$$(v_{1}(n_{1})^{2}) = \mathbb{E}[n_{1} n_{2}] - \mathbb{E}[n_{1}] \mathbb{E}[n_{2}]$$

$$= \mathbb{E}[n_{1} n_{2}] = \mathbb{E}[n_{1} (n_{1} + n_{1})]$$

$$= \mathbb{E}[n_{1}^{2}] + \mathbb{E}(n_{1}) \mathbb{E}[n_{1}]$$

$$= \mathbb{E}[n_{1}^{2}] + \mathbb{E}(n_{1}) \mathbb{E}[n_{1}]$$

$$= \mathbb{E}[n_{1} n_{3}] - \mathbb{E}[n_{1} \mathbb{E}[n_{2}]$$

$$\mathbb{E}[n_{1} n_{3}] = \mathbb{E}[n_{1} (n_{1} + n_{1} + n_{2})]$$

$$= \mathbb{E}[n_{1}^{2} + n_{1} n_{1} + n_{1} n_{2}]$$

$$= \varepsilon^{2}$$
Similarly
$$= \varepsilon^{2}$$
Similarly
$$= \mathbb{E}[n_{1} + n_{1} + n_{1} + n_{1} + n_{2} + n_{3}] - \mathbb{E}[n_{1}] \mathbb{E}[n_{1}]$$

$$= \varepsilon^{2}$$

$$(v_{1} n_{2} n_{1}) = \mathbb{E}[n_{2} n_{1}] - \mathbb{E}[n_{2}] \mathbb{E}[n_{1}]$$

$$= \mathbb{E}[(n_{1} + n_{1}) \times n_{1}] - \mathbb{E}[n_{2}] \mathbb{E}[n_{3}]$$

$$= \mathbb{E}[(n_{1} + n_{1}) \times n_{1}] - \mathbb{E}[n_{2}] \mathbb{E}[n_{3}]$$

$$= \mathbb{E}[(n_{1} + n_{1}) (n_{1} + n_{1} + n_{2}) = \mathbb{E}[n_{2}] \mathbb{E}[n_{3}]$$

$$= \mathbb{E}[n_{1}^{2}] + \mathbb{E}[n_{1}^{2}] + \mathbb{E}[n_{3}]$$

$$= \mathbb{E}[n_{1}^{2}] + \mathbb{E}[n_{1}] - \mathbb{E}[n_{2}] \mathbb{E}[n_{3}]$$

$$= \mathbb{E}[n_{1}^{2}] + n_{1} + n_{1} + n_{2} + n_{3} + n_{1}^{2} + n_{1} + n_{2} + n_{3}]$$

$$= \mathbb{E}[n_{1}^{2}] + n_{1} + n_{1} + n_{2} + n_{3} + n_{1}^{2} + n_{1} + n_{2} + n_{3}$$

$$= 2\varepsilon^{2}$$

$$Von(n_{2}) = \mathbb{E}[n_{2}^{2}]$$

= $\mathbb{E}\left(n_1 + n_1\right)\left(n_1 + n_1\right)$ = $\mathbb{E}\left[n_1^2 + n_1^2 + 2n_1 n_1\right] = 26^2$

row 1

 $Var(n_1) = \mathbb{E}[n_1^2] = 6^2$

From
$$3$$
 Var $(n_3) = \mathbb{E}(n_3^2) = \mathbb{E}(n_1 + n_1 + n_2)^2 = 36^2$

(ov $(n_3, n_1) = \mathbb{E}((n_1 + n_1 + n_2)(n_1)) = \mathbb{E}(n_1^2 + n_1 n_1 + n_2 n_1) = 6^2$

(or $(n_3, n_2) = \mathbb{E}((n_1 + n_1 + n_2)(n_1 + n_1)) = 86^2$

(or $(n_3, n_1) = \mathbb{E}(n_1 + n_1 + n_2)(n_1 + n_1 + n_2 + n_3) = 36^2$

From 3 (or $(n_1, n_1) = \mathbb{E}(n_1 + n_1 + n_2 + n_3)(n_1 + n_1) = 86^2$

(or $(n_1, n_2) = \mathbb{E}(n_1 + n_1 + n_2 + n_3)(n_1 + n_1) = 86^2$

(or $(n_1, n_2) = \mathbb{E}(n_1^2) = 46^2$

(or $(n_1, n_2) = \mathbb{E}(n_1^2) = 46^2$

(or $(n_1, n_2, n_3, n_1) = 6^2 =$

ConditionalDDPM

May 5, 2025

0.1 Setup

Similar to the previous projects, we will need some code to set up the environment.

First, run this cell that loads the autoreload extension. This allows us to edit .py source files and re-import them into the notebook for a seamless editing and debugging experience.

```
[3]: %load_ext autoreload %autoreload 2
```

0.1.1 Google Colab Setup

If you are not using Colab, please just skip this step.

Run the following cell to mount your Google Drive. Follow the link and sign in to your Google account (the same account you used to store this notebook!).

```
[2]: # from google.colab import drive # drive.mount('/content/drive')
```

Then enter your path of the project (for example, /content/drive/MyDrive/ConditionalDDPM)

```
[3]: # cd /content/drive/MyDrive/Graduate/ECE239_TA/ConditionalDDPM/skeleton
```

We will use GPUs to accelerate our computation in this notebook.

If you are using Colab, go to Runtime > Change runtime type and set Hardware accelerator to GPU. This will reset Colab. Rerun the top cell to mount your Drive again.

Run the following to make sure GPUs are enabled:

```
[4]: # set the device
import torch
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")

if torch.cuda.is_available():
   print('Good to go!')
else:
   print('Please set GPU!')
```

Good to go!

0.2 Conditional Denoising Diffusion Probabilistic Models

In the lectures, we have learnt about Denoising Diffusion Probabilistic Models (DDPM), as presented in the paper Denoising Diffusion Probabilistic Models. We went through both the training process and test sampling process of DDPM. In this project, you will use conditional DDPM to generate digits based on given conditions. The project is inspired by the paper Classifier-free Diffusion Guidance, which is a following work of DDPM. You are required to use MNIST dataset and the GPU device to complete the project.

0.2.1 What is a DDPM?

A Denoising Diffusion Probabilistic Model (DDPM) is a type of generative model inspired by the natural diffusion process. In the example of image generation, DDPM works in two main stages:

- Forward Process (Diffusion): It starts with an image sampled from the dataset and gradually adds noise to it step by step, until it becomes completely random noise. In implementation, the forward diffusion process is fixed to a Markov chain that gradually adds Gaussian noise to the data according to a variance schedule $\beta_1, ..., \beta_T$.
- Reverse Process (Denoising): By learning how the noise was added on the image step by step, the model can do the reverse process: start with random noise and step by step, remove this noise to generate an image.

0.2.2 Training and sampling of DDPM

As proposed in the DDPM paper, the training and sampling process can be concluded in the following steps:

```
[5]: from IPython.display import Image
Image(filename='pics/DDPM.png', width=800, height=200)
```

[5]:

Algorithm 1 Training	Algorithm 2 Sampling
1: repeat 2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$ 3: $t \sim \text{Uniform}(\{1, \dots, T\})$ 4: $\epsilon \sim \mathcal{N}(0, \mathbf{I})$ 5: Take gradient descent step on $\nabla_{\theta} \left\ \epsilon - \epsilon_{\theta} (\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t) \right\ ^2$ 6: until converged	1: $\mathbf{x}_{T} \sim \mathcal{N}(0, \mathbf{I})$ 2: $\mathbf{for} \ t = T, \dots, 1 \ \mathbf{do}$ 3: $\mathbf{z} \sim \mathcal{N}(0, \mathbf{I}) \ \text{if} \ t > 1$, else $\mathbf{z} = 0$ 4: $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$ 5: $\mathbf{end} \ \mathbf{for}$ 6: $\mathbf{return} \ \mathbf{x}_0$

Here we still use the example of image generation.

Algorithm 1 shows the training process of DDPM. Initially, an image \mathbf{x}_0 is sampled from the data distribution $q(\mathbf{x}_0)$, i.e. the dataset. Then a time step t is randomly selected from a uniform distribution across the predifined number of steps T.

A noise ϵ which has the same shape of the image is sampled from a standard normal distribution. According to the equation (4) in the DDPM paper and the new notation: $q(\mathbf{x}_t|\mathbf{x}_0) = N(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I}), \ \alpha_t := 1-\beta_t \text{ and } \bar{\alpha}_t := \prod_{s=1}^t \alpha_s$, we can get an intermediate state of

the diffusion process: $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\epsilon$. The model takes the \mathbf{x}_t and t as inputs, and predict a noise, i.e. $\epsilon_{\theta}(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\epsilon, t)$. The optimization of the model is done by minimizing the difference between the sampled noise and the model's prediction of noise.

Algorithm 2 shows the sampling process of DDPM, which is the complete procedure for generating an image. This process starts from noise x_T sampled from a standard normal distribution, and then uses the trained model to iteratively apply denoising for each time step from T to 1.

0.2.3 How to control the generation output?

As you may find, the vanilla DDPM can only randomly generate images which are sampled from the learned distribution of the dataset, while in some cases, we are more interested in controlling the generated images. Previous works mainly use an extra trained classifier to guide the diffusion model to generate specific images (Dhariwal & Nichol (2021)). Ho et al. proposed the Classifier-free Diffusion Guidance, which proposes a novel training and sampling method to achieve the conditional generation without extra models besides the diffusion model. Now let's see how it modify the training and sampling pipeline of DDPM.

Algorithm 1: Conditional training The training process is shown in the picture below. Some notations are modified in order to follow DDPM.

```
[6]: from IPython.display import Image
         Image(filename='pics/ConDDPM_1.png', width=800, height=240)
[6]:
                 Algorithm 1 Joint training a diffusion model with classifier-free guidance
                 Require: p_{uncond}: probability of unconditional training
                  1: repeat
                                                                                           > Sample data with conditioning from the dataset
                           (\mathbf{x}_0, \mathbf{c}_0) \sim q(\mathbf{x}_0, \mathbf{c}_0)
                  2:
                           \mathbf{c}_0 \leftarrow \emptyset with probability p_{\text{uncond}}
                                                                                > Randomly discard conditioning to train unconditionally
                  3:
                           t \sim \text{Uniform}(\{1, ..., T\})
                                                                                                                                    \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})
                  5:
                           \mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{(1 - \bar{\alpha}_t)} \boldsymbol{\epsilon}
                                                                                                       ▷ Corrupt data to the sampled time steps
                           Take gradient step on \nabla_{\theta} \| \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, \mathbf{c}_{0}, t) - \boldsymbol{\epsilon} \|^{2}
                                                                                                                Description Optimization of denoising model
                  8: until converged
```

Compared with the training process of vanilla DDPM, there are several modifications.

- In the training data sampling, besides the image \mathbf{x}_0 , we also sample the condition \mathbf{c}_0 from the dataset (usually the class label).
- There's a probabilistic step to randomly discard the conditions, training the model to generate data both conditionally and unconditionally. Usually we just set the one-hot encoded label as all -1 to discard the conditions.
- When optimizing the model, the condition \mathbf{c}_0 is an extra input.

Algorithm 2: Conditional sampling Below is the sampling process of conditional DDPM.

```
[7]: from IPython.display import Image Image(filename='pics/ConDDPM_2.png', width=500, height=250)
```

[7]:

Algorithm 2 Conditional sampling with classifier-free guidance

Require: w: guidance weight

Require: c: conditioning information for conditional sampling

- 1: $\mathbf{x}_T \sim \mathcal{N}(0, I)$
- 2: **for** t = T, ..., 1 **do**
- 3: $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \text{ if } t > 1, \text{ else } \mathbf{z} = 0$
- 4: $\tilde{\boldsymbol{\epsilon}}_t = (1+w)\boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, \mathbf{c}, t) w\boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t)$
- 5: $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \tilde{\boldsymbol{\epsilon}}_t \right) + \sigma_t \mathbf{z}$
- 6: end for
- 7: return x₀

Compared with the vanilla DDPM, the key modification is in step 4. Here the algorithm computes a corrected noise estimation, $\tilde{\epsilon}_t$, balancing between the conditional prediction $\epsilon_{\theta}(\mathbf{x}_t, \mathbf{c}, t)$ and the unconditional prediction $\epsilon_{\theta}(\mathbf{x}_t, t)$. The corrected noise $\tilde{\epsilon}_t$ is then used to update \mathbf{x}_t in step 5.

Here we follow the setting of DDPM paper and define $\sigma_t = \sqrt{\beta_t}$.

0.2.4 Conditional generation of digits

Now let's practice it! You will first asked to design a denoising network, and then complete the training and sampling process of this conditional DDPM.

In this project, by default, we resize all images to a dimension of 28×28 and utilize one-hot encoding for class labels. Also, please remember to normalize the time step t to the range 0-1 before inputting it into the denoising network as it will help the network have a more stable output.

First we define a configuration class DMConfig. This class contains all the settings of the model and experiment that may be useful later.

```
condition_mask_value: int = -1
                                        # unconditional condition mask value
                                        # number of classes in the dataset
  num_classes: int = 10
  T: int = 400
                                        # diffusion and denoising steps
                                        # variance schedule
  beta_1: float = 1e-4
  beta_T: float = 2e-2
  mask_p: float = 0.1
                                        # condition drop ratio
  num feat: int = 64
                                       # basic feature size of the UNet model
                                        # conditional guidance weight
  omega: float = 2.0
  batch_size: int = 256
                                        # training batch size
  epochs: int = 10
                                        # training epochs
  learning_rate: float = 1e-4
                                        # training learning rate
  multi_lr_milestones: List[int] = field(default_factory=lambda: [20]) #_J
→ learning rate decay milestone
  multi_lr_gamma: float = 0.1
                                        # learning rate decay ratio
```

Then let's prepare and visualize the dataset:

```
[9]: from utils import make_dataloader
     from torchvision import transforms
     import torchvision.utils as vutils
     import matplotlib.pyplot as plt
     # Define the data preprocessing and configuration
     transform = transforms.Compose([
             transforms.ToTensor(),
             transforms.Normalize((0.1307,), (0.3081,))
         ])
     config = DMConfig()
     # Create the train and test dataloaders
     train_loader = make_dataloader(transform = transform, batch_size = config.
      ⇔batch_size, dir = './data', train = True)
     test_loader = make_dataloader(transform = transform, batch_size = config.
      ⇔batch_size, dir = './data', train = False)
     # Visualize the first 100 images
     dataiter = iter(train_loader)
     images, labels = next(dataiter)
     images_subset = images[:100]
     grid = vutils.make_grid(images_subset, nrow = 10, normalize = True, padding=2)
     plt.figure(figsize=(6, 6))
     plt.imshow(grid.numpy().transpose((1, 2, 0)))
     plt.axis('off')
     plt.show()
```



1. Denoising network (6 points) The denoising network is defined in the file ResUNet.py. We have already provided some potentially useful layers or blocks, and you will be asked to complete the class ConditionalUnet.

Some hints:

- Please consider just using 2 down blocks and 2 up blocks. Using more blocks may improve the performance, while the training and sampling time may increase. Feel free to do some extra experiments in the creative exploring part later.
- An example structure of Conditional UNet is shown in the next cell. Here the initialization argument n_feat is set as 128. We provide all the potential useful components in the __init__ function. The simplest way to construct the network is to complete the forward function with these components.
- MODEL DESIGNING IS AN ART: You do not have to use this given structure. You can add/delete any blocks, or even design your own network from scratch. You are also free to change the way of adding the time step and condition.

Now let's check your denoising network using the following code.

Output shape: torch.Size([256, 1, 28, 28]) Dimension test passed!

- 2. Conditional DDPM With the correct denoising network, we can then start to build the pipeline of a conditional DDPM. You will be asked to complete the Conditional DDPM class in the file DDPM.py.
- **2.1 Variance schedule (4 points)** Let's first prepare the variance schedule β_t along with other potentially useful constants. You are required to complete the ConditionalDDPM.scheduler function in DDPM.py.

Given the starting and ending variances β_1 and β_T , the function should output one dictionary containing the following terms:

beta_t: variance of time step t_s , which is linearly interpolated between β_1 and β_T .

$$\label{eq:continuity} \begin{split} & \texttt{sqrt_beta_t:} \ \sqrt{\beta_t} \\ & \texttt{alpha_t:} \ \alpha_t = 1 - \beta_t \end{split}$$

```
oneover_sqrt_alpha: \frac{1}{\sqrt{\alpha_t}} alpha_t_bar: \bar{\alpha_t} = \prod_{s=1}^t \alpha_s sqrt_alpha_bar: \sqrt{\bar{\alpha_t}} sqrt_oneminus_alpha_bar: \sqrt{1-\bar{\alpha_t}} We set \beta_1 = 1e-4 and \beta_T = 2e-2. Let's check your solution!
```

All tests passed!

2.2 Training process (6 points) Recall the training algorithm we discussed above:

You will need to complete the ConditionalDDPM.forward function in the DDPM.py file. Then you can use the function utils.check_forward to test if it's working properly. The model will be trained for one epoch in this checking process. It should take around 1 min and return one curve showing a decreasing loss trend if your ConditionalDDPM.forward function is correct.

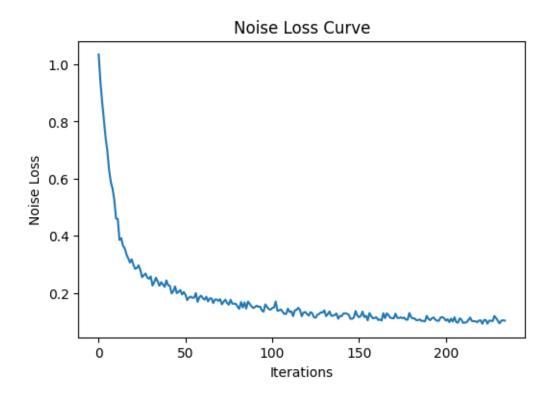
```
[17]: from IPython.display import Image Image(filename='pics/ConDDPM_1.png', width=800, height=240)
```

```
[17]:
                    Algorithm 1 Joint training a diffusion model with classifier-free guidance
                    Require: p_{uncond}: probability of unconditional training
                      1: repeat
                                                                                                      ▷ Sample data with conditioning from the dataset
                                (\mathbf{x}_0, \mathbf{c}_0) \sim q(\mathbf{x}_0, \mathbf{c}_0)
                                \mathbf{c}_0 \leftarrow \emptyset with probability p_{\text{uncond}}
                                                                                          ▶ Randomly discard conditioning to train unconditionally
                      3:
                               t \sim \text{Uniform}(\{1, ..., T\})

    Sample time steps

                               \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})
                      5:
                               \mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{(1 - \bar{\alpha}_t)} \boldsymbol{\epsilon}
                                                                                                                   Take gradient step on \nabla_{\theta} \| \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, \mathbf{c}_{0}, t) - \boldsymbol{\epsilon} \|^{2}
                                                                                                                            Description Optimization of denoising model
                      8: until converged
```

```
[18]: from utils import check_forward
  config = DMConfig()
  model = check_forward(train_loader, config, device)
```



2.3 Sampling process (6 points)

Now you are required to complete the ConditionalDDPM.sample function using the sampling process we mentioned above.

In the following cell, we will use the given utils.check_sample function to check the correctness. With the trained model in 2.2, the model should be able to generate some super-rough digits (you may not even see them as digits). The sampling process should take around 30s.

```
[19]: from IPython.display import Image Image(filename='pics/ConDDPM_2.png', width=500, height=250)
```

[19]:

Algorithm 2 Conditional sampling with classifier-free guidance

Require: w: guidance weight

Require: c: conditioning information for conditional sampling

- 1: $\mathbf{x}_T \sim \mathcal{N}(0, I)$
- 2: **for** t = T, ..., 1 **do**
- 3: $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \text{ if } t > 1, \text{ else } \mathbf{z} = 0$
- 4: $\tilde{\boldsymbol{\epsilon}}_t = (1+w)\boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, \mathbf{c}, t) w\boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t)$

5:
$$\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \tilde{\boldsymbol{\epsilon}}_t \right) + \sigma_t \mathbf{z}$$

- 6: end for
- 7: return \mathbf{x}_0

```
[35]: from utils import check_sample
  config = DMConfig()
  fig = check_sample(model, config, device)
```



2.4 Full training (8 points) As you might notice, the images generated are imperfect since the model trained for only one epoch has not yet converged. To improve the performance, we should proceed with a complete cycle of training and testing. You can utilize a provided **solver** function in this part.

Let's refresh all configurations:

```
[36]: train_config = DMConfig()
print(train_config)
```

DMConfig(input_dim=(28, 28), num_channels=1, condition_mask_value=-1, num_classes=10, T=400, beta_1=0.0001, beta_T=0.02, mask_p=0.1, num_feat=64, omega=2.0, batch_size=256, epochs=10, learning_rate=0.0001, multi_lr_milestones=[20], multi_lr_gamma=0.1)

Then we can use function utils.solver to train the model. You should also input your own experiment name, e.g. your_exp_name. The best-trained model will be saved as ./save/your_exp_name/best_checkpoint.pth. Furthermore, for each training epoch, one generated image will be stored in the directory ./save/your_exp_name/images as a validation.

