pulse2D_MLP

March 22, 2019

In [1]:
```
# Import packages

# Keras framework
from keras.layers import Input, Dense, Dropout, BatchNormalization
from keras.models import Model
from keras.callbacks import EarlyStopping, ReduceLROnPlateau, CSVLogger

# Scikit-learn
from sklearn.metrics import mean_squared_error

# data analysis packages
import numpy as np

# plotting tools
from matplotlib import rcParams  # next 3 lines set font family for plotting
rcParams['font.family'] = ['serif']
rcParams['font.sans-serif'] = ['Optima']
rcParams['font.serif'] = ['Didot']
import matplotlib.pyplot as plt
plt.rcParams.update({'font.size': 18})

# misc. packages
import os   # file navigation
import h5py
```

```
Using TensorFlow backend.
```

In [2]:
```
# SETTINGS FOR REPRODUCIBLE RESULTS DURING DEVELOPMENT

import tensorflow as tf
import random as rn

# The below is necessary in Python 3.2.3 onwards to
# have reproducible behavior for certain hash-based operations.
# See these references for further details:
# https://docs.python.org/3.4/using/cmdline.html#envvar-PYTHONHASHSEED
```

```
# https://github.com/keras-team/keras/issues/2280#issuecomment-306959926

#import os
os.environ['PYTHONHASHSEED'] = '0'

# The below is necessary for starting Numpy generated random numbers
# in a well-defined initial state.

np.random.seed(42)

# The below is necessary for starting core Python generated random numbers
# in a well-defined state.

rn.seed(12345)

# Force TensorFlow to use single thread.
# Multiple threads are a potential source of
# non-reproducible results.
# For further details, see: https://stackoverflow.com/questions/42022950/which-seeds-hav

session_conf = tf.ConfigProto(intra_op_parallelism_threads=1, inter_op_parallelism_threa

from keras import backend as K

# The below tf.set_random_seed() will make random number generation
# in the TensorFlow backend have a well-defined initial state.
# For further details, see: https://www.tensorflow.org/api_docs/python/tf/set_random_see

tf.set_random_seed(1234)

sess = tf.Session(graph=tf.get_default_graph(), config=session_conf)
K.set_session(sess)
```

In [3]:
```
# read in preprocessed data

with h5py.File('pulse2D_MLP_X.hdf5','r') as f:
    X_train = np.array(f['X_train'])
    X_test = np.array(f['X_test'])

with h5py.File('pulse2D_MLP_Y.hdf5','r') as f:
    Y_train = np.array(f['Y_train'])
    Y_test = np.array(f['Y_test'])
```

In [4]:
```
# misc parameters
Ndomain_nodes = 20  # number of 'timesteps', in this case is equal to the number of doma
XNfeatures = X_train.shape[1]  # static features
YNfeatures = Ndomain_nodes  # only one prediction of interest....(Cmax)
```

```
# HYPERPARAMETERS
epochs = 1000  # the number of forward/backward passes to train each model
batch_size = 5000  # number of samples to be trained at a time for batch processing
do = 0.1  # dropout rate - fraction of samples that do not receive updates per epoch, he
Nnodes = 5  # nodes per hidden layer
es_thresh = 0.001  # minimum improvement needed to avoid early stopping
lr_decay = 0.5  # factor by which to reduce the learning rate if it has not improved w/i
cb_patience = 15  # number of epochs to wait to activate callback functions
```

In [5]:
```
# build MLP model

# create input layer..........
main_input = Input(shape=(XNfeatures), # number features in the input dataset
                   dtype='float',  # number type - floating point, usually double precis
                   batch_shape=(batch_size,XNfeatures),  # shape of each batch size
                   name='main_input'  # name of input layer
                   )

#create hidden layers..........
hidden_layer1 = Dense(Nnodes, # number nodes in hidden layer
                      activation='tanh',  # activation function to apply to output of hi
                      name='hidden_layer1'  # name of hidden layer
                      )(main_input)
Dropout(do)(hidden_layer1)  # add dropout to hidden layer
hidden_layer1 = BatchNormalization()(hidden_layer1)  # add batch normalization
hidden_layer2 = Dense(Nnodes,
                      activation='tanh',
                      name='hidden_layer2'
                      )(hidden_layer1)
Dropout(do)(hidden_layer2)

# create output layer
main_output = Dense(YNfeatures, # number of features in output array
                    name='main_output'  # name of output layer
                    )(hidden_layer2)  # default activation is linear

# initialize the model, feed layers into model for training
model = Model(inputs=[main_input],
              outputs=[main_output]
              )

# compile the model with desired configuration
model.compile(loss='mean_squared_error',  # loss function to calculate at the end of eac
              optimizer='adam',  # optimization method to minimize cost function
              )

# one of several callbacks available in Keras, csv_logger saves metrics for every epoch
csv_logger = CSVLogger('trainingMLP_' + str(epochs) + '.log')
```

```python
        # if the model isn't improving, stop before the desired number epochs has been reached
        early_stop = EarlyStopping(monitor='val_loss', # quantity to monitor
                                   min_delta=es_thresh,  # min change to qualify as an improveme
                                   patience=cb_patience + 200, # stop after #epochs with no impr
                                   verbose=1)  # print messages

        # if the loss isn't decreasing, reduce the learning rate aid in optimization
        reduce_lr = ReduceLROnPlateau(monitor='val_loss',
                                      factor=lr_decay,  # reduction factor (new_lr = lr * factor
                                      patience=cb_patience, # stop after #epochs with no improve
                                      verbose=1)

        # train the model, and store training information in the history object
        history = model.fit([X_train],[Y_train],  # pass in training datasets
                            validation_data=(X_test, Y_test),  # pass in test data - not used in
                            # set hyperparameters and callbacks
                            epochs=epochs,
                            batch_size = batch_size,
        #                    callbacks=[csv_logger,reduce_lr]
                            callbacks=[reduce_lr,early_stop,csv_logger]
                            )

        histdict = history.history  # save the model output as a dictionary
        model.summary()  # print out a summary of layers/parameters
        config = model.get_config()  # detailed information about the configuration of each laye
```

```
Train on 90000 samples, validate on 10000 samples
Epoch 1/1000
90000/90000 [==============================] - 1s 7us/step - loss: 2.1564e-04 - val_loss: 0.0026
Epoch 2/1000
90000/90000 [==============================] - 0s 3us/step - loss: 1.0545e-04 - val_loss: 0.0165
Epoch 3/1000
90000/90000 [==============================] - 0s 3us/step - loss: 8.4252e-05 - val_loss: 0.0401
Epoch 4/1000
90000/90000 [==============================] - 0s 2us/step - loss: 7.1916e-05 - val_loss: 0.0603
Epoch 5/1000
90000/90000 [==============================] - 0s 3us/step - loss: 6.4008e-05 - val_loss: 0.0724

...
...

Epoch 00285: ReduceLROnPlateau reducing learning rate to 3.051757957450718e-08.
Epoch 286/1000
90000/90000 [==============================] - 0s 2us/step - loss: 3.6577e-05 - val_loss: 3.5927
Epoch 287/1000
90000/90000 [==============================] - 0s 2us/step - loss: 3.6577e-05 - val_loss: 3.5927
Epoch 288/1000
```

```
90000/90000 [==============================] - 0s 2us/step - loss: 3.6577e-05 - val_loss: 3.5927
Epoch 00288: early stopping
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
main_input (InputLayer)      (5000, 6)                 0
_________________________________________________________________
hidden_layer1 (Dense)        (5000, 5)                 35
_________________________________________________________________
batch_normalization_1 (Batch (5000, 5)                 20
_________________________________________________________________
hidden_layer2 (Dense)        (5000, 5)                 30
_________________________________________________________________
main_output (Dense)          (5000, 20)                120
=================================================================
Total params: 205
Trainable params: 195
Non-trainable params: 10
_________________________________________________________________
```

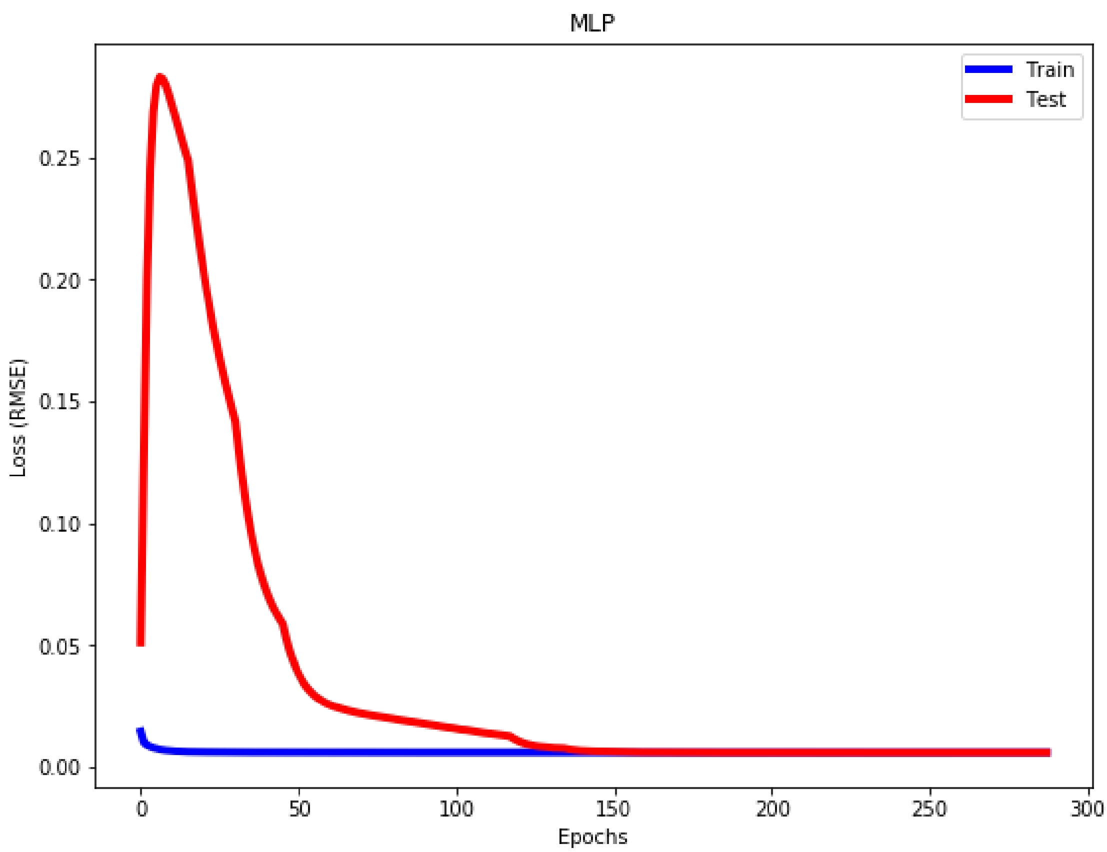
In [6]:
```
# evaluate the trained model on the test data set

# test how well the model can predict Cmax given only the reserved input test dataset
predict = model.predict([X_test],batch_size=batch_size)
Y_rmse = np.sqrt(mean_squared_error(predict,Y_test))
print('Y_rmse:   ',Y_rmse)
model.save('MLP_' + str(epochs) + 'epochs.h5')
```

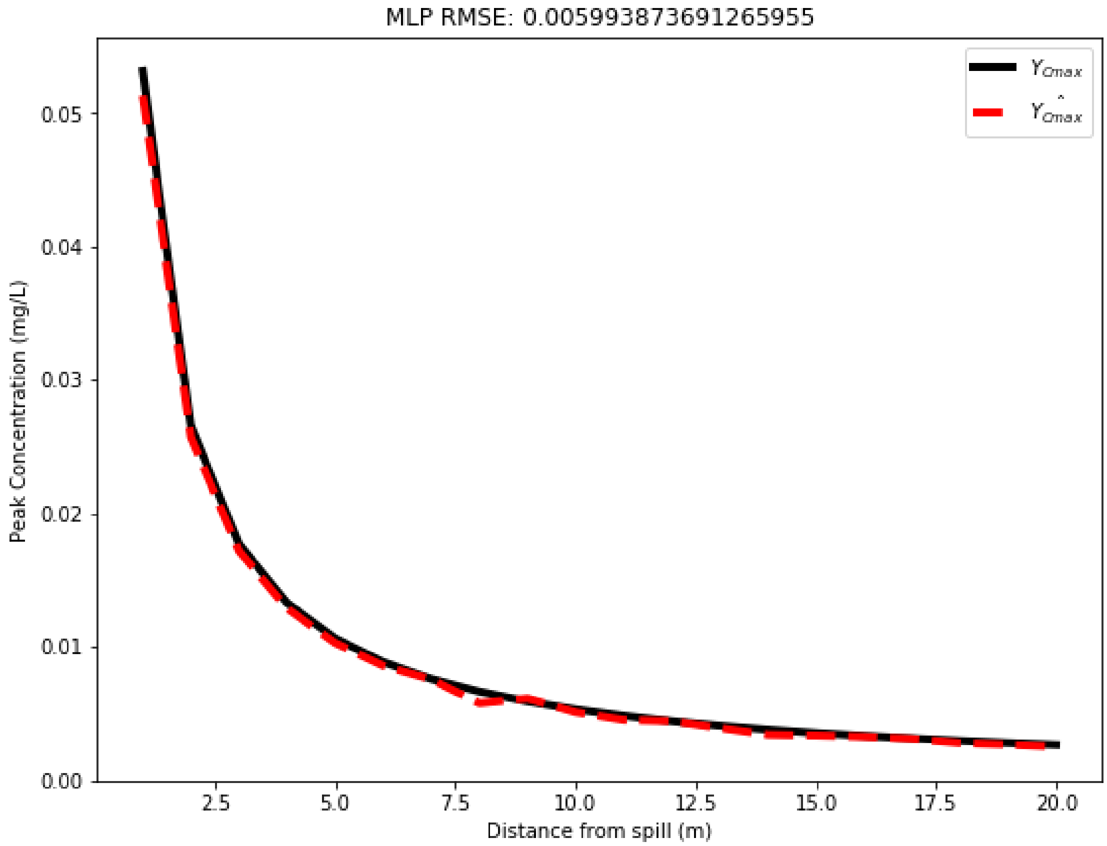
```
Y_rmse:    0.005993873691265955
```

In [7]:
```
# plot MLP output

loss_train = histdict['loss']
loss_test = histdict['val_loss']
xplot = list(range(len(loss_train)))

fig = plt.figure(num=1, figsize=(8,6))
ax = fig.add_subplot(111)
train = ax.plot(xplot,np.sqrt(loss_train),'b-', label='Train', linewidth=4)
test = ax.plot(xplot,np.sqrt(loss_test),'r-',label='Test',linewidth=4)
ax.set_xlabel('Epochs')
ax.set_ylabel('Loss (RMSE)')
curves = train + test
labels = [c.get_label() for c in curves]
ax.legend(curves, labels, loc=0)
plt.tight_layout()
```

```python
plt.title('MLP')
plt.savefig('MLPout' + str(epochs) + 'epochs.png')
plt.show()

xplot2 = list(range(1,21))
fig = plt.figure(num=2, figsize=(8,6))
ax = fig.add_subplot(111)
y_test = ax.plot(xplot2,Y_test[0],'k-', label=r'$Y_{Cmax}$', linewidth=4)
y_predict = ax.plot(xplot2,predict[0],'r--',label=r'$\hat{Y_{Cmax}}$',linewidth=4)
ax.set_xlabel('Distance from spill (m)')
ax.set_ylabel('Peak Concentration (mg/L)')
curves = y_test + y_predict
labels = [c.get_label() for c in curves]
ax.legend(curves, labels, loc=0)
plt.tight_layout()
plt.title('MLP RMSE: ' + str(Y_rmse))
plt.savefig('MLPpredict' + str(epochs) + 'epochs.png')
plt.show()
```

```
C:\Users\kathe\Anaconda3\lib\site-packages\matplotlib\font_manager.py:1238: UserWarning: findfon
  (prop.get_family(), self.defaultFamily[fontext]))
```




MLP RMSE: 0.005993873691265955
0.05
0.04
0.03
0.02
0.01
0.00
Peak Concentration (mg/L)
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
Distance from spill (m)
Y_{Cmax}
$\hat{Y_{Cmax}}$