1. X1 ~ N (0. 32)

xt xt-1~ N(xt-1, 62)

P(X1, X2, X3, X4) = P(X1) P(X2 | X1) P(X3 | X2) P(X4 | X3)

COV [x, Y]

= Cov[Y,x]

(X ~ N (Mx, 6x) Y ~ N (My, 6y)

X+Y ~ N(Mx+MY, 5x2+642)

one to C.L.T.

= E[XY - XETY] - ETX] Y + ETXJETY]

= E[xi] - E[i]E[x] - E[x]E[i] + E[x]E[i]

= E[xr] - E[x]E[r]

Var [x] = E[x2] - E[x]2

By def: $X_t = X_{t-1} + N(0, 6^2)$; $X_1 \sim N(0, 6^2)$

" X2 = X1+ N(0.62)

~ N(0, 252)

: Xs = X2+ N (0,52)

~ N(0,351)

×4 = x3 + N(0,50)

~ N (0,462)

: Var [x,] = 62

Var [X3] = 362

Var [x2] = 282

Var [X4] = 452

$$Cov[x,Y] = E[xY] - E[x]E[Y]$$

$$= E[x,x_2] - E[x,JE[x_2]$$

$$= E[x_1(x_1+Nco,6^2))] - O$$

$$= E[x_1^2 + x_1\cdot N(o,6^2)]$$

$$= E[x_1^2] + E[x_1\cdot N(o,6^2)]$$

$$= E[x_1^2] + E[x_1] \cdot E[Nco,6^2]$$

$$= E[x_1^2] + E[x_1] \cdot E[Nco,6^2]$$

$$= E[x_1^2] + O$$

$$= Var[x_1] - E[x_1]^2$$

$$= Var[x_1] - O$$

$$= 6^2$$

$$Cov [X_1, X_3] = E[X_1 X_3] = 0$$

$$= E[X_1 (X_1 + 2NCO, \delta^2))]$$

$$= E[X_1^2] + 2E[X_1]E[N(O, \delta^2)]$$

$$= E[X_1^2]$$

$$= \delta^2$$

Cov
$$[X_2, X_3] = E[X_2 X_3] - E[X_1]E[X_1]$$

$$= E[X_2^2]$$

$$= Var[X_1] - E[X_2]^2$$

$$= 26^2$$
Cov $[X_2, X_4] = E[X_2 X_4] - 0$

$$= E[X_2^2]$$

$$= 26^2$$

$$Cov \left[X_3, X_4 \right] = \left[E \left[X_3^2 \right] \right]$$
$$= 36^2$$

Cov Matrix
$$\Sigma = \begin{bmatrix} 6^2 & 6^2 & 6^2 & 6^2 \\ 6^2 & 26^2 & 26^2 & 26^2 \\ 6^2 & 26^2 & 36^2 & 36^2 \\ 6^2 & 26^2 & 36^2 & 46^2 \end{bmatrix}$$

$$\Sigma = \begin{bmatrix} 6^2 & 6^2 & 6^2 & 6^2 \\
6^2 & 26^2 & 26^2 & 26^2 \\
6^2 & 26^2 & 36^2 & 36^2 \\
6^2 & 26^2 & 36^2 & 36^2
\end{bmatrix} = 6^2 \begin{bmatrix} 1 & 1 & 1 & 1 \\
1 & 2 & 2 & 2 \\
1 & 2 & 3 & 3 \\
1 & 2 & 3 & 4 \end{bmatrix}$$

