

Jupyter (Python3) script to train 3-DOF neural network

This jupyter notebook provides an example workflow for training a neural network to predict forces on a spherical particle in an optical trap. This notebook requires the training data `input.mat` and produces two files: a trained network `nn3dof.h5` and information about the training run `results.pkl`. When run, this notebook also displays graphs showing how the error changes with training epoch.

Load the data

The training data was generated using the [optical tweezers toolbox](https://github.com/ilent2/ott) (<https://github.com/ilent2/ott>). The data is saved in a `.mat` file, so we use the `scipy.io.loadmat` function to load the data. The file contains 1000000 data points, each with 3 position and 3 force values. We scale the position and force data to be around unity, the position values in the data file are on the scale of microns so we multiply by 10^6 . The force values are in units of $1/c$, which is already near unity for the particular beam power.

In [1]:

```
from scipy.io import loadmat
import numpy as np
from scipy.constants import c

positions = np.transpose(loadmat('input.mat')['positions']) * 1e+6 # positions [um]
forces = np.transpose(loadmat('input.mat')['forces']) # forces [N * c]
```

Split validation and training data and shuffle

We randomly split the data into validation and training data. We use 10% of the data set for validation and reserve the rest for training.

In [2]:

```
number_train_samples = 900000
number_val_samples = 100000

feature_number = 3
tmp = np.concatenate((positions, forces), axis=1)
np.random.shuffle(tmp)

train_data = tmp[:number_train_samples, :feature_number]
train_targets = tmp[:number_train_samples, feature_number:]

val_data = tmp[number_train_samples:number_train_samples + number_val_samples, :feature_number]
val_targets = tmp[number_train_samples:number_train_samples + number_val_samples, feature_number:]
```

Setup keras model

For this problem, we use a dense neural network with 3 internal layers, 1 layer for inputs and 1 layer for outputs. We use different numbers of nodes on the internal layers, the effect of changing the number of nodes is shown in figure 1 in the paper: error improves at a cost of increased network size. For training, we use the [Adam \(https://keras.io/optimizers/#adam\)](https://keras.io/optimizers/#adam) optimiser and we use mean squared error for the loss function. We store mean average error and mean average percentage error for plotting.

In [3]:

```
from keras import models
from keras import layers

sz = 256;

model = models.Sequential()
model.add(layers.Dense(sz, activation='relu', input_shape=(train_data.shape[1],)))
model.add(layers.Dense(sz, activation='relu'))
model.add(layers.Dense(sz, activation='relu'))
model.add(layers.Dense(3))

model.compile(optimizer='adam', loss='mse', metrics=['mae', 'mape'])

model.summary()
```

Using TensorFlow backend.

WARNING:tensorflow:From C:\Users\uqilento\AppData\Local\Continuum\anaconda3\lib\site-packages\tensorflow\python\framework\op_def_library.py:263: colocate_with (from tensorflow.python.framework.ops) is deprecated and will be removed in a future version.
Instructions for updating:
Colocations handled automatically by placer.
Model: "sequential_1"

Layer (type)	Output Shape	Param #
dense_1 (Dense)	(None, 256)	1024
dense_2 (Dense)	(None, 256)	65792
dense_3 (Dense)	(None, 256)	65792
dense_4 (Dense)	(None, 3)	771
Total params: 133,379		
Trainable params: 133,379		
Non-trainable params: 0		

Train the model

We train the model using batches of increasing size. The batch size determines how many trial points are evaluated before updating the network weights. For each batch size, we pass over the entire data set `num_epochs` times, storing the error after each epoch. For reasonable accuracy, the number of epochs should be about 100 and we should start with small batches, however this can take a while so we have use a reduced number of batches in this example.

In [5]:

```
mae = []
mape = []
val_mae = []
val_mape = []

# Realistic number of batches/epochs (takes a while)
# batches = [32, 128, 1024, 4096, 16384]
# num_epochs = 100;

# Small number of batches/epochs for the example
batches = [4096, 16384]
num_epochs = 3;

for epochs, batch_size in zip([num_epochs]*len(batches), batches):
    print(">>> ")
    print(">>> ", batch_size, " <<<")
    print(">>> ")

    history = model.fit(train_data,
                        train_targets,
                        epochs=epochs,
                        batch_size=batch_size,
                        shuffle=True,
                        validation_data=(val_data, val_targets))

    mae.extend(history.history['mean_absolute_error'])
    mape.extend(history.history['mean_absolute_percentage_error'])
    val_mae.extend(history.history['val_mean_absolute_error'])
    val_mape.extend(history.history['val_mean_absolute_percentage_error'])
```

```

>>>
>>> 4096 <<<
>>>
Train on 900000 samples, validate on 100000 samples
Epoch 1/3
900000/900000 [=====] - 8s 9us/step - loss: 1.995
5e-05 - mean_absolute_error: 0.0026 - mean_absolute_percentage_error: 1138
57.2855 - val_loss: 1.5708e-05 - val_mean_absolute_error: 0.0024 - val_mea
n_absolute_percentage_error: 104343.0301
Epoch 2/3
900000/900000 [=====] - 8s 9us/step - loss: 1.361
9e-05 - mean_absolute_error: 0.0023 - mean_absolute_percentage_error: 9848
0.8455 - val_loss: 1.1861e-05 - val_mean_absolute_error: 0.0022 - val_mean
_absolute_percentage_error: 97935.9203
Epoch 3/3
900000/900000 [=====] - 8s 9us/step - loss: 1.518
0e-05 - mean_absolute_error: 0.0026 - mean_absolute_percentage_error: 1464
46.0980 - val_loss: 1.0419e-05 - val_mean_absolute_error: 0.0021 - val_mea
n_absolute_percentage_error: 112472.8664
>>>
>>> 16384 <<<
>>>
Train on 900000 samples, validate on 100000 samples
Epoch 1/3
900000/900000 [=====] - 9s 10us/step - loss: 9.23
73e-06 - mean_absolute_error: 0.0019 - mean_absolute_percentage_error: 878
96.7340 - val_loss: 8.7379e-06 - val_mean_absolute_error: 0.0019 - val_mea
n_absolute_percentage_error: 80990.5558
Epoch 2/3
900000/900000 [=====] - 9s 10us/step - loss: 1.25
29e-05 - mean_absolute_error: 0.0025 - mean_absolute_percentage_error: 142
193.3606 - val_loss: 1.5291e-05 - val_mean_absolute_error: 0.0029 - val_me
an_absolute_percentage_error: 193185.8469
Epoch 3/3
900000/900000 [=====] - 9s 10us/step - loss: 1.29
43e-05 - mean_absolute_error: 0.0026 - mean_absolute_percentage_error: 154
465.2171 - val_loss: 8.3032e-06 - val_mean_absolute_error: 0.0019 - val_me
an_absolute_percentage_error: 88445.0260

```

Look at the error

In [7]:

```
import matplotlib.pyplot as plt

def smooth_curve(points, factor=0.9, offset=200):

    # Doesn't work on small batch/epochs
    if len(points) < offset:
        return points

    smoothed_points = []
    for point in points:
        if len(smoothed_points) < offset:
            smoothed_points.append(points[offset])
        else:
            previous = smoothed_points[-1]
            smoothed_points.append(previous * factor + point * (1 - factor))
    return smoothed_points

def generate_plots(mae, mape, val_mae, val_mape):
    epochs = range(1, len(mae) + 1)

    plt.figure(figsize=(20, 8))

    plt.subplot(2, 2, 1)
    plt.semilogy(epochs, val_mae, 'r', label='Validation MAE')
    plt.semilogy(epochs, mae, 'b', label='Training MAE')
    plt.title('Training and validation MAE')
    plt.xlabel('Epochs')
    plt.ylabel('MAE')
    plt.legend()

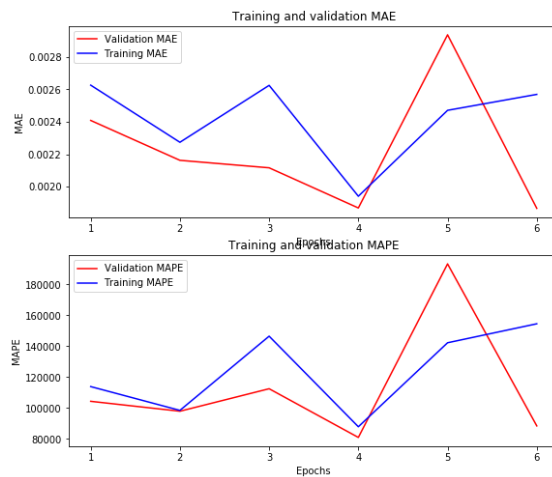
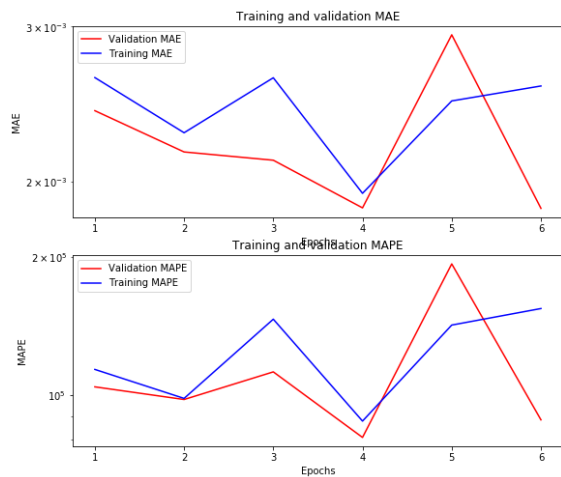
    plt.subplot(2, 2, 2)
    plt.plot(epochs, smooth_curve(val_mae), 'r', label='Validation MAE')
    plt.plot(epochs, smooth_curve(mae), 'b', label='Training MAE')
    plt.title('Training and validation MAE')
    plt.xlabel('Epochs')
    plt.ylabel('MAE')
    plt.legend()

    plt.subplot(2, 2, 3)
    plt.semilogy(epochs, val_mape, 'r', label='Validation MAPE')
    plt.semilogy(epochs, mape, 'b', label='Training MAPE')
    plt.title('Training and validation MAPE')
    plt.xlabel('Epochs')
    plt.ylabel('MAPE')
    plt.legend()

    plt.subplot(2, 2, 4)
    plt.plot(epochs, smooth_curve(val_mape), 'r', label='Validation MAPE')
    plt.plot(epochs, smooth_curve(mape), 'b', label='Training MAPE')
    plt.title('Training and validation MAPE')
    plt.xlabel('Epochs')
    plt.ylabel('MAPE')
    plt.legend()

    plt.show()

generate_plots(mae, mape, val_mae, val_mape)
```



Look at the predicted forces

Here we look at the validation data set and compare to the true data set, the validation data set is used for training the model so a better estimate of the error would use an additional data set that hasn't previously been seen by the model.

In [9]:

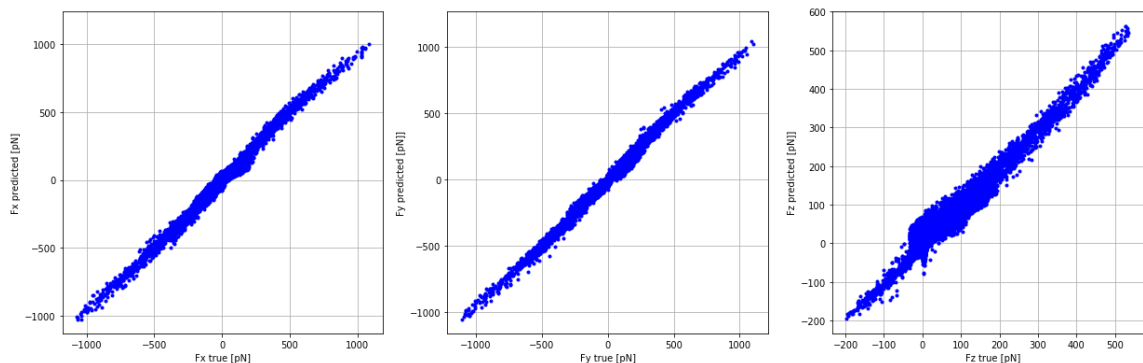
```
predictions = model.predict(val_data)

plt.figure(figsize=(21, 7))

plt.subplot(1, 3, 1)
plt.plot(val_targets[:, 0] / c * 1e+12,
         predictions[:, 0] / c * 1e+12,
         'b.')
plt.xlabel('Fx true [pN]')
plt.ylabel('Fx predicted [pN]')
plt.axis('equal')
plt.axis('square')
plt.grid(True)

plt.subplot(1, 3, 2)
plt.plot(val_targets[:, 1] / c * 1e+12,
         predictions[:, 1] / c * 1e+12,
         'b.')
plt.xlabel('Fy true [pN]')
plt.ylabel('Fy predicted [pN]')
plt.axis('equal')
plt.axis('square')
plt.grid(True)

plt.subplot(1, 3, 3)
plt.plot(val_targets[:, 2] / c * 1e+12,
         predictions[:, 2] / c * 1e+12,
         'b.')
plt.xlabel('Fz true [pN]')
plt.ylabel('Fz predicted [pN]')
plt.axis('equal')
plt.axis('square')
plt.grid(True)
```



Save the result

The output files can be loaded back into python or Matlab for later use.

In [11]:

```
save_file_name = "nn3dof.h5"  
model.save(save_file_name)  
  
import pickle  
  
save_file_name_pkl = "results.pkl"  
with open(save_file_name_pkl, 'wb') as f:  
    pickle.dump([mae, mape, val_mae, val_mape], f)
```

In []: