

Enhancing the Locality and Breaking the Memory Bottleneck of Transformer on Time Series Forecasting

Shiyang Li
UC Santa Barbara
shiyangli@ucsb.edu

Xiaoyong Jin
UC Santa Barbara
x_jin@ucsb.edu

Yao Xuan
UC Santa Barbara
yxuan@ucsb.edu

Xiyou Zhou
UC Santa Barbara
xiyou@ucsb.edu

Wenhu Chen
UC Santa Barbara
wenhuchen@ucsb.edu

Yu-Xiang Wang
UC Santa Barbara
yuxiangw@ucsb.edu

Xifeng Yan
UC Santa Barbara
xyan@cs.ucsb.edu

Abstract

Time series forecasting is an important problem across many domains, including predictions of solar plant energy output, electricity consumption, and traffic jam situation. In this paper, we propose to tackle such forecasting problem with *Transformer* [1]. Although impressed by its performance in our preliminary study, we found its two major weaknesses: (1) *locality-agnostics*: the point-wise dot-product self attention in canonical Transformer architecture is insensitive to local context, which can make the model prone to anomalies in time series; (2) *memory bottleneck*: space complexity of canonical Transformer grows quadratically with sequence length L , making modeling long time series infeasible. In order to solve these two issues, we first propose convolutional self attention by producing queries and keys with *causal convolution* so that local context can be better incorporated into attention mechanism. Then, we propose *LogSparse Transformer* with only $O(L(\log L)^2)$ memory cost, improving the time series forecasting in finer granularity under constrained memory budget. Our experiments on both synthetic data and real-world datasets show that it compares favorably to the state-of-the-art.

1 Introduction

Time series forecasting plays an important role in daily life to help people manage resources and make decisions. For example, in retail industry, probabilistic forecasting of product demand and supply based on historical data can help people do inventory planning to maximize the profit. Although still widely used, traditional time series forecasting models, such as State Space Models (SSMs) [2] and Autoregressive (AR) models, are designed to fit each time series independently. Besides, they also require practitioners' expertise in manually selecting trend, seasonality and other components. To sum up, these two major weaknesses have greatly hindered their applications in the modern large-scale time series forecasting tasks.

To tackle the aforementioned challenges, deep neural networks [3–6] have been proposed as an alternative solution, where Recurrent Neural Network (RNN) [7–9] has been employed to model time series in an autoregressive fashion. However, RNNs are notoriously difficult to train [10] because of gradient vanishing and exploding problem. Despite the emergence of various variants, including LSTM [11] and GRU [12], the issues still remain unresolved. As an example, [13] shows that language models using LSTM have an effective context size of about 200 tokens on average but are only able to sharply distinguish 50 tokens nearby, indicating that even LSTM struggles to capture long-term dependencies. On the other hand, real-world forecasting applications often have both long- and short-term repeating patterns [7]. For example, the hourly occupancy rate of a freeway has both

daily and hourly patterns. In such cases, how to model long-term dependencies becomes the critical step in achieving promising performances.

Recently, Transformer [1, 14] has been proposed as a brand new architecture which leverages attention mechanism to process a sequence of data. Unlike the RNN-based methods, Transformer allows the model to access any part of the history regardless of distance, making it potentially more suitable for grasping the recurring patterns with long-term dependencies. However, canonical dot-product self attention matches queries against keys insensitive to local context, which may make the model prone to anomalies and bring underlying optimization issues. More importantly, space complexity of canonical Transformer grows quadratically with the input length L , which causes the memory bottleneck on modeling long time series with fine granularity. We specifically delve into these two issues and investigate the applications of Transformer to time series forecasting. Our contributions are three fold:

- We successfully apply Transformer architecture to time series forecasting and perform extensive experiments on both synthetic and real datasets to validate Transformer’s potential value in better handling long-term dependencies than RNN-based models.
- We propose *convolutional* self attention by employing causal convolutions to produce queries and keys in the self attention layer. Query-key matching aware of local context, e.g. shapes, can help the model achieve lower training error and further improve its forecasting accuracy.
- We propose *LogSparse* Transformer, with only $O(L(\log L)^2)$ space complexity to break the memory bottleneck, not only making fine-grained long time series modeling feasible but also producing comparable or even better results with much less memory usage, compared to canonical Transformer.

2 Related Work

Due to the wide applications of forecasting, various methods have been proposed to solve the problem. One of the most prominent models is ARIMA [15]. Its statistical properties as well as the well-known Box-Jenkins methodology [16] in the model selection procedure make it the first attempt for practitioners. However, its linear assumption and limited scalability make it unsuitable for large-scale forecasting tasks. Further, information across similar time series cannot be shared since each time series is fitted individually. In contrast, [17] models related time series data as a matrix and deal with forecasting as a matrix factorization problem. [18] proposes hierarchical Bayesian methods to learn across multiple related count time series from the perspective of graph model.

Deep neural networks have been proposed to capture shared information across related time series for accurate forecasting. [3] fuses traditional AR models with RNNs by modeling a probabilistic distribution in an encoder-decoder fashion. Instead, [19] uses an RNN as an encoder and Multi-layer Perceptrons (MLPs) as a decoder to solve the so-called error accumulation issue and conduct multi-ahead forecasting in parallel. [6] uses a global RNN to directly output the parameters of a linear SSM at each step for each time series, aiming to approximate nonlinear dynamics with locally linear segments. In contrast, [9] deals with noise using a local Gaussian process for each time series while using a global RNN to model the shared patterns.

The well-known self attention-based Transformer [1] has recently been proposed for sequence modeling and has achieved great success. Several recent works apply it to translation, speech, music and image generation [1, 20–22]. However, scaling attention to extremely long sequences is computationally prohibitive since the time and space complexity of self attention grows quadratically with sequence length [20]. This becomes a serious issue in forecasting time series in fine granularity.

3 Background

Problem definition Suppose we have a collection of N related univariate time series $\{\mathbf{z}_{i,1:t_0}\}_{i=1}^N$, where $\mathbf{z}_{i,1:t_0} \triangleq [\mathbf{z}_{i,1}, \mathbf{z}_{i,2}, \dots, \mathbf{z}_{i,t_0}]$ and $\mathbf{z}_{i,t} \in \mathbb{R}$ denotes the value of time series i at time t . We are going to predict the next τ time steps for all time series, i.e. $\{\mathbf{z}_{i,t_0+1:t_0+\tau}\}_{i=1}^N$. Besides, let $\{\mathbf{x}_{i,1:t_0+\tau}\}_{i=1}^N$ be a set of associated time-based covariate vectors with dimension d that are assumed

to be known over the entire time period. We aim to model the following conditional distribution

$$p(\mathbf{z}_{i,t_0+1:t_0+\tau} | \mathbf{z}_{i,1:t_0}, \mathbf{x}_{i,1:t_0+\tau}; \Phi) = \prod_{t=t_0+1}^{t_0+\tau} p(\mathbf{z}_{i,t} | \mathbf{z}_{i,1:t-1}, \mathbf{x}_{i,1:t}; \Phi).$$

We reduce the problem to learning a one-step-ahead prediction model $p(\mathbf{z}_t | \mathbf{z}_{1:t-1}, \mathbf{x}_{1:t}; \Phi)$ ¹, where Φ denotes the learnable parameters shared by all time series in the collection. To fully utilize both the observations and covariates, we concatenate them to obtain an augmented matrix as follows:

$$\mathbf{y}_t \triangleq [\mathbf{z}_{t-1} \circ \mathbf{x}_t] \in \mathbb{R}^{d+1}, \quad \mathbf{Y}_t = [\mathbf{y}_1, \dots, \mathbf{y}_t]^T \in \mathbb{R}^{t \times (d+1)},$$

where $[\cdot \circ \cdot]$ represents concatenation. Note that we set \mathbf{z}_0 to be zero in all cases. An appropriate model $\mathbf{z}_t \sim f(\mathbf{Y}_t)$ is then explored to predict the distribution of \mathbf{z}_t given \mathbf{Y}_t .

Transformer We instantiate f with Transformer² by taking advantage of the multi-head self attention mechanism, since self attention enables Transformer to capture both long- and short-term dependencies, and different attention heads learn to focus on different aspects of temporal patterns. These advantages make Transformer a good candidate for time series forecasting. We briefly introduce its architecture here and refer readers to [1] for more details.

In the self attention layer, a multi-head self-attention sublayer simultaneously transforms \mathbf{Y} ³ into H distinct query matrices $\mathbf{Q}_h = \mathbf{Y}\mathbf{W}_h^Q$, key matrices $\mathbf{K}_h = \mathbf{Y}\mathbf{W}_h^K$, and value matrices $\mathbf{V}_h = \mathbf{Y}\mathbf{W}_h^V$ respectively, with $h = 1, \dots, H$. Here $\mathbf{W}_h^Q, \mathbf{W}_h^K \in \mathbb{R}^{(d+1) \times d_k}$ and $\mathbf{W}_h^V \in \mathbb{R}^{(d+1) \times d_v}$ are learnable parameters. After these linear projections, the scaled dot-product attention computes a sequence of vector outputs:

$$\mathbf{O}_h = \text{Attention}(\mathbf{Q}_h, \mathbf{K}_h, \mathbf{V}_h) = \text{softmax}\left(\frac{\mathbf{Q}_h \mathbf{K}_h^T}{\sqrt{d_k}} \cdot \mathbf{M}\right) \mathbf{V}_h.$$

Note that a mask matrix \mathbf{M} is applied to filter out rightward attention by setting all upper triangular elements to $-\infty$, in order to avoid future information leakage. Afterwards, $\mathbf{O}_1, \mathbf{O}_2, \dots, \mathbf{O}_H$ are concatenated and linearly projected again. Upon the attention output, a position-wise feedforward sublayer with two layers of fully-connected network and a ReLU activation in the middle is stacked.

4 Methodology

4.1 Enhancing the locality of Transformer

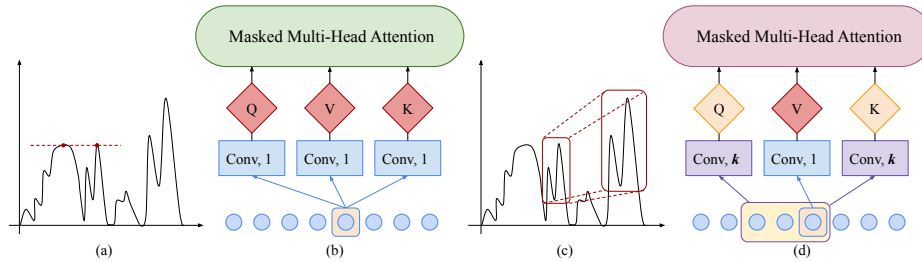


Figure 1: The comparison between canonical and our convolutional self attention layers. “Conv, 1” and “Conv, k ” mean convolution of kernel size $\{1, k\}$ with stride 1, respectively. Canonical self attention as used in Transformer is shown in (b), can wrongly match point-wise inputs as shown in (a). Convolutional self attention is shown in (d), which uses convolutional layers of kernel size k with stride 1 to transform inputs (with proper paddings) into queries/keys. Such locality awareness can correctly match the most relevant features based on shape matching in (c).

Patterns in time series may evolve with time significantly due to various events, e.g. holidays and extreme weather, so whether an observed point is an anomaly, change point or part of the patterns

¹Since the model is applicable to all time series, we omit the subscript i for simplicity and clarity.

²By referring to Transformer, we only consider the autoregressive Transformer-decoder in the following.

³At each time step the same model is applied, so we simplify the formulation with some abuse of notation.

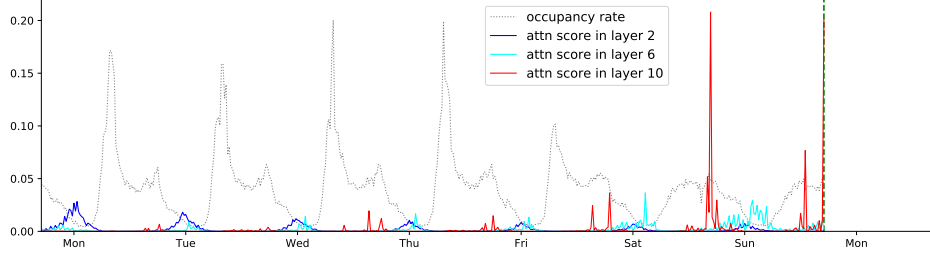


Figure 2: Learned attention patterns from a 10-layer canonical Transformer trained on `traffic-f` dataset with full attention. The green dashed line indicates the start time of forecasting and the gray dashed line on its left side is the conditional history. Blue, cyan and red lines correspond to attention patterns in layer 2, 6 and 10, respectively, for a head when predicting the value at the time corresponding to the green dashed line. a) Layer 2 tends to learn shared patterns in every day. b) Layer 6 focuses more on weekend patterns. c) Layer 10 further squeezes most of its attention on only several cells in weekends, causing most of the others to receive little attention.

is highly dependent on its surrounding context. However, in the self attention layers of canonical Transformer, the similarities between queries and keys are computed based on their point-wise values without fully leveraging local context like shape, as shown in Figure 1(a) and (b). Query-key matching agnostic of local context may confuse the self attention module in terms of whether the observed value is an anomaly, change point or part of patterns, and bring underlying optimization issues.

We propose convolutional self attention to ease the issue. The architectural view of proposed convolutional self attention is illustrated in Figure 1(c) and (d). Rather than using convolution of kernel size 1 with stride 1 (matrix multiplication), we employ *causal convolution* of kernel size k with stride 1 to transform inputs (with proper paddings) into queries and keys. Note that causal convolutions ensure that the current position never has access to future information. By employing causal convolution, generated queries and keys can be aware of local context and hence, compute their similarities by their local context information, e.g. local shapes, instead of point-wise values, which is helpful for accurate forecasting. Note that when $k = 1$, the convolutional self attention will degrade to canonical self attention, thus it can be seen as a generalization.

4.2 Breaking the memory bottleneck of Transformer

To motivate our approach, we first perform a qualitative assessment of the learned attention patterns with a canonical Transformer on `traffic-f` dataset. The `traffic-f` dataset contains occupancy rates of 963 car lanes of San Francisco bay area recorded every 20 minutes [6]. We trained a 10-layer canonical Transformer on `traffic-f` dataset with full attention and visualized the learned attention patterns. One example is shown in Figure 2. Layer 2 clearly exhibited global patterns, however, layer 6 and 10, only exhibited pattern-dependent sparsity, suggesting that some form of sparsity could be introduced without significantly affecting performance. More importantly, for a sequence with length L , computing attention scores between every pair of cells will cause $O(L^2)$ memory usage, making modeling long time series with fine granularity prohibitive.

We propose *LogSparse* Transformer, which only needs to calculate $O(\log L)$ dot products for each cell in each layer. Further, we only need to stack up to $O(\log L)$ layers and the model will be able to access every cell’s information. Hence, the total cost of memory usage is only $O(L(\log L)^2)$. We define I_l^k as the set of indices of the cells that cell l can attend to during the computation from k_{th} layer to $(k + 1)_{th}$ layer. In the standard self attention of Transformer, $I_l^k = \{j : j \leq l\}$, allowing every cell to attend to all of the past cells and its own as shown in Figure 3(a). However, such an algorithm suffers from the quadratic space complexity growth along with the input length. To alleviate such an issue, we propose to select a set of the indices $I_l^k \subset \{j : j \leq l\}$ so that $|I_l^k|$ does not grow too fast. An effective way of choosing indices is $|I_l^k| \propto \log L$.

Notice that cell l is a weighted combination of cells indexed by I_l^k in k_{th} self attention layer and can pass the information of cells indexed by I_l^k to its followings in the next layer. Let S_l^k be the set which contains indices of all the cells whose information has passed to cell l up to k_{th} layer. To ensure

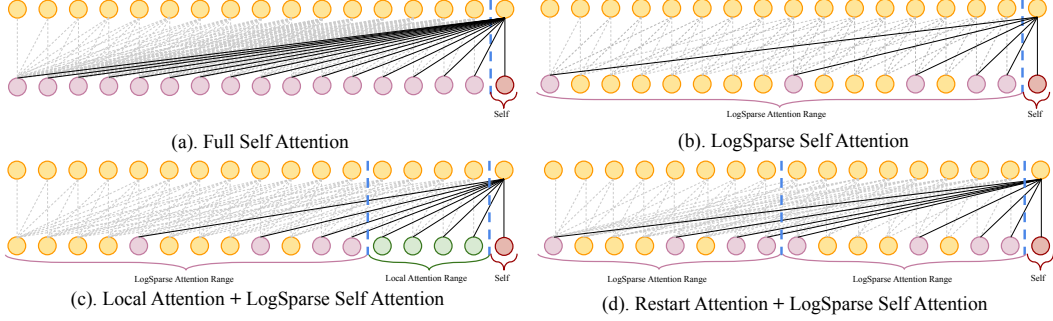


Figure 3: Illustration of different attention mechanism between adjacent layers in Transformer.

that every cell receives the information from all its previous cells and its own, the number of stacked layers \tilde{k}_l should satisfy that $S_l^{\tilde{k}_l} = \{j : j \leq l\}$ for $l = 1, \dots, L$. That is, $\forall l$ and $j \leq l$, there is a directed path $P_{jl} = (j, p_1, p_2, \dots, l)$ with \tilde{k}_l edges, where $j \in I_{p_1}^1, p_1 \in I_{p_2}^2, \dots, p_{\tilde{k}_l-1} \in I_l^{\tilde{k}_l}$.

We propose *LogSparse* self attention by allowing each cell only to attend to its previous cells with an exponential step size and itself. That is, $\forall k$ and l , $I_l^k = \{l - 2^{\lfloor \log_2 l \rfloor}, l - 2^{\lfloor \log_2 l \rfloor - 1}, l - 2^{\lfloor \log_2 l \rfloor - 2}, \dots, l - 2^0, l\}$, where $\lfloor \cdot \rfloor$ denotes the floor operation, as shown in Figure 3(b).⁴

Theorem 1. $\forall l$ and $j \leq l$, there is at least one path from cell j to cell l if we stack $\lfloor \log_2 l \rfloor + 1$ layers. Moreover, for $j < l$, the number of feasible unique paths from cell j to cell l increases at a rate of $O(\lfloor \log_2(l - j) \rfloor!)$.

The proof, deferred to Appendix A.1, uses a constructive argument.

Theorem 1 implies that despite an exponential decrease in the memory usage (from $O(L^2)$ to $O(L \log_2 L)$) in each layer, the information could still flow from any cell to any other cell provided that we go slightly “deeper” — take the number of layers to be $\lfloor \log_2 L \rfloor + 1$. Note that this implies an overall memory usage of $O(L(\log_2 L)^2)$ and addresses the notorious scalability bottleneck of Transformer under GPU memory constraint [1]. Moreover, as two cells become further apart, the number of paths increases at a rate of super-exponential in $\log_2(l - j)$, which indicates a rich information flow for modeling delicate long-term dependencies.

Local Attention We can allow each cell to densely attend to cells in its left window of size $O(\log_2 L)$ so that more local information, e.g. trend, can be leveraged for current step forecasting. Beyond the neighbor cells, we can resume our *LogSparse* attention strategy as shown in Figure 3(c).

Restart Attention Further, one can divide the whole input with length L into subsequences and set each subsequence length $L_{sub} \propto L$. For each of them, we apply the *LogSparse* attention strategy. One example is shown in Figure 3(d).

Employing *local attention* and *restart attention* won’t change the complexity of our sparse attention strategy but will create more paths and decrease the required number of edges in the path. Note that one can combine local attention and restart attention together.

5 Experiments

5.1 Synthetic datasets

To demonstrate Transformer’s capability to capture long-term dependencies, we conduct experiments on synthetic data. Specifically, we generate a piece-wise sinusoidal signals

$$f(x) = \begin{cases} A_1 \sin(\pi x/6) + 72 + N_x & x \in [0, 12), \\ A_2 \sin(\pi x/6) + 72 + N_x & x \in [12, 24), \\ A_3 \sin(\pi x/6) + 72 + N_x & x \in [24, t_0), \\ A_4 \sin(\pi x/12) + 72 + N_x & x \in [t_0, t_0 + 24). \end{cases}$$

⁴Applying other bases is trivial so we don’t discuss other bases here for simplicity and clarity.

A_1, A_2, A_3 are randomly generated by uniform distribution on $[0, 60]$, $A_4 = \max(A_1, A_2)$ and $N_x \sim \mathcal{N}(0, 1)$. Following the forecasting setting in Section 3, we aim to predict the last 24 steps given the previous t_0 data points. Intuitively, larger t_0 makes forecasting more difficult since the model is required to understand and remember the relation between A_1 and A_2 to make correct predictions after $t_0 - 24$ steps of irrelevant signals. Hence, we create 8 different datasets by varying the value of t_0 within $\{24, 48, 72, 96, 120, 144, 168, 192\}$. For each dataset, we generate 4.5K, 0.5K and 1K time series instances for training, validation and test set, respectively. An example time series with $t_0 = 96$ is shown in Figure 4(a).

In this experiment, we use a 3-layer canonical Transformer with standard self attention. For comparison, we employ DeepAR [3], an autoregressive model based on a 3-layer LSTM, as our baseline. Besides, to examine if larger capacity could improve performance of DeepAR, we also gradually increase its hidden size h as $\{20, 40, 80, 140, 200\}$. No further improvement is observed with larger hidden size. Following [3, 6], we evaluate both methods using ρ -quantile loss R_ρ with $\rho \in (0, 1)$,

$$R_\rho(\mathbf{x}, \hat{\mathbf{x}}) = \frac{2 \sum_{i,t} D_\rho(x_t^{(i)}, \hat{x}_t^{(i)})}{\sum_{i,t} |x_t^{(i)}|}, \quad D_\rho(x, \hat{x}) = (\rho - \mathbf{I}_{\{x \leq \hat{x}\}})(x - \hat{x}),$$

where \hat{x} is the empirical ρ -quantile of the predictive distribution and $\mathbf{I}_{\{x \leq \hat{x}\}}$ is an indicator function.

Figure 4(b) presents the performance of DeepAR and Transformer on the synthetic datasets. When $t_0 = 24$, both of them perform very well. But, as t_0 increases, especially when $t_0 \geq 96$, the performance of DeepAR drops significantly while Transformer keeps its accuracy, suggesting that Transformer can capture fairly long-term dependencies when LSTM fails to do so.

5.2 Real-world datasets

We further evaluate our model on several real-world datasets. The **electricity-f** (fine) dataset consists of electricity consumption of 370 customers recorded every 15 minutes and the **electricity-c** (coarse) dataset is the aggregated **electricity-f** by every 4 points, producing hourly electricity consumption. Similarly, the **traffic-f** (fine) dataset contains occupancy rates of 963 freeway in San Francisco recorded every 20 minutes and the **traffic-c** (coarse) contains hourly occupancy rates by averaging every 3 points in **traffic-f**. The **solar** dataset⁵ contains the solar power production records from January to August in 2006, which is sampled every hour from 137 PV plants in Alabama. The **wind**⁶ dataset contains daily estimates of 28 countries' energy potential from 1986 to 2015 as a percentage of a power plant's maximum output. The **M4-Hourly** contains 414 hourly time series from M4 competition [23].

Long-term and short-term forecasting We first show the effectiveness of canonical Transformer equipped with convolutional self attention in long-term and short-term forecasting in **electricity-c** and **traffic-c**. These two datasets exhibit both hourly and daily seasonal patterns. However, **traffic-c** demonstrates much greater difference between the patterns of weekdays and weekends compared to **electricity-c**. Hence, accurate forecasting in **traffic-c** dataset requires the model to capture both long- and short-term dependencies very well. As baselines, we use classical forecasting methods `auto.arima`, `ets` implemented in R's `forecast` package and the recent matrix

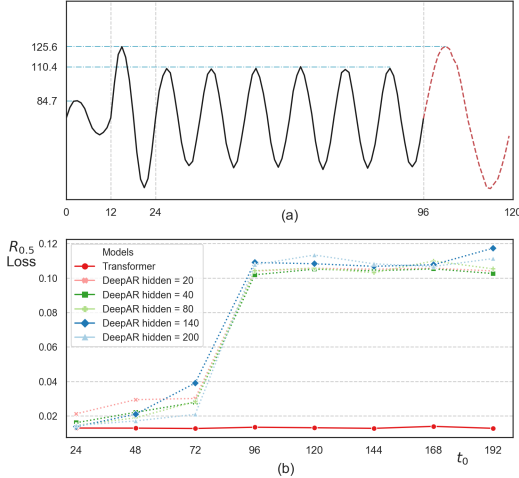


Figure 4: (a) An example time series with $t_0 = 96$. Black line is the conditional history while red dashed line is the target. (b) Performance comparison between DeepAR and canonical Transformer along with the growth of t_0 . The larger t_0 is, the longer dependencies the models need to capture for accurate forecasting.

⁵<https://www.nrel.gov/grid/solar-power-data.html>

⁶<https://www.kaggle.com/sohier/30-years-of-european-wind-generation>

Table 1: Results summary ($R_{0.5}/R_{0.9}$ -loss) of all methods. e-c and t-c represent electricity-c and traffic-c, respectively. In the 1st and 3rd row, we perform rolling-day prediction of 7 days while in the 2nd and 4th row, we directly forecast 7 days ahead. TRMF outputs points predictions, so we only report $R_{0.5}$. \diamond denotes results from [6].

	ARIMA	ETS	TRMF	DeepAR	DeepState	Ours
e- c_{1d}	0.154/0.102	0.101/0.077	0.084/-	0.075 $^\diamond$ /0.040 $^\diamond$	0.083 $^\diamond$ /0.056 $^\diamond$	0.059/0.028
e- c_{7d}	0.283 $^\diamond$ /0.109 $^\diamond$	0.121 $^\diamond$ /0.101 $^\diamond$	0.087/-	0.082/0.053	0.085 $^\diamond$ /0.052 $^\diamond$	0.080/0.039
t- c_{1d}	0.223/0.137	0.236/0.148	0.186/-	0.161 $^\diamond$ /0.099 $^\diamond$	0.167 $^\diamond$ /0.113 $^\diamond$	0.116/0.080
t- c_{7d}	0.492 $^\diamond$ /0.280 $^\diamond$	0.509 $^\diamond$ /0.529 $^\diamond$	0.202/-	0.179/0.105	0.168 $^\diamond$ /0.114 $^\diamond$	0.144/0.099

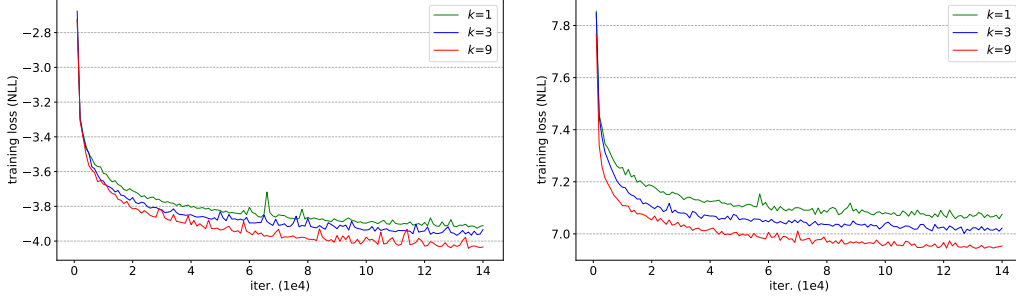


Figure 5: Training curve comparison among kernel size $k \in \{1, 3, 9\}$ in traffic-c (left) and electricity-c (right) dataset. Being aware of larger local context size, the model can achieve lower training error and converge faster.

factorization method TRMF [17], a RNN-based autoregressive model DeepAR and a RNN-based state space model DeepState [6]. For short-term forecasting, we evaluate rolling-day forecasts for seven days after training by following [7]. For long-term forecasting, we directly forecast 7 days ahead. As shown in Table 1, our models with convolutional self attention get better results in both long-term and short-term forecasting, especially in traffic-c dataset compared to strong baselines, partly due to the long-term dependency modeling ability of Transformer as shown in our synthetic data.

Convolutional self attention In this experiment, we conduct ablation study of our proposed convolutional self attention. We explore different kernel size $k \in \{1, 2, 3, 6, 9\}$ on the full attention model and fix all other settings. We still use rolling-day prediction for seven days on electricity-c and traffic-c datasets. The results of different kernel sizes are shown in Table 2. With larger k , the model can be aware of more local context information and help the model to forecast accurately and ease the training. Further, we plot the training loss of kernel size $k \in \{1, 3, 9\}$ in electricity-c and traffic-c datasets. We found that, in addition to getting better results, Transformer with convolutional self attention also converged faster and to lower error, as shown in Figure 5, proving that being aware of local context can ease the training process.

Table 2: Average $R_{0.5}/R_{0.9}$ -loss of different kernel sizes for rolling-day prediction of 7 days.

	$k = 1$	$k = 2$	$k = 3$	$k = 6$	$k = 9$
electricity- c_{1d}	0.064/0.030	0.058/0.029	0.059/0.030	0.057/0.032	0.059/0.028
traffic- c_{1d}	0.124/0.086	0.121/0.086	0.121/0.086	0.121/0.083	0.116/0.080

Sparse attention Further, we compare our proposed LogSparse Transformer to the full attention counterpart on fine-grained datasets, electricity-f and traffic-f. Note that time series in these two datasets have much longer periods and are noisier comparing to electricity-c and traffic-c. We first compare them under the same memory budget. For electricity-f dataset, we choose $L_{e_1} = 768$ with subsequence length $L_{e_1}/8$ and local attention length $\log_2(L_{e_1}/8)$ in each subsequence for our sparse attention model and $L_{e_2} = 284$ in the full attention counterpart. For traffic-f dataset, we select $L_{t_1} = 576$ with subsequence length $L_{t_1}/8$ and local attention length

Table 3: Average $R_{0.5}/R_{0.9}$ -loss comparisons between sparse attention and full attention models with/without convolutional self attention by rolling-day prediction of 7 days. “Full” means models are trained with full attention while “Sparse” means they are trained with our sparse attention strategy. “+ Conv” means models are equipped with convolutional self attention with kernel size $k = 6$.

Constraint	Dataset	Full	Sparse	Full + Conv	Sparse + Conv
Memory	electricity-f _{1d}	0.107/0.047	0.105/0.095	0.083/0.046	0.083/0.053
	traffic-f _{1d}	0.317/0.306	0.196/0.105	0.205/0.107	0.134/0.103
Length	electricity-f _{1d}	0.091/0.047	0.105/0.095	0.079/0.044	0.083/0.053
	traffic-f _{1d}	0.155/0.109	0.196/0.105	0.155/0.114	0.134/0.103

$\log_2(L_{t_1}/8)$ in each subsequence for our sparse attention model, and $L_{t_2} = 238$ in the full attention counterpart. The calculation of memory usage and other details can be found in Appendix A.4. We conduct experiments on aforementioned sparse and full attention models with/without convolutional self attention on both datasets. By following such settings, we summarize our results in Table 3 (Upper part). No matter equipped with convolutional self attention or not, our sparse attention models achieve competitive results on electricity-f but much better results on traffic-f compared to its full attention counterparts. Such performance gain on traffic-f could be the result of the dataset’s stronger long-term dependencies and our sparse model’s better capability of capturing these dependencies, which, under the same memory budget, the full attention model cannot match. In addition, both sparse and full attention models benefit from convolutional self attention, proving its effectiveness.

To explore how well our sparse attention model performs compared to full attention model with the same input length, we set $L_{e_2} = L_{e_1} = 768$ and $L_{t_2} = L_{t_1} = 576$ on electricity-f and traffic-f, respectively. Note that our sparse attention models use much less memory. The results of their comparisons are summarized in Table 3 (Lower part). As one expects, canonical full attention Transformer outperforms our sparse attention counterpart when both of them are not equipped with convolutional self attention. However, our sparse Transformer with convolutional self attention can get comparable results on electricity-f and, more interestingly, even better on traffic-f but with much less memory usage. We argue that in some cases sparse attention may help the model learn the most useful patterns in the noisy data and leave less useful things alone, hence, may get better generalization on test data compared to its full attention counterpart.

Further Exploration In our last experiment, we evaluate how our methods perform on datasets with various granularities compared to our baselines. All datasets except M4-Hourly are evaluated by rolling window 7 times since the test set of M4-Hourly has been provided. The results are shown in Table 4. These results further show that our method achieves the best performance overall.

Table 4: $R_{0.5}/R_{0.9}$ -loss of datasets with various granularities. The subscript of each dataset presents the forecasting horizon (days). TRMF is not applicable for M4-Hourly_{2d} and we leave it blank. For other datasets, TRMF outputs points predictions, so we only report $R_{0.5}$. $^\diamond$ denotes results from [10].

	electricity-f _{1d}	traffic-f _{1d}	solar _{1d}	M4-Hourly _{2d}	wind _{30d}
TRMF	0.094/-	0.213/-	0.241/-	-/-	0.311/-
DeepAR	0.082/0.063	0.230/0.150	0.222/0.093	0.090 $^\diamond$ /0.030 $^\diamond$	0.286/0.116
Ours	0.079/0.044	0.140/0.103	0.219 /0.085	0.054 /0.022	0.288/0.113

6 Conclusion

In this paper, we propose to apply Transformer in time series forecasting. Our experiments on both synthetic data and real datasets suggest that Transformer can capture long-term dependencies while LSTM may suffer. We also showed, on real-world datasets, that the proposed convolutional self attention further improves Transformer’s performance and achieves state-of-the-art in different settings in comparison with recent RNN-based methods, a matrix factorization method, as well as classic statistical approaches. In addition, with the same memory budget, our sparse attention models can

achieve better results on data with long-term dependencies. Exploring better sparsity in self attention and extending our method to better fit small datasets are our future research directions.

References

- [1] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. In *Advances in neural information processing systems*, pages 5998–6008, 2017.
- [2] James Durbin and Siem Jan Koopman. *Time series analysis by state space methods*. Oxford university press, 2012.
- [3] Valentin Flunkert, David Salinas, and Jan Gasthaus. Deepar: Probabilistic forecasting with autoregressive recurrent networks. *arXiv preprint arXiv:1704.04110*, 2017.
- [4] Alex Graves. Generating sequences with recurrent neural networks. *arXiv preprint arXiv:1308.0850*, 2013.
- [5] Ilya Sutskever, Oriol Vinyals, and Quoc V Le. Sequence to sequence learning with neural networks. In *Advances in neural information processing systems*, pages 3104–3112, 2014.
- [6] Syama Sundar Rangapuram, Matthias W Seeger, Jan Gasthaus, Lorenzo Stella, Yuyang Wang, and Tim Januschowski. Deep state space models for time series forecasting. In *Advances in Neural Information Processing Systems*, pages 7785–7794, 2018.
- [7] Guokun Lai, Wei-Cheng Chang, Yiming Yang, and Hanxiao Liu. Modeling long-and short-term temporal patterns with deep neural networks. In *The 41st International ACM SIGIR Conference on Research & Development in Information Retrieval*, pages 95–104. ACM, 2018.
- [8] Rose Yu, Stephan Zheng, Anima Anandkumar, and Yisong Yue. Long-term forecasting using tensor-train rnns. *arXiv preprint arXiv:1711.00073*, 2017.
- [9] Danielle C Maddix, Yuyang Wang, and Alex Smola. Deep factors with gaussian processes for forecasting. *arXiv preprint arXiv:1812.00098*, 2018.
- [10] Razvan Pascanu, Tomas Mikolov, and Yoshua Bengio. On the difficulty of training recurrent neural networks. In *International conference on machine learning*, pages 1310–1318, 2013.
- [11] Sepp Hochreiter and Jürgen Schmidhuber. Long short-term memory. *Neural computation*, 9(8):1735–1780, 1997.
- [12] Kyunghyun Cho, Bart Van Merriënboer, Dzmitry Bahdanau, and Yoshua Bengio. On the properties of neural machine translation: Encoder-decoder approaches. *arXiv preprint arXiv:1409.1259*, 2014.
- [13] Urvashi Khandelwal, He He, Peng Qi, and Dan Jurafsky. Sharp nearby, fuzzy far away: How neural language models use context. *arXiv preprint arXiv:1805.04623*, 2018.
- [14] Ankur P Parikh, Oscar Täckström, Dipanjan Das, and Jakob Uszkoreit. A decomposable attention model for natural language inference. *arXiv preprint arXiv:1606.01933*, 2016.
- [15] George EP Box and Gwilym M Jenkins. Some recent advances in forecasting and control. *Journal of the Royal Statistical Society. Series C (Applied Statistics)*, 17(2):91–109, 1968.
- [16] George EP Box, Gwilym M Jenkins, Gregory C Reinsel, and Greta M Ljung. *Time series analysis: forecasting and control*. John Wiley & Sons, 2015.
- [17] Hsiang-Fu Yu, Nikhil Rao, and Inderjit S Dhillon. Temporal regularized matrix factorization for high-dimensional time series prediction. In *Advances in neural information processing systems*, pages 847–855, 2016.
- [18] Nicolas Chapados. Effective bayesian modeling of groups of related count time series. *arXiv preprint arXiv:1405.3738*, 2014.
- [19] Ruofeng Wen, Kari Torkkola, Balakrishnan Narayanaswamy, and Dhruv Madeka. A multi-horizon quantile recurrent forecaster. *arXiv preprint arXiv:1711.11053*, 2017.
- [20] Cheng-Zhi Anna Huang, Ashish Vaswani, Jakob Uszkoreit, Noam Shazeer, Curtis Hawthorne, Andrew M Dai, Matthew D Hoffman, and Douglas Eck. An improved relative self-attention mechanism for transformer with application to music generation. *arXiv preprint arXiv:1809.04281*, 2018.

- [21] Daniel Povey, Hossein Hadian, Pegah Ghahremani, Ke Li, and Sanjeev Khudanpur. A time-restricted self-attention layer for asr. In *2018 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, pages 5874–5878. IEEE, 2018.
- [22] Niki Parmar, Ashish Vaswani, Jakob Uszkoreit, Łukasz Kaiser, Noam Shazeer, Alexander Ku, and Dustin Tran. Image transformer. *arXiv preprint arXiv:1802.05751*, 2018.
- [23] Spyros Makridakis, Evangelos Spiliotis, and Vassilios Assimakopoulos. The m4 competition: Results, findings, conclusion and way forward. *International Journal of Forecasting*, 34(4):802–808, 2018.
- [24] Tomaso Poggio, Hrushikesh Mhaskar, Lorenzo Rosasco, Brando Miranda, and Qianli Liao. Why and when can deep-but not shallow-networks avoid the curse of dimensionality: a review. *International Journal of Automation and Computing*, 14(5):503–519, 2017.
- [25] Kunihiro Fukushima. Neocognitron: A self-organizing neural network model for a mechanism of pattern recognition unaffected by shift in position. *Biological cybernetics*, 36(4):193–202, 1980.
- [26] Hrushikesh N Mhaskar and Tomaso Poggio. Deep vs. shallow networks: An approximation theory perspective. *Analysis and Applications*, 14(06):829–848, 2016.
- [27] Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.
- [28] Aäron Van Den Oord, Sander Dieleman, Heiga Zen, Karen Simonyan, Oriol Vinyals, Alex Graves, Nal Kalchbrenner, Andrew W Senior, and Koray Kavukcuoglu. Wavenet: A generative model for raw audio. *SSW*, 125, 2016.
- [29] Anastasia Borovykh, Sander Bohte, and Cornelis W Oosterlee. Conditional time series forecasting with convolutional neural networks. *arXiv preprint arXiv:1703.04691*, 2017.
- [30] Tim Cooijmans, Nicolas Ballas, César Laurent, Çağlar Gülçehre, and Aaron Courville. Recurrent batch normalization. *arXiv preprint arXiv:1603.09025*, 2016.
- [31] Rose Yu, Yaguang Li, Cyrus Shahabi, Ugur Demiryurek, and Yan Liu. Deep learning: A generic approach for extreme condition traffic forecasting. In *Proceedings of the 2017 SIAM International Conference on Data Mining*, pages 777–785. SIAM, 2017.
- [32] Guoqiang Zhang, B Eddy Patuwo, and Michael Y Hu. Forecasting with artificial neural networks:: The state of the art. *International journal of forecasting*, 14(1):35–62, 1998.
- [33] Rewon Child, Scott Gray, Alec Radford, and Ilya Sutskever. Generating long sequences with sparse transformers. *arXiv preprint arXiv:1904.10509*, 2019.
- [34] Peter J Liu, Mohammad Saleh, Etienne Pot, Ben Goodrich, Ryan Sepassi, Łukasz Kaiser, and Noam Shazeer. Generating wikipedia by summarizing long sequences. *arXiv preprint arXiv:1801.10198*, 2018.
- [35] Alec Radford, Karthik Narasimhan, Tim Salimans, and Ilya Sutskever. Improving language understanding by generative pre-training. URL https://s3-us-west-2.amazonaws.com/openai-assets/research-covers/languageunsupervised/language_understanding_paper.pdf, 2018.
- [36] Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. Bert: Pre-training of deep bidirectional transformers for language understanding. *arXiv preprint arXiv:1810.04805*, 2018.
- [37] Rewon Child, Scott Gray, Alec Radford, and Ilya Sutskever. Generating long sequences with sparse transformers. *arXiv preprint arXiv:1904.10509*, 2019.
- [38] Nikolay Laptev, Jason Yosinski, Li Erran Li, and Slawek Smyl. Time-series extreme event forecasting with neural networks at uber. In *International Conference on Machine Learning*, number 34, pages 1–5, 2017.

A Supplementary Materials

A.1 Proof of Theorem 1

Proof. According to the attention strategy in *LogSparse Transformer*, in each layer, cell l could attend to the cells with indices in $I_l^k = \{l - 2^{\lfloor \log_2 l \rfloor}, l - 2^{\lfloor \log_2 l \rfloor - 1}, l - 2^{\lfloor \log_2 l \rfloor - 2}, \dots, l - 2^0, l\}$. To ensure that every cell receives the information from all its previous cells and its own, the number of stacked layers \tilde{k}_l should satisfy that $S_l^{\tilde{k}_l} = \{j : j \leq l\}$ for $l = 1, \dots, L$. That is, $\forall l$ and $j \leq l$, there is a directed path $P_{jl} = (j, p_1, p_2, \dots, l)$ with \tilde{k}_l edges, where $j \in I_{p_1}^1, p_1 \in I_{p_2}^2, \dots, p_{\tilde{k}_l-1} \in I_l^{\tilde{k}_l}$. We prove the theorem by constructing a path from cell j to cell l , with length (number of edges) no larger than $\lfloor \log_2 l \rfloor + 1$. Case $j = l$ is trivial, we only need to consider $j < l$ case. Consider the binary representation of $l - j$, $l - j = \sum_{m=0}^{\lfloor \log_2(l-j) \rfloor} b_m 2^m$, where $b_m \in \{0, 1\}$. Suppose $\{m_{sub}\}$ is the subsequence $\{m | 0 \leq m \leq \lfloor \log_2(l-j) \rfloor, b_m = 1\}$ and m_p is the p_{th} element of $\{m_{sub}\}$. A feasible path from j to l is $P_{jl} = \{j, j + 2^{m_0}, j + 2^{m_0} + 2^{m_1}, \dots, l\}$. The length of this path is $|\{m_{sub}\}|$, which is no larger than $\lfloor \log_2(l-j) \rfloor + 1$. So

$$\min \{\tilde{k}_l | S_l^{\tilde{k}_l} = \{j : j \leq l\}\} \leq \max_{\{j | j < l\}} \lfloor \log_2(l-j) \rfloor + 1 \leq \lfloor \log_2 l \rfloor + 1.$$

Furthermore, by reordering $\{m_{sub}\}$, we can generate multiple different paths from cell j to cell l . The number of feasible paths increases at a rate of $O(\lfloor \log_2(l-j) \rfloor!)$ along with l . \square

A.2 Training

Table 5: Dataset statistics. "T", "M" and "S" represent the length, number and sample rate of the time series, respectively.

	electricity-c	electricity-f	traffic-c	traffic-f	wind	solar	M4-Hourly
T	32304	129216	4049	12435	10957	5832	748/1008
M	370	370	963	963	28	137	414
S	1 hour	15 mins	1 hour	20 mins	1 day	1 hour	1 hour

Similar to [3], our network directly predicts the parameters of the probability distribution for the next time point. In our experiments, we use Gaussian likelihood since our training datasets are real-valued data. Note that one can also use other likelihood models, e.g. negative-binomial likelihood for positive count data.

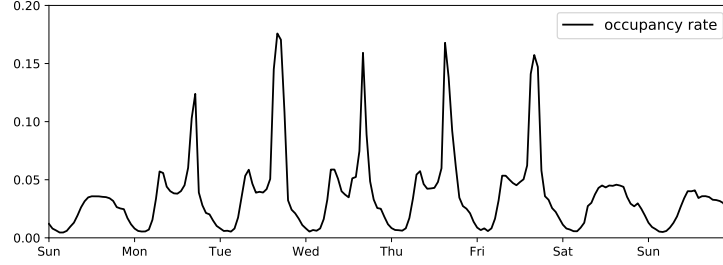
To learn the model, we are given a time series dataset $\{\mathbf{z}_{i,1:T}\}_{i=1}^M$ and its associated covariates $\{\mathbf{x}_{i,1:T}\}_{i=1}^M$, where T is the length of all available observations and M is the number of different time series. The dataset statistics is shown as Table 5. Following [3], we create training instances by selecting windows with fixed history length t_0 and forecasting horizon τ but varying the start point of forecasting from each of the original long time series. Note that during selecting training windows, data in the test set can never be accessed. As a result, we get a training dataset with N sliding windows $\{\mathbf{z}_{i,1:t_0+\tau}, \mathbf{x}_{i,1:t_0+\tau}\}_{i=1}^N$. During training, we use Adam optimizer [27] with early stopping to maximize the log-likelihood of each training instance.

For **electricity-c** and **traffic-c**, we take 500K training windows while for **electricity-f** and **traffic-f**, we select 200K and 125K training windows, respectively. For **wind**, **M4-Hourly** and **solar**, we choose 10K, 50K and 50K training windows, respectively. We sample and scale training windows following [3]. We use datetime information, e.g. month, weekday, hour, etc, as our time-based covariate vectors.

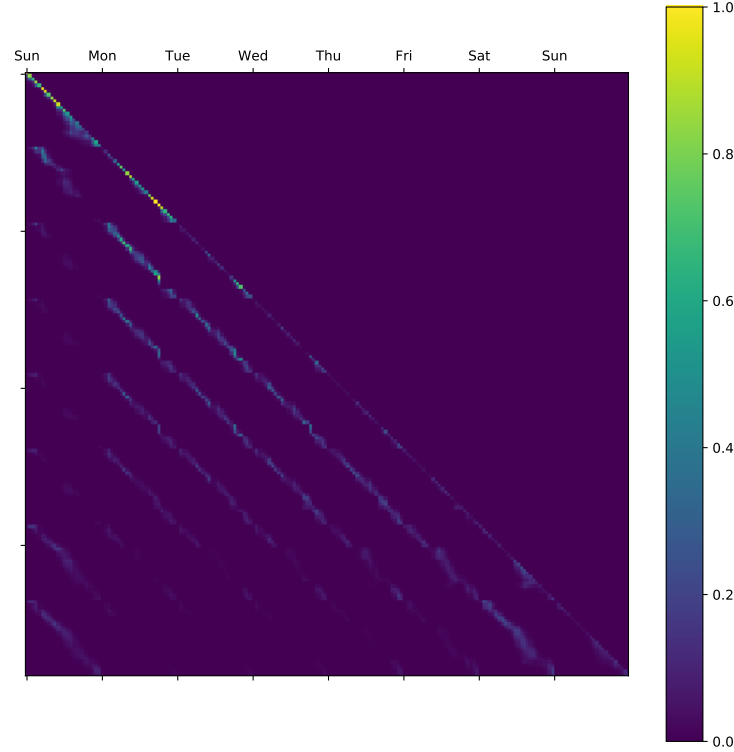
For our Transformer model, we don't tune hyperparameters heavily. All of them use $H = 8$ heads, $d_k = d_v = 20$. For other hyperparameters (e.g. learning rate and layers), a grid-search is used to find the best value. To do so, the data before the forecast start time is used as the training set and split into two partitions. For each hyper-parameter candidate, we fit our model on the first partition of the training set containing 90% of the data and we pick the one that has the minimal negative log-likelihood on the remaining 10%. All models are trained on GTX 1080 Ti GPUs.

A.3 Evaluation

We draw 200 samples to evaluate our method by the standard quantile loss. For **electricity-c**, **electricity-f**, **traffic-c**, **traffic-f** and **solar**, we leave the last 7 days as test sets. For **wind**, last 210 days are left as test set. For **M4-Hourly**, its training and test sets are already provided. Once the best sets of hyper parameters are found by aforementioned method, the evaluation metrics ($R_{0.5}$ and $R_{0.9}$) are then applied on the test sets.



(a)



(b)

Figure 6: (a): An example time series window in `traffic-c` dataset. (b): Corresponding learned attention patterns in the masked attention matrix of a head within the last layer.

A.4 Calculation of memory cost

For `electricity-f` dataset, we choose $L_{e_1} = 768$ with subsequence length $L_{sub}^{e_1} = L_{e_1}/8$ and local attention length $L_{loc}^{e_1} = \log_2(L_{e_1}/8)$ in each subsequence for our sparse attention model, and $L_{e_2} = 284$ in its full attention counterpart. We stack the same layers on both sparse attention and full attention models. Hence, we can guarantee that their memory usage is the same if they use the same memory in every layer. In sparse attention with local window, every cell attends to $2 * \log_2(L_{e_1}/8)$ cells in each subsequence. Since we have $8 = L_{e_1}/L_{sub}^{e_1}$ subsequences in total, then we get the memory usage of sparse attention in each layer is $L_{e_1} * 2 * \log_2(L_{sub}^{e_1}) * L_{e_1}/L_{sub}^{e_1} = 16 * L_{e_1} * \log_2(L_{sub}^{e_1}) = L_{e_2}^2$. Following such setting, the memory usage of the sparse attention model is comparable to that of the full attention model. For `traffic-f` dataset, one can follow the same procedure to check the memory usage.

A.5 Visualization of attention matrix

Here we show an example of learned attention patterns in the masked attention matrix of a head within canonical Transformer's last layer on `traffic-c` dataset. Figure 6 (a) is a time series window containing 8 days in `traffic-c`. The time series obviously demonstrates both hourly and daily patterns. From its corresponding

masked attention matrix, as shown in Figure 6 (b), we can see that for points in weekdays, they heavily attend to previous cells (including itself) at the same time in weekdays while points on weekends tend to only attend to previous cells (including itself) at the same time on weekends. Hence, the model automatically learned both hourly and daily seasonality, which is the key to accurate forecasting.