$$\sum_{i=1}^{x_{1}} \frac{x_{2}}{3^{2}} x_{3} x_{4}$$

$$\sum_{i=1}^{x_{1}} \frac{x_{2}}{3^{2}} x_{4}$$

$$\sum_{i=1}^{x_{1}} \frac{x_{2}}{3^{2}} x_{4}$$

$$\sum_{i=1}^{x_{2}} \frac{x_{3}}{3^{2}} x_{4}$$

$$\sum_{i=1}^{x_{2}} \frac{x_{3}}{3^{2}} x_{4}$$

$$\sum_{i=1}^{x_{2}} \frac{x_{3}}{3^{2}} x_{4}$$

$$= \frac{0.6 \times 0.9 \times 0.9 \times 0.9}{0.9 \times 0.9} = 0.54$$

$$= \frac{P(E^{+}, S^{+}, M^{+}, B^{+})}{P(B^{+}, E^{+}, S^{+})} = \frac{P(E^{+}) \cdot P(S^{+} | E^{+}, M^{+}) \cdot P(M^{+}) P(B^{+} | M^{+})}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)} = \frac{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)} = \frac{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)} = \frac{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)} = \frac{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)} = \frac{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)} = \frac{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)} = \frac{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)} = \frac{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)} = \frac{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)} = \frac{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)} = \frac{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)} = \frac{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)} = \frac{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)} = \frac{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)} = \frac{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)} = \frac{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}{\sum_{M} P(B^{+}, E^{+}, S^{+}, M)}$$

$$= \sum_{k=1}^{n} \int_{\mathbb{R}^{n}} \mathbb{E} x_{1} = x_{1},$$

(c) i. show : {B/M} IL { F. S/M} PEB, E, SIM] = PEBIM] PEE, SIM] P[B,E,SIM] = P[B,E,S,M] 1'IM7 = PEFJ · PESIE, M] · PEMJ · PEBIM] P[M] = P[E] . P[SIE, M] . P[BIM] PIBMJ. P[E] · P[SIE,M] = P[D+M] · P[E,S/M] PERJ. PESIE, M] : PERJ. PES. E. M] P. I.E. MI

= PEEJ · P [E. S/M] · PEM] PEF, MT

To Prove PEFJ. PESIE, M] = PEF, S/M] (=> Proving PLESTM] = P[F]. P[ESTM]. P[M] PEE, MT

(=) Proving PIE,M]: PEEJ. PEM]

To prove EILM (=> PIE,M] = PIE] PIM]

P[E,M] = Z Z P[E, S, M, B] (Marginal Dist.)

= Z Z P[E] P[SIE,M] P[M] P[BIM]

= PEE] P[M]. \(\frac{2}{5}\) P[S[EM] \(\frac{2}{5}\) P[B[M] \(\frac{2}{5}\) P[B[M] \(\frac{2}{5}\) P[B[M]

· P[E,m] = P[E] P[m]

: We can have PIEJ. PESIE, M] = PIE, S/M]

Can I'me P[B,E,S/M] = P[B/M] · P[E-S/M]

B/M IL E.S/M.

M(B) = M

E M.S IL 13/M.S

ii.

P[E,B|M,s] = P[E|M,s] P[B|M,s]

PEE,B/M,s] = PEE,B,M,S]
PEM,S]

= P[E] P[S|E,M] P[M] P[B|M]
P[M,S]

We've Proven po [E] P[M] : P[E, M]

PES, E, M] PEBIM] = PEEIMIS] · PEBIM]

ty to prove |'[B[M]= |'EB[M.s]

P[B|M,s]: P[B, M,s]

P[M,s]

= 1 = PERJ P[STR,M]P[BIM]

= 2 = P[B|M]

= P[B|M]

: P[E,B[M,S] = P[E[M,S] P[B]M.S]

iii

: M # Els

EILB / {M.S]

- MCE) = {MIS}

iv. No. Counter Example in 221.



