tutorial_ebm_CIFAR10

June 5, 2023

1 Tutorial on iterative image denoising with Langevine dynamics.

[ ]:
```
# Author: Róisín Luo
# Ref: https://uvadlc-notebooks.readthedocs.io/en/latest/tutorial_notebooks/
↪tutorial8/Deep_Energy_Models.html
```

2 Importing libraries

[143]:
```
import sys
import os
import random
import math

import numpy as np


import matplotlib
import matplotlib.pyplot as plt
from matplotlib import cm
from matplotlib import patches
#from matplotlib.colors import to_rgb
#from mpl_toolkits.mplot3d.axes3d import Axes3D
#from mpl_toolkits.mplot3d import proj3d

from tqdm import tqdm

#import csv
#import pandas as pd

import torch
import torch.nn as nn
import torch.nn.functional as F

import torchvision
from torchvision import transforms
from torchvision.utils import make_grid
```

```
from PIL import Image

from atomicwrites import atomic_write #we must guarantee the automicity of␣
↪write operation.
import pickle

%matplotlib inline
```

3 Find GPU

[144]:
```
def find_gpu():

    device = torch.device('cpu')

    if torch.cuda.is_available():
        print('# of CUDA devices: ', torch.cuda.device_count())

        for i in range(torch.cuda.device_count()):
            print()
            print(torch.cuda.get_device_name(i))
            print('CUDA memory Usage:')
            print('Allocated:', round(torch.cuda.memory_allocated(i)/
↪1024**3,1), 'GB')
            print('Cached:   ', round(torch.cuda.memory_reserved(i)/1024**3,1),␣
↪'GB')

        device = torch.device('cuda')

    # MacOS
    elif hasattr(torch, "backends") and \
          hasattr(torch.backends, "mps") and \
          torch.backends.mps.is_available():

        device = torch.device('mps')

    print()
    print("Detected GPU device is: ", device)

    return device
```

[145]:
```
device = find_gpu()
device
```

```
Detected GPU device is:  mps
```

[145]: device(type='mps')

4 Load dataset

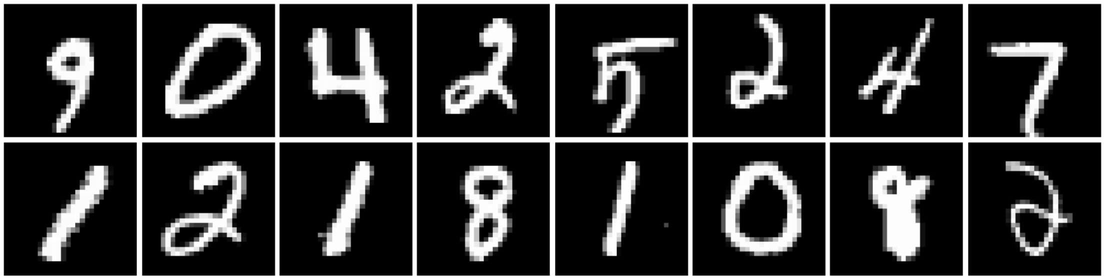
[150]:
```python
def plot_images(images, num_cols = 8, num_rows = 2):

    assert len(images) > num_cols * num_rows

    images = images[0: num_cols * num_rows]

    images = (images + 1) / 2

    #create grid with size by nrows x ncols
    img_grid = make_grid(tensor = images,
                    nrow = num_cols,
                    padding = 1,
                    pad_value = 1)

    #conver to channel last
    img_grid = img_grid.permute(1,2,0)

    plt.figure(figsize=(16, 16))
    plt.imshow(img_grid)
    plt.axis('off')
    plt.show()
```

[151]:
```python
transform = transforms.Compose([transforms.ToTensor(),
                                transforms.Normalize((0.5,), (0.5,)) #to [-1,+1]
                               ])

dataset = torchvision.datasets.MNIST(root="datasets",
                                     train=True,
                                     transform=transform,
                                     download=True)



dataloader = torch.utils.data.DataLoader(dataset,
                               batch_size=128,
                               shuffle=True,
                               #drop_last=True,
                               #num_workers=4,
                               #pin_memory=True
                            )
```

[152]:
```python
x,y = next(iter(dataloader))
x.shape
```

[152]: torch.Size([128, 1, 28, 28])

[153]:
```
plot_images(x)
```



5 Build energy model (simple)

[154]:
```
#we hope the energy model is smooth.
class Swish(nn.Module):
    def forward(self, x):
        return x * torch.sigmoid(x)

#As standard practice/convention, the outputs represent the negative energy.
class EBMSimple(nn.Module):

    def __init__(self, **kwargs):
        super().__init__()


        self.net = nn.Sequential(
            nn.Conv2d(1, 32, kernel_size=5, stride=2, padding=4),
            Swish(),

            nn.Conv2d(32, 64, kernel_size=3, stride=2, padding=1),
            Swish(),

            nn.Conv2d(64, 32, kernel_size=3, stride=2, padding=1),
            Swish(),

            nn.Conv2d(32, 32, kernel_size=3, stride=2, padding=1),
            Swish(),

            nn.Flatten(),
            nn.Linear(128, 100),
            Swish(),
```

```
            nn.Linear(100, 1)
        )


    def forward(self, x):
        x = self.net(x)
        return x
```

[155]:
```
model = EBMSimple()
print(model)

x = torch.rand(10, 1, 28, 28)
x = model(x)

print(x.shape)
print(x)
```

```
EBMSimple(
  (net): Sequential(
    (0): Conv2d(1, 32, kernel_size=(5, 5), stride=(2, 2), padding=(4, 4))
    (1): Swish()
    (2): Conv2d(32, 64, kernel_size=(3, 3), stride=(2, 2), padding=(1, 1))
    (3): Swish()
    (4): Conv2d(64, 32, kernel_size=(3, 3), stride=(2, 2), padding=(1, 1))
    (5): Swish()
    (6): Conv2d(32, 32, kernel_size=(3, 3), stride=(2, 2), padding=(1, 1))
    (7): Swish()
    (8): Flatten(start_dim=1, end_dim=-1)
    (9): Linear(in_features=128, out_features=100, bias=True)
    (10): Swish()
    (11): Linear(in_features=100, out_features=1, bias=True)
  )
)
torch.Size([10, 1])
tensor([[0.0904],
        [0.0904],
        [0.0907],
        [0.0905],
        [0.0906],
        [0.0905],
        [0.0906],
        [0.0905],
        [0.0904],
        [0.0902]], grad_fn=<AddmmBackward0>)
```

6 Build energy model (resnet based)

[156]:
```
#we hope the energy model is smooth.
class Swish(nn.Module):
    def forward(self, x):
        return x * torch.sigmoid(x)

#As standard practice/convention, the outputs represent the negative energy.
class EBMResNet(nn.Module):

    def __init__(self, **kwargs):
        super().__init__()

        self.decoder = torchvision.models.resnet18(pretrained = True)
        self.decoder.fc = nn.Identity()

        self.adapter = nn.Sequential(
            nn.Linear(512, 100),
            Swish(),

            nn.Linear(100, 1),

        )


    def forward(self, x):
        #self.decoder.eval()
        x = self.decoder(x)
        x = self.adapter(x)
        return x
```

[9]:
```
#model = EBMResNet()
#x = torch.rand(10, 3, 32, 32)
#x = model(x)
#
#print(x.shape)
```

7 Sampler for training and generating

[157]:
```
class EBMSampler:
    def __init__(self,
              #model,       #EBM
              image_size,  #image size
              sample_size, #sampling batch size.
              buffer_len = 8192):
```

```
        #self.model = model
        self.buffer_len = buffer_len
        self.image_size = image_size
        self.sample_size = sample_size
        self.sample_shape = (1,) + image_size

        self.buffer = [torch.rand((1, ) + image_size) * 2 - 1] * self.buffer_len

    #sample a batch for training.
    def train_sample(self,
                     model,
                     num_new = None,
                     iters = 60, step_size = 10, device = torch.device("cpu")):

        if num_new is None:
            num_new = np.random.binomial(self.sample_size, 0.05)

        if num_new == 0:
            num_new = 1

        num_old = self.sample_size - num_new

        new_images = torch.rand((num_new,) + self.image_size) * 2 - 1

        old_images = random.choices(self.buffer, k = num_old)
        old_images = torch.cat(old_images, dim = 0)

        images = torch.cat([new_images, old_images], dim = 0)
        images = images.detach().to(device)

        # Perform MCMC sampling
        images = self.langevine_dynamics_sample(model,
                                images,
                                iters = iters,
                                step_size = step_size,
                                device = device)

        self.buffer = list(images.to(torch.device("cpu")).chunk(self.
↪sample_size, dim=0)) + self.buffer
        self.buffer = self.buffer[:self.buffer_len]

        return images

    #MCMC sampling with Langevine dynamics.
    def langevine_dynamics_sample(self,
                model,
                images,
```

```
                iters = 60,
                step_size = 10,
                return_images_per_step = False,
                device = torch.device("cpu")):

    model.to(device)
    images = images.to(device)

    images.requires_grad = True


    noise = torch.randn(images.shape, device = images.device)

    images_per_step = []


    for _ in range(iters):

        noise.normal_(0, 0.005)
        images.data.add_(noise.data)
        images.data.clamp_(min=-1.0, max=1.0)

        outputs = -model(images)
        outputs = outputs.sum()

        #compute gradients wrt images.
        outputs.backward()

        #gradient clamp.
        images.grad.data.clamp_(-0.03, 0.03)

        # Towards the direction with low-energy
        images.data.add_(-step_size * images.grad.data)

        images.grad.detach_()
        images.grad.zero_()
        images.data.clamp_(min=-1.0, max=1.0)

        if return_images_per_step:
            images_per_step.append(images.clone().detach())


    if return_images_per_step:
        return torch.stack(images_per_step, dim=0)
    else:
        return images
```

[158]:
```python
model = EBMSimple()
sampler = EBMSampler(image_size = (1, 28, 28), sample_size = 10)

model.eval()
for p in model.parameters():
    p.requires_grad = False

images = sampler.train_sample(model = model, device = device)
images.shape
```

[158]: torch.Size([10, 1, 28, 28])

8 Training energy-based model for one epoch

[159]:
```python
%matplotlib inline

#from IPython.display import display, clear_output
from IPython import display

def EBM_train_one_epoch(
          model,
          device,
          dataloader,
          optimizer,
          epoch,
          sampler,
          sampler_iters = 60,
          sampler_step_size = 10,
          alpha = 0.2, #regularization weight.
          max_batches = None):

    # Enable gradient computing
    model.to(device)
    model.train()

    if max_batches is None:
        max_batches = len(dataloader)

    #averaged loss in current epoch.
    epoch_loss = 0.0
    total_loss_ = 0.0

    #contrastive divergence
    epoch_cdiv = 0.0
    total_cdiv_ = 0.0
```

```
    #regularization
    epoch_reg = 0.0
    total_reg_ = 0.0


    for batch_idx, batch in enumerate(dataloader, 1):

        real_images, _ = batch

        real_images = real_images.to(device)

        #simple data augmentation.
        noise = torch.randn_like(real_images) * 0.005
        #noise = torch.randn_like(real_images) * math.sqrt(eta)

        real_images.add_(noise).clamp_(min=-1.0, max=1.0)

        fake_images = sampler.train_sample(model = model,
                                           iters = sampler_iters,
                                           step_size = sampler_step_size,
                                           device = device)

        images = torch.cat([real_images, fake_images], dim = 0)

        optimizer.zero_grad()

        #model outputs negative energy.
        outputs = -model(images)

        real_outputs, fake_outputs = outputs.chunk(2, dim = 0)

        #computing batch loss.

        #we hope the minimum energy close to zero.
        batch_reg = alpha * (real_outputs**2 + fake_outputs**2).mean()
        batch_cdiv = real_outputs.mean() - fake_outputs.mean()
        batch_loss = batch_reg + batch_cdiv

        #computing gradients
        batch_loss.backward()

        #update weights.
        optimizer.step()

        #update statistics
        total_reg_ += batch_reg
        total_cdiv_ += batch_cdiv
```

```
        total_loss_ += batch_loss

        epoch_reg = total_reg_ / batch_idx
        epoch_cdiv = total_cdiv_ / batch_idx
        epoch_loss = total_loss_ / batch_idx


        #Updating training displays.
        display.clear_output(wait=True)

        display.display('Epoch {} [{}/{} ({:.0f}%)]'.format(
                    epoch, batch_idx,
                    len(dataloader),
                    100. * (batch_idx / len(dataloader))))

        display.display('* regularization batch {:.6f} epoch {:.6f}'.format(
                    batch_reg, epoch_reg))

        display.display('* contrastive divergence batch {:.6f} epoch {:.6f}'.
↪format(
                    batch_cdiv, epoch_cdiv))

        display.display('* loss batch {:.6f} epoch {:.6f}'.format(
                    batch_loss, epoch_loss))

        if batch_idx > max_batches:
            break

    return epoch_reg, epoch_cdiv, epoch_loss
```

[160]:
```
device = find_gpu()
print(device)
```

```
Detected GPU device is:  mps
mps
```

[161]:
```
batch_size = 128
model = EBMSimple()
sampler = EBMSampler(image_size = (1, 28, 28), sample_size = batch_size)
```

[162]:
```
dataloader = torch.utils.data.DataLoader(dataset,
                               batch_size=batch_size,
                               shuffle=True,
                               #drop_last=True,
                               #num_workers=4,
                               #pin_memory=True
```

```
                            )
```

[163]:
```
#for Adam the learning rate
#typically less than 0.001 for stabability.
learning_rate = 0.001


optimizer = torch.optim.Adam(
                        model.parameters(),
                        lr = learning_rate,
                        betas = (0.99, 0.999),
                        #momentum = 0.9,
                        #weight_decay = 5e-4
                      )

scheduler = torch.optim.lr_scheduler.StepLR(optimizer, 1, gamma=0.97) #␣
 ↪Exponential decay over epochs
```

[61]:
```
epoch_reg, epoch_cdiv, epoch_loss = EBM_train_one_epoch(
          model,
          device,
          dataloader,
          optimizer,
          epoch = 1,
          sampler = sampler,
          sampler_iters = 60,
          sampler_step_size = 10,
          alpha = 0.2,
          max_batches = None)
```

```
'Epoch 1 [469/469 (100%)]'

'* regularization batch 0.000214 epoch 0.012221'

'* contrastive divergence batch 0.010302 epoch -0.016724'

'* loss batch 0.010516 epoch -0.004503'
```

9 Save and load model from disk

[164]:
```
import os

def save_model(model, model_path):

    save_path = os.path.normpath(os.path.dirname(model_path)).rstrip(os.path.
 ↪sep)

    if not os.path.exists(save_path):
```

```
        os.makedirs(save_path)

    print("Save model weights to: ", model_path)
    torch.save(model.state_dict(), model_path)
```

[165]:
```
save_model(model, "models/ebm_simple.pth")
```

```
Save model weights to:  models/ebm_simple.pth
```

[166]:
```
def load_model(model_path, device):
    model = EBMSimple()

    if os.path.exists(model_path):
        #re-loading
        model.load_state_dict(torch.load(model_path, map_location = device))
        print("Loaded model weights from: ", model_path)
    else:
        print("Model weights not found.")

    return model
```

[167]:
```
model = load_model("models/ebm_simple.pth", device)
```

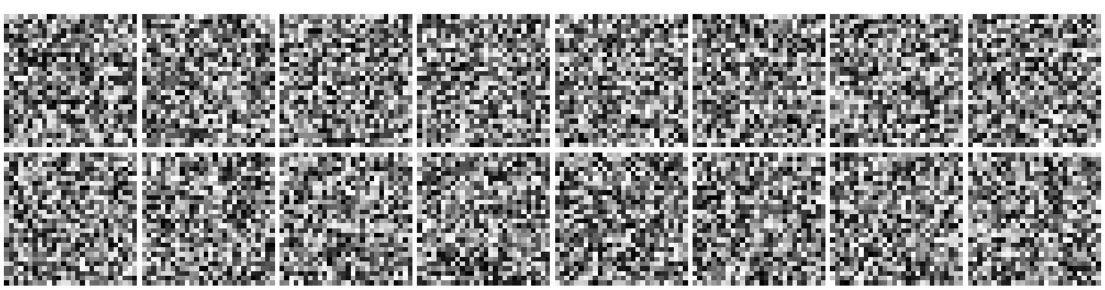
```
Loaded model weights from:  models/ebm_simple.pth
```

10 Generate samples

[168]:
```
def generate_samples(model,
                     sampler,
                     iters = 60,
                     step_size = 10,
                     num_samples = 16,
                     image_size = (1, 28, 28),
                     device = torch.device("cpu")):
    model.eval()
    model.to(device)

    for p in model.parameters():
        p.requires_grad = False


    images = torch.rand((16,) + image_size) * 2 - 1

    images = sampler.langevine_dynamics_sample(
               model,
               images,
               iters = iters,
```

```
                step_size = step_size,
                return_images_per_step = False,
                device = device)

    for p in model.parameters():
        p.requires_grad = True

    images = images.cpu().detach()
    #images.shape

    #visualize
    images = images[0:16]

    images = (images + 1) / 2

    #create grid with size by nrows x ncols
    img_grid = make_grid(tensor = images,
                     nrow = 8,
                     padding = 1,
                     pad_value = 1)

    #conver to channel last
    img_grid = img_grid.permute(1,2,0)

    plt.figure(figsize=(16, 16))
    plt.imshow(img_grid)
    plt.axis('off')
    plt.show()
```

[169]:
```
generate_samples(model,
                 sampler,
                 iters = 50,
                 step_size = 10,
                 num_samples = 16,
                 image_size = (1, 28, 28),
                 device = device)
```



11 Complete training

[75]:
```
def EBM_train(model,
          device,
          dataloader,
          optimizer,
          epochs,
          sampler,
          sampler_iters = 60,
          sampler_step_size = 10,
          alpha = 0.2, #regularization weight.
          scheduler = None,
          max_batches = None):

    #if model_path is not None and not os.path.exists(model_path):
    #    os.makedirs(model_path)

    loss_hist = []
    reg_hist = []
    cdiv_hist = []

    for epoch in range(1, epochs + 1):

        epoch_reg, epoch_cdiv, epoch_loss = EBM_train_one_epoch(
          model = model,
          device = device,
          dataloader = dataloader,
          optimizer = optimizer,
          epoch = epoch,
          sampler = sampler,
          sampler_iters = sampler_iters,
          sampler_step_size = sampler_step_size,
          alpha = alpha,
          max_batches = max_batches)

        if scheduler:
            #adjusting LR is necessary
            scheduler.step()

        loss_hist.append(epoch_loss)
        reg_hist.append(epoch_reg)
        cdiv_hist.append(epoch_cdiv)

    return reg_hist, cdiv_hist, loss_hist
```

[81]:
```
reg_hist, cdiv_hist, loss_hist = EBM_train(model,
          device,
```

```
            dataloader,
            optimizer,
            epochs = 20,
            sampler = sampler,
            sampler_iters = 60,
            sampler_step_size = 10,
            alpha = 0.2,
            scheduler = scheduler,
            max_batches = None)
```

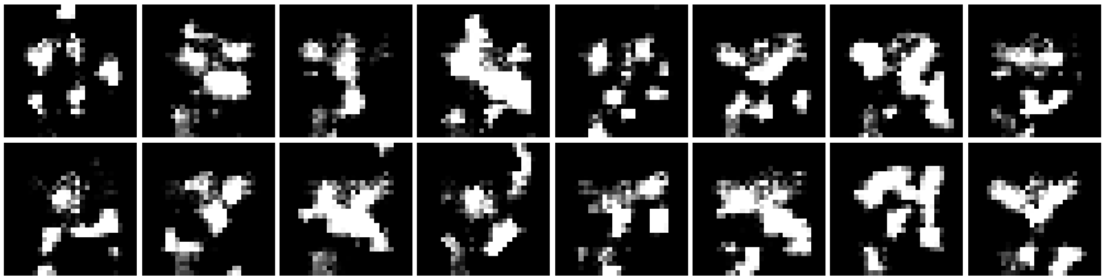
```
'Epoch 2 [127/469 (27%)]'

'* regularization batch 0.000421 epoch 0.000440'

'* contrastive divergence batch 0.020891 epoch 0.023432'

'* loss batch 0.021313 epoch 0.023872'
```

```
---------------------------------------------------------------------------
KeyboardInterrupt                         Traceback (most recent call last)
Cell In[81], line 1
----> 1 reg_hist, cdiv_hist, loss_hist = EBM_train(model,
      2           device,
      3           dataloader,
      4           optimizer,
      5           epochs = 20,
      6           sampler = sampler,
      7           sampler_iters = 60,
      8           sampler_step_size = 10,
      9           alpha = 0.2,
     10           scheduler = scheduler,
     11           max_batches = None)

Cell In[75], line 22, in EBM_train(model, device, dataloader, optimizer, epochs
 ↪sampler, sampler_iters, sampler_step_size, alpha, scheduler, max_batches)
     18 cdiv_hist = []
     20 for epoch in range(1, epochs + 1):
---> 22     epoch_reg, epoch_cdiv, epoch_loss = EBM_train_one_epoch(
     23         model = model,
     24         device = device,
     25         dataloader = dataloader,
     26         optimizer = optimizer,
     27         epoch = epoch,
     28         sampler = sampler,
     29         sampler_iters = sampler_iters,
     30         sampler_step_size = sampler_step_size,
     31         alpha = alpha,
     32         max_batches = max_batches)
     34     if scheduler:
```

```
     35         #adjusting LR is necessary
     36         scheduler.step()

Cell In[56], line 50, in EBM_train_one_epoch(model, device, dataloader,␣
↪optimizer, epoch, sampler, sampler_iters, sampler_step_size, alpha,␣
↪max_batches)
     46 #noise = torch.randn_like(real_images) * math.sqrt(eta)
     48 real_images.add_(noise).clamp_(min=-1.0, max=1.0)
---> 50 fake_images = sampler.train_sample(model = model,
     51                                  iters = sampler_iters,
     52                                  step_size = sampler_step_size,
     53                                  device = device)
     55 images = torch.cat([real_images, fake_images], dim = 0)
     57 optimizer.zero_grad()

Cell In[54], line 45, in EBMSampler.train_sample(self, model, num_new, iters,␣
↪step_size, device)
     38 # Perform MCMC sampling
     39 images = self.langevine_dynamics_sample(model,
     40                                         images,
     41                                         iters = iters,
     42                                         step_size = step_size,
     43                                         device = device)
---> 45 self.buffer = list(images.to(torch.device("cpu")).chunk(self.
↪sample_size, dim=0)) + self.buffer
     46 self.buffer = self.buffer[:self.buffer_len]
     48 return images

KeyboardInterrupt:
```

[105]:

```
generate_samples(model,
                 sampler,
                 iters = 80,
                 step_size = 100,
                 num_samples = 16,
                 image_size = (1, 28, 28),
                 device = device)
```



12 Image denoising with Langevine dynamics equation

[106]:
```
def denoise_samples(model,
                    images,
                    sampler,
                    iters = 60,
                    step_size = 10,
                    num_samples = 16,
                    image_size = (1, 28, 28),
                    device = torch.device("cpu")):
    model.eval()
    model.to(device)

    for p in model.parameters():
        p.requires_grad = False


    images = sampler.langevine_dynamics_sample(
                model,
                images,
                iters = iters,
                step_size = step_size,
                return_images_per_step = False,
                device = device)

    for p in model.parameters():
        p.requires_grad = True

    images = images.cpu().detach()
    #images.shape

    #visualize
    images = images[0:16]

    images = (images + 1) / 2

    #create grid with size by nrows x ncols
    img_grid = make_grid(tensor = images,
                         nrow = 8,
                         padding = 1,
                         pad_value = 1)

    #conver to channel last
    img_grid = img_grid.permute(1,2,0)
```

```
    plt.figure(figsize=(16, 16))
    plt.imshow(img_grid)
    plt.axis('off')
    plt.show()
```

[131]:
```
images, _ = next(iter(dataloader))
images = images[0:16]
images.shape
```

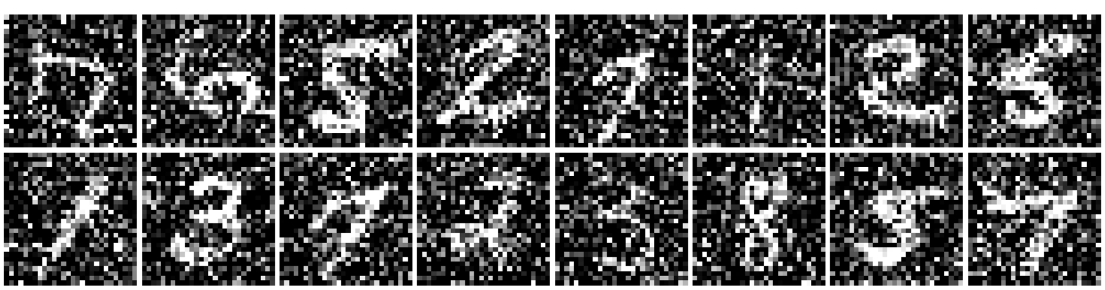
[131]: torch.Size([16, 1, 28, 28])

[133]:
```
plot_images(images)
```

[140]:
```
noise = torch.zeros_like(images)
noise.normal_(0, 1)
#noise = torch.rand(images.size())
noise = torch.randn(images.size())
images.data.add_(noise.data)
#noise_images = images + noise
noise_images = images.data.clamp_(min=-1.0, max=1.0)
noise_images.shape
```

[140]: torch.Size([16, 1, 28, 28])

[141]:
```
plot_images(noise_images)
```



[142]:

```
denoise_samples(model,
                noise_images,
                sampler,
                    iters = 200,
                    step_size = 10,
                    num_samples = 16,
                    image_size = (1, 28, 28),
                    device = device)
```

[ ]:

```

```