

Empirical Assessment of Transformer Based Neural Network Architecture in Forecasting Pollution Trends

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Abstract With rising pollution concerns in recent times, producing refined and accurate predictions as a part of United Nations Sustainable Development Goals 11 (Sustainable Cities and Communities) and 13 (Climate Action) have gained utmost importance. As new computational methods become available, it becomes difficult for an average policymaker to evaluate various techniques comprehensively. One such state-of-the-art architecture is the Transformer neural network which has shown an exceptional rise in various areas such as natural language processing and computer vision. This paper reviews the current literature and performance of such a Transformer based neural network (referred in the paper as PolTrans) in the domain of pollution forecasting. Experiments based on four univariate city pollution datasets (Delhi, Seoul, Skopje and Ulaanbaatar) and two multivariate datasets (Beijing PM_{2.5} and Beijing PM₁₀) are performed against other computational methods consisting of widely used statistical, machine learning and deep learning techniques. Experimental findings show that although PolTrans performs comparatively better compared to existing deep learning methods such as BiDirectional long short-term memory networks (LSTM), LSTM AutoEncoder, etc. for modelling pollution in cities such as Beijing, Delhi and Ulaanbaatar, in the majority of cases, the PolTrans architecture lags

behind statistical and machine learning methods such as AutoRegressive Integrated Moving Average (ARIMA), Random Forest Regression, Standard Vector Regression (SVR), etc. by a range of 1.5 - 15 units in terms of Root Mean Square Error.

Keywords Time Series Analysis · Air Pollution · Statistical Models · Deep Learning · Long Term Forecast

1 Introduction

Environmental risk assessment¹ aims to identify the likelihood of future environmental hazards and the long-term effects such events can pose to various communities and urban systems all over the planet. Out of multiple such possible hazards possessing a looming threat to modern human civilization, climate change and air quality degradation have been identified as the ones requiring prominent attention from key stakeholders. With leading nations now declaring urgent action to combat the ongoing climate change a key subject in their future government policies², the need for leading technological advancements to develop novel solutions to mitigate such climatic risks have become of utmost importance for long-term sustainability related causes. To develop leading edge computational approaches as efforts to address prominent environmental issues, new and exciting research under the umbrella of Computational Sustainability³ has gained traction in the last decade. With ideas from Artificial Intelligence (AI) coupled with numerous applications in interdisciplinary domains, research has shown that AI-based computing holds extensive promise in providing key actionable insights that can help society plan new policies to lessen the harm posed by future hazards.

With regards to modelling air quality in urban environments, methods from AI have presently become pervasive

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in recent times. Various versions of long short term memory (LSTM) networks along with regression models such as standard vector machines (SVM), linear regression coupled with models taken from econometrics such as autoregressive integrated moving average (ARIMA) are widely used in producing estimates with a fair amount of accuracy. Although LSTMs suffer from a lack of data in certain situations⁴, statistical models such as ARIMA and Holt-Winters have been found to perform substantially better in univariate time-series predictions. Fields of Natural Language Processing (NLP) and time-series modelling are inherently intertwined and advances made in one domain often find key applications in the other domain. For example, deep learning based methods such as recurrent neural networks (RNN) and LSTMs often are used in extensive applications such as sentiment analysis, spam detection and document summarization to name a few.

A recent key innovation in seq2seq modelling originally for NLP applications has been the Transformer⁵ neural network. Unlike LSTMs and RNNs, Transformers eliminate recurrence which helps decrease model complexity and also decrease training time as well. Further, due to the presence of independent components, Transformers can be easily parallelized thus improving computation efficiency when dealing with large sequence datasets. Taking motivation of the wide usage in NLP and recent Computer Vision related tasks⁶, this paper investigates the utility of Transformer neural networks in air quality modelling. Since the original auto-encoder architecture was specially designed for NLP related sequence modelling tasks, this paper builds upon the original model and utilizes an altered version (referred to as PolTrans in this paper) which is a modified architecture suited for tasks such as one-step ahead prediction usually used in pollution count estimation. Additionally, this paper also guides a detailed performance comparison of the time-series models used in air quality modelling and explores any relative improvement PolTrans provides over widely used baselines.

The organisation of the remaining parts of this paper is as follows : in Section 2, relevant research studies in this field are briefly discussed. Section 3 contains a detailed description of PolTrans. The results of the study along with a discussion of the data are laid out in Section 4. The conclusion of this study is ultimately presented in Section 5.

2 Related Works

This section presents a brief survey of related research studies and architectures proposed for temporal modelling of pollution time-series using various learning based methodologies.

2.0.1 Statistical Learning

Peng et al.⁷ thoroughly investigated through a simulation study on air pollution as well as mortality data to compare

the efficacies of various statistical approaches with respect to mean squared error. Koo et al.⁸ performed a comparative study on air pollution index in Kuala Lumpur using fuzzy time-series models and found them to outperform other approaches in error and computation time. Dominici et al.⁹ used generative-additive models to model time-series concerning air pollution and health effects. They found the estimates to be similar in Poisson regression and strict convergence parameter settings but upward biased in various default convergence counterparts. Reikard¹⁰ investigated the prediction performance of various models on SO₂ emissions by the Kilauea volcano in Hawaii and found methods such as ARIMA to produce accurate estimations on daily and hourly granularities. For PM, regressions and simple persistence methods were found to perform better. Fang et al.¹¹ used Bayesian Model Averaging (BMA) method and reported the GAMM+BMA combination to produce accurate estimates in learning the association between PM₁₀ and mortality.

2.0.2 Machine Learning

Dincer et al.¹² reported showing successful forecasting results using a proposed fuzzy based time-series model built on top of Fuzzy K-Medoid clustering algorithm. Shahriar et al.¹³ performed a comparative study of ML methods such as L-SVM, M-SVM Gaussian Process (GP) and Random Forest regression models and reported GP to perform significantly better in predictions of PM_{2.5} and PM₁₀. Chen et al.¹⁴ found SVMs to produce better results in prediction of CO₂ and TVOCs and were able to outperform GP, M5P and ANNs. Wang et al.¹⁵ et al. developed an improved version of SVM capable of online learning and used the model to estimate pollution levels based on the air pollutant database in Hong Kong. Staffogia et al.¹⁶ used an ensemble methodology to establish relationships between PM and satellite land use and meteorological parameters. Their study produces estimates in 1sq. km spatial resolution and reported finding improvements in the addition of small-scale predictors at monitor locations.

2.0.3 Deep Learning

Espinosa et al.¹⁷ based on exactness and robustness criteria compared multiple forecasting models such as 1DCNN, GRU, LSTM along with different linear regression models to create a multi-criteria methodology for air quality prediction. Niska et al.¹⁸ presented the use of parallel genetic algorithm (GA) to design the architecture of MLPs for forecasting NO₂ emissions reported in Helsinki. The findings showed promising results and found GA to be a capable tool in neural network design. Dunea¹⁹ proposed a wavelet-feed forward neural network architecture to predict pollutants such as O₃, NO₂ and PM. Their study reported improvements in ANN performance with wavelet integration and were found

to present positive results for O₃ and NO₂. Soh et.al²⁰ created an adaptive deep learning model which combined ANNs, CNNs and LSTMs which was used to extract spatio-temporal air quality relations for improved performance. Lei et al.²¹ performed a case study using a hybrid approach involving CNNs and Bi-LSTMs for spatio-temporal modelling of pollution counts in Fushung, Liaoning Province in China.

While extensive studies have been organized in the past, the majority of them have focussed on the utility of classical methodologies such as econometric models, shallow ML models and diverse versions of LSTM in emission modelling and forecasting. Due to the inherent nature of pollutant behaviour, majority studies were regional and lacked a global perspective. This paper aims to investigate the utility of a transformer based model PolTrans in air quality modelling and how the prediction performance varies with respect to widely used baselines in major pollution risk areas around the world.

3 Model Architecture

This section presents a description of the PolTrans model architecture outline in Fig. 1.

3.1 Input Data Pre-processing

3.1.1 In2Out Sequence Modelling

To convert the time-series data P_{data} into a series of sequences for supervised training, a new dataset is engineered from the original data by breaking into chunks using a rolling window λ_n of size n . As the window λ_n is slid over the 1-dimensional time-series P_{data} , the series $\{P_{data,k}\}_{k=i}^{k=n-i-1}$ is taken as the feature vector while $P_{data,n-i}$ is made to serve as the label for the i th row of the new dataset. Here, $1 \leq i \leq T - n + 1$ where T stands for the number of time-steps present in P_{data} . The new dataset Q_{data} can be then split and sampled into training, validation and test sets for evaluation purposes as and when needed.

3.1.2 Time2Vec Encoding

To create a model agnostic vector representation of time, the supervised feature vectors are passed through the Time2Vec²² Encoding layer. For a scalar time notion τ , the resulting Time2Vec encoding $t2v(\tau)$ is a vector of size n that can be defined as follows:

$$t2v(\tau)[j] = \mathfrak{F}(\omega_j\tau + \varphi_j), 1 \leq j \leq n \quad (1)$$

where \mathfrak{F} represents the periodic function, $t2v(\tau)[j]$ represents the j th element of $t2v(\tau)$. As the layer is trainable, φ_j

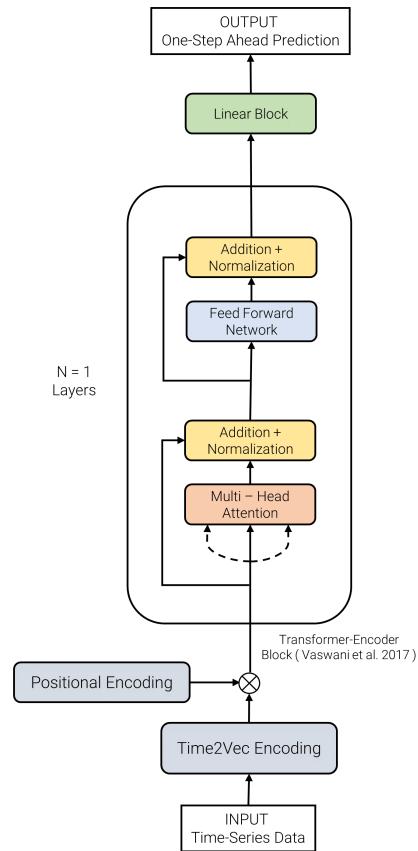


Fig. 1: PolTrans model architecture describing the flow of input, application of two kinds of encoding, modelling through the Transformer-Encoder block and output result as a one-step ahead forecast from the last linear block

and ω_j are taken to be the learnable parameters. In PolTrans, \mathfrak{F} is taken as the sine function, as in case of $\sin(\omega_j\tau + \varphi_j)$, being inherently periodic, recurrent behaviors can be captured without an explicit need for feature engineering. The benefit of the Time2Vec encoding lies in three main properties : periodicity, invariance to time rescaling and finally simplicity. Being easily consumable the $t2v(\tau)$ representation can be used inserted in any model with minimal overhead.

3.1.3 Positional Encoding

To inject relative or absolute positioning information about the elements in the vector representation derived from the Time2Vec layer, positional encodings are added to the input embeddings. As presented in the original paper⁵, PolTrans

also uses a similar encoding \mathfrak{P} given as functions of different frequencies.

$$\begin{aligned}\mathfrak{P}_{(\text{pos},2i)} &= \sin\left(\text{pos}/10000^{2i/d_{\text{model}}}\right) \\ \mathfrak{P}_{(\text{pos},2i+1)} &= \cos\left(\text{pos}/10000^{2i/d_{\text{model}}}\right)\end{aligned}\quad (2)$$

Here, pos refers to the position in the vector representation while i stands for the dimension. By converting each position to a sinusoid, the relative difference can be expressed as a linear function of $\mathfrak{P}_{\text{pos}}$ enabling the model to easily learn the relative positions.

3.2 Encoder and Decoder Layer Stack

3.2.1 Encoder

Unlike the NLP Transformer, PolTrans uses only a stack of $N = 1$ layer. The transformer encoder block has two sub-layers. The first sub-layer employs a multi-head attention wrapped around by a residual connection followed by a normalization layer. Using a multi-head attention layer helps the encoder to attend to all positions as well as parallelise through numerous attention layers, decreasing the overall computational cost. The second sub-layer uses the result from the first-layer and passes it through a fully connected feed-forward network wrapped around by a skip connection and followed by a normalization layer just like the first layer. The feed-forward network consists of two layers with the first layer containing a ReLU activation layer. The network output $y(x)$ with weights W_1, W_2 along with biases b_1 and b_2 can be mathematically expressed as follows :

$$y(x) = \text{ReLU}(xW_1 + b_1)W_2 + b_2 \quad (3)$$

In PolTrans the model dimension d_{model} is fixed to 250. As there are multiple residual connections involved along with various forms of encoding, a single d_{model} eases the tracking of dimensions.

3.2.2 Decoder

In contrast to the NLP Transformer, as the main output is concerned only with a single continuous output, the decoder block consists of only a single linear layer with an output dimension of $d_{\text{model}} \times 1$.

3.2.3 Multi-Head Attention

In the original Transformer paper⁵, multi-head attention promised extensive reductions in the total computational cost involved from values having dimension $d_v = d_{\text{model}}$ to $d_v = \frac{d_{\text{model}}}{h}$ where h is the number of parallel attention layers.

In this technique, attention is computed in parallel thereby producing value of dimension d_v . Since, multiple computations can be done simultaneously on parallel CPU cores, the computation cost effectively reduces to that of single-head attention with full dimensionality. The technique of multi-head attention can be mathematically expressed in the following equations as follows :

$$\begin{aligned}\text{MultiHead}(\mathcal{Q}, \mathcal{K}, \mathcal{V}) &= \text{Concatenate}(\mathcal{H}_1, \dots, \mathcal{H}_h) M^O \\ \mathcal{H}_i &= \text{Attention}(\mathcal{Q}M_i^Q, \mathcal{K}M_i^K, \mathcal{V}M_i^V) \\ \text{Attention}(\mathcal{Q}, \mathcal{K}, \mathcal{V}) &= \text{softmax}\left(\frac{\mathcal{Q}\mathcal{K}^T}{\sqrt{d_k}}\right)\mathcal{V}\end{aligned}\quad (4)$$

Here, the projections are parameter matrices $M_i^Q, M_i^K, M_i^V \in \mathbb{R}^{d_{\text{model}} \times d_v}$ and $M^O \in \mathbb{R}^{hd_v \times d_{\text{model}}}$. \mathcal{Q}, \mathcal{K} and \mathcal{V} stand for query, key and value matrices respectively while \mathcal{H}_i stands for the i th head out of a total of h heads.

4 Results

This section presents detailed insights into the experiments performed with the PolTrans model and its relative performance against various baselines.

4.1 Experimental Setting

4.1.1 Datasets

To test PolTrans on a wide range of regional variations, throughout the world, five highly polluted cities were chosen: Delhi, Seoul, Skopje, Ulaanbaatar and Beijing with the first four datasets being univariate while the last being multivariate in nature. Being the national capital of India, Delhi ($28.7041^\circ\text{N}, 77.1025^\circ\text{E}$) has been the hub for socio-economic activities. With lax pollution measures and a lack of social consensus, Delhi has been a regular feature in the world's most polluted cities list published annually by the World Health Organisation (WHO). Out of all developed cities, Seoul ($37.5665^\circ\text{N}, 126.9780^\circ\text{E}$) has been regarded to have the worst air quality among different developed cities around the world. The Korean government has been responsible for monitoring the pollution counts and has plans to decommission most of their coal power plants by 2025. Air pollution in Skopje, North Macedonia ($41.9981^\circ\text{N}, 21.4254^\circ\text{E}$) has been the highest in the European Union with pollutant levels sometime exceeding EU limits for more than 200 days in a year. Geographical location near a mountain and over-reliance on wood and coal are the main contributors to the pollution in the city. Ulaanbaatar ($47.8864^\circ\text{N}, 106.9057^\circ\text{E}$)

E), the capital city of Mongolia also is a regular feature of the most polluted cities list. With daily averages reaching to almost 27 times WHO recommended levels, the pollution in the city is a major public health emergency for the local government to solve in the coming years. Beijing (39.9042°N , 116.4074°E) before 2021 suffered from PM_{2.5} levels reaching 90 times WHO's recommended daily levels, with the sky mostly filled with haze and heavy air pollution. Such adverse effects lead to higher morbidity and mortality and became an important area of concern for the Chinese authorities. Although the situation has drastically improved now, the city still suffers from albeit short heavy pollution spells.

Most of the data sourced for these cities came from publicly available datasets. City wise data for the period of 2018 - 2020 from different datasets in Kaggle^{23 24 25 26} as well as from national air quality monitoring agencies such as Central Pollution Control Board²⁷ and AirNow²⁸ were used. The multivariate dataset for station in Tiantan, Beijing belonging to the period from 2013-2017 was sourced from UCI Machine Learning Repository^{29 30} containing various pollutants and other meteorological factors of which PM_{2.5}, PM₁₀, Temperature, Dew Point and Pressure were chosen with the pollutant (PM_{2.5} or PM₁₀) being the target variable.

4.1.2 Evaluation Metrics

As modelling time-series is inherently a regression task, the following four metrics: Root Mean Squared Error (RMSE), Mean Average Error (MAE) and Median Absolute Error (MedAE) were used to evaluate various method performances. For visualization purposes, Relative station-wise performance graphs in MedAE (only for univariate datasets since for Beijing, only a single station was used) along with Taylor diagrams were plotted to compare methods against each other.

4.1.3 Hardware and Software

The test setup used to carry out multiple experiments comprised of a 3.6 GHz 6C/12T processor with 16 GB 3000 MHz RAM and 8 GB RTX 2070 Super GPU for parallel matrix computation purposes. The project code was entirely based on Python with extensive support from libraries such as Py-Torch, TensorFlow, Sci-kit Learn, Statsmodels and NumPy.

4.1.4 Implementation Details

For PolTrans, because of ReLU, weights were first initialized using Kaiming (He) initialization³¹ method. A $n_{\text{heads}} = 10$ for multi-head attention in the encoder layer on extensive experimentation was found to provide optimum results. A learning rate $\alpha = 5 \times 10^{-3}$ was used inside an Adam optimizer³² with weight decay enabled. A learning rate scheduler with stepsize = 1 and $\gamma = 0.95$ were taken as parameters to help

in faster convergence. For experimental purposes PolTrans was trained with batchsize = 64 on 200 epochs. The In2Out sequences were constructed with window size $n = 2$. For testing purposes, the last 30% of the original time-samples was used as the test set while the first 70% was used for training and validation purposes.

4.1.5 Baselines

To measure the relative performance increase, three sets of evaluations were carried out. The first of evaluation placed PolTrans against popular deep learning methods such as Multi-Layer Perceptron (MLP), Bi-directional LSTM and LSTM Auto-Encoder. The second set and third set of evaluations involved using ML models such as SVM, Polynomial, Linear, Decision Tree and Random Forest regression along with statistical approaches such as ARIMA, AR and Holt-Winters respectively for each type of dataset. For multivariate datasets, in case of statistical approaches, ARIMAX and ARX were used due to their support for exogenous variables. For PolTrans the pollutant variable was used to perform modelling and subsequent forecasting in both kinds of datasets.

4.2 Performance in Univariate Time-Series Datasets

4.2.1 Comparison with Deep Learning Models

Upon performing detailed comparisons with various deep learning based methods, PolTrans (in terms of RMSE as can be seen in Table 1) was found to outperform competing deep learning models for Delhi and Ulaanbaatar. The biggest difference in MedAE performance was witnessed in Ulaanbaatar, where PolTrans fared significantly better than other deep learning models by a significant margin. For Ulaanbaatar, PolTrans managed an RMSE of around 61.167 compared to 64.7 - 67.6 as in the case for other deep learning methods. In the case of Seoul and Skopje, PolTrans performed around 1.09 - 3.87 units worse in comparison to the best performing deep learning model.

Inspecting the MedAE station-wise performance in Fig. 2, shows that PolTrans had mixed results in Delhi and Seoul. In Skopje, PolTrans consistently performed worse while in case of Ulaanbaatar, PolTrans consistently outperformed all other deep learning models in every station examined. In case of Seoul, for stations, SL119 and SL111, PolTrans showed MedAE deviation in the average of around 4 units from the competition. Conversely, in case of Ulaanbaatar, PolTrans showed improvements of as much as 60 units for UB012 in comparison. The two versions of LSTM used namely, LSTM Auto-Encoder and Bi-Directional LSTM were found to perform close to each other in almost all stations for all cities with minute differences separating the two.

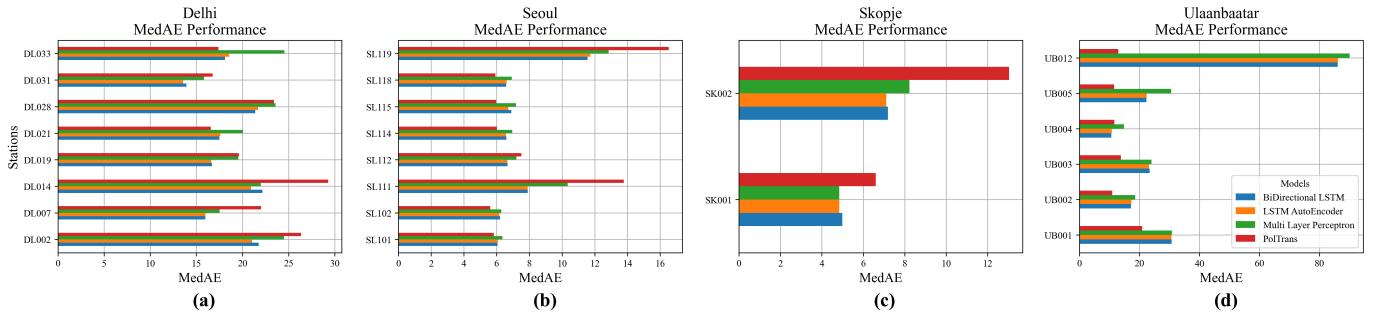


Fig. 2: MedAE performance of PolTrans vs other deep learning models (in $\mu\text{g}/\text{m}^3$) for different stations in (a) Delhi, (b) Seoul, (c) Skopje and (d) Ulaanbaatar cities

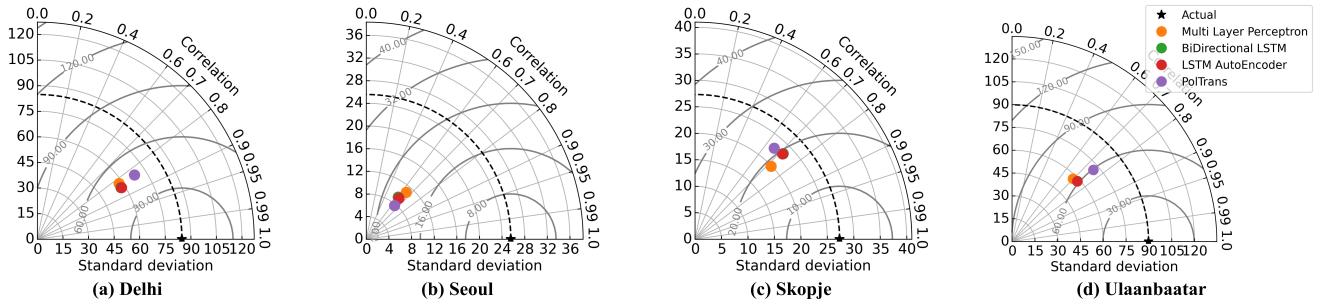


Fig. 3: Taylor diagrams comparing various deep learning methods vs PolTrans for (a) Delhi, (b) Seoul, (c) Skopje and (d) Ulaanbaatar cities

Table 1: Performance metrics averaged over all stations city-wise for deep learning methods and PolTrans

City	Model	MAE	RMSE	MedAE
Delhi	BiDirectional LSTM	31.958	49.658	18.439
	LSTM AutoEncoder	31.900	49.477	18.253
	Multi Layer Perceptron	34.017	51.746	20.956
	PolTrans	33.114	49.020	21.426
Seoul	BiDirectional LSTM	10.891	21.716	7.312
	LSTM AutoEncoder	10.869	21.538	7.305
	Multi Layer Perceptron	11.181	20.936	8.017
	PolTrans	11.855	22.597	8.398
Skopje	BiDirectional LSTM	11.491	19.416	6.086
	LSTM AutoEncoder	11.539	19.450	5.973
	Multi Layer Perceptron	11.726	18.942	6.533
	PolTrans	14.435	22.126	9.820
Ulaanbaatar	BiDirectional LSTM	43.269	64.750	31.713
	LSTM AutoEncoder	43.344	64.715	31.751
	Multi Layer Perceptron	46.575	67.627	34.814
	PolTrans	35.200	61.167	13.637

On examining the Taylor diagrams in Fig. 3, except in case of Seoul, PolTrans showed higher standard deviation in comparison to other deep learning models. Although RMSE and standard deviation performance might have been off w.r.t. competition, the correlation of predicted values in comparison to actual values could be found to be similar without much deviation.

4.2.2 Comparison with Machine Learning Methods

In this comparison, as evident from Table 2, PolTrans fared worse than its competition in every city examined. Although there does not seem to be present a clear winner, mostly SVR and Random Forest Regression performed the best out of all. Glancing overall comparisons PolTrans deviated with RMSE in the 2.19 - 4.09 units range. Out of all models experimented upon, Decision Tree Regression was found to perform the worst with RMSE values off by huge margins when compared to the best performing models.

Looking at individual station performances in Fig. 4, although PolTrans may not have performed the best, it certainly was also not the worst one being experimented upon. For station UB012, PolTrans was the best performing of all machine learning models tested. In majority of the stations, Decision Tree Regression showed the highest MedAE error among all with SVR and Random Forest being the best in almost all stations.

Taylor diagrams for this comparison in Fig. 7 show that the performance of machine learning methods (except Decision Tree Regression) and PolTrans were close to each other barring a few deviations. One notable observation can be found for Decision Tree Regression, wherein all cities the model consistently showed higher standard deviation coupled with lower correlation scores compared to others.

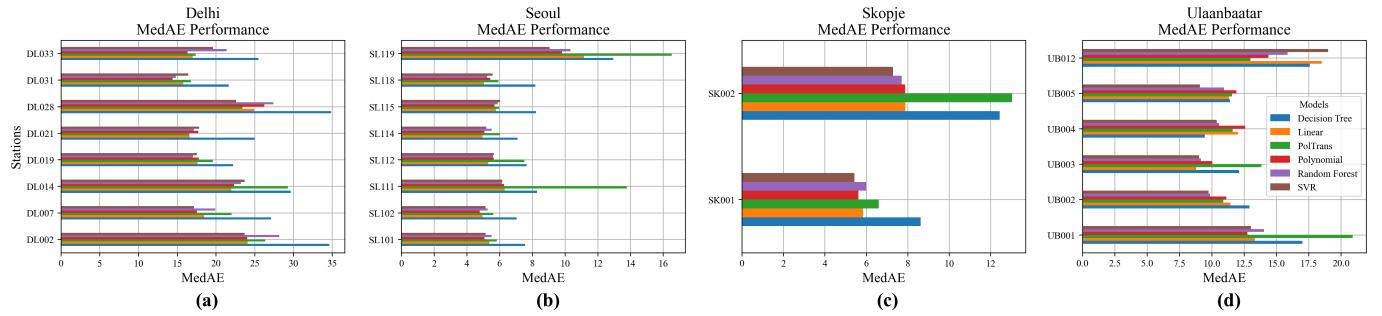


Fig. 4: MedAE performance of PolTrans (indicated in green) vs other machine learning models ($\mu\text{g}/\text{m}^3$) for different stations in (a) Delhi, (b) Seoul, (c) Skopje and (d) Ulaanbaatar cities

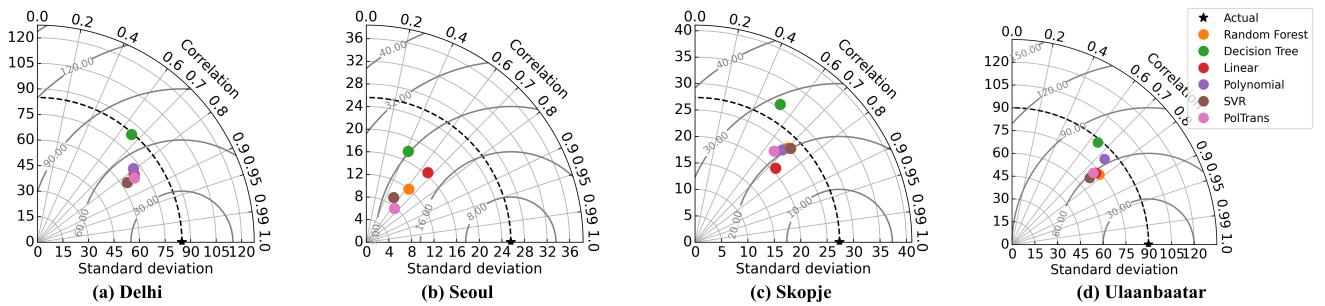


Fig. 5: Taylor diagrams comparing various machine learning methods vs PolTrans for (a) Delhi, (b) Seoul, (c) Skopje and (d) Ulaanbaatar cities

4.2.3 Comparison with Statistical Methods

Analysis of the performance metric in Table 3 shows that econometric methods such as AR and ARIMA consistently performed well in all stations experimented on. With RMSE deviations in the range from 1.16 - 4.37 units, PolTrans in comparison to statistical methods has been found to lag behind the best performing statistical counterpart by a narrow margin.

Even though in most stations, PolTrans (as evident from Fig. 6) has been found to show the highest MedAE error out of all, in specific stations such as DL028 and UB012 in the cities of Delhi and Ulaanbaatar respectively, PolTrans has been able to outperform the best performing statistical method used. Although the position of best performing model station-wise was jointly owned by AR, ARIMA and Holt-Winters in proportional amounts, for most of the Ulaanbaatar stations specifically UB012, UB005 and UB004, AR was found to show disproportionately high deviations in MedAE error compared to the competition.

Except Seoul, predictions made by PolTrans had correlations close to each other, along 0.6 - 0.8 levels as can be evident from Fig. 7. For Seoul, although correlations between predicted and actual values were almost the same along the 0.6 to 0.7 mark, standard deviations varied a lot, with Holt-

Winters and PolTrans being on the extreme ends with 24 to 8 units respectively.

4.3 Performance in Multivariate Time-Series Datasets

4.3.1 Comparison with Deep Learning Models

In the case of Beijing PM₁₀ and Beijing PM_{2.5} multivariate datasets, as evident from Table 4, PolTrans has been found to outperform other deep learning methods with great margin in all metrics of MAE, RMSE and MedAE. BiDirectional LSTM for both the multivariate Beijing datasets was found to perform consistently worse with RMSE values 83.391 and 75.782 respectively.

For Taylor diagrams in Fig. 8, even though most correlation values were in the range 0.6 - 0.7, the correlation for BiDirectional LSTM was found to be a little lower in the middle of 0.3 - 0.4 and alongside exhibited higher standard deviation compared other methods. The Multi Layer Perceptron method was found to show the lowest standard deviation for equivalent correlation values in comparison to the rest.

4.3.2 Comparison with Machine Learning Models

Similar to the scenario for univariate datasets mentioned in Section 4.2.2, PolTrans as evident from Table 5 was unsuc-

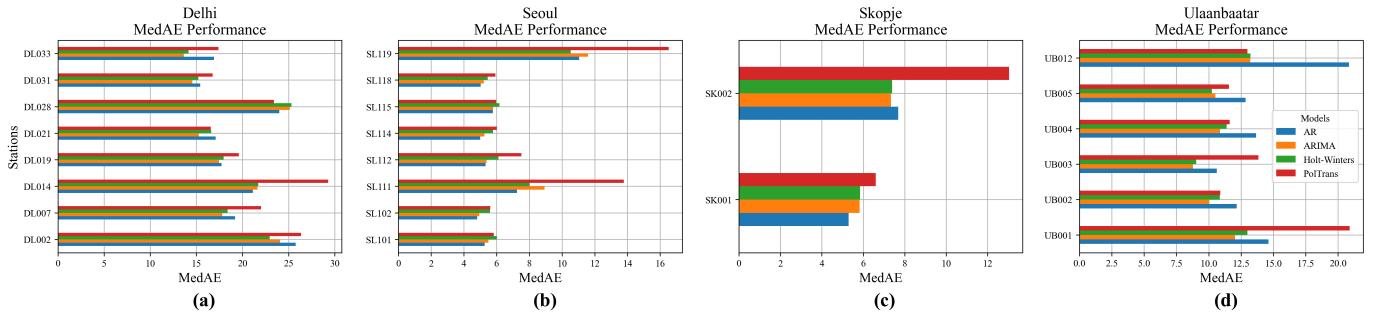


Fig. 6: MedAE performance of PolTrans (indicated in red) vs other statistical models ($\mu\text{g}/\text{m}^3$) for different stations in (a) Delhi, (b) Seoul, (c) Skopje and (d) Ulaanbaatar cities

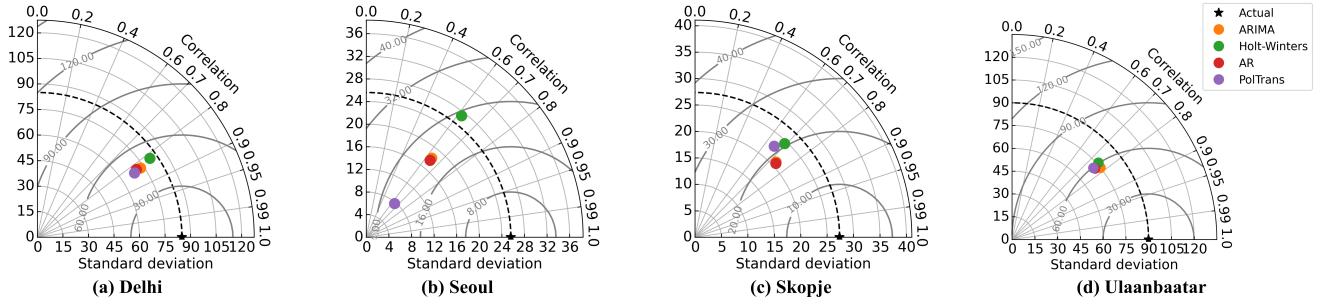


Fig. 7: Taylor diagrams comparing various statistical methods vs PolTrans for (a) Delhi, (b) Seoul, (c) Skopje and (d) Ulaanbaatar cities

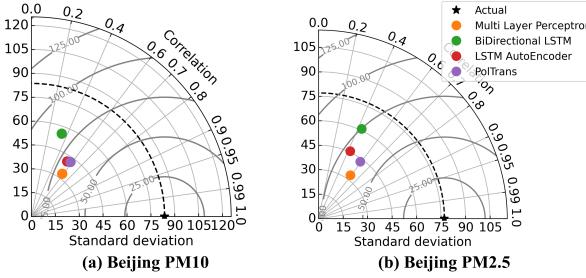


Fig. 8: Taylor diagrams comparing various deep learning methods vs PolTrans for (a) Beijing PM₁₀ and (b) Beijing PM_{2.5}

cessful in faring better than its machine learning counterparts. With SVR and Polynomial Regression dominating in terms of MAE and RMSE respectively, PolTrans was found to be off by around 2.7 units in RMSE and 0.75 units in MAE compared to the best performing counterparts. Out of all, Decision Tree Regression was found to perform worse in terms of RMSE and MAE with huge margins in comparison to others.

A similar picture prevailed for Taylor diagrams as well in Fig. 9. With Decision Tree Regression being left with a lower correlation in the 0.4 - 0.6 level and higher standard deviation around the 75 mark, other models clustered at stan-

dard deviation levels of 45 units with correlations in the 0.6 - 0.7 levels.

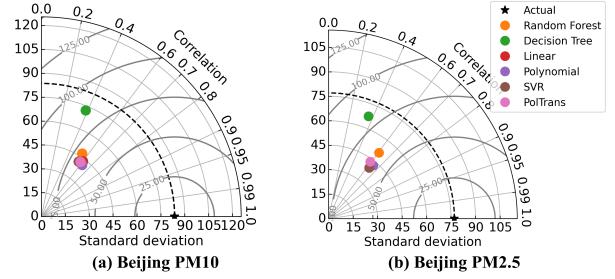


Fig. 9: Taylor diagrams comparing various machine learning methods vs PolTrans for (a) Beijing PM₁₀ and (b) Beijing PM_{2.5}

4.3.3 Comparison with Statistical Learning Models

The exogenous equipped ARIMAX outperformed all other models used in this specific comparison, as can be seen in Table 6. PolTrans was the worst performer of all three with a margin of 12 - 13 units in MAE and 14 - 15 units in RMSE errors. Although ARX was not the worst performing model in the experiments, the difference in the performance metrics

Table 2: Performance metrics averaged over all stations city-wise for machine learning methods and PolTrans

City	Model	MAE	RMSE	MedAE
Delhi	Decision Tree	45.666	69.912	27.575
	Linear	31.725	48.267	19.574
	PolTrans	33.114	49.020	21.426
	Polynomial	32.703	51.767	19.556
	Random Forest	32.667	49.121	21.138
	SVR	31.582	47.862	19.828
Seoul	Decision Tree	13.851	25.654	8.377
	Linear	10.269	20.407	6.109
	PolTrans	11.855	22.597	8.398
	Polynomial	16.712	52.338	5.973
	Random Forest	10.253	21.175	6.186
	SVR	10.502	22.834	5.991
Skopje	Decision Tree	17.365	28.644	10.532
	Linear	11.675	18.533	6.864
	PolTrans	14.435	22.126	9.820
	Polynomial	12.084	20.162	6.751
	Random Forest	12.185	20.502	6.852
	SVR	11.666	19.998	6.361
Ulaanbaatar	Decision Tree	41.375	76.775	13.412
	Linear	31.908	58.695	12.576
	PolTrans	35.200	61.167	13.637
	Polynomial	33.995	64.730	12.136
	Random Forest	31.017	57.071	11.744
	SVR	31.973	60.221	11.715

Table 3: Performance metrics averaged over all stations city-wise for statistical learning methods and PolTrans

City	Model	MAE	RMSE	MedAE
Delhi	AR	31.501	47.821	19.665
	ARIMA	30.994	47.234	18.698
	Holt-Winters	32.021	49.848	19.041
	PolTrans	33.114	49.020	21.426
	AR	10.452	21.431	6.187
	ARIMA	10.549	21.562	6.575
Seoul	Holt-Winters	12.102	26.199	6.711
	PolTrans	11.855	22.597	8.398
	AR	11.573	18.437	6.490
	ARIMA	11.531	18.601	6.575
	Holt-Winters	12.560	20.496	6.614
	PolTrans	14.435	22.126	9.820
Skopje	AR	32.491	58.698	14.128
	ARIMA	30.765	56.794	10.911
	Holt-Winters	31.843	59.312	11.291
	PolTrans	35.200	61.167	13.637

for ARX was lower compared to PolTrans and was close in the 5 - 6 units interval for MAE and RMSE.

The Taylor diagrams in Fig. 10 show a noticeable difference in the model performance for ARIMA, ARX and PolTrans. While PolTrans had correlation values around the 0.6 range, ARX and ARIMAX had values in the 0.7 and 0.8 mark. Regarding standard deviation, PolTrans showed lower values within 30 - 45 while ARX and ARIMAX had values ranging in 45 - 60 and 60 - 75 respectively.

Table 4: Performance metrics in muti-variate datasets for deep learning methods and PolTrans

City	Model	MAE	RMSE	MedAE
Beijing PM ₁₀	BiDirectional LSTM	56.432	83.391	39.139
	LSTM AutoEncoder	50.548	70.668	40.072
	Multi Layer Perceptron	50.877	70.085	42.114
	PolTrans	48.725	68.457	35.999
Beijing PM _{2.5}	BiDirectional LSTM	54.237	75.782	39.579
	LSTM AutoEncoder	51.290	71.671	38.711
	Multi Layer Perceptron	48.665	64.222	41.845
	PolTrans	45.161	62.305	34.179

Table 5: Performance metrics in muti-variate datasets for machine learning methods and PolTrans

City	Model	MAE	RMSE	MedAE
Beijing PM ₁₀	Decision Tree	61.370	87.291	43.240
	Linear	48.372	67.374	36.312
	PolTrans	48.725	68.457	35.999
	Polynomial	47.474	66.626	36.055
	Random Forest	49.589	70.555	37.424
	SVR	47.130	69.578	32.953
Beijing PM _{2.5}	Decision Tree	56.388	81.938	37.395
	Linear	44.928	61.244	34.881
	PolTrans	45.161	62.305	34.179
	Polynomial	43.586	59.532	34.757
	Random Forest	44.485	61.574	32.474
	SVR	42.830	61.028	30.583

Table 6: Performance metrics in muti-variate datasets for statistical learning methods and PolTrans

City	Model	MAE	RMSE	MedAE
Beijing PM ₁₀	ARIMAX	36.718	54.600	25.198
	ARX	41.590	60.391	29.748
	PolTrans	48.725	68.457	35.999
	AR	32.750	47.804	22.407
Beijing PM _{2.5}	ARIMAX	37.428	52.983	27.033
	PolTrans	45.161	62.305	34.179

4.4 Discussion

From the extensive experimentation performed in testing PolTrans against multiple baselines from areas of deep learning, machine learning and statistical methods, although PolTrans shows great promise as a deep learning method in forecasting time-series data in the pollution domain, other methods in the statistical and machine learning group of models perform better in the performance metrics used. However, the biggest advantage that PolTrans benefits from lies in its ability to rapidly train (w.r.t. other deep learning methods) as well as parallelize in distributed settings. When the volume of data increases (order $\geq 10^6$), statistical methods such as ARIMA, Holt-Winters, etc. take higher training times due to their inherent modelling characteristics.

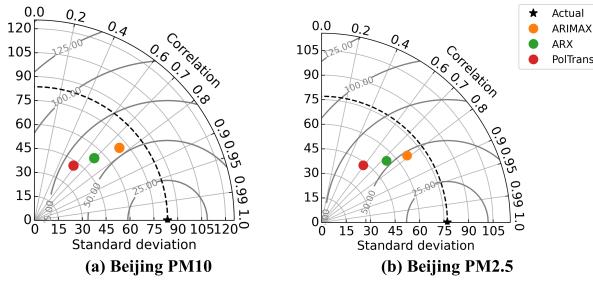


Fig. 10: Taylor diagrams comparing various statistical methods vs PolTrans for (a) Beijing PM₁₀ and (b) Beijing PM_{2.5}

Looking at the nature of predictions produced by PolTrans in Fig. 11, where ordinary deep learning models normally succumb to high variability and often lead to projections close to the mean, PolTrans was successfully able to model the variability fairly and predict with greater accuracy. The substantial superiority of statistical methods in providing more precise pollution counts can be attributed to their comparatively simple model parameter based architecture leading to low variance and a greater performance in producing close estimations.

Although the pollutants in focus were PM_{2.5} and PM₁₀, similar results could be expected in case of other major pollutants for different cities. In the experiments, the chief focus was made to pick cities which had high variation in pollution counts. In urban environments where the pollution scenario is relatively stable and shows regular periodicity (eg. New York City, London, Washington DC, etc.), PolTrans as well as other methods experimented, would help in production of much more refined and accurate insights with relatively higher accuracy.

5 Conclusion

In this paper, a transformer based deep learning approach (referred in this paper as PolTrans) based on the popular NLP Transformer was experimentally evaluated with respect to multiple baseline methods from statistical, machine learning and deep learning domains which are widely used in pollution modelling. Experiments were run on both univariate and multivariate datasets belonging to different major cities all around the world, and the results showed that although PolTrans shows good progress in comparison to other commonly used deep learning approaches such as BiDirectional LSTM, LSTM Auto-Encoder, MLP, etc. it still lags in comparison to machine learning and statistical approaches such as SVR, ARIMA, Holt-Winters, etc. Even though other models show greater advantage in estimation of pollution counts, in certain situations PolTrans especially those involving high volume environments, PolTrans shows extensive promise due

to high parallelizable nature of the underlying Transformer based architecture.

The study in the current form does not take into account infrequent pollution situations such as those involving complex temporal structures and heavy noise. Since missing values normally hinder models in estimation purposes, removal of such erroneous datapoints were already performed through various missing value imputation methods. As a future work, experiments can be proposed in situations especially close to industrial centres (eg. factories, coal mines, dumping grounds etc.) where sporadic spikes are a frequent occurrence.

As pollution modelling and monitoring becomes more important day by day, it is hoped that such a comparative evaluation made in this paper with different key urban settings in focus, will assist concerned policymakers (especially those working under SDG 11 and 13) in selecting appropriate pollution modelling strategies to gauge their own pollution scenarios effectively.

Data and Code Availability

The analysis code and data used for this paper upon publication can be found in the following link - <https://github.com/nathzi1505/PolTrans-Comparative-Study>.

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Conflict of Interest

The authors declare that they have no conflict of interest.

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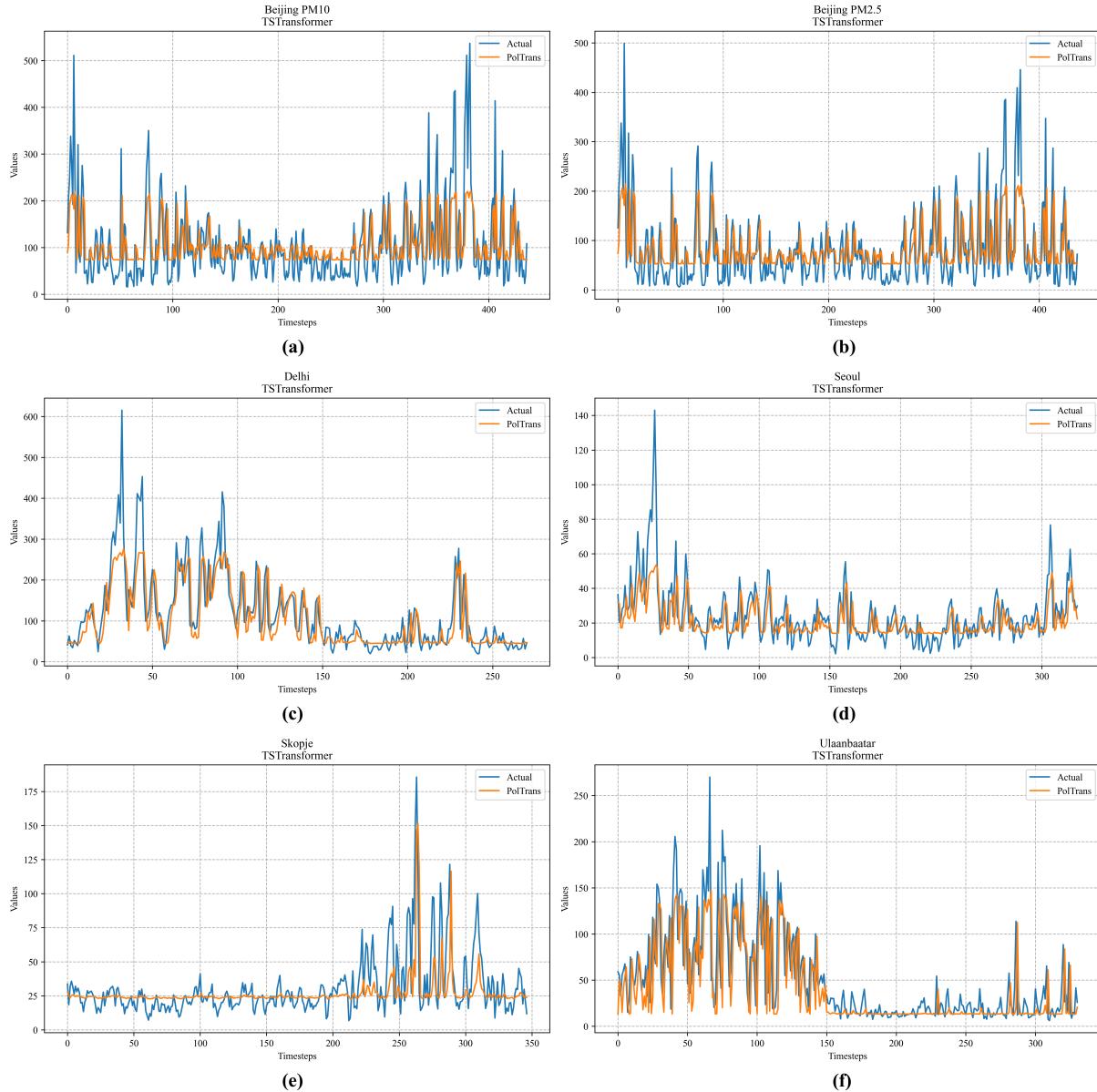


Fig. 11: Line plots demonstrating predictions made by PoTrans (indicated in orange) vs actual PM_{2.5} / PM₁₀ count as reported (in $\mu\text{g}/\text{m}^3$) for (a) Beijing PM₁₀, (b) Beijing PM_{2.5} and a sample station in each of (c) Delhi, (d) Seoul, (e) Skopje and (f) Ulaanbaatar datasets

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