RESUNET.PY

```
import torch
import torch.nn as nn
import math
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 / math.sqrt(2)
class UnetDown(nn.Module):
    UNet down block (encoding)
    def __init__(self, in_channels, out_channels):
        super().__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().__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().__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().__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().__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):
   Inputs:
       x: input images, with size (B,1,28,28)
       t: input time steps, 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) # 256
   temb2 = self.timeembed2(t).view(-1, self.n_feat, 1, 1) # 128
   # condition embedding
   cemb1 = self.conditionembed1(c).view(-1, self.n_feat * 2, 1, 1) # 256
   cemb2 = self.conditionembed2(c).view(-1, self.n_feat, 1, 1) # 128
   # 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))
   # =========== #
   down0 = self.init_conv(x)
   down1 = self.downblock1(down0)
   fusion1 = self.fusion1(down1, temb2, cemb2)
   down2 = self.downblock2(fusion1)
   fusion2 = self.fusion2(down2, temb1, cemb1)
   vec0 = self.to_vec(fusion2)
```

```
up0 = self.upblock0(vec0)
up1 = self.upblock1(up0, fusion2)
fusion3 = self.fusion3(up1, temb2, cemb2)
up2 = self.upblock2(fusion3, fusion1)
fusion4 = self.fusion4(up2, temb2, cemb2)
out = self.outblock(torch.cat((fusion4, down0), dim = 1))
```

return out

DDPM.PY

```
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
               f \setminus beta\_tf along with other potentially useful constants.
       device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
       beta = torch.linspace(beta_1, beta_T, T).to(device)
       beta_T = beta[t_s-1]
       sqrt_beta_t = torch.sqrt(beta_T)
       alpha_t = 1-beta_T
       oneover_sqrt_alpha = 1/torch.sqrt(alpha_t)
       alpha_t_bar = torch.cumprod(1-beta, dim=0)[t_s-1]
       sqrt_alpha_bar = torch.sqrt(alpha_t_bar)
       sqrt_oneminus_alpha_bar = torch.sqrt(1-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 .
   device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
   B = images.shape[0]
   t_s = torch.randint(1,T+1, size=(B,1)).to(device)
   t_s_norm = (t_s-1.0)/(T-1)
   noise = torch.randn_like(images).to(device)
   conditions = F.one_hot(conditions, num_classes=self.dmconfig.num_classes).to(device)
   drop_batch_idx = torch.rand(B).to(device) <= self.dmconfig.mask_p</pre>
   conditions[drop_batch_idx, :] = self.dmconfig.condition_mask_value
   scheduler = self.scheduler(t_s)
   sqrt_alpha_bar = scheduler['sqrt_alpha_bar'].reshape(-1,1,1,1)
   sqrt_oneminus_alpha_bar = scheduler['sqrt_oneminus_alpha_bar'].reshape(-1,1,1,1)
   x_t = sqrt_alpha_bar * images + sqrt_oneminus_alpha_bar * noise
   noise_loss = self.loss_fn(self.network(x_t, t_s_norm.reshape(-1,1,1,1),\)
                           conditions), noise)
   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 quidance weight.
   Outputs:
       generated_images
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
B = conditions.size(dim=0)
num_channels = self.dmconfig.num_channels
input_dim = self.dmconfig.input_dim
X_t = torch.randn(B, num_channels, input_dim[0], input_dim[1]).to(device)
my_condition = torch.full_like(conditions, self.dmconfig.condition_mask_value)\
                             .to(device)
with torch.no_grad():
   for t_s in torch.arange(T, 0, -1):
       time_step = torch.full((B,1), t_s).to(device)
       time\_step\_norm = (time\_step - 1.0) / (T-1)
       if t_s > 1:
           z = torch.randn_like(X_t).to(device)
           z = torch.zeros_like(X_t).to(device)
       cond_eps = self.network(X_t, time_step_norm.reshape(-1,1,1,1), conditions)
       uncond_eps = self.network(X_t, time_step_norm.reshape(-1,1,1,1),\
                                 my_condition)
       eps_t = (1+omega)*cond_eps - omega*uncond_eps
       scheduler = self.scheduler(time_step)
       oneover_sqrt_alpha = scheduler['oneover_sqrt_alpha'].reshape(-1,1,1,1)
       sqrt_oneminus_alpha_bar = scheduler['sqrt_oneminus_alpha_bar']\
                                 .reshape(-1,1,1,1)
       alpha_t = scheduler['alpha_t'].reshape(-1,1,1,1)
       sqrt_beta_t = scheduler['sqrt_beta_t'].reshape(-1,1,1,1)
       X_t = oneover_sqrt_alpha * (X_t-(1-alpha_t)/sqrt_oneminus_alpha_bar*eps_t)
             + sqrt_beta_t*z
# ----- #
generated_images = (X_t * 0.3081 + 0.1307).clamp(0,1) # denormalize the output image
```

return generated_images



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.

```
1 %load_ext autoreload
2 %autoreload 2
```

Google Colab Setup

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!).

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

```
1 %cd "/content/drive/MyDrive/Hw3_diffusion/ConditionalDDPM/ConditionalDDPM"
    /content/drive/MyDrive/Hw3_diffusion/ConditionalDDPM/ConditionalDDPM
```

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

```
1 # set the device
2 import torch
3 device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
4
5 if torch.cuda.is_available():
6  print('Good to go!')
7 else:
8  print('Please set GPU via the downward triangle in the top right corner.')
Good to go!
```

Conditional Denoising Diffusion Probabilistic Models

In the lectures, we have learnt about Denoising Diffusion Probabilistic Models (DDPM), as presented in the paper <u>Denoising Diffusion</u>

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 <u>Classifier-free Diffusion Guidance</u>, which is a following work of DDPM. You are required to use MNIST dataset and the GPU device to complete the project.

(It will take about 20~30 minutes (10 epochs) if you are using the free-version Google Colab GPU. Typically, realistic digits can be generated after around 2~5 epochs.)

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 β_1, \ldots, β_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.

Training and sampling of DDPM

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

Algorithm 1 Training	Algorithm 2 Sampling
1: repeat 2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$ 3: $t \sim \mathrm{Uniform}(\{1, \dots, T\})$ 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: for $t = T, \dots, 1$ do 3: $\mathbf{z} \sim \mathcal{N}(0, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = 0$ 4: $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_{t}}} \left(\mathbf{x}_{t} - \frac{1 - \alpha_{t}}{\sqrt{1 - \overline{\alpha_{t}}}} \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, t) \right) + \sigma_{t} \mathbf{z}$ 5: end for 6: 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: $q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\,\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I})$, $\alpha_t := 1-\beta_t$ 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 minimize 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.

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 content of 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.

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 2: $(\mathbf{x}_0, \mathbf{c}_0) \sim q(\mathbf{x}_0, \mathbf{c}_0)$ ▶ Randomly discard conditioning to train unconditionally 3: $\mathbf{c}_0 \leftarrow \emptyset$ with probability p_{uncond} $t \sim \text{Uniform}(\{1, ..., T\})$ 4: $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ ▷ Corrupt data to the sampled time steps $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{(1 - \bar{\alpha}_t)} \boldsymbol{\epsilon}$ 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

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 c_0 is an extra input.
- Algorithm 2: Conditional sampling

Below is the sampling process of conditional DDPM.

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: \mathbf{for}\ t = T, \dots, 1 do

3: \mathbf{z} \sim \mathcal{N}(\mathbf{0},\mathbf{I}) if t > 1, 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-\tilde{\alpha}_t}}\tilde{\boldsymbol{\epsilon}}_t\right) + \sigma_t\mathbf{z}

6: end for

7: return \mathbf{x}_0
```

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 $\sigma_t = \sqrt{\beta_t}$.

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.

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

```
1 from dataclasses import dataclass, field
2 from typing import List, Tuple
3 @dataclass
4 class DMConfig:
5
6
      Define the model and experiment settings here
7
8
      input_dim: Tuple[int, int] = (28, 28) # input image size
9
      num channels: int = 1
                                          # input image channels
10
      condition_mask_value: int = -1
                                           # unconditional condition mask value
11
      num_classes: int = 10
                                           # number of classes in the dataset
      T: int = 400
                                           # diffusion and denoising steps
12
13
      beta_1: float = 1e-4
                                          # variance schedule
      beta_T: float = 2e-2
14
      mask_p: float = 0.1
                                           # unconditional condition drop ratio
15
16
      num_feat: int = 128
                                           # feature size of the UNet model
17
      omega: float = 2.0
                                           # conditional guidance weight
18
19
      batch_size: int = 256
                                           # training batch size
20
      epochs: int = 10
                                            # training epochs
21
      learning_rate: float = 1e-4
                                            # training learning rate
      multi_lr_milestones: List[int] = field(default_factory=lambda: [20]) # learning rate decay milestone
22
23
      multi_lr_gamma: float = 0.1
                                            # learning rate decay ratio
```

Then let's prepare and visualize the dataset:

```
1 from utils import make_dataloader
2 from torchvision import transforms
3 import torchvision.utils as vutils
4 import matplotlib.pyplot as plt
6 # Define the data preprocessing and configuration
7 transform = transforms.Compose([
         transforms.ToTensor(),
8
9
          transforms.Normalize((0.1307,), (0.3081,))
     ])
10
11 config = DMConfig()
13 # Create the train and test dataloaders
14 train_loader = make_dataloader(transform = transform, batch_size = config.batch_size, dir = './data', train = True)
15 test_loader = make_dataloader(transform = transform, batch_size = config.batch_size, dir = './data', train = False)
17 # Visualize the first 100 images
18 dataiter = iter(train_loader)
19 images, labels = next(dataiter)
```

```
20 images_subset = images[:100]
21 grid = vutils.make_grid(images_subset, nrow = 10, normalize = True, padding=2)
22 plt.figure(figsize=(6, 6))
23 plt.imshow(grid.numpy().transpose((1, 2, 0)))
24 plt.axis('off')
25 plt.show()
```

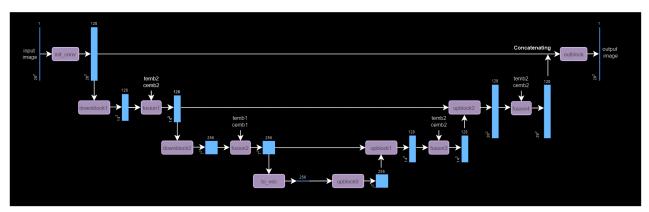


1. Denoising network (4 points)

The denoising network is defined in the file ResUNet.py. We have already provided some potentially useful 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
- You can design your own network and add any blocks. Feel free to modify or even remove the provided blocks or layers. You are also free to change the way of adding the time step and condition.
- 1 # Example structure of Conditional UNet
- 2 from IPython.core.display import SVG
- 3 SVG(filename='./pics/ConUNet.svg')



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

```
1 from ResUNet import ConditionalUnet
2 import torch
3 model = ConditionalUnet(in_channels = 1, n_feat = 128, n_classes = 10).to(device)
4 x = torch.randn((256,1,28,28)).to(device)
5 t = torch.randn((256,1,1,1)).to(device)
6 c = torch.randn((256,10)).to(device)
7 x_out = model(x,t,c)
8 assert x_out.shape == (256,1,28,28)
9 print('Output shape:', model(x,t,c).shape)
10 print('Dimension test passed!')

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

Before proceeding, please remember to normalize the time step t to the range 0-1 before inputting it into the denoising network for the next part of the project. It will help the network have a more stable output.

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 (3 points)

Let's first prepare the variance schedule β_t along with other potentially useful constants. You are required to complete the Conditional DDPM. 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 .

```
sqrt_beta_t: \sqrt{\beta_t}
alpha t: \alpha_t = 1 - \beta_t
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!
 1 from DDPM import ConditionalDDPM
 2 import torch
 3 torch.set_printoptions(precision=8)
 4 config = DMConfig(beta 1 = 1e-4, beta T = 2e-2)
 5 ConDDPM = ConditionalDDPM(dmconfig = config)
 6 \text{ schedule\_dict} = \text{ConDDPM.scheduler(t\_s} = \text{torch.tensor(77)}) \text{ } \text{ } \text{We use a specific time step (77) to check your output}
 7 assert torch.abs(schedule_dict['beta_t'] - 0.003890) <= 1e-5</pre>
 8 assert torch.abs(schedule_dict['sqrt_beta_t'] - 0.062374) <= 1e-5</pre>
 9 assert torch.abs(schedule_dict['alpha_t'] - 0.996110) <= 1e-5</pre>
10 assert torch.abs(schedule_dict['oneover_sqrt_alpha'] - 1.001951) <= 1e-5</pre>
11 assert torch.abs(schedule_dict['alpha_t_bar'] - 0.857414) <= 1e-5</pre>
12 assert torch.abs(schedule_dict['sqrt_oneminus_alpha_bar'] - 0.377606) <= 1e-5
13 print('All tests passed!')
      All tests passed!
```

2.2 Training process (5 points)

Recall the training algorithm we discussed above:

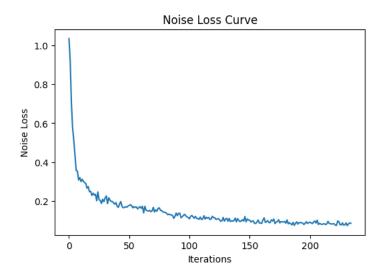
Algorithm 1 Joint training a diffusion model with classifier-free guidance

Require: p_{uncond} : probability of unconditional training

```
    ▷ Sample data with conditioning from the dataset

2:
          (\mathbf{x}_0, \mathbf{c}_0) \sim q(\mathbf{x}_0, \mathbf{c}_0)
3:
          \mathbf{c}_0 \leftarrow \emptyset with probability p_{uncond}
                                                                            > Randomly discard conditioning to train unconditionally
4:
          t \sim \text{Uniform}(\{1,...,T\})
                                                                                                                                           \epsilon \sim \mathcal{N}(\mathbf{0,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
6:
          Take gradient step on \nabla_{\theta} \| \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, \mathbf{c}_{0}, t) - \boldsymbol{\epsilon} \|^{2}
                                                                                                                   Description Optimization of denoising model
7:
8: until converged
```

```
1 from utils import check_forward
2 config = DMConfig()
3 model = check_forward(train_loader, config, device)
```



2.3 Sampling process (5 points)

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

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: \mathbf{for}\ t = T, \dots, 1\ \mathbf{do}

3: \mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})\ \text{if}\ t > 1, 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-\tilde{\alpha}_{t}}}\tilde{\boldsymbol{\epsilon}}_{t}\right) + \sigma_{t}\mathbf{z}

6: \mathbf{end}\ \mathbf{for}
```

7: return \mathbf{x}_0

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 about 1 minute.

```
1 from utils import check_sample
2 config = DMConfig()
3 fig = check_sample(model, config, device)
```



2.4 Full training (5 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 model's performance, we should proceed with a complete cycle of training and testing. You can utilize the provided solver function in this part.

Let's recall all model and experiment configurations:

```
1 train_config = DMConfig()
2 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_classes=10, T=400, beta_1=0.0001, beta_T=0.02, mask_p=0.1, num_classes=10, T=400, beta_1=0.0001, beta_T=0.02, mask_p=0.1, num_classes=10, T=400, beta_1=0.0001, beta_1=0.0001
```

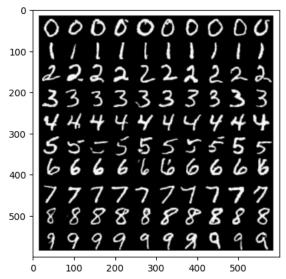
Then we can use function utils.solver to train the model. You should also input your own experiment name, e.g. your_exp_name. The best-trained model will be saved as ./save/your_exp_name/best_checkpoint.pth . Furthermore, for each training epoch, one generated image will be stored in the directory ./save/your_exp_name/images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

```
1 from utils import solver
2 solver(dmconfig = train_config,
        exp_name = '2.4_output',
3
        train_loader = train_loader,
5
        test_loader = test_loader)
   epoch 1/10
   train: train_noise_loss = 0.1377 test: test_noise_loss = 0.0784
   epoch 2/10
   train: train_noise_loss = 0.0751 test: test_noise_loss = 0.0668
   epoch 3/10
   train: train_noise_loss = 0.0661 test: test_noise_loss = 0.0627
   epoch 4/10
   train: train_noise_loss = 0.0615 test: test_noise_loss = 0.0593
   train: train_noise_loss = 0.0588 test: test_noise_loss = 0.0561
   epoch 6/10
    train: train_noise_loss = 0.0575 test: test_noise_loss = 0.0556
   epoch 7/10
   train: train_noise_loss = 0.0558 test: test_noise_loss = 0.0541
   epoch 8/10
   train: train_noise_loss = 0.0547 test: test_noise_loss = 0.0526
   epoch 9/10
    train: train_noise_loss = 0.0533 test: test_noise_loss = 0.0528
```

```
epoch 10/10
train: train noise loss = 0.0522 test: test noise loss = 0.0518
```

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

<matplotlib.image.AxesImage at 0x791f4f4139a0>



✓ 2.5 Exploring the conditional guidance weight (3 points)

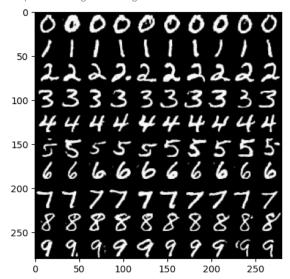
The generated images from the previous training-sampling process is using the default conditional guidance weight $\omega=2$. Now with the best checkpoint, please try at least 3 different ω values and visualize the generated images. You can use the provided function <code>sample_images</code> to get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

```
1 from utils import sample_images
 2 import matplotlib.pyplot as plt
 3 # ----- #
 4 # YOUR CODE HERE:
 5 # Try at least 3 different conditional guidance weights and visualize it.
     Example of using a different omega value:
 6 #
         sample_config = DMConfig(omega = ?)
 7 #
         fig = sample_images(config = sample_config, checkpoint_path = path_to_your_checkpoint)
 8 #
10 sample_config = DMConfig(omega = 0.1)
11 ckpt_dir = "/content/drive/MyDrive/Hw3_diffusion/\
12 ConditionalDDPM/ConditionalDDPM/save/2.4_output/best_checkpoint.pth"
13
14 fig = sample_images(config = sample_config, checkpoint_path = ckpt_dir)
15 plt.imshow(fig)
16
17 # ======== #
```

<matplotlib.image.AxesImage at 0x7ef57840be50>

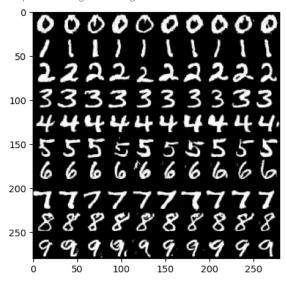
```
1 sample_config = DMConfig(omega = 5)
2 ckpt_dir = "/content/drive/MyDrive/Hw3_diffusion/\
3 ConditionalDDPM/ConditionalDDPM/save/2.4_output/best_checkpoint.pth"
4
5 fig = sample_images(config = sample_config, checkpoint_path = ckpt_dir)
6 plt.imshow(fig)
```

<matplotlib.image.AxesImage at 0x7ef0fa3677c0>



```
1 sample_config = DMConfig(omega = 10)
2 ckpt_dir = "/content/drive/MyDrive/Hw3_diffusion/\
3 ConditionalDDPM/ConditionalDDPM/save/2.4_output/best_checkpoint.pth"
4
5 fig = sample_images(config = sample_config, checkpoint_path = ckpt_dir)
6 plt.imshow(fig)
7
```

<matplotlib.image.AxesImage at 0x7ef0fa26f370>



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

Your answer: Higher conditional guidance weight leads to lower generation diversity and higher quality. The numbers has thicker brush strokes with higher guidance.

✓ 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=?, ...).

```
2 # YOUR CODE HERE:
3 #
     Your new configuration:
4 #
     train_config_new = DMConfig(...)
6 # class DMConfig:
7 #
8 #
        Define the model and experiment settings here
9 #
       input_dim: Tuple[int, int] = (28, 28) # input image size
10 #
11 #
       num_channels: int = 1
                                           # input image channels
12 #
       condition_mask_value: int = -1
                                           # unconditional condition mask value
13 #
       num classes: int = 10
                                            # number of classes in the dataset
14 #
        T: int = 400
                                            # diffusion and denoising steps
        beta_1: float = 1e-4
15 #
                                            # variance schedule
        beta_T: float = 2e-2
16 #
17 #
       mask_p: float = 0.1
                                            # unconditional condition drop ratio
        num_feat: int = 128
                                            # feature size of the UNet model
18 #
19 #
        omega: float = 2.0
                                            # conditional guidance weight
20
21 #
       batch_size: int = 256
                                            # training batch size
22 #
       epochs: int = 10
                                            # training epochs
23 #
        learning_rate: float = 1e-4
                                            # training learning rate
24 #
        multi_lr_milestones: List[int] = field(default_factory=lambda: [20]) # learning rate decay milestone
25 #
        multi lr gamma: float = 0.1
                                            # learning rate decay ratio
27 train_config_new = DMConfig(num_feat=256, T=800)
28 # ========= #
29 print(train_config_new)
```

3 4

5

```
8), num_channels=1, condition_mask_value=-1, num_classes=10, T=800, beta_1=0.0001, beta_T=0.02, mask_p=0.1, num_feat=256, omega=2.0, bat
```

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

```
1 from utils import solver
2 solver(dmconfig = train_config_new,
        exp_name = '2.6_feature',
        train_loader = train_loader,
        test_loader = test_loader)
   epoch 1/10
   train: train_noise_loss = 0.1068 test: test_noise_loss = 0.0558
   enoch 2/10
   train: train_noise_loss = 0.0531 test: test_noise_loss = 0.0464
   epoch 3/10
   train: train_noise_loss = 0.0462 test: test_noise_loss = 0.0445
   epoch 4/10
   train: train_noise_loss = 0.0433 test: test_noise_loss = 0.0412
   epoch 5/10
   train: train_noise_loss = 0.0411 test: test_noise_loss = 0.0414
   epoch 6/10
   train: train_noise_loss = 0.0398 test: test_noise_loss = 0.0398
   epoch 7/10
   train: train_noise_loss = 0.0384 test: test_noise_loss = 0.0383
   epoch 8/10
   train: train noise loss = 0.0380 test: test noise loss = 0.0377
   enoch 9/10
   train: train_noise_loss = 0.0373 test: test_noise_loss = 0.0360
   epoch 10/10
   train: train noise loss = 0.0368 test: test noise loss = 0.0369
```

Finally, show one image that you think has the best quality.

```
1 # ----- #
2 # YOUR CODE HERE:
3 # Among all images generated in the experiment,
    show the image that you believe has the best generation quality.
     You may use tools like matplotlib, PIL, OpenCV, ...
7 img_dir = "/content/drive/MyDrive/Hw3_diffusion/\
8 ConditionalDDPM/ConditionalDDPM/save/2.6_feature/images/generate_epoch_10.png"
10 best_result = mpimg.imread(img_dir)
11 plt.imshow(best_result)
12
13 # ========= #
```

<matplotlib.image.AxesImage at 0x791f4e7ccd00>

