Forecasting and Time Series Analysis with Air Quality from Beijing, China

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A series of data collected from the UCI Machine Learning Repository was collected from the Guanyuan suburb of Beijing, China measuring the hourly air quality between the dates of January 3, 2013 and February 28, 2017. PM2.5 and PM10 were two of the particle-matters observed in the air. Levels of PM10 were observed and analyzed along with temperature levels to see trends in change of particle-matter in Guanyuan, Beijing over time. A simple Recurrent Neural Network (RNN) and a Long Short-Term Memory (LSTM) were used to conduct this time-series analysis.

We started by working with the Guanyuan, Beijing data and filter the dataset down to records from 2015.

	No	ye ar	mo nth	d a y	h o ur	PM 2.5	P M 10	S O 2	N O 2	C	O 3	TE M P	PR ES	DE W P	R Al N	w d	WS PM	stati on
16 10 4	16 10 5	20 15	1	1	0	5.0	6. 0	1 3. 0	1 5. 0	30 0. 0	4 4. 0	1.0	10 27. 0	- 22. 4	0. 0	8 Z Z	4.4	Gua nyua n
16 10 5	16 10 6	20 15	1	1	1	7.0	8. 0	1 2. 0	1 3. 0	30 0. 0	4 6. 0	1.0	10 27. 0	- 23. 7	0. 0	N	5.6	Gua nyua n
16 10 6	16 10 7	20 15	1	1	2	3.0	6. 0	1 1. 0	1 0. 0	20 0. 0	4 8. 0	1.0	10 28. 0	- 23. 7	0. 0	N	4.2	Gua nyua n
16 10 7	16 10 8	20 15	1	1	3	4.0	8. 0	1 1. 0	1 2. 0	30 0. 0	4 7. 0	1.0	10 29. 0	- 24. 4	0. 0	N	4.4	Gua nyua n
16 10 8	16 10 9	20 15	1	1	4	3.0	5. 0	1 2. 0	1 2. 0	30 0. 0	4 8. 0	2.0	10 27. 0	- 23. 2	0. 0	E N E	1.4	Gua nyua n
16 10 9	16 11 0	20 15	1	1	5	5.0	12 .0	1 1. 0	2 5. 0	40 0. 0	3 4. 0	5.0	10 30. 0	- 23. 5	0. 0	N	1.1	Gua nyua n

	No	ye ar	mo nth	d a y	h o ur	PM 2.5	P M 10	S O 2	N O 2	CO	O 3	TE M P	PR ES	DE W P	R AI N	w d	WS PM	stati on
16 11 0	16 11 1	20 15	1	1	6	4.0	9. 0	9. 0	3 4. 0	40 0. 0	2 5. 0	6.0	10 29. 0	- 23. 8	0. 0	N E	1.6	Gua nyua n
16 11 1	16 11 2	20 15	1	1	7	6.0	9. 0	9. 0	4 1. 0	40 0. 0	1 9. 0	7.0	10 30. 0	- 24. 2	0. 0	N E	2.0	Gua nyua n
16 11 2	16 11 3	20 15	1	1	8	9.0	9. 0	1 3. 0	4 8. 0	50 0. 0	1 3. 0	6.0	10 28. 0	- 23. 8	0. 0	Е	0.9	Gua nyua n
16 11 3	16 11 4	20 15	1	1	9	9.0	9. 0	1 3. 0	4 8. 0	Na N	1 3. 0	5.0	10 26. 0	- 23. 5	0. 0	E N E	1.7	Gua nyua n

Figure 1: Data table displaying the air quality data that was collected from 2013-2017

Next a graph was plotted using the temperature data:

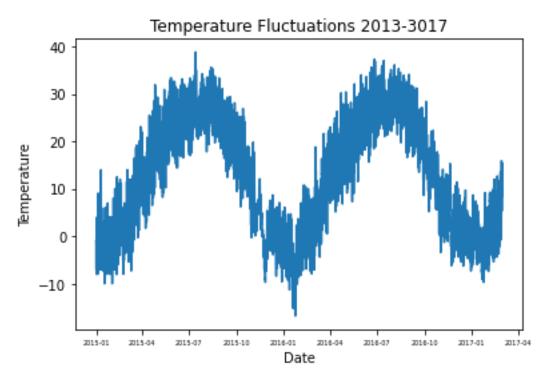


Figure 2: Temperature Fluctuations between 2013-2017

We are interested in attempting to forecast the 'PM' series, which are measurements of air pollution for several different districts. Note that there are occasional missing values in these series, which we can fill with simple linear interpolation. To start, we'll focus on the "PM10" series and interpolate the missing values.

```
df_Beijing['PM10'] = df_Beijing['PM10'].interpolate()
df_Beijing['TEMP'] = df_Beijing['TEMP'].interpolate()
df_Beijing['PM10'].head(10)
                                                                       Out[21]:
16104
        6.0
        8.0
16105
16106
        6.0
        8.0
16107
16108
        5.0
16109 12.0
16110 9.0
        9.0
16111
16112
        9.0
16113 9.0
Name: PM10, dtype: float64
def make data(row):
    return datetime(year = row['year'], month = row['month'], day = row['day'
], hour = row['hour'])
df_Beijing['date'] = df_Beijing.apply(make_data,axis=1)
df_Beijing.set_index(df_Beijing.date,inplace=True)
#quick plot of full time series
plt.figure(figsize = (15,5))
df Beijing['PM10'].plot()
plt.title('Particle Matter (PM) Fluctuations')
plt.ylabel('PM')
plt.xlabel('Date')
```

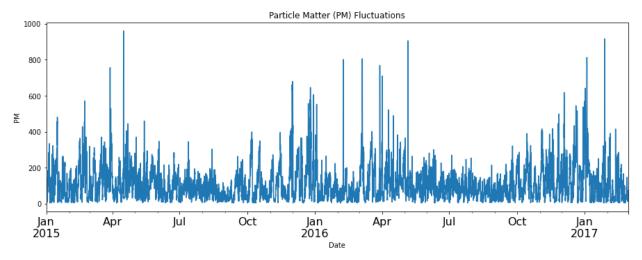


Figure 3: Particle Matter (PM) Fluctuations from January 2015 - February 2017

```
df Beijing['PM10']
date
2015-01-01 00:00:00
                         6.0
2015-01-01 01:00:00
                         8.0
2015-01-01 02:00:00
                         6.0
2015-01-01 03:00:00
                         8.0
2015-01-01 04:00:00
                         5.0
2017-02-28 19:00:00
                        37.0
2017-02-28 20:00:00
                        43.0
2017-02-28 21:00:00
                        33.0
2017-02-28 22:00:00
                        24.0
2017-02-28 23:00:00
                        27.0
Name: PM10, Length: 18960, dtype: float64
```

As usual, it's a good idea for us to generate a run-sequence plot before modeling the data. This way we can get a feel for what we're working with. We'll go ahead and define two utility functions that let us extract and plot the last n days of data (remember that this is an hourly time series, so each day has 24 time steps).

```
def get_n_last_days(df, series_name, n_days):

"""

Extract last n_days of an hourly time series

"""

return df[series_name][-(24*n_days):]

def plot_n_last_days(df, series_name, n_days):

"""

Plot last n_days of an hourly time series

"""
```

What do the last 6 weeks of data look like?

plot_n_last_days(df_Beijing, 'PM10', 42)

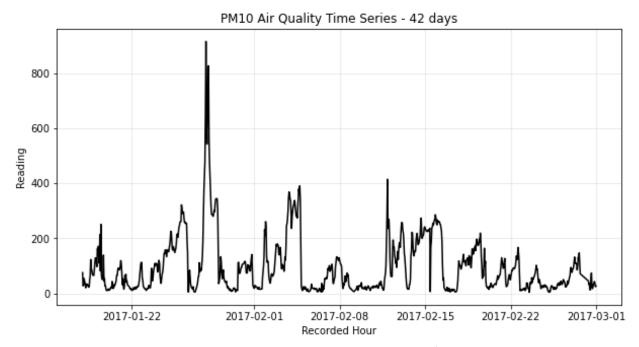


Figure 4: PM10 Air Quality Time Series during the last 42 days of the 4-year time-span.

Before we can train a neural network with keras, we need to process the data into a format that the library accepts. In particular, for keras RNNs and LSTMs, training samples should be stored in a 3D numpy array of shape (n_samples, time_steps, n_features). Since we'll be using only the series' history to predict its future, we'll only have 1 feature. Also, for the next-step prediction that we'll do, target values can be stored in a simple list.

To this end, we define utility functions that allow us to extract the formatted data. The get_train_test_data function gives us the flexibility to define the length of the extracted training and test sequences and the number of time steps to use for prediction -- we'll run simple tests of our models by holding out the end of the extracted sequence and generating predictions to compare against the ground truth.

Since our model will perform better with multiple training samples, we draw many slices from the entire training sequence, starting at different points in time. The gap between starting points of these slices is controlled by the sample_gap parameter.

```
def get keras format series (series):
    Convert a series to a numpy array of shape
    [n samples, time steps, features]
    series = np.array(series)
    return series.reshape(series.shape[0], series.shape[1], 1)
def get train test data(df, series name, series days, input hours,
                        test hours, sample gap=3):
    ** ** **
    Utility processing function that splits an hourly time series into
    train and test with keras-friendly format, according to user-specified
    choice of shape.
    arguments
    _____
    df (dataframe): dataframe with time series columns
    series name (string): column name in df
    series days (int): total days to extract
    input hours (int): length of sequence input to network
    test hours (int): length of held-out terminal sequence
    sample gap (int): step size between start of train sequences; default
5
    returns
    tuple: train X, test X init, train y, test y
    11 11 11
    forecast series = get n last days(df, series name, series days).values
# reducing our forecast series to last n days
    train = forecast series[:-test hours] # training data is remaining
days until amount of test hours
    test = forecast series[-test hours:] # test data is the remaining
test hours
    train X, train y = [], []
    # range 0 through # of train samples - input_hours by sample_gap.
    # This is to create many samples with corresponding
    for i in range(0, train.shape[0]-input hours, sample gap):
```

With the get_train_test_data utility function in hand, we're all set to extract keras-friendly arrays and start training simple RNN models. We run this function in the cell below. We use the last 56 days of the PM10 series, and will train a model that takes in 12 time steps in order to predict the next time step. We use the last day of data for visually testing the model.

Below we see that by taking multiple time slices, we get 436 training samples of 12 time steps each.

```
print('Training input shape: {}'.format(train_X.shape))
print('Training output shape: {}'.format(train_y.shape))
print('Test input shape: {}'.format(test_X_init.shape))
print('Test output shape: {}'.format(test_y.shape))

Training input shape: (436, 12, 1)
Training output shape: (436,)
Test input shape: (12,)
Test output shape: (12,)
```

Now we're ready to train! Since we'd like to repeatedly adjust our model's hyperparameters to see what works best, we'll write a reusable function for training a simple RNN model using keras.

```
!pip install keras
!pip install tensorflow
import tensorflow
import keras
from keras.models import Sequential
def fit_SimpleRNN(train_X, train_y, cell_units, epochs):
  Fit Simple RNN to data train_X, train_y
  arguments
  train X (array): input sequence samples for training
  train y (list): next step in sequence targets
  cell_units (int): number of hidden units for RNN cells
  epochs (int): number of training epochs
  # initialize model
  model = Sequential()
  # construct an RNN layer with specified number of hidden units
  # per cell and desired sequence input format
  model.add(SimpleRNN(cell_units, input_shape=(train_X.shape[1],1)))
  # add an output layer to make final predictions
  model.add(Dense(1))
  # define the loss function / optimization strategy, and fit
  # the model with the desired number of passes over the data (epochs)
  model.compile(loss='mean_squared_error', optimizer='adam')
  model.fit(train_X, train_y, epochs=epochs, batch_size=64, verbose=0)
  return model
```

Now let's use this function to fit a very simple baseline model.

```
from keras.layers import Activation, SimpleRNN, Dense model = fit_SimpleRNN(train_X, train_y, cell_units=10, epochs=10)
```

Not bad so far. But we need to work a bit harder to actually extract multi-step predictions from this model, as it was trained to predict only one future time step. For multi-step forecasting, we'll iteratively generate one prediction, append it to the end of the input sequence (and shift that sequence forward by one step), then feed the new sequence back to the model. We stop once we've generated all the time step predictions we need.

```
def predict(X_init, n_steps, model):
  Given an input series matching the model's expected format,
  generates model's predictions for next n steps in the series
  X_{init} = X_{init.copy().reshape(1,-1,1)}
  preds = []
  # iteratively take current input sequence, generate next step pred.
  # and shift input sequence forward by a step (to end with latest pred).
  # collect preds as we go.
  for in range(n steps):
     pred = model.predict(X_init)
    preds.append(pred)
    X init[:,:-1,:] = X init[:,1:,:] # replace first 11 values with 2nd through 12th
    X_init[:,-1,:] = pred # replace 12th value with prediction
  preds = np.array(preds).reshape(-1,1)
  return preds
def predict_and_plot(X_init, y, model, title):
  Given an input series matching the model's expected format,
  generates model's predictions for next n steps in the series,
  and plots these predictions against the ground truth for those steps
  arguments
  X_init (array): initial sequence, must match model's input shape
  y (array): true sequence values to predict, follow X_init
  model (keras.models.Sequential): trained neural network
  title (string): plot title
  y_preds = predict(test_X_init, n_steps=len(y), model=model) # predict through length of y
  # Below ranges are to set x-axes
  start_range = range(1, test_X_init.shape[0]+1) #starting at one through to length of test_X_init to
plot X_init
  predict range = range(test X init.shape[0], test hours) #predict range is going to be from end of
X_init to length of test_hours
  #using our ranges we plot X_init
```

```
plt.plot(start_range, test_X_init)
#and test and actual preds
plt.plot(predict_range, test_y, color='orange')
plt.plot(predict_range, y_preds, color='teal', linestyle='--')
plt.title(title)
plt.legend(['Initial Series','Target Series','Predictions'])
```

We can simply run the predict_and_plot function on the extracted test data as below, and inspect the resulting plot.

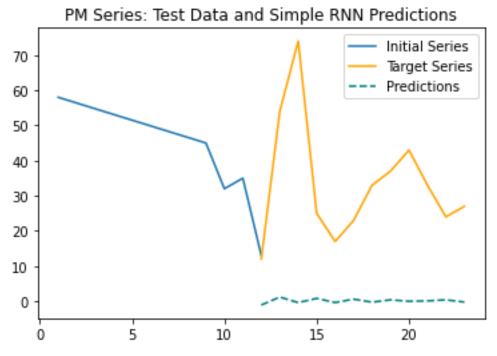


Figure 5: PM Series- Test Data and Simple RNN Predictions. It can be observed in this graph that the data is currently underfit.

It looks like our model is badly underfit and essentially just making constant predictions. That's ok, it was a very simple baseline and trained very quickly. We can improve by making the model more expressive, increasing cell_units. We can also pass over the training data many more times, increasing epochs, giving the model more opportunity to learn the patterns in the data. We'll try that below, it takes a longer time now since our training is more extensive. Note that there is a significant amount of randomness in neural network training - we may need to retrain the model a few times in order to get results that we're happy with.

model = fit_SimpleRNN(train_X, train_y, cell_units=30, epochs=1200) predict and plot(test X init, test y, model, 'PM Series: Test Data and Simple RNN Predictions')



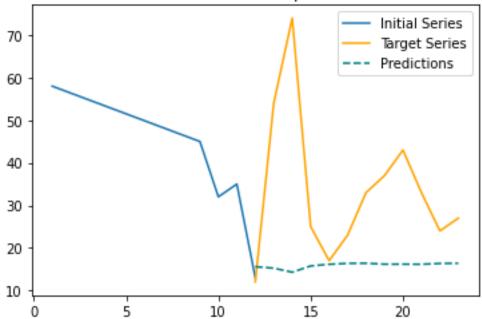


Figure 6: PM Series- Test Data and Simple RNN Predictions. It can be observed that the data-fit has improved in this graph.

We can definitely get better results than before. Note that the model has the capacity to forecast an upward trend based on the trough pattern that occured recently (the input sequence).

Once we've created a model object, we can also get information about its structure and number of parameters by using the summary function. This is a useful way to measure the complexity of the model and get a feel for how long it may take to train.

model.summary()

Model: "sequential 5"

Layer (type)	Output Shape	Param #
simple_rnn_3 (SimpleRNN)	(None, 30)	960
dense_2 (Dense)	(None, 1)	31 ======

Total params: 991 Trainable params: 991 Non-trainable params: 0

Note that even for this relatively simple model, we already have almost a thousand parameters to train. A larger number of cell units would increase the number of parameters - this is why the training process can become so time consuming.

Next, in this section, we'll build on our previous work by introducing LSTM models as an enhancement to the RNNs we've trained so far. Our first step will be to write a new function for fitting an LSTM with keras - notice that it's almost the same as our simple RNN function, with LSTM substituted for SimpleRNN.

```
def fit_LSTM(train_X, train_y, cell_units, epochs):
  .....
  Fit LSTM to data train_X, train_y
  arguments
  train X (array): input sequence samples for training
  train y (list): next step in sequence targets
  cell_units (int): number of hidden units for LSTM cells
  epochs (int): number of training epochs
  ....
  # initialize model
  model = Sequential()
  # construct a LSTM layer with specified number of hidden units
  # per cell and desired sequence input format
  model.add(LSTM(cell units, input shape=(train X.shape[1],1))) #,return sequences= True))
```

```
#model.add(LSTM(cell_units_l2, input_shape=(train_X.shape[1],1)))

# add an output layer to make final predictions

model.add(Dense(1))

# define the loss function / optimization strategy, and fit

# the model with the desired number of passes over the data (epochs)

model.compile(loss='mean_squared_error', optimizer='adam')

model.fit(train_X, train_y, epochs=epochs, batch_size=64, verbose=0)
```

With our new LSTM training function and all of our previously defined utility functions, adapting our code for LSTM forecasting will be fairly simple. We can extract the data as we did before, call the fit_LSTM function to build a model, and run the same predict_and_plot code.

Remember that one of the key benefits of LSTMs over simple RNNs is that they are better equipped to handle long input sequences and long-term dependencies. To see this evidence of this, we'll set input hours to 12 and test hours to 96 and see how our model predictions turn out with LSTM.

```
from tensorflow.keras.layers import LSTM
series_days = 50
input_hours = 12
test_hours = 96
```

model = fit_LSTM(train_X, train_y, cell_units=70, epochs=3000)

predict_and_plot(test_X_init, test_y, model,

'PM10 Series: Test Data and LSTM Predictions')

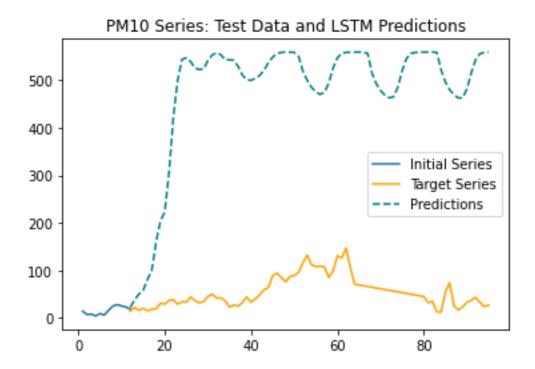


Figure 7: PM10 Series: Test Data and LSTM Predictions- It can be seen that the LSTMs can be more expressive than the SimpleRNNs.

In our prediction plot we can start to see how LSTMs can be more expressive than simple RNNs - instead of just extrapolating a simple trend like our previous RNN models did, this LSTM model can effectively anticipate inflection points.

Notice also that our model starts to struggle toward the end of the predicted sequence, becoming more conservative in its predictions. To improve the quality of forecasts over many time steps, we'd likely need to use more data and more sophisticated LSTM model structures.

model.summary()

Model: "sequential 8"

Layer	(type)	Output	Shape	Param	#
=====		======		=====	
lstm	(LSTM)	(None,	70)	20160	

dense 4 (Dense) 71 (None, 1)

Total params: 20,231 Trainable params: 20,231 Non-trainable params: 0

If enough repeated data analysis testing is conducted using SimpleRNN, it can be seen through these figures that SimpleRNN provides more correlation amongst the data to be discussed than the LSTM predictions. The repetition in data analysis possibly provides the machine-learning technique a chance to get more familiar with the data and thereby provide a better analysis. In Figure 6 it can be observed that both Target Levels and Initial Levels of the pollutant particle matter in the atmosphere elevate to much higher levels than the prediction estimates.

In conclusion, during the 4-year time-span particle-matter levels were recorded there were many fluctuations in the levels of PM10 in the atmosphere, with some of the time-periods containing hazardous amounts of PM10 that could affect Beijing citizens negatively over time. Exactly what negative effects will be due to this PM10 particle is uncertain. For possible improvements in this research, someone could try using longer chunks of the series for modeling (set series_days larger than 56), or modeling other series in the dataset. When training with more data, try increasing cell_units and running more training epochs. Finally, you could also try using longer input sequences with LSTM, and predicting a wider range of test hours.