TSSL Lab 4 - Recurrent Neural Networks

In this lab we will explore different RNN models and training procedures for a problem in time series prediction.

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```
import numpy as np
import tensorflow as tf
from tensorflow import keras
from tensorflow.keras import layers
import pandas
import matplotlib.pyplot as plt

plt.rcParams["figure.figsize"] = (10,6) # Increase default size of plots
```

Set the random seed, for reproducibility

1. Load and prepare the data

We will build a model for predicting the number of sunspots. We work with a data set that has been published on Kaggle, with the description:

Sunspots are temporary phenomena on the Sun's photosphere that appear as spots darker than the surrounding areas. They are regions of reduced surface temperature caused by concentrations of magnetic field flux that inhibit convection. Sunspots usually appear in pairs of opposite magnetic polarity. Their number varies according to the approximately 11-year solar cycle.

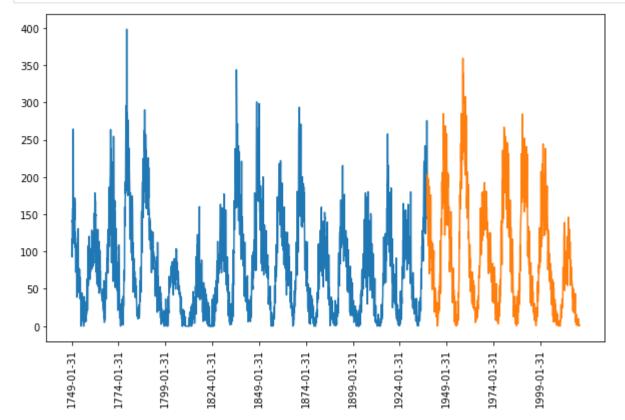
The data consists of the monthly mean total sunspot number, from 1749-01-01 to 2017-08-31.

```
# Read the data
data=pandas.read_csv('Sunspots.csv',header=0)
dates = data['Date'].values
y = data['Monthly Mean Total Sunspot Number'].values
ndata=len(y)
print(f'Total number of data points: {ndata}')

# We define a train/test split, here with 70 % training data
ntrain = int(ndata*0.7)
ntest = ndata-ntrain
print(f'Number of training data points: {ntrain}')
```

Total number of data points: 3252 Number of training data points: 2276

```
In [4]:
    plt.plot(dates[:ntrain], y[:ntrain])
    plt.plot(dates[ntrain:], y[ntrain:])
    plt.xticks(range(0, ndata, 300), dates[::300], rotation = 90); # Show only one tick even
```



There is a clear seasonality to the data, but the amplitude of the peaks very quite a lot. Also, we note that the data is nonnegative, which is natural since it consists of counts of sunspots. However, for simplicity we will not take this constraint into account in this lab assignment and allow ourselves to model the data using a Gaussian likelihood (i.e. using MSE as a loss function).

From the plot we see that the range of the data is roughly [0,400] so as a simple normalization we divide by the constant MAX_VAL=400 .

```
In [5]: MAX_VAL = 400
y = y/MAX_VAL
```

2. Baseline methods

Before constructing any sophosticated models using RNNs, let's consider two baseline methods,

- 1. The first baseline is a "naive" method which simply predicts $y_t = y_{t-1}$.
- 2. The second baseline is an AR(p) model (based on the implementation used for lab 1).

We evaluate the performance of these method in terms of mean-squared-error and mean-absoluteerror, to compare the more advanced models with later on.

```
In [6]:
         def evalutate_performance(y_pred, y, split_time, name=None):
             """This function evaluates and prints the MSE and MAE of the prediction.
             Parameters
             _____
             y_pred : ndarrary
                 Array of size (n,) with predictions.
             y : ndarray
                 Array of size (n,) with target values.
             split_time : int
                 The leading number of elements in y_pred and y that belong to the training data
                 The remaining elements, i.e. y_pred[split_time:] and y[split_time:] are treated
             # Compute error in prediction
             resid = y - y_pred
             # We evaluate the MSE and MAE in the original scale of the data, i.e. we add back MJ
             train_mse = np.mean(resid[:split_time]**2)*MAX_VAL**2
             test mse = np.mean(resid[split time:]**2)*MAX VAL**2
             train_mae = np.mean(np.abs(resid[:split_time]))*MAX_VAL
             test_mae = np.mean(np.abs(resid[split_time:]))*MAX_VAL
             # Print
             print(f'Model {name}\n Training MSE: {train_mse:.4f}, MAE: {train_mae:.4f}\n Te
```

Q1: Implement the naive baseline method which predicts according to $\hat{y}_{t|t-1} = y_{t-1}$. Since the previous value is needed for the prediction we do not get a prediction at t=1. Hence, we evaluate the method by predicting values at $t=2,\ldots,n$ (cf. an AR(p) model where we start predicting at t=p+1).

Model Naive Training MSE: 776.5437, MAE: 19.3285 Testing MSE: 708.6360, MAE: 19.2256

Next, we consider a slightly more advanced baseline method, namely an AR(p) model.

