

IM1102-232433M - Deep Neural Engineering assignment 2

Modifying the attention mechanism of transformers for time series forecasting

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Introduction

This report details the steps taken by Arne Lescrauwaet (852617312), Joachim Verschelde (852594432) and Alexander Van Hecke (852631385) for the second assignment of the 2023 Deep Neural Engineering course organised by the Open University (1).

For this assignment we look at different attention mechanisms in transformers (2) for use with time series data. The attention mechanism enables a transformer model to selectively focus on relevant parts of the input data. The goal is to be able to capture long range dependencies and relationships between items of the input data. This is particularly important for time series data containing recurring patterns, e.g. hourly traffic counts on busy highways and hourly power consumption of nations. We expect these types of data to contain clear and recurring patterns (i.e. traffic will typically be lower during weekends) and we want an attention mechanism to capture these patterns. In addition to capturing recurring patterns, we would also like to be able to capture the “local context” of a pattern to predict new values. That is, when encountering an event that is similar to a past event, we want to take the outcome of that past event into account in our prediction.

Different kinds of attention mechanisms exist. Convolutional self-attention is introduced in (3), which aims to capture the local context of input events, but does this using a symmetric convolution, thereby taking both input data leading to a particular event and the outcome of that event into account. A dual-stage attention mechanism is used for a Recurrent Neural Network (RNN) architecture in (4), using an input attention mechanism in an encoder step, and a temporal attention mechanism in a decoder step.

Even though transformers were originally designed in the field of natural language processing (NLP), a lot of work has been done to use transformers with time series data. An overview of different ways to adapt transformers to time series data is given in (5). The time2vec encoding mechanism is introduced in (6). The authors of this paper use transformer models to predict stock prices, and claim these models can be used both for short and long term predictions. The effectiveness of applying transformers to time series data is tested in (7).

The original transformer architecture introduces a quadratic time and space complexity. Much work has been done to improve on this. The LogSparse transformer is introduced in (3), which reduces the memory cost to $O(L(\log L)^2)$. The informer model (8) even achieves $O(L \log L)$ memory complexity. In this report we will focus on attention mechanisms in the context of time series forecasting, ignoring space and time complexity of the transformer algorithm.

Goal

In this paper, we focus on using transformers for time series forecasting. We aim to compare different attention mechanism and determine which mechanism best captures the outcome of past events. We formulate a first research question :

RQ 1 : When comparing regular self-attention, convoluted self-attention, right-padded convoluted self-attention and fourier transform based self-attention, which mechanism best predicts future values using mean square error (MSE) as metric?

The Elia dataset used is fully described in the dataset description section. It not only contains time series data, but also day+1 and day+7 predictions of the same data. We formulate a second research question :

RQ 2 : Is the MSE of a transformer model better than the Elia prediction model?

Firstly, this report will look at the characteristics of the dataset used and discuss pre-processing steps. Then, we will consider several attention mechanisms, discuss design and implementation details and finally evaluate the performance of these attention mechanisms on the dataset.

Data analysis

Dataset description

We use data from Elia (9), which operates the electricity transmission network in Belgium. In particular, we use the solar power forecast datasets. These contain time series of actual measured power in megawatt (MW), and also day+1 and day+7 predictions of solar power output in MW. Data is available in monthly datasets for the period of February 2013 to February 2024. Measurements and predictions are recorded every quarter of an hour. The measured value is always the amount of power equivalent to the running average measured for that particular quarter-hour. The layout of the dataset is fully described here (10). We recap the most important points in Table 1.

Table 1: Features captured per quarter-hour in (10)

feature	description	range
DateTime	Date and time per quarter hour	[00:00 - 24:00] in quarter hours
Measurement	Measured solar power production in MW	[0.0 - 6000.0]
Day+1 prediction	D+1 solar power forecast in MW	[0.0 - 6000.0]
Day+7 prediction	D+7 solar power forecast in MW	[0.0 - 6000.0]

Data general properties

Data is not normally distributed but highly regular and contains obvious day - night recurring patterns. Since we are using solar power production data, data typically shows no values in the early morning, building towards a peak around noon, and then slowly reducing values towards the evening. This is illustrated in Figure 1.

There are obvious differences in solar power generation between summer months and winter months, but the general pattern remains the same, as illustrated in Figure 2.

Data pre-processing

The Elia data (10) is very fine grained and contains $24 * 4 = 96$ measurements per day, resulting in $30 * 24 * 4 = 2880$ measurements for a 30 day month. In order to be able to limit memory and computational resources, we have added the possibility to aggregate this dataset. Possible choices are **(i)** no aggregation, **(ii)** hourly aggregation, **(iii)** aggregation every 4 hours (starting from 00:00, resulting in 6 values per day), and finally **(iv)** aggregation per day. Aggregation is done by averaging the values in the selected timeframe.

Elia provides a lot of historical data, going from February of 2013 to February of 2024. All data were taken into account, in order to maximize the possibility of finding interesting patterns in the data. Input length L has to be chosen carefully in basic transformer architectures because of the quadratic complexity in L . Taking too few measurements into account, it will be difficult to spot similar events in the past. Taking too many measurements into account, it will be prohibitively expensive in terms of memory and computational resources to train and evaluate the model. The model implemented allowed for easy selection of input length L . This is related to the level of aggregations in terms of how many hours or days this represents, i.e. when using hourly aggregation and taking 24 input measurements, we are looking at the data of exactly one day.

Outlier analysis

A visual outlier analysis yielded no abnormal or obviously wrong values. This makes sense, as the data contains actually measured solar power. Therefore, no values were discarded.

Methodology and Implementation

Research methodology

We started by examining the dataset (10). Outlier analysis yielded no results, and we performed a number of standard checks on the quality of the data and decided not to exclude any data from the dataset.

Given a basic transformer architecture, we implemented a number of attention mechanisms to investigate influence on prediction MSE. We first evaluated different models by varying some hyperparameters and by varying data aggregation (see Table 3). Given our limited computational resources, we chose a fixed set of hyperparameter and aggregation values for the rest of the experiments. All experiments used a forecast size of 1. Note that this is linked to the aggregation level, i.e. when using “1 day” aggregation, forecasting one value means forecasting the next day. When using 1h aggregation, forecasting one value means forecasting the next hour.

Data was split in a training part (63 %), a validation part (10 %), and a test part (27 %). To accomplish this split, all data was sorted chronologically. All data up to but not including 2020 served as training data, the data of 2020 up to but not including 2021 served as validation data, and data of 2021 and later served as test data. Models were first trained on the training dataset and then validated on the validation dataset for a maximum of 100 epochs. However, to limit computation, we kept track of the minimum average validation error across all epochs. An early stop was forced if the average validation error of the running epoch exceeded the minimum average validation error 5 consecutive times, as this would indicate the validation error was no longer decreasing. Each model was then tested on the testing set and all losses (training losses, validation losses and test losses) were kept for later analysis. In all cases, MSE was used as the loss metric.

In order to compare the prediction of the trained transformer models to the Elia predictions, we kept the Elia predictions in the test set as an additional feature. This feature was not used for training or validation. Elia predictions are done per quarter hour, and were aggregated using averaging where necessary to obtain the same aggregation as the input data.

Design elaboration

We decided to implement and evaluate the following attention mechanisms (Table 2) :

- regular self-attention (AM-1). This is the mechanism described in the original transformer paper (2).
- convoluted self-attention as described in (3) (AM-2). This mechanism generalizes the regular self-attention mechanism and uses a 1D convolution to transform the Query (Q) and Key (K) values before using them in the transformer architecture.
- right padded convoluted self-attention (AM-3). This is a variation of the mechanism described in (3). Whereas (3) uses a symmetric convolution, here we use a convolution that focuses on the right hand side to transform Q and K values before using them in the transformer architecture. Padding to the right is done to prevent looking at future values.
- fourier transform based self-attention (AM-4). This uses the fourier transform to decompose the input embedding in a vector of frequency values. These vectors are used as a measure of similarity between keys and values to determine where to direct attention.

Table 2: Attention mechanisms

attention mechanism	abbreviation
regular self-attention	AM-1
convoluted self-attention	AM-2
asymmetric convoluted self-attention	AM-3
fourier transform self-attention	AM-4

Transformer models have several tunable hyperparameters. We first experimented with variations of number of layers, number of heads, levels of forward expansion, convolution kernel sizes and aggregation levels of input data for the **base transformer model**, as detailed in Table 3. This yielded very small differences in average test loss (see Table 4). Given our limited computational resources, we decided to fix the number of layers to 2, the number of heads to 4, the forward expansion to 256 and the aggregation to “1 day”. For the models using a convolution (AM-2 and AM-3), we experimented with kernel sizes of [3, 6, 9]. In all scenarios, MSE was used as the measure to optimize for.

Table 3: Hyperparameters

attention mechanism	hyperparameters
AM-1	layers [2, 4, 6], heads [4, 8], forward expansion [256, 512], aggregation [1day, 4 hours]
AM-2	layers [2], heads [4], forward expansion [256], aggregation [1day], kernel size [3, 6, 9]
AM-3	layers [2], heads [4], forward expansion [256], aggregation [1day], kernel size [3, 6, 9]
AM-4	layers [2], heads [4], forward expansion [256], aggregation [1day], TODO

Feature embedding was done using a combination of both positional encoding and a more specific temporal encoding, taking into account hour of the day, day of the week, day of the month and month of the year of the data. The temporal encoding was added to the input vector and served as an additional clue for the transformer model to link similar events.

Implementation

All code and data is available in a github repository (11). All deep learning models were implemented using the pytorch python package, visualisation was done using matplotlib and seaborn. We recap the most important files here :

- `building_blocks.py` contains all pytorch modules and models, the different attention mechanism, input embedding and other support code to execute different scenarios.
- `datasets.py` contains the code to load and aggregate the Elia data into one pytorch dataloader.
- `figures.ipynb` is a jupyter notebook that contains code to generate figures.
- `stats.ipynb` is a jupyter notebook that contains code to check statistical validity and generate tables about statistics.
- `scenario-base-transformer.ipynb` is a jupyter notebook focusing on the execution of scenario using a vanilla transformer
- TODO andere notebooks

Evaluation and Results

Evaluation

Evaluation of RQ 1

In order to evaluate the first research question, we formulate the following H_0 hypothesis :

H_0 : There is no difference between AM-1 on the one hand, and AM-2, AM-3 and AM-4 on the other hand.

If the p-value is below $\alpha = 0.05$, we can reject H_0 and accept the alternative hypothesis, that there is indeed a difference between the standard self-attention mechanism on the one hand and the non-standard self-attention mechanisms on the other hand.

Evaluation of RQ 2

In order to evaluate the second research question, we formulate the following H_0 hypothesis :

H_0 : There is no difference between the prediction done by attention mechanisms AM-1, AM-2, AM-3 and AM-4 and the prediction done by Elia.

If the p-value is below $\alpha = 0.05$, we can reject H_0 and accept the alternative hypothesis, that there is indeed a difference between the transformer based predictions and the Elia predictions. Note that Elia provides no details on their prediction model, so this is in fact a comparison between the Elia prediction model and a transformer based prediction model.

Results

Results of RQ 1

Results of RQ 2

TODO resultaten beschrijven

Conclusions and Discussion

In this paper, we analysed the role of attention mechanisms in transformer models for forecasting values when using timeseries data. Several attention mechanisms were evaluated, **(i)** regular self-attention, **(ii)** convoluted self-attention, **(iii)** right padded convoluted self-attention and **(iv)** fourier transform based self-attention.

TODO some discussion

TODO future work

References

1. Startpagina - IM1102-232433M - Deep Neural Engineering [Internet]. [cited 2024 Mar 21]. Available from: <https://brightspace.ou.nl/d2l/home/8636>
2. Vaswani A, Shazeer N, Parmar N, Uszkoreit J, Jones L, Gomez AN, et al. Attention is All you Need. In: Advances in Neural Information Processing Systems [Internet]. Curran Associates, Inc.; 2017 [cited 2024 Mar 6]. Available from: https://proceedings.neurips.cc/paper_files/paper/2017/hash/3f5ee243547dee91fbd053c1c4a845aa-Abstract.html
3. Li S, Jin X, Xuan Y, Zhou X, Chen W, Wang YX, et al. Enhancing the Locality and Breaking the Memory Bottleneck of Transformer on Time Series Forecasting. In: Advances in Neural Information Processing Systems [Internet]. Curran Associates, Inc.; 2019 [cited 2024 Mar 10]. Available from: <https://proceedings.neurips.cc/paper/2019/hash/6775a0635c302542da2c32aa19d86be0-Abstract.html>
4. Qin Y, Song D, Chen H, Cheng W, Jiang G, Cottrell GW. A Dual-Stage Attention-Based Recurrent Neural Network for Time Series Prediction. In: Proceedings of the Twenty-Sixth International Joint Conference on Artificial Intelligence [Internet]. Melbourne, Australia: International Joint Conferences on Artificial Intelligence Organization; 2017 [cited 2024 Mar 6]. p. 2627–33. Available from: <https://www.ijcai.org/proceedings/2017/366>
5. Wen Q, Zhou T, Zhang C, Chen W, Ma Z, Yan J, et al. Transformers in Time Series: A Survey [Internet]. arXiv; 2023 [cited 2024 Mar 7]. Available from: <http://arxiv.org/abs/2202.07125>
6. Muhammad T, Aftab AB, Ibrahim M, Ahsan MdM, Muhu MM, Khan SI, et al. Transformer-Based Deep Learning Model for Stock Price Prediction: A Case Study on Bangladesh Stock Market. International Journal of Computational Intelligence and Applications [Internet]. 2023 Sep [cited 2024 Mar 16];22(03):2350013. Available from: <https://www.worldscientific.com/doi/full/10.1142/S146902682350013X>
7. Cholakov R, Kolev T. Transformers predicting the future. Applying attention in next-frame and time series forecasting [Internet]. arXiv; 2021 [cited 2024 Mar 16]. Available from: <http://arxiv.org/abs/2108.08224>
8. Zhou H, Zhang S, Peng J, Zhang S, Li J, Xiong H, et al. Informer: Beyond Efficient Transformer for Long Sequence Time-Series Forecasting [Internet]. arXiv; 2021 [cited 2024 Mar 7]. Available from: <http://arxiv.org/abs/2012.07436>
9. Elia: Belgian's Electricity System Operator [Internet]. Elia. [cited 2024 Mar 30]. Available from: <https://www.elia.be/en/>

10. Solar-PV power generation data [Internet]. [cited 2024 Mar 23]. Available from: <https://www.elia.be/en/grid-data/power-generation/solar-pv-power-generation-data>
11. Hecke AV, Lescrauwaet A, Verschelde J. Avhou/dne [Internet]. 2024. Available from: <https://github.com/avhou/dne>

Appendix A : Data general properties

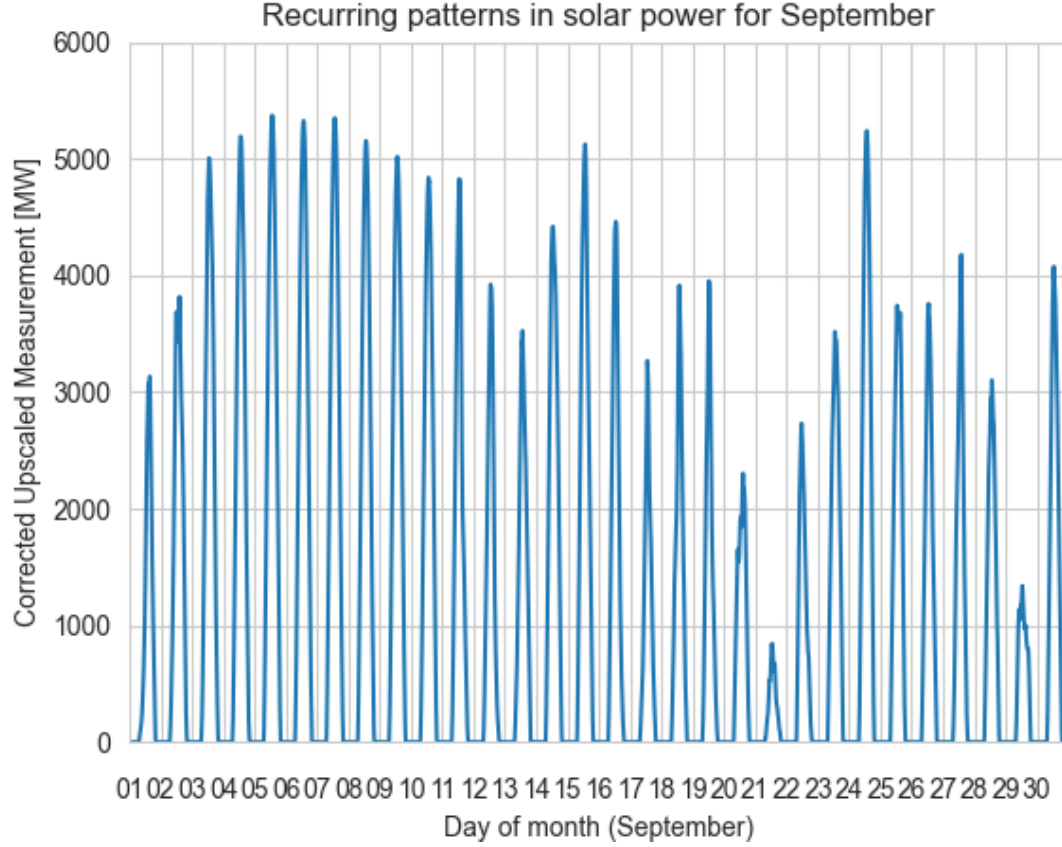


Figure 1: Typical recurrent patterns, here for September 2023

Appendix B : Average test losses (base transformer)

Table 4: Average test losses for base transformer hyperparameter variations

layers	heads	forward expansion	average	stddev
2	4	256	0.0799	0.0169
2	8	256	0.0906	0.0230
4	4	256	0.0875	0.0172
4	8	256	0.0841	0.0305
6	4	256	0.0877	0.0208
6	4	512	0.1086	0.0253
6	8	256	0.1038	0.0249

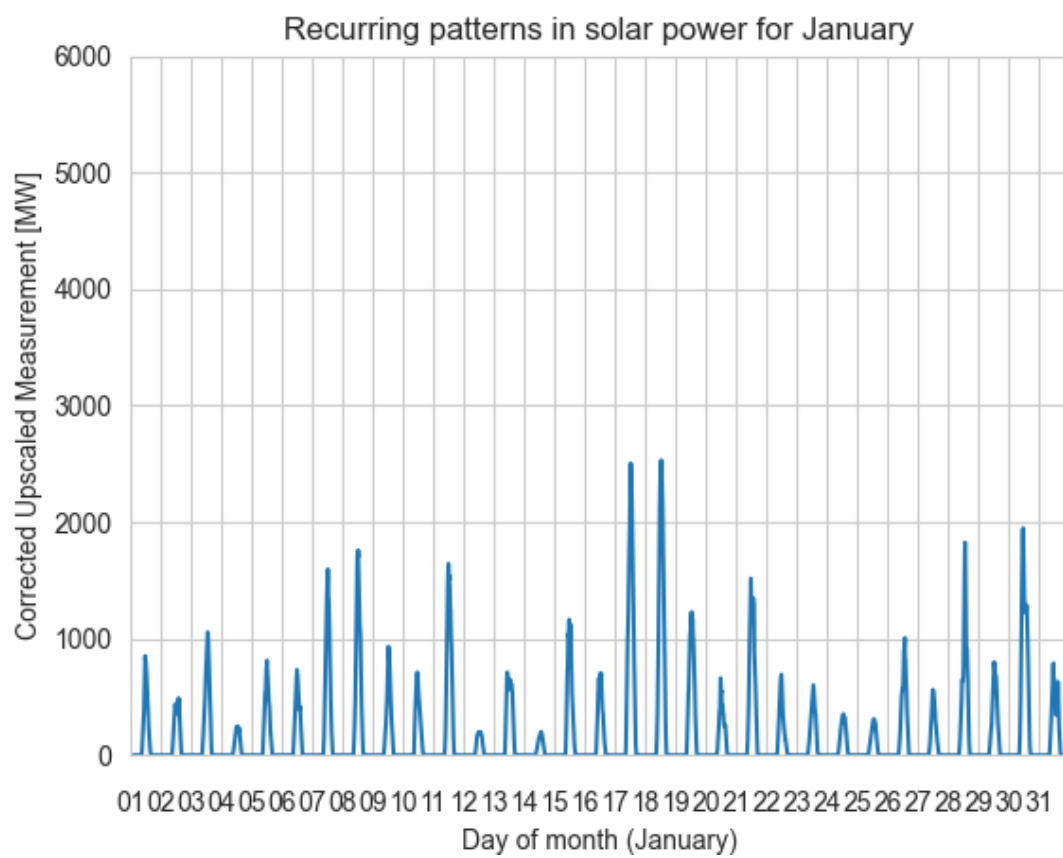


Figure 2: Typical recurrent patterns, here for January 2023