

NNC2P

November 21, 2022

Contents

1	Introduction	1
2	Generating training data	2
3	Getting data into PyTorch's DataLoader	4
4	Building the neural networks	5
5	Training the neural network	6
5.1	Results of training	38
6	Analyzing neural networks	39
6.1	Estimate the performance of the network	39
6.2	Estimate the performance on unseen/untrained cases:	40
6.2.1	When only one parameter gets outside of its range	40
6.2.2	When all parameters can go outside of their ranges	45
7	Get parameters of network out:	50

```
[154]: import numpy as np
import matplotlib.pyplot as plt
plt.rcParams['figure.dpi'] = 300
import random
import csv
import pandas as pd
import torch
from torch import nn
from torch.utils.data import Dataset, DataLoader
from torchvision.transforms import ToTensor
import matplotlib.cm as cm
```

1 Introduction

The conserved variables are (D, S_i, τ) and they are related to primitive variables, $w = (\rho, v^i, \epsilon, p)$, defined in the local rest frame of the fluid through (in units of light speed $c = 1$). The P2C is explicitly given:

$$D = \rho W, \quad S_i = \rho h W^2 v_i, \quad \tau = \rho h W^2 - p - D, \quad (1)$$

where we used

$$W = (1 - v^2)^{-1/2}, \quad h = 1 + \epsilon + \frac{p}{\rho}. \quad (2)$$

Our first goal is to reproduce the results from [this paper](#). A different notebook implemented the NNEOSB network. Here, we will implement the NNC2P network. We consider an **analytical Γ -law EOS** as a benchmark:

$$p(\rho, \epsilon) = (\Gamma - 1)\rho\epsilon, \quad (3)$$

and we fix $\Gamma = 5/3$ in order to fully mimic the situation of the paper.

2 Generating training data

```
[49]: # Define the three functions determining the output
def eos(rho, eps, Gamma = 5/3):
    """Computes the analytical gamma law EOS from rho and epsilon"""
    return (Gamma - 1) * rho * eps

def h(rho, eps, v):
    """Enthalpy"""
    p = eos(rho, eps)
    return 1 + eps + p/rho

def W(rho, eps, v):
    """Lorentz factor. Here, in 1D so v = v_x"""
    return (1-v**2)**(-1/2)

def D(rho, eps, v):
    """See eq 2 paper"""
    return rho*W(rho, eps, v)

def S(rho, eps, v):
    """See eq2 paper. Note: 1D only for now."""
    return rho*h(rho, eps, v)*((W(rho, eps, v))**2)*v

def tau(rho, eps, v):
    """See eq2 paper."""
    return rho*(h(rho, eps, v)*((W(rho, eps, v))**2) - eos(rho, eps) - D(rho,
↪eps, v))
```

We generate data as follows. We create a training set by randomly sampling as follows: - $\rho \in (0, 10.1)$, - $\epsilon \in (0, 2.02)$, - $v_x \in (0, 0.721)$.

```
[14]: # Define ranges of parameters to be sampled (see paper Section 2.1)
rho_min = 0
rho_max = 10.1
eps_min = 0
eps_max = 2.02
v_min = 0
```

```
v_max = 0.721
```

Note: the code in comment below was used to generate the data. It has now been saved separately in a folder called “data”.

```
[15]: # number_of_datapoints = 10000
# data = []

# for i in range(number_of_datapoints):
#     rho = random.uniform(rho_min, rho_max)
#     eps = random.uniform(eps_min, eps_max)
#     v     = random.uniform(v_min, v_max)

#     p           = eos(rho, eps)
#     Dvalue      = D(rho, eps, v)
#     Svalue      = S(rho, eps, v)
#     tauvalue    = tau(rho, eps, v)

#     new_row = [rho, eps, v, p, Dvalue, Svalue, tauvalue]

#     data.append(new_row)
```

Save the data in a csv file:

```
[16]: # header = ['rho', 'eps', 'v', 'p', 'D', 'S', 'tau']

# with open('data/NNC2P_data_test.csv', 'w', newline = '') as file:
#     writer = csv.writer(file)
#     # write header
#     writer.writerow(header)
#     # write data
#     writer.writerows(data)
```

```
[17]: # Import data
data_train = pd.read_csv("data/NNC2P_data_train.csv")
data_test = pd.read_csv("data/NNC2P_data_test.csv")
print("The training data has " + str(len(data_train)) + " instances")
print("The test data has " + str(len(data_test)) + " instances")
data_train
```

The training data has 80000 instances

The test data has 10000 instances

```
[17]:
```

	rho	eps	v	p	D	S	tau
0	0.662984	0.084146	0.218802	0.037192	0.679448	0.173724	0.077335
1	8.565808	0.205945	0.657351	1.176059	11.366755	13.318537	7.718100
2	4.387112	1.598809	0.021593	4.676103	4.388135	0.347321	7.020631
3	5.337054	0.530803	0.351307	1.888615	5.700396	4.031171	3.885760
4	1.133895	0.786717	0.079475	0.594703	1.137493	0.209600	0.905115

...
79995	8.101834	0.428605	0.616897	2.314990	10.294002	13.832316	9.813427
79996	7.841014	1.125480	0.209087	5.883268	8.018242	4.930289	9.678536
79997	4.628822	0.194190	0.237759	0.599248	4.765476	1.544018	1.129323
79998	9.913117	1.152242	0.477216	7.614874	11.280468	17.889657	18.592193
79999	9.717025	0.001552	0.163383	0.010052	9.849373	1.635352	0.149919

[80000 rows x 7 columns]

3 Getting data into PyTorch's DataLoader

Below: `all_data` is of the type $(\rho, \epsilon, v, p, D, S_x, \tau)$ as generated above.

```
[18]: class CustomDataset(Dataset):
    """See PyTorch tutorial: the following three methods HAVE to be
    implemented"""

    def __init__(self, all_data, transform=None, target_transform=None):
        self.transform = transform
        self.target_transform = target_transform

        # Separate features (rho and eps) from the labels (p, chi, kappa)
        # (see above to get how data is organized)
        features = []
        labels = []

        for i in range(len(all_data)):
            # Separate the features
            new_feature = [all_data['D'][i], all_data['S'][i],
            all_data['tau'][i]]
            features.append(torch.tensor(new_feature, dtype = torch.float32))
            # Separate the labels
            new_label = [all_data['p'][i]]
            labels.append(torch.tensor(new_label, dtype = torch.float32))

        # Save as instance variables to the dataloader
        self.features = features
        self.labels = labels

    def __len__(self):
        return len(self.labels)

    def __getitem__(self, idx):
        feature = self.features[idx]
        if self.transform:
            feature = transform(feature)
        label = self.labels[idx]
```

```

        if self.target_transform:
            feature = target_transform(label)

    return feature, label

```

Note that the following cell may be confusing. “data_train” refers to the data that was generated above, see the pandas table. “training_data” is defined similarly as in the PyTorch tutorial, see [this page](#) and this is an instance of the class CustomDataset defined above.

```

[19]: # Make training and test data, as in the tutorial
training_data = CustomDataset(data_train)
test_data = CustomDataset(data_test)

```

```

[20]: # Check if this is done correctly
print(training_data.features[:3])
print(training_data.labels[:3])

```

```

[tensor([0.6794, 0.1737, 0.0773]), tensor([11.3668, 13.3185, 7.7181]),
tensor([4.3881, 0.3473, 7.0206])]
[tensor([0.0372]), tensor([1.1761]), tensor([4.6761])]

```

```

[21]: # Now call DataLoader on the above CustomDataset instances:
train_dataloader = DataLoader(training_data, batch_size=32)
test_dataloader = DataLoader(test_data, batch_size=32)

```

4 Building the neural networks

We will follow [this part of the PyTorch tutorial](#). For more information, see the [documentation page of torch.nn](#). We take the parameters of NNEOS

```

[28]: # Define hyperparameters of the model here. Will first of all put two hidden
      ↪ layers
# total of 800 neurons for the one in the paper
device = "cpu"
size_HL_1 = 600
size_HL_2 = 200

# Implement neural network
class NeuralNetwork(nn.Module):
    def __init__(self):
        super(NeuralNetwork, self).__init__()
        #self.flatten = nn.Flatten()
        self.stack = nn.Sequential(
            nn.Linear(3, size_HL_1),
            nn.Sigmoid(),
            nn.Linear(size_HL_1, size_HL_2),
            nn.Sigmoid(),
            nn.Linear(size_HL_2, 1)

```

```

    )

    def forward(self, x):
        # No flatten needed, as our input and output are 1D?
        #x = self.flatten(x)
        logits = self.stack(x)
        return logits

```

5 Training the neural network

```

[29]: def train_loop(dataloader, model, loss_fn, optimizer, report_progress = False):
    """The training loop of the algorithm"""
    size = len(dataloader.dataset)
    for batch, (X, y) in enumerate(dataloader):
        # Compute prediction and loss
        pred = model(X)
        loss = loss_fn(pred, y)

        # Backpropagation
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        # If we want to report progress during training (not recommended -
        ↪obstructs view)
        if report_progress:
            if batch % 100 == 0:
                loss, current = loss.item(), batch * len(X)
                print(f"loss: {loss:>7f} [{current:>5d}/{size:>5d}]")

def test_loop(dataloader, model, loss_fn):
    """The testing loop of the algorithm"""
    num_batches = len(dataloader)
    test_loss = 0

    # Predict and compute losses
    with torch.no_grad():
        for X, y in dataloader:
            pred = model(X)
            test_loss += loss_fn(pred, y).item()

    average_test_loss = test_loss/num_batches
    return average_test_loss

```

Now we generate an instance of the above neural network in `model` (note: running this cell will create a ‘fresh’ model!).