It will take about $10\sim20$ minutes (10 epochs) if you are using the free-version Google Colab GPU. Typically, realistic digits can be generated after around $2\sim5$ epochs.

```
[37]: from utils import solver
      solver(dmconfig = train_config,
             exp_name = 'test_3',
             train_loader = train_loader,
             test_loader = test_loader)
     epoch 1/10
     train: train_noise_loss = 0.1909 test: test_noise_loss = 0.1088
     epoch 2/10
     train: train_noise_loss = 0.0901 test: test_noise_loss = 0.0835
     epoch 3/10
     train: train_noise_loss = 0.0787 test: test_noise_loss = 0.0770
     epoch 4/10
     train: train_noise_loss = 0.0722 test: test_noise_loss = 0.0739
     epoch 5/10
     train: train_noise_loss = 0.0682 test: test_noise_loss = 0.0713
     epoch 6/10
     train: train_noise_loss = 0.0666 test: test_noise_loss = 0.0645
     epoch 7/10
     train: train_noise_loss = 0.0640 test: test_noise_loss = 0.0666
     epoch 8/10
     train: train_noise_loss = 0.0624 test: test_noise_loss = 0.0612
     epoch 9/10
```

```
train: train_noise_loss = 0.0604 test: test_noise_loss = 0.0640
epoch 10/10
```

train: train_noise_loss = 0.0598 test: test_noise_loss = 0.0626

Now please show the image that you believe has the best generation quality in the following cell.



2.5 Exploring the conditional guidance weight (3 points) The generated images from the previous training-sampling process is using the default conditional guidance weight $\omega = 2$. Now with the best checkpoint, please try at least 3 different ω values and visualize the generated images. You can use the provided function sample_images to get a combined image each time.

```
fig = sample_images(config = sample_config, checkpoint_path =_
⇒path_to_your_checkpoint)
# Checkpoint path
checkpoint_path = "./save/test_2/best_checkpoint.pth"
torch.serialization.add_safe_globals([DMConfig])
# w values to test
omegas = [-1, 0.0, 0.5, 1.0, 2.0, 5.0, 10.0]
# Prepare test
fig, axes = plt.subplots(
   nrows=len(omegas),
   ncols=1,
   figsize=(6, 3 * len(omegas)),
   constrained_layout=True
# Loop over , sample and plot
for ax, w in zip(axes, omegas):
   config = DMConfig(omega=w)
   grid = sample_images(config=config, checkpoint_path=checkpoint_path)
   ax.imshow(grid)
   ax.set_title(f" = {w}")
   ax.axis("off")
plt.show()
# ============= #
```

00000000000 777777777 7 8

9997,999,999

7777777777 **6**5664**69**668 7977979999 $\omega = 10.0\,$

 $\omega = 5.0$

 $\omega = 1.0$

7474990947 $\omega = 0.5$

₩ = 0.0 ₩

Inline Question: Based on your experiment, discuss how the conditional guidance weight affects the quality and diversity of generation. (1 point)

Your answer:

The conditional guidance weight has a very large affect on the quality and diversity of generation in a few ways (summarized in the table below):

Guidance	O 1:4 0 CI	D: :	Class	NT 1
Weight	Quality & Sharpness	Diversi	tyFidelity	Notes
-1.0	Low	Very high	Low	highly rely on the unconditional network. so poor quality
0 - 0.5	Low (fuzzy, soft strokes)	Very high	Low	Poor digit legibility
1-2	Moderate (clear but natural)	ModerateHigh		Sweet spot—legible yet varied handwriting styles
5	High (very sharp, bold edges)	Low	Very high	Stereotyped, grid-like artifacts begin to appear
10	Very high (extreme sharpness)	Very low	Extremely high	Severe mode collapse; samples look almost identical

Overall - low conditional guidance weight (0.0-1.0) leads to increased digit diversity but low fidelity, as you increase w your fidelity increases substantially but your class diversity decreases proportionally.

2.6 Customize your own model (5 points) Now let's experiment by modifying some hyperparameters in the config and costomizing your own model. You should at least change one defalut setting in the config and train a new model. Then visualize the generation image and discuss the effects of your modifications.

Hint: Possible changes to the configuration include, but are not limited to, the number of diffusion steps T, the unconditional condition drop ratio mask_p, the feature size num_feat, the beta schedule, etc.

First you should define and print your modified config. Please state all the changes you made to the DMConfig class, i.e. DMConfig(T=?, num_feat=?, ...).

```
[14]: # train_config_new = DMConfig()
# print(train_config_new)

# default T = 400, mask_p = 0.1, num_feat = 64, beta_1 = 1e-4, beta_T= 2e-2
print(f"default config: {DMConfig()}")
train_config_new = DMConfig(T = 200, mask_p = 0.2, num_feat = 128, beta_1 = 0.1e-3, beta_T= 2e-1)
print(f"Modified config: {train_config_new}")
```

```
default config: DMConfig(input_dim=(28, 28), num_channels=1,
  condition_mask_value=-1, num_classes=10, T=400, beta_1=0.0001, beta_T=0.02,
  mask_p=0.1, num_feat=64, omega=2.0, batch_size=256, epochs=10,
  learning_rate=0.0001, multi_lr_milestones=[20], multi_lr_gamma=0.1)
  Modified config: DMConfig(input_dim=(28, 28), num_channels=1,
  condition_mask_value=-1, num_classes=10, T=200, beta_1=0.001, beta_T=0.2,
  mask_p=0.2, num_feat=128, omega=2.0, batch_size=256, epochs=10,
  learning_rate=0.0001, multi_lr_milestones=[20], multi_lr_gamma=0.1)
```

Then similar to 2.4, use solver funtion to complete the training and sampling process.

```
[15]: from utils import solver
      solver(dmconfig = train_config_new,
             exp_name = 'modified_env',
             train_loader = train_loader,
             test_loader = test_loader)
     epoch 1/10
     train: train_noise_loss = 0.0956 test: test_noise_loss = 0.0441
     epoch 2/10
     train: train_noise_loss = 0.0410 test: test_noise_loss = 0.0379
     epoch 3/10
     train: train_noise_loss = 0.0348 test: test_noise_loss = 0.0347
     epoch 4/10
     train: train_noise_loss = 0.0313 test: test_noise_loss = 0.0315
     epoch 5/10
     train: train_noise_loss = 0.0302 test: test_noise_loss = 0.0300
     epoch 6/10
     train: train_noise_loss = 0.0288 test: test_noise_loss = 0.0285
     epoch 7/10
     train: train_noise_loss = 0.0279 test: test_noise_loss = 0.0325
     epoch 8/10
```

```
train: train_noise_loss = 0.0267 test: test_noise_loss = 0.0276
epoch 9/10

train: train_noise_loss = 0.0256 test: test_noise_loss = 0.0245
epoch 10/10

train: train_noise_loss = 0.0252 test: test_noise_loss = 0.0274
Finally, show one image that you think has the best quality.
```



Inline Question: Discuss the effects of your modifications after you compare the generation performance under different configurations. (1 point)

Your answer:

```
Previous config: T = 400, mask_p = 0.1, num_feat = 64, beta_1 = 1e-4, beta_T = 2e-2
New config: T = 200, mask_p = 0.2, num_feat = 128, beta_1 = 1e-3, beta_T = 2e-1
```

As you can see, what we did are to decrease the num of timesteps but increase the features of U-Net and increase the beta_T. As the MNIST dataset is relatively simple to general rgb images, so decreasing T won't affect too much, but increase the num_features will enhance the network representation, and increase beta_T will make network better ability to generalization (ie. diversity)

```
import torch
import torch.nn as nn
class ResConvBlock(nn.Module):
   Basic residual convolutional block
   def init (self, in channels, out channels):
        super().__init__()
        self.in channels = in channels
        self.out_channels = out_channels
        self.conv1 = nn.Sequential(
            nn.Conv2d(in channels, out channels, 3, 1, 1),
            nn.BatchNorm2d(out channels),
            nn.GELU(),
        self.conv2 = nn.Sequential(
            nn.Conv2d(out channels, out channels, 3, 1, 1),
            nn.BatchNorm2d(out channels),
            nn.GELU(),
        )
   def forward(self, x):
       x1 = self.conv1(x)
       x2 = self.conv2(x1)
        if self.in channels == self.out channels:
           out = x + x2
       else:
           out = x1 + x2
        return out / torch.sqrt(torch.tensor(2.0, device=out.device))
class UnetDown(nn.Module):
   UNet down block (encoding)
   def init (self, in channels, out channels):
        super(UnetDown, self). init ()
        layers = [ResConvBlock(in channels, out channels), nn.MaxPool2d(2)]
        self.model = nn.Sequential(*layers)
   def forward(self, x):
       return self.model(x)
class UnetUp (nn.Module):
    UNet up block (decoding)
   def init (self, in channels, out channels):
        super(UnetUp, self).__init__()
        layers = [
            nn.ConvTranspose2d(in channels, out channels, 2, 2),
            ResConvBlock(out channels, out channels),
            ResConvBlock (out channels, out channels),
        self.model = nn.Sequential(*layers)
   def forward(self, x, skip):
        x = torch.cat((x, skip), 1)
       x = self.model(x)
       return x
class EmbedBlock(nn.Module):
   Embedding block to embed time step/condition to embedding space
```

```
def init (self, input dim, emb dim):
       super(EmbedBlock, self). init ()
       self.input_dim = input_dim
       layers = [
            nn.Linear(input dim, emb dim),
           nn.GELU(),
           nn.Linear(emb dim, emb dim),
       self.layers = nn.Sequential(*layers)
   def forward(self, x):
        # set embedblock untrainable
       for param in self.layers.parameters():
           param.requires grad = False
       x = x.view(-1, self.input dim)
       return self.layers(x)
class FusionBlock (nn.Module):
   Concatenation and fusion block for adding embeddings
   def init (self, in_channels, out_channels):
       super(FusionBlock, self). init ()
       self.layers = nn.Sequential(
            nn.Conv2d(in channels, out channels, 1),
            nn.BatchNorm2d(out channels),
           nn.GELU(),
   def forward(self, x, t, c):
       h, w = x.shape[-2:]
       return self.layers(torch.cat([x, t.repeat(1,1,h,w), c.repeat(1,1,h,w)], dim = 1))
class ConditionalUnet(nn.Module):
   def init (self, in channels, n feat = 128, n classes = 10):
       super(ConditionalUnet, self).__init__()
       self.in channels = in channels
       self.n feat = n feat
       self.n classes = n classes
        # embeddings
       self.timeembed1 = EmbedBlock(1, 2*n_feat)
       self.timeembed2 = EmbedBlock(1, 1*n_feat)
       self.conditionembed1 = EmbedBlock(n classes, 2*n feat)
       self.conditionembed2 = EmbedBlock(n classes, 1*n feat)
       # down path for encoding
       self.init conv = ResConvBlock(in channels, n feat)
       self.downblock1 = UnetDown(n feat, n feat)
       self.downblock2 = UnetDown(n_feat, 2 * n_feat)
       self.to vec = nn.Sequential(nn.AvgPool2d(7), nn.GELU())
        # up path for decoding
       self.upblock0 = nn.Sequential(
            nn.ConvTranspose2d(2 * n feat, 2 * n feat, 7, 7),
           nn.GroupNorm(8, 2 * n_feat),
           nn.ReLU(),
       )
       self.upblock1 = UnetUp(4 * n_feat, n_feat)
       self.upblock2 = UnetUp(2 * n feat, n feat)
       self.outblock = nn.Sequential(
            nn.Conv2d(2 * n feat, n feat, 3, 1, 1),
            nn.GroupNorm(8, n feat),
            nn.ReLU(),
            nn.Conv2d(n feat, self.in channels, 3, 1, 1),
```

```
)
   # fusion blocks
   self.fusion1 = FusionBlock(3 * self.n_feat, self.n_feat)
   self.fusion2 = FusionBlock(6 * self.n_feat, 2 * self.n_feat)
   self.fusion3 = FusionBlock(3 * self.n_feat, self.n_feat)
   self.fusion4 = FusionBlock(3 * self.n feat, self.n feat)
def forward(self, x, t, c):
   111
   Inputs:
     x: input images, with size (B,1,28,28)
      t: input time stepss, with size (B,1,1,1)
      c: input conditions (one-hot encoded labels), with size (B,10)
   t, c = t.float(), c.float()
   # time step embedding
   temb1 = self.timeembed1(t).view(-1, self.n feat * 2, 1, 1)
   temb2 = self.timeembed2(t).view(-1, self.n feat, 1, 1)
   # condition embedding
   cemb1 = self.conditionembed1(c).view(-1, self.n feat * 2, 1, 1)
   cemb2 = self.conditionembed2(c).view(-1, self.n feat, 1, 1)
   # ----- #
   # YOUR CODE HERE:
   # Define the process of computing the output of a
   # this network given the input x, t, and c.
   # The input x, t, c indicate the input image, time step
   # and the condition respectively.
   # A potential format is shown below, feel free to use your own ways to design it.
   # down0 =
   # down1 =
   \# down2 =
   # up0 =
   # up1 =
   # up2 =
   # out = self.outblock(torch.cat((up2, down0), dim = 1))
   # ========= #
   # Encoder
   down0 = self.init_conv(x)
                                                    # (B, 128, 28, 28)
   down1 = self.downblock1(down0)
                                                   # (B, 128, 14, 14)
   down1 = self.fusion1(down1, temb2, cemb2)
                                                   # (B, 128, 14, 14)
   down2 = self.downblock2(down1)
                                                   # (B, 256, 7, 7)
   down2 = self.fusion2(down2, temb1, cemb1)
                                                    # (B, 256, 7, 7)
   # Bottleneck
   hidden = self.to vec(down2)
                                                    # (B, 256, 1, 1)
   up0 = self.upblock0(hidden)
                                                    # (B, 256, 7, 7)
   # Decoder
   up1 = self.upblock1(up0, down2)
                                                   # (B, 128, 14, 14)
   up1 = self.fusion3(up1, temb2, cemb2)
                                                   # (B, 128, 14, 14)
   up2 = self.upblock2(up1, down1)
                                                   # (B, 128, 28, 28)
                                                   # (B, 128, 28, 28)
   up2 = self.fusion4(up2, temb2, cemb2)
   # Output
   out = self.outblock(torch.cat((up2, down0), dim=1)) # (B, 1, 28, 28)
```

```
import torch
import torch.nn as nn
import torch.nn.functional as F
from ResUNet import ConditionalUnet
from utils import *
device = torch.device("cuda" if torch.cuda.is available() else "cpu")
class ConditionalDDPM(nn.Module):
   def init (self, dmconfig):
       super().__init__()
       self.dmconfig = dmconfig
       self.loss fn = nn.MSELoss()
       self.network = ConditionalUnet(1, self.dmconfig.num feat, self.dmconfig.num classes)
   def scheduler(self, t_s):
       beta 1, beta T, T = self.dmconfig.beta 1, self.dmconfig.beta T, self.dmconfig.T
       # ============ #
       # YOUR CODE HERE:
       #
          Inputs:
       #
           t s: the input time steps, with shape (B,1).
       #
         Outputs:
       #
             one dictionary containing the variance schedule
               $\beta t$ along with other potentially useful constants.
       # Make sure t s is shape (B,1)
       if t s.dim() == 0:
           t s = t s.view(1,1)
       elif t s.dim() == 1:
           t s = t s.unsqueeze(-1)
       B = t s.size(0) # number of examples in the batch
       # Build the scheduler for the DDPM process
       device = t s.device
       betas = torch.linspace(beta_1, beta_T, T, device=device)
       alphas = 1.0 - betas
       alpha bars = torch.cumprod(alphas, dim=0)
       # Zero-base indices
       t = t s.squeeze(-1).long() - 1
       t = t.clamp(0, T-1)
       # Based on spec
       beta t = betas[t].view(B, 1, 1, 1)
       sqrt beta t = torch.sqrt(beta t)
       alpha t = alphas[t].view(B, 1, 1, 1)
       oneover_sqrt_alpha = 1.0 / torch.sqrt(alpha_t)
       alpha_t_bar = alpha_bars[t].view(B,1,1,1)
       sqrt alpha bar = torch.sqrt(alpha t bar)
       sqrt_oneminus_alpha_bar = torch.sqrt(1.0 - alpha_t_bar)
       # ----- #
       return {
           'beta t': beta t,
           'sqrt_beta_t': sqrt_beta_t,
           'alpha t': alpha t,
           'sqrt_alpha_bar': sqrt_alpha_bar,
           'oneover sqrt alpha': oneover sqrt alpha,
           'alpha t bar': alpha t bar,
           'sqrt_oneminus_alpha_bar': sqrt_oneminus_alpha_bar
       }
   def forward(self, images, conditions):
       T = self.dmconfig.T
       noise loss = None
       # ========== #
```

```
# YOUR CODE HERE:
       # Complete the training forward process based on the
       # given training algorithm.
       # Inputs:
       #
              images: real images from the dataset, with size (B,1,28,28).
       #
              conditions: condition labels, with size (B). You should
       #
                          convert it to one-hot encoded labels with size (B,10)
                          before making it as the input of the denoising network.
       #
          Outputs:
            noise loss: loss computed by the self.loss fn function .
       B, _, W = images.shape
       device = images.device
       # One-hot encode the labels
       c = F.one hot(conditions, num classes=self.dmconfig.num classes).float() # (B,
num classes)
       # Classifier-free masking
       p uncond = getattr(self.dmconfig, 'p uncond', 0.0)
       if p uncond > 0:
           mask = (torch.randn(B, device=device) 
           c[mask] = 0.0
       # Sample for each batch element
       t = torch.randint(1, T+1, (B,1), device=device)
       eps = torch.randn like(images)
       # Compute the noisy input
       sched = self.scheduler(t)
       x t = sched['sqrt alpha bar'] * images
           + sched['sqrt oneminus alpha bar'] * eps # broadcastâ(B,1,H,W)
       # Predict the noise
       noise_pred = self.network(x_t, t.squeeze(-1), c)
       # MSE loss
       noise loss = self.loss fn(noise pred, eps)
       # ============ #
       return noise_loss
   def sample(self, conditions, omega):
       T = self.dmconfig.T
       X t = None
       # ======== #
       # YOUR CODE HERE:
       # Complete the training forward process based on the
       # given sampling algorithm.
         Inputs:
       #
       #
            conditions: condition labels, with size (B). You should
       #
                         convert it to one-hot encoded labels with size (B, 10)
       #
                          before making it as the input of the denoising network.
       #
           omega: conditional guidance weight.
         Outputs:
            generated_images
       B = conditions.size(0)
       device = conditions.device
       # One-hot encode labels
       c = F.one hot(conditions, num_classes=self.dmconfig.num_classes).float()
       # Gaussian noise x T
       X t = torch.randn(B, 1, 28, 28, device=device)
```

```
# eval mode, no grad
   self.network.eval()
   with torch.no_grad():
       for t in range (T, 0, -1):
           # Build timeâstep tensors
          t batch = t vec.unsqueeze(-1)
           # Query scheduler
          sched = self.scheduler(t batch)
           # Predict noise
          eps cond = self.network(X t, t vec, c)
          eps uncond = self.network(X t, t vec, torch.zeros like(c))
           # Classifierâfree guidance
          eps hat = (1.0 + omega) * eps cond - omega * eps uncond
           # Compute the mean without noise
          coef = (1.0 - sched['alpha t']) / sched['sqrt oneminus alpha bar']
          X prev = sched['oneover sqrt alpha'] * (X t - coef * eps hat)
           # Add noise if t > 1
          if t > 1:
              z = torch.randn like(X t)
              X prev = X prev + sched['sqrt beta t'] * z
           # Step down
          X t = X prev
   # back to train mode
   self.network.train()
   # =========== #
   generated images = (X t * 0.3081 + 0.1307).clamp(0,1) # denormalize the output images
   return generated images
# def sample(self, conditions, omega):
    T = self.dmconfig.T
    X t = None
     # ----- #
#
     # YOUR CODE HERE:
#
    # Complete the training forward process based on the
#
     # given sampling algorithm.
#
       Inputs:
     #
           conditions: condition labels, with size (B). You should
                       convert it to one-hot encoded labels with size (B,10)
#
     #
                       before making it as the input of the denoising network.
    #
           omega: conditional guidance weight.
       Outputs:
     #
           generated images
    B = conditions.size(0)
     device = conditions.device
     # One-hot encode
     c = F.one hot(conditions, num classes=self.dmconfig.num classes).float()
     # Gaussian noise
     X t = torch.randn(B, 1, 28, 28, device=device)
     # put the network into eval & disable grads
     self.network.eval()
     with torch.no grad():
        # Denoise
```

#

#

#

#

#

#

#

```
for t in range(T, 0, -1):
   #
                t_batch = torch.full((B,1), t, device=device, dtype=torch.long)
                 sched = self.scheduler(t_batch)
                z = torch.randn\ like(X\ t)\ if\ t > 1\ else\ torch.zeros\ like(X\ t)
                eps_cond = self.network(X_t, t_batch.squeeze(-1),
                 eps uncond = self.network(X t, t batch.squeeze(-1), torch.zeros like(c))
                # Classifier-free guidance
   #
                eps_hat = (1.0 + omega) * eps_cond - omega * eps_uncond
                coef = (1.0 - sched['alpha t']) / sched['sqrt oneminus alpha bar']
                X_t = (
                    sched['oneover_sqrt_alpha']
                    * (X_t - coef * eps_hat)
                    + sched['sqrt beta t'] * z
   #
         # back to train mode
         self.network.train()
         # ----- #
   #
         generated images = (X t * 0.3081 + 0.1307).clamp(0,1) # denormalize the output
images
        return generated images
```