DT8122 - Assignment

Deadline: 2023 August 15 AoE (Anywhere on Earth)

Send a zip file with the notebook both as a .ipynb and as a .pdf file to dt8122@idi.ntnu.no. Label the file with your full name.

The task is to implement conditional DDPM for MNIST images. Your implementation should take as input a digit and be able to generate 28x28 grayscale handwritten image of said digit.

You can add additional cells anywhere in the notebook to make your code more readable.

DDPM: https://arxiv.org/abs/2006.11239

Classifier-free conditional DDPM: https://arxiv.org/abs/2207.12598

The notebook should be run when it is turned in so all plots are visible. All code should be contained in the notebook.

Install necessary libraries

Any additional libraries you make use of should be installed in this cell.

Import libraries

All import statements should be contained here.

In [1]:
```
import random
import math

import matplotlib.pyplot as plt
import torch

from torch.utils.data import DataLoader
from torchvision.transforms import Compose, ToTensor, Lambda
from torchvision.datasets.mnist import MNIST

from typing import Optional, Tuple, TypeVar
import numpy as np
from tqdm import tqdm
```

Define constants here

Constants such as number of epochs, device, and learning rate and other hyperparameters should be defined here.

In [2]:
```
SEED = 0
random.seed(SEED)
torch.manual_seed(SEED)

batch_size = 128
##number of steps for defusion and denoising
N = 500
BMIN = 0.0001
BMAX = 0.02
guidence_w = 0.5
device = "cuda:0"
```

Functionality for loading and visualizing dataset

We have provided some functionality for loading and visualizing the dataset. You may add more cells/functions here.

In [3]:
```
## from 0-1 to -1-1
transform = Compose([
    ToTensor(),
    Lambda(lambda x: (x - 0.5) * 2)]
)
dataset = MNIST("./datasets", download=True, train=True, transform=transform)
loader = DataLoader(dataset, batch_size, shuffle=True)
```

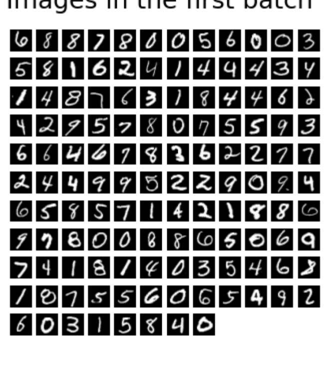
In [4]:
```
"""
This function plots images in a grid. Input is a Tensor.
See show_first_batch to see how it is used.
"""
def show_images(images, title=""):
    images = images.detach().cpu().numpy()
    fig = plt.figure(figsize=(4, 4))
    cols = math.ceil(len(images) ** (1 / 2))
    rows = math.ceil(len(images) / cols)
    for r in range(rows):
        for c in range(cols):
            idx = cols * r + c
            ax = fig.add_subplot(rows, cols, idx + 1)
            ax.axis('off')
            if idx < len(images):
                ax.imshow(images[idx][0], cmap="gray")
    fig.suptitle(title, fontsize=18)
    plt.show()

## we gnerate the 10*n_sample conditioned images, so we resize it to the same size in the plt
def show_images_custom(images, title=""):
    images = images.detach().cpu().numpy()
    fig = plt.figure(figsize=(4, 8))
    rows = 11
    cols = math.ceil(len(images) / rows)
    for r in range(rows):
        for c in range(cols):
            plot_idx = r * cols + c
            ax = fig.add_subplot(rows, cols, plot_idx + 1)
            ax.axis('off')
            img_idx = plot_idx
            if img_idx < len(images):
                ax.imshow(images[img_idx][0], cmap="gray")
    fig.suptitle(title, fontsize=18)
    plt.show()
```

In [5]:
```
def show_first_batch(loader):
    for batch_feats,batch_labels in loader:
        print(batch_labels)
        print(batch_feats.shape)
        show_images(batch_feats, "Images in the first batch")
        break
show_first_batch(loader)
```

```
tensor([6, 8, 8, 7, 8, 0, 0, 5, 6, 0, 0, 3, 5, 8, 1, 6, 2, 4, 1, 4, 9, 4, 3, 4,
        1, 4, 8, 7, 6, 3, 1, 8, 4, 4, 6, 2, 4, 2, 9, 5, 7, 8, 0, 7, 5, 5, 9, 3,
        6, 6, 4, 6, 7, 8, 3, 6, 2, 2, 7, 7, 2, 4, 4, 9, 9, 5, 2, 2, 9, 0, 9, 4,
        6, 5, 8, 5, 7, 1, 4, 2, 1, 8, 8, 6, 9, 7, 8, 0, 0, 8, 8, 6, 5, 0, 6, 9,
        7, 4, 1, 8, 1, 4, 0, 3, 5, 4, 6, 8, 1, 8, 7, 5, 5, 6, 0, 6, 5, 4, 9, 2,
        6, 0, 3, 1, 5, 8, 4, 0])
torch.Size([128, 1, 28, 28])
```

Images in the first batch



Your conditional DDPM implementation should go here

This includes functionality for adding noise to the image.

In [6]:
```
class Forward_pass:
    def __init__(self) -> None:
        #number of steps
        self.N = N
        self.beta_min = BMIN
        self.beta_max = BMAX
        self._betas, self._alphas, self._alpha_bars = (0, 0 ,0)
        self.get_coefs()

    ##linear steps
    def get_coefs(self):
        """Get the coefficients for the noise schedule.
        Returns:
            Tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]:
                betas, alphas, alpha_bars
        """
        self._betas = torch.linspace(self.beta_min, self.beta_max, self.N)
        self._alphas = 1 - self._betas
        self._alpha_bars = torch.cumprod(self._alphas, dim=0)

    #return the coef for initializing the denoising model
    def ret_coefs(self) -> Tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]:

        return (self._betas,self._alphas,self._alpha_bars)

    def _q_mean(
        self,
        z: torch.FloatTensor,
        t: torch.LongTensor,
    ) -> torch.FloatTensor:
        # mean of the distribution q(z_t | z_0)
        sqrt_alpha_bars = torch.sqrt(self._alpha_bars[t.tolist()])
        return sqrt_alpha_bars.view(-1,1,1,1) * z

    def _q_std(
        self,
        z: torch.FloatTensor,
        t: torch.LongTensor,
    ) -> torch.FloatTensor:
        # std of the distribution q(z_t | z_0)
        std = torch.sqrt(1.0 - self._alpha_bars[t.tolist()])
        return std.view(-1,1,1,1)

    def q_sample(
        self,
        z: torch.FloatTensor,
        t: torch.LongTensor,
    ) -> Tuple[torch.FloatTensor, torch.FloatTensor]:
        # Sample from q(z_t | z_0)

        mean = self._q_mean(z, t)
        std = self._q_std(z, t)
        epsilon = torch.randn_like(z)
        z_t = epsilon * std + mean

        return z_t, epsilon

    ##for training, sample random n timesteps for each input, return the repeated features, times-steps sampl
    def q_sample_random(
        self,
        z: torch.FloatTensor,
        lables: torch.FloatTensor,
        n_timesteps = 5,
    ) -> Tuple[torch.FloatTensor, torch.FloatTensor,   torch.IntTensor, torch.IntTensor]:
        # Sample from q(z_t | z_0)
        #we use the same times steps for all the samples in this batch for simplicity
        times = list(torch.randint(0, self.N-1, (n_timesteps,)))
        print(times)
        times_list = [torch.Tensor([i]).repeat(z.shape[0]).to(torch.int64) for i in times ]
        times_repeated = torch.cat(times_list)
        lables_repeated = lables.repeat(n_timesteps)
        z_repeated = z.repeat(n_timesteps,1,1,1) #shape=(batch_size*5, 1, 28, 28)
        mean = self._q_mean(z_repeated, times_repeated)  #shape=(batch_size, 1, 28, 28)
        std = self._q_std(z_repeated, times_repeated)
        epsilon = torch.randn_like(z_repeated)

        z_out = epsilon * std + mean

        return z_out, epsilon, times_repeated, lables_repeated


    ##for training, sample randomly one timestep for each img, return the repeated features, times-steps samp
    def q_sample_random2(
        self,
        z: torch.FloatTensor,
        lables: torch.FloatTensor,
    ) -> Tuple[torch.FloatTensor, torch.FloatTensor,  torch.IntTensor, torch.IntTensor]:
        # Sample from q(z_t | z_0)
        #we use the same times steps for all the samples in this batch for simplicity
        times = torch.randint(0, self.N-1, (z.shape[0],))
        mean = self._q_mean(z, times)  #shape=(batch_size, 1, 28, 28)
        std = self._q_std(z, times)
        epsilon = torch.randn_like(z)

        z_out = epsilon * std + mean

        return z_out, epsilon, times, lables
```

The implementation of the neural network used to estimate the noise should go here

The network should make use of both time and context embedding.

Any functions/methods used for time and context embeddings should also go here.

In [7]:
```
## I tried some simpler models but they don't seeem to work well, so finally I use the same Unet implementati
## The difference is we use simple embedding that has only one linear layer and adds to the input image featu
class ResidualConvBlock(torch.nn.Module):
    def __init__(
        self, in_channels: int, out_channels: int, is_res: bool = False
    ) -> None:
        super().__init__()
        '''
        standard ResNet style convolutional block
        '''
        self.same_channels = in_channels==out_channels
        self.is_res = is_res
        self.conv1 = torch.nn.Sequential(
            torch.nn.Conv2d(in_channels, out_channels, 3, 1, 1),
            torch.nn.BatchNorm2d(out_channels),
            torch.nn.GELU(),
        )
        self.conv2 = torch.nn.Sequential(
            torch.nn.Conv2d(out_channels, out_channels, 3, 1, 1),
            torch.nn.BatchNorm2d(out_channels),
            torch.nn.GELU(),
        )

    def forward(self, x: torch.Tensor) -> torch.Tensor:
        if self.is_res:
            x1 = self.conv1(x)
            x2 = self.conv2(x1)
            # this adds on correct residual in case channels have increased
            if self.same_channels:
                out = x + x2
            else:
                out = x1 + x2
            return out / 1.414
        else:
            x1 = self.conv1(x)
            x2 = self.conv2(x1)
            return x2

class UnetDown(torch.nn.Module):
    def __init__(self, in_channels, out_channels):
        super(UnetDown, self).__init__()
        '''
        process and downscale the image feature maps
        '''
        layers = [ResidualConvBlock(in_channels, out_channels), torch.nn.MaxPool2d(2)]
        self.model = torch.nn.Sequential(*layers)

    def forward(self, x):
        return self.model(x)


class UnetUp(torch.nn.Module):
    def __init__(self, in_channels, out_channels):
        super(UnetUp, self).__init__()
        '''
        process and upscale the image feature maps
        '''
        layers = [
            torch.nn.ConvTranspose2d(in_channels, out_channels, 2, 2),
            ResidualConvBlock(out_channels, out_channels),
            ResidualConvBlock(out_channels, out_channels),
        ]
        self.model = torch.nn.Sequential(*layers)

    def forward(self, x, skip):
        x = torch.cat((x, skip), 1)
        x = self.model(x)
        return x


class EmbedFC(torch.nn.Module):
    def __init__(self, input_dim, emb_dim):
        super(EmbedFC, self).__init__()
        '''
        generic one layer FC NN for embedding things
        '''
        self.input_dim = input_dim
        layers = [
            torch.nn.Linear(input_dim, emb_dim),
            torch.nn.GELU(),
            torch.nn.Linear(emb_dim, emb_dim),
        ]
        self.model = torch.nn.Sequential(*layers)

    def forward(self, x):
        x = x.view(-1, self.input_dim)
        return self.model(x)

class ConditionedBackbone(torch.nn.Module):
    def __init__(self, in_channels = 1, hidden_channels = 256, image_size = 28, n_classes=11, num_timesteps=N
        super(ConditionedBackbone, self).__init__()

        self.in_channels = in_channels
        self.n_feat = hidden_channels
        self.image_size = image_size
        self.num_timesteps = num_timesteps
        self.n_classes = n_classes  #the classes are 0-9 plus a "empty/unconditional" lable, they are encodec

        ## trainable embeddings for lable and time, not working if using a simple linear transformation, so t
        #self.time_emb = torch.nn.Linear(1, self.n_feat*2)
        #self.lable_emb = torch.nn.Linear(self.n_classes, self.n_feat*2)

        self.time_emb = EmbedFC(1, self.n_feat * 2)
        self.lable_emb = EmbedFC(self.n_classes, self.n_feat * 2)

        self.init_conv = ResidualConvBlock(in_channels, self.n_feat, is_res=True)
        self.down1 = UnetDown(self.n_feat, self.n_feat)
        self.down2 = UnetDown(self.n_feat, 2 * self.n_feat)

        self.to_vec = torch.nn.Sequential(torch.nn.AvgPool2d(7), torch.nn.GELU())

        self.up0 = torch.nn.Sequential(
            torch.nn.ConvTranspose2d(6 * self.n_feat, 2 * self.n_feat, 7, 7),
            torch.nn.GroupNorm(8, 2 * self.n_feat),
            torch.nn.ReLU(),
        )

        self.up1 = UnetUp(4 * self.n_feat, self.n_feat)
        self.up2 = UnetUp(2 * self.n_feat, self.n_feat)
        self.out = torch.nn.Sequential(
            torch.nn.Conv2d(2 * self.n_feat, self.n_feat, 3, 1, 1),
            torch.nn.GroupNorm(8, self.n_feat),
            torch.nn.ReLU(),
            torch.nn.Conv2d(self.n_feat, self.in_channels, 3, 1, 1),
        )


    def forward(self, x, lables, t) -> float:
        # x is (noisy) image batch (from the Forward_pass for training and from the N(0,1) for sampling),  (b
        # diff_noise are the corresponding noise in the forward pass,
        #labels are the numbers from 0-10, 10 represents the unconditioned sample, t is the timestep usually


        x = self.init_conv(x)
        down1 = self.down1(x)
        down2 = self.down2(down1)
        hiddenvec = self.to_vec(down2)

        #I tried several embedding methods, the concatenation seems to be the best
        #map to the vector size
        time_emb = self.time_emb(t.type(torch.float32).view(-1,1)).view(-1, self.n_feat * 2, 1 ,1)
        lable_one_hot = torch.nn.functional.one_hot(lables, num_classes=self.n_classes).type(torch.float)
        lable_emb  = self.lable_emb(lable_one_hot).view(-1, self.n_feat * 2, 1 ,1)

        #hiddenvec = hiddenvec + lable_emb

        up1 = self.up0(torch.cat((time_emb, lable_emb, hiddenvec), 1))
        up2 = self.up1(up1, down2)
        up3 = self.up2(up2, down1)
        e_pred = self.out(torch.cat((up3, x), 1))

        return e_pred

class Reverse_pass(torch.nn.Module):
    def __init__(self, model, alphas, alpha_bars, betas, num_classes = 11 ) -> None:
        super().__init__()
        self.model = model.to(device)
        self.N = N
        self.num_classes = num_classes
        ##for computing the samples
        self.alphas = alphas
        self.sqrt_1_minus_alpha_bars = torch.sqrt(1-alpha_bars)
        ##we use the simpler version of sigma for the reverse pass
        self.sigmas = torch.sqrt(betas)

        #loss
        self.mse = torch.nn.MSELoss()

    def sample(self, n_samples = 3, image_size = 28, guidence_w = guidence_w):
        ## sample "n" samples for each number “0-9” (including the unditional label "10") using 'Classifier-F
        with torch.no_grad():
            #sample noised images and arrange labels
            batch_size = n_samples*self.num_classes
            #x_batch = torch.randn(batch_size, 1, image_size, image_size).to(device)
            x_batch = torch.randn(batch_size, 1, image_size, image_size).to(device)
            ##labels = [0,0,0,1,1,1,2,2,2....]
            labels = [ torch.tensor([i], device=device).repeat(n_samples) for i in range(self.num_classes)]
            #labels = torch.cat(labels).to(device)
            labels = torch.cat(labels)
            # unconditioned labels for interpolation (label = 10)
            labels_uncon = torch.full_like(labels, self.num_classes-1)
            labels = torch.cat((labels, labels_uncon))
            last_batch = x_batch
            for i in range(self.N, 0, -1):
                print(f'sampling timestep {i}\n')
                #current_t = torch.tensor([i]).to(device)
                current_t = torch.tensor([i-1],device=device)  #i-1 for one-hot encoding
                t_batch = current_t.repeat(batch_size) #(batch_size)

                # duplicate the current img for unconditioned sampling
                x_doubled = last_batch.repeat(2,1,1,1) #(2*batch_size, channel, img_size, img_size)
                t_doubled = t_batch.repeat(2) #(2*batch_size)

                # predict the diffusion noise, and interpolate
                diff_noise = self.model(x_doubled, labels, t_doubled)
                diff_con = diff_noise[:batch_size]
                diff_uncon = diff_noise[batch_size:]
                diff_noise_final = (1+guidence_w)*diff_con - guidence_w*diff_uncon
                # predict x_t-1
                #observation_noise = torch.randn(batch_size, 1, image_size, image_size).to(device) if i > 1 e
                observation_noise = torch.randn(batch_size, 1, image_size, image_size).to(device) if i > 1 el
                x_predict = (1/torch.sqrt(self.alphas[i-1])) * (last_batch - diff_noise_final * (1 - self.alp

                last_batch = x_predict
            return last_batch

    def compute_loss(self, batch_input, batch_noise, batch_time, batch_lables):
        #a batch of diffused input (by the forward process), with its difuusion noise,  timesteps and labels
        # return the loss of this batch for training the model

        predicted_noise = self.model(batch_input.to(device), batch_lables.to(device), batch_time.to(device))
        return self.mse(batch_noise.to(device), predicted_noise)
```

Show that you can generate images before the model is trained

This should demonstrate that the backwards pass works. The generated images are expected to be noise.

In [8]:
```
model = ConditionedBackbone(hidden_channels = 128)
forward = Forward_pass()
betas,alphas,alpha_bars = forward.ret_coefs()
reverse = Reverse_pass(model, alphas, alpha_bars, betas)
return_batch = reverse.sample(n_samples=5)
show_images_custom(return_batch, "Images generated from the untrained model")
```

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Images generated from the untrained model

Implement training loop

Train the model here. There should be some indication of how long the model took to train, both total and per epoch. For good results you will want to train the model for several epochs, but with a good implementation you should expect to see something that looks like digits after only a single epoch.

In [9]:

```python
def train_conditionedDDPM(n_epochs = 10, learning_rate = 1e-4):
    print(f"{sum(p.numel() for p in reverse.parameters() if p.requires_grad)} parameters to train")
    optimizer = torch.optim.Adam(reverse.parameters(), lr=learning_rate)
    for i in range(n_epochs):
        print(f"Training epoch: {i+1}")
        progress_loader = tqdm(loader)
        total_loss = 0
        for batch_feats,batch_labels in progress_loader:
            optimizer.zero_grad()
            #sample with forward pass
            #z_out, epsilon_target, times, labels= forward.q_sample_random(batch_feats, batch_labels)
            z_out, epsilon_target, times, labels= forward.q_sample_random2(batch_feats, batch_labels)
            loss = reverse.compute_loss(z_out, epsilon_target, times, labels)
            total_loss += loss
            loss.backward()
            optimizer.step()

        print(f'Loss for the current epoch is {total_loss}')
```

Train and visualize the model

We want to see several generated examples of each digit.

In [10]:

```python
model = ConditionedBackbone(hidden_channels = 128)
forward = Forward_pass()
betas,alphas,alpha_bars = forward.ret_coefs()
reverse = Reverse_pass(model, alphas, alpha_bars, betas)
train_conditionedDDPM(n_epochs = 10)
```

```
12973697 parameters to train
Training epoch: 1
100%|██████████| 469/469 [00:27<00:00, 17.12it/s]
Loss for the current epoch is 43.41958236694336
Training epoch: 2
100%|██████████| 469/469 [00:27<00:00, 16.85it/s]
Loss for the current epoch is 24.419374465942383
Training epoch: 3
100%|██████████| 469/469 [00:28<00:00, 16.44it/s]
Loss for the current epoch is 21.434226989746094
Training epoch: 4
100%|██████████| 469/469 [00:30<00:00, 15.54it/s]
Loss for the current epoch is 19.79697608947754
Training epoch: 5
100%|██████████| 469/469 [00:31<00:00, 15.00it/s]
Loss for the current epoch is 18.852949142456055
Training epoch: 6
100%|██████████| 469/469 [00:30<00:00, 15.20it/s]
Loss for the current epoch is 18.14109992980957
Training epoch: 7
100%|██████████| 469/469 [00:28<00:00, 16.37it/s]
Loss for the current epoch is 17.489013671875
Training epoch: 8
100%|██████████| 469/469 [00:28<00:00, 16.67it/s]
Loss for the current epoch is 17.0726318359375
Training epoch: 9
100%|██████████| 469/469 [00:28<00:00, 16.75it/s]
Loss for the current epoch is 16.6922550201416
Training epoch: 10
100%|██████████| 469/469 [00:27<00:00, 16.78it/s]
Loss for the current epoch is 16.3807373046875
```

In [12]:

```python
return_batch1 = reverse.sample( n_samples = 5, guidence_w = 0.5)
show_images_custom(return_batch1, "Imgs from 0-9, the last row is the unconditioned sampling")
```

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Imgs from 0-9, the last row is the unconditioned sampling