Recurrent Neural Networks for Time Series Prediction

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Abstract

Recently recurrent neural networks due to their ability to capture time-dependent features have been applied to time series forecasting showing important improvements with respect to previous methods. Simple RNN architectures though suffer from vanishing/exploding gradient problems and cannot discriminate exogenous series in case these are given as input. In this work we analyse a solution based on LSTM networks and multiple attention mechanisms, which was originally proposed by [1], and compare it to simpler models including an encoder architecture to show the effectiveness of the method proposed.

1 Introduction and Related Work

Nonlinear autoregressive exogenous models (NARX) aim to predict the current value y_T of a time series y based on its collected knowledge coming from the past $T-1$ values (T also denoted as window size) of the time series $(y_1, y_2, ..., y_{T-1})$ and the current and past T values of n exogenous time series $(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_T)$, $\mathbf{x}_t \in \mathbb{R}^n$ where $\mathbf{x}_t = (x_t^1, x_t^2, ..., x_t^n)^\top$ are the values of each driving series at timestep t and $\mathbf{x}^k = (x_1^k, x_2^k, ..., x_T^k)$ are the values of the k-th time series in a given window. Exogenous time series are data that may be correlated to the series under consideration, so they are also called *driving series*. A good NARX algorithm should be able to choose which of the series are to be considered driving when predicting the current value of the target series. At the same time, a good algorithm should be able to capture long-term temporal dependencies.

In this work we analyse a deep-learning-based model that tries to tackle these two issues through the usage of recurrent neural networks and a carefully combined system of attention mechanisms. We perform an ablation study that wasn't directly reported in the authors' paper to validate the effectiveness of the approach proposed and compare the result with other possible approaches to the same problem using again recurrent networks. Classic statistical models, though effective for some real word applications, do not perform very well since they cannot model nonlinear relationships and do not differentiate between driving terms, or they model nonlinear relationships but with a predefined nonlinear relationship which is not necessarily the true underlying one.

2 Dataset

We used the same datasets as the authors' in order to try to compare our results with the ones reported.

The first dataset is SML 2010; its task is to predict the temperature of indoor environments. The data is collected from sensors of a system mounted in a domestic house for a total time of 40 days. The data is sampled every minute and was smoothed with 15 minutes mean. The target series we select is the room temperature and we collect 17 driving series by filtering out series which are constant. We use 80 percent of the dataset for training and we split evenly the remaining between validation and test.

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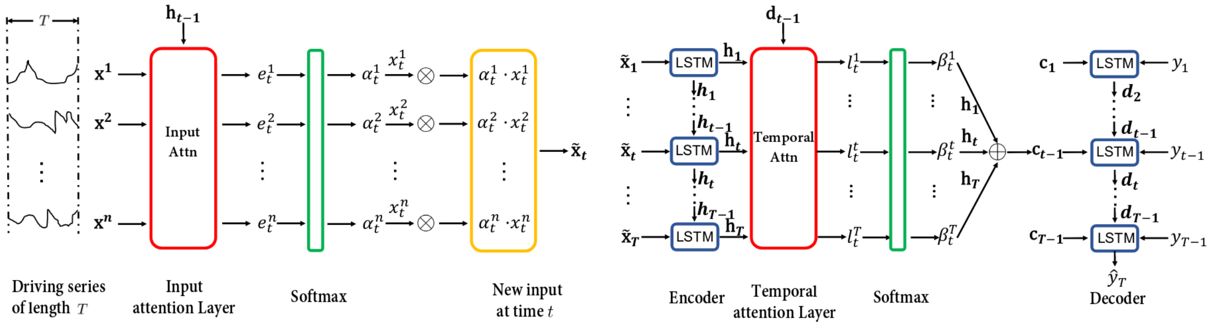
The second dataset is the NASDAQ 100 Stock dataset which is characterised by a larger number of driving series and stronger variations. This dataset is made public by the same authors of the original paper and is a collection of prices of 81 major corporations under NASDAQ 100 used as driving time series. The target series used is the value of the NASDAQ 100 index. The frequency of the data is minute-by-minute and covers 105 days from July 26, 2016 to December 22, 2016. We use 80 percent of the dataset for training, and the remaining is split into validation and test.

Both datasets are transformed into overlapping windows of a given size T (with the last value of the target series being the one we aim to predict), with stride 1.



(a) Input Attention Mechanism

(b) Temporal Attention Mechanism

Figure 1: DA-RNN model

3 Dual-stage attention model

The proposed model of the reference paper, which is illustrated in Figure 1, introduces two attention mechanisms in a LSTM-based encoder and decoder architecture. The first attention, *Input Attention*, is trained to independently weight the driving series at each timestep producing

$$(\tilde{\mathbf{x}}_1, \tilde{\mathbf{x}}_2, ..., \tilde{\mathbf{x}}_T) = A_{in}((\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_T)) = (\boldsymbol{\alpha}_1 \odot \mathbf{x}_1, \boldsymbol{\alpha}_2 \odot \mathbf{x}_2, ..., \boldsymbol{\alpha}_T \odot \mathbf{x}_T)$$

with $\boldsymbol{\alpha}_i \in \mathbb{R}^n$ and $\|\boldsymbol{\alpha}_i\|_1 = 1$. This helps in highlighting which series are useful for the prediction of the target series.

The weighted driving series are than passed to a one layer LSTM encoder of which hidden states (cell state and hidden state) are used in the Input Attention mechanism.

For each timestep the encoder maps the "attentioned" input $\tilde{\mathbf{x}}_t$ to a vector $\mathbf{h}_t \in \mathbb{R}^m$ which is the hidden state of the LSTM at timestep t. The operations involved in this mapping are the ones that take place in the update of a LSTM cell and can be summarised as follows:

$$\begin{aligned}
\mathbf{f}_t &= \sigma(\mathbf{W}_f[\mathbf{h}_{t-1}; \tilde{\mathbf{x}}_t] + \mathbf{b}_f) \\
\mathbf{i}_t &= \sigma(\mathbf{W}_i[\mathbf{h}_{t-1}; \tilde{\mathbf{x}}_t] + \mathbf{b}_i) \\
\mathbf{o}_t &= \sigma(\mathbf{W}_o[\mathbf{h}_{t-1}; \tilde{\mathbf{x}}_t] + \mathbf{b}_o) \\
\mathbf{s}_t &= \mathbf{f}_t \odot \mathbf{s}_t + \mathbf{i}_t \odot \tanh(\mathbf{W}_s[\mathbf{h}_{t-1}; \tilde{\mathbf{x}}_t] + \mathbf{b}_s) \\
\mathbf{h}_t &= \mathbf{o}_t \odot \tanh(\mathbf{s}_t)
\end{aligned} \tag{1}$$

Where $[\mathbf{h}_{t-1}; \tilde{\mathbf{x}}_t] \in \mathbb{R}^{m+n}$ is a concatenation of the hidden state of the previous timestep and the input of the current timestep; $\mathbf{W}_f, \mathbf{W}_i, \mathbf{W}_o, \mathbf{W}_s \in \mathbb{R}^{m \times (m+n)}$, and $\mathbf{b}_f, \mathbf{b}_i, \mathbf{b}_o, \mathbf{b}_s \in \mathbb{R}^m$ are parameters to learn; σ and $\odot$ are a logistic sigmoid function and an element-wise multiplication, respectively.

The second attention mechanism introduced, *Temporal Attention*, adaptively selects relevant encoder hidden states across the timesteps of the window producing

$$(\mathbf{c}_1, \mathbf{c}_2, ..., \mathbf{c}_T) = A_{temp}((\mathbf{h}_1, \mathbf{h}_2, ..., \mathbf{h}_T)) = \left(\sum_{i=1}^{T} \beta_1^i \mathbf{h}_i, \sum_{i=1}^{T} \beta_2^i \mathbf{h}_i, ..., \sum_{i=1}^{T} \beta_T^i \mathbf{h}_i \right)$$

where β_t^i represents the importance of the i-th encoder hidden state for the prediction.

The t-th "attentioned" encoder hidden state $\mathbf{c}_t$ is then concatenated with y_t, given in input to a dense layer of which output is then fed in input to the decoder. When $t = T$ instead, the "attentioned" encoder hidden state is concatenated to the hidden state of the decoder and passed to two dense layers to obtain the predicted value.

For the Input Attention, the following operations are taken to obtain the weights α_t^k

$$
\begin{aligned}
e_t^k &= \mathbf{v}_e^\top \tanh(\mathbf{W_e}[\mathbf{h}_{t-1}; \mathbf{s}_{t-1}] + \mathbf{U_e}\mathbf{x}^k), && 1 \leq k \leq n \\
\alpha_t^k &= \frac{\exp(e_t^k)}{\sum_{i=1}^n \exp(e_t^i)},
\end{aligned}
$$

where $\mathbf{h}_{t-1}, \mathbf{s}_{t-1}$ are the hidden and cell states of the encoder, $\mathbf{x}^k$ is one driving series, $\mathbf{v}_e \in \mathbb{R}^T, \mathbf{W}_e \in \mathbb{R}^{T \times 2m}$ and $\mathbf{U}_e \in \mathbb{R}^{T \times T}$ (with m the hidden size of the encoder) are learnable parameters.

For the Temporal Attention, the following operations are taken to obtain the weights β_t^i

$$
\begin{aligned}
l_t^i &= \mathbf{v}_d^\top \tanh(\mathbf{W_d}[\mathbf{d}_{t-1}; \mathbf{s}'_{t-1}] + \mathbf{U_d}\mathbf{h}_i), && 1 \leq i \leq T \\
\beta_t^i &= \frac{\exp(l_t^i)}{\sum_{i=1}^n \exp(e_t^i)},
\end{aligned}
$$

where $\mathbf{d}_{t-1}, \mathbf{s}'_{t-1} \in \mathbb{R}^p$ are the hidden and cell states of the decoder, $\mathbf{h}_i$ is the i-th hidden state of the encoder, $\mathbf{v}_d \in \mathbb{R}^m, \mathbf{W}_d \in \mathbb{R}^{m \times 2p}$ and $\mathbf{U}_d \in \mathbb{R}^{m \times m}$ (with p the hidden size of the decoder) are learnable parameters.

3.1 Implementation details

We used Tensorflow 1.12 as the target framework to implement the model just described. The reason behind this choice is that we could easily translate the equations of the model directly into the code and define each step of the model pragmatically.

For the encoder network we used the `LSTMCell` class from `tensorflow.python.ops.rnn_cell_impl`. We initially instantiated a zero state for the cell and the hidden states. Then for each timestep we defined the Tensorflow computational graph nodes, in particular the nodes for the Input Attention implementation and the `LSTMCell`, which takes as input the hidden state of the previous timestep and the output of the Input Attention. During this process we collect the output hidden states of the cell for the various timesteps, that is finally reshaped to be the input of the Temporal Attention.

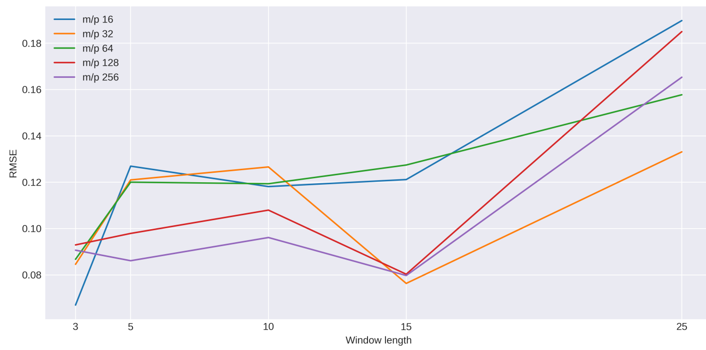
For the decoder network implementation we instantiated a zero state for the cell and the hidden state and we defined the nodes for the Temporal attention. The target series value at time t is concatenated with the output of the temporal attention at time t and passed to a dense layer. The newly computed vector is used for the update of the decoder hidden state in the `LSTMCell`. For y_T, which is what we aim to predict, the "attentioned" encoder hidden state at time T is concatenated to the last hidden state of the decoder and fed to two dense layers.

To make the experimentation modular we defined a data class that loads all the parameters and file paths from JSON configuration files.

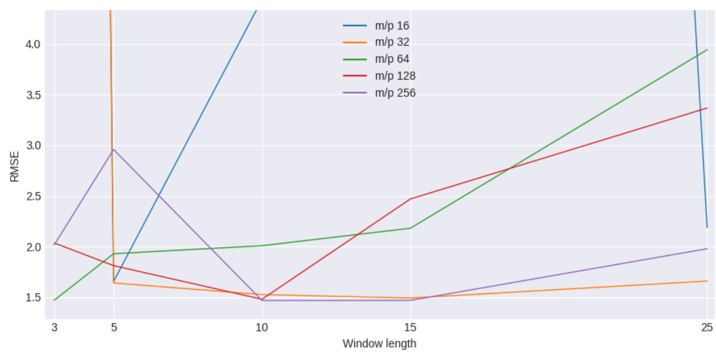
Initially, in order to ensure the correctness of the formulas being implemented we used the Eager Execution model offered by Tensorflow which allows to easily debug and quickly iterate over the core of the model.

We used Tensorboard to graphically visualize the value of the loss across the training steps and the values of the evaluation metrics on the validation set at every epoch of training.

Finally we exploited the checkpointing facilities offered by the framework to save two main set of values: the data needed to restart the training on a successive run of the training and the weights of the model that achieved the best performance in all the evaluation sessions. The final tests indeed are done by loading the weights of the best model even if the training ran for longer or later incurred in overfitting.



(a) SML 2010 validation set



(b) NASDAQ 100 validation set

Figure 2: RMSE score across the dataset for different window lengths T and encoder/decoder hidden state sizes, m and p respectively

3.2 Hyper parameter tuning

We validated our implementation using the same set of metrics as the original authors (RMSE, MAE, MAPE) and we performed some hyper-parameter tuning running the training with different configuration files.

All the models were trained for 150 epochs using two Adam optimisers one for the encoder and one for the decoder, which sped up the training. We used a starting learning rate of 0.001 and exponential decay with objective function the Mean Squared Error. We applied clipping of the gradients to prevent exploding gradients messing up the parameters during training. The models trained on the SML 2010 dataset were trained with batch size 32 while the ones trained on NASDAQ 100 with batch size 128. In both cases a grid search is performed over $T \in \{3, 5, 10, 15, 25\}$ and $m = p \in \{16, 32, 64, 128, 256\}$. The model with the best performance on the validation set is then used for further analysis. In Figure 2 the RMSE scores as the parameters vary are shown. The other scores (MAE, MAPE) follow a similar trend. As can be noticed, in general better scores are achieved for small window size and as it grows a drop in performance arises which is typical of encoder decoder networks [2].

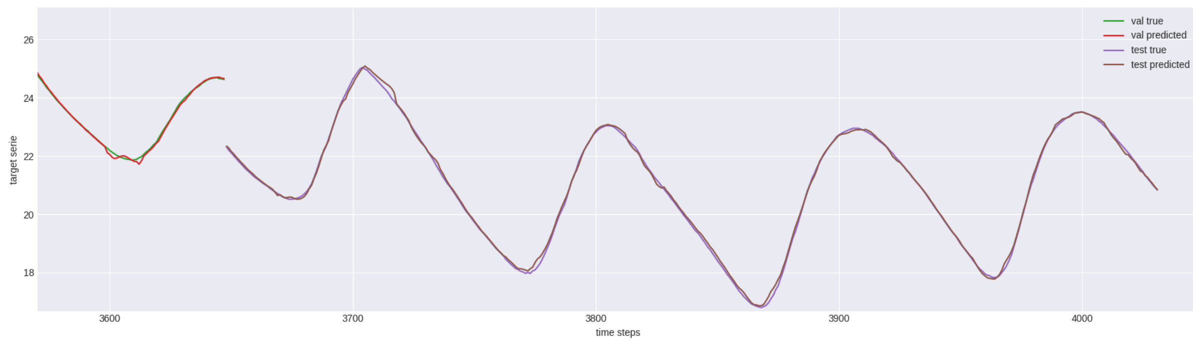
For SML 2010 dataset, given the simplicity of the series to predict, the RMSE is small even for small values of the window length. However, since a small window length cannot capture long-term dependencies and will also weaken the usefulness of the Temporal Attention, we decided to take for test $T = 15$ and $m = p = 32$.

For NASDAQ 100 dataset, $T = 3$ and $m = p = 16$ or $m = p = 32$ have high RMSE, since a small window size combined with small hidden state sizes does not result effective enough for the prediction. For evaluation we take the ones that achieves the best performance, $T = 15$ and $m = p = 256$.

After we have obtained a good hyper-parameters setting for the various models we compare their performance on our reference datasets. In Table 1 we show the scores achieved. As can be seen, the results slightly differ from the ones of the authors which can be either because of the difference in the number of epochs or because of a data normalisation which we did not perform.

	Train			Validation			Test		
	RMSE	MAE	MAPE	RMSE	MAE	MAPE	RMSE	MAE	MAPE
NASDAQ100	1.7095	0.9537	0.01991	1.4689	0.9550	0.0198	1.5810	1.0477	0.0212
SML2010	0.0644	0.0434	0.2279	0.0763	0.0601	0.2561	0.0863	0.0666	0.3248

Table 1: Results over SML2010 and NASDAQ100



(a) SML 2010

(b) NASDAQ 100

Figure 3: Predicted time series and true time series plotted for portions of the time steps

The results of the predictions are displayed in Figure 3. As can be noticed, the model produces a prediction close to the last seen value of the target series, with some small variations.

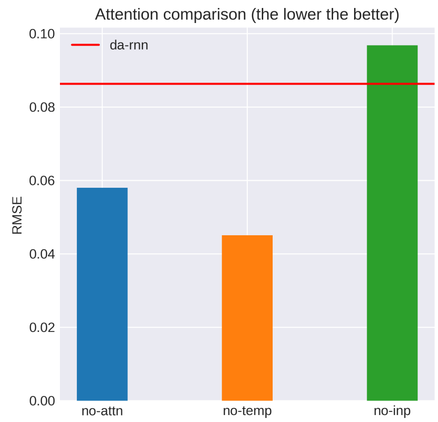
3.3 Ablation Study

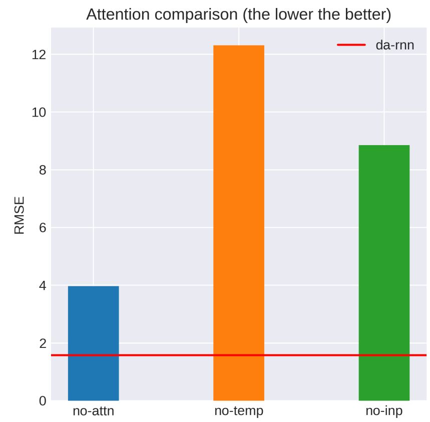
To validate the usefulness and correctness of the dual-stage attention approach we perform an ablation study of the model and report the values of the resulting three systems comparing them against the model with both attention mechanisms active and hyperparameters said above. We notice that here we include the temporal-attention-only model together with the input-attention-only model that was not evaluated in our original reference paper.

In Figure 4 the comparison between the model without any attention mechanism, without the temporal attention and without the input attention respectively is shown against the line representing the dual attention model of the authors'.

Figure 4a shows that the temporal attention is ineffective for this task (green bar and red line representing models with temporal attention enabled higher than models where the temporal attention is disabled). This is probably due to the sinusoidal shape of the target series of which timesteps have equal importance.

Figure 4b highlights the effectiveness of the dual-stage attention mechanism. In the NASDAQ100 dataset the models without one of the attention mechanisms are not able to produce remarkable results due to both the large number of driving series and the strong variations of the series over the timesteps.





(a) SML 2010 test set

(b) NASDAQ 100 test set

Figure 4: Comparison of the performances by switching off the attention mechanisms. The red line shows the RMSE score of the model with both attentions (input and temporal attention) enabled. In blue the RMSE score with both the input and temporal attentions disabled. In orange the score with only the temporal attention disabled and in green the score with only the input attention disabled. Similar plots for the other metrics.

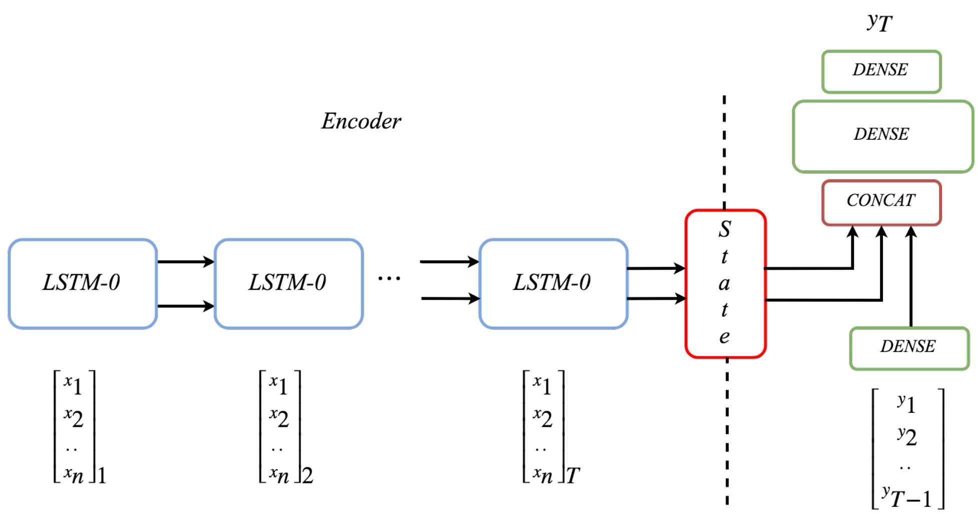


Figure 5: Encoder model

4 Simple encoder network baseline

In this paragraph we introduce a simple model we used as a baseline.

We initially developed a model composed of an encoder and a decoder with the goal of producing a network that could be easily extended to a multistep-ahead environment where we could predict accurately the future values for more than a single timestep. The encoder of this original network was composed of two stacked LSTM layers, taking as input the driving series' sequence, and we collected the final hidden state and cell state of each layer that were used as the initial states for the decoder. The number of layers of the decoder had to be the same as the encoder, as well as the dimension of the hidden state, to directly use the encoder states. We then gave as input to the decoder LSTM the vector containing the past history of the target series; for multi-step ahead forecasting the vector was simply fed a number of time equal to the number of steps to predict. The hidden states of the decoder were finally fed to a dense layer to obtain the final predictions.

Discouraged by the difficulties this network had in learning to predict values for the NASDAQ 100 dataset (although the model still performed well on the SML 2010 dataset) we decided to make the network simpler focusing only on the single step target series value forecasting. Given this choice we dropped completely the decoder part replacing it with two feed-forward neural networks. The first one is composed of one dense layer and it is used to encode the target series history. The other one takes the concatenation of the encoder output and the cell state of the final LSTM iteration with the output of the other network and maps it to the predicted value of the target series.

The encoder network was mostly left unchanged but we reduced the number of LSTM layers from 2 to 1; the choice of keeping the encoder makes sense since we still want to capture time dependencies in the driving series and encode this information in a fixed size representation. On the other hand the window of past values is considered altogether applying a dense layer to the input vector. The complete architecture is shown in Figure 5.

4.1 Implementation details

For this simple encoder model we took advantage of Keras interface. We instantiated a `LSTMCell` and gave it as argument to a `RNN` layer. Using the functional API we applied this layer to the driving series' input and collected the final state. We set the size of the output equal to 128. As in the original architecture the input to the LSTM at each timestep is a vector of n values of the n driving series values in that timestep.

The encoder last hidden and cell states were concatenated to the values of the past history of the target series, after being fed to the dense layer with output size 64. The concatenation is passed to two final `Dense` layers, of output size respectively 256 and 1, with the last one being the predicted value.

We defined a callback in the `fit()` function call to make the training stop if the value of the loss doesn't improve for a certain number of consecutive steps (the level of patience was empirically adjusted).

We trained for a total of 100 epochs with an Adam optimizer without any learning rate decay, with input window size $T = 10$.

4.2 Results

As can be seen from Table 2 the scores achieved in the various metrics are not as good as the ones of the dual-stage attention RNN described in the previous sections. This validates the ideas by the original authors and finally justifies the complexity of the network with an improvement in the performance.

	Train			**Validation**			**Test**		
	RMSE	MAE	MAPE	RMSE	MAE	MAPE	RMSE	MAE	MAPE
NASDAQ100	4.5726	3.5723	0.0744	4.0200	3.1977	0.0658	4.0803	3.1980	0.0647
SML2010	0.1049	0.0746	0.3858	0.1714	0.1714	0.5728	0.1026	0.0750	0.3497

Table 2: Results over SML2010 and NASDAQ100

5 Conclusion

In this paper we analysed the work done in [1], re-implementing the dual-stage attention mechanism building a model that is able to select both relevant driving series and relevant timesteps from the past time window. We reported a large number of experiments to validate the performances described in [1], including a complete ablation study of the original attention based model and the development of a novel baseline model based on a simple encoder and a set of feed-forward networks. Our implementations use modern APIs at both low level (Tensorflow) and high (Keras functional API) and we put much effort in writing a modular and readable code that makes as easy as possible to reproduce the results we presented in this work.

References

[1] Qin, Yao, et al. "A Dual-Stage Attention-Based Recurrent Neural Network for Time Series Prediction." Proceedings of the Twenty-Sixth International Joint Conference on Artificial Intelligence, 2017.

[2] Cho, Kyunghyun, et al. "On the Properties of Neural Machine Translation: Encoder–Decoder Approaches." Proceedings of SSST-8, Eighth Workshop on Syntax, Semantics and Structure in Statistical Translation, 2014.