Deep Learning — Assignment 11

Assignment for week 11 of the 2023 Deep Learning course (NWI-IMC070) of the Radboud University.

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Instructions:

- Fill in your names and the name of your group.
- Answer the questions and complete the code where necessary.
- Keep your answers brief, one or two sentences is usually enough.
- Re-run the whole notebook before you submit your work.
- Save the notebook as a PDF and submit that in Brightspace together with the `.ipynb` notebook file.
- The easiest way to make a PDF of your notebook is via File > Print Preview and then use your browser's print option to print to PDF.

Objectives

In this assignment you will

1. Build a diffusion model
2. Extend the model to a class-conditional version

Required software

As before you will need these libraries:

- `torch` and `torchvision` for PyTorch,
- `d2l`, the library that comes with Dive into deep learning book.

All libraries can be installed with `pip install`.

In [2]:
```
%config InlineBackend.figure_formats = ['png']
%matplotlib inline

from d2l import torch as d2l
import itertools
import numpy as np
import matplotlib.pyplot as plt
import torch
from torch import nn
from torch.nn import functional as F
from torchvision import datasets, transforms

device = d2l.try_gpu()
```

11.1 MNIST dataset

In this assignment we will once again use the MNIST digit dataset. This dataset consists of 28×28 binary images and has 60000 training examples divided over 10 classes. We split this into 55000 images for training and 5000 images for validation.

As preprocessing, we pad the images to 32x32 pixels and scale the intensities to [-1, +1].

(a) Run the code below to load the MNIST dataset.

In [3]:
```
transform = transforms.Compose([
    transforms.ToTensor(),
    transforms.Pad(2),                # pad to 32x32 pixels
    transforms.Normalize(0.5, 0.5),  # normalize to [-1, +1]
])
train_val_data = datasets.MNIST('data', train=True, download=True, transform=transform)
# Split into train and validation set
train_data, validation_data = torch.utils.data.random_split(train_val_data, [55000, 5000])
# Create data loaders
train_iter      = torch.utils.data.DataLoader(train_data, batch_size=128, shuffle=True)
validation_iter = torch.utils.data.DataLoader(validation_data, batch_size=1000)
num_classes = 10
```

11.2 Training images (4 points)

We will implement a model from the paper Denoising Diffusion Probabilistic Models by Ho et al., 2020.

We reuse some parameter settings from the paper:

In [4]:
```
diffusion_steps = 1000
beta = torch.linspace(1e-4, 0.02, diffusion_steps)
alpha = 1.0 - beta
alpha_bar = torch.cumprod(alpha, dim=0)
```

Using these settings, we can generate a sequence of noisy images with

$$\mathbf{x}_t = \sqrt{\alpha_t}\mathbf{x}_{t-1} + \sqrt{1-\alpha_t}\boldsymbol{\epsilon}_{t-1} \qquad \text{where } \boldsymbol{\epsilon}_{t-1}, \boldsymbol{\epsilon}_{t-2}, \dots \sim \mathcal{N}(\mathbf{0}, \mathbf{I}).$$

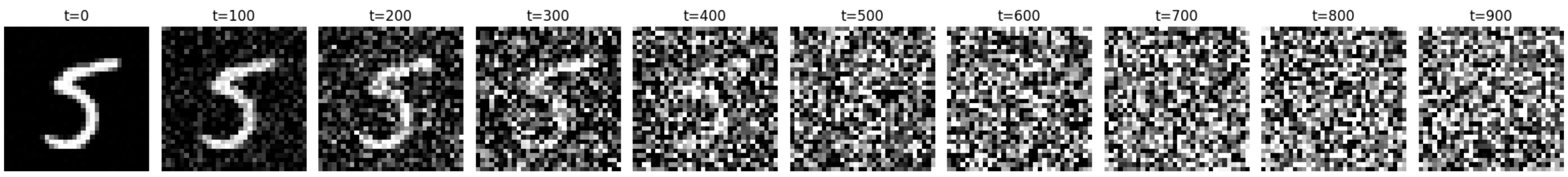
There is a closed-form solution to compute x_t directly from x_0 (see the paper or this blog):

$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon} \qquad \text{where } \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}).$$

(a) Implement this closed-form solution in the code below to generate random images. **(1 point)**

Expected output: you should see some images with recognizable shapes and some images with noise.

In [5]:
```
# sample some original images
x_0, y = next(iter(train_iter))

plt.figure(figsize=(19, 21))
for i, t in enumerate(range(0, diffusion_steps, 100)):
    # TODO generate random noise
    noise = torch.randn_like(x_0)

    # TODO add noise to the original image to compute x_t
    x_t = torch.sqrt(alpha_bar[t]) * x_0 + torch.sqrt(1-alpha_bar[t]) * noise
    x_t = torch.clamp(x_t, -1, 1)

    plt.subplot(3, diffusion_steps // 100, i + 1)
    plt.imshow(x_t[0, 0], cmap='gray')
    plt.axis('off')
    plt.title(f't={t}')
plt.tight_layout()
```



(b) Describe how we should interpret these images, and how they can be used to train the diffusion model. **(2 points)**

The following images represent a Markov process where transition distribution is given by $q(x_t|x_{t-1})$, given properties of Markov chains we can compute the closed-form solution, we do not know the $q(x_{t-1}|x_t)$ since that would require the whole dataset. We can use the realization of this process to learn a distribution $p_\theta(x_{t-1}|x_t)$ which approximates the backward transition $q(x_{t-1}|x_t)$ and gives us the ability to generate x_0 given a noisy image x_T.

During training, we will need a minibatch with multiple images and multiple time steps.

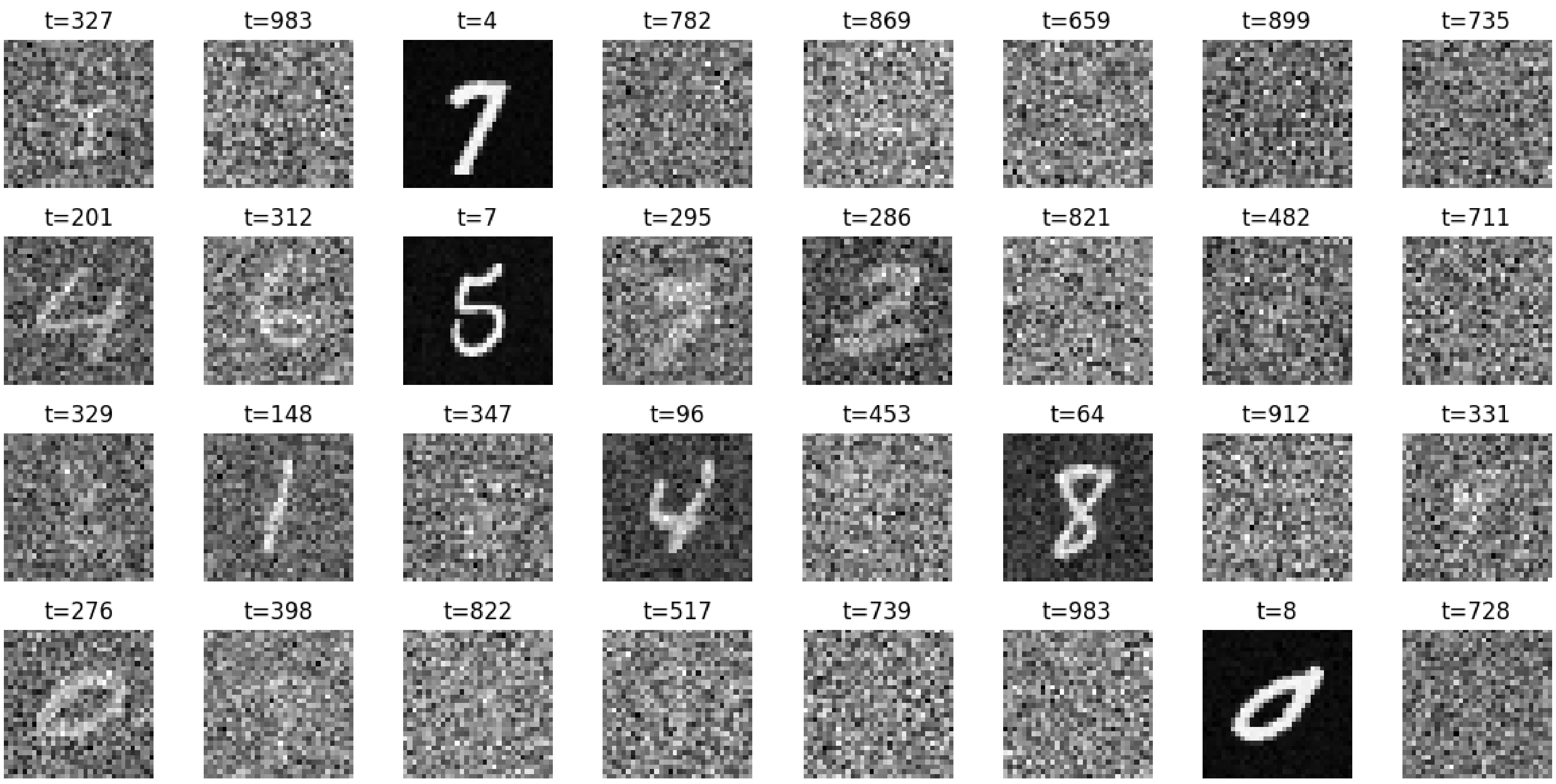
(c) Complete the function below to add noise to a minibatch of images. **(1 point)**

In [6]:
```
def generate_noisy_samples(x_0, beta, device=device):
    '''
    Create noisy samples for the minibatch x_0.
    Return the noisy image, the noise, and the time for each sample.
    '''
    device = x_0.device
    beta = beta.to(device)
    alpha = 1.0 - beta
    alpha_bar = torch.cumprod(alpha, dim=0)

    # sample a random time t for each sample in the minibatch
    t = torch.randint(beta.shape[0], size=(x_0.shape[0],), device=alpha_bar.device)
    # TODO generate noise
    noise = torch.randn_like(x_0).to(device)
    # TODO add the noise to each sample
    alpha_bar = alpha_bar[t].view(x_0.shape[0], 1, 1, 1).to(device)
    x_t = torch.sqrt(alpha_bar) * x_0 + torch.sqrt(1-alpha_bar) * noise
    return x_t, noise, t
```

(d) Try out your new function by generating a few noisy samples.

Expected output: you should see the samples in the minibatch with different levels of noise, depending on the time t for each sample.

In [7]:
```
x_0, y = next(iter(train_iter))
x_0 = x_0.to(device)
x_t, noise, sampled_t = generate_noisy_samples(x_0, beta)
assert x_t.shape == x_0.shape
assert noise.shape == x_0.shape
assert sampled_t.shape == (x_0.shape[0],)

plt.figure(figsize=(12, 6))
for i in range(32):
    plt.subplot(4, 8, i + 1)
    plt.imshow(x_t[i, 0].detach().cpu().numpy(), cmap='gray')
    plt.axis('off')
    plt.title(f't={sampled_t[i]}')
plt.tight_layout()
```



11.3 Helper functions

We will use some predefined components to construct our model, based on an existing implementation on GitHub.

In [8]:
```
class SelfAttention(nn.Module):
    def __init__(self, h_size):
        super(SelfAttention, self).__init__()
        self.h_size = h_size
        self.mha = nn.MultiheadAttention(h_size, 4, batch_first=True)
        self.ln = nn.LayerNorm([h_size])
        self.ff_self = nn.Sequential(
            nn.LayerNorm([h_size]),
            nn.Linear(h_size, h_size),
            nn.GELU(),
            nn.Linear(h_size, h_size),
        )

    def forward(self, x):
        x_ln = self.ln(x)
        attention_value, _ = self.mha(x_ln, x_ln, x_ln)
        attention_value = attention_value + x
        attention_value = self.ff_self(attention_value) + attention_value
        return attention_value

class SAWrapper(nn.Module):
    def __init__(self, h_size, num_s):
        super(SAWrapper, self).__init__()
        self.sa = nn.Sequential(*[SelfAttention(h_size) for _ in range(1)])
        self.num_s = num_s
        self.h_size = h_size

    def forward(self, x):
        x = x.view(-1, self.h_size, self.num_s * self.num_s).swapaxes(1, 2)
        x = self.sa(x)
        x = x.swapaxes(2, 1).view(-1, self.h_size, self.num_s, self.num_s)
        return x
```

```
# U-Net code adapted from: https://github.com/milesial/Pytorch-UNet

class DoubleConv(nn.Module):
    def __init__(self, in_channels, out_channels, mid_channels=None, residual=False):
        super().__init__()
        self.residual = residual
        if not mid_channels:
            mid_channels = out_channels
        self.double_conv = nn.Sequential(
            nn.Conv2d(in_channels, mid_channels, kernel_size=3, padding=1, bias=False),
            nn.GroupNorm(1, mid_channels),
            nn.GELU(),
            nn.Conv2d(mid_channels, out_channels, kernel_size=3, padding=1, bias=False),
            nn.GroupNorm(1, out_channels),
        )

    def forward(self, x):
        if self.residual:
            return F.gelu(x + self.double_conv(x))
        else:
            return self.double_conv(x)

class Down(nn.Module):
    def __init__(self, in_channels, out_channels):
        super().__init__()
        self.maxpool_conv = nn.Sequential(
            nn.MaxPool2d(2),
            DoubleConv(in_channels, in_channels, residual=True),
            DoubleConv(in_channels, out_channels),
        )

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

class Up(nn.Module):
    def __init__(self, in_channels, out_channels, bilinear=True):
        super().__init__()

        # if bilinear, use the normal convolutions to reduce the number of channels
        if bilinear:
            self.up = nn.Upsample(scale_factor=2, mode="bilinear", align_corners=True)
            self.conv = DoubleConv(in_channels, in_channels, residual=True)
            self.conv2 = DoubleConv(in_channels, out_channels, in_channels // 2)
        else:
            self.up = nn.ConvTranspose2d(
                in_channels, in_channels // 2, kernel_size=2, stride=2
            )
            self.conv = DoubleConv(in_channels, out_channels)

    def forward(self, x1, x2):
        x1 = self.up(x1)
        # input is CHW
        diffY = x2.size()[2] - x1.size()[2]
        diffX = x2.size()[3] - x1.size()[3]

        x1 = F.pad(x1, [diffX // 2, diffX - diffX // 2, diffY // 2, diffY - diffY // 2])
        x = torch.cat([x2, x1], dim=1)
        x = self.conv(x)
        x = self.conv2(x)
        return x

class OutConv(nn.Module):
    def __init__(self, in_channels, out_channels):
        super(OutConv, self).__init__()
        self.conv = nn.Conv2d(in_channels, out_channels, kernel_size=1)

    def forward(self, x):
        return self.conv(x)
```

11.4 Diffusion model (5 points)

Similar to Ho et al. and to several online implementations, we will use a U-Net with self-attention and positional embedding as our diffusion model.

(a) Familiarize yourself with the architecture of this U-Net.

In [9]:
```
class UNet(nn.Module):
    def __init__(self, c_in=1, c_out=1, device="cuda"):
        super().__init__()
        self.device = device

        bilinear = True
        self.inc = DoubleConv(c_in, 64)
        self.down1 = Down(64, 128)
        self.down2 = Down(128, 256)
```

```
        factor = 2 if bilinear else 1
        self.down3 = Down(256, 512 // factor)
        self.up1 = Up(512, 256 // factor, bilinear)
        self.up2 = Up(256, 128 // factor, bilinear)
        self.up3 = Up(128, 64, bilinear)
        self.outc = OutConv(64, c_out)
        self.sa1 = SAWrapper(256, 8)
        self.sa2 = SAWrapper(256, 4)
        self.sa3 = SAWrapper(128, 8)

    def pos_encoding(self, t, channels, embed_size):
        inv_freq = 1.0 / (
            10000
            ** (torch.arange(0, channels, 2, device=self.device).float() / channels)
        )
        pos_enc_a = torch.sin(t[:, None].repeat(1, channels // 2) * inv_freq)
        pos_enc_b = torch.cos(t[:, None].repeat(1, channels // 2) * inv_freq)
        pos_enc = torch.cat([pos_enc_a, pos_enc_b], dim=-1)
        return pos_enc.view(-1, channels, 1, 1).repeat(1, 1, embed_size, embed_size)

    def forward(self, x, t):
        """
        Model is U-Net with added positional encodings and self-attention layers.
        """
        x1 = self.inc(x)
        x2 = self.down1(x1) + self.pos_encoding(t, 128, 16)
        x3 = self.down2(x2) + self.pos_encoding(t, 256, 8)
        x3 = self.sa1(x3)
        x4 = self.down3(x3) + self.pos_encoding(t, 256, 4)
        x4 = self.sa2(x4)
        x = self.up1(x4, x3) + self.pos_encoding(t, 128, 8)
        x = self.sa3(x)
        x = self.up2(x, x2) + self.pos_encoding(t, 64, 16)
        x = self.up3(x, x1) + self.pos_encoding(t, 64, 32)
        output = self.outc(x)
        return output
```

(b) What does the positional encoding encode? Why would this be useful? **(2 points)**

It encode the position in the Markov Chain. It is useful to know because the model needs to predict the amount of noise which has a different variance for every state of the chain.

(c) Describe how this model will be used. What do the inputs and outputs represent? **(3 points)**

Used for: To predict the noise added at step t. We will learn to model this noise as best as we can giving use the ability to predict images.

Inputs: The noisy input image at any stage of the forward diffusion process and time step

Outputs: Prediction of a noise added at time step t

11.5 Training the model (7 points)

We will train our diffusion model using Algorithm 1 from the paper Denoising Diffusion Probabilistic Models by Ho et al., 2020.

(a) The algorithm uses $\mathbf{x}_0$. How do you obtain $\mathbf{x}_0$ during training? **(1 point)**

x_0 is sampled from $q(x_0)$. In other words a random image from the dataset, or a batch of images.

(b) Which two values are compared in the loss on line 5 of the algorithm? **(1 point)**

We are comparing the noise added in the forward process and the noise predicted by the model at time t since our model only needs to predict the noise at each timestep.

(c) Implement this procedure in the training loop below. **(3 points)**

In [10]:
```
def train(model, beta, num_epochs=10, lr=1e-3):
    """Train a diffusion model"""
    optimizer = torch.optim.Adam(model.parameters(), lr=lr)
    animator = d2l.Animator(xlabel='epoch', xlim=[1, num_epochs], figsize=(10, 5),
                            legend=['train loss', 'validation loss'])
    beta = beta.to(device)
    alpha = 1.0 - beta
    alpha_bar = torch.cumprod(alpha, dim=0).to(device)
    loss_fn = torch.nn.functional.mse_loss
    for epoch in range(num_epochs):
        metric = d2l.Accumulator(2)
        model.train()
        for x, y in train_iter:
            x = x.to(device)
            optimizer.zero_grad()
```

```
            # TODO compute the loss for minibatch x
            # hint: we already have a function to generate noisy images
            x_t, noise, t = generate_noisy_samples(x, beta)
            pred_noise = model(x_t, t)

            loss = loss_fn(pred_noise, noise)

            # Optimize
            loss.backward()
            optimizer.step()

            # Track our progress
            metric.add(loss.detach() * x.shape[0], x.shape[0])
        train_loss = metric[0] / metric[1]

        # Compute validation loss
        validation_loss = test(model, validation_iter, beta)

        # Plot
        animator.add(epoch + 1, (train_loss, validation_loss))
    print(f'training loss {train_loss:.3g}, validation loss {validation_loss:.3g}')

def test(model, test_iter, beta):
    """Test a diffusion model by computing the loss."""
    metric = d2l.Accumulator(2)
    model.eval()
    for x, y in test_iter:
        x = x.to(device)
        with torch.no_grad():
            # TODO compute the loss for minibatch x
            x_t, noise, t = generate_noisy_samples(x, beta, alpha_bar)
            pred_noise = model(x_t, t)
            loss = torch.nn.functional.mse_loss(noise, pred_noise)
            metric.add(loss.detach() * x.shape[0], x.shape[0])
    return metric[0] / metric[1]
```

(d) How does the training time depend on the number of diffusion steps T? **(1 point)**

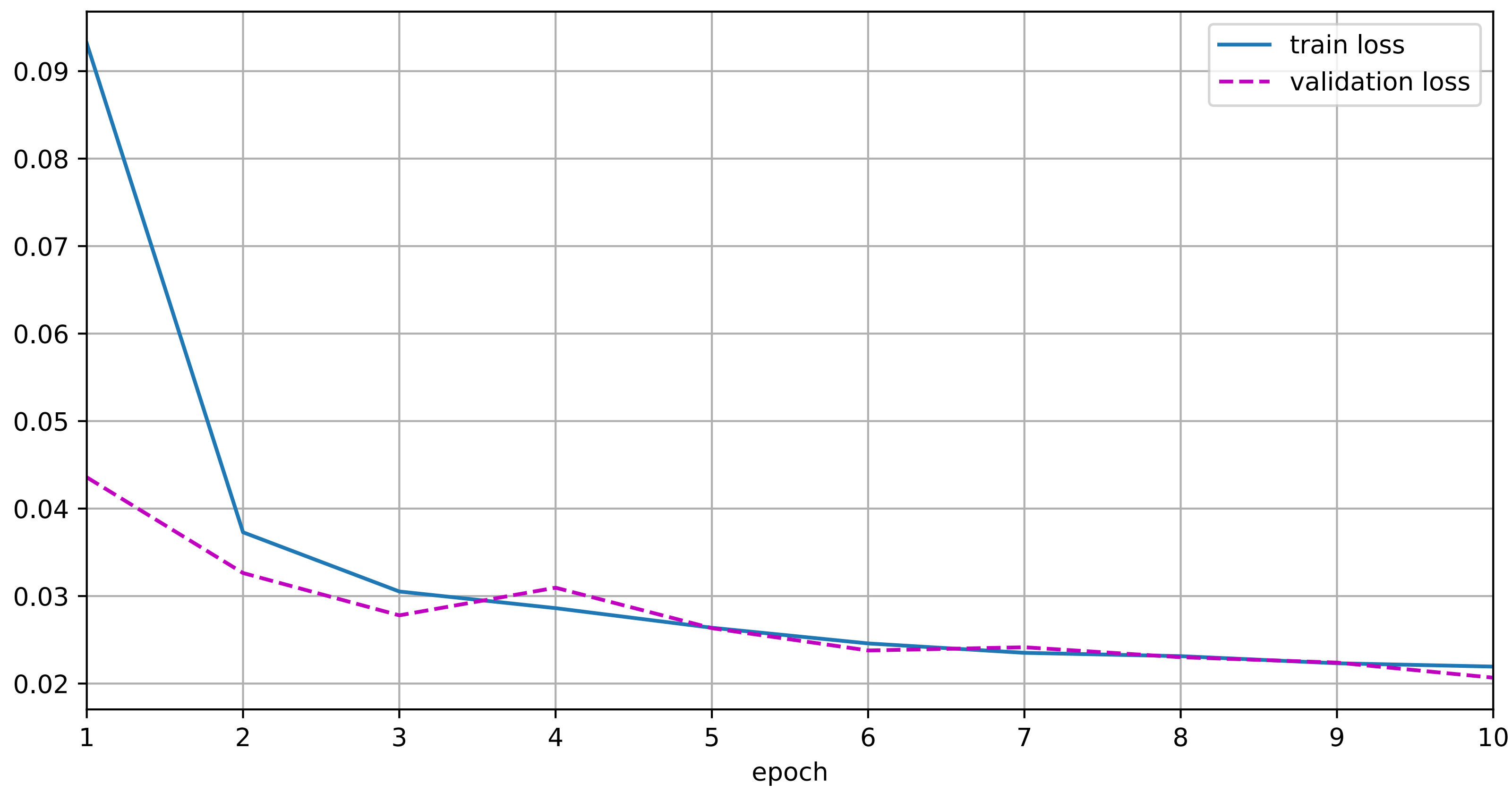
To calculate the x_t at any time requires us to compute $\bar{\alpha}_t$ which requires linear time though that can be done in negligible time. The UNet itself does not depend on size of t so the only increase in time is the time it took us to calculate $\bar{\alpha}_t$.

(e) Train the model.

Expected output: in our implementation, the training loss started at around 0.1 and went down quickly to 0.03 and lower.

In [18]:
```
device = d2l.try_gpu()

model = UNet().to(device)
train(model, beta, num_epochs=10, lr=1e-4)
#model = torch.load("model.pth", map_location=device)
```

```
training loss 0.0219, validation loss 0.0207
```



In [20]:
```
torch.save(model, "model.pth")
```

(f) Has the training converged? Do you think we should train longer? **(1 point)**

The losses are still decreasing by the look of the plot, so it has not fully converged. We could increase the number of epochs to say for certainty that it has converged when we see the flat line of losses.

11.6 Sampling from the model (9 points)

Once the model is trained, we can sample from it using Algorithm 2 from paper Denoising Diffusion Probabilistic Models:

Algorithm 2:
1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: for $t = T, \ldots, 1$ do
3: $\quad \mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
4: $\quad \mathbf{x}_{t-1} = \frac{1}{\sqrt{a_t}}\left(\mathbf{x}_t - \frac{1-a_t}{\sqrt{1-\bar{a}_t}}\epsilon_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$
5: end for
6: return $\mathbf{x}_0$

(a) In step 3 of algorithm 2, $\mathbf{z}$ is set to 0 some times. What is the effect of this? **(1 point)**

In the stochastic gradient Langevin dynamics Gaussian noise is injected into the parameter updates to avoid to avoid collapse into a local minima.

(b) In step 4 of algorithm 2, $\mathbf{x}_{t-1}$ is computed based on three ingredients: $\mathbf{x}_t$, $\epsilon_\theta(\mathbf{x}_t, t)$, and $\mathbf{z}$. What do these represent? **(2 points)**

- $\mathbf{x}_t$: Image with removed noise after t steps.
- $\epsilon_\theta(\mathbf{x}_t, t)$: The predicted noise at time step t.
- $\mathbf{z}$: Random noise added to the dynamics to avoid collapse into the local minima.

(c) How does the sampling time depend on the number of diffusion steps T? **(1 point)**

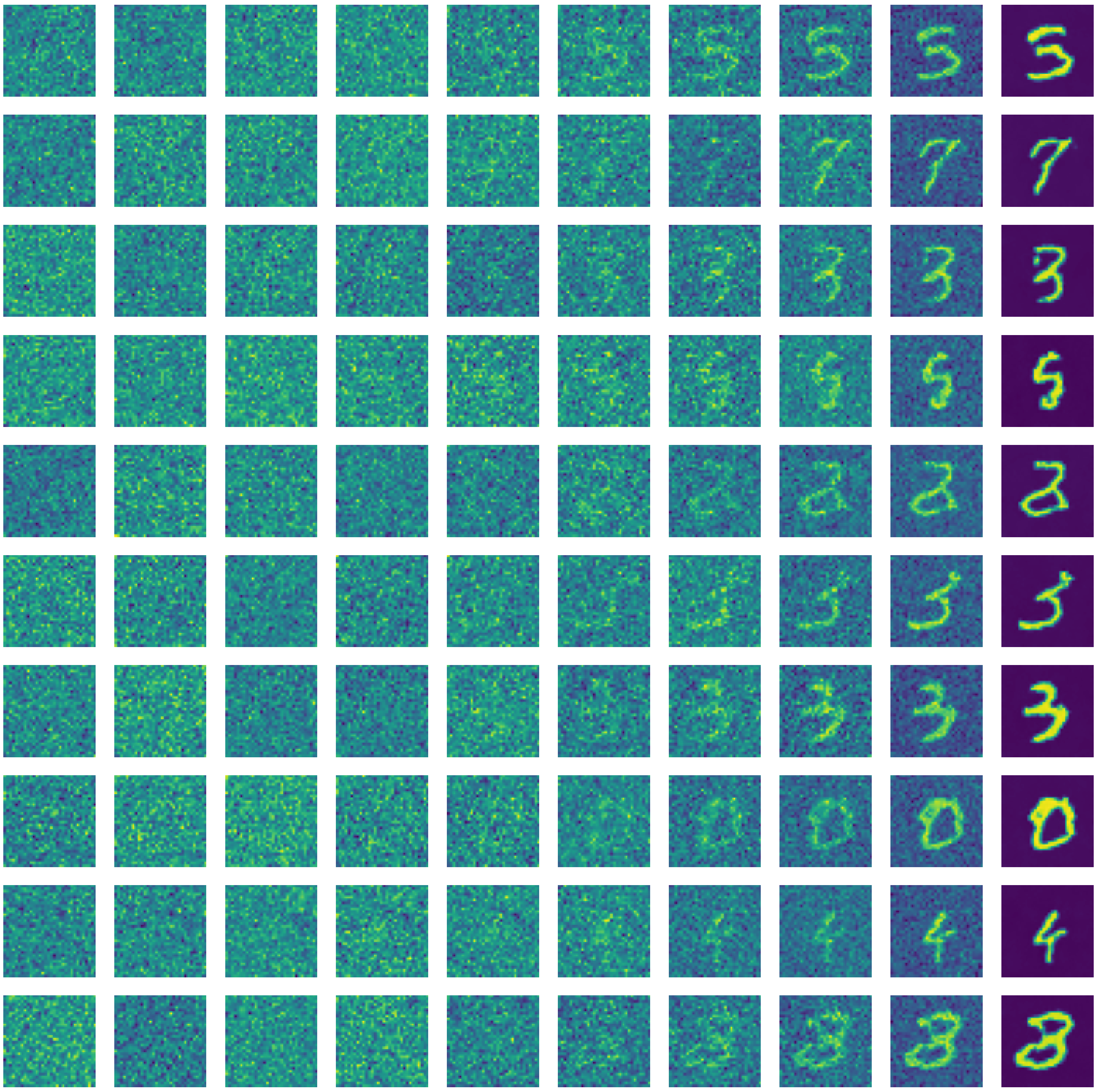
It depends linearly, increase in T increases the sampling time and vice-versa.

(d) Complete the code below to sample a minibatch from the model. **(2 points)**

- Use the equations in Algorithm 2.
- Use $\sigma_t = \sqrt{\beta_t}$, as suggested in the paper.
- Keep in mind that Algorithm 2 uses $t = 1$ as the first time step, whereas we use $t = 0$.

Expected output: after training, your model should generate fairly realistic, clean images when given random inputs.

In [22]:
```
def sample_from_model(x, model, beta):
    # keep track of x at different time steps
    x_hist = []
    beta=beta.to(device)
    alpha = 1 - beta
    alpha_bar = torch.cumprod(alpha, dim=0)
    with torch.no_grad():
        # loop over all time steps in reverse order
        for i in reversed(range(0, beta.shape[0])):
            # copy the time step for each sample in the minibatch
            z = torch.randn_like(x) if i!=0 else 0
            t = (torch.ones(x.shape[0]) * i).long().to(device)
            alpha_t = alpha[t].view(-1, 1, 1, 1).to(device)
            alpha_bar_t = alpha_bar[t].view(-1, 1, 1, 1).to(device)
            beta_t = beta[t].view(-1,1,1,1).to(device)
            # TODO compute the next value of x
            epsilon = model(x, t)
            x = 1.0/torch.sqrt(alpha_t) * (x - (1-alpha_t)/torch.sqrt(1-alpha_bar_t) * epsilon) + torch.sqrt(beta_t)*z
            if i % 100 == 0:
                x_hist.append(x.detach().cpu().numpy())
    return x, x_hist

def plot_x_hist(x_hist):
    # plot the generated images
    plt.figure(figsize=(10, 10))
    for i in range(len(x_hist)):
        for j in range(10):
            plt.subplot(10, 10, j * 10 + i + 1)
            plt.imshow(x_hist[i][j, 0])
            plt.axis('off')

# TODO initialize x with the right values
# shape: [10, 1, 32, 32]
x = torch.randn_like(x_0[:10]).to(device)

x, x_hist = sample_from_model(x, model, beta)
plot_x_hist(x_hist)
```



(e) Explain the X and Y axes of this figure. **(1 point)**

Y axis is each of the 10 random generated images. X axis is the time step from T-1 to 0.

(f) In a variational autoencoder or a GAN, the output is determined by the latent representation. How does that work for this diffusion model? **(1 point)**

In a diffusion model, the output is generated by iteratively transforming an initial noise distribution to resemble the target data distribution. This is done through a reversible diffusion process over multiple steps, with no explicit latent representation like in GANs. The diffusion model's focus is on the process of transforming noise to generate realistic samples rather than sampling from a latent space. Due to the noise added in reverse process we avoid deterministic sampling and thus same intialization gives a different image which is not the case for GANs and VAE

(g) Look at the generated intermediate samples over time in question (d). Do we need all of the steps? Why/why not? **(1 point)**

No, we can clearly see the outline on the digits before the last step and sometimes those outlines are clearer than in the last step. We can use some image filters to extract the digit before the sampling removes all the noise giving us a clearer image. On the other hand we cannot see the visible digits in early denoising steps which could imply to use more noise at the end of forward diffusion to reduce the time to sample an image.

11.7 Experiments (5 points)

Fixed initialization

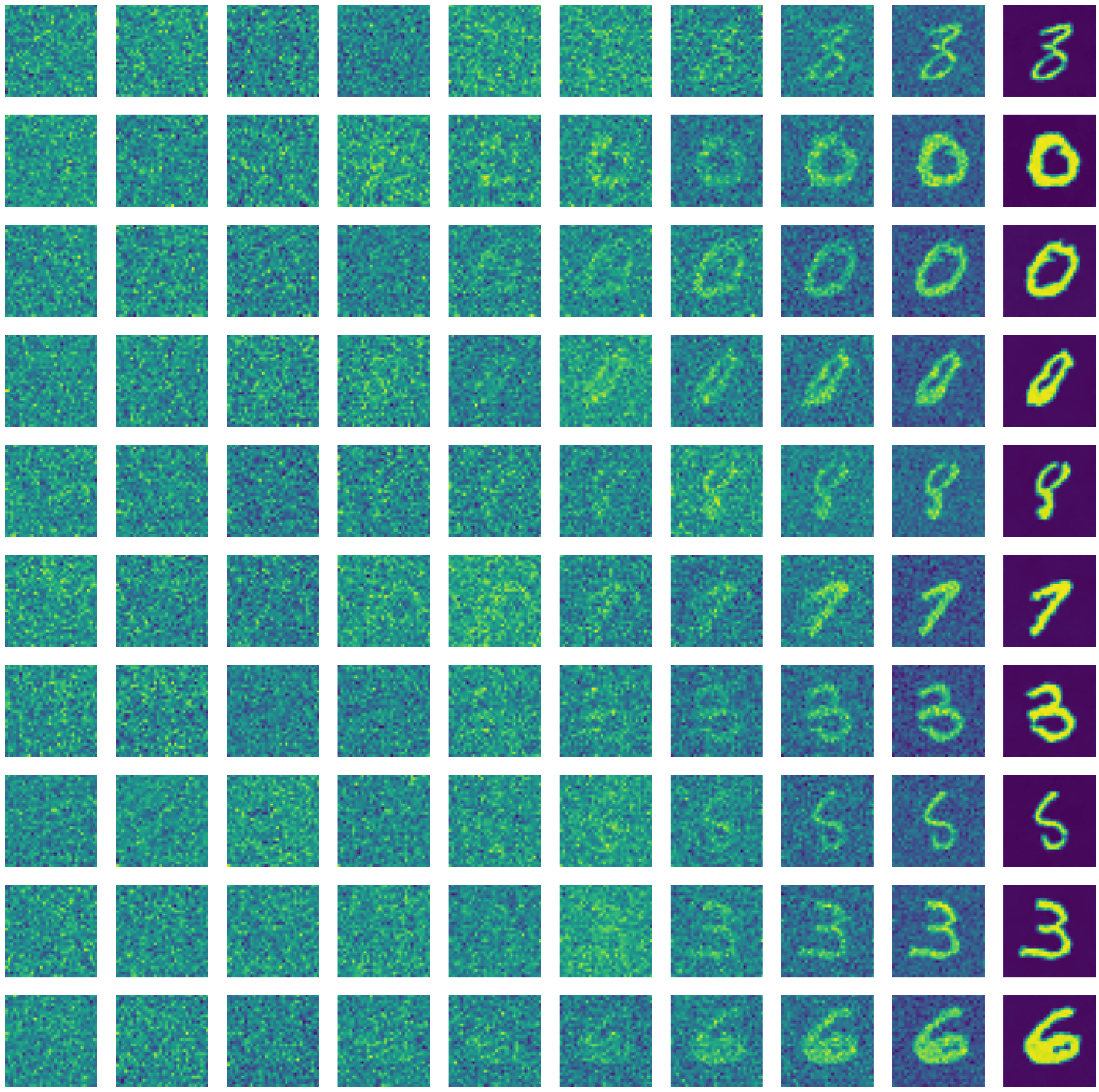
How does the end result depend on the initialization? We will generate multiple images from the same initial noise to find out.

(a) Complete and run the code below.

Expected output: the model should still produce recognizable shapes.

In [23]:
```
# TODO initialize x=x_T with the right values for one image
# (see earlier question)
# shape: [1, 1, 32, 32]
# x = generate_noisy_samples(torch.zeros_like(x_0[:1]).to(device), beta)[0] # TODO: change
```

```
x = torch.randn_like(x_0[:1]).to(device)
# repeat this to generate 10 images from the same initialization
x = x.repeat(10, 1, 1, 1)

x, x_hist = sample_from_model(x, model, beta)
plot_x_hist(x_hist)
```



(b) Does the model always produce the same output from the same initial input? Why, or why not? **(2 points)**

No, as we can see from the generated images, the model does not always produce the same output from the same initial input. This is because of the noise added (z), that is different every time, and the randomness in the sampling process.

No randomness between time steps

To check the influence of noise during sampling, we can remove the term $\sigma_t \mathbf{z}$ from Algorithm 2.

(c) Create a new function `deterministic_sample_from_model`, based on `sample_from_model`, that does not include this term. **(2 points)**

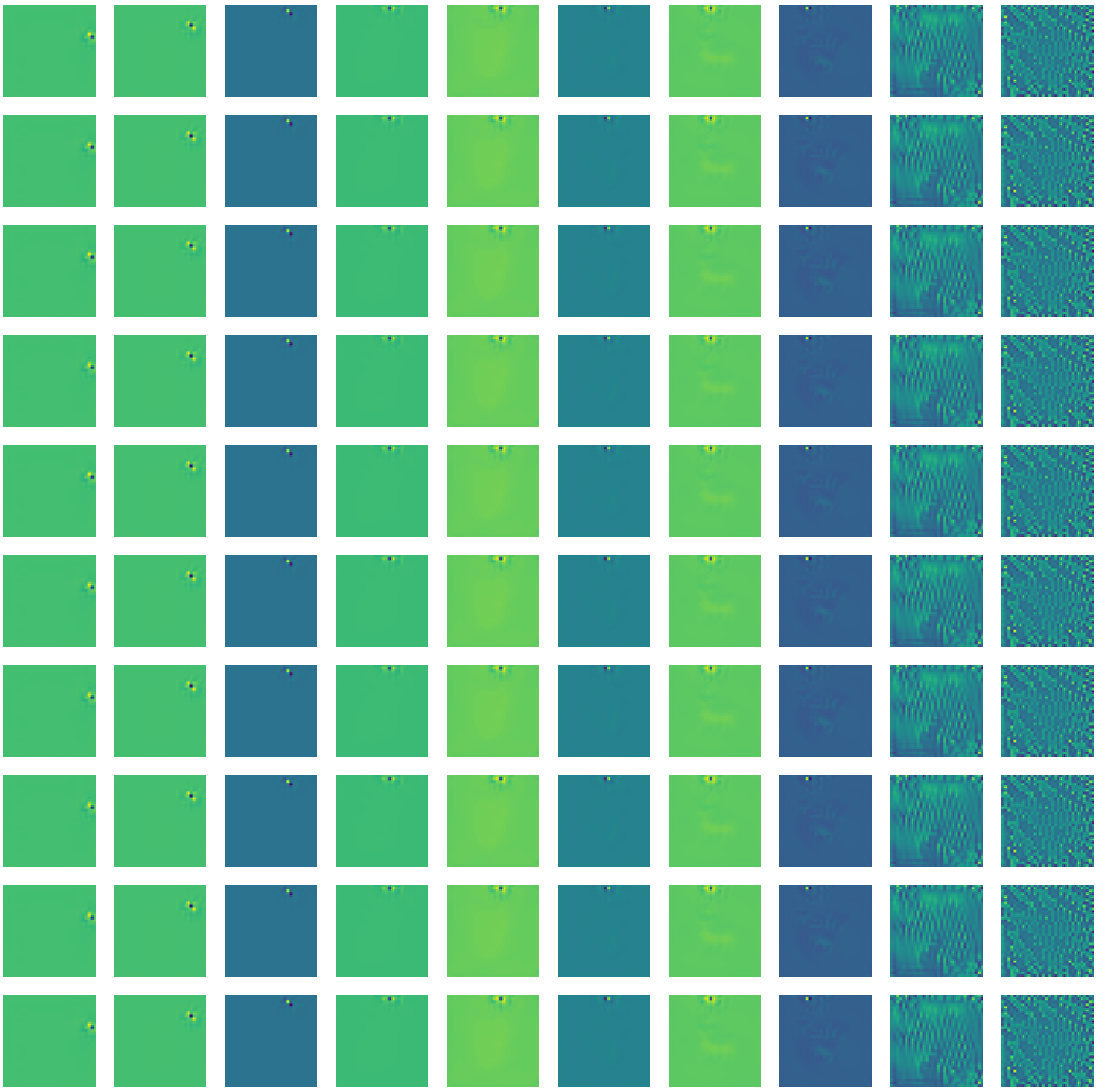
In [24]:
```
def deterministic_sample_from_model(x, model, beta):
    # TODO copy sample_from_model and remove the random term sigma * z
    x_hist = []
    beta=beta.to(device)
    alpha = 1 - beta
    alpha_bar = torch.cumprod(alpha, dim=0)
    with torch.no_grad():
        # loop over all time steps in reverse order
        for i in reversed(range(0, beta.shape[0])):
            # copy the time step for each sample in the minibatch
            z = torch.randn_like(x) if i!=0 else 0
            t = (torch.ones(x.shape[0]) * i).long().to(device)
            alpha_t = alpha[t].view(-1, 1, 1, 1).to(device)
            alpha_bar_t = alpha_bar[t].view(-1, 1, 1, 1).to(device)
            beta_t = beta[t].view(-1,1,1,1).to(device)
            # TODO compute the next value of x
            epsilon = model(x, t)
            x = 1.0/torch.sqrt(alpha_t) * (x - (1-alpha_t)/torch.sqrt(1-alpha_bar_t) * epsilon)
            if i % 100 == 0:
```

```
            x_hist.append(x.detach().cpu().numpy())
    return x, x_hist
```

(d) Generate some samples using the new function.

Expected output: you should get a different result than before.

In [27]:
```
# TODO initialize x with the right values
# (see earlier questions)
# shape: [10, 1, 32, 32]
x = torch.randn_like(x_0[:1]).to(device)
x= x.repeat(10, 1, 1, 1)

x, x_hist = deterministic_sample_from_model(x, model, beta)
plot_x_hist(x_hist)
```



(e) What can you conclude from these results? Is the random noise during sampling important? (1 point)

By removing the noise from the sampling process we can see that it's generating random noise (z). So the random noise, during the sampling, is important because the output will depend only on the input (and on the parameters), and also it helps the model to avoid local minima.

11.8 Making the model conditional (6 points)

Similar to the conditional VAE in the previous assignment, we can make the diffusion model conditional by including class labels. This allows us to generate samples from a specific digit.

We will include the class information alongside the existing positional encoding, using a `torch.nn.Embedding` layer to map the 10 digits to a higher-dimensional space.

Conditional model

(a) Study the implemenation of UNetConditional to see how this works.

In [28]:
```
class UNetConditional(nn.Module):
    def __init__(self, c_in=1, c_out=1, n_classes=10, device=device):
        super().__init__()
```

```
        self.device = device

        bilinear = True
        self.inc = DoubleConv(c_in, 64)
        self.down1 = Down(64, 128)
        self.down2 = Down(128, 256)
        factor = 2 if bilinear else 1
        self.down3 = Down(256, 512 // factor)
        self.up1 = Up(512, 256 // factor, bilinear)
        self.up2 = Up(256, 128 // factor, bilinear)
        self.up3 = Up(128, 64, bilinear)
        self.outc = OutConv(64, c_out)
        self.sa1 = SAWrapper(256, 8)
        self.sa2 = SAWrapper(256, 4)
        self.sa3 = SAWrapper(128, 8)

        self.label_embedding = nn.Embedding(n_classes, 256)

    def pos_encoding(self, t, channels, embed_size):
        inv_freq = 1.0 / (
            10000
            ** (torch.arange(0, channels, 2, device=self.device).float() / channels)
        )
        pos_enc_a = torch.sin(t[:, None].repeat(1, channels // 2) * inv_freq)
        pos_enc_b = torch.cos(t[:, None].repeat(1, channels // 2) * inv_freq)
        pos_enc = torch.cat([pos_enc_a, pos_enc_b], dim=-1)
        return pos_enc.view(-1, channels, 1, 1).repeat(1, 1, embed_size, embed_size)

    def label_encoding(self, label, channels, embed_size):
        return self.label_embedding(label)[:, :channels, None, None].repeat(1, 1, embed_size, embed_size)

    def forward(self, x, t, label):
        """
        Model is U-Net with added positional encodings and self-attention layers.
        """
        x1 = self.inc(x)
        x2 = self.down1(x1) + self.pos_encoding(t, 128, 16) + self.label_encoding(label, 128, 16)
        x3 = self.down2(x2) + self.pos_encoding(t, 256, 8) + self.label_encoding(label, 256, 8)
        x3 = self.sa1(x3)
        x4 = self.down3(x3) + self.pos_encoding(t, 256, 4) + self.label_encoding(label, 256, 4)
        x4 = self.sa2(x4)
        x = self.up1(x4, x3) + self.pos_encoding(t, 128, 8) + self.label_encoding(label, 128, 8)
        x = self.sa3(x)
        x = self.up2(x, x2) + self.pos_encoding(t, 64, 16) + self.label_encoding(label, 64, 16)
        x = self.up3(x, x1) + self.pos_encoding(t, 64, 32) + self.label_encoding(label, 64, 32)
        output = self.outc(x)
        return output
```

(b) As in the paper by Ho et al., the position and label encoding are added in every layer of the model, instead of as an input to the first layer only. Why do you think the authors made this choice? (1 point)

The positional and label encoding is added in every layer to encode the position of the image in the diffusion process, to guide each layer during the forward.

Conditional training loop

(c) Create a new function `train_conditional` to train this model. (1 point)

In [29]:
```
def train_conditional(model, beta, num_epochs=10, lr=1e-3):
    # TODO implement the training loop, based on your earlier train function
    optimizer = torch.optim.Adam(model.parameters(), lr=lr)
    animator = d2l.Animator(xlabel='epoch', xlim=[1, num_epochs], figsize=(10, 5),
                            legend=['train loss', 'validation loss'])
    beta = beta.to(device)
    alpha = 1.0 - beta
    alpha_bar = torch.cumprod(alpha, dim=0).to(device)
    loss_fn = torch.nn.functional.mse_loss
    for epoch in range(num_epochs):
        metric = d2l.Accumulator(2)
        model.train()
        for x, y in train_iter:
            x = x.to(device)
            y = y.to(device)
            optimizer.zero_grad()

            # TODO compute the loss for minibatch x
            # hint: we already have a function to generate noisy images
            x_t, noise, t = generate_noisy_samples(x, beta)
            pred_noise = model(x_t, t, y)

            loss = loss_fn(pred_noise, noise)

            # Optimize
            loss.backward()
```

```
            optimizer.step()

            # Track our progress
            metric.add(loss.detach() * x.shape[0], x.shape[0])
        train_loss = metric[0] / metric[1]

        # Compute validation loss
        validation_loss = test_conditional(model, validation_iter, beta)

        # Plot
        animator.add(epoch + 1, (train_loss, validation_loss))
    print(f'training loss {train_loss:.3g}, validation loss {validation_loss:.3g}')

def test_conditional(model, test_iter, beta):
    # TODO implement the testing loop, based on your earlier test function
    metric = d2l.Accumulator(2)
    model.eval()
    for x, y in test_iter:
        x = x.to(device)
        with torch.no_grad():
            # TODO compute the loss for minibatch x
            x_t, noise, t = generate_noisy_samples(x, beta, alpha_bar)
            y = y.to(device)
            pred_noise = model(x_t, t, y)
            loss = torch.nn.functional.mse_loss(noise, pred_noise)
            metric.add(loss.detach() * x.shape[0], x.shape[0])
    return metric[0] / metric[1]
```

(d) Train the conditional model.

Expected output: in our implementation, the training loss started at around 0.1 and went down quickly to 0.03 and lower.

In [31]:
```
#model_conditional = UNetConditional().to(device)
#train_conditional(model_conditional, beta, num_epochs=10, lr=1e-4)
model_conditional = torch.load("model_conditional.pth", map_location=device)
```

Conditional sampling

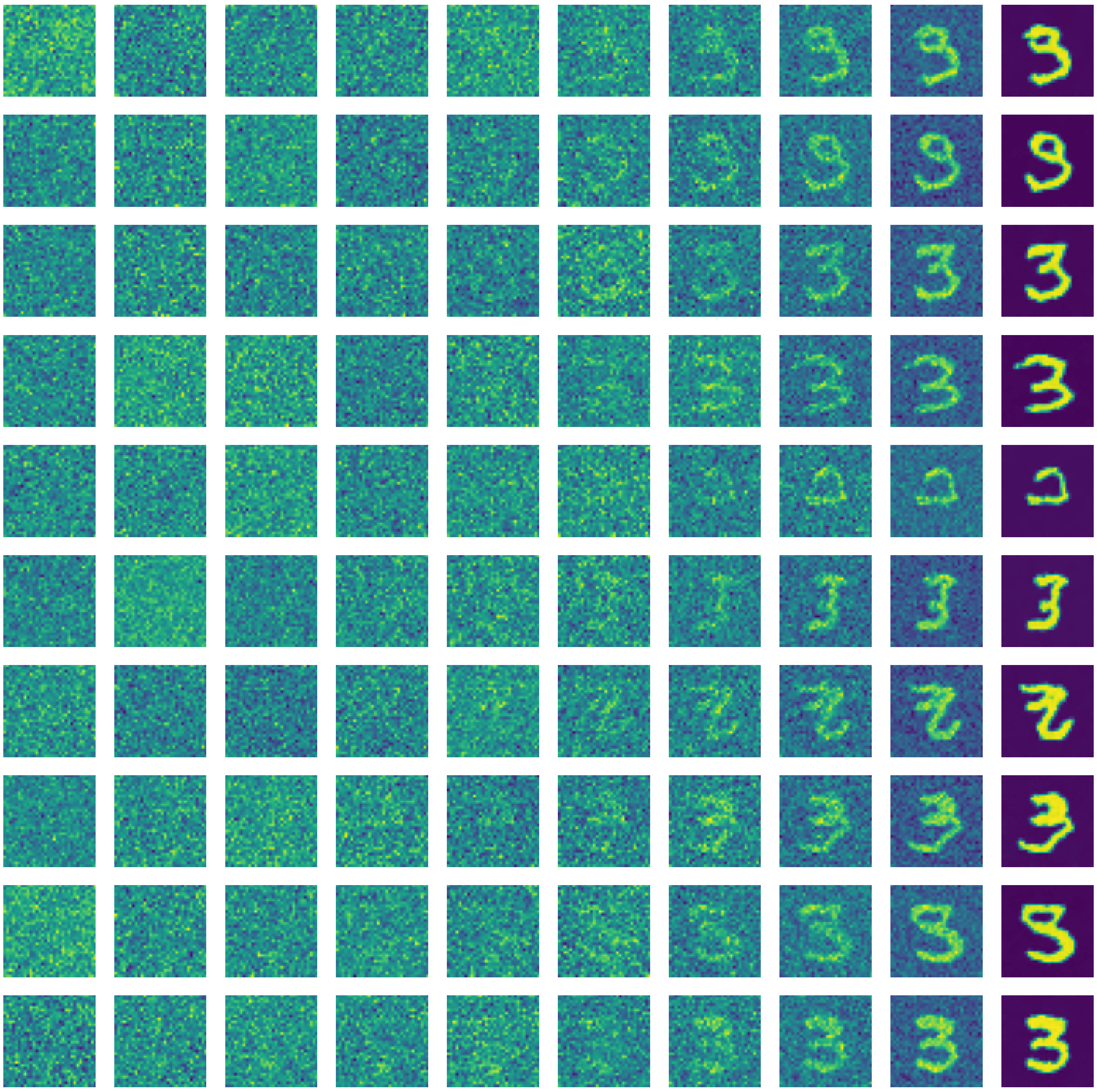
(e) Modify the sampling function to include a label. **(1 point)**

In [32]:
```
def sample_from_model_conditional(x, model, beta, label):
    # keep track of x at different time steps
    x_hist = []
    beta=beta.to(device)
    alpha = 1 - beta
    alpha_bar = torch.cumprod(alpha, dim=0)
    label = torch.tensor([int(label)]).to(device)
    with torch.no_grad():
        # loop over all time steps in reverse order
        for i in reversed(range(0, beta.shape[0])):
            # copy the time step for each sample in the minibatch
            z = torch.randn_like(x) if i!=0 else 0
            t = (torch.ones(x.shape[0]) * i).long().to(device)
            alpha_t = alpha[t].view(-1, 1, 1, 1).to(device)
            alpha_bar_t = alpha_bar[t].view(-1, 1, 1, 1).to(device)
            beta_t = beta[t].view(-1,1,1,1).to(device)
            # TODO compute the next value of x
            epsilon = model(x, t, label)
            x = 1.0/torch.sqrt(alpha_t) * (x - (1-alpha_t)/torch.sqrt(1-alpha_bar_t) * epsilon) + torch.sqrt(beta_t)*z
            if i % 100 == 0:
                x_hist.append(x.detach().cpu().numpy())
    return x, x_hist
```

(f) Sample a few digits with label `3`. **(1 point)**

Expected output: you should see recognizable images with the number you requested.

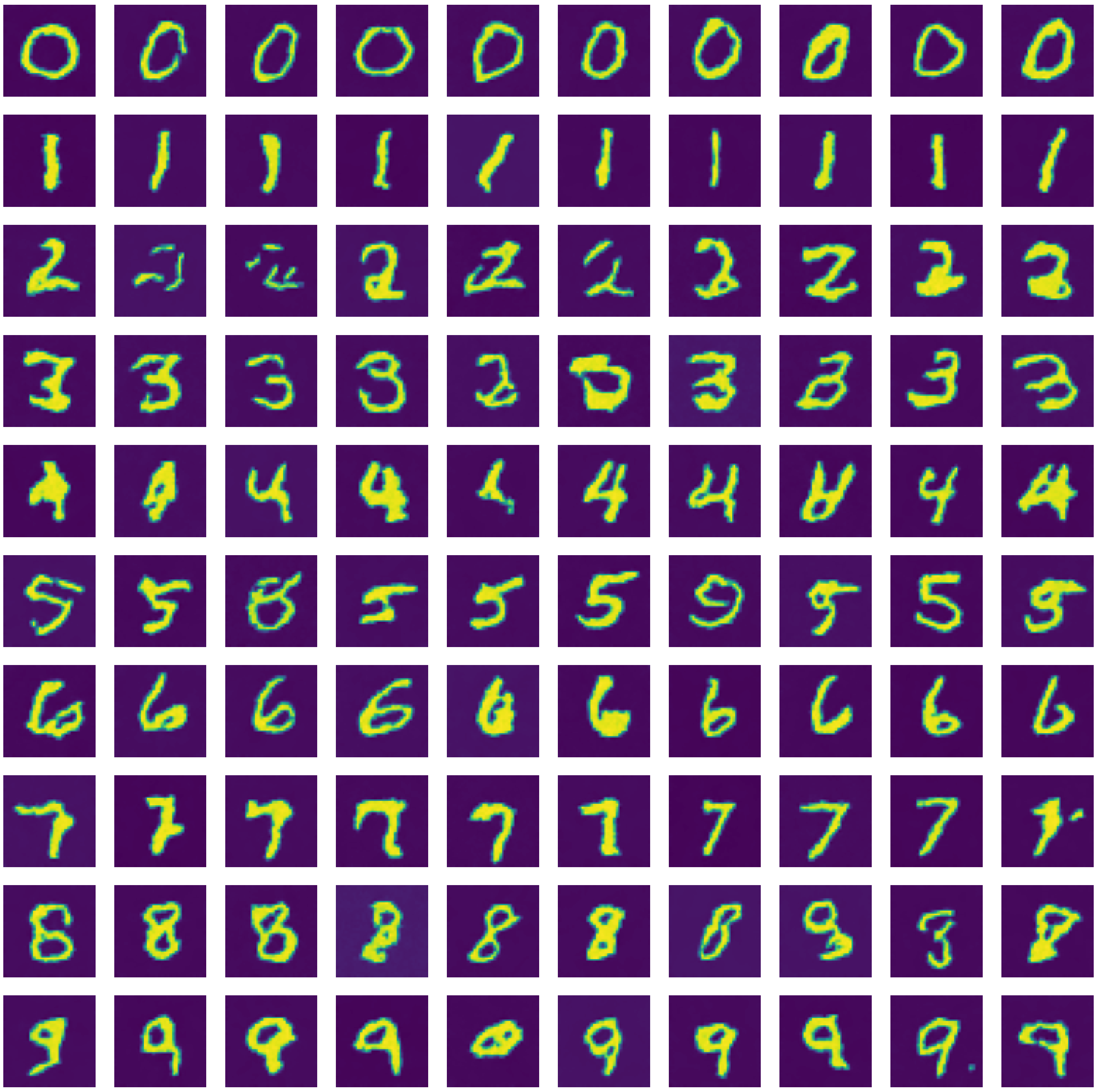
In [33]:
```
# TODO sample some digits
x = torch.randn_like(x_0[:10]).to(device)

x, x_hist = sample_from_model_conditional(x, model_conditional, beta, "3")
plot_x_hist(x_hist)
```



(g) Complete the code to sample and plot 10 samples for every digit. **(1 point)**

In [35]:
```
x_per_class = []
for label in range(10):
    # sample 10 digits with this label
    x = torch.randn_like(x_0[:10]).to(device)
    x, x_hist = sample_from_model_conditional(x, model_conditional, beta, label)
    x_per_class.append(x.detach().cpu().numpy())
```

In [36]:
```
plt.figure(figsize=(10, 10))
for i in range(10):
    for j in range(10):
        plt.subplot(10, 10, j * 10 + i + 1)
        plt.imshow(x_per_class[j][i, 0])
        plt.axis('off')
```



(h) Compare the output of the conditional model with that of the unconditional model. Which one is better? **(1 point)**

The images of the unconditional model seem to be slightly better looking while conditional model might combine 2 digits into one making them unrecognizable. But in the conditional model we can choose which digit we want.

11.9 Discussion (6 points)

(a) Compare the sources of randomness in our diffusion model with that in the variational autoencoder and the GAN in earlier assignments. What are the main differences? **(1 point)**

The source of randomness in diffusion model is of the same dimension as the output image, this source is not equivalent to the latent variable z in the input of GANs and VAEs. Since diffusion models do not model the input from the latent space to the space of images.

(b) Would you be able to train a good digit classification model on the initial input to the sampling function? Why, or why not? **(1 point)**

Hint: for variational autoencoders and GANs, there is a clear link between the input (a latent feature vector) and the output of the decoder. How does this work for our diffusion model?

No, we would not be able to train a digit classifier given a normally distributed initial image due to the fact that image has no meaningful representation, diffusion models do not map the Normal Gaussian distribution to the set of images but use a diffusion process to denoise the random image into a visible one. We've seen that initial image gives a different sampled image.

(c) When loading the data, we normalized the image intensities to [-1, +1], instead of [0, 1] or [0, 255]. Why is this a good input range for this diffusion model? **(1 point)**

This is done so that the image has roughly the same range as standard gaussian. It is equally probable for gaussian to take on a negative value so it is necessary to have include in the range negative values.

(d) In this assignment, we use a β schedule that has a small $\beta = 0.0004$ at the initial time steps ($t = 0$), and a larger $\beta = 0.02$ at the end ($t = T$). Why is it useful to choose an increasing β? **(1 point)**

With a static and small beta, we are not adding enough noise to the images. So a increasing beta is useful to add more noise to the images as we go through the diffusion process, without adding too much noise at the beginning (that would be the consequence of using a bigger static beta).

(e) What would happen if we made β very small? **(1 point)**

The data would stay closer to its original distribution for more steps, as less noise is being added. This could potentially make it easier for the model to learn the denoising function, as the data would be less noisy.

(f) What would happen if we made β very large? **(1 point)**

The data would quickly become very noisy, moving away from its original distribution faster. This could make it harder for the model to learn the denoising function, as the data would be more distorted.

The end

Well done! Please double check the instructions at the top before you submit your results.

This assignment has 42 points.

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