

# Final Project

April 21, 2022

## 1 Introduction

For this final project, I am making a trajectory prediction for the ball in a simulated physics environment. For the simulation, I am using the Phyre benchmark simulator. For machine learning, I am training the Echo State Networks.

This submission consists of three parts:

1. **Simulator Demo.** In this section, I will make a short demo of how the Phyre simulator works and what kind of output we can get from it.
2. **Data preparation.** In this section, I am creating the dataset of simulations using Phyre. This consists of two parts:
  - Generating a dataset using Phyre.
  - Creating a set of PyTorch Dataset classes that will be used to feed the data into a machine learning model. **NOTE:** these classes are defined and implemented in a separate file named `PhyreDataset.py`. I will include the code in the end of the PDF submission; this file will also come in a zip archive in a secondary submission.
3. **ESN Training.** In this section I am training three Echo State Networks.
  - One takes the entire scene, frame by frame, as an input, and predicts the entire scene as an output.
  - One takes the entire scene as an input, where the flattened data from three consecutive frames is combined as a single input row, and predicts the trajectory of one of the balls as an output.
  - One takes the flattened data from three consecutive frames as an input (just three frames), and provides a single pair of coordinates for one ball on the following frame as an output.

I have to note here that a big part of this project was trying to replicate existing tutorials but on the Phyre dataset. I will attach notes to which parts of the code was borrowed and in which way it was modified to satisfy my project goals.

## 2 Simulator Demo

```
[1]: import matplotlib.pyplot as plt
import numpy as np
from tqdm import tqdm_notebook
import random
import math

import phyre
```

Let's start with a short simulator demo. The code below is taken from Phyre example notebook. You can find the tutorial using the link below:

[https://github.com/facebookresearch/phyre/blob/main/examples/01\\_phyre\\_intro.ipynb](https://github.com/facebookresearch/phyre/blob/main/examples/01_phyre_intro.ipynb)

```
[2]: # Choosing a setup where only one ball is needed
eval_setup = 'ball_cross_template'

# Getting just one fold of scenarios from the simulator
fold_id = 0

# Getting the tasks split into training, validation, and test
train_tasks, dev_tasks, test_tasks = phyre.get_fold(eval_setup, fold_id)
print('Size of resulting splits:\n train:', len(train_tasks), '\n dev:',
      len(dev_tasks), '\n test:', len(test_tasks))
```

Size of resulting splits:

```
train: 1600
dev: 400
test: 500
```

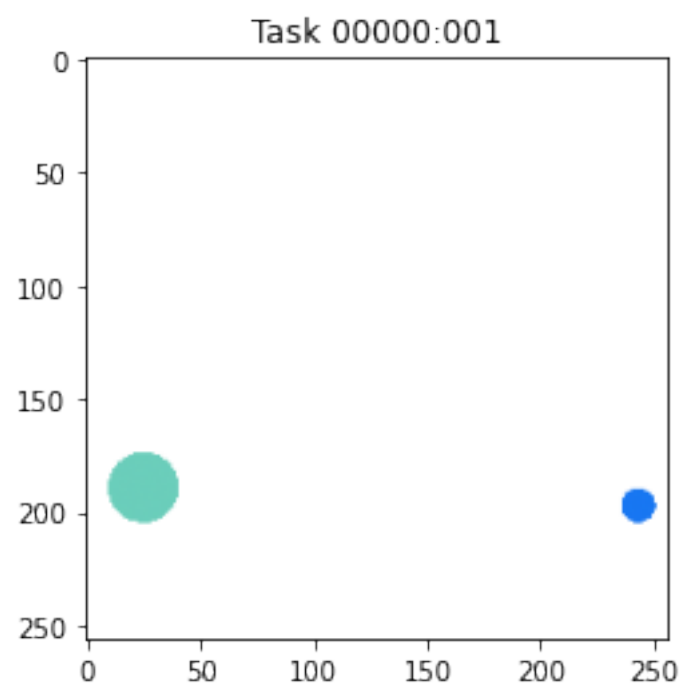
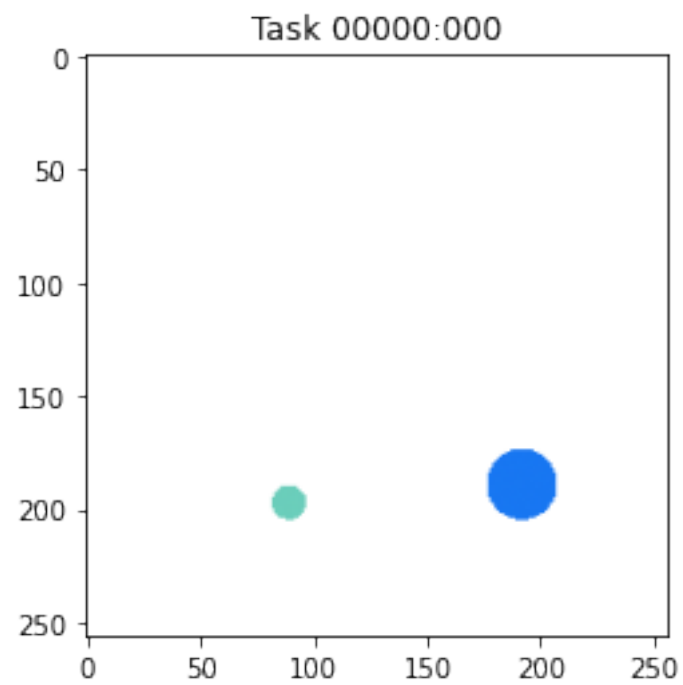
```
[3]: # Getting action tier for our tasks - a single ball
action_tier = phyre.eval_setup_to_action_tier(eval_setup)
print('Action tier for', eval_setup, 'is', action_tier)
```

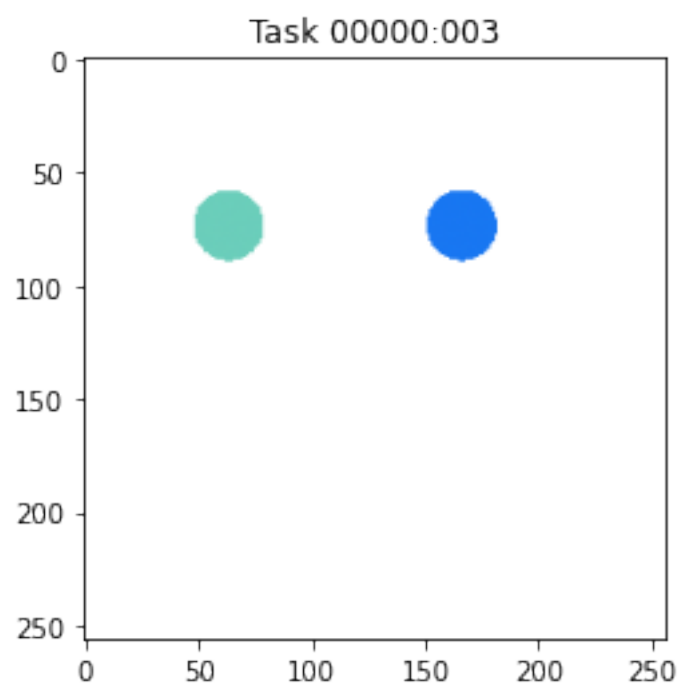
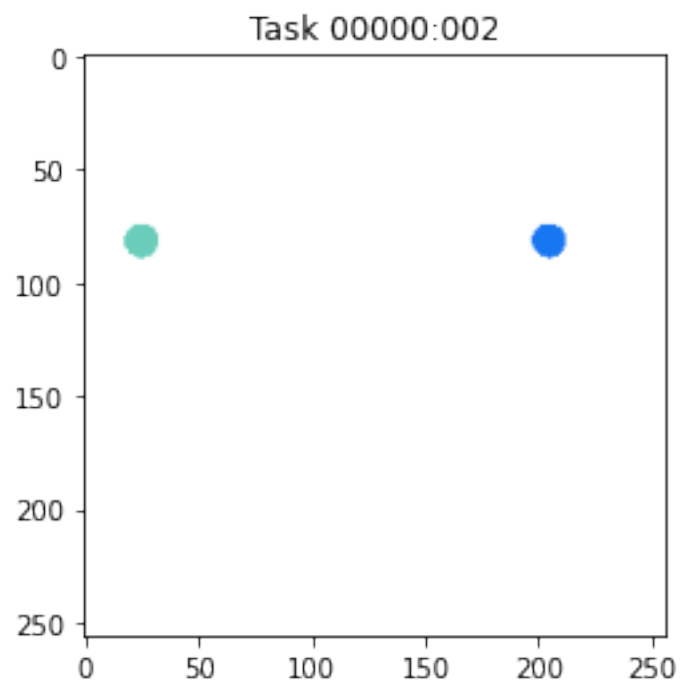
Action tier for ball\_cross\_template is ball

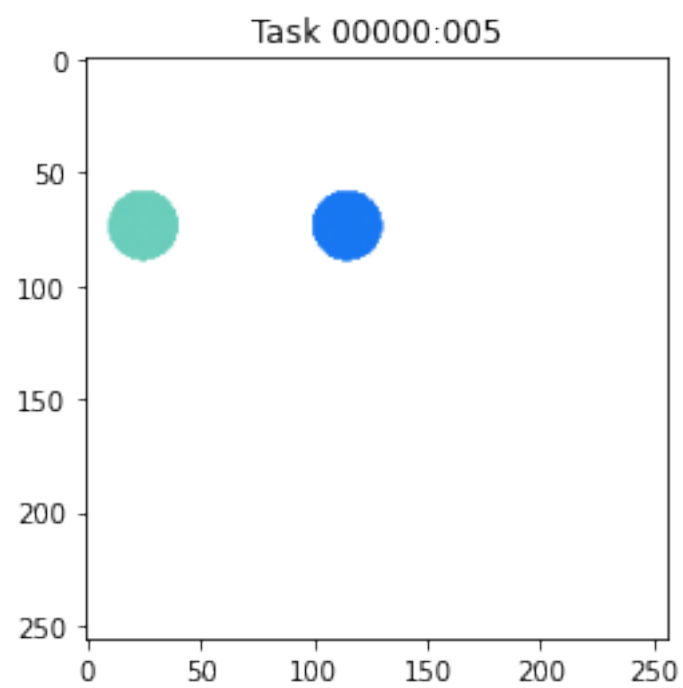
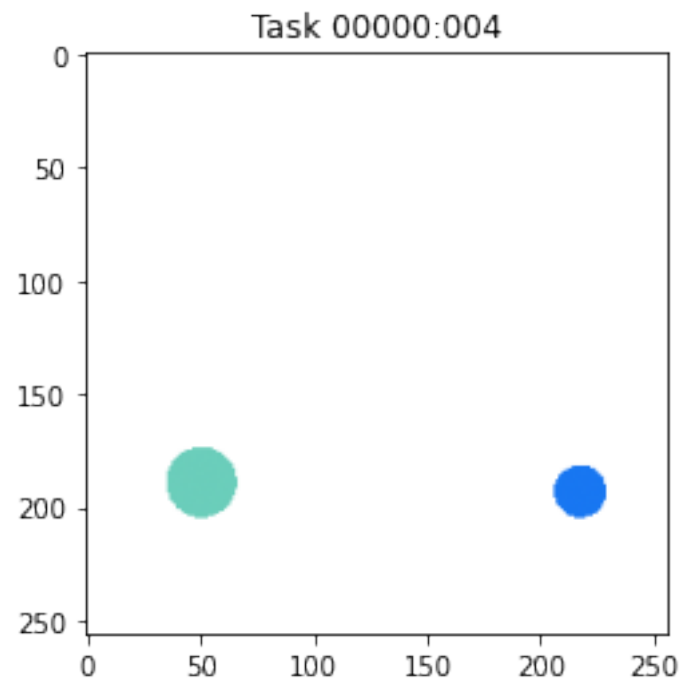
```
[4]: # Let's set our tasks to first 50 of the dev set
tasks = dev_tasks[:50]

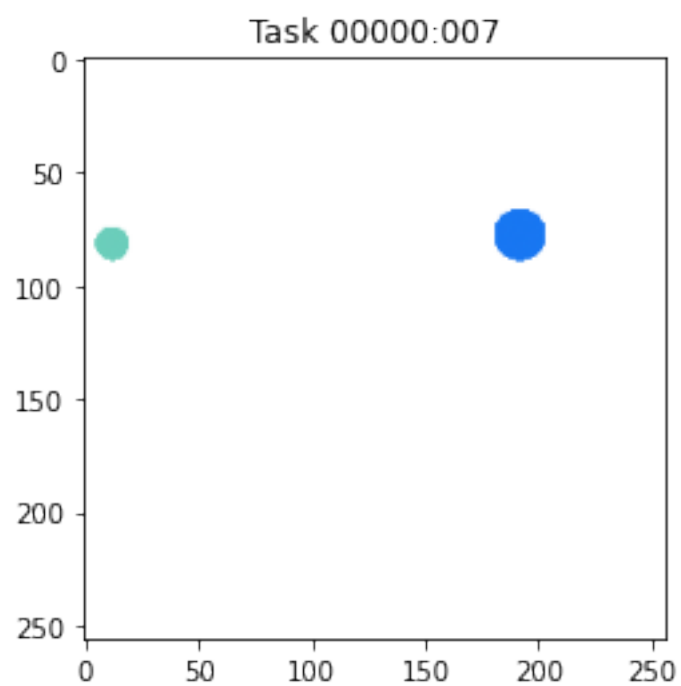
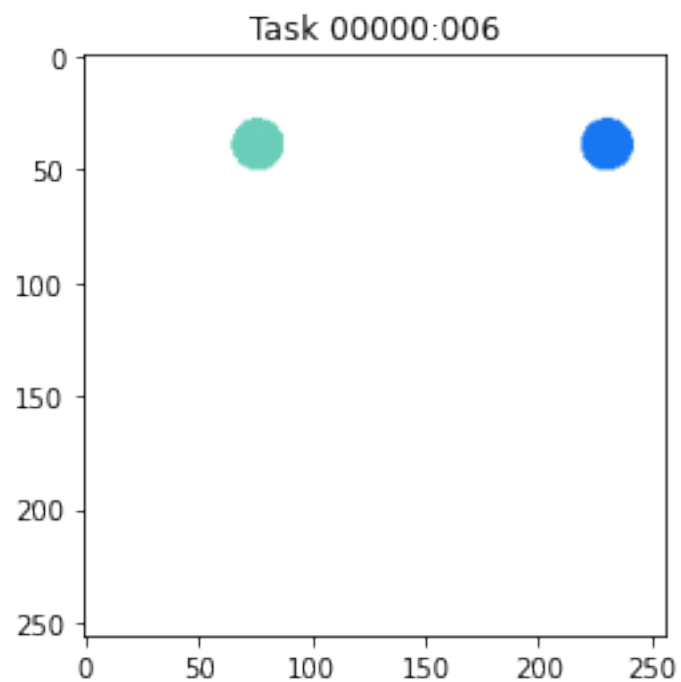
# Create the simulator from the tasks and tier.
simulator = phyre.initialize_simulator(tasks, action_tier)
```

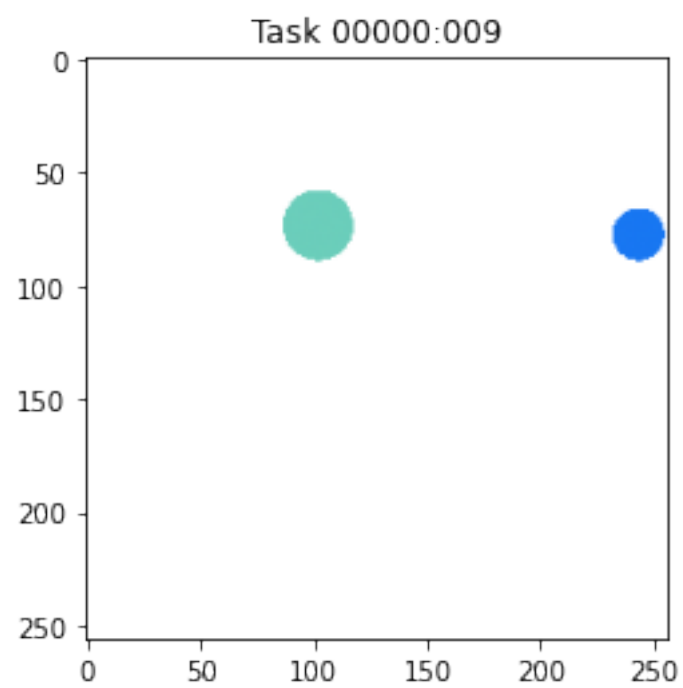
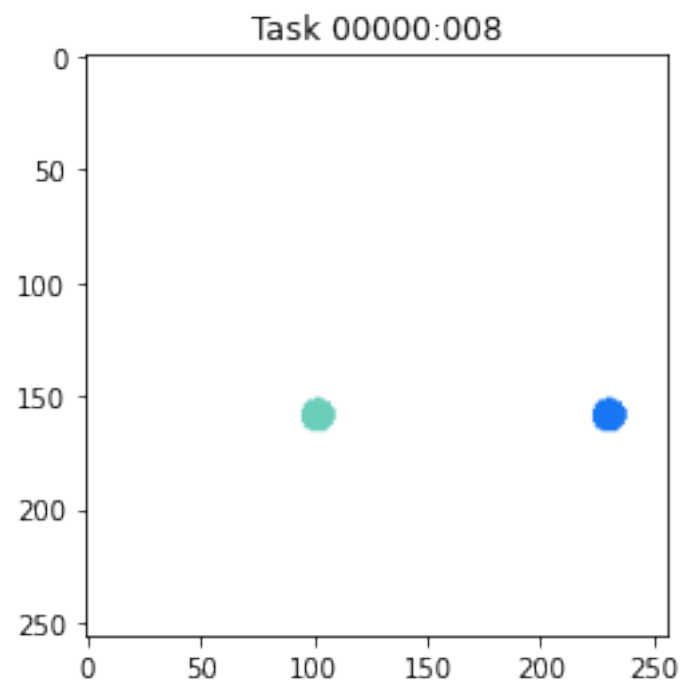
```
[5]: # Showing initial stages of the first 10 scenes
for task_index in range(min(10, len(tasks))):
    initial_scene = simulator.initial_scenes[task_index]
    plt.imshow(phyre.observations_to_float_rgb(initial_scene))
    plt.title(f'Task {simulator.task_ids[task_index]}');
    plt.show()
```











```
[6]: # getting a 100 actions from a simulator
# it uniformly samples actions skipping invalid ones
# Action dimensions: 3 (x, y, radius)

actions = simulator.build_discrete_action_space(max_actions=100)

# Let's simulate for the random actions
action = random.choice(actions)

[7]: # Simulating for the first sampled action
task_index = 0
simulation = simulator.simulate_action(task_index, action, need_images=True,
    ↪need_featurized_objects=True)

[8]: # Checking the simulator response
print('Result of taking action', action, 'on task', tasks[task_index], 'is:',
      simulation.status)
print('Does', action, 'solve task', tasks[task_index], '?', simulation.status.
    ↪is_solved())
print('Is', action, 'an invalid action on task', tasks[task_index], '?',
      simulation.status.is_invalid())
```

Result of taking action [0.86354185 0.74712164 0.55624023] on task 00000:000 is:  
SimulationStatus.SOLVED  
Does [0.86354185 0.74712164 0.55624023] solve task 00000:000 ? True  
Is [0.86354185 0.74712164 0.55624023] an invalid action on task 00000:000 ?  
False

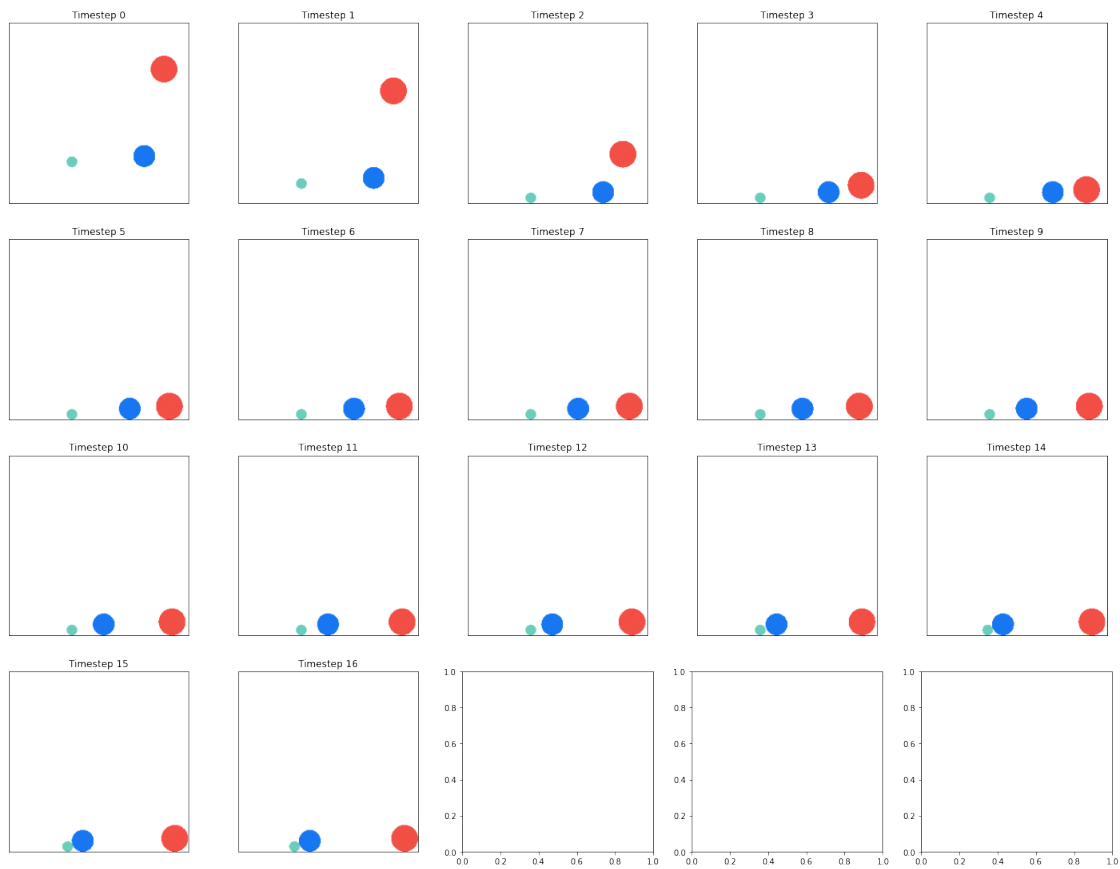
```
[9]: # Displaying the simulation
print('Number of observations returned by simulator:', len(simulation.images))

num_across = 5
height = int(math.ceil(len(simulation.images) / num_across))
fig, axs = plt.subplots(height, num_across, figsize=(20, 15))
fig.tight_layout()
plt.subplots_adjust(hspace=0.2, wspace=0.2)

# We can visualize the simulation at each timestep.
for i, (ax, image) in enumerate(zip(axs.flatten(), simulation.images)):
    # Convert the simulation observation to images.
    img = pyre.observations_to_float_rgb(image)
    ax.imshow(img)
    ax.title.set_text(f'Timestep {i}')
    ax.get_xaxis().set_ticks([])
    ax.get_yaxis().set_ticks([])
```

Number of observations returned by simulator: 17





For my data preparation, I am interested in saving three features for each ball: x and y coordinates and the balls' diameters. Let's take a look on the form of output that we can get for this purpose.

```
[10]: # We can get the response from the simulator in a matrix form
featurized_objects = simulation.featurized_objects

# I am interested in saving coordinates and diameters for every object
# This is because I am limiting my model to work only with balls, so these
#   ↳ features are enough
# The last component of the output corresponds to the red ball - the one we are
#   ↳ interested in

# X-coordinates by frame
print('X-coordinates by frame')
print(featurized_objects.xs)
print()

# Y-coordinates by frame
print('Y-coordinates by frame')
print(featurized_objects.ys)
```

```
print()

# Diameters
print('Diameters')
print(featurized_objects.diameters)
```

X-coordinates by frame

```
[[0.35      0.75      0.859375 ]
 [0.35      0.75      0.859375 ]
 [0.35      0.75      0.859375 ]
 [0.35      0.7283796 0.9079187 ]
 [0.35      0.6991054 0.8859483 ]
 [0.35      0.6699288 0.8889642 ]
 [0.35      0.64084935 0.89197004]
 [0.35      0.6118668 0.8949659 ]
 [0.35      0.58298075 0.89795136]
 [0.35      0.554191  0.900927  ]
 [0.35      0.52549726 0.9038928 ]
 [0.35      0.49689907 0.9068488 ]
 [0.35      0.4683962  0.90979505]
 [0.35      0.43998826 0.9127316 ]
 [0.33897987 0.42306018 0.91565806]
 [0.32555503 0.4096508  0.9185748 ]
 [0.31217507 0.39628595 0.92148185]]
```

Y-coordinates by frame

```
[[0.22923309 0.26048306 0.7421237 ]
 [0.10864712 0.1398971  0.62153774]
 [0.02942147 0.06066259 0.27126455]
 [0.02942147 0.06066405 0.0988986  ]
 [0.02942147 0.06066405 0.07438174]
 [0.02942147 0.06066405 0.07438174]
 [0.02942147 0.06066405 0.07438174]
 [0.02942147 0.06066405 0.07438174]
 [0.02942147 0.06066405 0.07438174]
 [0.02942147 0.06066405 0.07438174]
 [0.02942147 0.06066405 0.07438174]
 [0.02942147 0.06066405 0.07438174]
 [0.02942147 0.06066405 0.07438174]
 [0.02942147 0.06066405 0.07438174]
 [0.02941406 0.06075586 0.07438174]
 [0.02941406 0.06075586 0.07438174]
 [0.02941406 0.06075586 0.07438174]]
```

Diameters

```
[0.05859375 0.12109375 0.1484375 ]
```

All the numbers here are normalized by the width and height of the scene, so are bound between

0 and 1.

From the output above we can see that the first component corresponds to the green ball, the second - to the blue ball, and the third - to the red ball.

### 3 Data preparation

So my data preparation consists of the following steps:

1. Simulate a bunch of scenarios
2. For each scenario and for each frame save the position and diameter of each ball.

So the data that I save has the following dimensions: (n\_frames, n\_objects, 3), where 3 corresponds to (x, y, diameter). I will save the output in a separate file for each single simulation - thus, I will have `n_tasks * n_valid_actions` files.

Also, in the process of making this assignment, I noticed that more than 90% of all simulations consists of 17 frames. Thus, I decided to throw out all of the other ones to make all my data consistent.

```
[11]: for task_index in range(len(tasks)):
        for action_index in range(len(actions)):
            simulation = simulator.simulate_action(task_index,
            ↪actions[action_index], need_images=True, need_featurized_objects=True)

            # if action was invalid, don't solve and continue to next
            if simulation.status.is_invalid(): continue

            featurized_objects = simulation.featurized_objects

            data = []
            for frame_number in range(len(featurized_objects.features)):
                features = []
                features.append(featurized_objects.xs[frame_number])
                features.append(featurized_objects.ys[frame_number])
                features.append(featurized_objects.diameters)
                features = np.array(features).T
                data.append(features)

            # Also skip if not 17 frames in a simulation
            if len(data) != 17: continue

            np.save(f'data/task-{task_index}-action-{action_index}', data)
```

We just ended up saving 4,178 simulations. Let's try to load one of the files to assure that the data saves correctly.

```
[12]: np.load('data/task-0-action-0.npy')
```

[illegible]

```

[[0.35      , 0.02942147, 0.05859375],
 [0.75      , 0.06066405, 0.12109375],
 [0.4140625 , 0.00793899, 0.015625  ]],

[[0.35      , 0.02942147, 0.05859375],
 [0.75      , 0.06066405, 0.12109375],
 [0.4140625 , 0.00793899, 0.015625  ]],

[[0.35      , 0.02942147, 0.05859375],
 [0.75      , 0.06066405, 0.12109375],
 [0.4140625 , 0.00793899, 0.015625  ]],

[[0.35      , 0.02942147, 0.05859375],
 [0.75      , 0.06066405, 0.12109375],
 [0.4140625 , 0.00793899, 0.015625  ]],

[[0.35      , 0.02942147, 0.05859375],
 [0.75      , 0.06066405, 0.12109375],
 [0.4140625 , 0.00793899, 0.015625  ]], dtype=float32)

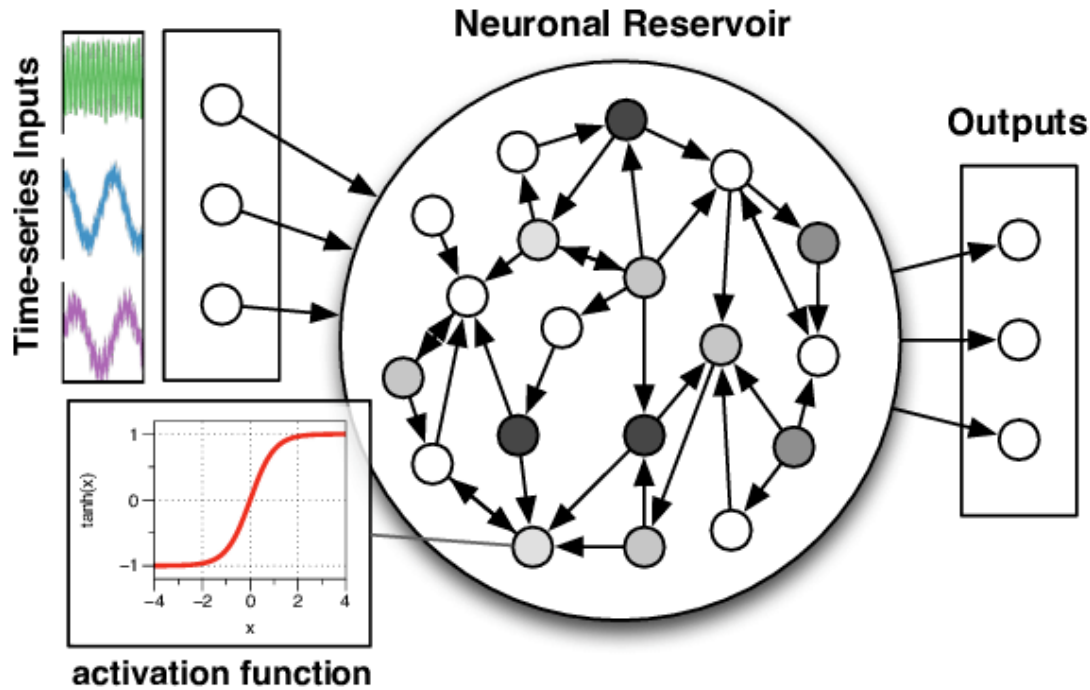
```

Yay, great success. We can now go ahead and setup the models.

## 4 ESN Training

Let's first try to summarize briefly what is an Echo State Network and why it might be good for this kind of tasks.

So ESN is a three layer network, where the first layer is an input, the last layer is an output, and the hidden layer is a big reservoir of randomly interconnected neurons (including some that are recurrent). The first two layers are not trainable; the only thing that is trainable is the matrix that matches the output of reservoir to the output layer. Here is a beautiful picture that shows the structure of ESN.



Retrieved from [https://www.researchgate.net/figure/Echo-State-Network-ESN-In-the-typical-setup-the-inputs-are-fully-connected-to-a\\_fig1\\_263124732](https://www.researchgate.net/figure/Echo-State-Network-ESN-In-the-typical-setup-the-inputs-are-fully-connected-to-a_fig1_263124732)

The fact that there is a recurrency present in the model should make it a good choice for time-series prediction. For the intuitive physics problems (that I plan to focus on), this fact is given as a result in the DeepMind paper “Learning Intuitive Physics Through Objects” (<https://www.deepmind.com/publications/learning-intuitive-physics-through-objects>). The “reservoir” in ESN is pretty much one big recurrent layer, which supposedly should do a good job for the trajectory prediction. This assumption is what I plan to test in my final project.

```
[13]: import torch
import echotorch
import echotorch.nn.reservoir as etrs
import echotorch.utils.matrix_generation as mg
from torch.autograd import Variable
from torch.utils.data.dataloader import DataLoader

# These are the PyTorch Dataset objects that I created in a separate file.
# Reminder: code for these in the end of the PDF
from PhyreDataset import
    ↳PhyreSequentialDataset_EntireSceneInput_EntireSceneOutput as SceneDataset, \
        PhyreSequentialDataset_ThreeFrameSceneInput_TrajectoryOutput as
    ↳TrajectoryDataset, \
        PhyreSequentialDataset_ThreeFramesInput_OneFrame as FrameDataset
```

### 4.1 Predicting the time evolution of the entire scene

For this step, we will use the SceneDataset. Here, the input to the network will be a tensor, each row of which is a flattened matrix of features of all balls on the scene, and each row corresponds to a frame of a simulation. The output is a similar tensor, but each row is a prediction of the scene state on the following frame.

Let's first load the data.

```
[14]: # Loading data
train_dataset, test_dataset = SceneDataset.train_test_split('data', 0.2)

train_test_split response: test fraction rounded to 0.19985639061752034 (835
simulations)
```

How about taking a look at one of the data instances.

[illegible]

```

0.0156],
    [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,
0.0156]])
output:  tensor([[0.3500, 0.1086, 0.0586, 0.7500, 0.1399, 0.1211, 0.4141,
0.5942, 0.0156],
    [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.2439,
0.0156],
    [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0362,
0.0156],
    [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,
0.0156],
    [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,
0.0156],
    [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,
0.0156],
    [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,
0.0156],
    [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,
0.0156],
    [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,
0.0156],
    [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,
0.0156],
    [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,
0.0156],
    [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,
0.0156],
    [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,
0.0156],
    [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,
0.0156],
    [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,
0.0156],
    [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,
0.0156]])

```

And let's also get the input and output dimensions, both for gazing on them for a second and to get some hyperparameters for the ESN.

```

[16]: # Setting up input and output dimensions for the network
input_dim = len(train_dataset.__getitem__(0)[0][0])
output_dim = len(train_dataset.__getitem__(0)[1][0])

print(input_dim, output_dim)

```

9 9

I am also tired from data already, but we need a PyTorch Dataloader that will feed the data to the network.



```
[17]: # Data loader
trainloader = DataLoader(train_dataset, batch_size=1, shuffle=False,
    ↪num_workers=2)
testloader = DataLoader(test_dataset, batch_size=1, shuffle=False,
    ↪num_workers=2)

trainloader
```

```
[17]: <torch.utils.data.dataloader.DataLoader at 0x1a2862b400>
```

Let's also specify some hyperparameters of the network. Here, we will focus on the following:

- Spectral radius - defines the rate at which signal from neurons changes when passed to other neurons within the reservoir.
- Leaky rate - defines the rate at which signal from neurons changes over time. (The product of this with spectral radius should be kept under 1).
- Reservoir size - defines the number of neurons in the reservoir.
- Connectivity - defines the connectivity rate between neurons.

The values for the hyperparameters here (except reservoir size) are taken from the EchoState timeseries prediction example that you can find below:

[https://github.com/nschaetti/EchoTorch/blob/dev/examples/timeserie\\_prediction/narma10\\_esn.py](https://github.com/nschaetti/EchoTorch/blob/dev/examples/timeserie_prediction/narma10_esn.py)

```
[18]: # Reservoir hyper-parameters
spectral_radius = 1.07
leaky_rate = 0.9261
reservoir_size = 500
connectivity = 0.1954
```

Let's initialize the matrices that we will feed into the network. This part is borrowed from the same example as above.

```
[19]: # Internal matrix
w_generator = mg.NormalMatrixGenerator(
    connectivity=connectivity,
    spectral_radius=spectral_radius
)

# Input weights
win_generator = mg.NormalMatrixGenerator(
    connectivity=connectivity,
    apply_spectral_radius=False
)

# Bias vector
wbias_generator = mg.NormalMatrixGenerator(
    connectivity=connectivity,
```

```
    apply_spectral_radius=False
)
```

Finally, let's initialize the ESN.

```
[20]: esn = etrs.LiESN(
        input_dim=input_dim,
        hidden_dim=reservoir_size,
        output_dim=output_dim,
        leaky_rate=leaky_rate,
        learning_algo='inv',
        w_generator=w_generator,
        win_generator=win_generator,
        wbias_generator=wbias_generator,
    )
```

/usr/local/anaconda3/envs/phyre/lib/python3.6/site-packages/echotorch/utils/utility\_functions.py:410: UserWarning: torch.eig is deprecated in favor of torch.linalg.eig and will be removed in a future PyTorch release.

torch.linalg.eig returns complex tensors of dtype cfloat or cdouble rather than real tensors mimicking complex tensors.

L, \_ = torch.eig(A)

should be replaced with

L\_complex = torch.linalg.eigvals(A)

and

L, V = torch.eig(A, eigenvectors=True)

should be replaced with

L\_complex, V\_complex = torch.linalg.eig(A) (Triggered internally at  
../aten/src/ATen/native/BatchLinearAlgebra.cpp:2894.)

return torch.max(torch.abs(torch.eig(m)[0])).item()

Finally, we can train the model. This step consists of three parts:

- Getting the data from the dataloader
- Converting it into the PyTorch Variables
- Feeding it into the network

Traditionally, the code is adapted from the example

```
[21]: for data in trainloader:
        # Inputs and outputs
        inputs, targets = data

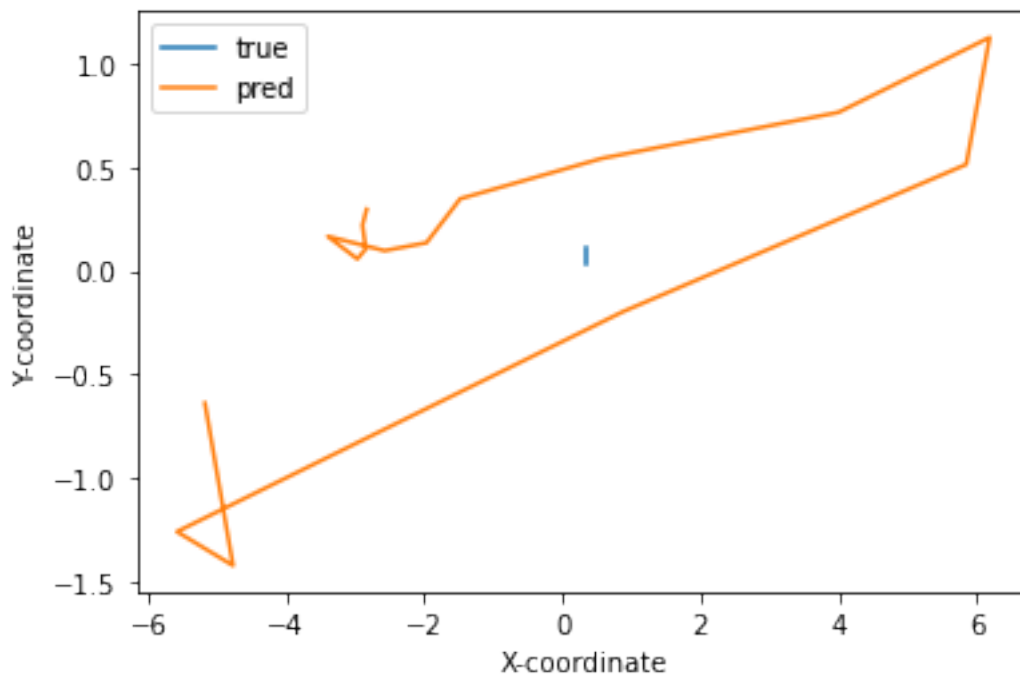
        # Transform data to Variables
        inputs, targets = Variable(inputs), Variable(targets)

        # ESN need inputs and targets
        esn(inputs, targets)
```

```
[22]: # Now we finalize the training by computing the output matrix Wout.  
esn.finalize()
```

Let's take a look at one of the predicted trajectories from the training sample.

```
[23]: dataiter = iter(trainloader)  
train_u, train_y = dataiter.next()  
train_u, train_y = Variable(train_u), Variable(train_y)  
  
y_predicted = esn(train_u)  
  
x_true = []  
x_pred = []  
y_true = []  
y_pred = []  
  
for frame in range(len(y_predicted[0])):  
    x_true.append(train_y[0][frame].numpy()[0])  
    y_true.append(train_y[0][frame].numpy()[1])  
    x_pred.append(y_predicted[0][frame].numpy()[0])  
    y_pred.append(y_predicted[0][frame].numpy()[1])  
  
plt.plot(x_true, y_true, label='true')  
plt.plot(x_pred, y_pred, label='pred')  
plt.xlabel('X-coordinate')  
plt.ylabel('Y-coordinate')  
plt.legend()  
plt.show()
```



Terrible and disgusting, but it is what it is :((

How about test datapoint?

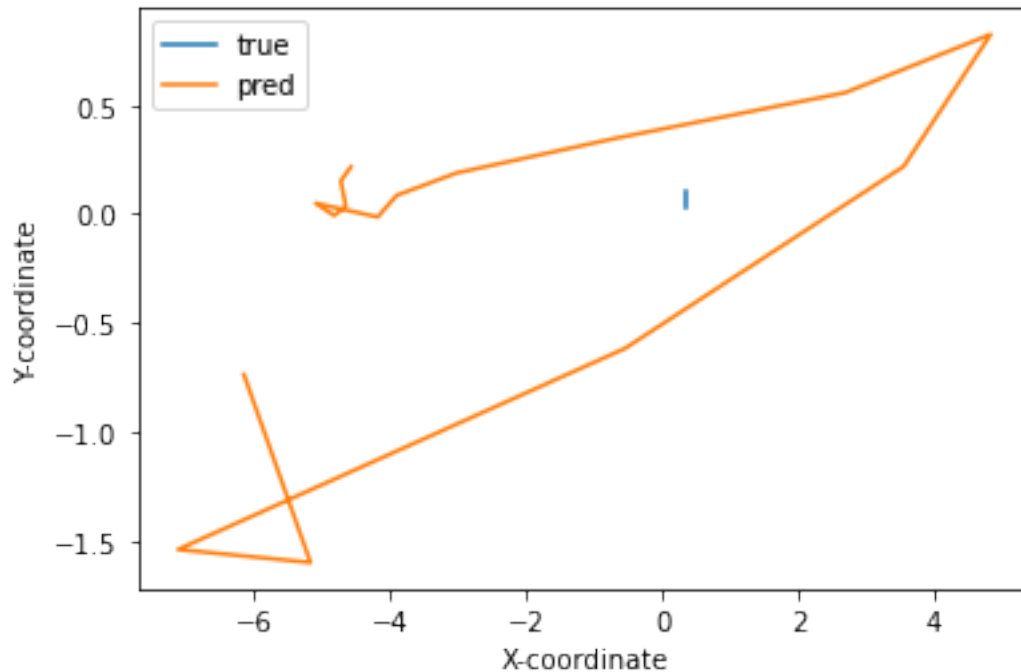
```
[24]: dataiter = iter(testloader)
test_u, test_y = dataiter.next()
test_u, test_y = Variable(test_u), Variable(test_y)

# Make a prediction with our trained ESN
y_predicted = esn(test_u)

x_true = []
x_pred = []
y_true = []
y_pred = []

for frame in range(len(y_predicted[0])):
    x_true.append(test_y[0][frame].numpy()[0])
    y_true.append(test_y[0][frame].numpy()[1])
    x_pred.append(y_predicted[0][frame].numpy()[0])
    y_pred.append(y_predicted[0][frame].numpy()[1])

plt.plot(x_true, y_true, label='true')
plt.plot(x_pred, y_pred, label='pred')
plt.xlabel('X-coordinate')
plt.ylabel('Y-coordinate')
plt.legend()
plt.show()
```



If, by any chance, you thought it can't get worse, then here it is, the “worse”.

Let's now calculate the RMSE for training and testing datasets.

```
[25]: dataiter = iter(trainloader)

mse = 0

for train_u, train_y in dataiter:
    train_u, train_y = Variable(train_u), Variable(train_y)

    y_predicted = esn(train_u)

    mse += echotorch.utils.mse(y_predicted.data, train_y.data)

mse /= len(trainloader)

print('RMSE on train set:', math.sqrt(mse))
```

RMSE on train set: 16.07510224769264

```
[26]: dataiter = iter(testloader)

mse = 0

for test_u, test_y in dataiter:
```

Surprisingly, RMSE on the testing set is smaller.

Now we just repeat the same set of steps but for the dataset that has flattened data from three frames as a single input row instead of one.

```
train_test_split response: test fraction rounded to 0.19985639061752034 (835
simulations)
```

```
input: tensor([[0.3500, 0.2292, 0.0586, 0.7500, 0.2605, 0.1211, 0.4141, 0.7148,  
0.0156,  
          0.3500, 0.1086, 0.0586, 0.7500, 0.1399, 0.1211, 0.4141, 0.5942, 0.0156,  
          0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.2439,  
0.0156],  
          [0.3500, 0.1086, 0.0586, 0.7500, 0.1399, 0.1211, 0.4141, 0.5942, 0.0156,  
          0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.2439, 0.0156,  
          0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0362,  
0.0156],  
          [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.2439, 0.0156,  
          0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0362, 0.0156,  
          0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,  
0.0156],  
          [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0362, 0.0156,  
          0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079, 0.0156,  
          0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,  
0.0156],  
          [0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079, 0.0156,  
          0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079, 0.0156,  
          0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.4141, 0.0079,
```

[illegible]

```

[0.4141, 0.0079],
[0.4141, 0.0079],
[0.4141, 0.0079]])

```

```

[29]: # Setting up input and output dimensions for the network
input_dim = len(train_dataset.__getitem__(0)[0][0])
output_dim = len(train_dataset.__getitem__(0)[1][0])

print(input_dim, output_dim)

```

27 2

```

[30]: # Data loader
trainloader = DataLoader(train_dataset, batch_size=1, shuffle=False,
    ↪num_workers=2)
testloader = DataLoader(test_dataset, batch_size=1, shuffle=False,
    ↪num_workers=2)

trainloader

```

[30]: <torch.utils.data.dataloader.DataLoader at 0x1a2862b6a0>

```

[31]: # Internal matrix
w_generator = mg.NormalMatrixGenerator(
    connectivity=connectivity,
    spectral_radius=spectral_radius
)

# Input weights
win_generator = mg.NormalMatrixGenerator(
    connectivity=connectivity,
    apply_spectral_radius=False
)

# Bias vector
wbias_generator = mg.NormalMatrixGenerator(
    connectivity=connectivity,
    apply_spectral_radius=False
)

```

```

[32]: esn = etrs.LiESN(
    input_dim=input_dim,
    hidden_dim=reservoir_size,
    output_dim=output_dim,
    leaky_rate=leaky_rate,
    learning_algo='inv',
    w_generator=w_generator,
    win_generator=win_generator,

```

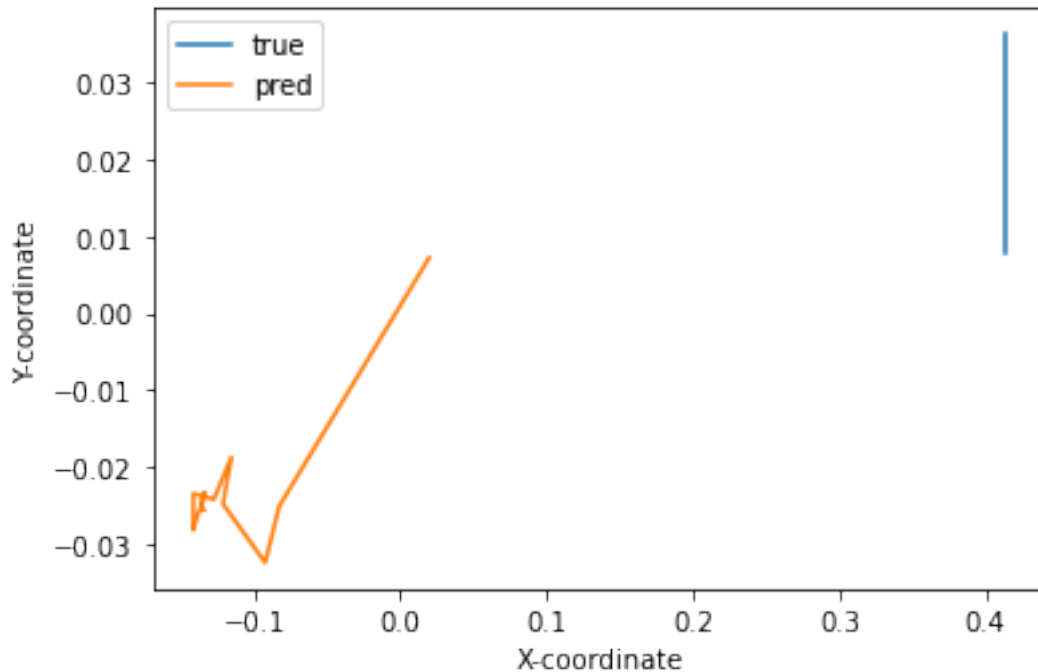


```
wbias_generator=wbias_generator,  
)
```

```
[33]: for data in trainloader:  
      # Inputs and outputs  
      inputs, targets = data  
  
      # Transform data to Variables  
      inputs, targets = Variable(inputs), Variable(targets)  
  
      # ESN need inputs and targets  
      esn(inputs, targets)
```

```
[34]: # Now we finalize the training by computing the output matrix Wout.  
      esn.finalize()
```

```
[35]: dataiter = iter(trainloader)  
      train_u, train_y = dataiter.next()  
      train_u, train_y = Variable(train_u), Variable(train_y)  
  
      y_predicted = esn(train_u)  
  
      x_true = []  
      x_pred = []  
      y_true = []  
      y_pred = []  
  
      for frame in range(len(y_predicted[0])):  
          x_true.append(train_y[0][frame].numpy()[0])  
          y_true.append(train_y[0][frame].numpy()[1])  
          x_pred.append(y_predicted[0][frame].numpy()[0])  
          y_pred.append(y_predicted[0][frame].numpy()[1])  
  
      plt.plot(x_true, y_true, label='true')  
      plt.plot(x_pred, y_pred, label='pred')  
      plt.xlabel('X-coordinate')  
      plt.ylabel('Y-coordinate')  
      plt.legend()  
      plt.show()
```



We can't see the true trajectory, because it is bound between 0 and 1, remember? Sometimes the predicted numbers here are quite not between 0 and 1 :(

```
[36]: dataiter = iter(testloader)
test_u, test_y = dataiter.next()
test_u, test_y = Variable(test_u), Variable(test_y)

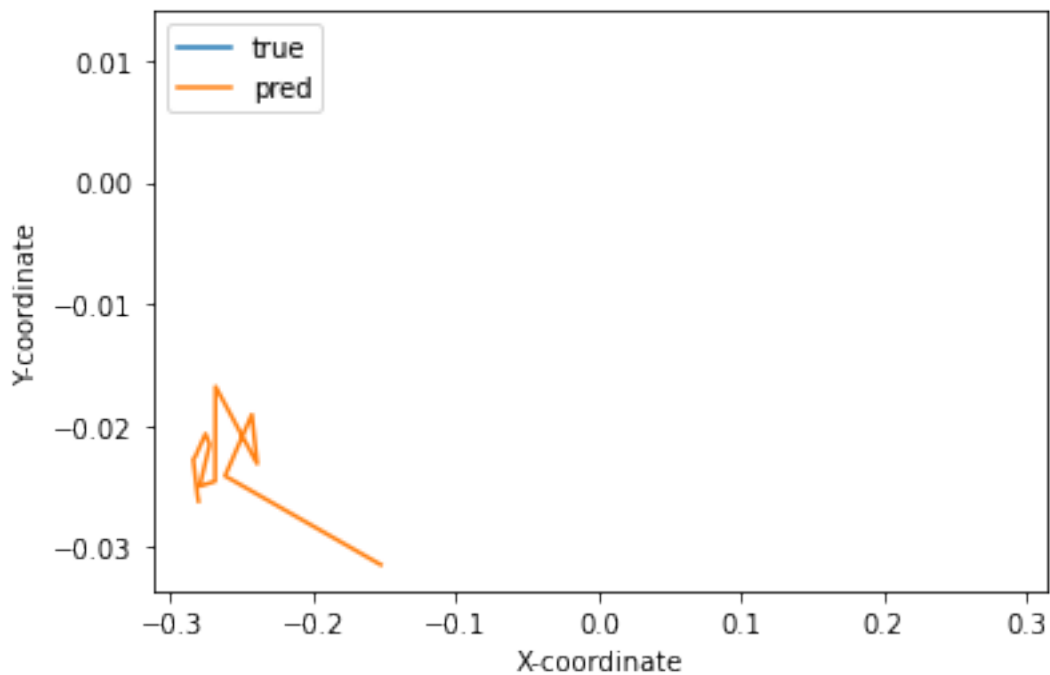
# Make a prediction with our trained ESN
y_predicted = esn(test_u)

x_true = []
x_pred = []
y_true = []
y_pred = []

for frame in range(len(y_predicted[0])):
    x_true.append(test_y[0][frame].numpy()[0])
    y_true.append(test_y[0][frame].numpy()[1])
    x_pred.append(y_predicted[0][frame].numpy()[0])
    y_pred.append(y_predicted[0][frame].numpy()[1])

plt.plot(x_true, y_true, label='true')
plt.plot(x_pred, y_pred, label='pred')
plt.xlabel('X-coordinate')
plt.ylabel('Y-coordinate')
```

```
plt.legend()
plt.show()
```



```
[37]: dataiter = iter(trainloader)

mse = 0

for train_u, train_y in dataiter:
    train_u, train_y = Variable(train_u), Variable(train_y)

    y_predicted = esn(train_u)

    mse += echotorch.utils.mse(y_predicted.data, train_y.data)

mse /= len(trainloader)

print('RMSE on train set:', math.sqrt(mse))
```

RMSE on train set: 0.3518182419747111

```
[38]: dataiter = iter(testloader)

mse = 0

for test_u, test_y in dataiter:
```

```

test_u, test_y = Variable(test_u), Variable(test_y)

y_predicted = esn(test_u)

mse += echotorch.utils.mse(y_predicted.data, test_y.data)

mse /= len(testloader)

print('RMSE on test set:', math.sqrt(mse))

```

RMSE on test set: 0.3507439254057791

Doing disgustingly terrible here, yeah?

## 5.1 Predicting a single pair of next coordinates from three preceeding frames

I have to say that I did not expect this method to be working. When I was trying it out before writing this final project report, the weight matrix after training was non-singular and could not be inverted, which means that the training could not be finalized.

I set the spectral radius to 1 and leaky rate to .9999999, so that after 50,000 iterations the signal rate is still slightly under 1. The only thing that I changed since my previous attempts is reducing the reservoir size from 1000 to 500. Even now sometimes I get the non-singular matrix error, but at least most of the times the training finishes successfully. You can see that the code cell numbers below don't follow the sequence above - I had to rerun these a few times to get a working output.

```

[57]: # Loading data
train_dataset, test_dataset = FrameDataset.train_test_split('data', 0.2)

```

train\_test\_split response: test fraction rounded to 0.19985639061752034 (835 simulations)

```

[58]: # Checking if what loaded is indeed what we need
print('input: ', train_dataset.__getitem__(0)[0])
print('output: ', train_dataset.__getitem__(0)[1])

```

```

input:  tensor([[0.3500, 0.2292, 0.0586, 0.7500, 0.2605, 0.1211, 0.2773, 0.7851,
0.0391,
            0.3500, 0.1086, 0.0586, 0.7500, 0.1399, 0.1211, 0.2773, 0.6645, 0.0391,
            0.3500, 0.0294, 0.0586, 0.7500, 0.0607, 0.1211, 0.2773, 0.3142,
0.0391]])
output:  tensor([[0.2773, 0.0498]])

```

```

[59]: # Setting up input and output dimensions for the network
input_dim = len(train_dataset.__getitem__(0)[0])
output_dim = len(train_dataset.__getitem__(0)[1])

print(input_dim, output_dim)

```

27 2

```
[60]: # Data loader
trainloader = DataLoader(train_dataset, batch_size=1, shuffle=False,
    ↪num_workers=2)
testloader = DataLoader(test_dataset, batch_size=1, shuffle=False,
    ↪num_workers=2)

trainloader
```

```
[60]: <torch.utils.data.dataloader.DataLoader at 0x1a2660c550>
```

```
[61]: # Reservoir hyper-parameters
spectral_radius = 1
leaky_rate = 0.9999999
reservoir_size = 500
connectivity = 0.1954
```

```
[62]: # Internal matrix
w_generator = mg.NormalMatrixGenerator(
    connectivity=connectivity,
    spectral_radius=spectral_radius
)

# Input weights
win_generator = mg.NormalMatrixGenerator(
    connectivity=connectivity,
    apply_spectral_radius=False
)

# Bias vector
wbias_generator = mg.NormalMatrixGenerator(
    connectivity=connectivity,
    apply_spectral_radius=False
)
```

```
[63]: esn = etrs.LiESN(
    input_dim=input_dim,
    hidden_dim=reservoir_size,
    output_dim=output_dim,
    leaky_rate=leaky_rate,
    learning_algo='inv',
    w_generator=w_generator,
    win_generator=win_generator,
    wbias_generator=wbias_generator,
)
```

```
[64]: for data in trainloader:
    # Inputs and outputs
```

```

inputs, targets = data

# Transform data to Variables
inputs, targets = Variable(inputs), Variable(targets)

# ESN need inputs and targets
esn(inputs, targets)

```

```

[65]: # Now we finalize the training by computing the output matrix Wout.
esn.finalize()

```

```

[67]: dataiter = iter(trainloader)

mse = 0

for train_u, train_y in dataiter:
    train_u, train_y = Variable(train_u), Variable(train_y)

    y_predicted = esn(train_u)

    mse += echotorch.utils.mse(y_predicted.data, train_y.data)

mse /= len(trainloader)

print('RMSE on train set:', math.sqrt(mse))

```

RMSE on train set: 0.30667686450375065

```

[68]: dataiter = iter(testloader)

mse = 0

for test_u, test_y in dataiter:
    test_u, test_y = Variable(test_u), Variable(test_y)

    y_predicted = esn(test_u)

    mse += echotorch.utils.mse(y_predicted.data, test_y.data)

mse /= len(testloader)

print('RMSE on test set:', math.sqrt(mse))

```

RMSE on test set: 0.308805027574426

Let's visualize the training and testing trajectories.

```
[69]: dataiter = iter(trainloader)

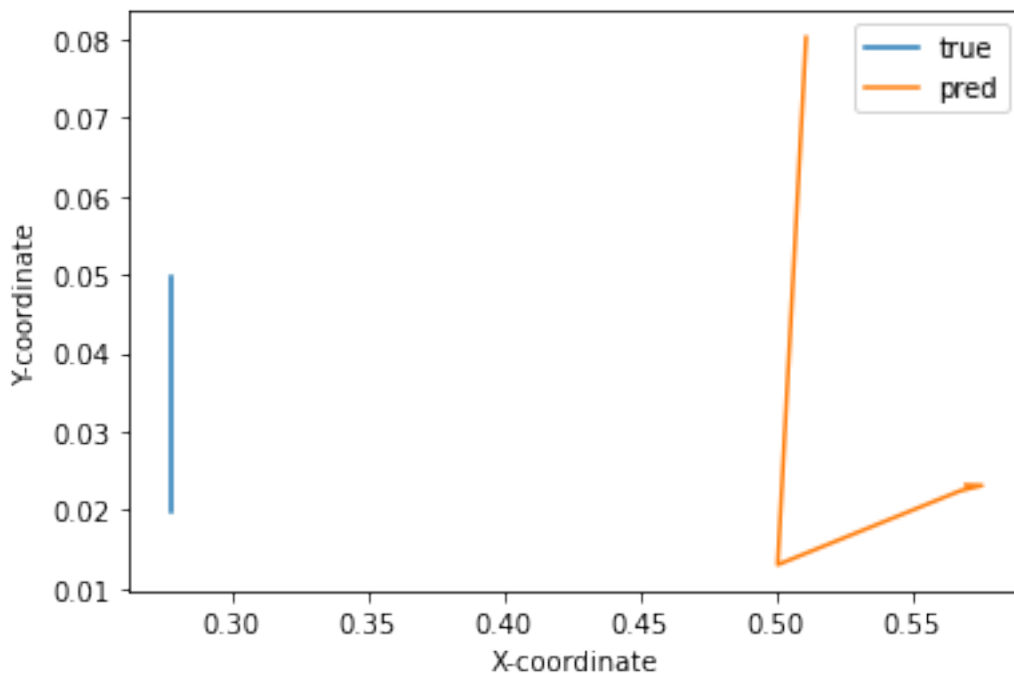
x_true = []
x_pred = []
y_true = []
y_pred = []

# One scene consists of 14 windows of 3 frames each, so I can take the first 14
→to visualize
# the first trajectory.
for i in range(14):
    train_u, train_y = dataiter.next()
    train_u, train_y = Variable(train_u), Variable(train_y)

    y_predicted = esn(train_u)

    x_true.append(train_y[0][0].numpy()[0])
    y_true.append(train_y[0][0].numpy()[1])
    x_pred.append(y_predicted[0][0].numpy()[0])
    y_pred.append(y_predicted[0][0].numpy()[1])

plt.plot(x_true, y_true, label='true')
plt.plot(x_pred, y_pred, label='pred')
plt.xlabel('X-coordinate')
plt.ylabel('Y-coordinate')
plt.legend()
plt.show()
```



```

[77]: dataiter = iter(testloader)

x_true = []
x_pred = []
y_true = []
y_pred = []

# One scene consists of 14 windows of 3 frames each, so I can take the first 14
→to visualize
# the first trajectory.
for i in range(14):
    test_u, test_y = dataiter.next()
    test_u, test_y = Variable(test_u), Variable(test_y)

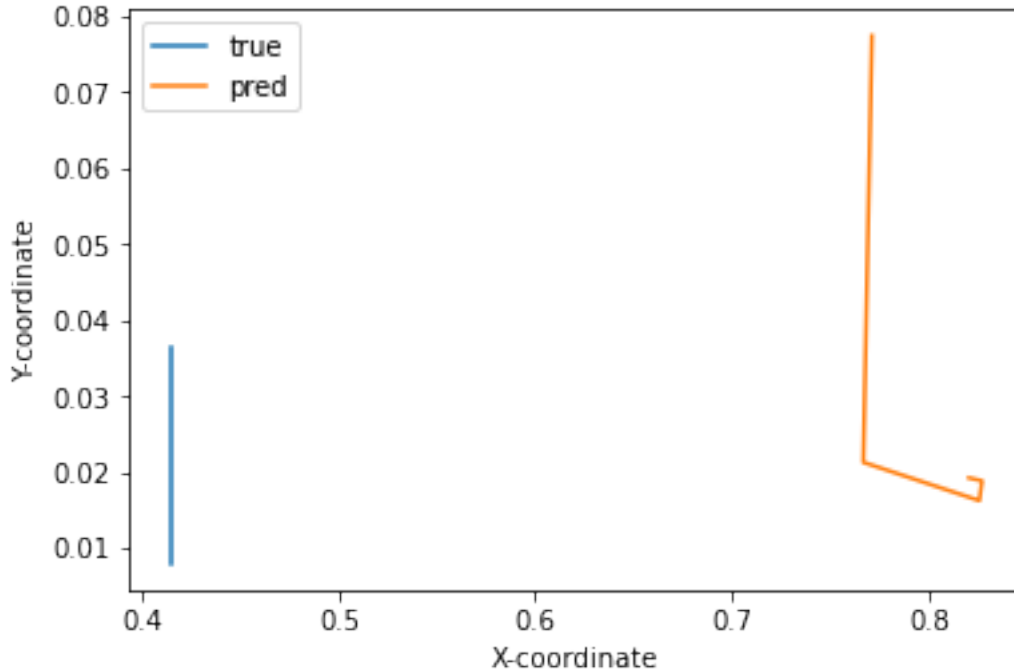
    y_predicted = esn(test_u)

    x_true.append(test_y[0][0].numpy()[0])
    y_true.append(test_y[0][0].numpy()[1])
    x_pred.append(y_predicted[0][0].numpy()[0])
    y_pred.append(y_predicted[0][0].numpy()[1])

plt.plot(x_true, y_true, label='true')
plt.plot(x_pred, y_pred, label='pred')
plt.xlabel('X-coordinate')
plt.ylabel('Y-coordinate')
plt.legend()
plt.show()

```





## 6 Conclusion

In this assignment I trained three ESN models to predict the trajectory of the ball falling, including interactions with two other balls on the scene. Here are the results that I obtained:

- RMSE for the first model (predicting the scene evolution):
  - Training set: 16.07510224769264
  - Testing set: 16.02451024208921
  - The predicted trajectories are not bound in the range of normalized coordinates and visually don't match the ground truth at all.
- RMSE for the second model (predicting a ball trajectory on the entire scene having scene states at three frames as an input instance):
  - Training set: 0.3518182419747111
  - Testing set: 0.3507439254057791
  - The predicted trajectories are much closer to the ground truth but are still ugly. The values are much closer to the normalized coordinates bounds.
- RMSE for the third model (predicting the coordinates of one ball on the next frame given the scene states at three preceeding frames as an input):
  - Training set: 0.30667686450375065
  - Testing set: 0.308805027574426

- Predicted trajectories, while are not matching, at least have a somewhat similar shapes, which is a great success already.
- This model, however, doesn't necessarily converge, which means it still requires some improvement.

Judging only from the results here, I think the third model would be the best choice. It has the smallest error rates, and the predicted trajectory visually has a shape close to what should be in the reality.

Next steps, that will be a part of the capstone journey, would be exploring the performance of such networks on the deterministic free fall trajectories.

[ ]:

```

import torch
from torch.utils.data.dataset import Dataset
from glob import glob
import math
import random
import numpy as np

class PhyreSequentialDataset_ThreeFramesInput_OneFrame(Dataset):
    @staticmethod
    def train_test_split(path, test_frac=0):
        data_glob = glob(path + '/*')

        test_size = int(math.floor(test_frac * len(data_glob)))

        if test_size != test_frac * len(data_glob):
            print(f'train_test_split response: test fraction rounded to ' +
                  f'{test_size/len(data_glob)} ({test_size} simulations)')

        all_indices = list(range(len(data_glob)))
        test_indices = random.choices(all_indices, k=test_size)
        train_indices = [i for i in all_indices if i not in test_indices]

        # returns tuple(train_dataset, test_dataset)
        return (PhyreSequentialDataset_ThreeFramesInput_OneFrame(path,
data_file_indices=train_indices), \
                PhyreSequentialDataset_ThreeFramesInput_OneFrame(path,
data_file_indices=test_indices))

    def __init__(self, path, data_file_indices=None):
        self.data_path = path + '/*'
        self.data_file_indices = data_file_indices

        self.inputs = []
        self.outputs = []

        self.process_data()

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

```

```

def __getitem__(self, idx):
    return self.inputs[idx], self.outputs[idx]

def process_data(self):
    path_glob = sorted(glob(self.data_path))

    for file_idx in range(len(path_glob)):
        if file_idx not in self.data_file_indices: continue

        data = np.load(path_glob[file_idx])

        for frame_number in range(len(data)-3):
            input_instance = []
            output_instance = []

            input_instance.append(data[frame_number])
            input_instance.append(data[frame_number+1])
            input_instance.append(data[frame_number+2])

            input_instance = np.array(input_instance).flatten()
            output_instance = np.array(data[frame_number+3])[2,0:2].flatten()

            input_instance = torch.FloatTensor(np.expand_dims(input_instance,
axis=0))

            output_instance = torch.FloatTensor(np.expand_dims(output_instance,
axis=0))

            self.inputs.append(input_instance)
            self.outputs.append(output_instance)

class PhyreSequentialDataset_ThreeFrameSceneInput_TrajectoryOutput(Dataset):
    @staticmethod
    def train_test_split(path, test_frac=0):
        data_glob = glob(path + '/*')

        test_size = int(math.floor(test_frac * len(data_glob)))

        if test_size != test_frac * len(data_glob):

```

```

        print(f'train_test_split response: test fraction rounded to ' +
              f'{test_size/len(data_glob)} ({test_size} simulations)')

    all_indices = list(range(len(data_glob)))
    test_indices = random.choices(all_indices, k=test_size)
    train_indices = [i for i in all_indices if i not in test_indices]

    # returns tuple(train_dataset, test_dataset)
    return (PhyreSequentialDataset_ThreeFrameSceneInput_TrajectoryOutput(path,
data_file_indices=train_indices), \
           PhyreSequentialDataset_ThreeFrameSceneInput_TrajectoryOutput(path,
data_file_indices=test_indices))

def __init__(self, path, data_file_indices=None):
    self.data_path = path + '/*'
    self.data_file_indices = data_file_indices

    self.inputs = []
    self.outputs = []

    self.process_data()

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

def __getitem__(self, idx):
    return self.inputs[idx], self.outputs[idx]

def process_data(self):
    path_glob = sorted(glob(self.data_path))

    for file_idx in range(len(path_glob)):
        if file_idx not in self.data_file_indices: continue

        data = np.load(path_glob[file_idx])

        input_instance = []

```

```

        output_instance = []
        for frame_number in range(len(data)-3):
            temp_input = []
            temp_input.append(data[frame_number])
            temp_input.append(data[frame_number+1])
            temp_input.append(data[frame_number+2])

            input_instance.append(np.array(temp_input).flatten())
            output_instance.append(np.array(data[frame_number+3])[2,0:2].flatten())

        input_instance = torch.FloatTensor(np.array(input_instance))
        output_instance = torch.FloatTensor(np.array(output_instance))

        self.inputs.append(input_instance)
        self.outputs.append(output_instance)

class PhyreSequentialDataset_EntireSceneInput_EntireSceneOutput(Dataset):
    @staticmethod
    def train_test_split(path, test_frac=0):
        data_glob = glob(path + '/*')

        test_size = int(math.floor(test_frac * len(data_glob)))

        if test_size != test_frac * len(data_glob):
            print(f'train_test_split response: test fraction rounded to ' +
                  f'{test_size/len(data_glob)} ({test_size} simulations)')

        all_indices = list(range(len(data_glob)))
        test_indices = random.choices(all_indices, k=test_size)
        train_indices = [i for i in all_indices if i not in test_indices]

        # returns tuple(train_dataset, test_dataset)
        return (PhyreSequentialDataset_EntireSceneInput_EntireSceneOutput(path,
data_file_indices=train_indices), \
               PhyreSequentialDataset_EntireSceneInput_EntireSceneOutput(path,
data_file_indices=test_indices))

    def __init__(self, path, data_file_indices=None):
        self.data_path = path + '/*'

```

```

self.data_file_indices = data_file_indices

self.inputs = []
self.outputs = []

self.process_data()

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

def __getitem__(self, idx):
    return self.inputs[idx], self.outputs[idx]

def process_data(self):
    path_glob = sorted(glob(self.data_path))

    for file_idx in range(len(path_glob)):
        if file_idx not in self.data_file_indices: continue

        data = np.load(path_glob[file_idx])

        input_instance = []
        output_instance = []
        for frame_number in range(len(data)-1):

            input_instance.append(np.array(data[frame_number]).flatten())
            output_instance.append(np.array(data[frame_number+1]).flatten())

        input_instance = torch.FloatTensor(np.array(input_instance))
        output_instance = torch.FloatTensor(np.array(output_instance))

        self.inputs.append(input_instance)
        self.outputs.append(output_instance)

```