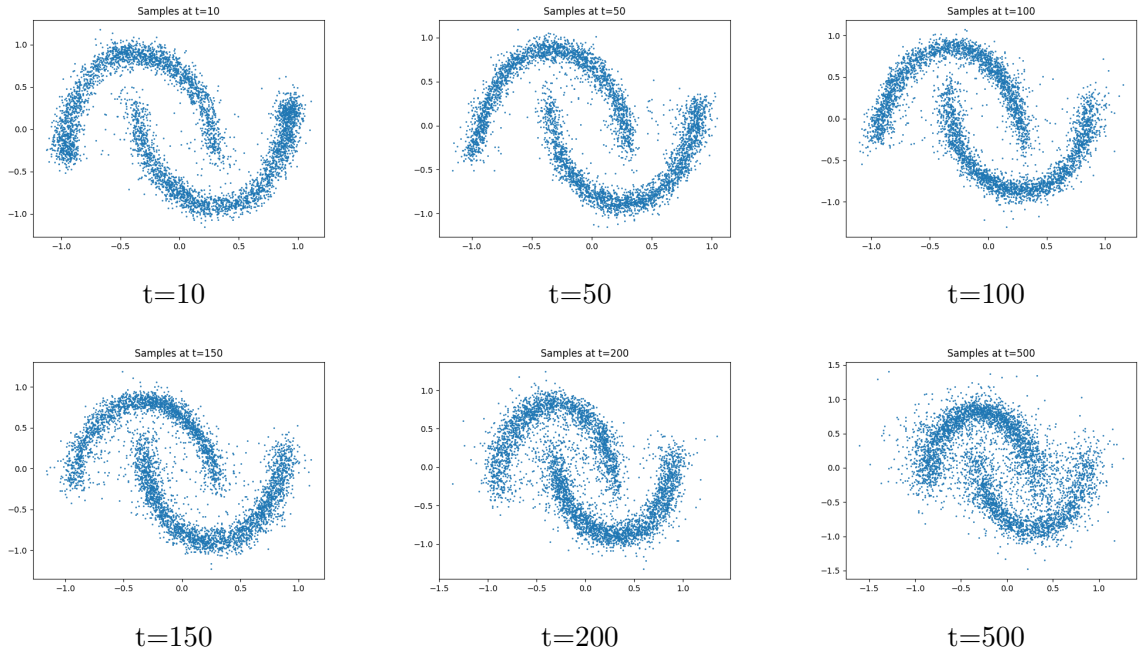
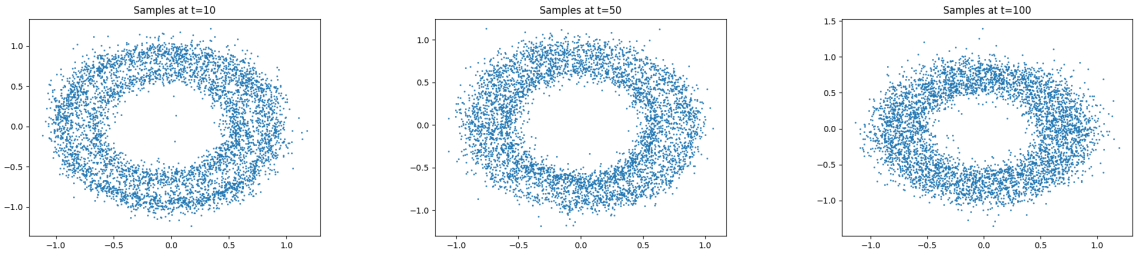
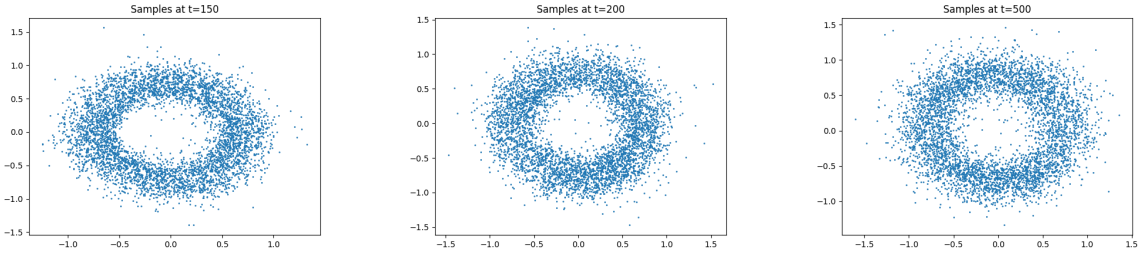


Figure 1: Samples generated by DDPM with **varying timesteps** for the Moons dataset.

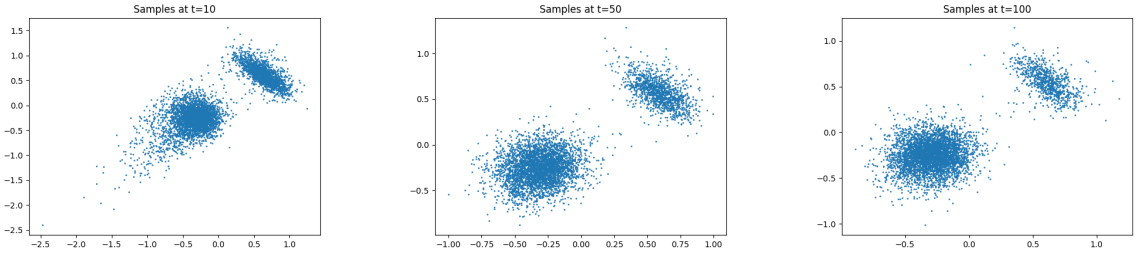


t=10 t=50 t=100

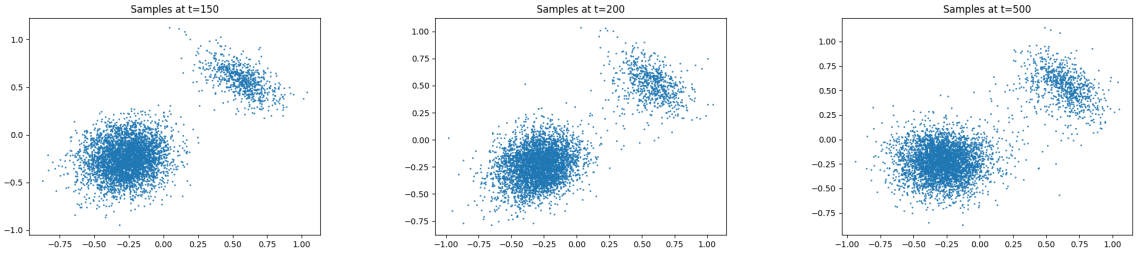


t=150 t=200 t=500

Figure 2: Samples generated by DDPM with **varying timesteps** for the Circles dataset.

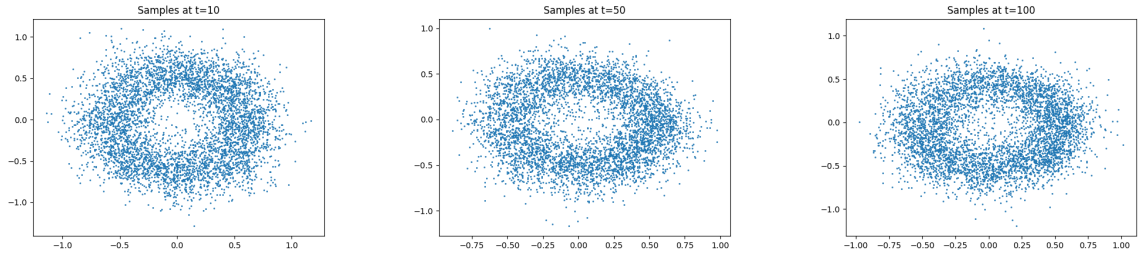


t=10 t=50 t=100

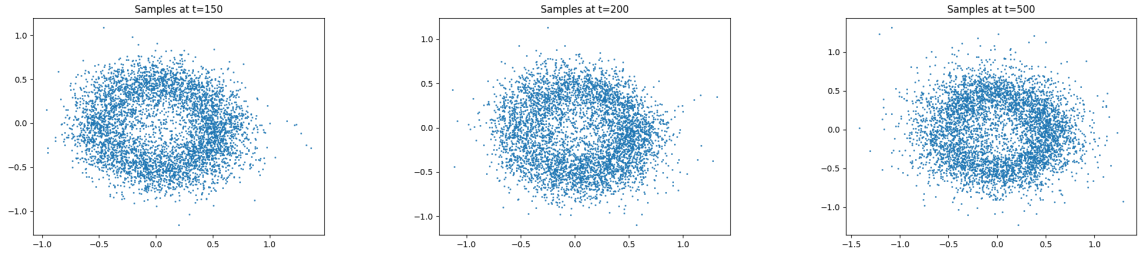


t=150 t=200 t=500

Figure 3: Samples generated by DDPM with **varying timesteps** for the Blobs dataset.

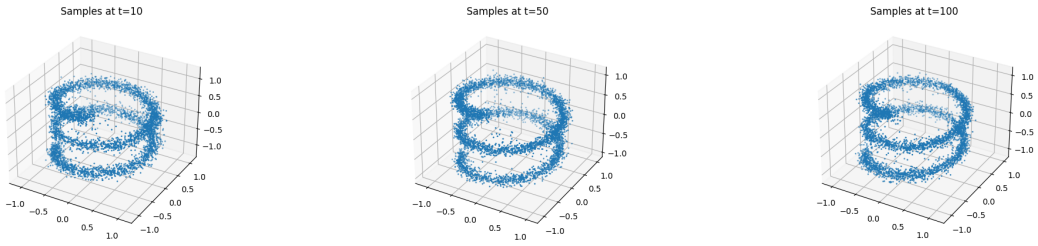


t=10 t=50 t=100

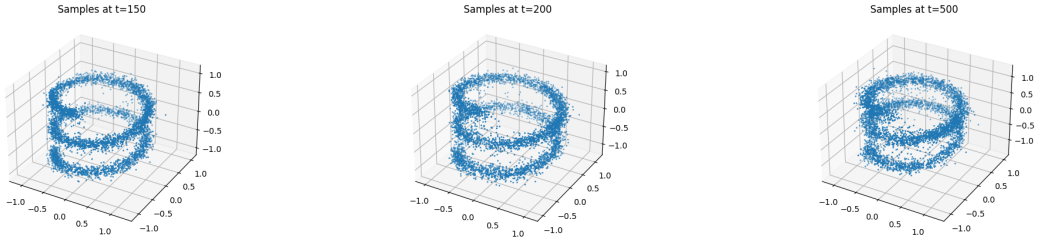


t=150 t=200 t=500

Figure 4: Samples generated by DDPM with **varying timesteps** for the Manycircles dataset.



t=10 t=50 t=100



t=150 t=200 t=500

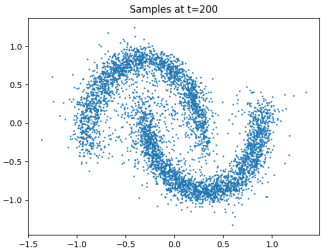
Figure 5: Samples generated by DDPM with **varying timesteps** for the Helix dataset.

1.2.2 Varying Beta Schedule

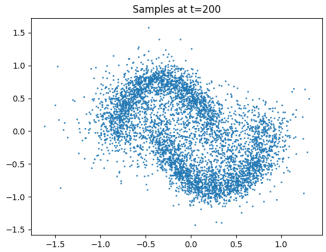
Here, timesteps = 200.

Dataset	**Metric**	**Beta Schedule (lbeta→ubeta)**					
		1e-4→0.02	**1e-3→0.2**	**1e-5→0.002**	**1e-5→0.02**	**1e-4→0.2**	**1e-5→0.2**

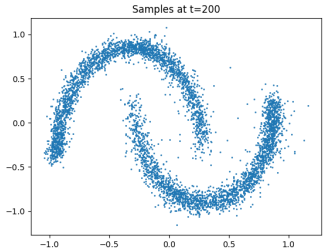
Moons	EMD	30.55	35.57	34.76	**30.48**	33.48	33.62
	NLL	0.94	**0.93**	0.98	0.95	0.95	0.94
Circles	EMD	38.62	38.03	**33.03**	38.36	36.52	37.45
	NLL	1.01	**1.00**	1.02	**1.00**	1.01	1.01
Blobs	EMD	**17.17**	20.35	62.98	**17.17**	19.59	19.62
	NLL	0.01	0.02	0.20	0.01	0.01	**0.00**
Manycircles	EMD	30.98	28.75	**26.55**	31.82	29.40	29.92
	NLL	0.54	**0.52**	0.58	0.53	0.53	0.54
Helix	EMD	58.87	**56.25**	57.31	58.29	57.34	58.72
	NLL	1.53	**1.52**	1.54	1.53	1.53	1.52



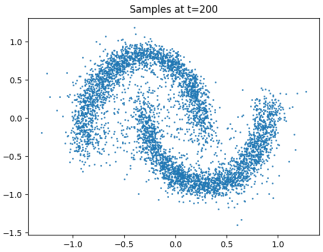
β = 1e-4 $\rightarrow$ 0.02



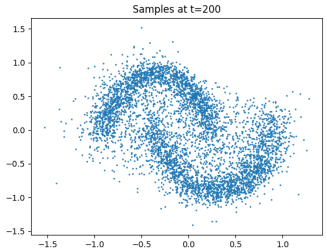
β = 1e-3 $\rightarrow$ 0.2



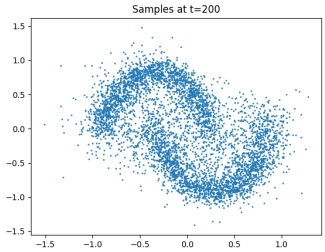
β = 1e-5 $\rightarrow$ 0.002



β = 1e-5 $\rightarrow$ 0.02

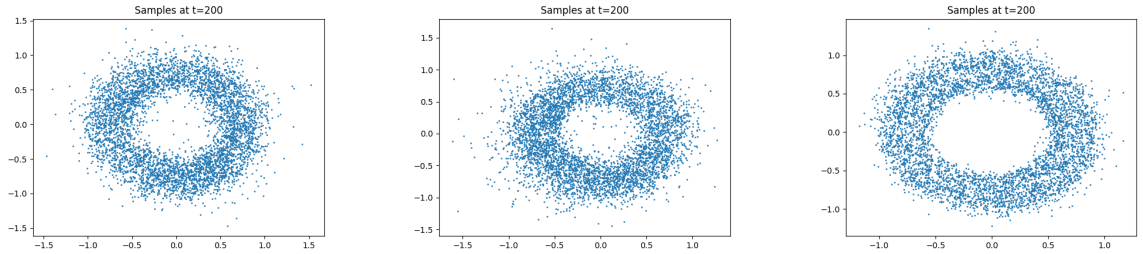


β = 1e-4 $\rightarrow$ 0.2

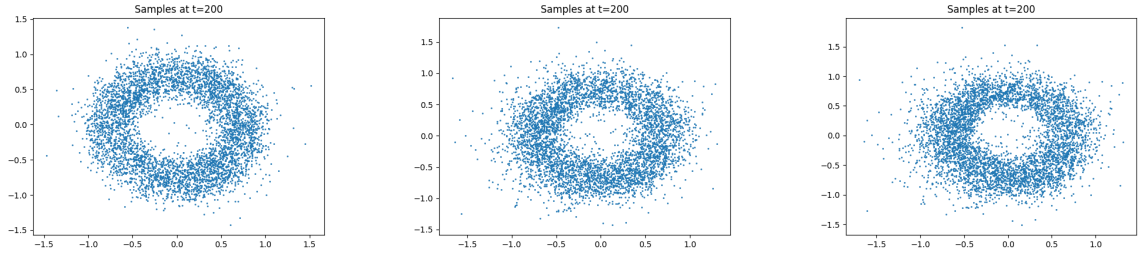


β = 1e-5 $\rightarrow$ 0.2

Figure 6: Samples generated by DDPM with **varying beta schedules** for the Moons dataset.

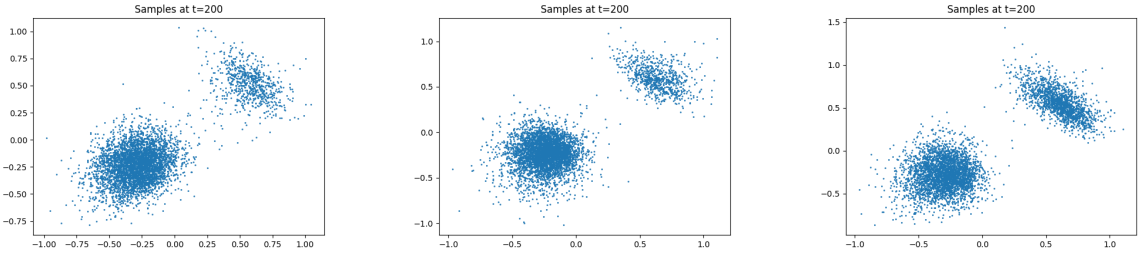


$\beta = \text{1e-4} \rightarrow 0.02$ $\beta = \text{1e-3} \rightarrow 0.2$ $\beta = \text{1e-5} \rightarrow 0.002$

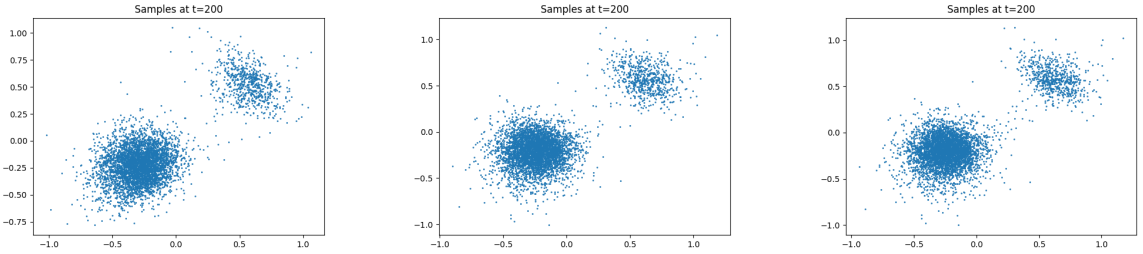


$\beta = \text{1e-5} \rightarrow 0.02$ $\beta = \text{1e-4} \rightarrow 0.2$ $\beta = \text{1e-5} \rightarrow 0.2$

Figure 7: Samples generated by DDPM with **varying beta schedules** for the Circles dataset.

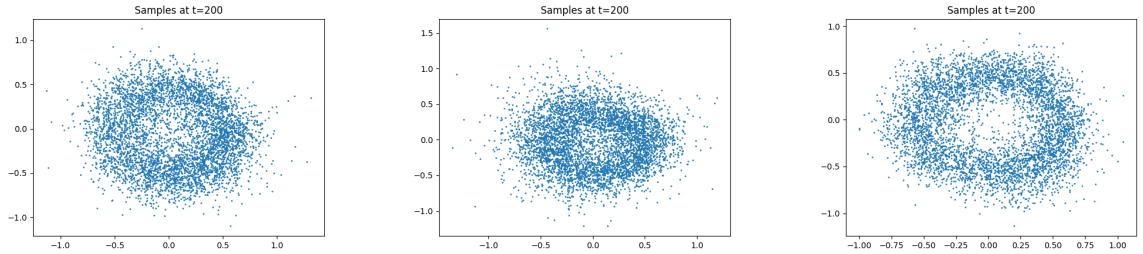


$\beta = \text{1e-4} \rightarrow 0.02$ $\beta = \text{1e-3} \rightarrow 0.2$ $\beta = \text{1e-5} \rightarrow 0.002$

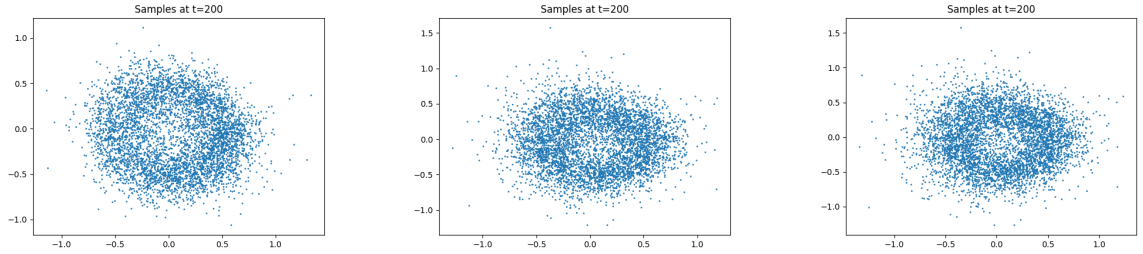


$\beta = \text{1e-5} \rightarrow 0.02$ $\beta = \text{1e-4} \rightarrow 0.2$ $\beta = \text{1e-5} \rightarrow 0.2$

Figure 8: Samples generated by DDPM with **varying beta schedules** for the Blobs dataset.

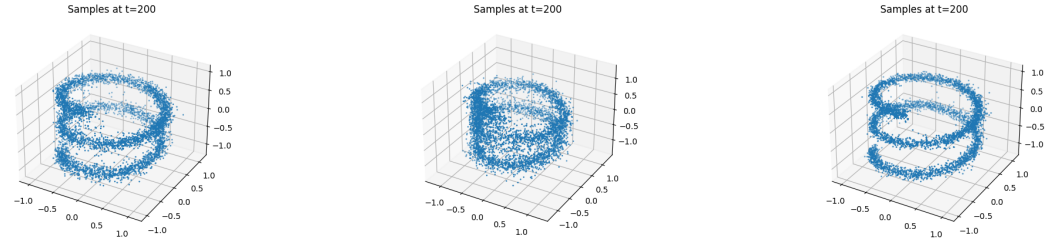


$\beta = 1\text{e-}4 \rightarrow 0.02$ $\beta = 1\text{e-}3 \rightarrow 0.2$ $\beta = 1\text{e-}5 \rightarrow 0.002$

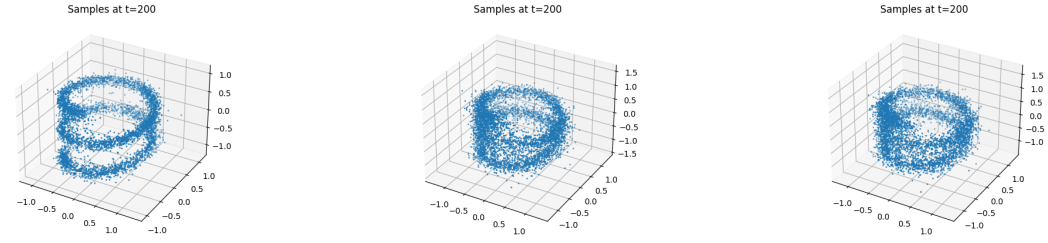


$\beta = 1\text{e-}5 \rightarrow 0.02$ $\beta = 1\text{e-}4 \rightarrow 0.2$ $\beta = 1\text{e-}5 \rightarrow 0.2$

Figure 9: Samples generated by DDPM with **varying beta schedules** for the Manycircles dataset.



$\beta = 1\text{e-}4 \rightarrow 0.02$ $\beta = 1\text{e-}3 \rightarrow 0.2$ $\beta = 1\text{e-}5 \rightarrow 0.002$



$\beta = 1\text{e-}5 \rightarrow 0.02$ $\beta = 1\text{e-}4 \rightarrow 0.2$ $\beta = 1\text{e-}5 \rightarrow 0.2$

Figure 10: Samples generated by DDPM with **varying beta schedules** for the Helix dataset.

1.2.3 Training Albatross

The hyperparameters used for training Albatross are as follows:

- **Timesteps**: 150
- **Beta Schedule**: 1e-4→0.02

2 Classifier-Free Guidance

For EMD calculation, the number of subsamples is set to 250 and the number of iterations is set to 5.

For all training runs, the hyperparameters used are as follows:

- **Epochs**: 100
- **Batch Size**: 64
- **Learning Rate**: 1e-3
- **lbeta**: 0.0001
- **ubeta**: 0.02
- **p_uncond** (required for CFG training): 0.2

2.1 Guided vs. Conditional Sampling

- **Training:** Conditional sampling requires the model to be trained with explicit labels, while guided sampling can work even with an unconditional model.
- **Control:** Conditional sampling directly conditions the model on labels, whereas guided sampling modifies the noise prediction using a guidance scale.
- **Flexibility:** Conditional sampling is fixed after training, while guided sampling allows dynamic tuning of the guidance strength during inference.
- **Diversity:** Conditional sampling maintains diversity in generated samples, but guided sampling can reduce diversity if the guidance scale is too high.
- **Best Use Case:** Conditional sampling is ideal when training a model from scratch, while guided sampling is useful when modifying an already trained model.

2.2 Architecture

The model architecture for Classifier-Free Guidance (CFG) is similar to DDPM, with the modification of concatenating a class embedding to the input layer. The class embedding is a sinusoidal position embedding similar to the time embedding used in DDPM.

2.3 Conditional DDPM Results

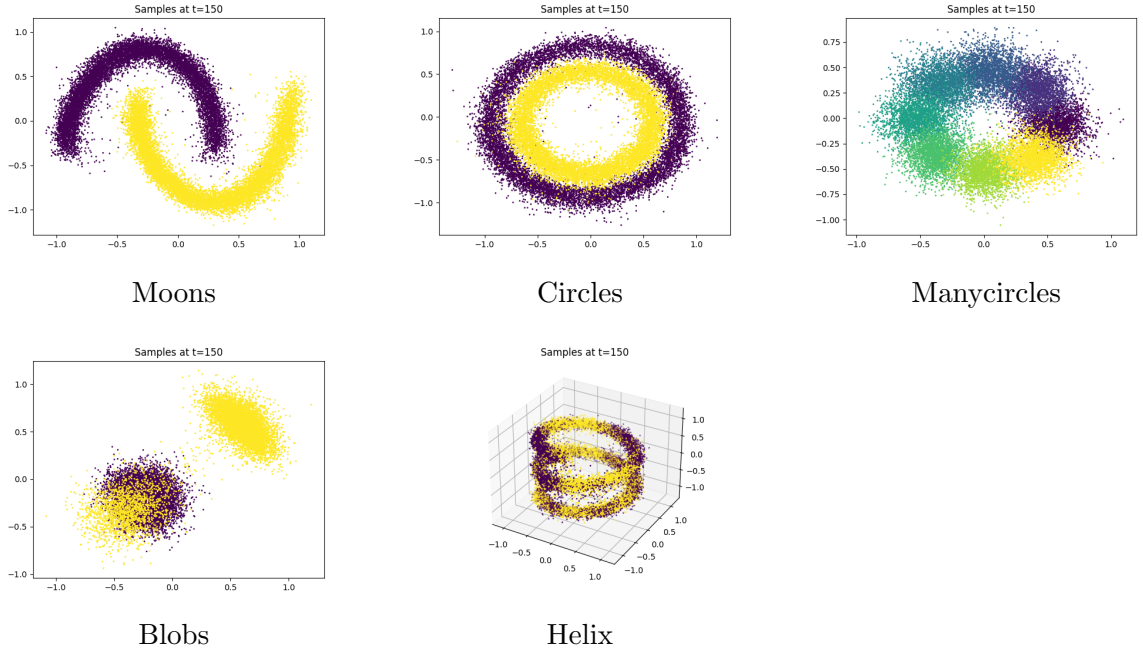
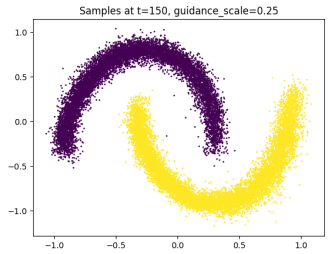


Figure 11: Samples generated by **conditional** DDPM for various datasets.

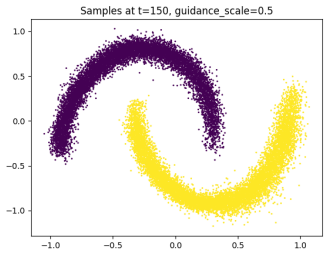
2.4 Classifier-Free Guidance Results

Dataset	**Metric**	**Guidance Scale**				
		0.25	**0.5**	**1.0**	**2.0**	**4.0**
Moons	EMD	**27.23**	31.77	44.57	63.59	82.62
	Accuracy	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**
Circles	EMD	40.60	**40.33**	40.65	42.87	56.30
	Accuracy	0.97	0.99	**1.00**	**1.00**	**1.00**
Blobs	EMD	**20.27**	26.16	39.27	55.48	77.69
	Accuracy	0.95	0.98	0.99	**1.00**	**1.00**
Manycircles	EMD	**12.16**	14.62	18.97	25.14	34.04
	Accuracy	0.92	0.96	0.98	**1.00**	**1.00**
Helix	EMD	**56.82**	58.13	63.17	74.67	97.19
	Accuracy	0.73	0.76	0.82	0.88	**0.94**

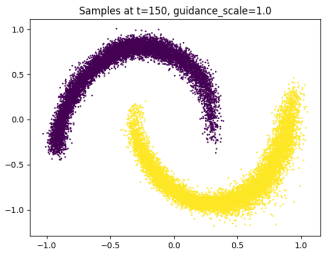
We observe a clear trade-off between sample quality (measured by EMD) and conditional accuracy across all datasets. As the guidance scale increases, the accuracy generally improves. However, this comes at the cost of increasing EMD values, suggesting that the generated samples may stray further from the true data distribution.



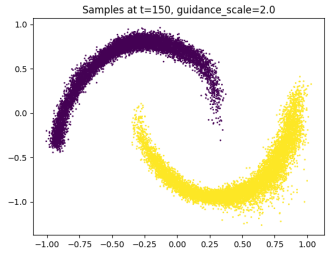
guidance=0.25



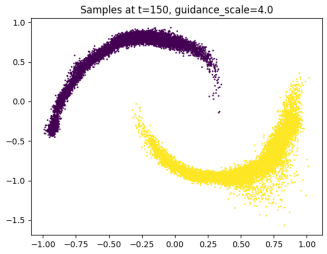
guidance=0.5



guidance=1.0

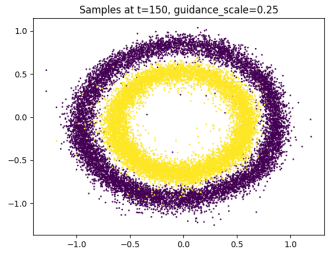


guidance=2.0

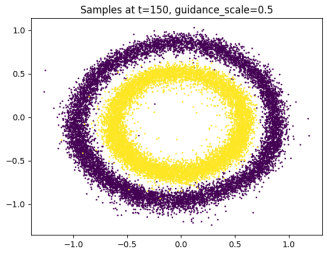


guidance=4.0

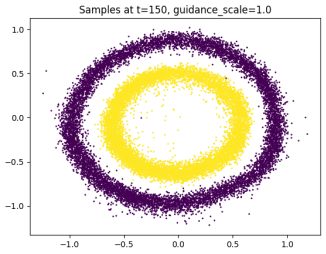
Figure 12: Samples generated by DDPM with **varying guidance scales** for the Moons dataset.



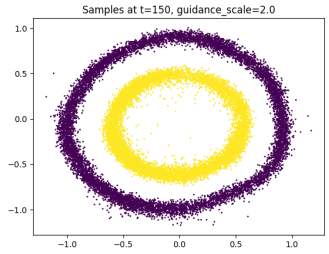
guidance=0.25



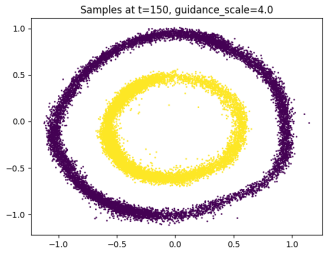
guidance=0.5



guidance=1.0

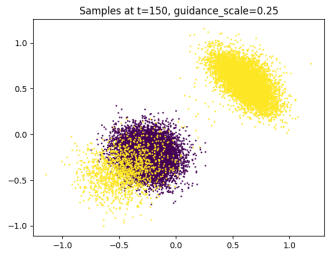


guidance=2.0

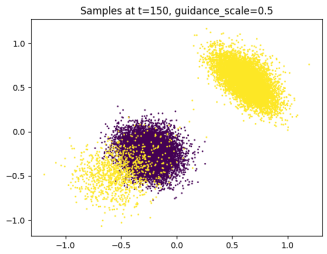


guidance=4.0

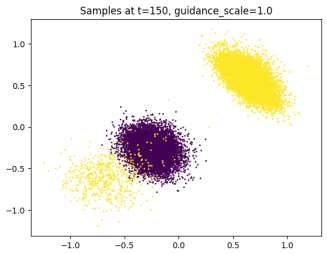
Figure 13: Samples generated by DDPM with **varying guidance scales** for the Circles dataset.



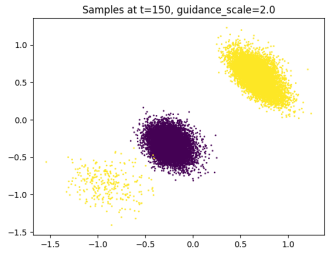
guidance=0.25



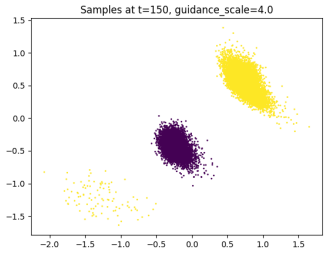
guidance=0.5



guidance=1.0

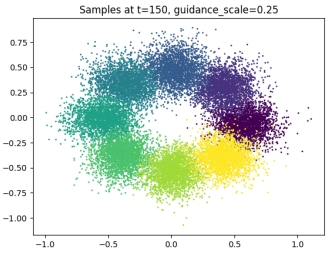


guidance=2.0

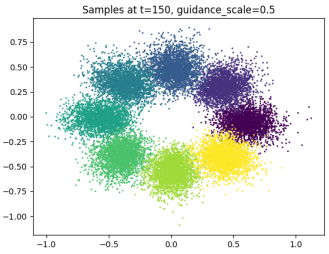


guidance=4.0

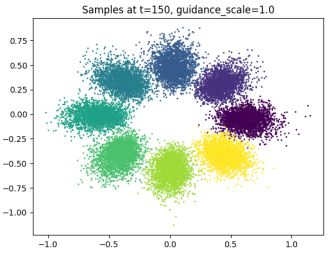
Figure 14: Samples generated by DDPM with **varying guidance scales** for the Blobs dataset.



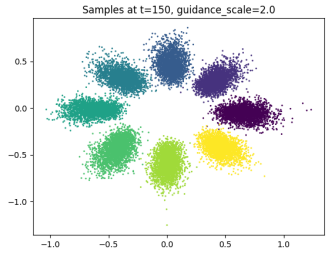
guidance=0.25



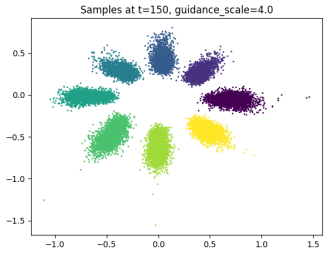
guidance=0.5



guidance=1.0

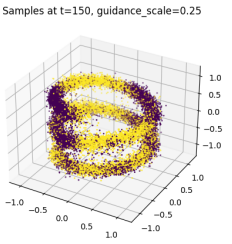


guidance=2.0

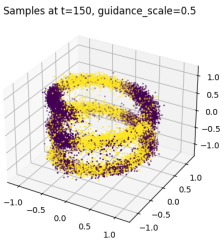


guidance=4.0

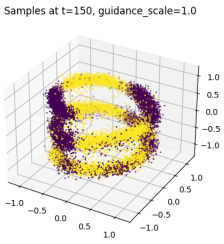
Figure 15: Samples generated by DDPM with **varying guidance scales** for the Manycircles dataset.



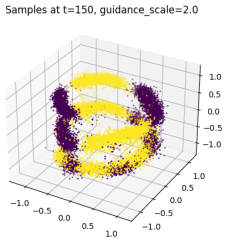
guidance=0.25



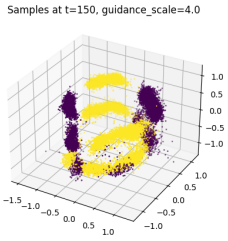
guidance=0.5



guidance=1.0



guidance=2.0



guidance=4.0

Figure 16: Samples generated by DDPM with **varying guidance scales** for the Helix dataset.

2.5 Training Free Classifier

For this we are using the KNN classifier with 100 neighbors. The classifier uses 20000 samples made using the ConditionalDDPM model. We are comparing its performance with an MLP classifier with 2 hidden layers of 100 and 50 units respectively.

Dataset	**KNN**	**MLP**
Moons	1.00	1.00
Circles	0.99	1.00
Blobs	0.87	0.86
Manycircles	0.95	0.97
Helix	0.77	0.80