```
# We import two functions that were written as part of lab 1
from tssltools_lab4 import fit_ar, predict_ar_1step

p=30 # Order of the AR model (set by a few manual trials)
ar_coef = fit_ar(y[:ntrain], p) # Fit the model to the training data
# Predict. Note that y contains both training and validation data,
```

```
# and the prediction is for the values y_{p+1}, ..., y_{n}.
y_pred_ar = predict_ar_1step(ar_coef, y)
```

```
In [9]:
```

```
evalutate_performance(y_pred_ar,  # The prediction array is of length n-p y[p:],  # Corresponding target values ntrain-p, # Number of leading elements in the input arrays correspondence='AR')
```

Model AR

Training MSE: 603.8656, MAE: 17.3420 Testing MSE: 590.3732, MAE: 17.6221

3. Simple RNN

We will now construct a model based on a recurrent neural network. We will initially use the SimpleRNN class from *Keras*, which correspond to the basic Jordan-Elman network presented in the lectures.

Q2: Assume that we construct an "RNN cell" using the call layers.SimpleRNN(units = d, return_sequences=True). Now, assume that an array X with the dimensions [Q,M,P] is fed as the input to the above object. We know that X contains a set of sequences (time series) with equal lengths. Specify which of the symbols Q, M, P that corresponds to each of the items below:

- The length of the sequences (number of time steps)
- The number of features (at each time step), i.e. the dimension of each time series
- The number of sequences

Furthermore, specify the values of Q, M, P for the data at hand (treated as a single time series).

Hint: Read the documentation for SimpleRNN to find the answer.

A2: From the documentation inputs is A 3D tensor, with shape [batch, timesteps, feature]. which means Q is the number of sequences. M is the length of the sequences (number of time steps). P is the number of features (at each tipe step), i.e. the dimension of each time step.

Q3: Continuing the question above, answer the following:

- What is the meaning of setting units = d?
- Assume that we pass a single time series of length n as input to the layer. Then what is the dimension of the *output*?
- If we would had set the parameter return_sequences=False when constructing the layer, then what would be the answer to the previous question?

A3:

What is the meaning of setting units = d?

Dimensionality of the output space, in another words the hidden layers

 Assume that we pass a single time series of length n as input to the layer. Then what is the dimension of the output? The output will be in dimension d

• If we would had set the parameter return_sequences=False when constructing the layer, then what would be the answer to the previous question?

The parameter used to whether to return the last output in the output sequence, or the full sequence. thus if we set it as false we will have output of dimensionality 1 instead of d.

In *Keras*, each layer is created separately and are then joined by a Sequential object. It is very easy to construct stacked models in this way. The code below corresponds to a simple Jordan-Elman Network on the form,

$$egin{aligned} \mathbf{h}_t &= \sigma(W\mathbf{h}_{t-1} + Uy_{t-1} + b), \ \hat{y}_{t|t-1} &= C\mathbf{h_t} + c, \end{aligned}$$

Note: It is not necessary to explicitly specify the input shape, since this can be inferred from the input on the first call. However, for the summary function to work we need to tell the model what the dimension of the input is so that it can infer the correct sizes of the involved matrices. Also note that in *Keras* you can sometimes use None when some dimensions are not known in advance.

```
In [10]:
    d = 10  # hidden state dimension

model0=keras.Sequential([
        # Simple RNN Layer
        layers.SimpleRNN(units = d, input_shape=(None,1), return_sequences=True, activation
        # A Linear output Layer
        layers.Dense(units = 1, activation='linear')
])

# We store the initial weights in order to get an exact copy of the model when trying d
model0.summary()
init_weights = model0.get_weights().copy()
```

Model: "sequential"

```
Layer (type)
Output Shape
Param #

simple_rnn (SimpleRNN) (None, None, 10)

dense (Dense)
(None, None, 1)

Total params: 131
Trainable params: 131
Non-trainable params: 0
```

Q4: From the model summary we can see the number of paramters associated with each layer. Relate these numbers to the dimensions of the weight matrices and bias vectors $\{W,U,b,C,c\}$ in the mathematical model definition above.

A4:

```
In [11]:
    print("C Dimension = ",model0.weights[0].shape)
    print("W Dimension = ",model0.weights[1].shape)
```

```
print("b Dimension = ",model0.weights[2].shape)
print("U Dimension = ",model0.weights[3].shape)
print("c Dimension = ",model0.weights[4].shape)

C Dimension = (1, 10)
W Dimension = (10, 10)
b Dimension = (10,)
U Dimension = (10, 1)
c Dimension = (1,)
```

4. Training the RNN model

In this section we will consider a few different ways of handling the data when training the simple RNN model constructed above. As a first step, however, we construct explicit input and target (output) arrays for the training and test data, which will simplify the calls to the training procedures below.

The task that we consider in this lab is one-step prediction, i.e. at each time step we compute a prediction $\hat{y}_{t|t-1} \approx y_t$ which depend on the previous observations $y_{1:t-1}$. However, when working with RNNs, the information contained in previous observations is aggregated in the *state* of the RNN, and we will only use y_{t-1} as the *explicit input* at time step t.

Furthermore, when addressing a problem of time series prediction it is often a good idea to introduce an explicit skip connection from the input y_{t-1} to the prediction $\hat{y}_{t|t-1}$. Equivalently, we can define the target value at time step t to be the residual $\tilde{y}_t := y_t - y_{t-1}$. Indeed, if the model can predict the value of the residual, then we can simply add back y_{t-1} to get a prediction of y_t .

Taking this into consideration, we define explicit input and output arrays as shifted versions of the data series $y_{1:n}$.

```
# Training data
x_train = y[:ntrain-1] # Input is denoted by x, training inputs are x[0]=y[0], ..., x[i
yt_train = y[1:ntrain] - x_train # Output is denoted by yt, training outputs are yt[0]:

# Test data
x_test = y[ntrain-1:-1] # Test inputs are x_test[0] = y[ntrain-1], ..., x_test[ntest]:
yt_test = y[ntrain:] - x_test # Test outputs are yt_test[0] = y[ntrain]-y[ntrain-1], .

# Reshape the data
x_train = x_train.reshape((1,ntrain-1,1))
yt_train = yt_train.reshape((1,ntrain-1,1))
x_test = x_test.reshape((1,ntest,1))
yt_test = yt_test.reshape((1,ntest,1))
```

Option 1. Process all data in each gradient computation ("do nothing")

The first option is to process all data at each iteration of the gradient descent method.

```
model1 = keras.models.clone_model(model0) # This creates a new instance of the same model1.set_weights(init_weights) # We set the initial weights to be the same for all models.
```

Q5: What should we set the *batch size* to, in order to compute the gradient based on the complete training data sequnce at each iteration? Complete the code below!

Note: You can set verbose=1 if you want to monitor the training progress, but if you do, please clear the output of the cell before generating a pdf with your solutions, so that we don't get multiple pages with training errors in the submitted reports.

We plot the training and test error vs the iteration (epoch) number, using a helper function from the tssltools lab4 module.

Q6: Finally we compute the predictions of $\{y_t\}$ for both the training and test data uning the model's predict function. Complete the code below to compute the predictions.

100

Epoch

75

50

25

125

150

175

200

Hint: You need to reshape the data when passing it to the predict to comply with the input shape used in *Keras* (cf. above).

Hint: Since the model is trained on the residuals \tilde{y}_t , don't forget to add back y_{t-1} when predicting y_t . However, make sure that you dont "cheat" by using a non-causal predictor (i.e. using y_t when predicting y_t)!

```
In [17]: # Predict on all data using the final model.

# We predict using y_1,...,y_{n-1} as inputs, resulting in predictions of the values y_x
# That is, y_pred1 should be an (n-1,) array where element y_pred[t] is based only on vo
y_pred1 = model1.predict(y[:ndata-1].reshape((1,ndata-1,1))).flatten() + y[:ndata-1] #
```

```
Using the prediction computed above we can plot them and evaluate the performance of the model
         in terms of MSE and MAE.
In [18]:
           def plot prediction(y pred):
               # Plot prediction on test data
               plt.plot(dates[ntrain:], y[ntrain:])
               plt.plot(dates[ntrain:], y_pred[ntrain-1:])
               plt.xticks(range(0, ntest, 300), dates[ntrain::300], rotation = 90); # Show only o
               plt.legend(['Data','Prediction'])
               plt.title('Predictions on test data')
In [19]:
           # Plot prediction
           plot_prediction(y_pred1)
           # Evaluate MSE and MAE (both training and test data)
           evalutate_performance(y_pred1, y[1:], ntrain-1, name='Simple RNN, "do nothing"')
          Model Simple RNN, "do nothing"
            Training MSE: 617.8157,
                                       MAE: 17.8616
            Testing MSE: 573.7734,
                                        MAE: 17.7223
                                             Predictions on test data
                                                                                        Data
                                                                                        Prediction
          0.8
          0.6
          0.4
          0.2
          0.0
                                                                                       2013-09-30
                1938-09-30
```

Option 2. Random windowing

Instead of using all the training data when computing the gradient for the numerical optimizer, we can speed it up by restricting the gradient computation to a smaller window of consecutive time steps. Here, we sample a random window within the traing data and "pretend" that this window is independent from the observations outside the window. Specifically, when processing the observations within each window the hidden state of the RNN is initialized to zero at the first time point in the window.

To implement this method in Python, we will make use of a *generator function*. A generator is a function that can be paused, return an intermediate value, and then resumed to continue its execution. An intermediate return value is produces using the yield keyword.

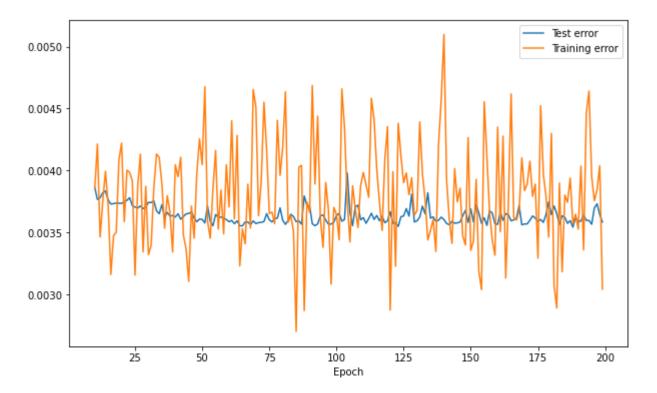
Generators are used in *Keras* to implement inifinite loops that feed the training procedure with training data. Specifically, the <code>yield</code> statement of the generator should return a pair <code>x</code>, <code>y</code> with inputs and corresponding targets from the training data. Each epoch of the training procedure will then call the generator for a total of <code>steps_per_epoch</code> such <code>yield</code> statements.

```
In [20]:
    def generator_train(window_size):
        while True:
            """The upper value is excluded in randint, so the maximum value that we can get
            Hence, the maximum end point of a window is ntrain-1, in agreement with the fact
            when working with one-step-ahead prediction."""
            start_of_window = np.random.randint(0, ntrain - window_size) # First time index
            end_of_window = start_of_window + window_size # Last time index of window (exc
            yield x_train[:,start_of_window:end_of_window,:], yt_train[:,start_of_window:end_of_window], yt_train[:,start_of_window:end_of_window], yt_train[:,start_of_window], yt_train[:,start_of_window]
```

Q7: Assume that we process a window of observations of length window_size at each iteration. Then, how many gradient steps per epoch can we afford, for computational cost per epoch to be comparable to the method considered in Option 1? Set the steps_per_epoch parameter of the fitting function based on your answer.

Similarly to above we plot the error curves vs the iteration (epoch) number.

```
In [23]: plot_history(history, start_at)
```



Q8: Comparing this error plot to the one you got for training Option 1, can you see any *qualitative* differences? Explain the reason for the difference.

A8: The error plot we generated in the first option clearly demonstrates convergence as the number of errors increases. However, this trend is not evident in option 2, where we observe the error zigzagging as the epochs are incremented.

Q9: Compute a prediction for all values of $\{y_2, \ldots, y_n\}$ analogously to **Q6**.

Testing MSE: 570.0144, MAE: 17.3017

In [24]:

```
# Predict on all data using the final model.

# We predict using y_1,...,y_{n-1} as inputs, resulting in predictions of the values y_ y_pred2 = model2.predict(y[:ndata-1].reshape((1,ndata-1,1))).flatten() + y[:ndata-1]

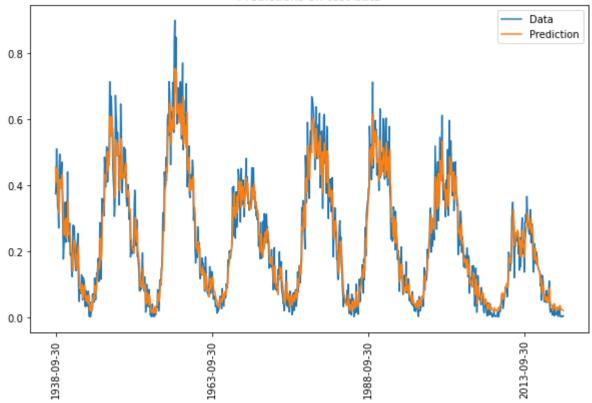
In [25]:

# Plot prediction on test data
plot_prediction(y_pred2)

# Evaluate MSE and MAE (both training and test data)
evalutate_performance(y_pred2, y[1:], ntrain-1, name='Simple RNN, windowing')

Model Simple RNN, windowing
Training MSE: 602.6192, MAE: 17.5562
```





Option 3. Sequential windowing with stateful training

As a final option we consider a model aimed at better respecting the temporal dependencies between consequtive windows. This is based on "statefulness" which simply means that the RNN remembers its hidden state between calls. That is, if model is in stateful mode and is used to process two sequences of inputs after each other, then the final state from the first sequence is used as the initial state for the second sequence.

```
# To enable stateful training, we need to create model where we set stateful=True in the
model3=keras.Sequential([
    # Simple RNN layer with stateful=True
    layers.SimpleRNN(units = d, batch_input_shape=(1,None,1), return_sequences=True, st
    # A linear output layer
    layers.Dense(1, activation='linear')
])
model3.set_weights(init_weights)
```

Q10: When working with stateful training we need to make some adjustments to the training data generator.

1. First, the RNN model doesn't keep track of the actual time indices of the different windows that it is fed. Hence, if we feed the model randomly selected windows, it will still treat them as if they were consecutive, and retain the state from one window to the next. To avoid this, we therefore need to make sure that the generator outputs windows of training data that are indeed consecutive (and not ranomdly selected as above).

2. When training the model we will process the whole training data multiple times (i.e. we train for multiple epochs). However, if we have statefulness between epochs this would effectively result in a "circular dependence", where the final state at time step $t=n_{\rm train}$ would be used as the initial state at time t=1. To avoid this, we can manually reset the state of the model by calling model.reset_states() .

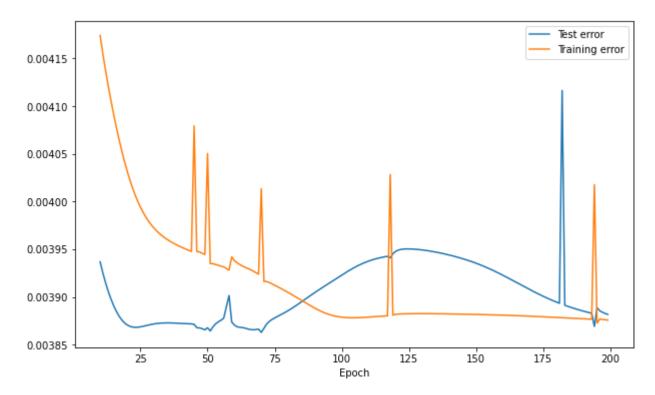
Taking this two points into consideration, complete the code for the stateful data generator below.

```
In [27]:
          def generator_train_stateful(window_size, model):
              """In addition to the window size, the generator also takes the model as input so
              that we can reset the RNN states at appropriate intervals."""
              # Compute the total number of windows of length window size that we need to cover a
              # Note 1. The length of x_train (and yt_train) is ntrain-1 since we work with 1-ste
              # Note 2. The final window could be smaller than window size, if (ntrain-1) is not
              number of windows = int( ntrain/window size )
              while True:
                  for i in range(number of windows):
                      # First time index of window (inclusive)
                      start of window = window size * i
                      # Last time index of window (exclusive, i.e. this is the index to the first
                      # Note 3. Python allows using end of window > ntrain-1, it will simply trun
                      end_of_window = start_of_window + window_size
                      yield x_train[:,start_of_window:end_of_window,:], yt_train[:,start_of_window]
                      model.reset_states()
              """NOTE! In addition to replacing the ????? with the correct code, you need to move
              """to the correct place in the function definition above!"""
```

With the generator defined we can train the model.

Similarly to above we plot the error curves vs the iteration (epoch) number.

```
In [29]: plot_history(history, start_at)
```



Q11: Comparing this error plot to the one you got for training Options 1 and 2, can you see any *qualitative* differences?

Optional: If you have a theory regarding the reason for the observed differences, feel free to explain!

A11: It's evident that our error is converging after a certain number of epochs, unlike the results we obtained earlier. This could be attributed to the window size we utilized and the nature of the stateful method, where we retain the hidden state from the previous sub-sequence when processing the next one.

Q12: Compute a prediction for all values of $\{y_2, \ldots, y_n\}$ analogously to **Q6**.

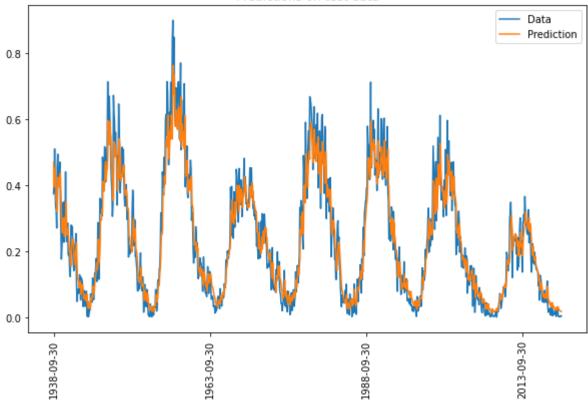
```
In [30]: # Predict on all data using the final model.
    # We predict using y_1,...,y_{n-1} as inputs, resulting in predictions of the values y_
    y_pred3 = model3.predict(y[:ndata-1].reshape((1,ndata-1,1))).flatten() + y[:ndata-1]

In [31]: # Plot prediction on test data
    plot_prediction(y_pred3)

# Evaluate MSE and MAE (both training and test data)
    evalutate_performance(y_pred3, y[1:], ntrain-1, name='Simple RNN, windowing/stateful')

Model Simple RNN, windowing/stateful
    Training MSE: 623.7272, MAE: 17.8705
    Testing MSE: 614.3817, MAE: 18.0474
```





5. Reflection

Q13: Which model performed best? Did you manage to improve the prediction compared to the two baseline methods? Did the RNN models live up to your expectations? Why/why not? Please reflect on the lab using a few sentences.

A13: In my opinion, the first model performed exceptionally well. This is because there are instances where taking no action or maintaining the current approach yields the best outcome. In this specific example, we did not enhance the model's performance by attempting alternative models, emphasizing the effectiveness of the initial model.

6. A more complex network (OPTIONAL)

If you are interested, feel free to play around with more complex models and see if you can improve the predictive performance! It is very easy to build stacked models in *Keras*, see the example below.

```
# A stacked model with 3 layers of LSTM cells, two Dense layers with Relu activation and
model4 = tf.keras.models.Sequential([
    tf.keras.layers.LSTM(64, batch_input_shape=(1,None,1), return_sequences=True, statefu
    tf.keras.layers.LSTM(64, batch_input_shape=(1,None,1), return_sequences=True, statefu
    tf.keras.layers.LSTM(64, batch_input_shape=(1,None,1), return_sequences=True, statefu
    tf.keras.layers.Dense(32, activation="relu"),
    tf.keras.layers.Dense(16, activation="relu"),
    tf.keras.layers.Dense(1),
])
model4.summary()
```

Model: "sequential 2"

Layer (type)	Output Shape	Param #
lstm (LSTM)	(1, None, 64)	16896
lstm_1 (LSTM)	(1, None, 64)	33024
lstm_2 (LSTM)	(1, None, 64)	33024
dense_2 (Dense)	(1, None, 32)	2080
dense_3 (Dense)	(1, None, 16)	528
dense_4 (Dense)	(1, None, 1)	17
T-+-1 05 560		:=========

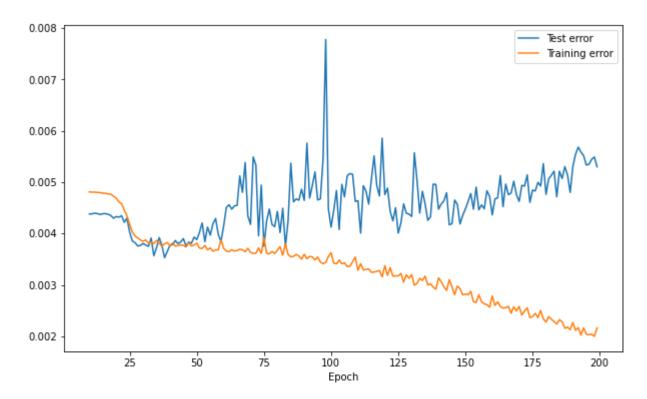
Total params: 85,569
Trainable params: 85,569
Non-trainable params: 0

We can store the best model in a file, so that we can load it after analyisng the training procedure.

```
checkpoint_filepath = './'
model_checkpoint_callback = tf.keras.callbacks.ModelCheckpoint(
    filepath=checkpoint_filepath,
    save_weights_only=True,
    monitor='val_loss',
    save_best_only=True) # Save only the best model, determined by the validation loss
```

Train the model

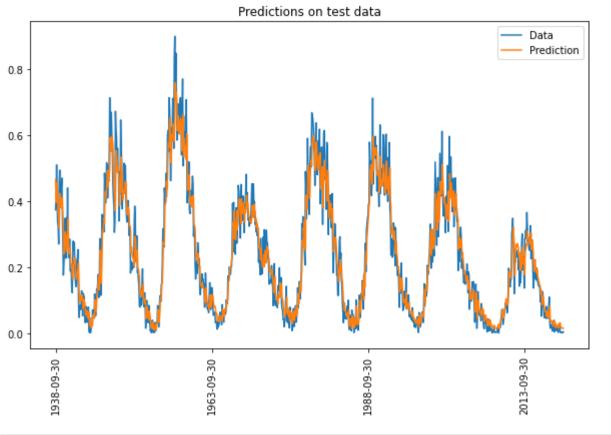
```
In [35]: plot_history(history, start_at)
```



Q14 (optional): Based on the training and test error plots, are there signs of over- or underfitting? **A14:**

We load the best model from checkpoint.

```
In [36]:
          model4.load_weights(checkpoint_filepath)
          <tensorflow.python.training.tracking.util.CheckpointLoadStatus at 0x2751eb15610>
Out[36]:
In [37]:
          # Predict on all data using the final model.
          # We predict using y_1, \ldots, y_{n-1} as inputs, resulting in predictions of the values y_n
          y pred4 = model4.predict(y[:ndata-1].reshape((1,ndata-1,1))).flatten() + y[:ndata-1]
In [38]:
          # Predict on all data using the final model.
          # We predict using y_1, \ldots, y_{n-1} as inputs, resulting in predictions of the values y_n
          y_pred4 = model4.predict(y[:-1].reshape(1, ndata-1, 1)).flatten() + y[:-1]
In [39]:
          # Plot prediction on test data
          plot_prediction(y_pred4)
          # Evaluate MSE and MAE (both training and test data)
          evalutate_performance(y_pred4, y[1:], ntrain-1, name='Stacked RNN, windowing/stateful')
         Model Stacked RNN, windowing/stateful
           Training MSE: 601.3257,
                                     MAE: 17.6311
           Testing MSE: 558.3778,
                                    MAE: 17.2574
```



In []: