# **NNEOSB**

# November 2, 2022

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	in point in	<pre>mport numpy as np mport matplotlib.pyplot as plt lt.rcParams['figure.dpi'] = 300 mport random mport csv mport pandas as pd mport torch rom torch import nn # pytorch neural networks rom torch.utils.data import Dataset, DataLoader # pytorch dataset structures rom torch.utils.data import ToTensor # pytorch transformer from torch.utils.data import DataLoader from torchvision import datasets from torchvision.transforms import ToTensor</pre>	

# 1 Introduction

The conserved variables are  $(D, S_i, \tau)$  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:

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

where we used

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

Our first goal is to reproduce the results from this paper. We first focus on what they call **NNEOS** networks. These are networks which are trained to infer information on the equation of state (EOS). In its simplest form, the EOS is the thermodynamical relation connecting the pressure to the fluid's rest-mass density and internal energy  $p = \bar{p}(\rho, \epsilon)$ . We consider an **analytical**  $\Gamma$ -law **EOS** as a benchmark:

$$\bar{p}(\rho,\varepsilon) = (\Gamma - 1)\rho\epsilon$$
, (3)

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

# 2 Generating training data

We generate training data for the NNEOS networks as follows. We create a training set by randomly sampling the EOS on a uniform distribution over  $\rho \in (0, 10.1)$  and  $\epsilon \in (0, 2.02)$ . Below, we first focus on the implementation of **NNEOSB** as called in the paper, meaning we also make the derivatives of the EOS part of the output. So we compute three quantities:

- p, using the EOS defined above
- $\chi := \partial p/\partial \rho$ , inferred from the EOS
- $\kappa := \partial p/\partial \epsilon$ , inferred from the EOS

```
[2]: # 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 chi(rho, eps, Gamma = 5/3):
    """Computes dp/drho from EOS"""
    return (Gamma - 1) * eps

def kappa(rho, eps, Gamma = 5/3):
    """Computes dp/deps from EOS"""
    return (Gamma - 1) * rho
```

```
[3]: # 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
```

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

```
[4]: # number_of_datapoints = 10000 # 80 000 for train, 10 000 for test
# data = []

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

```
# new_row = [rho, eps, eos(rho, eps), chi(rho, eps), kappa(rho, eps)]
# data.append(new_row)
```

```
[5]: # header = ['rho', 'eps', 'p', 'chi', 'kappa']

# with open('NNEOS_data_test.csv', 'w', newline = '') as file:

# writer = csv.writer(file)

# # write header

# writer.writerow(header)

# # write data

# writer.writerows(data)
```

```
[6]: # Import data
data_train = pd.read_csv("data/NNEOS_data_train.csv")
data_test = pd.read_csv("data/NNEOS_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

```
[6]:
                 rho
                                              chi
                                                      kappa
                           eps
                                      р
    0
            9.770794 0.809768 5.274717 0.539845 6.513863
    1
           10.093352 0.575342 3.871421 0.383561 6.728901
    2
            1.685186 1.647820 1.851255
                                         1.098547 1.123457
    3
            1.167718  0.408377  0.317913  0.272251  0.778479
            7.750848 1.069954 5.528700 0.713303 5.167232
            3.985951 1.642317 4.364131 1.094878 2.657301
    79995
    79996
            6.948815  0.809021  3.747824  0.539347  4.632543
    79997
            8.423227 1.125142 6.318217 0.750095 5.615485
    79998
            4.748173 0.774870 2.452810 0.516580 3.165449
    79999
            2.927483   0.616751   1.203686   0.411167   1.951655
```

[80000 rows x 5 columns]

In case we want to visualize the datapoints (not useful, nothing significant happening).

```
[7]: # rho = data_train['rho']
# eps = data_train['eps']

# plt.figure(figsize = (12,10))
# plt.plot(rho, eps, 'o', color = 'black', alpha = 0.005)
# plt.grid()
# plt.xlabel(r'$\rho$')
```

```
# plt.ylabel(r'$\epsilon$')
# plt.title('Training data')
# plt.show()
```

# 3 Getting data into PyTorch's DataLoader

Below: all\_data is of the type  $(\rho, \epsilon, p, \chi, \kappa)$  as generated above.

```
[8]: class CustomDataset(Dataset):
         """See PyTorch tutorial: the following three methods HAVE to be\Box
      \hookrightarrow 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['rho'][i], all_data['eps'][i]]
                 features.append(torch.tensor(new_feature, dtype = torch.float32))
                 # Separate the labels
                 new_label = [all_data['p'][i], all_data['chi'][i],__
      →all_data['kappa'][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)
         # TODO: I don't understand transform and target_transform --- but this is_{\sqcup}
      ⇔not used now!
         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.

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

[10]: # Check if this is done correctly
    print(training_data.features[:2])
    print(training_data.labels[:2])
    print(training_data.__len__())
    print(test_data.__len__())

[tensor([9.7708, 0.8098]), tensor([10.0934, 0.5753])]
    [tensor([5.2747, 0.5398, 6.5139]), tensor([3.8714, 0.3836, 6.7289])]
    80000
    10000

[11]: # Now call DataLoader on the above CustomDataset instances:
    train dataloader = DataLoader(training data, batch size=32)
```

# 4 Building the neural networks

test\_dataloader = DataLoader(test\_data, batch\_size=32)

We will follow this part of the PyTorch tutorial. For more information, see the documentation page of torch.nn. We take the parameters of NNEOSB in the paper, see Table 1. Question: I'm not sure how the ReLU at the output layer is done... For now, we just use sigmoids in the hidden layers. To do check other activation functions.

# 5 Training the neural network

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

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

NeuralNetwork(
    (stack): Sequential(
        (0): Linear(in_features=2, out_features=400, bias=True)
        (1): Sigmoid()
        (2): Linear(in_features=400, out_features=600, bias=True)
        (3): Sigmoid()
        (4): Linear(in_features=600, out_features=3, bias=True)
        )
}
```

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. Question: how many epochs should be used? What size for the batches,...

```
[14]: # Save hyperparameters here --- see paper!!!
learning_rate = 6e-4
batch_size = 32
epochs = 200
# Initialize the loss function
loss_fn = nn.MSELoss()
optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)
```

The train and test loops are implemented below (copy pasted from this part of the tutorial):

```
[15]: 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 \neg\sqcup
 ⇔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
```

The following function allows us to select a subset of the training data with the same size as the training set (if desired) and use it as a separate test set. **Question:** will the authors have computed the loss on the *whole* training set, or 10 000 random instances sampled from the training set?

```
[16]: def get_subset_train_dataloader(data_train, size = 10000):

"""Creates a 'subset' of dataloader for computing loss on training data.

This way we can 'test' on training data too - to check the claim of the

paper about overfitting. """

# Get random ids to sample

random_ids = np.random.choice(len(data_train), size, replace=False)

# the following is a pandas dataframe

sampled_train_data = data_train.iloc[random_ids]
```

```
# relabel the indices
          sampled_train_data.index = [i for i in range(len(sampled_train_data))]
          new_dataset = CustomDataset(sampled_train_data)
          # Make it a dataloader and return it
          new_dataloader = DataLoader(new_dataset, batch_size=32)
          return new_dataloader
[17]: # Testing to see if this works!
      hey = [i for i in range(15)]
      print(hey)
      print(hey[-5:], len(hey[-5:]))
      print(hey[-10:-5], len(hey[-10:-5]))
     [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]
     [10, 11, 12, 13, 14] 5
     [5, 6, 7, 8, 9] 5
[18]: # Train the model!
      test_losses = []
      train_losses = []
      counter = -5 # we skip the very first few iterations before changing learning ⊔
       \rightarrowrate
      adaptation_threshold = 0.0005 # 0.05 % (paper)
      adaptation_indices = []
      print("Training the model . . .")
      for t in range(epochs):
          # Train
          train_loop(train_dataloader, model, loss_fn, optimizer)
          average_test_loss = test_loop(test_dataloader, model, loss_fn)
          test_losses.append(average_test_loss)
          # Also test on the training data
          subset = get_subset_train_dataloader(data_train)
          # test on this subset
          average_train_loss = test_loop(subset, model, loss_fn)
          train_losses.append(average_train_loss)
          # Update the learning rate - see Appendix B of the paper
          # only check if update needed after 10 epochs
          if counter >= 10:
              current_average = np.mean(test_losses[-5:])
              previous average = np.mean(test losses[-10:-5])
              # If we did not improve the test loss sufficiently, going to adapt LR
```

```
if current_average/previous_average >= 0.05:
             # Reset counter (note: will increment later, so set to -1 st it_{\sqcup}
  ⇒becomes 0)
            counter = -1
            learning_rate = 0.5*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(t)
    # Another epoch passed - increment counter
    counter += 1
    # Report progress:
    print(f"\n Epoch {t+1} \n -----")
    print(f"Average loss of: {average_test_loss} for test data")
    print(f"Average loss of: {average_train_loss} for train data")
print("Done!")
Training the model . . .
Epoch 1
Average loss of: 0.0017823913499501686 for test data
Average loss of: 0.0017260212710457513 for train data
Epoch 2
 _____
Average loss of: 0.0004918487218488305 for test data
Average loss of: 0.0004916590779421691 for train data
Epoch 3
Average loss of: 0.0001674860643060021 for test data
Average loss of: 0.00016857311222553492 for train data
Epoch 4
Average loss of: 6.980137053972703e-05 for test data
Average loss of: 6.803461293455216e-05 for train data
Epoch 5
Average loss of: 0.0017871337313466846 for test data
Average loss of: 0.0017906745680765555 for train data
```

# Epoch 6 \_\_\_\_\_ Average loss of: 0.00014033970706549417 for test data Average loss of: 0.00014054515291084968 for train data Epoch 7 Average loss of: 0.0010092918587753328 for test data Average loss of: 0.0009967701188987866 for train data Epoch 8 Average loss of: 4.778926101837347e-05 for test data Average loss of: 4.679444930933679e-05 for train data Epoch 9 Average loss of: 0.003728222890426747 for test data Average loss of: 0.0037496253839149453 for train data Epoch 10 Average loss of: 0.00043513274912651 for test data Average loss of: 0.00043189073890483325 for train data Epoch 11 \_\_\_\_\_ Average loss of: 0.0010971768069997453 for test data Average loss of: 0.0010885801900865529 for train data Epoch 12 Average loss of: 0.00010233953938363477 for test data Average loss of: 0.00010126772785400109 for train data Epoch 13 Average loss of: 3.383543650871113e-05 for test data Average loss of: 3.406924012572893e-05 for train data Epoch 14 \_\_\_\_\_ Average loss of: 9.073701172098391e-06 for test data Average loss of: 8.823581257905326e-06 for train data

Epoch 15

Average loss of: 1.1161160966349443e-05 for test data

Average loss of: 1.1051952772565613e-05 for train data

#### Epoch 16

-----

Average loss of: 0.00010027311113133012 for test data Average loss of: 9.89542253528009e-05 for train data

#### Epoch 17

\_\_\_\_\_

Average loss of: 1.7420071030712348e-05 for test data Average loss of: 1.702395224791357e-05 for train data

## Epoch 18

-----

Average loss of: 1.013671858388919e-05 for test data Average loss of: 9.70077214475668e-06 for train data Adapting learning rate to 0.0003

## Epoch 19

-----

Average loss of: 1.0052255467203845e-05 for test data Average loss of: 9.654529601455568e-06 for train data

## Epoch 20

\_\_\_\_\_

Average loss of: 8.374545058658508e-06 for test data Average loss of: 8.199265211530587e-06 for train data

#### Epoch 21

-----

Average loss of: 1.2378793755964546e-05 for test data Average loss of: 1.2429277864376867e-05 for train data

# Epoch 22

-----

Average loss of: 5.489215645604836e-06 for test data Average loss of: 5.447202713225787e-06 for train data

# Epoch 23

-----

Average loss of: 5.141209373705758e-06 for test data Average loss of: 5.073710837951075e-06 for train data

#### Epoch 24

\_\_\_\_\_

Average loss of: 4.148107721015514e-06 for test data Average loss of: 4.072896935338013e-06 for train data

# Epoch 25 \_\_\_\_\_ Average loss of: 5.263829167413936e-06 for test data Average loss of: 5.160126716763074e-06 for train data Epoch 26 Average loss of: 3.522602074821343e-06 for test data Average loss of: 3.4254739040797302e-06 for train data Epoch 27 Average loss of: 7.905531073136578e-06 for test data Average loss of: 7.949140630728924e-06 for train data Epoch 28 Average loss of: 6.235866153518076e-06 for test data Average loss of: 6.179988064488248e-06 for train data Epoch 29 Average loss of: 2.9153932721931542e-06 for test data Average loss of: 2.8753999995620315e-06 for train data Adapting learning rate to 0.00015 Epoch 30 \_\_\_\_\_ Average loss of: 7.88133109718371e-06 for test data Average loss of: 7.816045280677893e-06 for train data Epoch 31 Average loss of: 4.24673103457818e-06 for test data Average loss of: 4.179012048059002e-06 for train data Epoch 32 Average loss of: 2.6462546912762408e-06 for test data Average loss of: 2.575691082101069e-06 for train data Epoch 33

Average loss of: 4.111713299668821e-06 for test data Average loss of: 4.103939334137872e-06 for train data

Epoch 34 ----- Average loss of: 1.5616023918660074e-06 for test data Average loss of: 1.4305276898756365e-06 for train data

#### Epoch 35

-----

Average loss of: 2.921958694335912e-06 for test data Average loss of: 2.9321225867487448e-06 for train data

#### Epoch 36

\_\_\_\_\_

Average loss of: 2.6446220128067166e-06 for test data Average loss of: 2.635567590969643e-06 for train data

#### Epoch 37

-----

Average loss of: 4.141676849606109e-06 for test data Average loss of: 4.150908116949118e-06 for train data

#### Epoch 38

-----

Average loss of: 1.9740436819381593e-06 for test data Average loss of: 1.9758612170219024e-06 for train data

## Epoch 39

\_\_\_\_\_

Average loss of: 3.6239909652718464e-06 for test data Average loss of: 3.6384054204008223e-06 for train data

#### Epoch 40

-----

Average loss of: 1.1076798044816238e-06 for test data Average loss of: 1.0783792916186393e-06 for train data Adapting learning rate to 7.5e-05

#### Epoch 41

-----

Average loss of: 1.6888753684100356e-06 for test data Average loss of: 1.6698498466967677e-06 for train data

#### Epoch 42

-----

Average loss of: 2.6453087931773093e-06 for test data Average loss of: 2.6791487947740882e-06 for train data

# Epoch 43

\_\_\_\_\_

Average loss of: 3.4960457836999336e-06 for test data Average loss of: 3.5052631543707024e-06 for train data

## Epoch 44

\_\_\_\_\_

Average loss of: 2.464926109069303e-06 for test data Average loss of: 2.450544416089728e-06 for train data

#### Epoch 45

\_\_\_\_\_

Average loss of: 2.6518469312054477e-06 for test data Average loss of: 2.5819985313746337e-06 for train data

#### Epoch 46

\_\_\_\_\_

Average loss of: 3.906813404659661e-06 for test data Average loss of: 3.942644100559486e-06 for train data

## Epoch 47

-----

Average loss of: 1.8710323491921273e-06 for test data Average loss of: 1.813160674290835e-06 for train data

#### Epoch 48

-----

Average loss of: 2.0092966489331543e-06 for test data Average loss of: 2.011616749940457e-06 for train data

#### Epoch 49

-----

Average loss of: 1.8069462299309452e-06 for test data Average loss of: 1.796225814659077e-06 for train data

#### Epoch 50

-----

Average loss of: 2.2076530924165743e-06 for test data Average loss of: 2.1852336277761104e-06 for train data

## Epoch 51

-----

Average loss of: 2.1473438889011153e-06 for test data Average loss of: 2.1259425527289435e-06 for train data Adapting learning rate to 3.75e-05

#### Epoch 52

-----

Average loss of: 2.0926544916488845e-06 for test data Average loss of: 2.0251650464826188e-06 for train data

## Epoch 53

-----

Average loss of: 2.713061472043943e-06 for test data Average loss of: 2.7216986704509135e-06 for train data

Epoch 54

\_\_\_\_\_

Average loss of: 2.6419167255381108e-06 for test data Average loss of: 2.6403614972256302e-06 for train data

Epoch 55

-----

Average loss of: 2.7357749519133256e-06 for test data Average loss of: 2.743939059071479e-06 for train data

Epoch 56

-----

Average loss of: 2.7603601431848347e-06 for test data Average loss of: 2.754117815765931e-06 for train data

Epoch 57

-----

Average loss of: 1.4894148708204018e-06 for test data Average loss of: 1.4259529771094186e-06 for train data

Epoch 58

-----

Average loss of: 9.381144171713615e-07 for test data Average loss of: 9.058513226594363e-07 for train data

Epoch 59

-----

Average loss of: 1.1697984415315758e-06 for test data Average loss of: 1.1630199945904487e-06 for train data

Epoch 60

-----

Average loss of: 2.636883913112161e-06 for test data Average loss of: 2.6388132946144345e-06 for train data

Epoch 61

-----

Average loss of: 8.593646336053664e-07 for test data Average loss of: 8.434105359755719e-07 for train data

Epoch 62

-----

Average loss of: 2.7426770142215964e-06 for test data Average loss of: 2.774399296632704e-06 for train data

## Adapting learning rate to 1.875e-05

# Epoch 63 Average loss of: 1.0521505595179608e-06 for test data Average loss of: 1.0382492573539051e-06 for train data Epoch 64 Average loss of: 1.6617349013321715e-07 for test data Average loss of: 1.619047445830639e-07 for train data Epoch 65 Average loss of: 1.6254727866296412e-07 for test data Average loss of: 1.5548895876777393e-07 for train data Epoch 66 \_\_\_\_\_ Average loss of: 1.583920994420305e-07 for test data Average loss of: 1.4738991364702552e-07 for train data Epoch 67 Average loss of: 1.54470954303945e-07 for test data Average loss of: 1.4565095642883143e-07 for train data Epoch 68 Average loss of: 1.5080221739578183e-07 for test data Average loss of: 1.5114684005491002e-07 for train data Epoch 69 Average loss of: 1.4854311697041693e-07 for test data Average loss of: 1.4063483666078695e-07 for train data Epoch 70 Average loss of: 1.4985146002447638e-07 for test data Average loss of: 1.5024343019822496e-07 for train data Epoch 71 \_\_\_\_\_ Average loss of: 1.5591955552020643e-07 for test data Average loss of: 1.4740863653891698e-07 for train data

Epoch 72

-----

Average loss of: 1.5990364150997055e-07 for test data Average loss of: 1.5477942037168526e-07 for train data

#### Epoch 73

\_\_\_\_\_

Average loss of: 1.6269609886513208e-07 for test data Average loss of: 1.540805494694639e-07 for train data Adapting learning rate to 9.375e-06

#### Epoch 74

-----

Average loss of: 1.6322777613319418e-07 for test data Average loss of: 1.5965061597050784e-07 for train data

#### Epoch 75

-----

Average loss of: 9.422505023723553e-08 for test data Average loss of: 9.148482027026743e-08 for train data

#### Epoch 76

\_\_\_\_\_

Average loss of: 9.287588048722953e-08 for test data Average loss of: 1.0558500117811261e-07 for train data

#### Epoch 77

-----

Average loss of: 9.144670154803124e-08 for test data Average loss of: 8.615748381685762e-08 for train data

#### Epoch 78

-----

Average loss of: 9.014431044713714e-08 for test data Average loss of: 7.97972905019968e-08 for train data

#### Epoch 79

\_\_\_\_\_

Average loss of: 8.894785228988123e-08 for test data Average loss of: 8.56435939078856e-08 for train data

#### Epoch 80

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Average loss of: 8.782052637675057e-08 for test data Average loss of: 7.94265366803171e-08 for train data

#### Epoch 81

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Average loss of: 8.677367845211048e-08 for test data

Average loss of: 7.672331003104686e-08 for train data Epoch 82 Average loss of: 8.57994585964535e-08 for test data Average loss of: 7.825783039273108e-08 for train data Epoch 83 Average loss of: 8.487612235193012e-08 for test data Average loss of: 9.672973851084766e-08 for train data Epoch 84 Average loss of: 8.407245267302331e-08 for test data Average loss of: 7.617923517700953e-08 for train data Adapting learning rate to 4.6875e-06 Epoch 85 Average loss of: 8.323489942440007e-08 for test data Average loss of: 8.372315954611971e-08 for train data Epoch 86 Average loss of: 1.549247231375997e-07 for test data Average loss of: 1.5142827758775555e-07 for train data Epoch 87 \_\_\_\_\_ Average loss of: 1.5179634415042924e-07 for test data Average loss of: 1.4680651595052638e-07 for train data Epoch 88 Average loss of: 1.498851235756562e-07 for test data Average loss of: 1.4200734175793707e-07 for train data Epoch 89

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Average loss of: 1.4797051439306498e-07 for test data Average loss of: 1.4385175560642492e-07 for train data

#### Epoch 90

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Average loss of: 1.45942886396429e-07 for test data Average loss of: 1.3684024449598502e-07 for train data

# Epoch 91 \_\_\_\_\_ Average loss of: 1.4386466575931485e-07 for test data Average loss of: 1.3683084256272398e-07 for train data Epoch 92 Average loss of: 1.4193656847790687e-07 for test data Average loss of: 1.429411714133575e-07 for train data Epoch 93 Average loss of: 1.3997328777624642e-07 for test data Average loss of: 1.3591397828422371e-07 for train data Epoch 94 Average loss of: 1.380518514584189e-07 for test data Average loss of: 1.330039069466112e-07 for train data Epoch 95 Average loss of: 1.3591591940525403e-07 for test data Average loss of: 1.2512529931024535e-07 for train data Adapting learning rate to 2.34375e-06 Epoch 96 \_\_\_\_\_ Average loss of: 1.3420203670673033e-07 for test data Average loss of: 1.2480804601951466e-07 for train data Epoch 97 Average loss of: 7.771917037376326e-08 for test data Average loss of: 7.679740332768518e-08 for train data Epoch 98 Average loss of: 7.715280965328293e-08 for test data Average loss of: 7.793844612077288e-08 for train data Epoch 99 Average loss of: 7.683872578042201e-08 for test data

Average loss of: 7.340215814364232e-08 for train data

Epoch 100

\_\_\_\_\_

Average loss of: 7.663336409465386e-08 for test data Average loss of: 6.966425524624923e-08 for train data

#### Epoch 101

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Average loss of: 7.634261311722412e-08 for test data Average loss of: 8.452858307377894e-08 for train data

#### Epoch 102

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Average loss of: 7.610083760316677e-08 for test data Average loss of: 7.336873950269585e-08 for train data

#### Epoch 103

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Average loss of: 7.586449169120926e-08 for test data Average loss of: 7.487711635245961e-08 for train data

#### Epoch 104

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Average loss of: 7.565269290822448e-08 for test data Average loss of: 7.12564616555654e-08 for train data

## Epoch 105

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Average loss of: 7.541054304257019e-08 for test data Average loss of: 7.695784856518579e-08 for train data

#### Epoch 106

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Average loss of: 7.51300265138567e-08 for test data Average loss of: 7.124799089650495e-08 for train data Adapting learning rate to 1.171875e-06

#### Epoch 107

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Average loss of: 7.492553573101236e-08 for test data Average loss of: 6.874477850868906e-08 for train data

#### Epoch 108

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Average loss of: 6.163545001040671e-08 for test data Average loss of: 5.933509895273888e-08 for train data

# Epoch 109

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Average loss of: 6.146454257594714e-08 for test data Average loss of: 6.209007592772356e-08 for train data

# Epoch 110

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Average loss of: 6.126443677820057e-08 for test data Average loss of: 6.768837962409705e-08 for train data

#### Epoch 111

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Average loss of: 6.106516586249326e-08 for test data Average loss of: 5.514449438650693e-08 for train data

#### Epoch 112

\_\_\_\_\_

Average loss of: 6.08722306497812e-08 for test data Average loss of: 5.191489921658147e-08 for train data

## Epoch 113

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Average loss of: 6.067255266459459e-08 for test data Average loss of: 5.859620533481149e-08 for train data

#### Epoch 114

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Average loss of: 6.048404754395846e-08 for test data Average loss of: 6.384966706860315e-08 for train data

#### Epoch 115

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Average loss of: 6.028839948816168e-08 for test data Average loss of: 5.5383320569334204e-08 for train data

# Epoch 116

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Average loss of: 6.009513993993201e-08 for test data Average loss of: 6.275539051850579e-08 for train data

## Epoch 117

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Average loss of: 5.98883693705045e-08 for test data Average loss of: 5.6670732373759845e-08 for train data Adapting learning rate to 5.859375e-07

#### Epoch 118

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Average loss of: 5.971109745379877e-08 for test data Average loss of: 5.524138541277055e-08 for train data

Epoch 119

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Average loss of: 6.134069216784973e-08 for test data Average loss of: 5.5001194931138e-08 for train data

Epoch 120

\_\_\_\_\_

Average loss of: 6.125862537856075e-08 for test data Average loss of: 5.807539750912075e-08 for train data

Epoch 121

\_\_\_\_\_

Average loss of: 6.115835866137404e-08 for test data Average loss of: 5.3733612058960745e-08 for train data

Epoch 122

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Average loss of: 6.109268607366529e-08 for test data Average loss of: 5.397005337773878e-08 for train data

Epoch 123

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Average loss of: 6.099362266514181e-08 for test data Average loss of: 5.963830268536057e-08 for train data

Epoch 124

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Average loss of: 6.091591657083152e-08 for test data Average loss of: 5.3983016611349225e-08 for train data

Epoch 125

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Average loss of: 6.08261716976018e-08 for test data Average loss of: 6.010159674165646e-08 for train data

Epoch 126

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Average loss of: 6.073820716524503e-08 for test data Average loss of: 5.435300137834744e-08 for train data

Epoch 127

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Average loss of: 6.065200877425702e-08 for test data Average loss of: 5.939154980241344e-08 for train data

Epoch 128

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Average loss of: 6.055743566665836e-08 for test data Average loss of: 5.5611680451988466e-08 for train data

# Adapting learning rate to 2.9296875e-07

#### Epoch 129

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Average loss of: 6.047857805612103e-08 for test data Average loss of: 6.383471852637659e-08 for train data

## Epoch 130

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Average loss of: 5.3099046744218374e-08 for test data Average loss of: 5.101478875260433e-08 for train data

#### Epoch 131

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Average loss of: 5.3044042711650826e-08 for test data Average loss of: 5.031307970887555e-08 for train data

#### Epoch 132

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Average loss of: 5.3015164393383774e-08 for test data Average loss of: 4.6317751031819105e-08 for train data

#### Epoch 133

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Average loss of: 5.297976562533491e-08 for test data Average loss of: 5.1795664146769556e-08 for train data

#### Epoch 134

\_\_\_\_\_

Average loss of: 5.2942649727475316e-08 for test data Average loss of: 5.144164699464809e-08 for train data

#### Epoch 135

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Average loss of: 5.2905538034984475e-08 for test data Average loss of: 4.695262778220978e-08 for train data

#### Epoch 136

\_\_\_\_\_

Average loss of: 5.286636715899899e-08 for test data Average loss of: 5.115338599846048e-08 for train data

#### Epoch 137

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Average loss of: 5.2829917565212023e-08 for test data Average loss of: 4.363461437114951e-08 for train data

Epoch 138

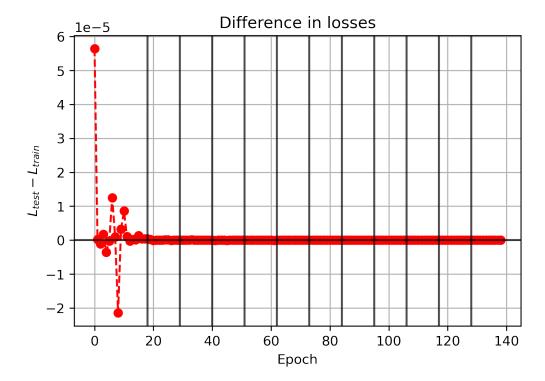
```
Average loss of: 5.279018041731254e-08 for test data
Average loss of: 4.9564207982441874e-08 for train data

Epoch 139
------
Average loss of: 5.2751628360486974e-08 for test data
Average loss of: 5.573700895355884e-08 for train data
```

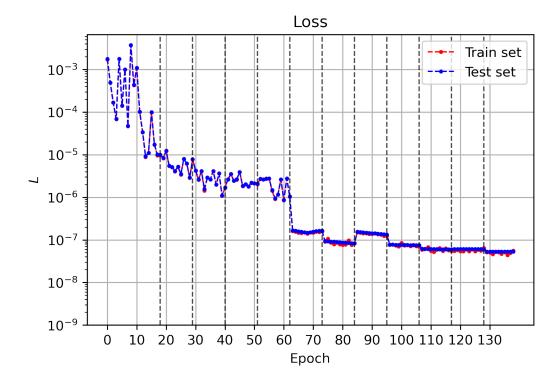
```
KeyboardInterrupt
                                          Traceback (most recent call last)
Input In [18], in <cell line: 9>()
      8 print("Training the model . . .")
      9 for t in range(epochs):
          # Train
     10
---> 11
            train_loop(train_dataloader, model, loss_fn, optimizer)
     12
            # Test
            average_test_loss = test_loop(test_dataloader, model, loss_fn)
Input In [15], in train_loop(dataloader, model, loss_fn, optimizer, u
 →report_progress)
      7 loss = loss_fn(pred, y)
      9 # Backpropagation
---> 10 optimizer.zero_grad()
     11 loss.backward()
     12 optimizer.step()
File D:\Anaconda3\lib\site-packages\torch\optim\optimizer.py:267, in Optimizer.
 \rightarrow zero_grad(self, set_to_none)
    265 if foreach:
            per_device_and_dtype_grads = defaultdict(lambda: defaultdict(list))
--> 267 with torch.autograd.profiler.record_function(self.
 →_zero_grad_profile_name):
    268
            for group in self.param_groups:
                for p in group['params']:
    269
File D:\Anaconda3\lib\site-packages\torch\autograd\profiler.py:488, in_
 ⇔record_function.__enter__(self)
    487 def __enter__(self):
--> 488
            self.handle = torch.ops.profiler._record_function_enter(self.name,_
 ⇔self.args)
    489
           return self
KeyboardInterrupt:
```

# 5.1 Results of training

```
[20]: # Get the difference (need np.array)
      test_losses_as_array = np.array(test_losses)
      train_losses_as_array = np.array(train_losses)
      difference = test_losses_as_array - train_losses_as_array
      # Plot it
      plt.figure()
      plt.plot(difference, 'o--', color = 'red', label = "Difference")
      plt.grid()
      plt.xlabel("Epoch")
      plt.ylabel(r'$L_{test} - L_{train}$')
     plt.axhline(0, color = 'black', alpha = 0.7)
      plt.title("Difference in losses")
      # Plot when we adapted learning rate
      for t in adaptation_indices:
         plt.axvline(t, color = 'black', alpha = 0.7)
      plt.show()
```



```
plt.plot(train_losses, 'o--', color = 'red', label = "Train set", lw = lw, ms = u
 ⊶ms)
plt.plot(test_losses, 'o--', color = 'blue', label = "Test set", lw = lw, ms = u
 ⊶ms)
plt.legend()
plt.grid()
plt.xlabel("Epoch")
xt_step = 10
xt = [i*xt_step for i in range(len(train_losses)//xt_step+1)]
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, linestyle = "--", color = 'black', alpha = 0.7, lw = 1)
plt.yscale('log')
plt.ylim(10**(-9))
plt.show()
```



# 5.2 Save the neural network

[]: torch.save(model, 'NNEOSBvO.pth')
[]: