MathDNN Homework 10

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Problem 1

Expansion over the expectation operator gives the following.

$$\begin{aligned}
\nabla_\phi \mathbb{E}_{Z\sim q_\phi(z)}\left[\log\left(\frac{h(Z)}{q_\phi(Z)}\right)\right] &= \nabla_\phi \int_{\mathbb{R}^k} \log\left(\frac{h(z)}{q_\phi(z)}\right) q_\phi(z)dz \\
&= \int_{\mathbb{R}^k} \left(\nabla_\phi \log\left(\frac{h(z)}{q_\phi(z)}\right) q_\phi(z) + \log\left(\frac{h(z)}{q_\phi(z)}\right)\nabla_\phi q_\phi(z)\right)dz \\
&= \int_{\mathbb{R}^k} \left(-\frac{\nabla_\phi q_\phi(z)}{q_\phi(z)} q_\phi(z) + \log\left(\frac{h(z)}{q_\phi(z)}\right)\nabla_\phi q_\phi(z)\right)dz \\
&= \int_{\mathbb{R}^k} \log\left(\frac{h(z)}{q_\phi(z)}\right)\nabla_\phi q_\phi(z)dz = \int_{\mathbb{R}^k} \log\left(\frac{h(z)}{q_\phi(z)}\right)\frac{\nabla_\phi q_\phi(z)}{q_\phi(z)} q_\phi(z)dz \\
&= \mathbb{E}_{Z\sim q_\phi(z)}\left[(\nabla_\phi \log q_\phi(Z))\log\left(\frac{h(Z)}{q_\phi(Z)}\right)\right]
\end{aligned}$$

Problem 2

Since $C = \left\{x \in \mathbb{R}^2 \,|\, x_1 = a,\, 0 \le x_2 \le 1\right\}$, we obtain the following.

$$\begin{aligned}
\Pi_C(y) &= \underset{x\in C}{\operatorname{argmin}}\, \|x-y\|^2 = \underset{x\in C}{\operatorname{argmin}} \left\{(a-y_1)^2 + (x_2-y_2)^2\right\} = \underset{x\in C}{\operatorname{argmin}}\, (x_2-y_2)^2 \\
&= \begin{bmatrix} a \\ \min\{\max\{y_2, 0\}, 1\} \end{bmatrix} \quad (\because 0 \le x_2 \le 1)
\end{aligned}$$

Problem 4

(a) Since $f_1(x) = Ax = PL(U + \operatorname{diag}(s))x$, we obtain the following.

$$\begin{aligned}
\log\left|\frac{\partial f_1}{\partial x}\right| &= \log|A| = \log|PL(U+\operatorname{diag}(s))| = \log(|P||L||U+\operatorname{diag}(s)|) = \log|\operatorname{diag}(s)| \\
&= \sum_{i=1}^{C} \log|s_i|
\end{aligned}$$

(b) Different choices of reshape results differ by permutations, i.e., multiplying a permutation matrix to one result of reshape gives another possible result of reshape. Let $x, y \in \mathbb{R}^{abc}$, and $P \in \mathbb{R}^{abc}$ a permutation matrix. We obtain the following.

$$\left|\frac{\partial(Py)}{\partial(Px)}\right| = \left|\frac{\partial(Py)}{\partial y}\frac{\partial y}{\partial x}\frac{\partial x}{\partial(Px)}\right| = |P|\left|\frac{\partial y}{\partial x}\right|\frac{1}{|P|} = \left|\frac{\partial y}{\partial x}\right|$$

Therefore Jacobian determinants between two vectors or between their permutations give the same result. Therefore the choice of reshape does not matter in the given calculation.

(c) Select the reshape operator as reshaping $X \in \mathbb{R}^{C\times m\times n}$ into

$$(X_{1,1,1}, X_{2,1,1}, \cdots, X_{C,1,1}, X_{1,2,1}, X_{2,2,1}, \cdots, X_{C,2,1}, \cdots, X_{1,m,n}, X_{2,m,n}, \cdots, X_{C,m,n}).$$

Then we know

$$f_2(X \mid P, L, U, s).\text{reshape}(Cmn) = \begin{bmatrix} A & & 0 \\ & \ddots & \\ 0 & & A \end{bmatrix} X.\text{reshape}(Cmn)$$

where the As in the diagonal are repeated mn times. Therefore using the result of (a), we obtain the following.

$$\begin{aligned} \log\left|\frac{\partial f_2(X \mid P, L, U, s)}{\partial X}\right| &= \log\left|\frac{\partial f_2(X \mid P, L, U, s).\text{reshape}(Cmn)}{\partial X.\text{reshape}(Cmn)}\right| \\ &= \log\begin{vmatrix} A & & 0 \\ & \ddots & \\ 0 & & A \end{vmatrix} = \log|A|^{mn} = mn\log|A| = mn\sum_{i=1}^{C}\log|s_i| \end{aligned}$$

(d) Select the reshape operator as reshaping $X \in \mathbb{R}^{2C\times m\times n}$ into

$$(X_{1,1,1}, \cdots, X_{C,1,1}, \cdots, X_{1,m,n}, \cdots, X_{C,m,n}, X_{C+1,1,1}, \cdots, X_{2C,1,1}, \cdots, X_{C+1,m,n}, \cdots, X_{2C,m,n}).$$

Then we know

$$Z.\text{reshape}(2Cmn) = \begin{bmatrix} I & & & 0 \\ & A & & \\ & & \ddots & \\ 0 & & & A \end{bmatrix} X.\text{reshape}(2Cmn)$$

where $I \in \mathbb{R}^{Cmn\times Cmn}$ and the As in the diagonal are repeated mn times. Therefore using the result of (a), we obtain the following.

$$\begin{aligned} \log\left|\frac{\partial Z}{\partial X}\right| &= \log\left|\frac{\partial Z.\text{reshape}(2Cmn)}{\partial X.\text{reshape}(2Cmn)}\right| \\ &= \log\begin{vmatrix} I & & & 0 \\ & A & & \\ & & \ddots & \\ 0 & & & A \end{vmatrix} = \log|A|^{mn} = mn\log|A| = mn\sum_{i=1}^{C}\log|s_i| \end{aligned}$$

Problem 3

[1]:
```
import torch
import torch.nn as nn
import torch.nn.functional as F
import torchvision
from torchvision import datasets, transforms
from torchvision.utils import save_image, make_grid
import numpy as np
import matplotlib.pyplot as plt
```

[2]:
```
batch_size = 128
(full_dim, mid_dim, hidden) = (1 * 28 * 28, 1000, 5)
lr = 1e-3
epochs = 100
device = torch.device("cpu")
```

[3]:
```
############################################
# STEP 1: Define dataset and preprocessing #
############################################

#####################################
# STEP 2: Define prior distribution #
#####################################

class Logistic(torch.distributions.Distribution):
    def __init__(self):
        super(Logistic, self).__init__()

    def log_prob(self, x):
        return -(F.softplus(x) + F.softplus(-x))

    def sample(self, size):
        z = torch.distributions.Uniform(0., 1.).sample(size).to(device)
        return torch.log(z) - torch.log(1. - z)
```

[4]:
```
####################################
# STEP 3: Implement Coupling Layer #
####################################

class Coupling(nn.Module):
    def __init__(self, in_out_dim, mid_dim, hidden, mask_config):
        super(Coupling, self).__init__()
        self.mask_config = mask_config

        self.in_block = nn.Sequential(nn.Linear(in_out_dim//2, mid_dim), nn.ReLU())
        self.mid_block = nn.ModuleList([nn.Sequential(nn.Linear(mid_dim, mid_dim), nn.
↪ReLU())
                                                        for _ in range(hidden␣
↪- 1)])
        self.out_block = nn.Linear(mid_dim, in_out_dim//2)

    def forward(self, x, reverse=False):
```

```
        [B, W] = list(x.size())
        x = x.reshape((B, W//2, 2))
        if self.mask_config:
            on, off = x[:, :, 0], x[:, :, 1]
        else:
            off, on = x[:, :, 0], x[:, :, 1]

        off_ = self.in_block(off)
        for i in range(len(self.mid_block)):
            off_ = self.mid_block[i](off_)
        shift = self.out_block(off_)

        if reverse:
            on = on - shift
        else:
            on = on + shift

        if self.mask_config:
            x = torch.stack((on, off), dim=2)
        else:
            x = torch.stack((off, on), dim=2)
        return x.reshape((B, W))

class Scaling(nn.Module):
    def __init__(self, dim):
        super(Scaling, self).__init__()
        self.scale = nn.Parameter(torch.zeros((1, dim)), requires_grad=True)

    def forward(self, x, reverse=False):
        log_det_J = torch.sum(self.scale)
        if reverse:
            x = x * torch.exp(-self.scale)
        else:
            x = x * torch.exp(self.scale)
        return x, log_det_J
```

[5]:

```
##########################
# STEP 4: Implement NICE #
##########################

class NICE(nn.Module):
    def __init__(self,in_out_dim, mid_dim, hidden, mask_config=1.0, coupling=4):
        super(NICE, self).__init__()
        self.prior = Logistic()
        self.in_out_dim = in_out_dim

        self.coupling = nn.ModuleList([
            Coupling(in_out_dim=in_out_dim,
                     mid_dim=mid_dim,
                     hidden=hidden,
                     mask_config=(mask_config+i)%2) \
            for i in range(coupling)])
```

```
        self.scaling = Scaling(in_out_dim)

    def g(self, z):
        x, _ = self.scaling(z, reverse=True)
        for i in reversed(range(len(self.coupling))):
            x = self.coupling[i](x, reverse=True)
        return x

    def f(self, x):
        for i in range(len(self.coupling)):
            x = self.coupling[i](x)
        z, log_det_J = self.scaling(x)
        return z, log_det_J

    def log_prob(self, x):
        z, log_det_J = self.f(x)
        log_ll = torch.sum(self.prior.log_prob(z), dim=1)
        return log_ll + log_det_J

    def sample(self, size):
        z = self.prior.sample((size, self.in_out_dim)).to(device)
        return self.g(z)

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

[6]:
```
# Load pre-trained NICE model onto CPU
model = NICE(in_out_dim=784, mid_dim=1000, hidden=5).to(device)
model.load_state_dict(torch.load('nice.pt',map_location=torch.device('cpu')))

# Since we do not update model, set requires_grad = False
model.requires_grad_(False)

# Get an MNIST image
testset = torchvision.datasets.MNIST(root='./', train=False, download=True,␣
 ↪transform=torchvision.transforms.ToTensor())
test_loader = torch.utils.data.DataLoader(testset, batch_size=1, shuffle=False)
pass_count = 6
itr = iter(test_loader)
for _ in range(pass_count+1):
    image,_ = itr.next()

fig, (ax1, ax2, ax3) = plt.subplots(1, 3, figsize=(12, 4))
ax1.set_title('Original Image')
ax1.imshow(make_grid(image.squeeze().detach()).permute(1,2,0))
# ax1.savefig('plt1.png')

# Create mask
mask = torch.ones_like(image,dtype=torch.bool)
mask[:,:,5:12,5:20] = 0

# Partially corrupt the image
image[mask.logical_not()] = torch.ones_like(image[mask.logical_not()])
```

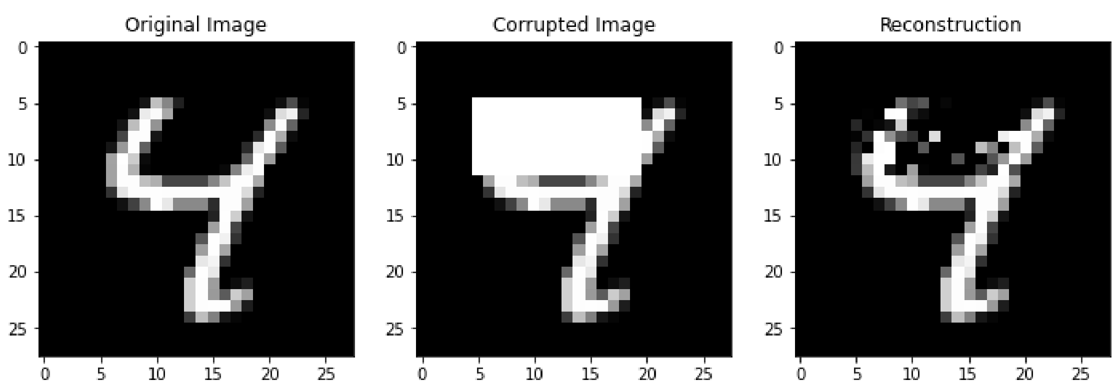
```
ax2.set_title('Corrupted Image')
ax2.imshow(make_grid(image.squeeze()).permute(1,2,0))
# ax2.savefig('plt2.png')

# Plot reconstruction
X = image.clone().requires_grad_(True)
for i in range(300):
    X.data = X.data.view(-1, 28*28)
    loss = -model(X)
    loss.backward()
    X.data = torch.clamp(X.data - lr * X.grad, min=0, max=1)
    X.data[mask.view(-1, 28*28).logical_not().logical_not()] = image.view(-1,␣
 ↪28*28)[mask.view(-1, 28*28).logical_not().logical_not()]
X.data = X.data.view(image.size())

ax3.set_title('Reconstruction')
ax3.imshow(make_grid(X.squeeze().detach()).permute(1,2,0))
# ax3.savefig('plt3.png')

plt.show()
```

```
/Library/Frameworks/Python.framework/Versions/3.8/lib/python3.8/site-
packages/torch/distributions/distribution.py:44: UserWarning: <class
'__main__.Logistic'> does not define `arg_constraints`. Please set
`arg_constraints = {}` or initialize the distribution with `validate_args=False`
to turn off validation.
  warnings.warn(f'{self.__class__} does not define `arg_constraints`. ' +
```



Problem 5

[7]:
```
import torch
import math

N = 3000
p = 18. / 37.
q = 0.55
max_play = 600
```

```
def f(X_i):
    return p**X_i * (1-p)**(1-X_i)

def g(Y_i):
    return q**Y_i * (1-q)**(1-Y_i)

samp = []
for _ in range(N):
    Y = torch.bernoulli(q * torch.ones(max_play))
    balance = 100
    s = 1
    for i in range(max_play):
        balance += 2*Y[i]-1
        s *= f(Y[i]) / g(Y[i])
        if balance == 0 or balance == 200:
            break
    s *= (balance == 200).float()
    samp.append(s)

samp = torch.Tensor(samp)
Ihat,s = samp.mean(), samp.var()
print(f"Estimate: {Ihat:.6f} ± {math.sqrt(s/N):.6f}")
```

```
Estimate: 0.000002 ± 0.000000
```

Problem 6

(a)

[8]:
```
import torch
import math

lr = 1e-3
B = 16
iterations = 500
mu = torch.tensor([0.])
tau = torch.tensor([0.])

for itr in range(iterations):
    X = torch.normal(0, 1, size=(B,)) * tau.exp() + mu
    mu -= lr * (torch.sum(X * X.sin() * (X - mu) / tau.exp()**2) / B + mu - 1)
    tau -= lr * (torch.sum(X * X.sin() * ((X - mu)**2 / tau.exp() - 1)) / B + tau.exp()
 ↪- 1)

print(f"mu = {mu[0]}")
print(f"sigma = {tau.exp()[0]}")
```

```
mu = 0.32686325907707214
sigma = 0.8322127461433411
```

(b)

[9]:
```
import torch
import math

lr = 1e-3
B = 16
iterations = 500
mu = torch.tensor([0.])
tau = torch.tensor([0.])

for itr in range(iterations):
    Y = torch.normal(0, 1, size=(B,))
    X = mu + tau.exp() * Y
    mu -= lr * (torch.sum(X.sin() + X * X.cos()) / B + mu - 1)
    tau -= lr * (torch.sum((X.sin() + X * X.cos()) * Y) / B + tau.exp() - 1)

print(f"mu = {mu[0]}")
print(f"sigma = {tau.exp()[0]}")
```

```
mu = 0.3241511881351471
sigma = 0.7526840567588806
```