Save hyperparameters and loss function - note that we follow the paper. I think that their loss function agrees with [MSELoss](#). The paper uses the [Adam optimizer](#). More details on optimizers can be found [here](#). Required argument `params` can be filled in by calling `model` which contains the neural network. For simplicity we will train for 10 epochs here.

```
[30]: model = NeuralNetwork().to(device)
print(model)

# Save hyperparameters, loss function and optimizer here (see paper for details)
learning_rate = 6e-3
batch_size = 32
adaptation_threshold = 0.9995
adaptation_multiplier = 0.5

loss_fn = nn.MSELoss()
optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)
```

```
NeuralNetwork(
  (stack): Sequential(
    (0): Linear(in_features=3, out_features=600, bias=True)
    (1): Sigmoid()
    (2): Linear(in_features=600, out_features=200, bias=True)
    (3): Sigmoid()
    (4): Linear(in_features=200, out_features=1, bias=True)
  )
)
```

Training:

```
[27]: # Restart training by changing this parameter:
restart = True
abort = False
max_number_epochs = 500

# Initialize lists in case we start a new training loop
if restart:
    confirmation = input("Are you sure you want to restart? Press y >> ")
    if confirmation == "y":
        test_losses = []
        train_losses = []
        train_losses_subset = []
        adaptation_indices = []
        counter = -5 # we skip the very first few iterations before changing_
↪ learning rate
    else:
        print("Aborting training.")
        abort = True
```

```

# Actual training loop is done:
if abort is False:
    epoch_counter = len(train_losses) + 1

    print("Training the model . . .")
    if restart is False:
        print("(Continued)")

# Training:
while epoch_counter < max_number_epochs:
    print(f"\n Epoch {epoch_counter} \n -----")
    # Train
    train_loop(train_dataloader, model, loss_fn, optimizer)
    # Test on the training data
    average_train_loss = test_loop(train_dataloader, model, loss_fn)
    train_losses.append(average_train_loss)
    # Test on testing data
    average_test_loss = test_loop(test_dataloader, model, loss_fn)
    test_losses.append(average_test_loss)

    # Update the learning rate - see Appendix B of the paper
    # only check if update needed after 10 new epochs
    if counter >= 10:
        current = np.min(train_losses[-5:])
        previous = np.min(train_losses[-10:-5])

        # If we did not improve the test loss sufficiently, going to adapt
        ↪LR
        if current/previous >= adaptation_threshold:
            # Reset counter (note: will increment later, so set to -1 st it
            ↪becomes 0)
            counter = -1
            learning_rate = adaptation_multiplier*learning_rate
            print(f"Adapting learning rate to {learning_rate}")
            # Change optimizer
            optimizer = torch.optim.Adam(model.parameters()),
            ↪lr=learning_rate)
            # Add the epoch time for plotting later on
            adaptation_indices.append(epoch_counter)

    # Report progress:
    # print(f"Average loss of: {average_test_loss} for test data")
    print(f"Average loss of: {average_train_loss} for train data")

    # Another epoch passed - increment counter
    counter += 1
    epoch_counter += 1

```



```
print("Done!")
```

Are you sure you want to restart? Press y >> y

Training the model . . .

Epoch 1

Average loss of: 0.0008374712398741394 for train data

Epoch 2

Average loss of: 0.0028390558508457615 for train data

Epoch 3

Average loss of: 0.00176264596353285 for train data

Epoch 4

Average loss of: 0.0018434447112260386 for train data

Epoch 5

Average loss of: 0.012840801018476487 for train data

Epoch 6

Average loss of: 0.005599299266841263 for train data

Epoch 7

Average loss of: 0.0009573062956158537 for train data

Epoch 8

Average loss of: 0.0012745201862009708 for train data

Epoch 9

Average loss of: 0.021164815479889514 for train data

Epoch 10

Average loss of: 0.0014400066701695323 for train data

Epoch 11

Average loss of: 0.002986287210625596 for train data

Epoch 12

Average loss of: 0.01286850904924795 for train data

Epoch 13

Average loss of: 0.009362233091238886 for train data

Epoch 14

Average loss of: 0.0024174958161078393 for train data

Epoch 15

Average loss of: 0.0029913834168808534 for train data

Epoch 16

Adapting learning rate to 0.003

Average loss of: 0.002275881057837978 for train data

Epoch 17

Average loss of: 0.0010866594808292575 for train data

Epoch 18

Average loss of: 0.000685571559582604 for train data

Epoch 19

Average loss of: 0.0010815738166682423 for train data

Epoch 20

Average loss of: 0.0004254248633369571 for train data

Epoch 21

Average loss of: 0.0004163259977358393 for train data

Epoch 22

Average loss of: 0.0003321605166856898 for train data

Epoch 23

```
-----
Average loss of: 0.0003036793719133129 for train data

Epoch 24
-----
Average loss of: 0.0007284642843645997 for train data

Epoch 25
-----
Average loss of: 0.0008030698567803484 for train data

Epoch 26
-----
Average loss of: 0.0005154055201157462 for train data

Epoch 27
-----
Average loss of: 0.00023526176397281232 for train data

Epoch 28
-----
Average loss of: 0.0016246155150874983 for train data

Epoch 29
-----
Average loss of: 0.00047035179757804146 for train data

Epoch 30
-----
Average loss of: 0.0027680852412246167 for train data

Epoch 31
-----
Average loss of: 0.00034685198436200154 for train data

Epoch 32
-----
Adapting learning rate to 0.0015
Average loss of: 0.0014031593533873092 for train data

Epoch 33
-----
Average loss of: 0.00016790372807736276 for train data

Epoch 34
-----
Average loss of: 0.00019431638129608473 for train data
```

Epoch 35

Average loss of: 0.0006761802385153715 for train data

Epoch 36

Average loss of: 0.00034298850800842045 for train data

Epoch 37

Average loss of: 0.00033999654359940905 for train data

Epoch 38

Average loss of: 0.0003540729997854214 for train data

Epoch 39

Average loss of: 0.0006684789749269839 for train data

Epoch 40

Average loss of: 0.00012168349831554224 for train data

Epoch 41

Average loss of: 0.00022992139270354528 for train data

Epoch 42

Average loss of: 0.0001759395051325555 for train data

Epoch 43

Average loss of: 0.00035280449390702413 for train data

Epoch 44

Average loss of: 0.00013466744584729896 for train data

Epoch 45

Adapting learning rate to 0.00075
Average loss of: 0.0002512213310634252 for train data

Epoch 46

Average loss of: 6.713904162243125e-05 for train data

Epoch 47

Average loss of: 6.219180659791163e-05 for train data

Epoch 48

Average loss of: 6.577019045362249e-05 for train data

Epoch 49

Average loss of: 6.114968546899036e-05 for train data

Epoch 50

Average loss of: 5.172770523859071e-05 for train data

Epoch 51

Average loss of: 4.91537233836425e-05 for train data

Epoch 52

Average loss of: 5.328337369501241e-05 for train data

Epoch 53

Average loss of: 6.457944684661924e-05 for train data

Epoch 54

Average loss of: 9.008280789712444e-05 for train data

Epoch 55

Average loss of: 9.268357945547905e-05 for train data

Epoch 56

Adapting learning rate to 0.000375
Average loss of: 0.00011167042215529364 for train data

Epoch 57

Average loss of: 2.859411746940168e-05 for train data

Epoch 58

Average loss of: 2.518275689035363e-05 for train data

Epoch 59

Average loss of: 2.4122865337631083e-05 for train data

Epoch 60

Average loss of: 2.4452574419956363e-05 for train data

Epoch 61

Average loss of: 2.4061113363131882e-05 for train data

Epoch 62

Average loss of: 2.1571091255100326e-05 for train data

Epoch 63

Average loss of: 2.0228936509374763e-05 for train data

Epoch 64

Average loss of: 1.980204531992058e-05 for train data

Epoch 65

Average loss of: 1.944150442541286e-05 for train data

Epoch 66

Average loss of: 1.9019129154366965e-05 for train data

Epoch 67

Average loss of: 1.8600023055296335e-05 for train data

Epoch 68

Average loss of: 1.820302260493918e-05 for train data

Epoch 69

Average loss of: 1.7844117978893338e-05 for train data

Epoch 70

Average loss of: 1.7507765450864097e-05 for train data

Epoch 71

Average loss of: 1.7196891020466864e-05 for train data

Epoch 72

Average loss of: 1.6902474209928187e-05 for train data

Epoch 73

Average loss of: 1.6627590232565126e-05 for train data

Epoch 74

Average loss of: 1.6366952178213977e-05 for train data

Epoch 75

Average loss of: 1.6121911657683085e-05 for train data

Epoch 76

Average loss of: 1.5872540604505046e-05 for train data

Epoch 77

Average loss of: 1.5624181948442127e-05 for train data

Epoch 78

Average loss of: 1.5338656873973378e-05 for train data

Epoch 79

Average loss of: 1.4991375871250056e-05 for train data

Epoch 80

Average loss of: 1.455777868959558e-05 for train data

Epoch 81

Average loss of: 1.4019853218997013e-05 for train data

Epoch 82

Average loss of: 1.342473424738273e-05 for train data

Epoch 83

Average loss of: 1.286168643309793e-05 for train data

Epoch 84

Average loss of: 1.2367646779239294e-05 for train data

Epoch 85

Average loss of: 1.1940011171009246e-05 for train data

Epoch 86

Average loss of: 1.1547774174505322e-05 for train data

Epoch 87

Average loss of: 1.1217158741601452e-05 for train data

Epoch 88

Average loss of: 1.0938955255551263e-05 for train data

Epoch 89

Average loss of: 1.0744831578267622e-05 for train data

Epoch 90

Average loss of: 1.0587547819432076e-05 for train data

Epoch 91

Average loss of: 1.0417071637220943e-05 for train data

Epoch 92

Average loss of: 1.0254595713558955e-05 for train data

Epoch 93

Average loss of: 1.00566246102062e-05 for train data

Epoch 94

Average loss of: 9.850346663370147e-06 for train data

Epoch 95

Average loss of: 9.683224149193847e-06 for train data

Epoch 96

Average loss of: 9.478459651109006e-06 for train data

Epoch 97

Average loss of: 9.27343222710988e-06 for train data

Epoch 98

Average loss of: 9.09457401594409e-06 for train data

Epoch 99

Average loss of: 8.949953785213437e-06 for train data

Epoch 100

Average loss of: 8.823468472473906e-06 for train data

Epoch 101

Average loss of: 8.69367549648814e-06 for train data

Epoch 102

Average loss of: 8.566825740308559e-06 for train data

Epoch 103

Average loss of: 8.452927098824148e-06 for train data

Epoch 104

Average loss of: 8.347954696819216e-06 for train data

Epoch 105

Average loss of: 8.246156070708822e-06 for train data

Epoch 106

Average loss of: 8.156023010269564e-06 for train data

Epoch 107

Average loss of: 8.068066925261519e-06 for train data

Epoch 108

Average loss of: 7.989396141147154e-06 for train data

Epoch 109

Average loss of: 7.9113305946521e-06 for train data

Epoch 110

Average loss of: 7.840624469008617e-06 for train data

Epoch 111

Average loss of: 7.772283887061348e-06 for train data

Epoch 112

Average loss of: 7.705822829393583e-06 for train data

Epoch 113

Average loss of: 7.645670363581303e-06 for train data

Epoch 114

Average loss of: 7.587451477957074e-06 for train data

Epoch 115

Average loss of: 7.528351131350064e-06 for train data

Epoch 116

Average loss of: 7.476396489164472e-06 for train data

Epoch 117

Average loss of: 7.4204914752954206e-06 for train data

Epoch 118

Average loss of: 7.371865952882217e-06 for train data

Epoch 119

Average loss of: 7.314280705759302e-06 for train data

Epoch 120

Average loss of: 7.260753952778032e-06 for train data

Epoch 121

Average loss of: 7.199779112670513e-06 for train data

Epoch 122

Average loss of: 7.133341466851561e-06 for train data

Epoch 123

Average loss of: 7.057825559786579e-06 for train data

Epoch 124

Average loss of: 6.975392372078204e-06 for train data

Epoch 125

Average loss of: 6.891693763509466e-06 for train data

Epoch 126

Average loss of: 6.810985768015599e-06 for train data

Epoch 127

Average loss of: 6.734880648400576e-06 for train data

Epoch 128

Average loss of: 6.6641130418702235e-06 for train data

Epoch 129

Average loss of: 6.594504514441724e-06 for train data

Epoch 130

Average loss of: 6.52456226657705e-06 for train data

Epoch 131

Average loss of: 6.4551132864835385e-06 for train data

Epoch 132

Average loss of: 6.384176859955915e-06 for train data

Epoch 133

Average loss of: 6.30825466364513e-06 for train data

Epoch 134

Average loss of: 6.2243470185421756e-06 for train data

Epoch 135

Average loss of: 6.1436157258413e-06 for train data

Epoch 136

Average loss of: 6.09942012083593e-06 for train data

Epoch 137

Average loss of: 6.100279466818393e-06 for train data

Epoch 138

Average loss of: 6.0959003561492866e-06 for train data

Epoch 139

Average loss of: 6.0467620578037896e-06 for train data

Epoch 140

Average loss of: 5.991876803091145e-06 for train data

Epoch 141

Average loss of: 5.949278629896071e-06 for train data

Epoch 142

Average loss of: 5.887109353352571e-06 for train data

Epoch 143

Average loss of: 5.795303950208108e-06 for train data

Epoch 144

Average loss of: 5.729388220788678e-06 for train data

Epoch 145

Average loss of: 5.807249706504081e-06 for train data

Epoch 146

Average loss of: 5.78118533126144e-06 for train data

Epoch 147

Average loss of: 5.668733869651987e-06 for train data

Epoch 148

Average loss of: 5.547868486564766e-06 for train data

Epoch 149

Average loss of: 5.542695759004346e-06 for train data

Epoch 150

Average loss of: 5.5565302712238914e-06 for train data

Epoch 151

Average loss of: 5.477469120251044e-06 for train data

Epoch 152

Average loss of: 5.476664339539639e-06 for train data

Epoch 153

Average loss of: 5.433030142421558e-06 for train data

Epoch 154

Average loss of: 5.384247737629267e-06 for train data

Epoch 155

Average loss of: 5.364854617391756e-06 for train data

Epoch 156

Average loss of: 5.347203180599535e-06 for train data

Epoch 157

Average loss of: 5.3365975296401304e-06 for train data

Epoch 158

Average loss of: 5.309060895660878e-06 for train data

Epoch 159

Average loss of: 5.280717278810698e-06 for train data

Epoch 160

Average loss of: 5.257382112358755e-06 for train data

Epoch 161

Average loss of: 5.243267094783732e-06 for train data

Epoch 162

Average loss of: 5.223805030982476e-06 for train data

Epoch 163

Average loss of: 5.202360179782772e-06 for train data

Epoch 164

Average loss of: 5.176662967505763e-06 for train data

Epoch 165

Average loss of: 5.154846010782421e-06 for train data

Epoch 166

Average loss of: 5.13309890943674e-06 for train data

Epoch 167

Average loss of: 5.107650152694987e-06 for train data

Epoch 168

Average loss of: 5.0800397762486685e-06 for train data

Epoch 169

Average loss of: 5.0536835059574515e-06 for train data

Epoch 170

Average loss of: 5.0238561767855576e-06 for train data

Epoch 171

Average loss of: 4.9914669439203865e-06 for train data

Epoch 172

Average loss of: 4.957455329258664e-06 for train data

Epoch 173

Average loss of: 4.917579126504279e-06 for train data

Epoch 174

Average loss of: 4.877017398212047e-06 for train data

Epoch 175

Average loss of: 4.8366932282988275e-06 for train data

Epoch 176

Average loss of: 4.79528993000713e-06 for train data

Epoch 177

Average loss of: 4.7543924693854934e-06 for train data

Epoch 178

Average loss of: 4.714597207339466e-06 for train data

Epoch 179

Average loss of: 4.6793685037755495e-06 for train data

Epoch 180

Average loss of: 4.64627201354233e-06 for train data

Epoch 181

Average loss of: 4.620893368110046e-06 for train data

Epoch 182

Average loss of: 4.595793011685601e-06 for train data

Epoch 183

Average loss of: 4.573902602805901e-06 for train data

Epoch 184

Average loss of: 4.555271559775065e-06 for train data

Epoch 185

Average loss of: 4.5400204931866025e-06 for train data

Epoch 186

Average loss of: 4.526925647996905e-06 for train data

Epoch 187

Average loss of: 4.515965297696311e-06 for train data

Epoch 188

Average loss of: 4.508190486740204e-06 for train data

Epoch 189

Average loss of: 4.501978736107048e-06 for train data

Epoch 190

Average loss of: 4.4978812655244835e-06 for train data

Epoch 191

Average loss of: 4.4980569061863205e-06 for train data

Epoch 192

Average loss of: 4.497184923638997e-06 for train data

Epoch 193

Average loss of: 4.505026607876061e-06 for train data

Epoch 194

Average loss of: 4.509637728506277e-06 for train data

Epoch 195

Adapting learning rate to 0.0001875

Average loss of: 4.519046373070523e-06 for train data

Epoch 196

Average loss of: 4.798816825541507e-06 for train data

Epoch 197

Average loss of: 4.7493514348389e-06 for train data

Epoch 198

Average loss of: 4.7283954053455095e-06 for train data

Epoch 199

Average loss of: 4.699353774731208e-06 for train data

Epoch 200

Average loss of: 4.666806319710304e-06 for train data

Epoch 201

Average loss of: 4.6347091022198585e-06 for train data

Epoch 202

Average loss of: 4.603078894297142e-06 for train data

Epoch 203

Average loss of: 4.574633784159232e-06 for train data

Epoch 204

Average loss of: 4.543875713943635e-06 for train data

Epoch 205

Average loss of: 4.514921182817488e-06 for train data

Epoch 206

Average loss of: 4.487483666753178e-06 for train data

Epoch 207

Average loss of: 4.458408622895149e-06 for train data

Epoch 208

Average loss of: 4.432577651004976e-06 for train data

Epoch 209

Average loss of: 4.4061749761112875e-06 for train data

Epoch 210

Average loss of: 4.380593842870439e-06 for train data

Epoch 211

Average loss of: 4.355165206197853e-06 for train data

Epoch 212

Average loss of: 4.331876931109946e-06 for train data

Epoch 213

Average loss of: 4.308266906900826e-06 for train data

Epoch 214

Average loss of: 4.285617262712549e-06 for train data

Epoch 215

Average loss of: 4.2647557330838025e-06 for train data

Epoch 216

Average loss of: 4.241707698747632e-06 for train data

Epoch 217

Average loss of: 4.22214540863024e-06 for train data

Epoch 218

Average loss of: 4.201621145330137e-06 for train data

Epoch 219

Average loss of: 4.181467027456165e-06 for train data

Epoch 220

Average loss of: 4.164766159146893e-06 for train data

Epoch 221

Average loss of: 4.145655386855651e-06 for train data

Epoch 222

Average loss of: 4.127958874369142e-06 for train data

Epoch 223

Average loss of: 4.111037539360041e-06 for train data

Epoch 224

Average loss of: 4.093716415627569e-06 for train data

Epoch 225

Average loss of: 4.077746243092406e-06 for train data

Epoch 226

Average loss of: 4.063467345940808e-06 for train data
Epoch 227

Average loss of: 4.046672023241627e-06 for train data
Epoch 228

Average loss of: 4.030415008446653e-06 for train data
Epoch 229

Average loss of: 4.017784879442843e-06 for train data
Epoch 230

Average loss of: 4.004089162117453e-06 for train data
Epoch 231

Average loss of: 3.9904496365579686e-06 for train data
Epoch 232

Average loss of: 3.978054924027674e-06 for train data
Epoch 233

Average loss of: 3.965862314453262e-06 for train data
Epoch 234

Average loss of: 3.954346607542902e-06 for train data
Epoch 235

Average loss of: 3.94436814913206e-06 for train data
Epoch 236

Average loss of: 3.9309113998115205e-06 for train data
Epoch 237

Average loss of: 3.92147844640931e-06 for train data
Epoch 238

Average loss of: 3.909480834499845e-06 for train data

Epoch 239

Average loss of: 3.90025293513645e-06 for train data

Epoch 240

Average loss of: 3.892321731018455e-06 for train data

Epoch 241

Average loss of: 3.8806628784186615e-06 for train data

Epoch 242

Average loss of: 3.8733174015305846e-06 for train data

Epoch 243

Average loss of: 3.8634403361811566e-06 for train data

Epoch 244

Average loss of: 3.8544762806850485e-06 for train data

Epoch 245

Average loss of: 3.847848664281628e-06 for train data

Epoch 246

Average loss of: 3.837962621219049e-06 for train data

Epoch 247

Average loss of: 3.831052545001512e-06 for train data

Epoch 248

Average loss of: 3.822655921112528e-06 for train data

Epoch 249

Average loss of: 3.8126320198443863e-06 for train data

Epoch 250

Average loss of: 3.8070793309998408e-06 for train data

Epoch 251

Average loss of: 3.798285595030393e-06 for train data

Epoch 252

Average loss of: 3.7926820317352393e-06 for train data

Epoch 253

Average loss of: 3.784649699309739e-06 for train data

Epoch 254

Average loss of: 3.780779546696067e-06 for train data

Epoch 255

Average loss of: 3.7735328501184994e-06 for train data

Epoch 256

Average loss of: 3.7668829627364173e-06 for train data

Epoch 257

Average loss of: 3.7598787323076976e-06 for train data

Epoch 258

Average loss of: 3.755612909708361e-06 for train data

Epoch 259

Average loss of: 3.7492410499453398e-06 for train data

Epoch 260

Average loss of: 3.7439031388203146e-06 for train data

Epoch 261

Average loss of: 3.742016051819519e-06 for train data

Epoch 262

Average loss of: 3.7345511792409523e-06 for train data

Epoch 263

Average loss of: 3.7305419338281353e-06 for train data

Epoch 264

Average loss of: 3.7250204735755686e-06 for train data

Epoch 265

Average loss of: 3.7208038557764668e-06 for train data

Epoch 266

Average loss of: 3.7177993399836852e-06 for train data

Epoch 267

Average loss of: 3.712640654475763e-06 for train data

Epoch 268

Average loss of: 3.709693020027771e-06 for train data

Epoch 269

Average loss of: 3.7067859343096645e-06 for train data

Epoch 270

Average loss of: 3.702502267287855e-06 for train data

Epoch 271

Average loss of: 3.7005157046678505e-06 for train data

Epoch 272

Average loss of: 3.697227060820296e-06 for train data

Epoch 273

Average loss of: 3.694460673568756e-06 for train data

Epoch 274

Average loss of: 3.6925376539329593e-06 for train data

Epoch 275

Average loss of: 3.6885646137761795e-06 for train data

Epoch 276

Average loss of: 3.6852043720045914e-06 for train data

Epoch 277

Average loss of: 3.684051525169707e-06 for train data

Epoch 278

Average loss of: 3.67937466744479e-06 for train data

Epoch 279

Average loss of: 3.678786688533364e-06 for train data

Epoch 280

Average loss of: 3.6779632584512e-06 for train data

Epoch 281

Average loss of: 3.676450811235554e-06 for train data

Epoch 282

Average loss of: 3.6730487507156796e-06 for train data

Epoch 283

Average loss of: 3.6701292106045004e-06 for train data

Epoch 284

Average loss of: 3.6667008759195596e-06 for train data

Epoch 285

Average loss of: 3.6655883911407727e-06 for train data

Epoch 286

Average loss of: 3.666807380204773e-06 for train data
Epoch 287

Average loss of: 3.661311399901024e-06 for train data
Epoch 288

Average loss of: 3.662442101585839e-06 for train data
Epoch 289

Average loss of: 3.661395195967998e-06 for train data
Epoch 290

Average loss of: 3.6588935571671756e-06 for train data
Epoch 291

Average loss of: 3.65584195901647e-06 for train data
Epoch 292

Average loss of: 3.6557770094987065e-06 for train data
Epoch 293

Average loss of: 3.6515163474177827e-06 for train data
Epoch 294

Average loss of: 3.6525194370824467e-06 for train data
Epoch 295

Average loss of: 3.6489028341748054e-06 for train data
Epoch 296

Average loss of: 3.6487563101673003e-06 for train data
Epoch 297

Average loss of: 3.646621759799018e-06 for train data
Epoch 298

```
-----
Average loss of: 3.6462795758325227e-06 for train data

Epoch 299
-----
Average loss of: 3.643792116736222e-06 for train data

Epoch 300
-----
Average loss of: 3.645119373231864e-06 for train data

Epoch 301
-----
Average loss of: 3.643942443659398e-06 for train data

Epoch 302
-----
Average loss of: 3.6461167494053372e-06 for train data

Epoch 303
-----
Average loss of: 3.6451727042276616e-06 for train data

Epoch 304
-----
Adapting learning rate to 9.375e-05
Average loss of: 3.64919813441702e-06 for train data

Epoch 305
-----
Average loss of: 2.8318906649246855e-06 for train data

Epoch 306
-----
Average loss of: 2.9349710265250905e-06 for train data

Epoch 307
-----
Average loss of: 2.939577935262605e-06 for train data

Epoch 308
-----
Average loss of: 2.9206538072230616e-06 for train data

Epoch 309
-----
Average loss of: 2.8892379717490257e-06 for train data
```

Epoch 310

Average loss of: 2.8449544700379192e-06 for train data

Epoch 311

Average loss of: 2.7950253873541443e-06 for train data

Epoch 312

Average loss of: 2.738999089729077e-06 for train data

Epoch 313

Average loss of: 2.677050098077416e-06 for train data

Epoch 314

Average loss of: 2.61227552971377e-06 for train data

Epoch 315

Average loss of: 2.5506822186343926e-06 for train data

Epoch 316

Average loss of: 2.4872603275298387e-06 for train data

Epoch 317

Average loss of: 2.4265045177571663e-06 for train data

Epoch 318

Average loss of: 2.367329883804814e-06 for train data

Epoch 319

Average loss of: 2.311564687761347e-06 for train data

Epoch 320

Average loss of: 2.25548002144933e-06 for train data

Epoch 321

Average loss of: 2.206101162073537e-06 for train data

Epoch 322

Average loss of: 2.157522434094972e-06 for train data

Epoch 323

Average loss of: 2.1141210996574956e-06 for train data

Epoch 324

Average loss of: 2.0709267296524557e-06 for train data

Epoch 325

Average loss of: 2.035054795328506e-06 for train data

Epoch 326

Average loss of: 1.99908435351972e-06 for train data

Epoch 327

Average loss of: 1.9694231193625456e-06 for train data

Epoch 328

Average loss of: 1.9407838193501448e-06 for train data

Epoch 329

Average loss of: 1.9143136281854823e-06 for train data

Epoch 330

Average loss of: 1.8910067440856438e-06 for train data

Epoch 331

Average loss of: 1.8695493971335964e-06 for train data

Epoch 332

Average loss of: 1.8517013028713335e-06 for train data

Epoch 333

Average loss of: 1.8337185065320228e-06 for train data

Epoch 334

Average loss of: 1.8190200801427637e-06 for train data

Epoch 335

KeyboardInterrupt Traceback (most recent call last)

Input In [27], in <cell line: 20>()

29 print(f"\n Epoch {epoch_counter} \n -----")

30 # Train

---> 31 train_loop(train_dataloader, model, loss_fn, optimizer)

32 # Test on the training data

33 average_train_loss = test_loop(train_dataloader, model, loss_fn)

Input In [22], in train_loop(dataloader, model, loss_fn, optimizer,

↪report_progress)

9 # Backpropagation

10 optimizer.zero_grad()

---> 11 loss.backward()

12 optimizer.step()

14 # If we want to report progress during training (not recommended -

↪obstructs view)

File D:\Anaconda3\lib\site-packages\torch_tensor.py:487, in Tensor.

↪backward(self, gradient, retain_graph, create_graph, inputs)

477 if has_torch_function_unary(self):

478 return handle_torch_function(
479 Tensor.backward,
480 (self,),
(...)

485 inputs=inputs,
486)

--> 487 torch.autograd.backward(
488 self, gradient, retain_graph, create_graph, inputs=inputs
489)

489)

485 inputs=inputs,
486)

--> 487 torch.autograd.backward(
488 self, gradient, retain_graph, create_graph, inputs=inputs
489)

489)

488 self, gradient, retain_graph, create_graph, inputs=inputs
489)

File D:\Anaconda3\lib\site-packages\torch\autograd_init_.py:197, in

↪backward(tensors, grad_tensors, retain_graph, create_graph, grad_variables,

↪inputs)

192 retain_graph = create_graph

194 # The reason we repeat same the comment below is that

195 # some Python versions print out the first line of a multi-line function
196 # calls in the traceback and some print out the last line

196 # calls in the traceback and some print out the last line

--> 197

↪Variable._execution_engine.run_backward(# Calls into the C++ engine to run the backward pass

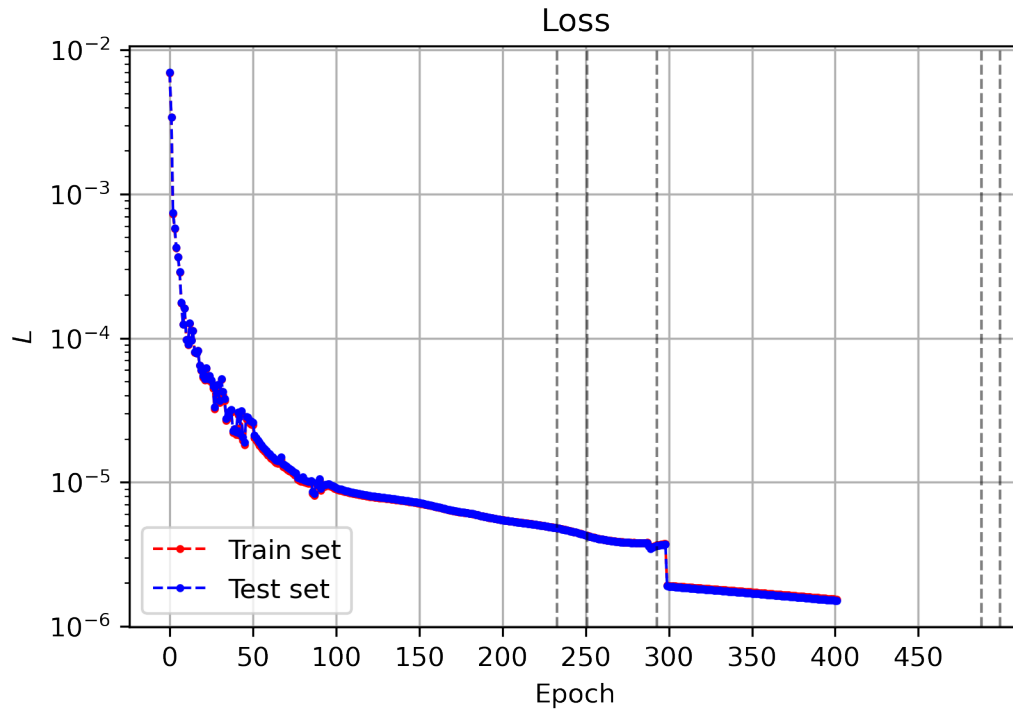
198 tensors, grad_tensors_, retain_graph, create_graph, inputs,

```
199 allow_unreachable=True, accumulate_grad=True)
```

KeyboardInterrupt:

5.1 Results of training

```
[20]: # Plot it
plt.figure()
lw = 1
ms = 2
plt.plot(train_losses, 'o--', color = 'red', label = 'Train set', lw = lw, ms = 2)
plt.plot(test_losses, 'o--', color = 'blue', label = "Test set", lw = lw, ms = 2)
plt.legend()
plt.grid()
plt.xlabel("Epoch")
xt_step = 50
xt = [i*xt_step for i in range(len(train_losses)//xt_step+2)]
plt.xticks(xt)
plt.ylabel(r'$L$')
plt.axhline(0, color = 'black', alpha = 0.7)
plt.title("Loss")
# Plot when we adapted learning rate
for t in adaptation_indices:
    plt.axvline(t+200, linestyle = "--", color = 'black', alpha = 0.5, lw = 1)
plt.yscale('log')
# plt.ylim(10**(-9))
# plt.savefig("Plots/NNC2Pv1.pdf", bbox_inches = 'tight')
plt.show()
```



6 Analyzing neural networks

We import NNC2Pv0, which beats the performance of the models in the paper.

```
[39]: NNC2P = torch.load('Models/NNC2Pv0.pth')
      model = NNC2P
```

6.1 Estimate the performance of the network

```
[40]: def L1_norm(predictions, y):
      """Here, predictions and y are arrays for one specific quantity, eg_
      ↪pressure. See table 1"""
      return sum(abs(predictions - y))/len(predictions)
```

```
[41]: def Linfty_norm(predictions, y):
      """Here, predictions and y are arrays for one specific quantity, eg_
      ↪pressure. See table 1"""
      return max(abs(predictions - y))
```

```
[67]: # Get features and labels
      test_features = test_data.features
      test_labels = test_data.labels
      test_features[:4]
```

```
[67]: [tensor([10.2041, 12.0266, 22.1313]),
      tensor([ 7.0046, 22.3374, 21.0772]),
      tensor([ 9.5747, 10.5188, 10.0152]),
      tensor([0.7725, 1.8519, 1.8100])]
```

```
[68]: test_features[0]
```

```
[68]: tensor([10.2041, 12.0266, 22.1313])
```

```
[43]: # Get predictions
      with torch.no_grad():
          p_hat= np.array([])
          for input_values in test_features:
              prediction = model(input_values)
              p_hat = np.append(p_hat, prediction[0].item())
```

```
[44]: # Get labels as np arrays
      p = np.array([])
      for value in test_labels:
          p = np.append(p, value[0].item())
```

```
[45]: # Get the errors:
      delta_p_L1 = L1_norm(p_hat, p)
      delta_p_Linf = Linfty_norm(p_hat, p)
```

```
[46]: print("Errors for p: %e with L1 and %e with Linfty" % (delta_p_L1,
      ↪delta_p_Linf))
```

Errors for p: 3.610137e-04 with L1 and 8.646600e-03 with Linfty

```
[67]: # torch.save(model, 'Models/NNC2Pv0.pth')
```

6.2 Estimate the performance on unseen/untrained cases:

Here, we check the performance whenever we use the model on values on which it wasn't trained. Is there a large error compared to the case of seen data?

6.2.1 When only one parameter gets outside of its range

```
[104]: # We are going to save the performance according to the ranges specified:
      # this dict is filled with the errors we found above
      errors_dict = {
          "rho_max": [rho_max],
          "eps_max": [eps_max],
          "v_max": [v_max],
          "L1": [delta_p_L1],
          "Linfty": [delta_p_Linf]}
```



```

# Get the parameters we are going to test

# This is how we are going to increment the upper bound each run
delta_rho = 0.01
delta_eps = 0.01
delta_v    = 0.001

number_of_runs = 100

# Construct the parameters
rho_list = [[rho_max + i*delta_rho, eps_max, v_max] for i in range(1,
↪number_of_runs)]
eps_list = [[rho_max, eps_max + i*delta_eps, v_max] for i in range(1,
↪number_of_runs)]
v_list = [[rho_max, eps_max, v_max + i*delta_v] for i in range(1,
↪number_of_runs)]

parameters_list = rho_list + eps_list + v_list

```

```

[105]: number_of_datapoints = 10000

p = []
phat = []

with torch.no_grad():
    # Iterate over all parameter bounds
    for [rho_bound, eps_bound, v_bound] in parameters_list:
        # Save current value:
        errors_dict["rho max"].append(rho_bound)
        errors_dict["eps max"].append(eps_bound)
        errors_dict["v max"].append(v_bound)

        # Now get 10 000 new cases and predictions
        for i in range(number_of_datapoints):

            # Sample randomly from the new range
            rho = random.uniform(rho_min, rho_bound)
            eps = random.uniform(eps_min, eps_bound)
            v    = random.uniform(v_min,          v_bound)

            # Get true value
            p.append(eos(rho, eps))

            # Get the prediction

            # Compute features (D, S, tau)
            Dvalue    = D(rho, eps, v)

```

```

Svalue      = S(rho, eps, v)
tauvalue    = tau(rho, eps, v)

# Get prediction
prediction = model(torch.tensor([Dvalue, Svalue, tauvalue]))
phat.append(prediction[0].item())

# All values computed, store the errors we found
L1 = L1_norm(np.array(p), np.array(phat))
errors_dict["L1"].append(L1)
Linfty= Linfty_norm(np.array(p), np.array(phat))
errors_dict["Linfty"].append(Linfty)

```

```

[110]: df = pd.DataFrame(errors_dict)
df

```

```

[110]:      rho max  eps max  v max      L1      Linfty
0      10.10     2.02  0.721  0.000361  0.008647
1      10.11     2.02  0.721  0.000368  0.008856
2      10.12     2.02  0.721  0.000367  0.010107
3      10.13     2.02  0.721  0.000370  0.010107
4      10.14     2.02  0.721  0.000367  0.010107
..      ...      ...      ...      ...      ...
293    10.10     2.02  0.816  0.004811  3.184771
294    10.10     2.02  0.817  0.004801  3.184771
295    10.10     2.02  0.818  0.004790  3.184771
296    10.10     2.02  0.819  0.004780  3.184771
297    10.10     2.02  0.820  0.004771  3.184771

```

[298 rows x 5 columns]

```

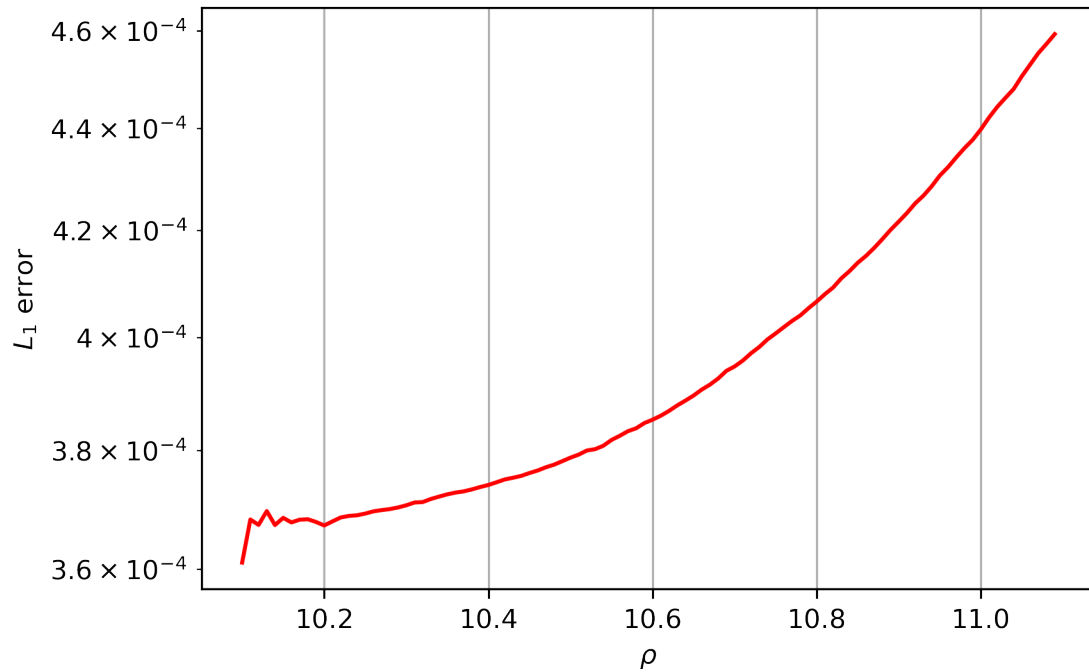
[114]: sub_df_rho = df.loc[(df["eps max"] == eps_max) & (df["v max"] == v_max)]
sub_df_eps = df.loc[(df["rho max"] == rho_max) & (df["v max"] == v_max)]
sub_df_v = df.loc[(df["rho max"] == rho_max) & (df["eps max"] == eps_max)]

```

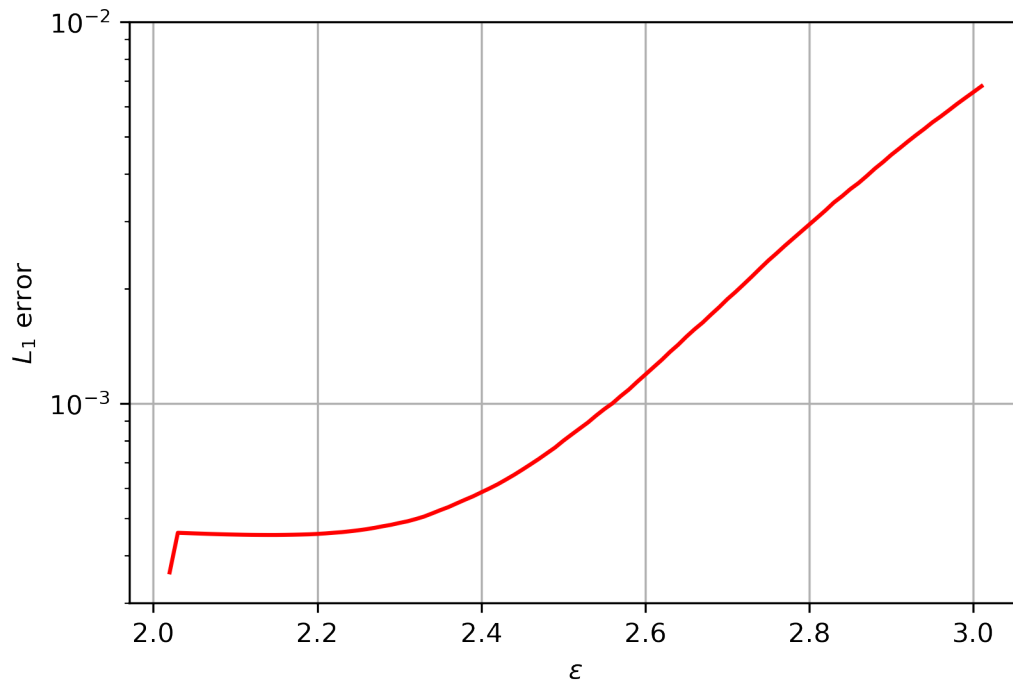
```

[119]: plt.plot(sub_df_rho["rho max"], sub_df_rho["L1"], color='red', label='rho')
# plt.legend()
plt.xlabel(r"$\rho$")
plt.ylabel(r"$L_1$ error")
plt.yscale('log')
plt.grid()
plt.savefig("error_analysis_v1_rho.pdf", bbox_inches='tight')
plt.show()

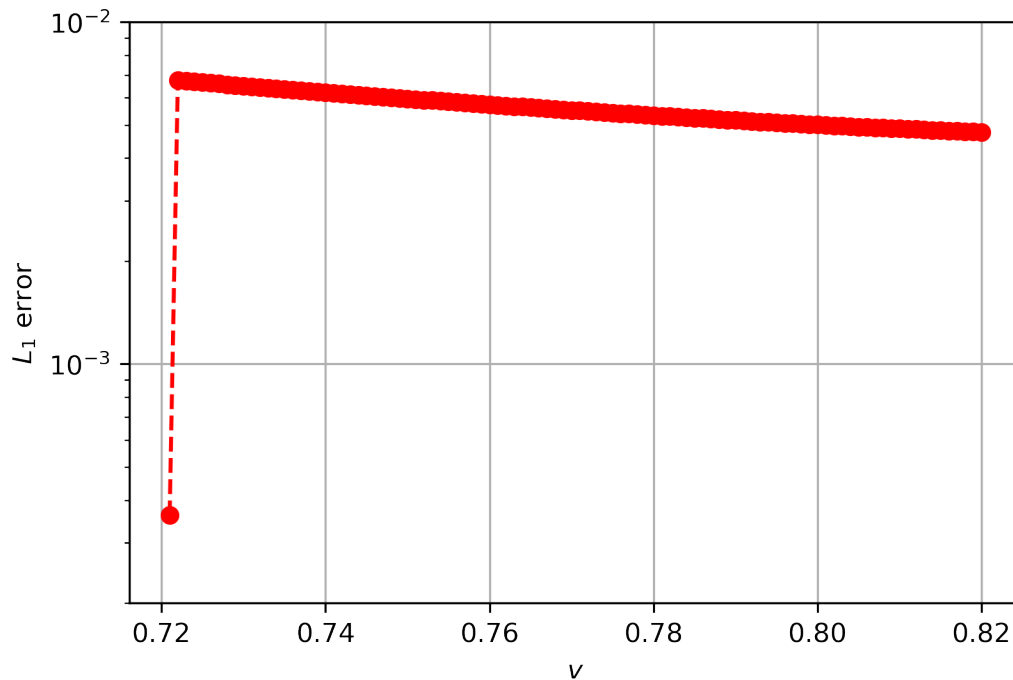
```



```
[130]: plt.plot(sub_df_eps["eps max"], sub_df_eps["L1"], color='red', label='rho')
# plt.legend()
plt.xlabel(r"$\epsilon$")
plt.ylabel(r"$L_1$ error")
plt.yscale('log')
plt.ylim(3*10**(-4), 10**(-2))
plt.grid()
plt.savefig("error_analysis_v1_eps.pdf", bbox_inches='tight')
plt.show()
```



```
[129]: plt.plot(sub_df_v["v max"], sub_df_v["L1"], '--o', color='red', label='rho')
# plt.legend()
plt.xlabel(r"$v$")
plt.ylabel(r"$L_1$ error")
plt.yscale('log')
plt.ylim(2*10**(-4), 10**(-2))
plt.grid()
plt.savefig("error_analysis_v1_v.pdf", bbox_inches='tight')
plt.show()
```



Save this data to process later on:

```
[107]: # df.to_csv("Data/errors_analysis_v2.csv")
```

```
[ ]:
```

6.2.2 When all parameters can go outside of their ranges

```
[136]: # We are going to save the performance according to the ranges specified:
# this dict is filled with the errors we found above
errors_dict = {
    "rho max": [rho_max],
    "eps max": [eps_max],
    "v max": [v_max],
    "L1": [delta_p_L1],
    "Linfty": [delta_p_Linfty]}

# Get the parameters we are going to test

# This is how we are going to increment the upper bound each run
delta_rho = 0.02
delta_eps = 0.02
delta_v    = 0.002

number_of_runs = 10
```

```

# Construct the parameters
rho_list = [rho_max + i*delta_rho for i in range(1, number_of_runs)]
eps_list = [eps_max + i*delta_eps for i in range(1, number_of_runs)]
v_list     = [v_max      + i*delta_v for i in range(1, number_of_runs)]

```

```

[138]: number_of_datapoints = 10000

p = []
phat = []

with torch.no_grad():
    # Iterate over all parameter bounds
    for rho_bound in rho_list:
        for eps_bound in eps_list:
            for v_bound in v_list:
                # Save current values:
                errors_dict["rho max"].append(rho_bound)
                errors_dict["eps max"].append(eps_bound)
                errors_dict["v max"].append(v_bound)

                # Now get 10 000 new cases and predictions
                for i in range(number_of_datapoints):

                    # Sample randomly from the new range
                    rho = random.uniform(rho_min, rho_bound)
                    eps = random.uniform(eps_min, eps_bound)
                    v     = random.uniform(v_min,          v_bound)

                    # Get true value
                    p.append(eos(rho, eps))

                    # Get the prediction

                    # Compute features (D, S, tau)
                    Dvalue = D(rho, eps, v)
                    Svalue = S(rho, eps, v)
                    tauvalue = tau(rho, eps, v)

                    # Get prediction
                    prediction = model(torch.tensor([Dvalue, Svalue, tauvalue]))

                    phat.append(prediction[0].item())

                # All values computed, store the errors we found
                L1 = L1_norm(np.array(p), np.array(phat))
                errors_dict["L1"].append(L1)

```

```

Linfty= Linfty_norm(np.array(p), np.array(phat))
errors_dict["Linfty"].append(Linfty)

```

```

[139]: df = pd.DataFrame(errors_dict)
df

```

```

[139]:      rho max  eps max  v max      L1      Linfty
0      10.10     2.02  0.721  0.000361  0.008647
1      10.12     2.04  0.723  0.000368  0.009280
2      10.12     2.04  0.725  0.000369  0.009725
3      10.12     2.04  0.727  0.000371  0.009725
4      10.12     2.04  0.729  0.000373  0.009725
..      ...      ...      ...      ...      ...
725    10.28     2.20  0.731  0.000463  0.135447
726    10.28     2.20  0.733  0.000463  0.135447
727    10.28     2.20  0.735  0.000463  0.135447
728    10.28     2.20  0.737  0.000464  0.135447
729    10.28     2.20  0.739  0.000464  0.135447

```

[730 rows x 5 columns]

```

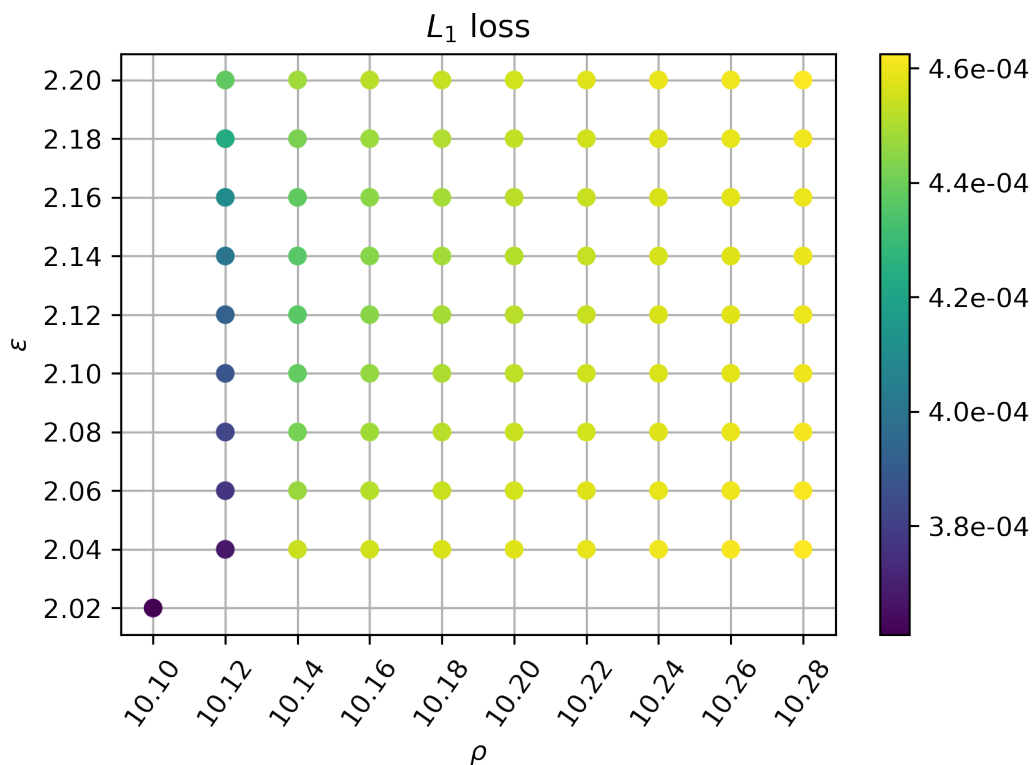
[150]: sub_df_rho_eps = df.loc[(df["v max"] == v_max) | (df["v max"] == v_max+delta_v)]
sub_df_rho_v = df.loc[(df["eps max"] == eps_max) | (df["eps max"] ==
↳eps_max+delta_eps)]
sub_df_eps_v = df.loc[(df["rho max"] == rho_max) | (df["rho max"] ==
↳rho_max+delta_rho)]

```

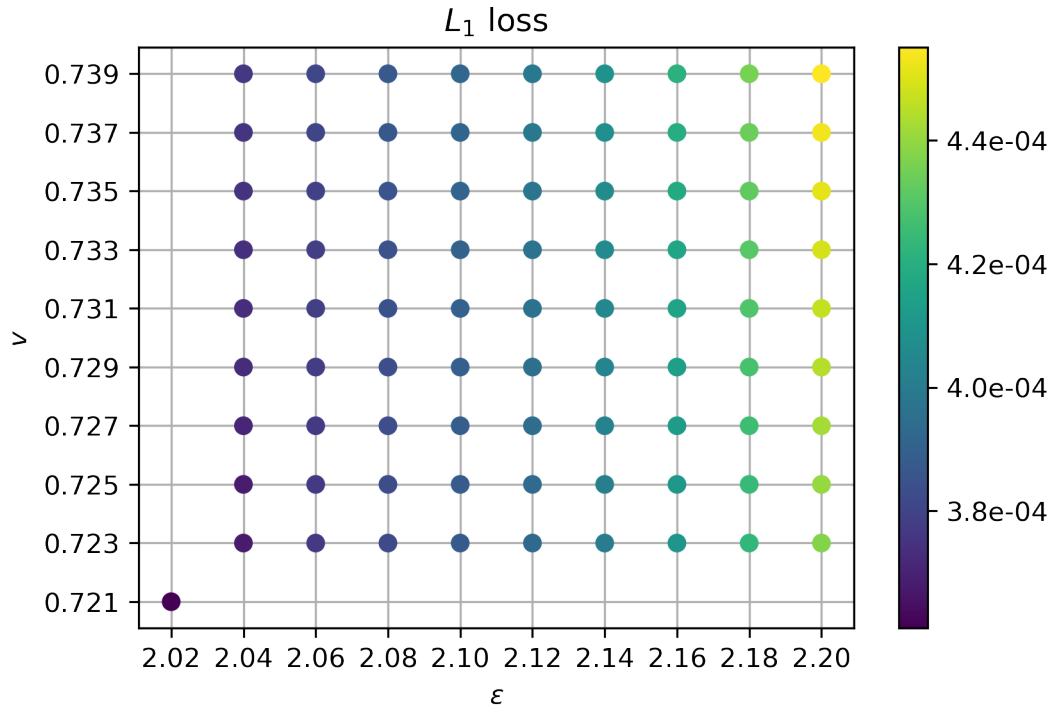
```

[178]: plt.scatter(sub_df_rho_eps["rho max"], sub_df_rho_eps["eps max"],
↳c=sub_df_rho_eps["L1"], zorder=5)
plt.colorbar(format='%0.1e')
plt.xlabel(r"$\rho$")
plt.ylabel(r"$\varepsilon$")
plt.xticks(list(set(sub_df_rho_eps["rho max"])), rotation=55)
plt.yticks(list(set(sub_df_rho_eps["eps max"])))
plt.grid()
plt.title(r"$L_1$ loss")
plt.savefig("error_analysis_rho_eps.pdf", bbox_inches='tight')
plt.show()

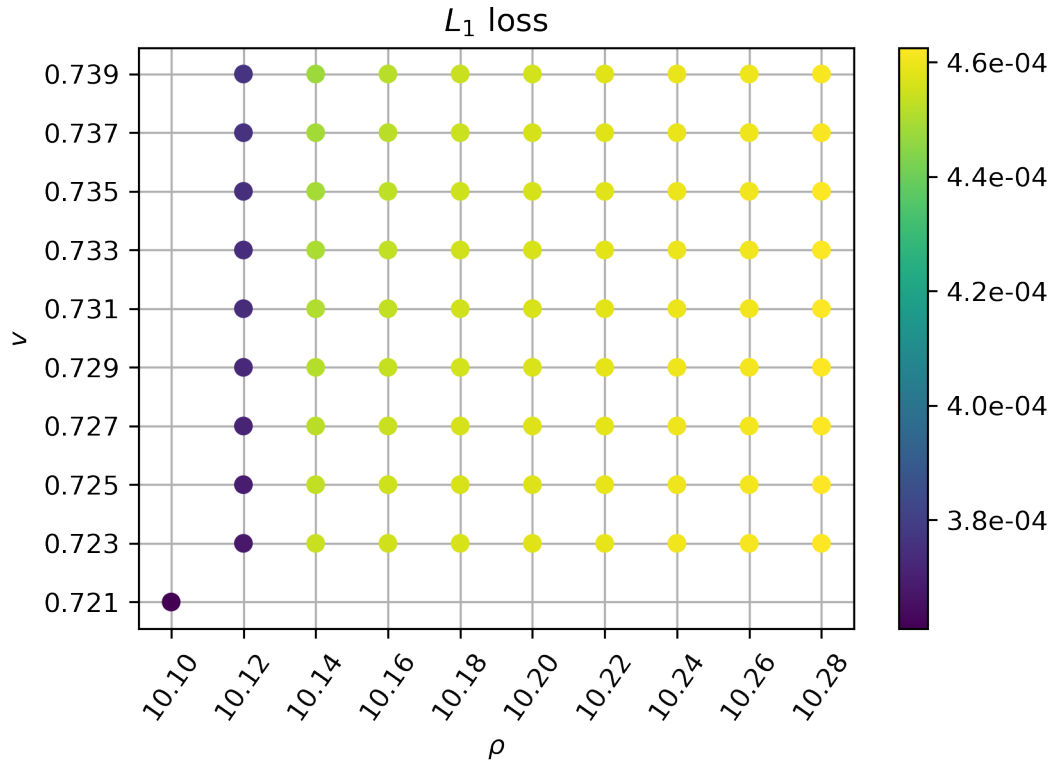
```



```
[180]: plt.scatter(sub_df_eps_v["eps max"], sub_df_eps_v["v max"],
                  c=sub_df_eps_v["L1"], zorder=5)
plt.colorbar(format='%0.1e')
plt.xticks(list(set(sub_df_eps_v["eps max"])))
plt.yticks(list(set(sub_df_eps_v["v max"])))
plt.grid()
plt.xlabel(r"$\varepsilon$")
plt.ylabel(r"$v$")
plt.title(r"$L_1$ loss")
plt.savefig("error_analysis_eps_v.pdf", bbox_inches='tight')
plt.show()
```

```
[184]: plt.scatter(sub_df_rho_v["rho max"], sub_df_rho_v["v max"], c=
    ↪sub_df_rho_v["L1"], zorder=5)
plt.colorbar(format='%0.1e')
plt.xlabel(r"$\rho$")
plt.xticks(list(set(sub_df_rho_v["rho max"])), rotation=55)
plt.yticks(list(set(sub_df_rho_v["v max"])))
plt.grid()
plt.ylabel(r"$v$")
plt.title(r"$L_1$ loss")
plt.savefig("error_analysis_rho_v.pdf", bbox_inches='tight')
plt.show()
```



```
[ ]: # plt.pcolormesh(X, Y, Z, cmap=plt.cm.get_cmap('Blues'))
```

Save this data to process later on:

```
[140]: # df.to_csv("Data/errors_analysis_v2.csv")
```

7 Get parameters of network out:

```
[47]: with torch.no_grad():
      for param in NNC2P.parameters():
          print(param)
```

Parameter containing:

```
tensor([[ -0.3637,  0.4540, -0.4355],
        [ 0.0066,  0.6949,  0.4879],
        [ 0.1112, -0.0925,  0.1091],
        ...,
        [ 0.5306, -0.4535, -0.3026],
        [-0.4308, -0.1415,  0.2810],
        [ 0.6349, -0.2947,  0.0561]], requires_grad=True)
```

Parameter containing:

```
tensor([ 0.5675,  0.2904, -0.7667, -0.3078, -0.1945,  0.0523,  0.0514, -0.4138,
```

0.2312, -0.5222, 0.2495, -0.3197, -0.4844, -0.5024, -0.3668, -0.2699,
 0.7860, 0.7489, 0.1024, 0.8798, 0.1536, -0.4353, -0.3389, -0.5969,
 -0.4334, -0.7355, -0.4756, -0.4140, -0.1220, -0.1788, -0.7250, -0.0075,
 0.2842, 0.1193, 0.5405, -0.1805, -0.0228, -0.3408, -0.1134, -0.2822,
 0.5498, -0.1406, 0.3311, -0.5858, 0.0567, -0.2661, 0.3879, 0.8417,
 -0.2426, 0.5311, 0.0035, 0.1361, -0.3355, 0.2191, -0.3657, 0.0739,
 -0.7668, -0.7611, -0.4528, 0.7155, 0.4711, 0.1546, -0.7966, -0.6006,
 0.5338, -0.4438, -0.5507, 0.2647, -0.5531, -0.1843, 0.6857, -0.1058,
 -0.2366, 0.5566, -0.2539, -0.0841, -0.2701, 0.1520, -0.3656, -0.0887,
 -0.3681, -0.4994, 0.1562, 0.0979, -0.1539, -0.2539, -0.3159, 0.2476,
 0.1437, 0.1037, -0.6092, -0.4861, 0.6079, -0.1717, 0.3969, -0.8278,
 -0.7750, 0.4500, 0.1029, 0.0236, 0.3942, -0.0011, -0.5502, -0.6392,
 -0.1455, -0.5056, -0.4315, -0.6536, -0.8086, 0.8507, -0.4151, -0.7212,
 -0.0891, 0.1468, -0.0913, 0.1593, -0.3147, -0.7297, 0.2530, -0.1589,
 -0.1999, 0.4665, -0.5153, -0.6170, -0.3868, 0.0854, 0.5496, 0.1570,
 -0.5972, 0.1290, -0.2804, -0.1617, -0.4747, -0.1994, 0.1695, -0.2299,
 0.5255, -0.7798, 0.7290, -0.1372, -0.0409, 0.4159, 0.2687, -0.6314,
 0.1840, -0.6343, -0.7727, 0.0432, 0.1978, 0.0018, -0.2912, 0.5889,
 0.1239, -0.5980, -0.3289, -0.4699, 0.1432, 0.6450, -0.4566, 0.6617,
 -0.5549, -0.7374, 0.2306, 0.9800, 0.1920, 0.5020, 0.2284, 0.2587,
 0.6900, 0.2306, 0.7923, -0.1113, 0.2198, 0.6304, 0.3187, 0.0511,
 -0.5725, -0.6510, -0.7051, -0.3080, -0.2263, -0.5543, -0.2684, -0.2800,
 -0.5838, 0.6659, -0.0447, -0.3244, -0.2777, 0.1524, 0.8192, -0.0718,
 -0.1331, 0.0362, -0.3517, 0.2572, 0.0893, -0.3430, -0.6010, -0.2209,
 0.4120, -0.5042, 0.1973, 0.0020, 0.2477, 0.2700, -0.6794, -0.2675,
 -0.3750, 0.3425, -0.0609, -0.0658, 0.3587, -0.2422, 0.3080, -0.7774,
 -0.0425, -0.1093, -0.6006, -0.4135, 0.0222, 0.0549, 0.4497, 0.2517,
 -0.0629, 0.4377, 0.3117, 0.3804, -0.8146, -0.1727, -0.0757, -0.4479,
 -0.3724, 0.2646, 0.2722, 0.2111, -0.4963, -0.7829, -0.1263, 0.1045,
 -0.4437, -0.4764, 0.0316, -0.6644, 0.0834, 0.5011, 0.3411, 0.3595,
 -0.5658, -0.4027, -0.5273, 0.2064, -0.2696, 0.1704, -0.7847, -0.4299,
 -0.5457, -0.2170, 0.5040, 0.1638, -0.2259, -0.1841, 0.3940, -0.1587,
 -0.0681, -0.5532, 0.0486, -0.0708, -0.0685, -0.1967, -0.6578, -0.0085,
 -0.5584, 0.3869, -0.3360, 0.0781, -0.4732, -0.4988, 0.5257, -0.0463,
 -0.5861, 0.0443, 0.3502, -0.3827, -0.0767, -0.4918, -0.0975, 0.0335,
 0.0242, -0.1530, 0.2708, 0.3870, -0.0407, -0.7733, -0.3965, 0.7103,
 -0.5266, -0.8473, -0.2814, 0.0634, -0.0469, 0.2093, -0.5929, 0.3147,
 0.7441, -0.2883, -0.4244, -0.4688, 0.7391, -0.2475, -0.2986, -0.7846,
 -0.5749, 0.6449, 0.5729, 0.0330, -0.7806, -0.3968, -0.1973, 0.8683,
 0.2063, 0.0795, -0.2172, -0.3743, -0.1792, 0.0273, -0.2719, -0.1724,
 0.5487, -0.2173, -0.5166, -0.8283, -0.5187, -0.2308, 0.0458, -0.0205,
 -0.0467, -0.6538, -0.0829, 0.0589, 0.0573, 0.3710, 0.1821, -0.6651,
 0.0139, 0.1801, -0.3490, -0.5684, 0.5960, 0.6916, -0.5211, -0.0705,
 -0.0245, 0.5548, -0.4998, 0.1310, 0.0123, 0.1382, 0.5340, -0.1300,
 0.0042, 0.0777, -0.8929, -0.2648, 0.1318, 0.1760, 0.0599, -0.4066,
 0.3279, 0.2792, -0.3842, 0.1425, -0.0647, -0.6798, -0.9598, 0.3412,
 -0.4429, -0.3725, 0.2720, 0.5411, 0.0429, -0.7045, 0.4488, 0.2515,
 0.4915, -0.2986, -0.0725, 0.8208, 0.0345, -0.4975, 0.2115, -0.3730,

```

-0.1543, 0.4633, -0.7425, 0.3975, -0.1460, -0.0902, 0.5782, -0.5746,
-0.0736, -0.8905, -0.1959, 0.3797, 0.6835, 0.4984, -0.0769, 0.2039,
0.5143, -0.4893, -0.5451, -0.5868, 0.8137, 0.5941, 0.1640, 0.2265,
-0.6311, 0.3958, -0.2065, -0.4971, -0.0210, -0.3891, -0.2294, -0.3468,
0.7438, -0.1030, 0.7179, -0.7436, -0.5150, 0.0701, -0.2541, 0.5022,
-0.7572, 0.0990, 0.1417, 0.1436, 0.0180, 0.0168, -0.4819, 0.8244,
-0.0125, -0.1109, -0.6625, 0.7918, -0.4478, -0.2006, 0.1864, -0.3666,
0.2405, 0.2242, -0.0725, -0.1479, -0.2050, 0.4549, 0.2757, -0.2656,
0.5447, 0.2885, 0.0163, -0.5062, -0.3655, -0.4252, -0.2810, -0.6262,
0.4720, -0.5443, -0.2816, 0.7436, 0.7959, -0.2127, 0.6045, 0.2159,
0.0723, 0.8628, 0.0749, 0.1937, -0.5478, -0.1131, 0.3797, 0.4071,
-0.5809, -0.6407, -0.6400, -0.3935, -0.7474, -0.2790, 0.1554, 0.1401,
0.4752, -0.2307, -0.5861, 0.6426, -0.3433, -0.5701, 0.1752, 0.4724,
-0.3654, 0.4743, 0.5474, 0.2260, -0.3306, -0.1384, 0.3962, -0.3417,
-1.0276, -0.4299, 0.2657, 0.1818, 0.3824, 0.1642, -0.1071, -0.1129,
0.1338, 0.3750, -0.0246, 0.2682, 0.6734, -0.4917, -0.8268, 0.1484,
-0.6909, -0.3862, 0.1191, 0.2251, 0.4636, -0.0899, 0.5847, -0.5227,
0.0309, -0.1919, -0.4084, 0.0564, 0.2178, 0.1525, -0.4559, -0.0342,
-0.1900, -0.2373, -0.0560, 0.3202, -0.2350, -0.1091, -0.2436, -0.0595,
-0.0075, 0.0434, 0.4786, 0.4589, -0.7814, -0.4575, -0.1438, 0.7816,
0.6213, -0.3059, -0.0335, 0.5486, -0.8782, -0.7016, 0.6680, -0.4792,
0.2301, 0.0706, -0.1901, -0.2882, -0.1218, 0.3371, -0.1424, -0.5664,
-0.3493, 0.2683, -0.4209, -0.1263, 0.1663, 0.3661, 0.0221, -0.0802,
0.8377, -0.8028, 0.1312, 0.5930, 0.0925, 0.5772, -0.3172, -0.2318,
0.3839, -0.3587, -0.1506, -0.2225, -0.3813, 0.3004, 0.5387, -0.0993,
0.1397, -0.2269, -0.4488, 0.6487, -0.3429, 0.7323, -0.6757, -0.1690],
requires_grad=True)
Parameter containing:
tensor([[[-0.2088, 0.0383, 0.0544, ..., -0.1030, 0.0783, -0.0014],
[ 0.0470, -0.0564, -0.0553, ..., 0.0203, -0.1165, -0.0557],
[-0.0048, -0.0284, -0.0800, ..., -0.0789, -0.0413, -0.0859],
...,
[ 0.0504, -0.0565, -0.0705, ..., 0.0052, -0.0812, -0.0857],
[ 0.0676, -0.0898, -0.0730, ..., 0.0324, -0.0613, -0.0054],
[-0.1756, 0.0118, 0.0710, ..., -0.0210, 0.0434, 0.0014]]],
requires_grad=True)
Parameter containing:
tensor([[-0.0270, -0.0241, -0.0302, -0.0111, -0.0253, 0.0092, -0.0516, -0.0816,
0.0336, -0.0337, -0.0481, 0.0434, -0.0189, 0.0027, -0.0539, -0.0060,
-0.0646, -0.0440, -0.0354, -0.0596, -0.0734, -0.0540, -0.0820, -0.0217,
-0.0141, -0.0055, -0.0674, 0.0044, -0.0344, -0.0741, 0.0176, -0.0616,
-0.0446, -0.0020, -0.0306, -0.0233, -0.0305, -0.0373, -0.0475, -0.0744,
0.0541, -0.0632, -0.0144, -0.0232, -0.0255, 0.0226, -0.0348, -0.0434,
-0.0581, 0.0095, -0.0401, -0.0386, -0.0368, 0.0169, 0.0336, -0.0220,
0.0518, -0.0205, 0.0081, -0.0749, -0.0333, -0.0069, -0.0173, 0.0392,
0.0175, -0.0278, 0.0328, 0.0343, -0.0011, -0.0501, -0.0517, -0.0325,
-0.0284, -0.0531, 0.0279, -0.0292, 0.0079, -0.0678, -0.0238, -0.0258,
-0.0790, 0.0158, -0.0643, 0.0079, -0.0183, 0.0297, 0.0061, 0.0364,

```

```

-0.0228, -0.0035, 0.0068, -0.0856, -0.0804, 0.0039, -0.0382, -0.0563,
-0.0724, 0.0061, -0.0240, -0.0852, -0.0255, -0.0267, 0.0112, -0.0661,
-0.0289, -0.0278, -0.0946, 0.0428, -0.0398, -0.0250, -0.0035, 0.0147,
-0.0032, -0.0094, -0.0720, -0.0195, -0.0702, -0.0429, 0.0336, -0.0590,
0.0109, 0.0078, -0.0717, -0.0769, -0.0308, -0.0152, 0.0234, 0.0287,
-0.0626, -0.0299, 0.0259, 0.0166, -0.0485, -0.0169, -0.0319, 0.0128,
0.0126, 0.0150, -0.0164, 0.0116, -0.0582, 0.0241, -0.0376, 0.0374,
-0.0056, -0.0238, -0.0540, 0.0336, -0.0016, -0.0473, -0.0338, -0.0415,
-0.0025, -0.0549, 0.0414, -0.0718, -0.0048, -0.0709, 0.0092, -0.0428,
-0.0446, -0.0539, 0.0246, -0.0199, -0.0679, -0.0330, -0.0509, -0.0346,
-0.0404, 0.0587, 0.0257, 0.0199, 0.0176, 0.0247, -0.0360, 0.0113,
-0.0526, 0.0746, -0.0126, 0.0148, -0.0180, 0.0308, -0.0730, 0.0025,
-0.0178, -0.0758, 0.0204, -0.0438, 0.0013, 0.0851, -0.0482, -0.0559,
-0.0076, -0.0415, 0.0245, 0.0066, 0.0124, -0.0645, -0.0227, -0.0411],
requires_grad=True)
Parameter containing:
tensor([[ 0.1627, -0.0709, 0.0123, 0.3133, -0.0664, 0.1463, 0.1598, -0.0656,
         0.1418, 0.1590, -0.0636, 0.1596, -0.0613, 0.1870, 0.2146, 0.1589,
        -0.0531, 0.1655, 0.2035, -0.0812, 0.2130, -0.0660, -0.0634, 0.1614,
        -0.0514, 0.1856, -0.0662, -0.0870, -0.0564, -0.0592, -0.0726, 0.2121,
        -0.0452, -0.0451, -0.0661, 0.1536, -0.0549, -0.0531, -0.0767, -0.0604,
         0.0218, 0.1820, -0.0688, -0.0404, 0.1659, 0.1630, 0.1711, 0.1666,
        -0.0629, 0.1867, 0.1757, -0.0653, -0.0009, -0.0835, 0.1746, 0.1658,
         0.1263, 0.1652, 0.1826, 0.2197, -0.0461, -0.0854, 0.1609, 0.1759,
         0.1829, 0.1776, 0.1510, 0.1660, 0.1700, 0.2523, -0.0616, 0.1798,
         0.2320, 0.1671, 0.1840, -0.0574, 0.1818, 0.1700, -0.0544, -0.0604,
        -0.0597, 0.1765, 0.1576, 0.1636, 0.1670, 0.1743, 0.1496, 0.1805,
        -0.0265, -0.0614, 0.1608, -0.0620, -0.0661, -0.0646, -0.0664, -0.0510,
        -0.0638, 0.1882, 0.1827, -0.0636, 0.1784, 0.1607, 0.1750, -0.0586,
         0.2005, 0.1738, -0.0557, 0.1631, -0.0659, -0.0593, 0.1661, 0.2004,
         0.1617, -0.0612, -0.0625, -0.0604, -0.0643, 0.1516, 0.1590, -0.0466,
         0.1747, -0.0753, 0.2033, -0.0531, -0.0683, -0.0731, 0.1523, 0.1447,
         0.1618, -0.0730, 0.1459, 0.1990, -0.0332, -0.0622, -0.0709, 0.1701,
         0.1877, -0.0721, -0.0712, 0.1784, 0.1617, -0.0757, 0.1658, 0.1736,
         0.1609, -0.0745, 0.0118, 0.1497, 0.2044, 0.1691, 0.1669, 0.1960,
        -0.0650, 0.1632, 0.1851, -0.0569, 0.1556, 0.1992, 0.1768, -0.0513,
        -0.0658, 0.1782, 0.2142, 0.1588, -0.0646, 0.1558, 0.1586, -0.0601,
        -0.0669, 0.0652, 0.1553, -0.0779, 0.1668, 0.1606, -0.0585, 0.1972,
        -0.0570, 0.2067, 0.1678, 0.1546, -0.0296, 0.1642, -0.0804, -0.0662,
        -0.0473, -0.0452, 0.1472, -0.0654, 0.1412, 0.1047, -0.0688, -0.0658,
        -0.0858, 0.2038, 0.1444, 0.1963, 0.1914, -0.0606, -0.0622,
        0.1813]],
requires_grad=True)
Parameter containing:
tensor([0.1309], requires_grad=True)

```

[]: