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How to Tune LSTM Hyperparameters with Keras for Time Series Forecasting

by **Jason Brownlee** on April 12, 2017 in **Long Short-Term Memory Networks**

Configuring neural networks is difficult because there is no good theory on how to do it.

You must be systematic and explore different configurations both from a dynamical and an objective results point of a view to try to understand what is going on for a given predictive modeling problem.

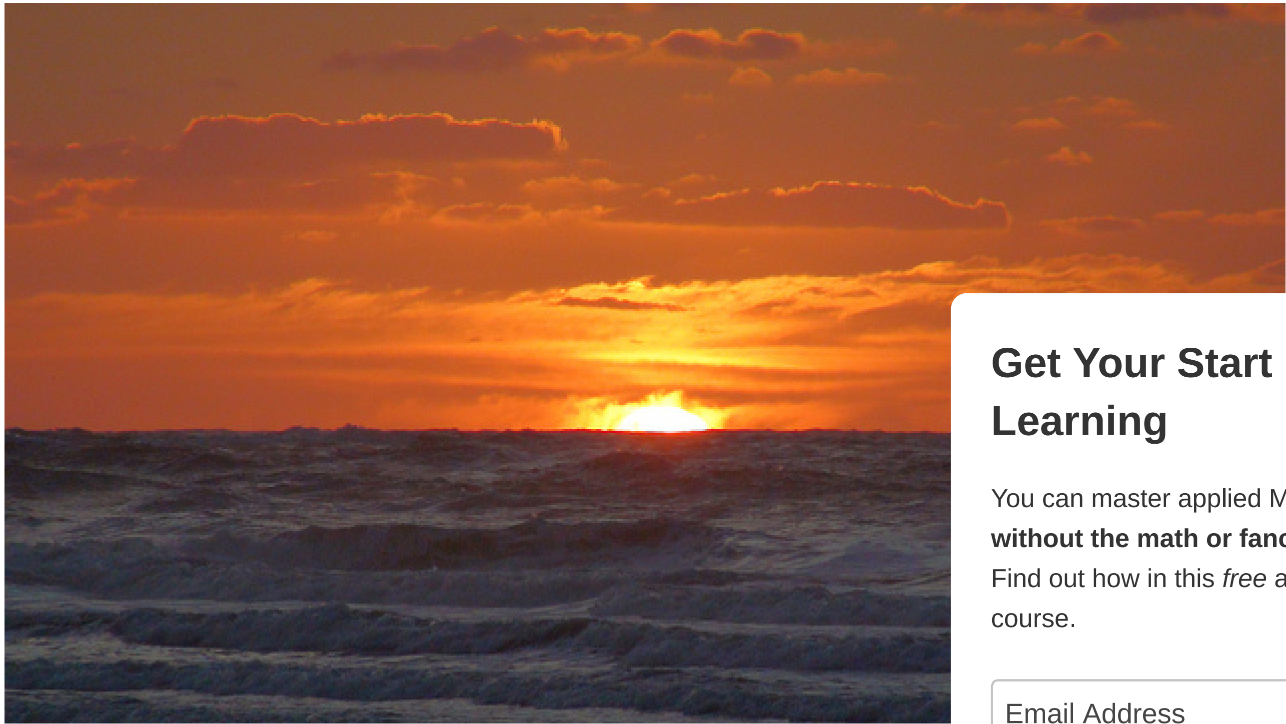
In this tutorial, you will discover how you can explore how to configure an LSTM network on a time series forecasting problem.

After completing this tutorial, you will know:

- How to tune and interpret the results of the number of training epochs.

- How to tune and interpret the results of the size of training batches.
- How to tune and interpret the results of the number of neurons.

Let’s get started.



How to Tune LSTM Hyperparameters with Keras for Time Series Fo
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Tutorial Overview

This tutorial is broken down into 6 parts; they are:

1. Shampoo Sales Dataset
2. Experimental Test Harness
3. Tuning the Number of Epochs
4. Tuning the Batch Size

Environment

This tutorial assumes you have a Python SciPy environment installed. You can use either Python 2 or 3 with this example.

This tutorial assumes you have Keras v2.0 or higher installed with either the TensorFlow or Theano backend.

The tutorial also assumes you have scikit-learn, Pandas, NumPy and Matplotlib installed.

If you need help setting up your Python environment, see this post:

- How to Setup a Python Environment for Machine Learning and Deep Learning with Anaconda

Shampoo Sales Dataset

This dataset describes the monthly number of sales of shampoo over a 3-year period.

The units are a sales count and there are 36 observations. The original dataset is credited to Makrid

You can download and learn more about the dataset here.

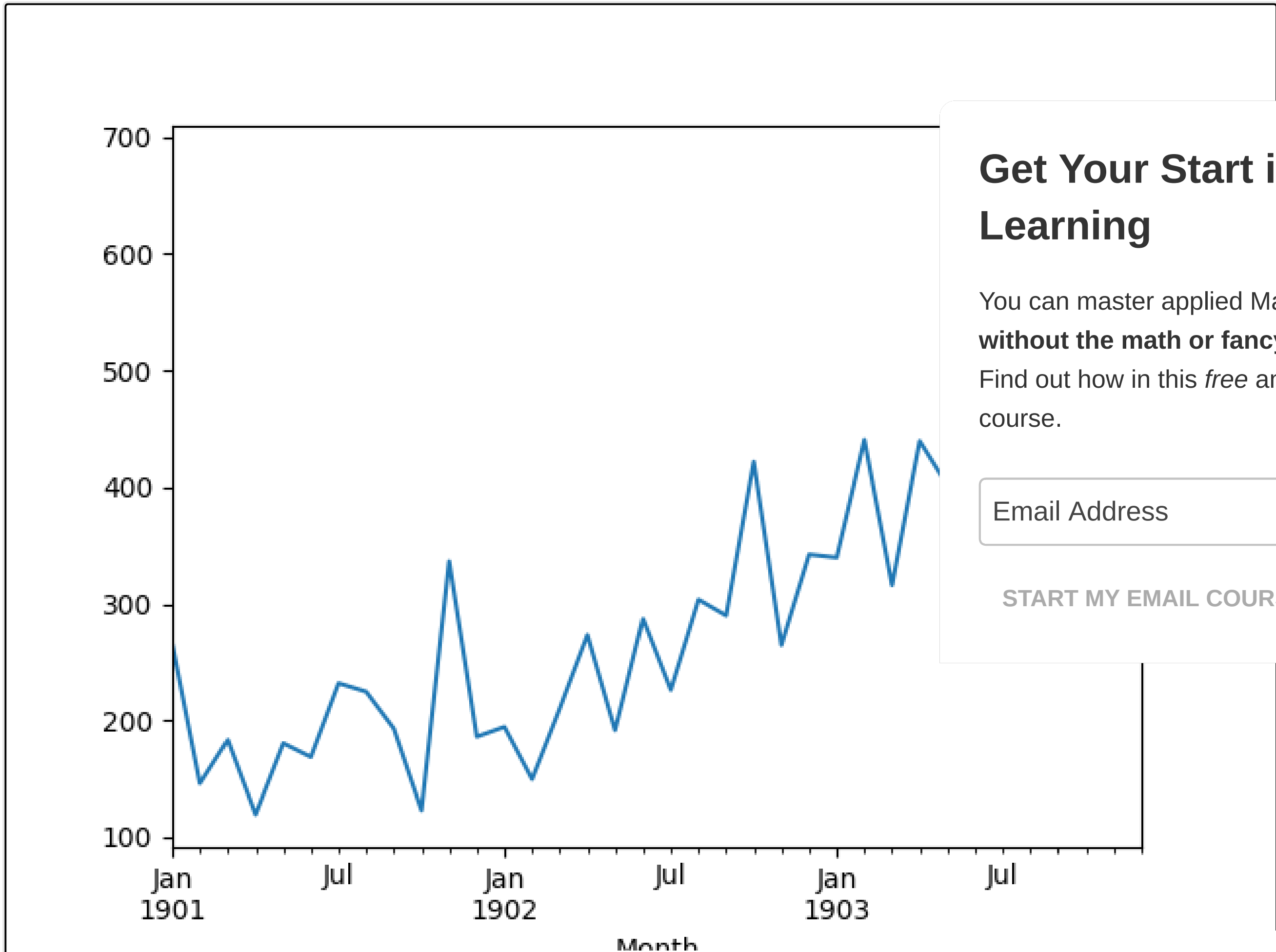
The example below loads and creates a plot of the loaded dataset.

```
# load and plot dataset
from pandas import read_csv
from pandas import datetime
from matplotlib import pyplot
# load dataset
def parser(x):
    return datetime.strptime('190'+x, '%Y-%m')
series = read_csv('shampoo-sales.csv', header=0, parse_dates=[0], index_col=0, squeeze=True, date_parser=parser)
# summarize first few rows
print(series.head())
# line plot
series.plot()
pyplot.show()
```

Running the example loads the dataset as a Pandas Series and prints the first 5 rows.

```
Month
1901-01-01 266.0
1901-02-01 145.9
1901-03-01 183.1
1901-04-01 119.3
1901-05-01 180.3
Name: Sales, dtype: float64
```

A line plot of the series is then created showing a clear increasing trend.



Line Plot of Shampoo Sales Dataset

Next, we will take a look at the LSTM configuration and test harness used in the experiment.

Experimental Test Harness

This section describes the test harness used in this tutorial.

Data Split

We will split the Shampoo Sales dataset into two parts: a training and a test set.

The first two years of data will be taken for the training dataset and the remaining one year of data w

Models will be developed using the training dataset and will make predictions on the test dataset.

The persistence forecast (naive forecast) on the test dataset achieves an error of 136.761 monthly shampoo sales. This provides a lower acceptable bound of performance on the test set.

Model Evaluation

A rolling-forecast scenario will be used, also called walk-forward model validation.

Each time step of the test dataset will be walked one at a time. A model will be used to make a forec[redacted]ue from the test set will be taken and made available to the model for the forecast on the next time step.

This mimics a real-world scenario where new Shampoo Sales observations would be available each month and used in the forecasting of the following month.

This will be simulated by the structure of the train and test datasets. We will make all of the forecasts in a one-shot method.

All forecasts on the test dataset will be collected and an error score calculated to summarize the skill of the model. The root mean squared error (RMSE) will be used as it punishes large errors and results in a score that is in the same units as the forecast data, namely monthly shampoo sales.

Data Preparation

Before we can fit an LSTM model to the dataset, we must transform the data.

The following three data transforms are performed on the dataset prior to fitting a model and making

1. Transform the time series data so that it is stationary. Specifically, a lag=1 differencing to remov
2. Transform the time series into a supervised learning problem. Specifically, the organization of da observation at the previous time step is used as an input to forecast the observation at the curre
3. Transform the observations to have a specific scale. Specifically, to rescale the data to values b tangent activation function of the LSTM model.

These transforms are inverted on forecasts to return them into their original scale before calculating

Experimental Runs

Each experimental scenario will be run 10 times.

The reason for this is that the random initial conditions for an LSTM network can result in very different results each time a given configuration is trained.

A diagnostic approach will be used to investigate model configurations. This is where line plots of model skill over time (training iterations called epochs) will be created and studied for insight into how a given configuration performs and how it may be adjusted to elicit better performance.

The model will be evaluated on both the train and the test datasets at the end of each epoch and the

The train and test RMSE scores at the end of each scenario are printed to give an indication of progress.

