DHOscillator_FFNN_tuning

March 10, 2024

[36]:

```
# import numpy, scipy, and matplotlib
import numpy as np
import scipy as sp
import matplotlib.pyplot as plt

from itables import init_notebook_mode

init_notebook_mode(all_interactive=True)

from sklearn.model_selection import train_test_split


# import from scipy solve_ivp
from scipy.integrate import solve_ivp
import torch
%matplotlib widget

from ray import train, tune
from ray.train import Checkpoint, session, report
from ray.tune.schedulers import ASHAScheduler

import os
import tempfile
```

```
<IPython.core.display.HTML object>
```

[37]:

```
path = os.getcwd()
results_dir = os.path.join(path, "../tuning")
os.makedirs(results_dir, exist_ok=True)
```

1 Tuning of the PINN for the Damped Harmonic Oscillator ODE

In this notebook we tune the hyperparamenters of the PINN.

1.1 Load data

[38]:

```
# import data
# data are generated by "src/DHOscillator_data_gen.py"
data = np.load('../data/DHOscillator_data.npy')
data_X = data[:,0]
data_Y = data[:,1:]
```

[39]:

```
def data_loader(X, Y, batch_size):
    """
    Function to load data and divide it in batches
    input: X, Y, batch_size
    output: train_X_batches, train_Y_batches, val_X, val_Y, test_X, test_Y
    """

    # divide in train, validation and test
    train_frac = 0.7
    val_frac = 0.15
    test_frac = 0.15

    train_val_X = X[:int((train_frac+val_frac)*len(X))]
    train_val_Y = Y[:int((train_frac+val_frac)*len(X)), :]
    train_X, val_X, train_Y, val_Y = train_test_split(
        train_val_X,
        train_val_Y,
        test_size=val_frac/(train_frac+val_frac),
        random_state=42
        )

    test_X = X[int((train_frac+val_frac)*len(X)):]
    test_Y = Y[int((train_frac+val_frac)*len(X)):, :]

    # convert to torch tensor
    train_X = torch.tensor(train_X, dtype=torch.float32).view(-1, 1)
    train_Y = torch.tensor(train_Y, dtype=torch.float32)
    val_X = torch.tensor(val_X, dtype=torch.float32).view(-1, 1)
    val_Y = torch.tensor(val_Y, dtype=torch.float32)
    test_X = torch.tensor(test_X, dtype=torch.float32).view(-1, 1)
    test_Y = torch.tensor(test_Y, dtype=torch.float32)

    # divide in batches train
    train_X_batches = torch.split(train_X, batch_size)
    train_Y_batches = torch.split(train_Y, batch_size)


    return train_X_batches, train_Y_batches, val_X, val_Y, test_X, test_Y
```

1.2 Define hyper model

[40]:

```
#  define the model
class FFNN(torch.nn.Module):
    def __init__(self, n_layers, n_neurons):
        super(FFNN, self).__init__()
        layers = []
        for i in range(n_layers):
            if i == 0:
                layers.append(torch.nn.Linear(1, n_neurons))
            else:
                layers.append(torch.nn.Linear(n_neurons, n_neurons))
            layers.append(torch.nn.Tanh())
        layers.append(torch.nn.Linear(n_neurons, 2))
        self.model = torch.nn.Sequential(*layers)
    def forward(self, x):
        return self.model(x)
```

1.3 Define the Objective

[41]:

```
def objective(config):
    net = FFNN(config["n_layers"], config["n_neurons"])

    device = "cpu"

    criterion = torch.nn.MSELoss()
    optimizer = torch.optim.Adam(net.parameters(), lr=config["lr"])
    scheduler = torch.optim.lr_scheduler.ReduceLROnPlateau(
        optimizer,
        'min',
        factor=config["factor"],
        patience=config["patience"]
    )

    train_X_batches, train_Y_batches, val_X, val_Y, test_X, test_Y =␣
 ↪data_loader(data_X, data_Y, config["batch_size"])

    for epoch in range(50000):
        for i, (X, Y) in enumerate(zip(train_X_batches, train_Y_batches)):
            optimizer.zero_grad()
            Y_pred = net(X)
            loss = criterion(Y_pred, Y)
            loss.backward()
            optimizer.step()
            optimizer.step()
            scheduler.step(loss)
        val_loss = criterion(net(val_X), val_Y).item()

        report(metrics={"loss": val_loss})

        if epoch % 100 == 0:
            torch.save(net.state_dict(), "./model.pth")
```

1.4 Tuning

[42]:

```
# configuration space and sampling method
config = {
    "n_layers": tune.randint(1, 5),
    "n_neurons": tune.randint(10, 50),
    "lr" : tune.loguniform(1e-4, 1e-1),
    "factor": tune.uniform(0.1, 0.9),
    "patience": tune.randint(100, 1000),
    "batch_size": tune.randint(32, 595)
}



# schedueler ASHA
scheduler = ASHAScheduler(
    metric="loss",
    mode="min",
    max_t=10000,
    grace_period=2500,
    reduction_factor=2
    )


tuner = tune.Tuner(
    objective,
    param_space=config,
    tune_config=tune.TuneConfig(
        num_samples=16,
        scheduler=scheduler,
    ),
    run_config=train.RunConfig(
        name="DHO_FFNN_tuning",
        storage_path=results_dir
    )
)
```

[43]:

```
results = tuner.fit()
```

```
<IPython.core.display.HTML object>
```

```
2024-03-10 21:00:02,695 INFO tune.py:1042 -- Total run time: 458.79 seconds
(458.50 seconds for the tuning loop).
```

[57]:

```
df = results.get_dataframe()
df
```

[57]:

```
        loss   timestamp checkpoint_dir_name  done  training_iteration  \
0   0.000061  1710100674                None  True               10000
1   0.033320  1710100583                None  True               10000
2   0.044591  1710100405                None  True                2500
3   0.005030  1710100603                None  True               10000
4   0.000005  1710100634                None  True               10000
5   0.188000  1710100414                None  True                2500
6   0.073328  1710100440                None  True                2500
7   0.000062  1710100604                None  True               10000
8   0.001768  1710100758                None  True                5000
9   0.000910  1710100546                None  True                5000
10  0.010280  1710100568                None  True                5000
11  0.002539  1710100802                None  True                5000
12  0.091638  1710100641                None  True                2500
13  0.062574  1710100664                None  True                2500
14  0.082134  1710100684                None  True                2500
15  0.087197  1710100661                None  True                2500

       trial_id                 date  time_this_iter_s  time_total_s    pid  \
0   b6cbc_00000  2024-03-10_20-57-54          0.015730    169.932873  10459
1   b6cbc_00001  2024-03-10_20-56-23          0.021216     65.895605  10491
2   b6cbc_00002  2024-03-10_20-53-25          0.011742     18.122798  10493
3   b6cbc_00003  2024-03-10_20-56-43          0.010067     84.705609  10494
4   b6cbc_00004  2024-03-10_20-57-14          0.016839    120.658826  10495
5   b6cbc_00005  2024-03-10_20-53-34          0.010947     26.572859  10496
6   b6cbc_00006  2024-03-10_20-54-00          0.024073     48.955651  10497
7   b6cbc_00007  2024-03-10_20-56-44          0.010854     89.195537  10525
8   b6cbc_00008  2024-03-10_20-59-18          0.039083    294.712348  10493
9   b6cbc_00009  2024-03-10_20-55-46          0.008236     44.852540  10496
10  b6cbc_00010  2024-03-10_20-56-08          0.007587     41.369596  10497
11  b6cbc_00011  2024-03-10_21-00-02          0.027495    225.069007  10496
12  b6cbc_00012  2024-03-10_20-57-21          0.013911     37.032490  10497
13  b6cbc_00013  2024-03-10_20-57-44          0.017209     50.915546  10491
14  b6cbc_00014  2024-03-10_20-58-04          0.013014     59.925988  10494
15  b6cbc_00015  2024-03-10_20-57-41          0.008908     30.493110  10525

    …        node_ip time_since_restore  iterations_since_restore  \
0   …  192.168.50.220         169.932873                     10000
1   …  192.168.50.220          65.895605                     10000
2   …  192.168.50.220          18.122798                      2500
3   …  192.168.50.220          84.705609                     10000
```

```
4   …  192.168.50.220         120.658826                     10000
5   …  192.168.50.220          26.572859                      2500
6   …  192.168.50.220          48.955651                      2500
7   …  192.168.50.220          89.195537                     10000
8   …  192.168.50.220         294.712348                      5000
9   …  192.168.50.220          44.852540                      5000
10  …  192.168.50.220          41.369596                      5000
11  …  192.168.50.220         225.069007                      5000
12  …  192.168.50.220          37.032490                      2500
13  …  192.168.50.220          50.915546                      2500
14  …  192.168.50.220          59.925988                      2500
15  …  192.168.50.220          30.493110                      2500

    config/n_layers  config/n_neurons  config/lr  config/factor  \
0                 4                13   0.001922       0.208865
1                 1                34   0.000929       0.889070
2                 1                11   0.011040       0.298420
3                 2                21   0.063401       0.446048
4                 4                12   0.012718       0.509175
5                 2                40   0.099443       0.840646
6                 2                23   0.000160       0.467883
7                 2                37   0.001539       0.634394
8                 4                26   0.026397       0.875736
9                 2                38   0.027298       0.114808
10                2                10   0.009679       0.496178
11                4                31   0.000573       0.258035
12                2                14   0.000152       0.814966
13                4                18   0.000203       0.645737
14                3                31   0.000140       0.737743
15                1                38   0.000247       0.778915

    config/patience  config/batch_size       logdir
0               651                258  b6cbc_00000
1               232                367  b6cbc_00001
2               132                257  b6cbc_00002
3               260                356  b6cbc_00003
4               558                454  b6cbc_00004
5               628                253  b6cbc_00005
6               853                139  b6cbc_00006
7               297                460  b6cbc_00007
8               272                 53  b6cbc_00008
9               284                409  b6cbc_00009
10              192                389  b6cbc_00010
11              198                 57  b6cbc_00011
12              239                246  b6cbc_00012
13              238                290  b6cbc_00013
14              513                174  b6cbc_00014
```

```
15              840                313  b6cbc_00015

[16 rows x 21 columns]
```

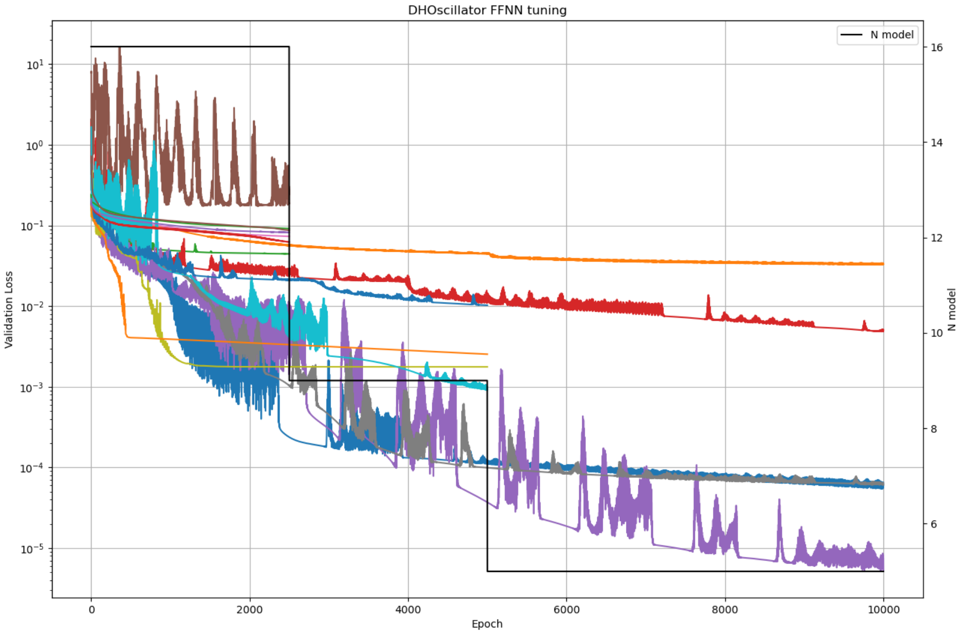
[65]:

```
def get_alive_model(df, max_epoch):
    """
    Function to get the number of alive models at each epoch
    input: df, max_epoch
    output: alive_model
    """
    # get traininig_iteration vector
    training_iteration = df["training_iteration"]
    training_iteration = training_iteration.to_numpy()
    # alive_model = number of entries of training_iteration > epoch
    # epoch = (0, max_epoch)
    alive_model = np.zeros(max_epoch)
    for i in range(max_epoch):
        alive_model[i] = np.sum(training_iteration > i)
    return alive_model

alive_model = get_alive_model(df, 10000)
```

[93]:

```
# show results
dfs = {result.path: result.metrics_dataframe for result in results}

# twinx plot alive_model and validation loss
fig, ax1 = plt.subplots(figsize=(15, 10))
# plot the validation loss
for path, df in dfs.items():
    ax1.plot(df["training_iteration"], df["loss"], label=path)
ax1.set_yscale("log")
ax1.set_xlabel("Epoch")
ax1.set_ylabel("Validation Loss")
ax1.grid()

# plot the alive model
ax2 = ax1.twinx()
ax2.plot(alive_model, label="N model", color="black")
ax2.set_ylabel("N model")
ax2.legend()
ax2.grid()


plt.title("DHOscillator FFNN tuning")
plt.grid()

# save the plot
```

```
plt.savefig("../plot/DHOscillator_FFNN_tuning.png")
```



[92]:

```
# get best model
best_result = results.get_best_result("loss", mode="min")
logdir = best_result.path
state_dict = torch.load(os.path.join(logdir, "model.pth"))
best_model = FFNN(best_result.config["n_layers"], best_result.
 ↪config["n_neurons"])

best_model.load_state_dict(state_dict)

# save best model
torch.save(best_model, "../models/DHO_FFNN_tuned.pt")
```

[52]:

```
# print validation and test loss
train_X_batches, train_Y_batches, val_X, val_Y, test_X, test_Y = data_loader(
    data_X,
    data_Y,
    best_result.config["batch_size"]
    )


val_loss = torch.nn.MSELoss()(best_model(val_X), val_Y).item()
```

```
test_loss = torch.nn.MSELoss()(best_model(test_X), test_Y).item()

print(f"Validation Loss: {val_loss}")
print(f"Test Loss: {test_loss}")
```

```
Validation Loss: 7.342151548073161e-06
Test Loss: 0.09691622108221054
```

1.5 Restore results

[85]:

```
# restore results
experiment_path = os.path.join(results_dir, "DHO_FFNN_tuning")
experiment_path
```

[85]:

```
'/home/luigi/Documents/PHYSICS/ML/Project1/src/../ray_results/DHO_FFNN_tuning'
```

[89]:

```
restored_tuner = tune.Tuner.restore(experiment_path, objective)
restored_results = restored_tuner.get_results()
```

[90]:

```
restored_df = restored_results.get_dataframe()
restored_df
```

[90]:

```
        loss   timestamp checkpoint_dir_name  done  training_iteration  \
0   0.001768  1710100758                None  True                5000   
1   0.062574  1710100664                None  True                2500   
2   0.082134  1710100684                None  True                2500   
3   0.087197  1710100661                None  True                2500   
4   0.091638  1710100641                None  True                2500   
5   0.000062  1710100604                None  True               10000   
6   0.073328  1710100440                None  True                2500   
7   0.000061  1710100674                None  True               10000   
8   0.002539  1710100802                None  True                5000   
9   0.044591  1710100405                None  True                2500   
10  0.005030  1710100603                None  True               10000   
11  0.000910  1710100546                None  True                5000   
12  0.033320  1710100583                None  True               10000   
13  0.010280  1710100568                None  True                5000   
14  0.188000  1710100414                None  True                2500   
15  0.000005  1710100634                None  True               10000   

       trial_id                 date  time_this_iter_s  time_total_s    pid  \
0   b6cbc_00008  2024-03-10_20-59-18          0.039083    294.712348  10493   
1   b6cbc_00013  2024-03-10_20-57-44          0.017209     50.915546  10491   
2   b6cbc_00014  2024-03-10_20-58-04          0.013014     59.925988  10494   
3   b6cbc_00015  2024-03-10_20-57-41          0.008908     30.493110  10525   
4   b6cbc_00012  2024-03-10_20-57-21          0.013911     37.032490  10497   
5   b6cbc_00007  2024-03-10_20-56-44          0.010854     89.195537  10525   
```

```
6   b6cbc_00006  2024-03-10_20-54-00          0.024073    48.955651  10497
7   b6cbc_00000  2024-03-10_20-57-54          0.015730   169.932873  10459
8   b6cbc_00011  2024-03-10_21-00-02          0.027495   225.069007  10496
9   b6cbc_00002  2024-03-10_20-53-25          0.011742    18.122798  10493
10  b6cbc_00003  2024-03-10_20-56-43          0.010067    84.705609  10494
11  b6cbc_00009  2024-03-10_20-55-46          0.008236    44.852540  10496
12  b6cbc_00001  2024-03-10_20-56-23          0.021216    65.895605  10491
13  b6cbc_00010  2024-03-10_20-56-08          0.007587    41.369596  10497
14  b6cbc_00005  2024-03-10_20-53-34          0.010947    26.572859  10496
15  b6cbc_00004  2024-03-10_20-57-14          0.016839   120.658826  10495

    …         node_ip time_since_restore  iterations_since_restore  \
0   …  192.168.50.220         294.712348                      5000   
1   …  192.168.50.220          50.915546                      2500   
2   …  192.168.50.220          59.925988                      2500   
3   …  192.168.50.220          30.493110                      2500   
4   …  192.168.50.220          37.032490                      2500   
5   …  192.168.50.220          89.195537                     10000   
6   …  192.168.50.220          48.955651                      2500   
7   …  192.168.50.220         169.932873                     10000   
8   …  192.168.50.220         225.069007                      5000   
9   …  192.168.50.220          18.122798                      2500   
10  …  192.168.50.220          84.705609                     10000   
11  …  192.168.50.220          44.852540                      5000   
12  …  192.168.50.220          65.895605                     10000   
13  …  192.168.50.220          41.369596                      5000   
14  …  192.168.50.220          26.572859                      2500   
15  …  192.168.50.220         120.658826                     10000   

    config/n_layers  config/n_neurons  config/lr  config/factor  \
0                 4                26   0.026397       0.875736   
1                 4                18   0.000203       0.645737   
2                 3                31   0.000140       0.737743   
3                 1                38   0.000247       0.778915   
4                 2                14   0.000152       0.814966   
5                 2                37   0.001539       0.634394   
6                 2                23   0.000160       0.467883   
7                 4                13   0.001922       0.208865   
8                 4                31   0.000573       0.258035   
9                 1                11   0.011040       0.298420   
10                2                21   0.063401       0.446048   
11                2                38   0.027298       0.114808   
12                1                34   0.000929       0.889070   
13                2                10   0.009679       0.496178   
14                2                40   0.099443       0.840646   
15                4                12   0.012718       0.509175   
```

```
    config/patience  config/batch_size       logdir
0               272                 53  b6cbc_00008
1               238                290  b6cbc_00013
2               513                174  b6cbc_00014
3               840                313  b6cbc_00015
4               239                246  b6cbc_00012
5               297                460  b6cbc_00007
6               853                139  b6cbc_00006
7               651                258  b6cbc_00000
8               198                 57  b6cbc_00011
9               132                257  b6cbc_00002
10              260                356  b6cbc_00003
11              284                409  b6cbc_00009
12              232                367  b6cbc_00001
13              192                389  b6cbc_00010
14              628                253  b6cbc_00005
15              558                454  b6cbc_00004

[16 rows x 21 columns]
```

[ ]: