Transformers for Time Series Forecasting

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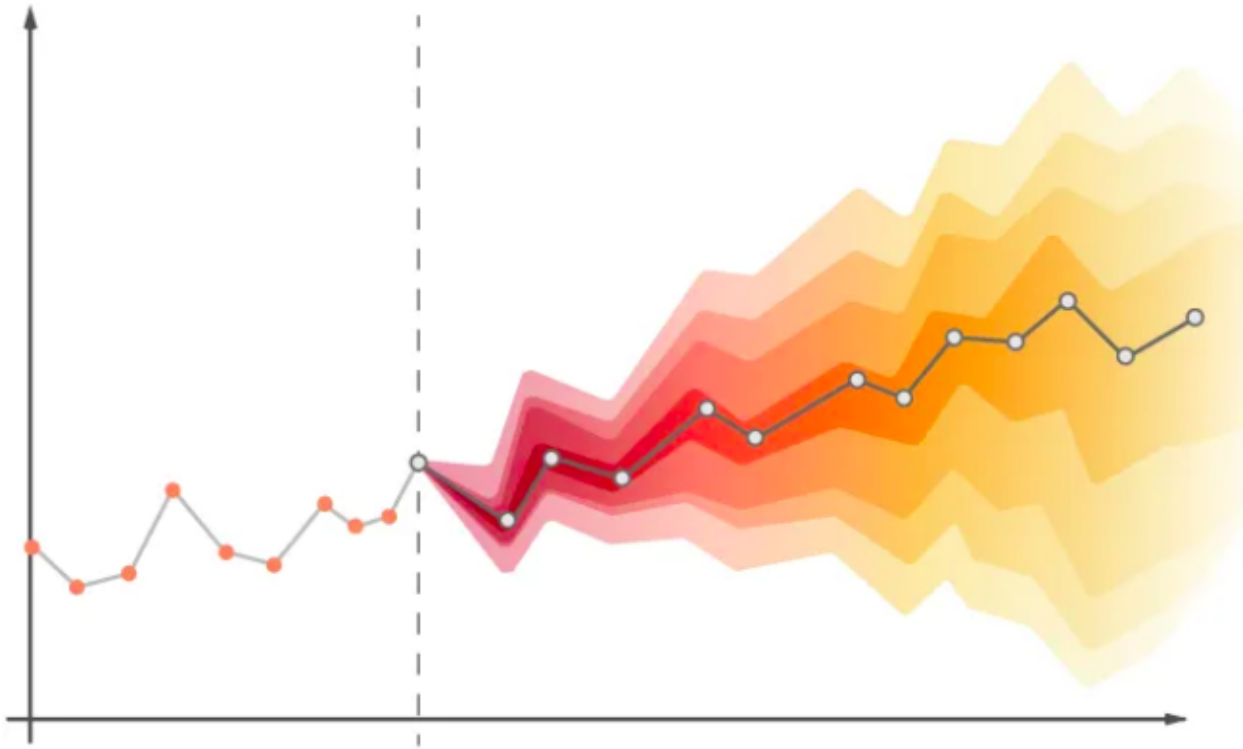
Contents

1. The TSF Problem

Time series forecasting (TSF) is the task of predicting future values of a given sequence based on previously observed values.



The TSF problem may be essentially identified by the following aspects:

- **Prediction objective**: point forecasting vs probabilistic forecasting
- **Forecast horizon**: short-term vs long-term forecasting
- **Input-Output dimension**: univariate vs multivariate forecasting
- **Forecasting task**: single-step vs multi-step forecasting

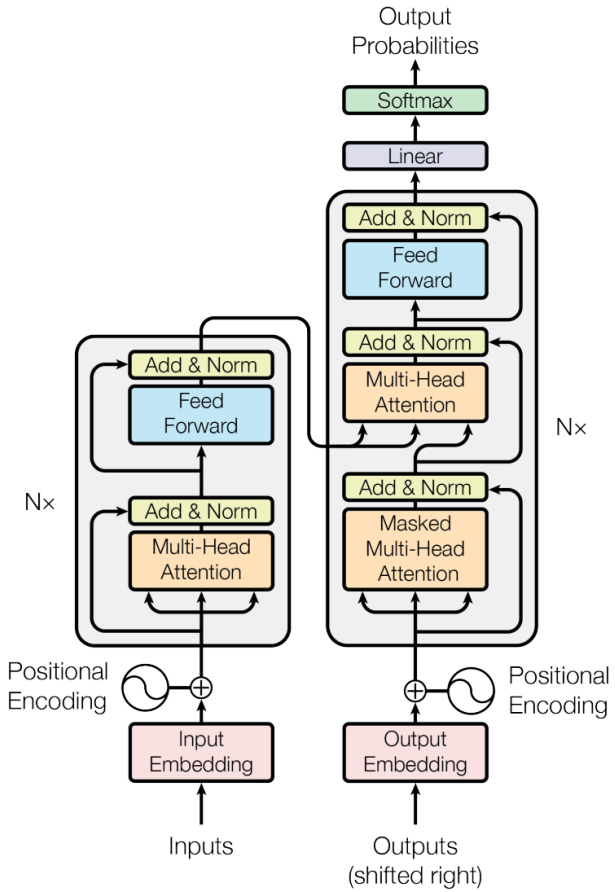
The TSF problem is usually faced with statistical models (ARIMA, ETS) or deep learning models (RNN, LSTM).

The main challenges of the TSF problem are:

- **uncertainty** increases as the forecast horizon increases
- difficulty in capturing **multiple complex patterns** over time
- difficulty in capturing **long-term dependencies** (critical for long-term forecasting)
- difficulty to handle **long input sequences**

2. Vanilla Transformer

- Based on Encoder-Decoder architecture
- Uses self-attention mechanism to access any part of the sequence history
- Positional encoding allows to account for element positions
- Residual connections and layer normalization help to stabilize the learning process
- Each encoder and decoder layer is composed of a self-attention layer and a feed-forward layer



Can vanilla Transformers be used for TSF?

The TSF problem can be seen as a sequence learning problem such as machine translation.

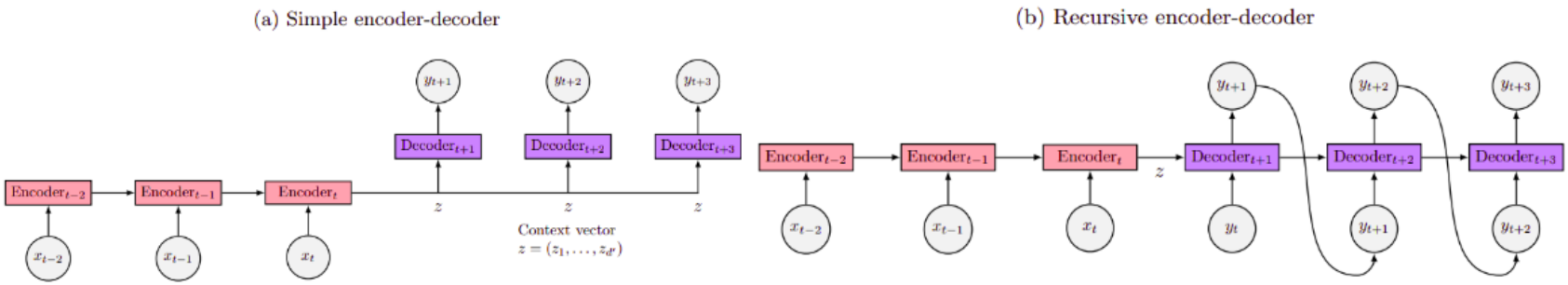
Main ingredients allowing to use vanilla Transformers for TSF:

- **Multi-head Self-attention** mechanism allows to access any part of the sequence history, capturing both short-term and long-term dependencies (but it is invariant to the order of elements in a sequence)
- **Positional encoding** allows to account for the sequence ordering
- **Masked self-attention** allows to avoid information leakage from future

Can vanilla Transformers be used for TSF?

Just few changes are needed to adapt Transformers to TSF:

- **Remove the final activation** function (softmax) from the output layer and set the dimension of the linear layer equal to the forecasting horizon
- **Adapt the structure** to the desired forecasting task (single-step or multi-step)



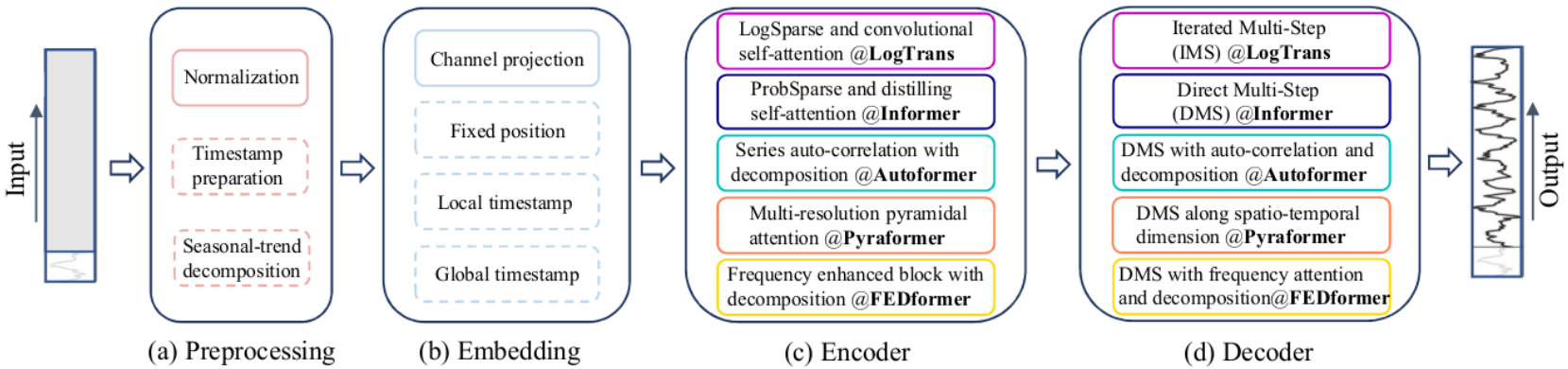
Problems with vanilla Transformers

- **Positional encoding**: only the order in which two elements occur is taken into account, but their temporal distance is not
- **Computational complexity**: given a sequence of length L, the time and memory burden is $O(L^2)$, making it difficult to learn patterns in long time series
- **Simple Architecture**: the architecture does not include any component of typical importance in TSF (e.g. autocorrelation, decomposition, recurrent layers, etc.)

3. TSF Transformers

Transformers are **very appealing for long-term TSF** due to their ability to learn long-range dependencies.

Many solutions have been proposed to adapt Transformers to TSF, mainly in the direction to adopt more efficient attention and expand the architecture.

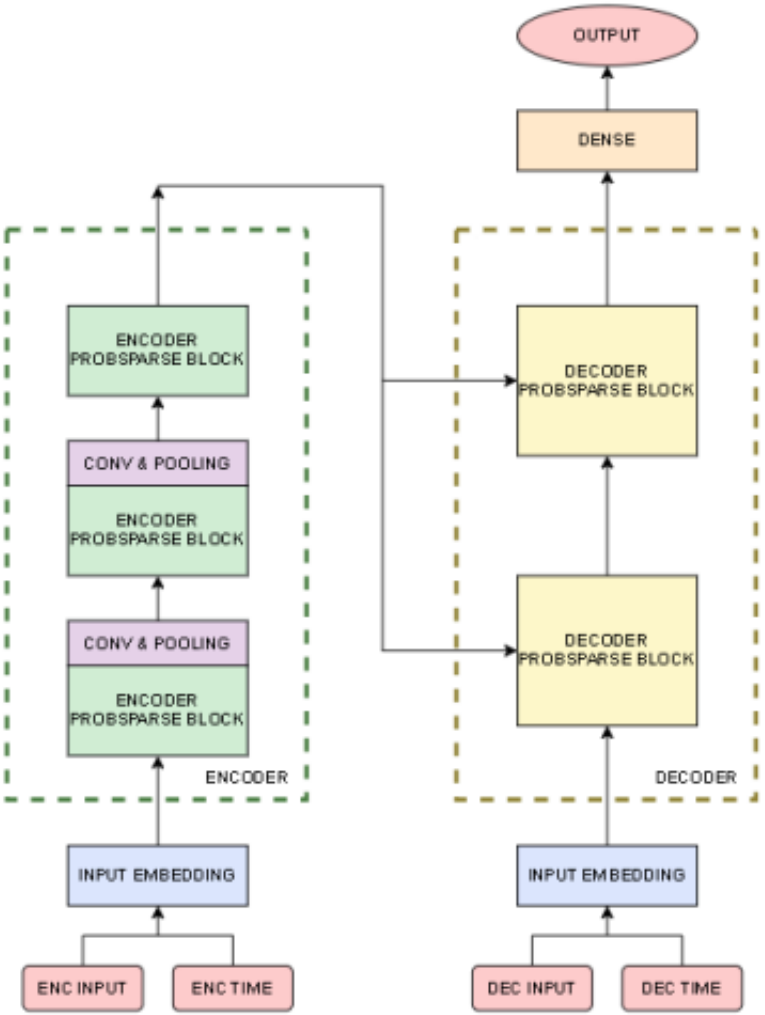


Informer

Informer employs two major improvements:

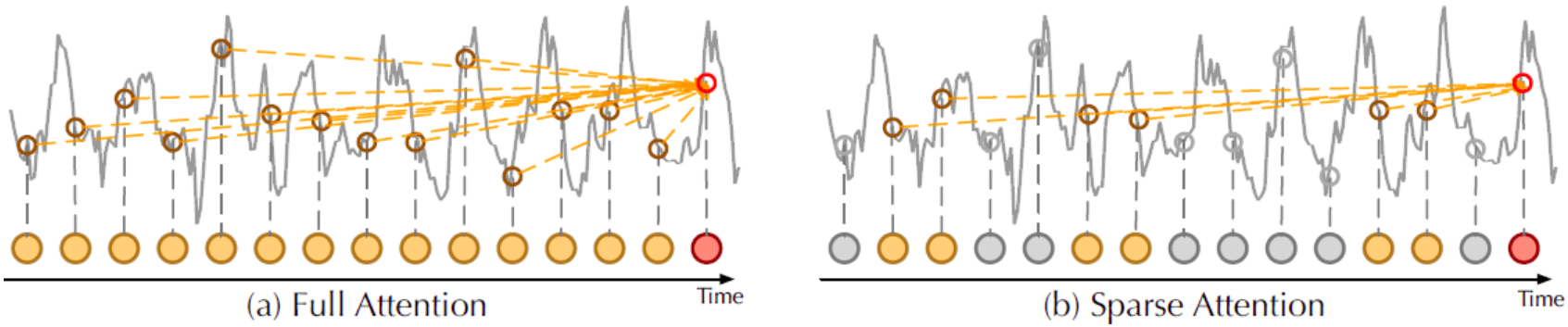
- **ProbSparse Attention Mechanism**, which replaces the standard self-attention used in the vanilla transformer with a sparse attention so to achieve $O(LlogL)$ complexity
- **Distilling Module**, which reduces the input size between encoder layers into its half slice, removing redundancy and reducing the computational burden

Informer - Architecture



Informer - ProbSparse Attention

The main idea of **ProbSparse** is that just a small subset of queries ("active") effectively contribute to the attention mechanism. The ProbSparse attention selects the "active" queries, and creates a reduced query matrix, which is then used to calculate the attention weights, reaching $O(LlogL)$ complexity.



In practice, the KL divergence is used to define a sparsity measure, since active queries distribution diverges from uniform, and a random sample of K is used to obtain a sparse matrix of keys.

Informer - Convolution Layers

Because of the ProbSparse self-attention, the encoder's feature map has some redundancy that can be removed. The **distilling** operation is used to reduce the input size between encoder layers.

In practice, Informer's distilling operation just adds **1D convolution layers**, along the time dimension, with max pooling between each of the encoder layers.

$$X_{n+1} = MaxPool(\, ELU(\, Conv1d(Xn)\,)\,)$$

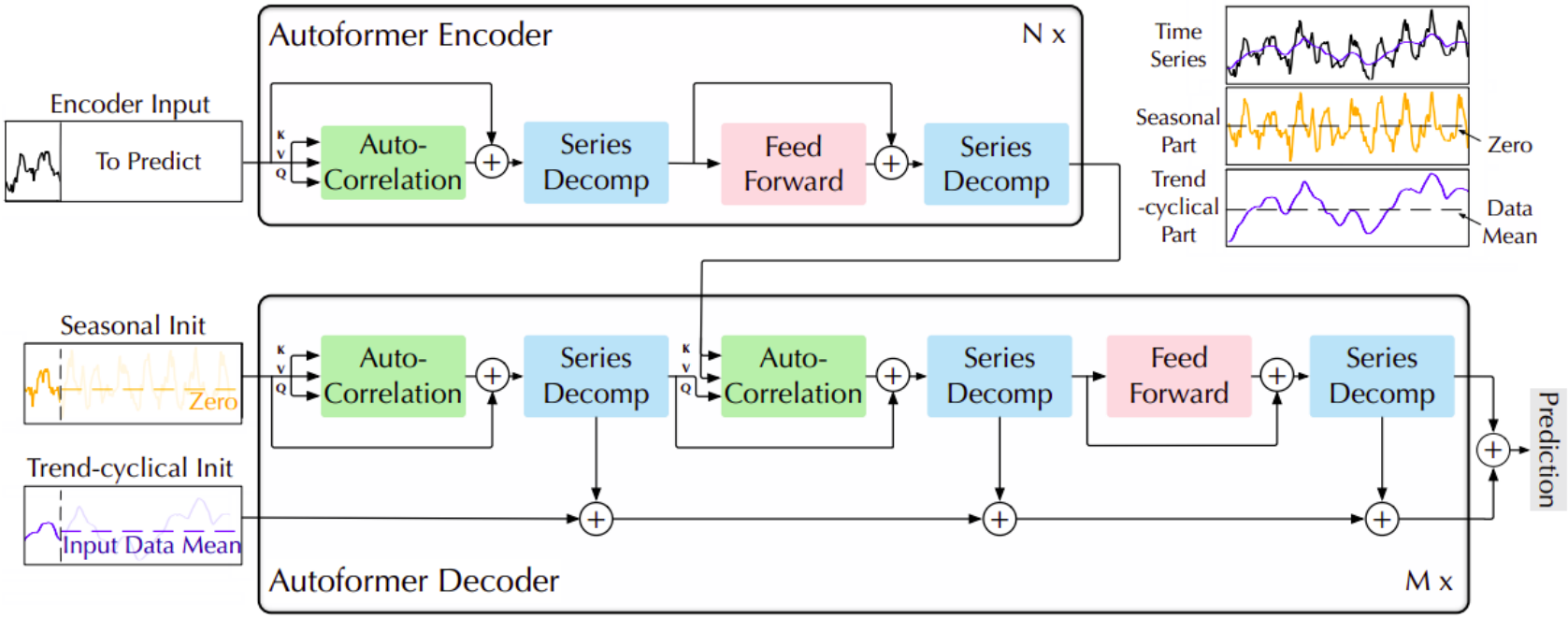
This reduces by half the size of the data between the feature space, improving both memory and computational efficiency.

Autoformer

Autoformer builds upon two traditional time series analysis methods:

- **Decomposition Layer**, which allows to decompose the time series into seasonality and trend-cycle components, enhancing the model's ability to capture these components accurately
- **Autocorrelation Attention Mechanism**, which replaces the standard self-attention used in the vanilla transformer with an autocorrelation mechanism, allowing to capture the temporal dependencies in the frequency domain and achieving $O(LlogL)$ complexity

Autoformer - Architecture



Autoformer - Decomposition Layer

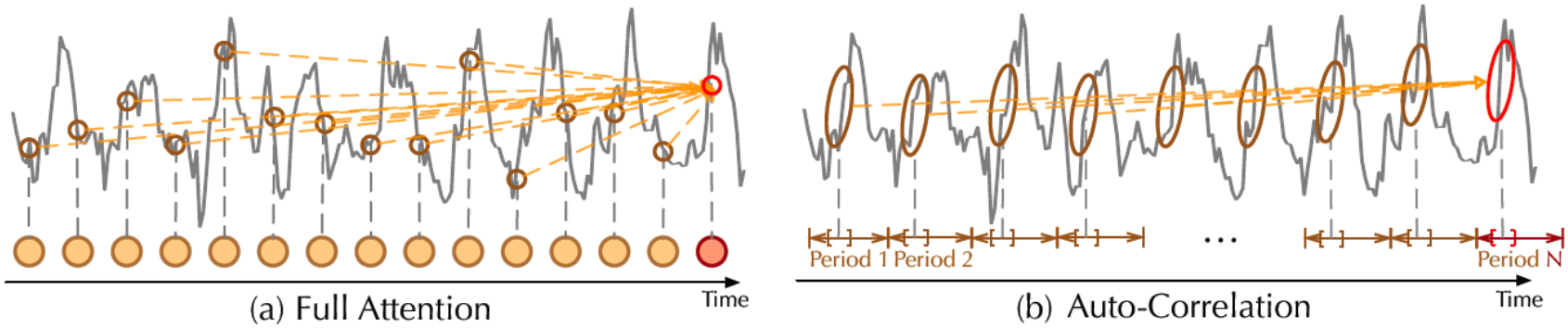
Autoformer incorporates **decomposition blocks** as an inner operation of the model.

Encoder and decoder use decomposition blocks to extract and aggregate the trend-cyclical and seasonal components from the series progressively, so to make raw data easier to predict.

For an input series X_t with length L, the decomposition layer returns X_{trend} and $X_{seasonal}$, both of length L. In practice, X_{trend} is extracted using some form of moving-average and $X_{seasonal}$ is then obtained by difference.

Autoformer - Autocorrelation Attention

Autoformer uses **autocorrelation within the self-attention** layer, extracting frequency-based dependencies from (Q, K). The autocorrelation block measures the **time-delay similarity** and aggregates the top n similar sub-series to reduce complexity.



In practice, autocorrelation of the queries and keys for all lags is calculated at once by Fast Fourier Transform, so to achieve $O(LlogL)$ time complexity (similar to Informer).

4. Conclusions

Conclusions

- Transformers are very appealing for TSF due to their ability to learn long-range dependencies
- Many solutions have been proposed to adapt Transformers to TSF, mainly in the direction to adopt more efficient attention and expand the architecture
- Informer and Autoformer are two of the most successful solutions, and they both achieve $O(LlogL)$ complexity
- Empirical results show that Transformer models are able to reach SOTA performance in TSF, and are among the best methods for long-term forecasting

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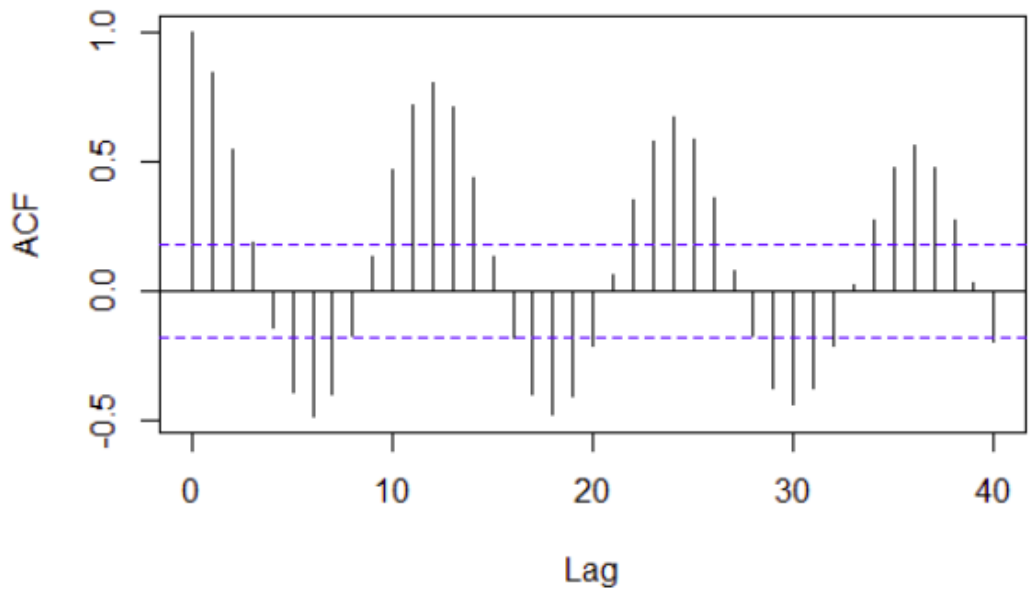
Thank you!

Appendix

Autocorrelation

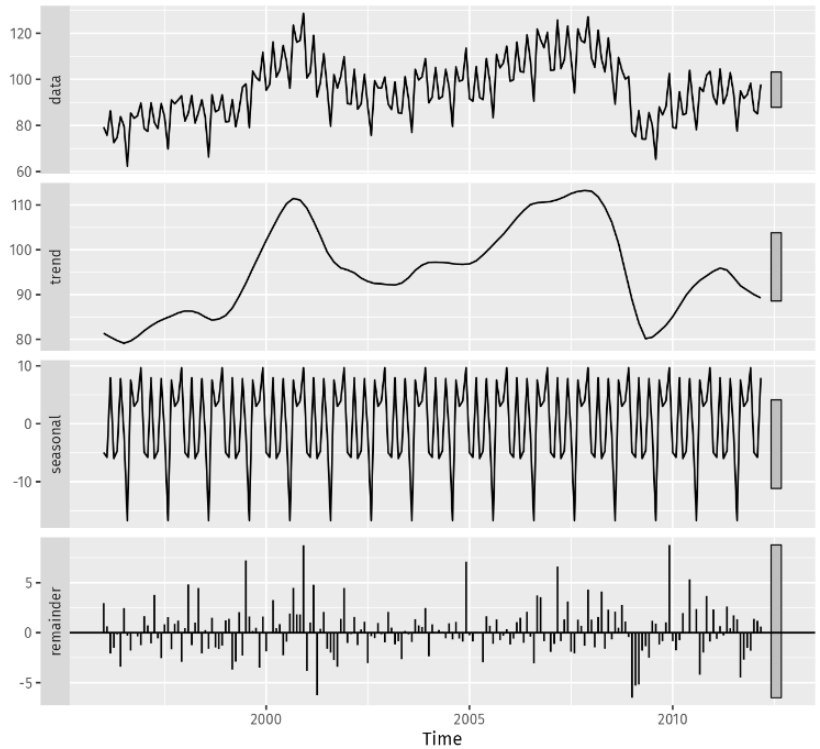
In theory, given a time lag τ, **autocorrelation** for a single discrete variable Y is used to measure the "relationship" between the variable at time t to its past value at time $t - \tau$.

$$Autocorrelation(\tau) = \mathcal{R}(\tau) = Corr(Y_t, Y_{t-\tau})$$



Time Series Decomposition

In time series analysis, **decomposition** is a method of breaking down a time series into three systematic components: **trend-cycle**, **seasonal variations**, and **random fluctuations**.



Time2Vec Embedding

Time2Vec is a method of encoding time information into a vector and has three important properties:

1. **Periodicity**, captures periodic and non-periodic patterns
2. **Invariant to time rescaling**
3. **Model-agnostic**, can be combined with many models

For a given scalar time τ, $t2v$ of τ is defined as:

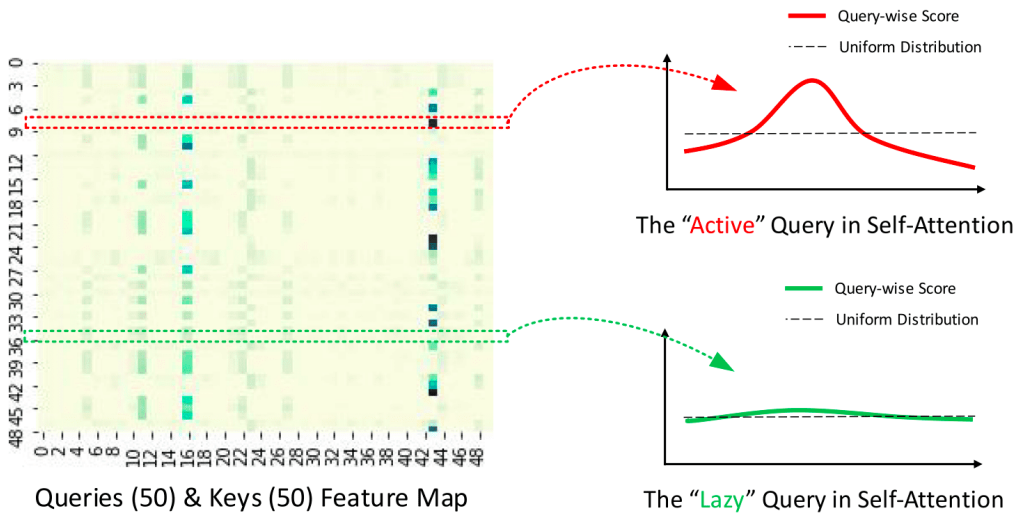
$$t2v(\tau)[i] = \begin{cases} \omega_i \tau + \phi_i, & \text{if } i = 0 \\ \mathcal{F}(\omega_i \tau + \phi_i), & \text{if } 1 \leq i \leq k \end{cases}$$

where $\mathcal{F}$ is a periodic activation function, and ω_i and ϕ_i are learnable parameters.

Informer - ProbSparse Attention

$$Attention(Q, K, V) = softmax(\frac{Q_{reduced} K^T}{\sqrt{d_k}})V$$

$$M(q_i, K) = \max_j \frac{q_i K_j^T}{\sqrt{d_k}} - \frac{1}{L_k} \sum_{j=1}^{L_k} \frac{q_i K_j^T}{\sqrt{d_k}}$$



Autoformer - Autocorrelation Attention

$$\tau_1, ..., \tau_k = arg\ Top - k\ (\mathcal{R}_{Q,K}(\tau))$$

$$Attention(Q, K, V) = \sum_{i=1}^{k} Roll(V, \tau_i) \times softmax(\mathcal{R}_{Q,K}(\tau_i))$$