The series of train and test RMSE scores are plotted at the end of a run as a line plot. Train scores are colored blue and test scores are colored orange.

Let's dive into the results.

Tuning the Number of Epochs

The first LSTM parameter we will look at tuning is the number of training epochs.

The model will use a batch size of 4, and a single neuron. We will explore the effect of training this configuration for different numbers of training epochs.

Diagnostic of 500 Epochs

The complete code listing for this diagnostic is listed below.

The code is reasonably well commented and should be easy to follow. This code will be the basis fo
changes made in each subsequent experiment will be listed.

```
from pandas import DataFrame
from pandas import Series
from pandas import concat
from pandas import read_csv
from pandas import datetime
from sklearn.metrics import mean_squared_error
from sklearn.preprocessing import MinMaxScaler
from keras.models import Sequential
from keras.layers import Dense
from keras.layers import LSTM
from math import sqrt
import matplotlib
# be able to save images on server
matplotlib.use('Agg')
from matplotlib import pyplot
import numpy

# date-time parsing function for loading the dataset
def parser(x):
    return datetime.strptime('190'+x, '%Y-%m')

```

```
# frame a sequence as a supervised learning problem
def timeseries_to_supervised(data, lag=1):
    df = DataFrame(data)
    columns = [df.shift(i) for i in range(1, lag+1)]
    columns.append(df)
    df = concat(columns, axis=1)
    df = df.drop(0)
    return df

# create a differenced series
def difference(dataset, interval=1):
    diff = list()
    for i in range(interval, len(dataset)):
        value = dataset[i] - dataset[i - interval]
        diff.append(value)
    return Series(diff)

# scale train and test data to [-1, 1]
def scale(train, test):
    # fit scaler
    scaler = MinMaxScaler(feature_range=(-1, 1))
    scaler = scaler.fit(train)
    # transform train
    train = train.reshape(train.shape[0], train.shape[1])
    train_scaled = scaler.transform(train)
    # transform test
    test = test.reshape(test.shape[0], test.shape[1])
    test_scaled = scaler.transform(test)
    return scaler, train_scaled, test_scaled

# inverse scaling for a forecasted value
def invert_scale(scaler, X, yhat):
    new_row = [x for x in X] + [yhat]
    array = numpy.array(new_row)
    array = array.reshape(1, len(array))
    inverted = scaler.inverse_transform(array)
    return inverted[0, -1]

# evaluate the model on a dataset, returns RMSE in transformed units
def evaluate(model, raw_data, scaled_dataset, scaler, offset, batch_size):
    # separate
    X, y = scaled_dataset[:,0:-1], scaled_dataset[:,-1]
    # reshape
    reshaped = X.reshape(len(X), 1, 1)
    # forecast dataset
    output = model.predict(reshaped, batch_size=batch_size)
    # invert data transforms on forecast
```

```
    predictions = list()
    for i in range(len(output)):
        yhat = output[i,0]
        # invert scaling
        yhat = invert_scale(scaler, X[i], yhat)
        # invert differencing
        yhat = yhat + raw_data[i]
        # store forecast
        predictions.append(yhat)
    # report performance
    rmse = sqrt(mean_squared_error(raw_data[1:], predictions))
    return rmse

# fit an LSTM network to training data
def fit_lstm(train, test, raw, scaler, batch_size, nb_epoch, neurons):
    X, y = train[:, 0:-1], train[:, -1]
    X = X.reshape(X.shape[0], 1, X.shape[1])
    # prepare model
    model = Sequential()
    model.add(LSTM(neurons, batch_input_shape=(batch_size, X.shape[1], X.shape[2]), stc
    model.add(Dense(1))
    model.compile(loss='mean_squared_error', optimizer='adam')
    # fit model
    train_rmse, test_rmse = list(), list()
    for i in range(nb_epoch):
        model.fit(X, y, epochs=1, batch_size=batch_size, verbose=0, shuffle=False)
        model.reset_states()
        # evaluate model on train data
        raw_train = raw[-(len(train)+len(test)+1):-len(test)]
        train_rmse.append(evaluate(model, raw_train, train, scaler, 0, batch_size))
        model.reset_states()
        # evaluate model on test data
        raw_test = raw[-(len(test)+1):]
        test_rmse.append(evaluate(model, raw_test, test, scaler, 0, batch_size))
        model.reset_states()
    history = DataFrame()
    history['train'], history['test'] = train_rmse, test_rmse
    return history

# run diagnostic experiments
def run():
    # load dataset
    series = read_csv('shampoo-sales.csv', header=0, parse_dates=[0], index_col=0, squeeze=True, date_parser=parser)
    # transform data to be stationary
    raw_values = series.values
    diff_values = difference(raw_values, 1)
    # transform data to be supervised learning
```

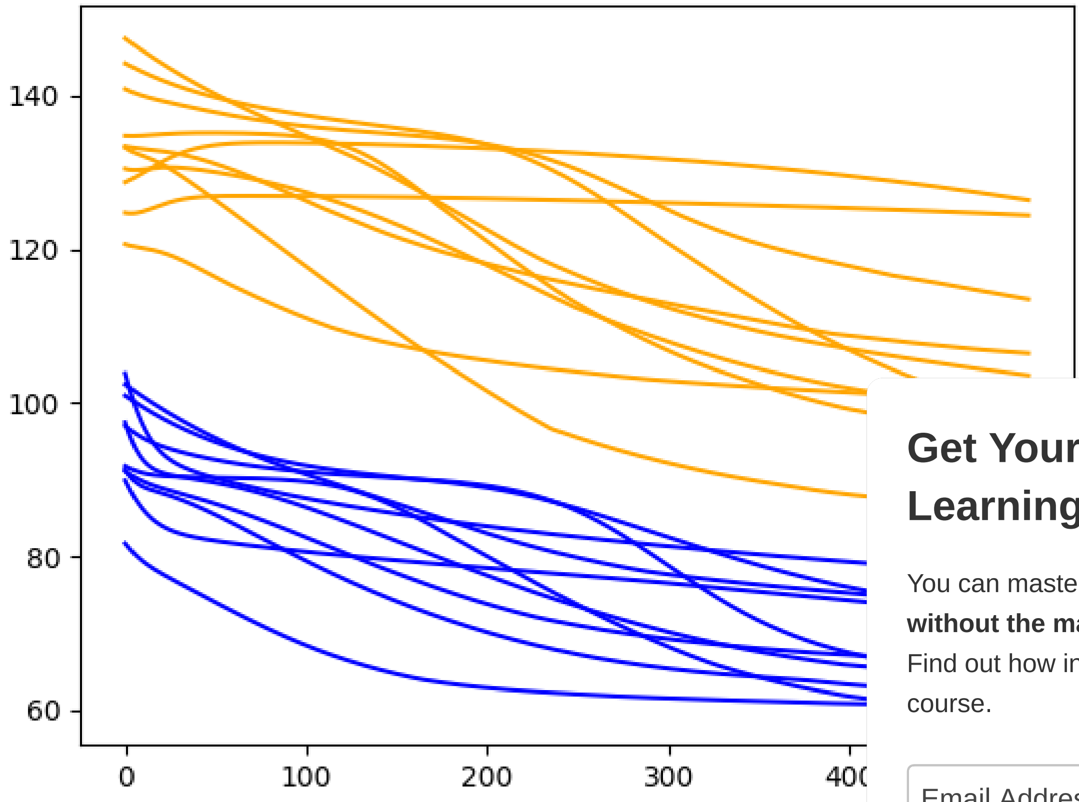
```
    supervised = timeseries_to_supervised(diff_values, 1)
    supervised_values = supervised.values
    # split data into train and test-sets
    train, test = supervised_values[0:-12], supervised_values[-12:]
    # transform the scale of the data
    scaler, train_scaled, test_scaled = scale(train, test)
    # fit and evaluate model
    train_trimmed = train_scaled[2:, :]
    # config
    repeats = 10
    n_batch = 4
    n_epochs = 500
    n_neurons = 1
    # run diagnostic tests
    for i in range(repeats):
        history = fit_lstm(train_trimmed, test_scaled, raw_values, scaler, n_batch, n_epochs, n_neurons)
        pyplot.plot(history['train'], color='blue')
        pyplot.plot(history['test'], color='orange')
        print('%d) TrainRMSE=%f, TestRMSE=%f' % (i, history['train'].iloc[-1], history[
    pyplot.savefig('epochs_diagnostic.png')

# entry point
run()
```

Running the experiment prints the RMSE for the train and the test sets at the end of each of the 10 e

```
0) TrainRMSE=63.495594, TestRMSE=113.472643
1) TrainRMSE=60.446307, TestRMSE=100.147470
2) TrainRMSE=59.879681, TestRMSE=95.112331
3) TrainRMSE=66.115269, TestRMSE=106.444401
4) TrainRMSE=61.878702, TestRMSE=86.572920
5) TrainRMSE=73.519382, TestRMSE=103.551694
6) TrainRMSE=64.407033, TestRMSE=98.849227
7) TrainRMSE=72.684834, TestRMSE=98.499976
8) TrainRMSE=77.593773, TestRMSE=124.404747
9) TrainRMSE=71.749335, TestRMSE=126.396615
```

A line plot of the series of RMSE scores on the train and test sets after each training epoch is also created.



Diagnostic Results with 500 Epochs

The results clearly show a downward trend in RMSE over the training epochs for almost all of the experimental runs.

This is a good sign, as it shows the model is learning the problem and has some predictive skill. In fact, all of the final test scores are below the error of a simple persistence model (naive forecast) that achieves an RMSE of 136.761 on this problem.

The results suggest that more training epochs will result in a more skillful model.

Let's try doubling the number of epochs from 500 to 1000.

Diagnostic of 1000 Epochs

In this section, we use the same experimental setup and fit the model over 1000 training epochs.

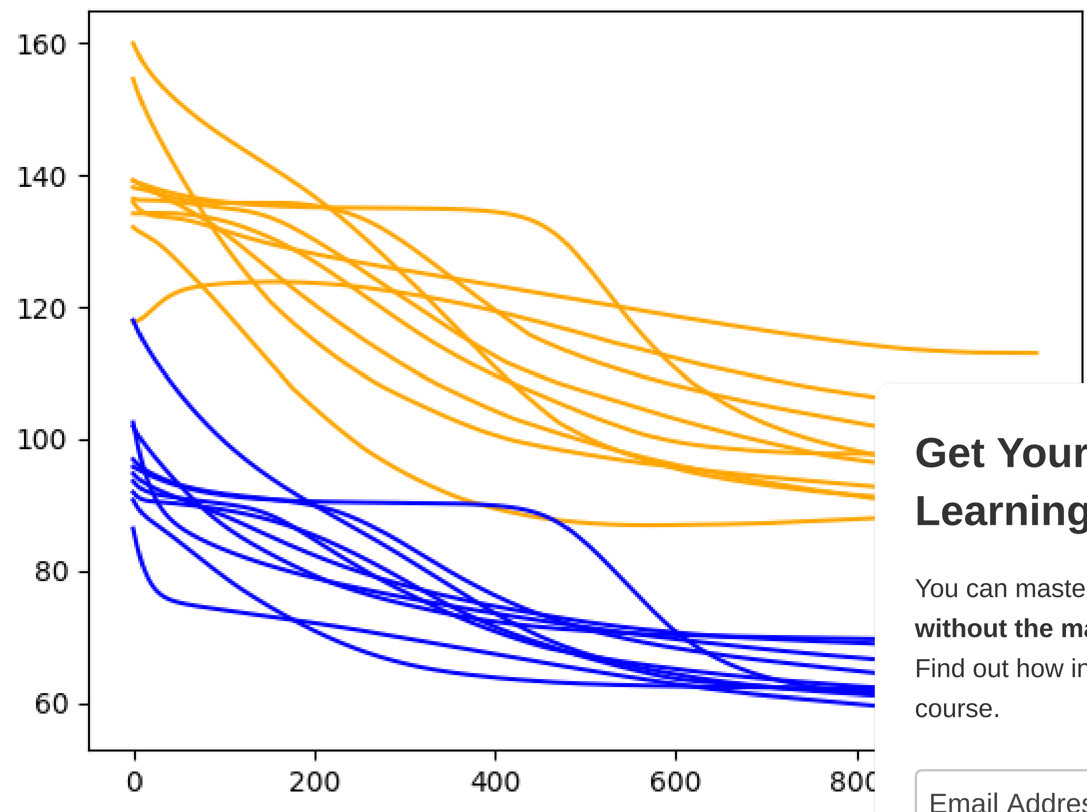
Specifically, the *n_epochs* parameter is set to *1000* in the *run()* function.

```
n_epochs = 1000
```

Running the example prints the RMSE for the train and test sets from the final epoch.

```
0) TrainRMSE=69.242394, TestRMSE=90.832025
1) TrainRMSE=65.445810, TestRMSE=113.013681
2) TrainRMSE=57.949335, TestRMSE=103.727228
3) TrainRMSE=61.808586, TestRMSE=89.071392
4) TrainRMSE=68.127167, TestRMSE=88.122807
5) TrainRMSE=61.030678, TestRMSE=93.526607
6) TrainRMSE=61.144466, TestRMSE=97.963895
7) TrainRMSE=59.922150, TestRMSE=94.291120
8) TrainRMSE=60.170052, TestRMSE=90.076229
9) TrainRMSE=62.232470, TestRMSE=98.174839
```

A line plot of the test and train RMSE scores each epoch is also created.



Diagnostic Results with 1000 Epochs

We can see that the downward trend of model error does continue and appears to slow.

The lines for the train and test cases become more horizontal, but still generally show a downward trend, although at a lower rate of change. Some examples of test error show a possible inflection point around 600 epochs and may show a rising trend.

It is worth extending the epochs further. We are interested in the average performance continuing to improve on the test set and this may continue.

Let's try doubling the number of epochs from 1000 to 2000.

Diagnostic of 2000 Epochs

In this section, we use the same experimental setup and fit the model over 2000 training epochs.

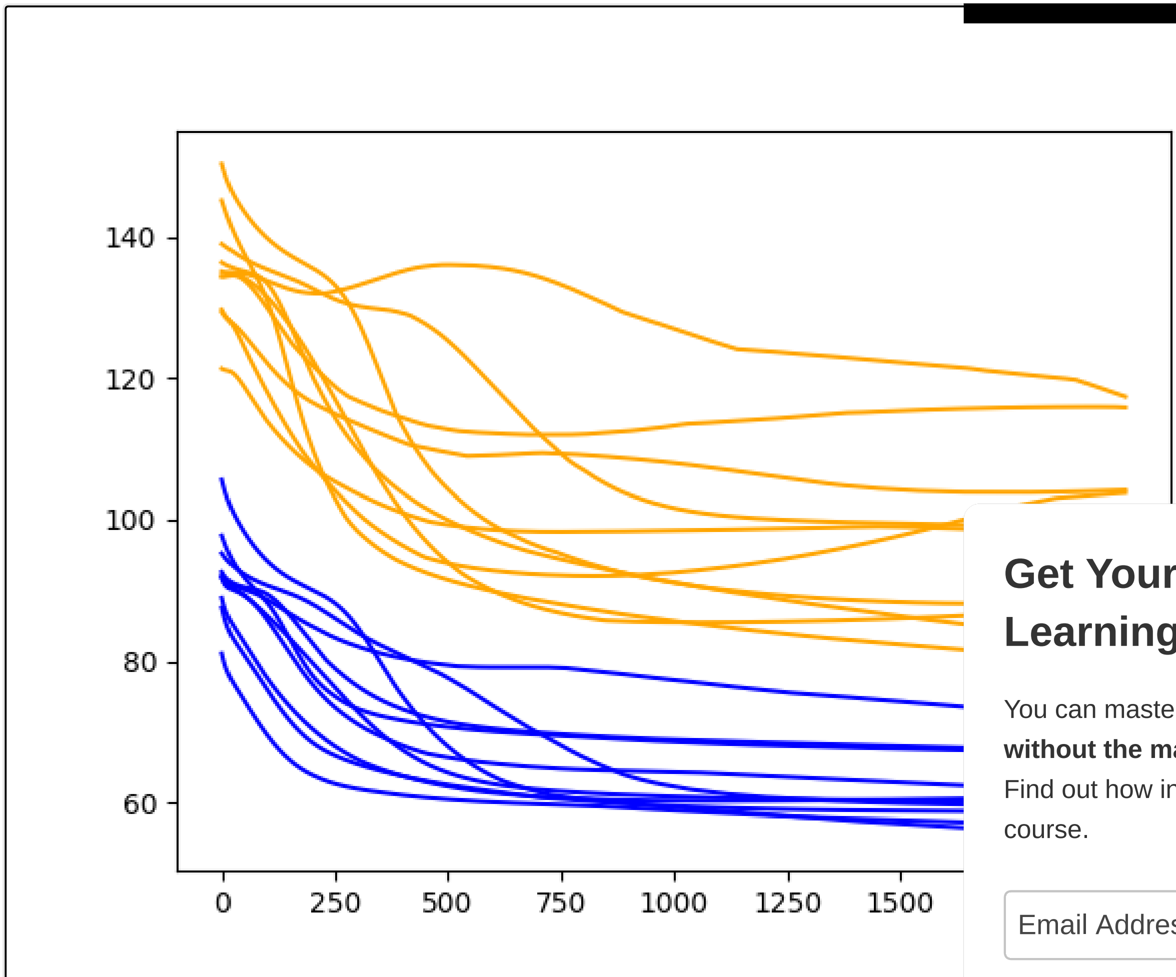
Specifically, the *n_epochs* parameter is set to 2000 in the *run()* function.

```
n_epochs = 2000
```

Running the example prints the RMSE for the train and test sets from the final epoch.

```
0) TrainRMSE=67.292970, TestRMSE=83.096856
1) TrainRMSE=55.098951, TestRMSE=104.211509
2) TrainRMSE=69.237206, TestRMSE=117.392007
3) TrainRMSE=61.319941, TestRMSE=115.868142
4) TrainRMSE=60.147575, TestRMSE=87.793270
5) TrainRMSE=59.424241, TestRMSE=99.000790
6) TrainRMSE=66.990082, TestRMSE=80.490660
7) TrainRMSE=56.467012, TestRMSE=97.799062
8) TrainRMSE=60.386380, TestRMSE=103.810569
9) TrainRMSE=58.250862, TestRMSE=86.212094
```

A line plot of the test and train RMSE scores each epoch is also created.



Diagnostic Results with 2000 Epochs

As one might have guessed, the downward trend in error continues over the additional 1000 epochs on both the train and test datasets.

Of note, about half of the cases continue to decrease in error all the way to the end of the run, whereas the rest show signs of an increasing trend.

The increasing trend is a sign of overfitting. This is when the model overfits the training dataset at the cost of worse performance on the test dataset. It is exemplified by continued improvements on the training dataset and improvements followed by an inflection point and worsting skill in the test dataset. A little less than half of the runs show the beginnings of this type of pattern on the test dataset.

Nevertheless, the final epoch results on the test dataset are very good. If there is a chance we can [redacted] explore it.

Let's try doubling the number of epochs from 2000 to 4000.

Diagnostic of 4000 Epochs

In this section, we use the same experimental setup and fit the model over 4000 training epochs.

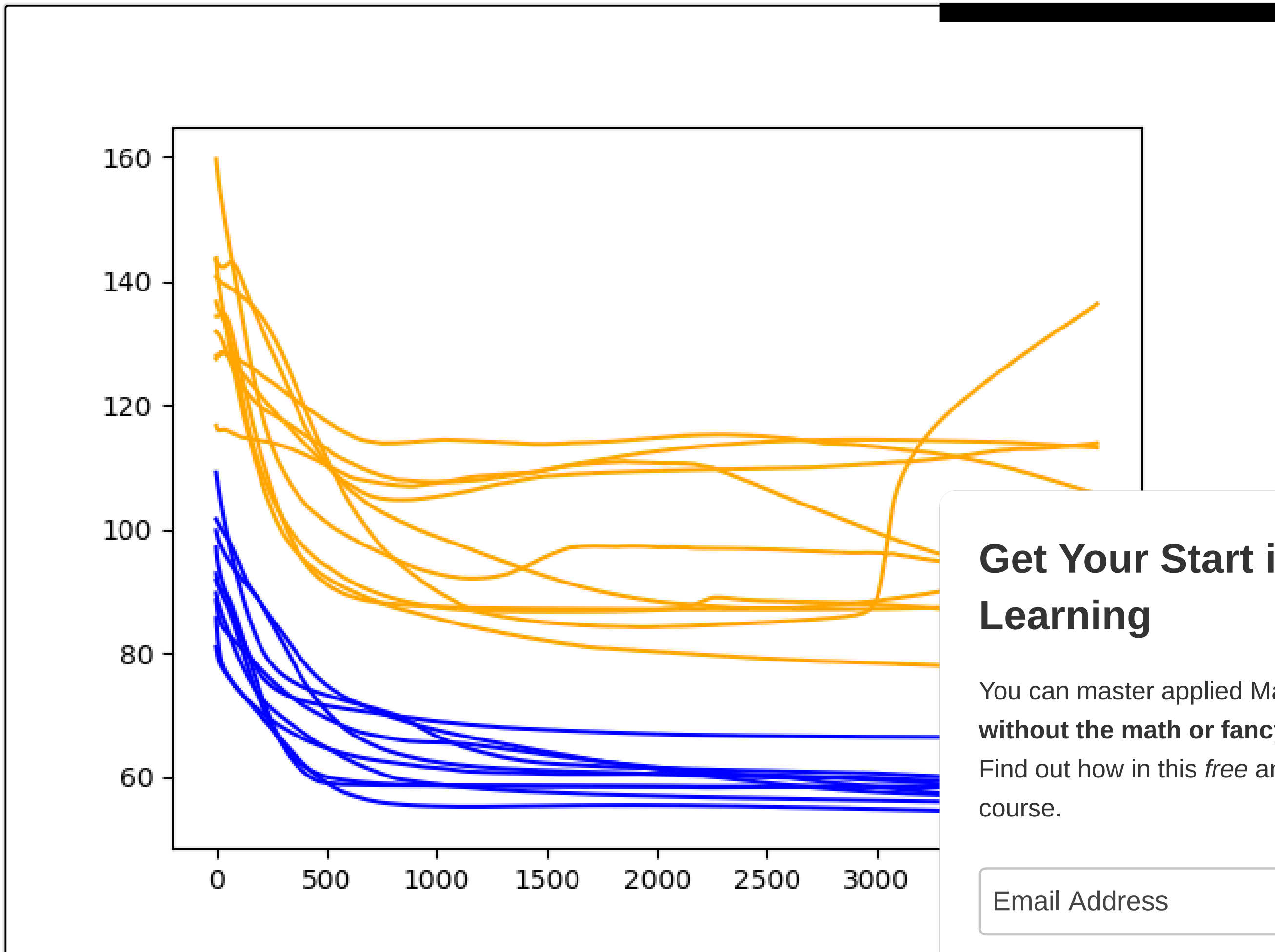
Specifically, the *n_epochs* parameter is set to 4000 in the *run()* function.

```
n_epochs = 4000
```

Running the example prints the RMSE for the train and test sets from the final epoch.

```
0) TrainRMSE=58.889277, TestRMSE=99.121765
1) TrainRMSE=56.839065, TestRMSE=95.144846
2) TrainRMSE=58.522271, TestRMSE=87.671309
3) TrainRMSE=53.873962, TestRMSE=113.920076
4) TrainRMSE=66.386299, TestRMSE=77.523432
5) TrainRMSE=58.996230, TestRMSE=136.367014
6) TrainRMSE=55.725800, TestRMSE=113.206607
7) TrainRMSE=57.334604, TestRMSE=90.814642
8) TrainRMSE=54.593069, TestRMSE=105.724825
9) TrainRMSE=56.678498, TestRMSE=83.082262
```

A line plot of the test and train RMSE scores each epoch is also created.



Diagnostic Results with 4000 Epochs

A similar pattern continues.

There is a general trend of improving performance, even over the 4000 epochs. There is one case of severe overfitting where test error rises sharply.

Again, most runs end with a “good” (better than persistence) final test error.

Summary of Results

The diagnostic runs above are helpful to explore the dynamical behavior of the model, but fall short (e.

We can address this by repeating the same experiments and calculating and comparing summary [redacted] were completed of the epoch values 500, 1000, 2000, 4000, and 6000.

The idea is to compare the configurations using summary statistics over a larger number of runs and see exactly which of the configurations might perform better on average.

The complete code example is listed below.

```
from pandas import DataFrame
from pandas import Series
from pandas import concat
from pandas import read_csv
from pandas import datetime
from sklearn.metrics import mean_squared_error
from sklearn.preprocessing import MinMaxScaler
from keras.models import Sequential
from keras.layers import Dense
from keras.layers import LSTM
from math import sqrt
import matplotlib
# be able to save images on server
matplotlib.use('Agg')
from matplotlib import pyplot
import numpy

# date-time parsing function for loading the dataset
def parser(x):
    return datetime.strptime('190'+x, '%Y-%m')

# frame a sequence as a supervised learning problem
def timeseries_to_supervised(data, lag=1):
    df = DataFrame(data)
    columns = [df.shift(i) for i in range(1, lag+1)]
    columns.append(df)
    df = concat(columns, axis=1)
    df = df.drop(0)
    return df

# create a differenced series
def difference(dataset, interval=1):
    diff = list()
    for i in range(interval, len(dataset)):
        value = dataset[i] - dataset[i - interval]
        diff.append(value)
```

```
    return Series(diff)

# invert differenced value
def inverse_difference(history, yhat, interval=1):
    return yhat + history[-interval]

# scale train and test data to [-1, 1]
def scale(train, test):
    # fit scaler
    scaler = MinMaxScaler(feature_range=(-1, 1))
    scaler = scaler.fit(train)
    # transform train
    train = train.reshape(train.shape[0], train.shape[1])
    train_scaled = scaler.transform(train)
    # transform test
    test = test.reshape(test.shape[0], test.shape[1])
    test_scaled = scaler.transform(test)
    return scaler, train_scaled, test_scaled

# inverse scaling for a forecasted value
def invert_scale(scaler, X, yhat):
    new_row = [x for x in X] + [yhat]
    array = numpy.array(new_row)
    array = array.reshape(1, len(array))
    inverted = scaler.inverse_transform(array)
    return inverted[0, -1]

# fit an LSTM network to training data
def fit_lstm(train, batch_size, nb_epoch, neurons):
    X, y = train[:, 0:-1], train[:, -1]
    X = X.reshape(X.shape[0], 1, X.shape[1])
    model = Sequential()
    model.add(LSTM(neurons, batch_input_shape=(batch_size, X.shape[1], X.shape[2]), st
    model.add(Dense(1))
    model.compile(loss='mean_squared_error', optimizer='adam')
    for i in range(nb_epoch):
        model.fit(X, y, epochs=1, batch_size=batch_size, verbose=0, shuffle=False)
        model.reset_states()
    return model

# run a repeated experiment
def experiment(repeats, series, epochs):
    # transform data to be stationary
    raw_values = series.values
    diff_values = difference(raw_values, 1)
    # transform data to be supervised learning
    supervised = timeseries_to_supervised(diff_values, 1)
```

```
    supervised_values = supervised.values
    # split data into train and test-sets
    train, test = supervised_values[0:-12], supervised_values[-12:]
    # transform the scale of the data
    scaler, train_scaled, test_scaled = scale(train, test)
    # run experiment
    error_scores = list()
    for r in range(repeats):
        # fit the model
        batch_size = 4
        train_trimmed = train_scaled[2:, :]
        lstm_model = fit_lstm(train_trimmed, batch_size, epochs, 1)
        # forecast the entire training dataset to build up state for forecasting
        train_reshaped = train_trimmed[:, 0].reshape(len(train_trimmed), 1, 1)
        lstm_model.predict(train_reshaped, batch_size=batch_size)
        # forecast test dataset
        test_reshaped = test_scaled[:,0:-1]
        test_reshaped = test_reshaped.reshape(len(test_reshaped), 1, 1)
        output = lstm_model.predict(test_reshaped, batch_size=batch_size)
        predictions = list()
        for i in range(len(output)):
            yhat = output[i,0]
            X = test_scaled[i, 0:-1]
            # invert scaling
            yhat = invert_scale(scaler, X, yhat)
            # invert differencing
            yhat = inverse_difference(raw_values, yhat, len(test_scaled)+1-i)
            # store forecast
            predictions.append(yhat)
        # report performance
        rmse = sqrt(mean_squared_error(raw_values[-12:], predictions))
        print('%d) Test RMSE: %.3f' % (r+1, rmse))
        error_scores.append(rmse)
    return error_scores


# load dataset
series = read_csv('shampoo-sales.csv', header=0, parse_dates=[0], index_col=0, squeeze=True, date_parser=parser)
# experiment
repeats = 30
results = DataFrame()
# vary training epochs
epochs = [500, 1000, 2000, 4000, 6000]
for e in epochs:
    results[str(e)] = experiment(repeats, series, e)
# summarize results
print(results.describe())
```

```
# save boxplot
results.boxplot()
pyplot.savefig('boxplot_epochs.png')
```

Running the code first prints summary statistics for each of the 5 configurations. Notably, this includes the mean and standard deviations of the RMSE scores from each population of results.

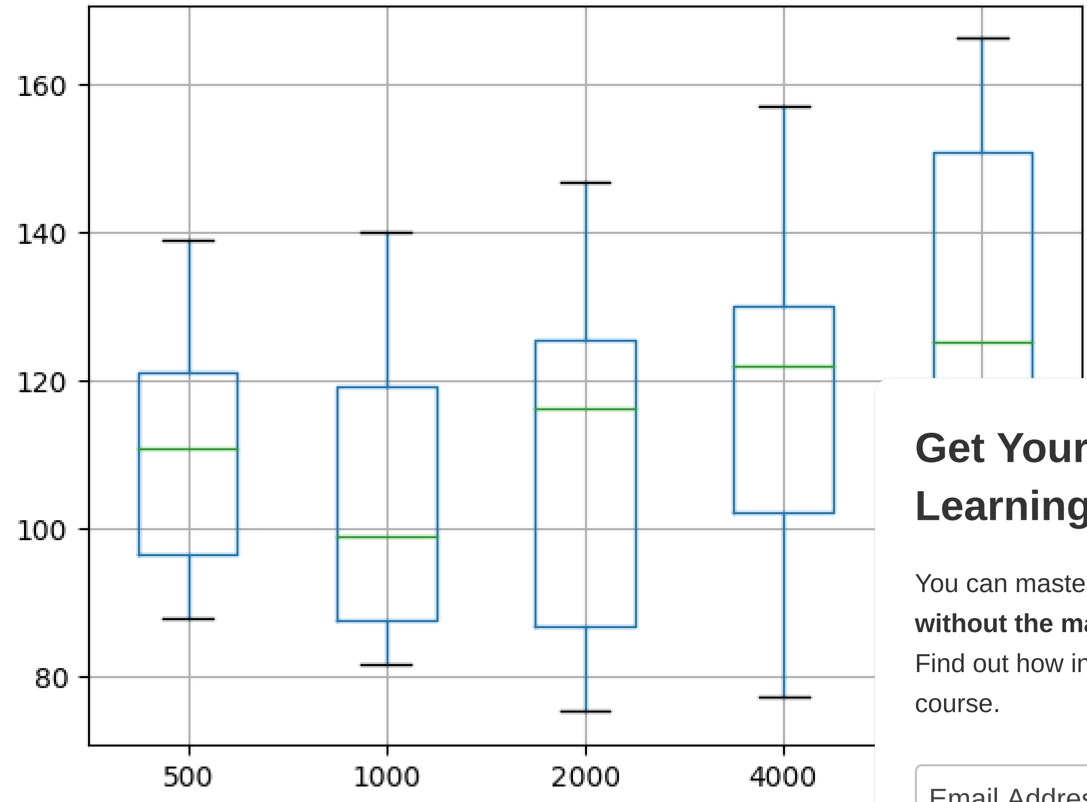
The mean gives an idea of the average expected performance of a configuration, whereas the standard deviation gives an idea of the variance. The min and max RMSE scores also give an idea of the range of possible best and worst case examples that might be expected.

Looking at just the mean RMSE scores, the results suggest that an epoch configured to 1000 may be better. The results also suggest further investigations may be warranted of epoch values between 1000 and 2000.

	500	1000	2000	4000	6000
count	30.000000	30.000000	30.000000	30.000000	30.000000
mean	109.439203	104.566259	107.882390	116.339792	127.618305
std	14.874031	19.097098	22.083335	21.590424	24.866763
min	87.747708	81.621783	75.327883	77.399968	90.512409
25%	96.484568	87.686776	86.753694	102.127451	105.861881
50%	110.891939	98.942264	116.264027	121.898248	125.273050
75%	121.067498	119.248849	125.518589	130.107772	150.832313
max	138.879278	139.928055	146.840997	157.026562	166.111151

The distributions are also shown on a box and whisker plot. This is helpful to see how the distributior

The green line shows the median and the box shows the 25th and 75th percentiles, or the middle 50 ie choice of setting epochs to 1000 is better than the tested alternatives. It also shows that the best pos of 2000 or 4000, at the cost of worse performance on average.



Box and Whisker Plot Summarizing Epoch Results

Next, we will look at the effect of batch size.

Tuning the Batch Size

Batch size controls how often to update the weights of the network.

Importantly in Keras, the batch size must be a factor of the size of the test and the training dataset.

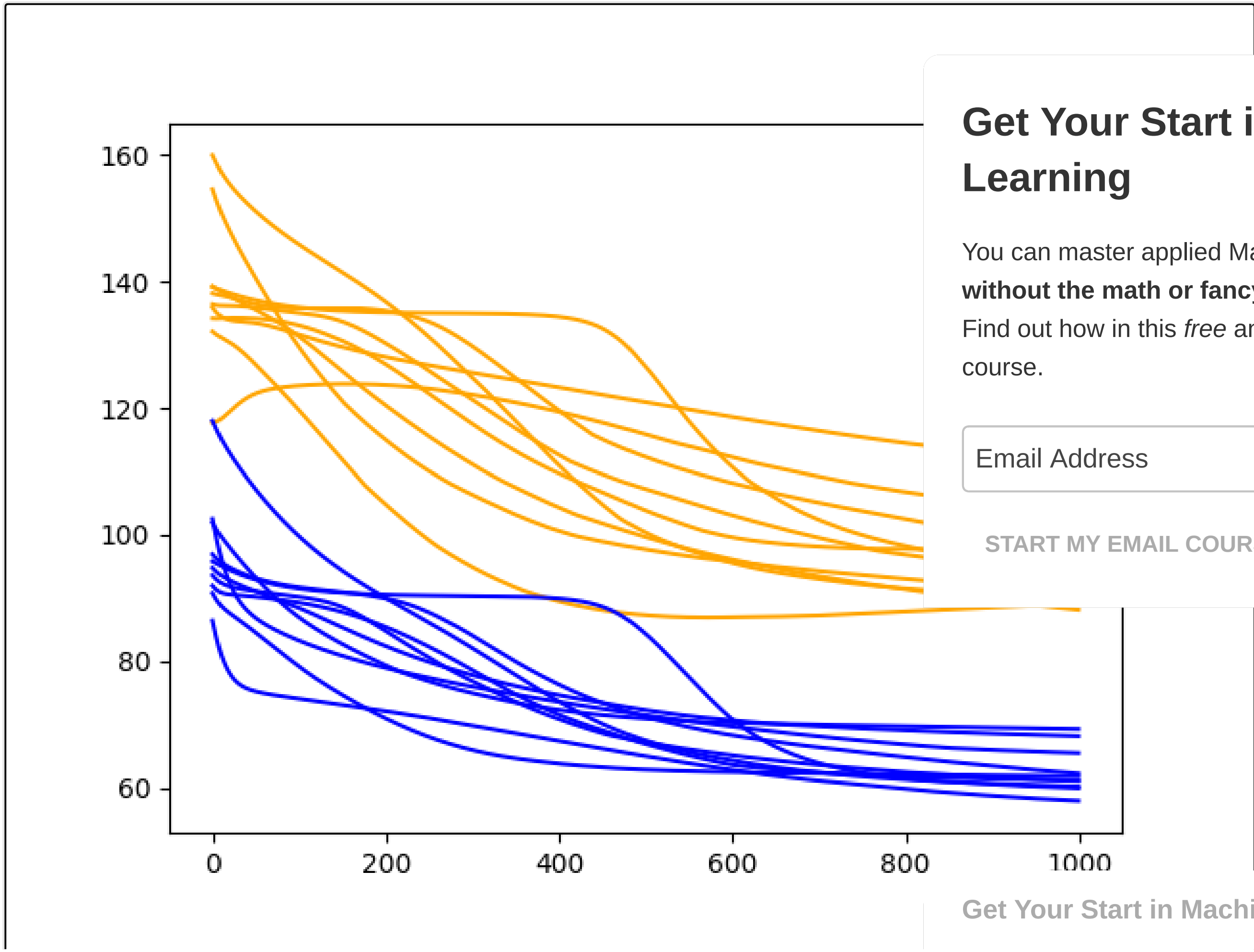
In the previous section exploring the number of training epochs, the batch size was fixed at 4, which [redacted] 12) and in a truncated version of the test dataset (with the size of 20).

In this section, we will explore the effect of varying the batch size. We will hold the number of training epochs constant at 1000.

Diagnostic of 1000 Epochs and Batch Size of 4

As a reminder, the previous section evaluated a batch size of 4 in the second experiment with a number of epochs of 1000.

The results showed a downward trend in error that continued for most runs all the way to the final training epoch.



Diagnostic Results with 1000 Epochs

Diagnostic of 1000 Epochs and Batch Size of 2

In this section, we look at halving the batch size from 4 to 2.

This change is made to the *n_batch* parameter in the *run()* function; for example:

```
n_batch = 2
```

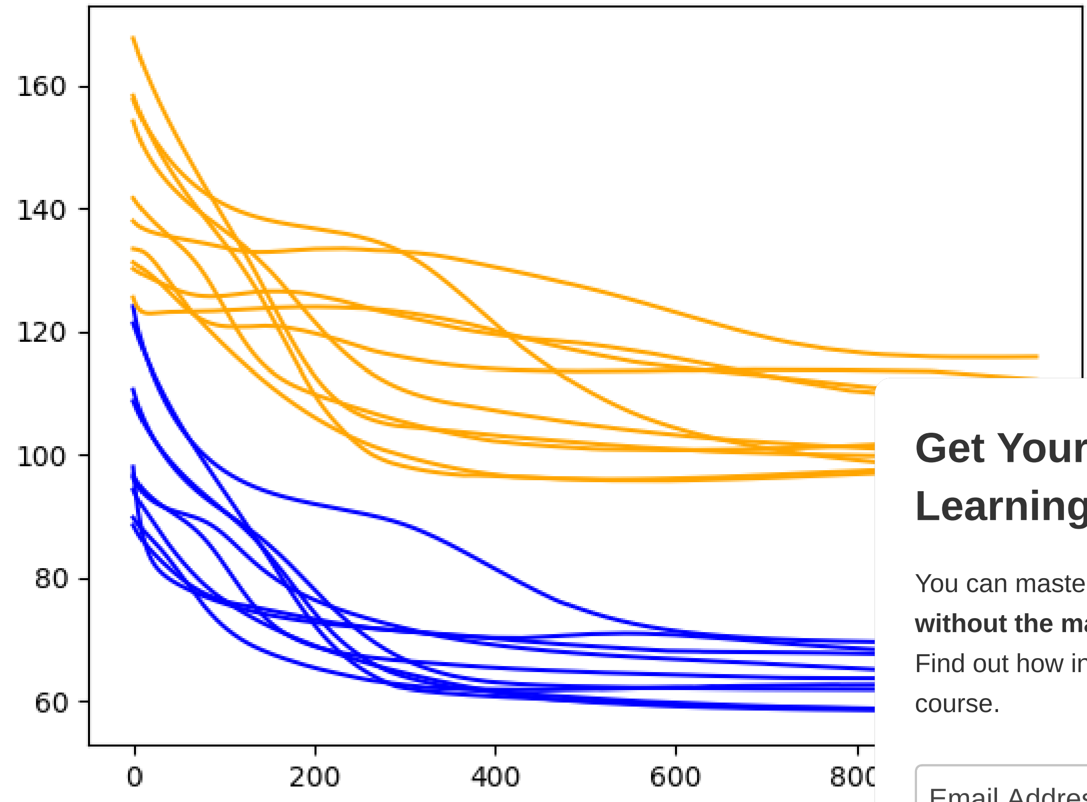
Running the example shows the same general trend in performance as a batch size of 4, perhaps with a higher RMSE on the final epoch.

The runs may show the behavior of stabilizing the RMES sooner rather than seeming to continue the downward trend.

The RSME scores from the final exposure of each run are listed below.

```
0) TrainRMSE=63.510219, TestRMSE=115.855819
1) TrainRMSE=58.336003, TestRMSE=97.954374
2) TrainRMSE=69.163685, TestRMSE=96.721446
3) TrainRMSE=65.201764, TestRMSE=110.104828
4) TrainRMSE=62.146057, TestRMSE=112.153553
5) TrainRMSE=58.253952, TestRMSE=98.442715
6) TrainRMSE=67.306530, TestRMSE=108.132021
7) TrainRMSE=63.545292, TestRMSE=102.821356
8) TrainRMSE=61.693847, TestRMSE=99.859398
9) TrainRMSE=58.348250, TestRMSE=99.682159
```

A line plot of the test and train RMSE scores each epoch is also created.



Diagnostic Results with 1000 Epochs and Batch Size of 2

Let's try having the batch size again.

Diagnostic of 1000 Epochs and Batch Size of 1

A batch size of 1 is technically performing online learning.

That is where the network is updated after each training pattern. This can be contrasted with batch learning, where the weights are only updated at the end of each epoch.

We can change the *n_batch* parameter in the *run()* function; for example:

```
n_batch = 1
```

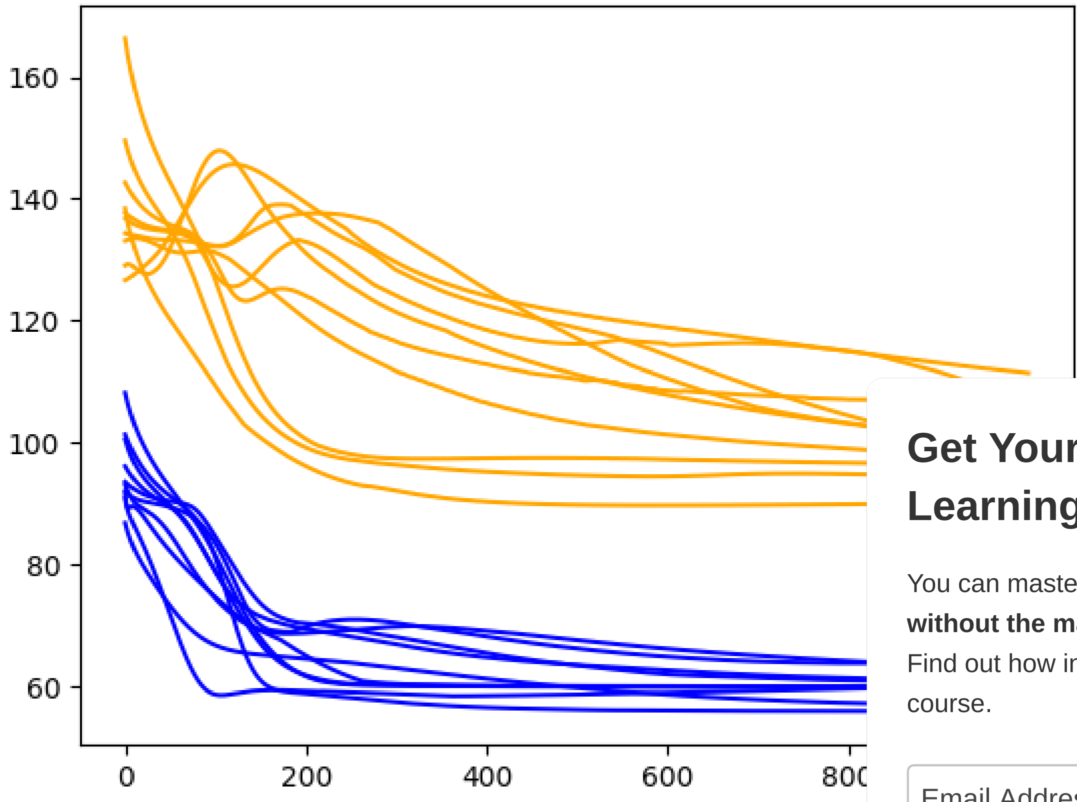
Again, running the example prints the RMSE scores from the final epoch of each run.

```
0) TrainRMSE=60.349798, TestRMSE=100.182293
1) TrainRMSE=62.624106, TestRMSE=95.716070
2) TrainRMSE=64.091859, TestRMSE=98.598958
3) TrainRMSE=59.929993, TestRMSE=96.139427
4) TrainRMSE=59.890593, TestRMSE=94.173619
5) TrainRMSE=55.944968, TestRMSE=106.644275
6) TrainRMSE=60.570245, TestRMSE=99.981562
7) TrainRMSE=56.704995, TestRMSE=111.404182
8) TrainRMSE=59.909065, TestRMSE=90.238473
9) TrainRMSE=60.863807, TestRMSE=105.331214
```

A line plot of the test and train RMSE scores each epoch is also created.

The plot suggests more variability in the test RMSE over time and perhaps a train RMSE that stabiliz increased variability in the test RMSE is to be expected given the large changes made to the networ

The graph also suggests that perhaps the decreasing trend in RMSE may continue if the configuratio



Diagnostic Results with 1000 Epochs and Batch Size of 1

Summary of Results

As with training epochs, we can objectively compare the performance of the network given different batch sizes.

Each configuration was run 30 times and summary statistics calculated on the final results.

```
...

# run a repeated experiment
def experiment(repeats, series, batch_size):
```

```
    # transform data to be stationary
    raw_values = series.values
    diff_values = difference(raw_values, 1)
    # transform data to be supervised learning
    supervised = timeseries_to_supervised(diff_values, 1)
    supervised_values = supervised.values
    # split data into train and test-sets
    train, test = supervised_values[0:-12], supervised_values[-12:]
    # transform the scale of the data
    scaler, train_scaled, test_scaled = scale(train, test)
    # run experiment
    error_scores = list()
    for r in range(repeats):
        # fit the model
        train_trimmed = train_scaled[2:, :]
        lstm_model = fit_lstm(train_trimmed, batch_size, 1000, 1)
        # forecast the entire training dataset to build up state for forecasting
        train_reshaped = train_trimmed[:, 0].reshape(len(train_trimmed), 1, 1)
        lstm_model.predict(train_reshaped, batch_size=batch_size)
        # forecast test dataset
        test_reshaped = test_scaled[:,0:-1]
        test_reshaped = test_reshaped.reshape(len(test_reshaped), 1, 1)
        output = lstm_model.predict(test_reshaped, batch_size=batch_size)
        predictions = list()
        for i in range(len(output)):
            yhat = output[i,0]
            X = test_scaled[i, 0:-1]
            # invert scaling
            yhat = invert_scale(scaler, X, yhat)
            # invert differencing
            yhat = inverse_difference(raw_values, yhat, len(test_scaled)+1-i)
            # store forecast
            predictions.append(yhat)
        # report performance
        rmse = sqrt(mean_squared_error(raw_values[-12:], predictions))
        print('%d) Test RMSE: %.3f' % (r+1, rmse))
        error_scores.append(rmse)
    return error_scores


# load dataset
series = read_csv('shampoo-sales.csv', header=0, parse_dates=[0], index_col=0, squeeze=True, date_parser=parser)
# experiment
repeats = 30
results = DataFrame()
# vary training batches
batches = [1, 2, 4]
```

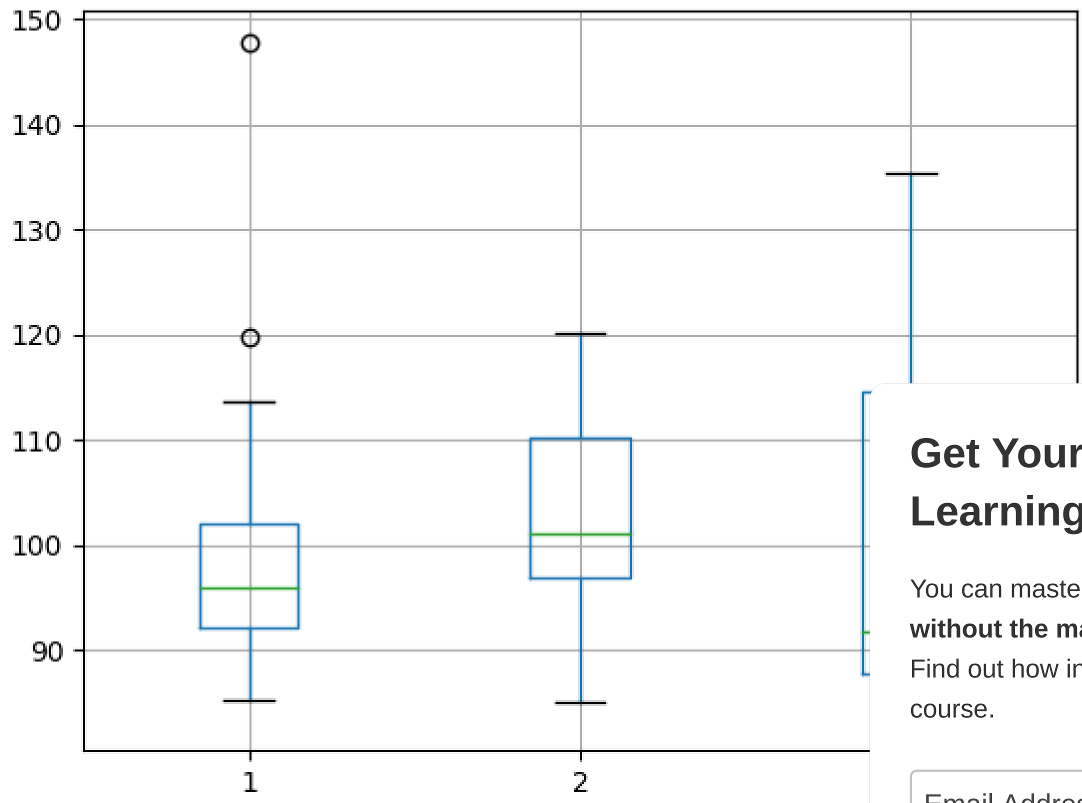
```
for b in batches:
    results[str(b)] = experiment(repeats, series, b)
# summarize results
print(results.describe())
# save boxplot
results.boxplot()
pyplot.savefig('boxplot_batches.png')
```

From the mean performance alone, the results suggest lower RMSE with a batch size of 1. As was noted in the previous section, this may be improved further with more training epochs.

```
                1           2           4
count   30.000000   30.000000   30.000000
mean    98.697017  102.642594  100.320203
std     12.227885    9.144163   15.957767
min     85.172215   85.072441   83.636365
25%     92.023175   96.834628   87.671461
50%     95.981688  101.139527   91.628144
75%    102.009268  110.171802  114.660192
max    147.688818  120.038036  135.290829
```

A box and whisker plot of the data was also created to help graphically compare the distributions. Th line where a batch size of 4 shows both the largest variability and also the lowest median RMSE.

Tuning a neural network is a tradeoff of average performance and variability of that performance, wit variability, meaning that it is generally good and reproducible.



Box and Whisker Plot Summarizing Batch Size Results

Tuning the Number of Neurons

In this section, we will investigate the effect of varying the number of neurons in the network.

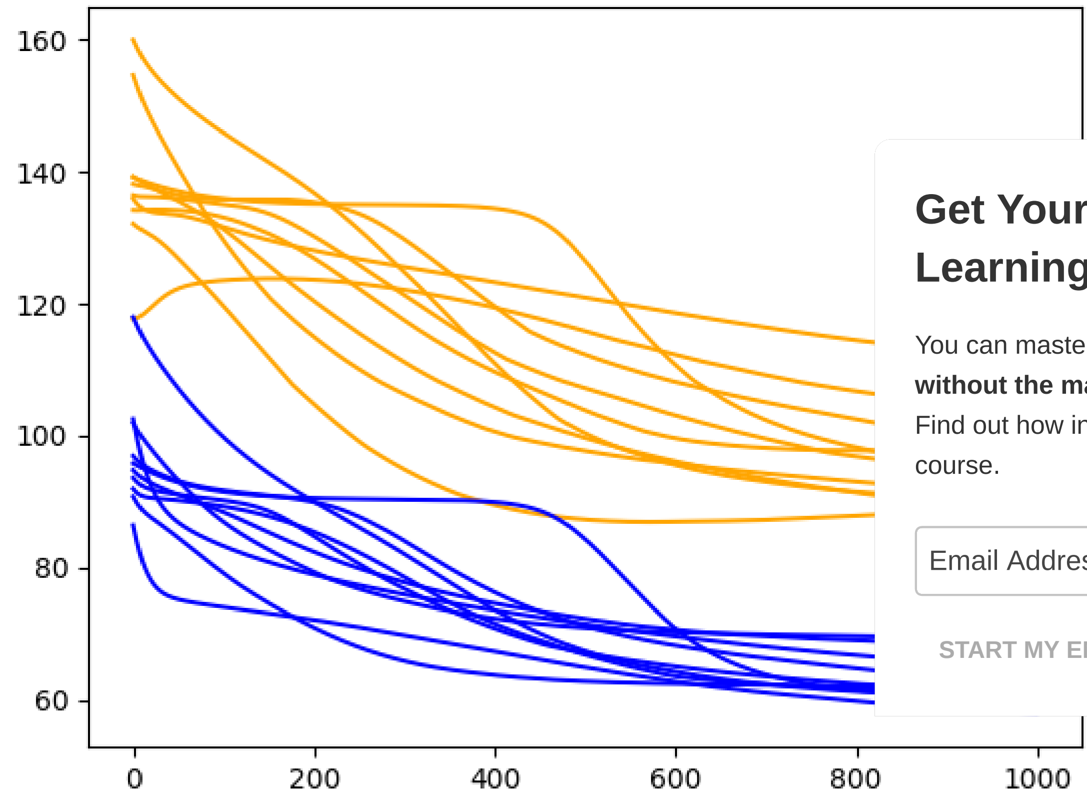
The number of neurons affects the learning capacity of the network. Generally, more neurons would be able to learn more structure from the problem at the cost of longer training time. More learning capacity also creates the problem of potentially overfitting the training data.

We will use a batch size of 4 and 1000 training epochs.

Diagnostic of 1000 Epochs and 1 Neuron

We will start with 1 neuron.

As a reminder, this is the second configuration tested from the epochs experiments.



Diagnostic Results with 1000 Epochs

Diagnostic of 1000 Epochs and 2 Neurons

We can increase the number of neurons from 1 to 2. This would be expected to improve the learning

We can do this by changing the *n_neurons* variable in the *run()* function.

```
n_neurons = 2
```

Running this configuration prints the RMSE scores from the final epoch of each run.

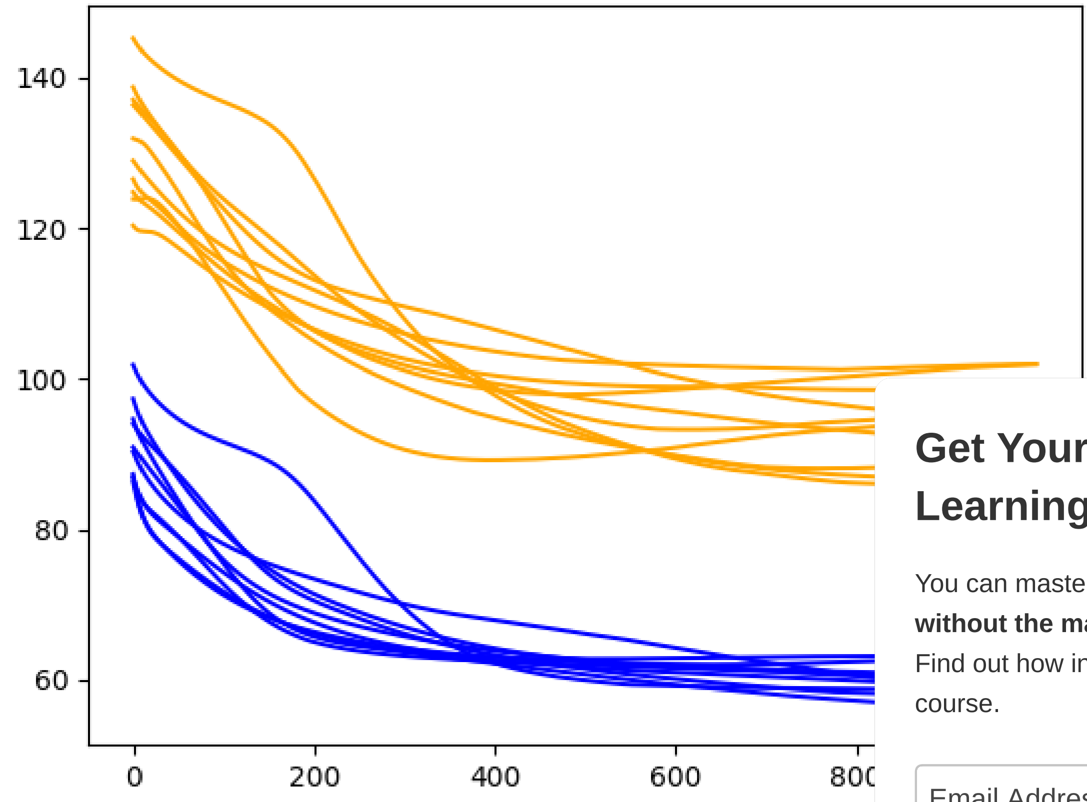
The results suggest a good, but not great, general performance.

```
0) TrainRMSE=59.466223, TestRMSE=95.554547
1) TrainRMSE=58.752515, TestRMSE=101.908449
2) TrainRMSE=58.061139, TestRMSE=86.589039
3) TrainRMSE=55.883708, TestRMSE=94.747927
4) TrainRMSE=58.700290, TestRMSE=86.393213
5) TrainRMSE=60.564511, TestRMSE=101.956549
6) TrainRMSE=63.160916, TestRMSE=98.925108
7) TrainRMSE=60.148595, TestRMSE=95.082825
8) TrainRMSE=63.029242, TestRMSE=89.285092
9) TrainRMSE=57.794717, TestRMSE=91.425071
```

A line plot of the test and train RMSE scores each epoch is also created.

This is more telling. It shows a rapid decrease in test RMSE to about epoch 500-750 where an inflec s the board on all runs. Meanwhile, the training dataset shows a continued decrease to the final epoch

These are good signs of overfitting of the training dataset.



Diagnostic Results with 1000 Epochs and 2 Neurons

Let's see if this trend continues with even more neurons.

Diagnostic of 1000 Epochs and 3 Neurons

This section looks at the same configuration with the number of neurons increased to 3.

We can do this by setting the *n_neurons* variable in the *run()* function.

```
n_neurons = 3
```

Running this configuration prints the RMSE scores from the final epoch of each run.

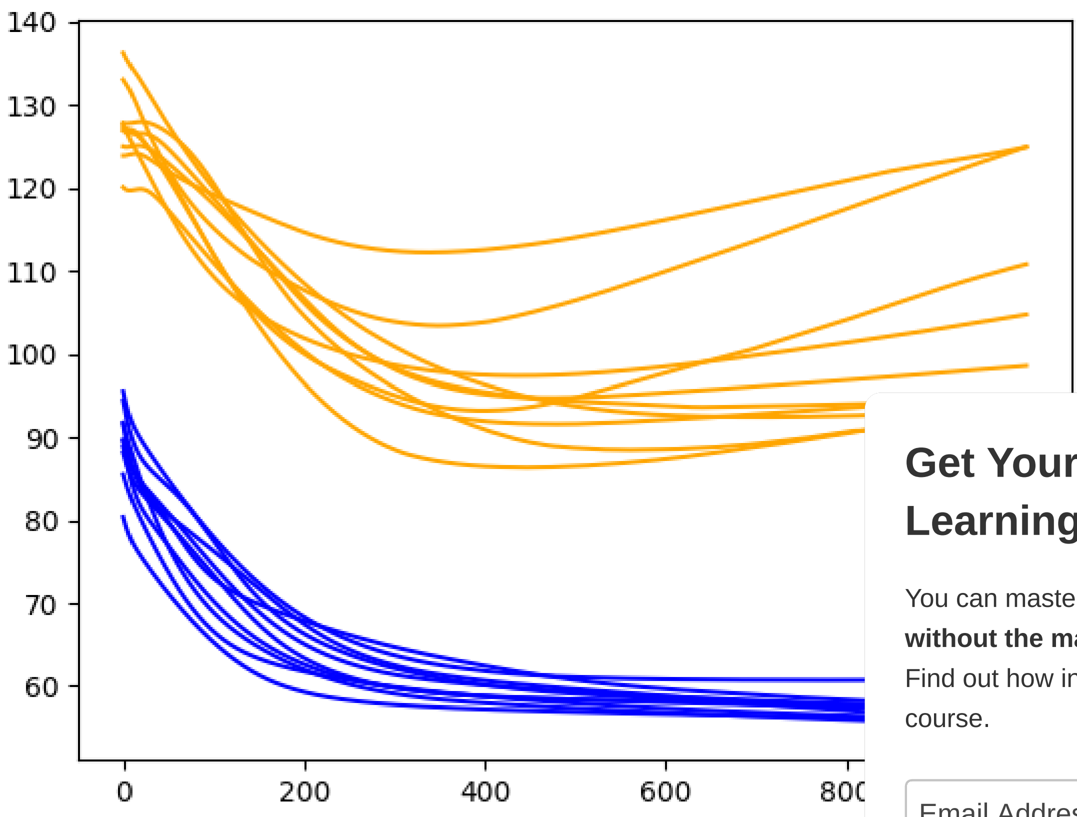
The results are similar to the previous section; we do not see much general difference between the final epoch test scores for 2 or 3 neurons. The final train scores do appear to be lower with 3 neurons, perhaps showing an acceleration of overfitting.

The inflection point in the training dataset seems to be happening sooner than the 2 neurons experiment, perhaps at epoch 300-400.

These increases in the number of neurons may benefit from additional changes to slowing down the rate of learning. Such as the use of regularization methods like dropout, decrease to the batch size, and decrease to the number of training epochs.

```
0) TrainRMSE=55.686242, TestRMSE=90.955555
1) TrainRMSE=55.198617, TestRMSE=124.989622
2) TrainRMSE=55.767668, TestRMSE=104.751183
3) TrainRMSE=60.716046, TestRMSE=93.566307
4) TrainRMSE=57.703663, TestRMSE=110.813226
5) TrainRMSE=56.874231, TestRMSE=98.588524
6) TrainRMSE=57.206756, TestRMSE=94.386134
7) TrainRMSE=55.770377, TestRMSE=124.949862
8) TrainRMSE=56.876467, TestRMSE=95.059656
9) TrainRMSE=57.067810, TestRMSE=94.123620
```

A line plot of the test and train RMSE scores each epoch is also created.



Diagnostic Results with 1000 Epochs and 3 Neurons

Summary of Results

Again, we can objectively compare the impact of increasing the number of neurons while keeping all other network configurations fixed.

In this section, we repeat each experiment 30 times and compare the average test RMSE performance with the number of neurons ranging from 1 to 5.

```
...

# run a repeated experiment
def experiment(repeats, series, neurons):
```

```
    # transform data to be stationary
    raw_values = series.values
    diff_values = difference(raw_values, 1)
    # transform data to be supervised learning
    supervised = timeseries_to_supervised(diff_values, 1)
    supervised_values = supervised.values
    # split data into train and test-sets
    train, test = supervised_values[0:-12], supervised_values[-12:]
    # transform the scale of the data
    scaler, train_scaled, test_scaled = scale(train, test)
    # run experiment
    error_scores = list()
    for r in range(repeats):
        # fit the model
        batch_size = 4
        train_trimmed = train_scaled[2:, :]
        lstm_model = fit_lstm(train_trimmed, batch_size, 1000, neurons)
        # forecast the entire training dataset to build up state for forecasting
        train_reshaped = train_trimmed[:, 0].reshape(len(train_trimmed), 1, 1)
        lstm_model.predict(train_reshaped, batch_size=batch_size)
        # forecast test dataset
        test_reshaped = test_scaled[:,0:-1]
        test_reshaped = test_reshaped.reshape(len(test_reshaped), 1, 1)
        output = lstm_model.predict(test_reshaped, batch_size=batch_size)
        predictions = list()
        for i in range(len(output)):
            yhat = output[i,0]
            X = test_scaled[i, 0:-1]
            # invert scaling
            yhat = invert_scale(scaler, X, yhat)
            # invert differencing
            yhat = inverse_difference(raw_values, yhat, len(test_scaled)+1-i)
            # store forecast
            predictions.append(yhat)
        # report performance
        rmse = sqrt(mean_squared_error(raw_values[-12:], predictions))
        print('%d) Test RMSE: %.3f' % (r+1, rmse))
        error_scores.append(rmse)
    return error_scores


# load dataset
series = read_csv('shampoo-sales.csv', header=0, parse_dates=[0], index_col=0, squeeze=True, date_parser=parser)
# experiment
repeats = 30
results = DataFrame()
# vary neurons
```

```
neurons = [1, 2, 3, 4, 5]
for n in neurons:
    results[str(n)] = experiment(repeats, series, n)
# summarize results
print(results.describe())
# save boxplot
results.boxplot()
pyplot.savefig('boxplot_neurons.png')
```

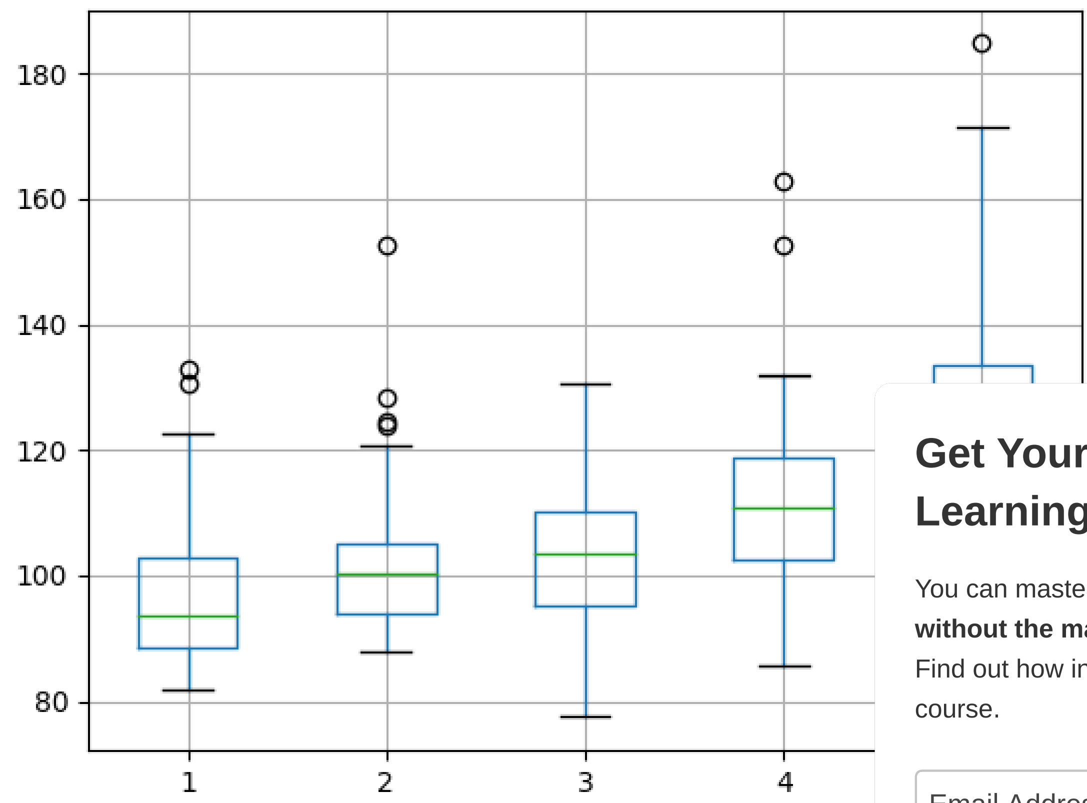
Running the experiment prints the summary statistics for each configuration.

From the mean performance alone, the results suggest a network configuration with 1 neuron as having the best performance over 1000 epochs with a batch size of 4. This configuration also shows the tightest variance.

```
                1           2           3           4           5
count   30.000000   30.000000   30.000000   30.000000   30.000000
mean    98.344696  103.268147  102.726894  112.453766  122.843032
std     13.538599   14.720989   12.905631   16.296657   25.586013
min     81.764721   87.731385   77.545899   85.632492   85.955093
25%     88.524334   94.040807   95.152752  102.477366  104.192588
50%     93.543948  100.330678  103.622600  110.906970  117.022724
75%    102.944050  105.087384  110.235754  118.653850  133.343669
max    132.934054  152.588092  130.551521  162.889845  184.678185
```

The box and whisker plot shows a clear trend in the median test set performance where the increase

the test RMSE.



Box and Whisker Plot Summarizing Neuron Results

Summary of All Results

We completed quite a few LSTM experiments on the Shampoo Sales dataset in this tutorial.

Generally, it seems that a stateful LSTM configured with 1 neuron, a batch size of 4, and trained for 1000 epochs might be a good configuration.

The results also suggest that perhaps this configuration with a batch size of 1 and fit for more epochs may be worthy of further exploration.

Tuning neural networks is difficult empirical work, and LSTMs are proving to be no exception.

This tutorial demonstrated the benefit of both diagnostic studies of configuration behavior over time, as well as objective studies of test RMSE.

Nevertheless, there are always more studies that could be performed. Some ideas are listed in the next section.

Extensions

This section lists some ideas for extensions to the experiments performed in this tutorial.

If you explore any of these, report your results in the comments; I'd love to see what you come up with.

- **Dropout**. Slow down learning with regularization methods like dropout on the recurrent LSTM connections.
- **Layers**. Explore additional hierarchical learning capacity by adding more layers and varied num
- **Regularization**. Explore how weight regularization, such as L1 and L2, can be used to slow dov configurations.
- **Optimization Algorithm**. Explore the use of alternate optimization algorithms, such as classica to speed up or slow down learning can lead to benefits.
- **Loss Function**. Explore the use of alternative loss functions to see if these can be used to lift p
- **Features and Timesteps**. Explore the use of lag observations as input features and input time ut can improve learning and/or predictive capability of the model.
- **Larger Batch Size**. Explore larger batch sizes than 4, perhaps requiring further manipulation of

Summary

In this tutorial, you discovered how you can systematically investigate the configuration for an LSTM network for time series forecasting.

Specifically, you learned:

- How to design a systematic test harness for evaluating model configurations.
- How to use model diagnostics over time, as well as objective prediction error to interpret model behavior.
- How to explore and interpret the effects of the number of training epochs, batch size, and number of neurons.

Do you have any questions about tuning LSTMs, or about this tutorial?
Ask your questions in the comments below and I will do my best to answer.

About Jason Brownlee

Dr. Jason Brownlee is a husband, proud father, academic researcher, author, professional developer and a machine learning practitioner. He is dedicated to helping developers get started and get good at applied machine learning. Learn more.

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23 Responses to *How to Tune LSTM Hyperparameters with Keras for Time Series Forecasting*

John Richards April 12, 2017 at 8:51 am #

REPLY

Awesome Work!

Jason Brownlee April 12, 2017 at 9:34 am #

Thanks John!

Kunpeng Zhang April 12, 2017 at 10:51 am #

line 137, in
results[str(e)] = experiment(repeats, series, e)
line 104, in experiment
lstm_model = fit_lstm(train_trimmed, batch_size, epochs, 1)
line 81, in fit_lstm
model.fit(X, y, epochs=1, batch_size=batch_size, verbose=0, shuffle=False)
File "C:\Anaconda3\lib\site-packages\keras\models.py", line 654, in fit
str(kwargs))
TypeError: Received unknown keyword arguments: {'epochs': 1}
Is there something wrong?

Jason Brownlee April 13, 2017 at 9:54 am # REPLY

You need to upgrade to Keras v2.0 or higher.

Logan May 17, 2017 at 12:28 am # REPLY

You should replace model.fit(X, y, epochs=1, …) for model.fit(X, y, nb_epoch=1…) It worked perfectly for me.

Jason Brownlee May 17, 2017 at 8:25 am #

The example was updated to use Keras v2.0 which changed the "nb_epochs" argumen

Leo April 12, 2017 at 6:12 pm #

Nice blog post once again. What is the size of the data set that you are using? What is the max
I have a system with 8GB RAM?

Jason Brownlee April 13, 2017 at 9:56 am # REPLY

The examples use small <1 MB datasets.

The size of supported datasets depends on data types, number of rows and number of columns.

Consider doing some experiments with synthetic data to find the limits of your system.

Lorenzo April 13, 2017 at 1:08 am # REPLY

Amazing tutorial as always. Would you have an example of running the LSTM on a multivariate regression problem like the Walmart's on Kaggle (https://www.kaggle.com/c/walmart-recruiting-store-sales-forecasting) ?

Jason Brownlee April 13, 2017 at 10:02 am # REPLY

There should be some examples on the blog soon.

Tykimos April 13, 2017 at 4:28 am #

Great work! I have a question regarding batch_size. I think that only one batch_size is reasonal
is 4, there are 4 states separately. That means 4 states don't share each other. Although every sample h
sample is connected the quaternary next sample.

For example,
1 > 5 > 9
2 > 6 > 10
3 > 7 > 11
4 > 8 > 12

Jason Brownlee April 13, 2017 at 10:12 am # REPLY

Sorry, I'm not sure I understand your question, perhaps you can restate it.

We are using stateful LSTMs and regardless of the batch size, state is only reset when we reset it explicitly with a call to model.reset_states()

tykimos April 14, 2017 at 1:56 am #

REPLY

I think that the batch_size depends on not user tuning parameter but dataset design relative to the number of sequence set.

When batch_size is 4 and stateful is true, output of LSTM is weight_count * batch_size. This means that there are 4 different and independent states.
It seems good for the following dataset :
A1-B1-C1-D1-A2-B2-C2-D2-A3-B3-C3-D3
– sample is 12
– batch_size is 4
– sequence set is 4
Because A isn't relative to others in sequence, the next of A1 should be not B1 but A2. For this we have to choose batch_size as 4.

For each epoch,
A1-A2-A3 and reset
B1-B2-B3 and reset
C1-C2-C3 and reset
D1-D2-D3 and reset

Your example is one sequence set like:
A1-A2-A3-A4-A5-A6-A7-A8-A9-A10-A11-A12
If we set batch_size as 4, state is transferred as the following:
A1-A5-A9 and reset
A2-A6-A10 and reset
A3-A7-A11 and reset
A4-A8-A12 and reset

So, I think that batch_size should be 1 in your dataset. Other batch_size values are invalid.

Jason Brownlee April 14, 2017 at 8:53 am #

REPLY

I agree with the first part, it makes sense to reset state at the natural end of a sequence.

I also agree that with the dataset used that there is no natural end to the sequence other tha

I disagree that you “have to have” a batch size of 1. We can have a batch size of 1. We can [redacted]

My previous point is that batch size does not matter when stateful=True because we manage exactly when the state is reset. It does not matter what batch size is used, as long as the state is reset at the natural end of the sequence.

Yes, you are right, there is a bug. The regime of resetting state after each batch of 4 input patterns does not make sense. I’ll schedule time to fix the examples and re-run the experiments.

Thanks for pointing this out and thanks for having the patients to help me see what you saw.

UPDATE: There is no fault, all weight updates are occurring within one epoch regardless of batch size.

Jason Brownlee April 24, 2017 at 8:02 am #

Update I have taken a much closer look at this code (it was written months ago

I believe there is no fault.

Take a close look at the loop for running manual epochs.

Although the batch sizes vary, we are performing one entire epoch + all weight updates

Sebastian April 13, 2017 at 7:51 pm #

Great blog post!

Jason Brownlee April 14, 2017 at 8:44 am #

REPLY

Thanks Sebastian.

Jesse April 26, 2017 at 4:54 pm #

REPLY

Hi Jason,

Cool post! I already learnt a lot from your blogs.

I have 2 questions regarding this post, I hope you can help me:

1. Why aren't you specifying activation functions in your model layers (for the LSTM layer for example?) I read on the keras docs that no activation function is used if you don't pass one. It seems to me that a tanh activation would fit the [-1,1] scaling?
2. Do you always remove the increasing trend from the data?

Thanks a lot!

Jason Brownlee April 27, 2017 at 8:35 am #

I am using the default for LSTMs which are tanh and sigmoid.

Yes, making time series data stationary is a recommended in general.

Sebastian June 16, 2017 at 12:10 am #

Hi Jason,

very nice post, but still got a question.

When reversing difference for predicitions, isn't it wrong to reverse it using the raw values? Instead, shouldn't you use the last prediction to reverse the difference?
Like, instead of yhat = yhat + history[-interval] it is yhat = yhat + predictions[-interval]?

Or am I misunderstanding something?

Freetings

Jason Brownlee June 16, 2017 at 8:02 am # REPLY

Yes, but if you have the real observations for a past time step, we should use them instead to better reflect the "real" level.

Does that help?

Sepideh September 30, 2017 at 7:42 am # REPLY

Thank you Dr. Jason for the great blog. Is it possible to use GPU for this example? If so, how can I apply it! I appreciate your help. The reason I want to use GPU is that I need to get results faster. I am using google compute engine with 6vCPUs and 39 GB memory.

Jason Brownlee September 30, 2017 at 7:48 am #

Perhaps. The GPU configuration is controlled by the library used by Keras, such as Tensor

I have found that it is better to run models sequentially on the GPU and instead use multiple GPUs/s

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Email (will not be published) (required)

Website

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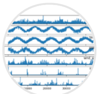
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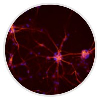
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