tssl lab4

October 14, 2023

1 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.

```
[1]: 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

```
[2]: np.random.seed(42)
tf.random.set_seed(42)
```

1.1 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.

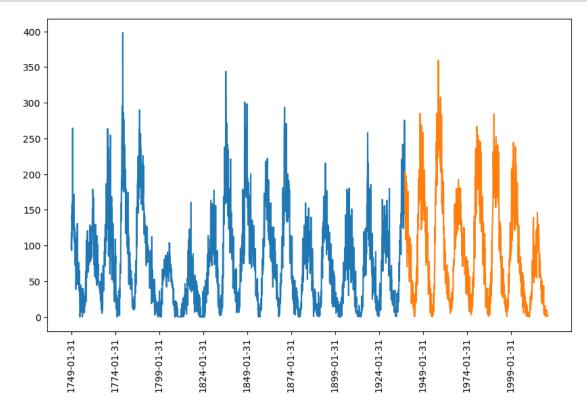
```
[3]: # Read the data
data=pandas.read_csv('Sunspots.csv',header=0)
dates = data['Date'].values
y = data['Monthly Mean Total Sunspot Number'].values
ndata=len(y)
print(f'Total number of data points: {ndata}')

# 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

```
[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 every 25th year for clarity
```



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.

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

1.2 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-absolute-error, to compare the more advanced models with later on.

```
[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_
      \hookrightarrow training data set.
            The remaining elements, i.e. y pred[split_time:] and y[split_time:] are__
      →treated as test data.
         nnn
        # 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 MAX VAL
        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:.
      MAE: {test mae:.4f}')
```

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, ..., n (cf. an AR(p) model where we start predicting at t = p + 1).

```
[7]: # Store the predictions in an array of length ndata-1. Note that there is an ashift in the indices
# between the prediction and the observation sequence, since there is non apprediction available for the first observation.
```

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.

```
[8]: # 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)
```

```
[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 corrsponding to training data points
name='AR')
```

Model AR

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

1.3 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: X is a 3D tensor where:

- The number of sequences Q
- \bullet The length of the sequences (number of time steps) ${f M}$
- The number of features (at each time step), i.e. the dimension of each time series P

Dimension $\dim(X) = [Q, M, P] = [1,3252, 1]$

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: - units = d, refers to the dimensionality of the output space. - The dimension output will be [1,3252,d], in this case d is 1 - Return sequence refers to return the last output in the output sequence, or the full sequence. [1,d] in this case d is 1

```
[10]: inputs = np.random.random([1, 3252, 1]).astype(np.float32)
simple_rnn = tf.keras.layers.SimpleRNN(4)

output = simple_rnn(inputs) # The output has shape `[32, 4]`.
print(len(simple_rnn.get_weights()))
#output.shape
```

3

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,

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

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.

Model: "sequential_3"

Layer (type)	Output Shape	Param #
simple_rnn_4 (SimpleRNN)	(None, None, 10)	120
dense_3 (Dense)	(None, None, 1)	11

Total params: 131 (524.00 Byte)
Trainable params: 131 (524.00 Byte)
Non-trainable params: 0 (0.00 Byte)

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:

$$W = (10, 10) = 100$$
, $U = (10, 1) = 10$, $b = (1, 10) = 10$

Parameters = 120

$$C = (10,) = 10, c = (1,) = 1$$

Parameters = 11

Total number of parameters = 131

1.4 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 $y_{1:n}$.

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

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

1.4.1 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.

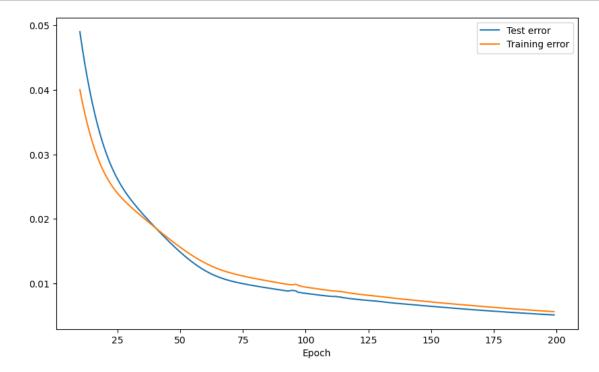
Q5: What should we set the *batch size* to, in order to compute the gradient based on the complete training data sequence at each iteration? Complete the code below!

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.

```
[24]: from tssltools_lab4 import plot_history
start_at = 10  # Skip the first few epochs for clarity
plot_history(history, start_at)
```



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.

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)!

```
# 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_2, ..., y_n.

# That is, y_pred1 should be an (n-1,) array where element y_pred[t] is based only on values y[:t]

y_pred1 = model1.predict( y[0:len(y)-1].reshape((1,len(y)-1,1)) ).flatten() + onp.append(x_train,x_test)
```

```
1/1 [=======] - Os 260ms/step
```

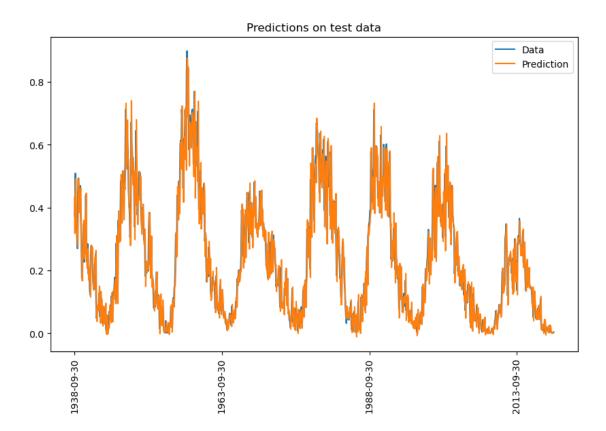
Using the prediction computed above we can plot them and evaluate the performance of the model in terms of MSE and MAE.

```
[27]: # Plot prediction
plot_prediction(y_pred1)

# Evaluate MSE and MAE (both training and test data)
evaluate_performance(y_pred1, y[1:], ntrain-1, name='Simple RNN, "do nothing"')
```

Model Simple RNN, "do nothing"

Training MSE: 896.7628, MAE: 20.9268 Testing MSE: 810.1569, MAE: 20.4308



1.4.2 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 yield statement of the generator should return a pair x, y with inputs and corresponding targets from the training data. Each epoch of the training procedure will then call the generator for a total of steps_per_epoch such yield statements.

```
[28]: def generator_train(window_size):
    while True:
        """The upper value is excluded in randint, so the maximum value that we
        →can get is tt = ntrain-window_size-1.
```

```
Hence, the maximum end point of a window is ntrain-1, in agreement with_

the fact that the size of input/output is ntrain-1

when working with one-step-ahead prediction."""

start_of_window = np.random.randint(0, ntrain - window_size) # First_

time index of window (inclusive)

end_of_window = start_of_window + window_size # Last time index of_

window (exclusive, i.e. this is really the first index_after_ the window)

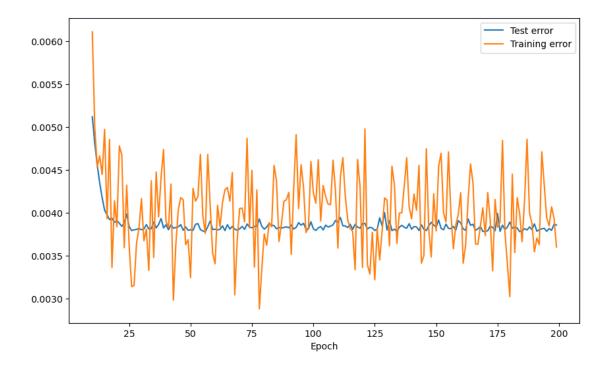
yield x_train[:,start_of_window:end_of_window,:], yt_train[:

,start_of_window:end_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.

```
[31]: 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 on the "do nothing" from option 1 has a smoother behaviour but the error is bigger. The random window option has a lot of jumps on both error, which represent inconssistency in orders words not so good results.

The reason for this peaks on the error is that when doing random windowing, the current sequence of data being process will take the last state of the last sequence as his first state, this means that it is passing time dependencies that may not be present on the current sequence, so that is why there is a lot of inconsistency on the error.

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

```
[32]: # 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_2, ..., y_n

y_pred2 = model2.predict( y[0:len(y)-1].reshape((1,len(y)-1,1)) ).flatten() +

np.append(x_train,x_test)
```

```
1/1 [======] - Os 211ms/step
```

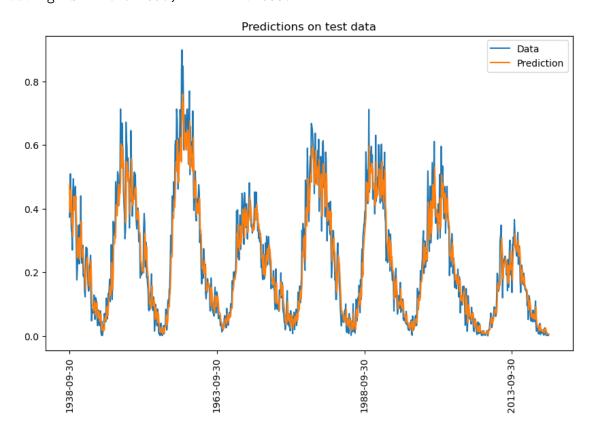
```
[33]: # Plot prediction on test data
plot_prediction(y_pred2)

# 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: 633.1413, MAE: 17.7039 Testing MSE: 616.2596, MAE: 17.8356



1.4.3 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.

```
[34]: # To enable stateful training, we need to create model where we set ustateful=True in the RNN layer

model3=keras.Sequential([
    # Simple RNN layer with stateful=True
    layers.SimpleRNN(units = d, batch_input_shape=(1,None,1),ustateful=True, activation='tanh'),
    # 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.

```
[35]: def generator_train_stateful(window_size, model):
          """In addition to the window_size, the generator also takes the model as_{\sqcup}
       \hookrightarrow 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 \Box
       ⇔cover all the training data.
          # Note 1. The length of x_{train} (and yt_{train}) is ntrain-1 since we work.
       ⇔with 1-step prediction.
          # Note 2. The final window could be smaller than window_size, ifu
       ⇔(ntrain-1) is not evenly divisable by the window_size.
          number_of_windows = int(ntrain//window_size)
          while True:
              end_of_window=0
              for i in range(number_of_windows):
                  # First time index of window (inclusive)
                  start_of_window = end_of_window
                  # Last time index of window (exclusive, i.e. this is the index to,)
       → the first time step after the window)
                  # Note 3. Python allows using end_of_window > ntrain-1, it will_
       simply truncate the indexing at the final element of the array!
                  end_of_window = start_of_window + window_size
                  #print(start_of_window, end_of_window)
                  yield x_train[:,start_of_window:end_of_window,:], yt_train[:
       →,start_of_window:end_of_window,:]
```

```
model.reset_states()

"""NOTE! In addition to replacing the ????? with the correct code, you need

→to move the line"""

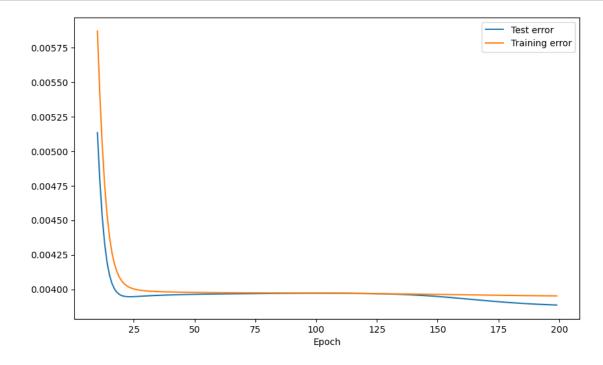
# model.reset_states()

"""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.

[37]: 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:

Both errors for this option are smaller than in option 1 and 2, and it can be seen it has more consistency, without having any peaks. Comparing it with Option 1, it reaches faster of in less epochs, the smaller values and where it stabalize it. Also there is no overfitting.

Reason:

When we do sequential windowing with stateful training, the sequence of the data is mantain in comparison with random windowing, resulting in mantaining the time dependencies of the data when the RNN pass the final state of a sequence into the new sequence to process, avoiding the peaks in the errors. And by partitioning the whole sequence into multiple sequences of the same lenght, we allowed the RNN to calculate more times the gradient, basically it computes the gradient for each sequence available, so in addition to calculate more times the gradients, the RNN is computing it in a "more fine grain" sense.

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

```
[38]: # 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_2,..., y_n

y_pred3 = model3.predict( y[0:len(y)-1].reshape((1,len(y)-1,1))).flatten() + np.

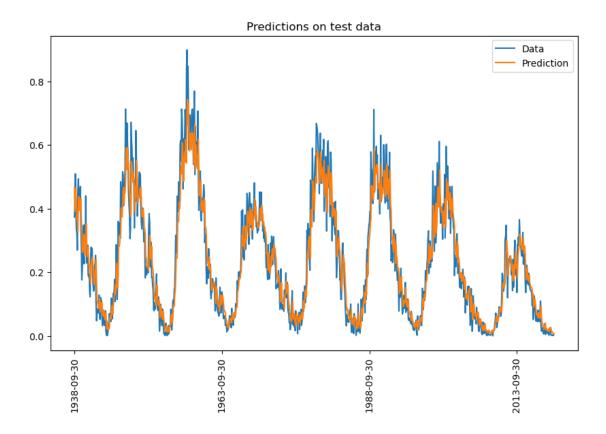
append(x_train,x_test)
```

```
1/1 [======] - Os 203ms/step
```

```
[39]: # Plot prediction on test data
plot_prediction(y_pred3)

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

Model Simple RNN, windowing/stateful Training MSE: 630.9376, MAE: 17.8626 Testing MSE: 616.8604, MAE: 18.0725



1.5 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:

The Ar(p) model, of order 30, performed better than the RNN methods. It was not possible to improve the prediction compared to the two baseline models, perhaps because a more fine tunning of the hyperparameters is needed. RNN models did not fullfil our expectations, as we believe it would performed better, because neural networks can learn complex patterns even with simpler asrchitectures.

1.6 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.

```
[40]: # A stacked model with 3 layers of LSTM cells, two Dense layers with Relument activation and a final linear output layer
model4 = tf.keras.models.Sequential([
```

```
tf.keras.layers.LSTM(64, batch_input_shape=(1,None,1), return_sequences=True,u
stateful=True),
tf.keras.layers.LSTM(64, batch_input_shape=(1,None,1), return_sequences=True,u
stateful=True),
tf.keras.layers.LSTM(64, batch_input_shape=(1,None,1), return_sequences=True,u
stateful=True),
tf.keras.layers.Dense(32, activation="relu"),
tf.keras.layers.Dense(16, activation="relu"),
tf.keras.layers.Dense(1),
])
model4.summary()
```

Model: "sequential_5"

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_5 (Dense)	(1, None, 32)	2080
dense_6 (Dense)	(1, None, 16)	528
dense_7 (Dense)	(1, None, 1)	17

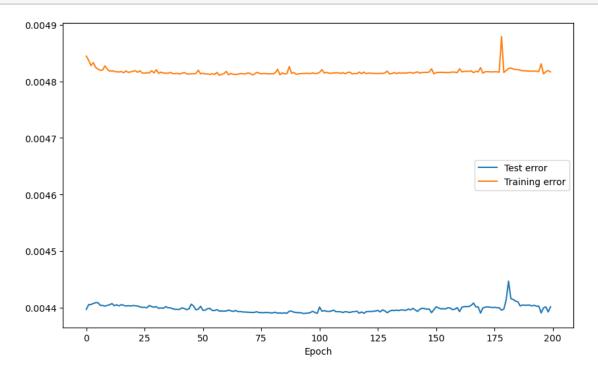
Total params: 85569 (334.25 KB)
Trainable params: 85569 (334.25 KB)
Non-trainable params: 0 (0.00 Byte)

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

```
[41]: 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

[48]: plot_history(history, 0)



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

Appears to be an overfitting because even from step 0 both error are splitted. But the error is still low, if it was underfitting both errors will be high and the model will not be able to predict neither the training and test data.

We load the best model from checkpoint.

```
[44]: model4.load_weights(checkpoint_filepath)
```

[44]: <tensorflow.python.checkpoint.checkpoint.CheckpointLoadStatus at 0x1ea994744f0>

```
[45]: # 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_2, ..., y_n

y_pred4 = model4.predict( y[0:len(y)-1].reshape((1,len(y)-1,1)) ).flatten() +
□
□ np.append(x_train,x_test)
```

1/1 [======] - 1s 1s/step

```
[46]: # 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_2,..., y_n

y_pred4 = model4.predict(y[:-1].reshape(1, ndata-1, 1)).flatten() + y[:-1]
```

1/1 [======] - Os 443ms/step

```
[47]: # Plot prediction on test data
plot_prediction(y_pred4)

# Evaluate MSE and MAE (both training and test data)
evaluate_performance(y_pred4, y[1:], ntrain-1, name='Stacked RNN, windowing/
stateful')
```

Model Stacked RNN, windowing/stateful Training MSE: 773.3623, MAE: 19.3492 Testing MSE: 701.8990, MAE: 19.1796

