Evaluation of Transformer Based Neural Nets in Pollution Forecasting Tasks

Pritthijit Nath, Asif Iqbal Middya and Sarbani Roy

***Abstract*—With rising pollution concerns in recent times, producing refined and accurate predictions as a part of UN SDG 11 (Sustainable Cities and Communities) and 13 (Climate Action) has gained utmost importance. In this paper, taking inspiration from the famous Transformer neural network architecture and its wide applications in areas such as natural language processing and computer vision, a novel approach PolTrans is proposed that introduces the transformer architecture to the domain of pollution count estimation. Experiments on four important city pollution datasets (Delhi, Seoul, Skopje and Ulaanbaatar) show PolTrans to outperform the most widely used methods in the statistical, machine and deep learning domains with significant margins. PolTrans managed to achieve RMSE values in the range of 21.462 (Skopje) to 61.134 (Ulaanbaatar), thereby improving over other baselines with as much as 34.7 units compared to the worst performing models in the experiments. With substantial parallelism and reduced training time, PolTrans presents extensive scaling opportunities for high-data intensive real-world pollution modelling tasks.**

***Index Terms*—Deep Learning, Air Quality, Transformer Neural Network, Time-Series**

I. Introduction

ENVIRONMENTAL risk assessment [1] aims to identify the likelihood of future environmental hazards and the long-term effects such 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 policies [2], 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 Sustainability [3] 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 has presently became pervasive 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 fair amount of accuracy. Although LSTMs suffer from lack of data in certain situations [4], statistical models such as ARIMA and Holt-Winters have been found to perform substantially better in univariate time-series predictions. Advances made originally in the field of Natural Language Processing (NLP) often find key applications especially in time-series modelling. 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 orginally for NLP applications has been the Transformer [5] neural network. Unlike LSTMs and RNNs, Transformers eliminates recurrence which help decrease model complexity and 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 tasks [6], 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 modeling tasks, this paper builds upon the original model and utilizes a modified version (entitled as PolTrans for references purposes) 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 modeling 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 II, relevant research studies in this field are briefly discussed. Section III contains a detailed description of the proposed pollution time-series transformer model PolTrans . The results of the study along with a discussion of the data are laid out Section IV. The conclusion and the broad impact of the study are ultimately presented in Section V.

II. 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.

Pritthijit Nath, Asif Iqbal Middya and Sarbani Roy are affiliated with the Department of Computer Science and Engineering, Jadavpur University, Kolkata, India. (e-mail: sarbani.roy@jadavpuruniversity.in)

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. Their study reported to find estimate biases to decrease on addition of more smoothing rendering selection methods not suitable for obtaining low bias estimates. 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. Reikard [10] investigated the prediction performance of various models on SO_2 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 PM_{10} and mortality.

2) Machine Learning: Dincer at 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 PM_{10}. Chen et al. [14] found SVMs to produce better results in prediction of CO_2 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 to find improvements on addition of small-scale predictors at monitor locations.

3) Deep Learning: Espinosa et al. [17] based on exactness and robustness criteria compared multiple forecasing 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 NO_2 emissions reported in Helsinki. The findings showed promising results and found GA to be a capable tool in neural network design. Dunea [19] proposed a wavelet-feed forward neural network architecture to predict pollutants such as O_3, NO_2 and PM. Their study reported improvements in ANN performance with wavelet integration and were found to present positive results for O_3 and NO_2. Soh et.al [20] 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 modeling of pollution counts in Fushung, Liaoning Province in China.

While extensive studies have been organized in the past, 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 in nature and lacked a global perspective. This paper aims to investigate the utility of the proposed 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.

III. Model Architecture

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

A. Input Data Pre-processing

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 orginal 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.

2) Time2Vec Encoding: To create a model agnostic vector representation of time, the supervised feature vectors are passed through the Time2Vec [22] Encoding layer. For a scalar time notion τ, the resulting Time2Vec encoding $\mathbf{t2v}(\tau)$ is a vector of size n that can be defined as follows:

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

where $\mathfrak{F}$ represents the periodic function, $\mathbf{t2v}(\tau)[j]$ represents the j th element of $\mathbf{t2v}(\tau)$. As the layer is trainable, φ_j and ω_j are taken to be the learnable parameters. In PolTrans , $\mathfrak{F}$ is taken as the sine function, as in case of $\sin\left(\omega_j \tau + \varphi_j\right)$, 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 $\mathbf{t2v}(\tau)$ representation can be used inserted in any model with minimal overhead.

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 paper [5], PolTrans also uses a similar encoding $\mathfrak{P}$ given as functions of various different frequencies.

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

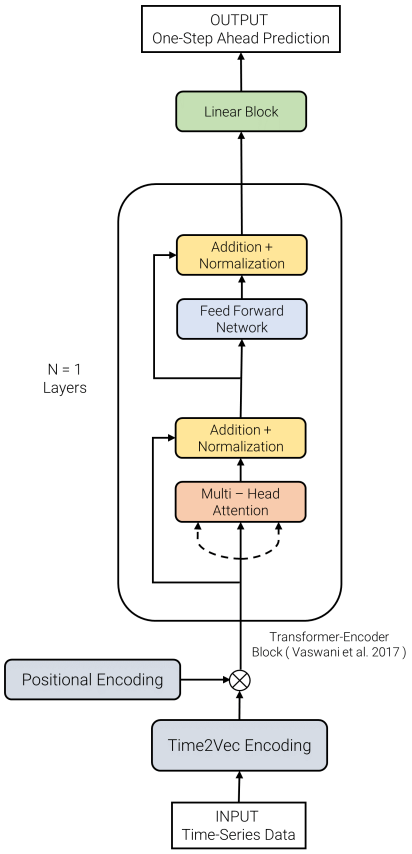


Fig. 1. PolTrans model architecture describing the flow of input, application of two kinds of encoding, modelling through the Transformer-Encoder block and output result as a one-step ahead forecast from the last linear block

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.

B. Encoder and Decoder Layer Stack

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 form 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 :

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

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.

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) Multi-Head Attention: In the original Transformer paper [5], 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 :

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

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.

IV. Results

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

A. Experimental Setting

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°N, 77.1025°E) has been the hub for socio-economic activities. With lax pollution measures and 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°N, 126.9780°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 have plans to decommission most of their coal power plants by 2025. Air pollution in Skopje, North Macedonia (41.9981°N, 21.4254°E) has been the highest in the European Union with pollutant levels sometiming exceeding EU limits for more than 200 days in a year. Geographical location near a mountain and over reliance

on wood and coal are main contributors to the pollution in the city. Ulaanbaatar (47.8864° N, 106.9057° 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 Chinease authorities. Although situation has drastically improved after 2021, the city still suffers from albeit short heavy pollution spells.

Most of the data sourced for the 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 Board [27] and AirNow [28] 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 $PM_{2.5}$, PM_{10}, Temperature, Dew Point and Pressure were chosen with the pollutant ($PM_{2.5}$ or PM_{10}) being the target variable.

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 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.

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 PyTorch, TensorFlow, Sci-kit Learn, Statsmodels and NumPy.

4) Implementation Details: For PolTrans, because of ReLU, weights were first initialized using Kaiming (He) initialization [31] 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 optimizer [32] with weight decay enabled. A learning rate scheduler with $\text{stepsize} = 1$ and $\gamma = 0.95$ were taken as parameters to help in faster convergence. For experimental purposes PolTrans was trained with $\text{batchsize} = 64$ 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.

5) Baselines: To measure the relative performance increase, three sets of evaluation 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 mulitvariate datasets, in case of statistical approaches, ARIMAX and ARX were used for their support of exogenous variables. For PolTrans the pollutant variable was used to perform modelling and subsequent forecasting in ooth kinds of datasets.

B. Performance in Univariate Time-Series Datasets

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 I) was found to outperform comparing 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 case for other deep learning methods. In case of Seoul and Skopje, PolTrans performed around 1.09-3.87 units worse in comparison to the best performing deep learning model.

TABLE I
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**

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 average 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.

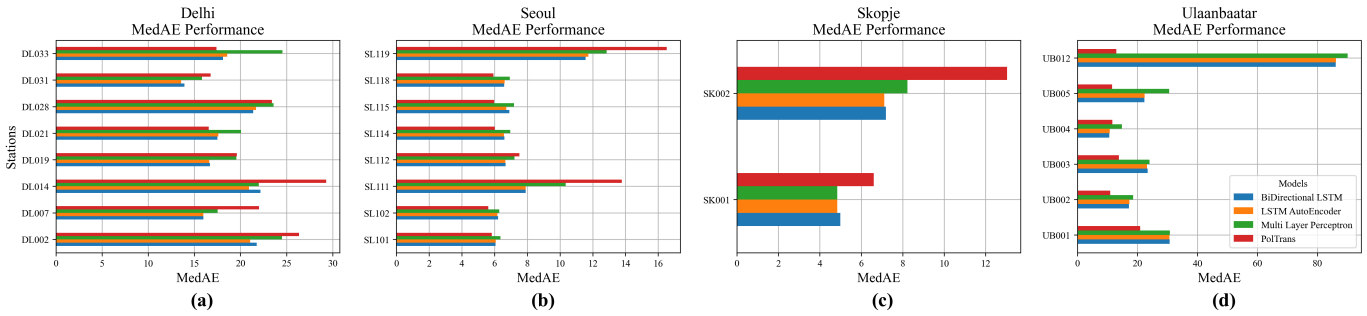


Fig. 2. MedAE performance of PolTrans vs other deep learning models (in $\mu g/m^3$) for different stations in (a) Delhi, (b) Seoul, (c) Skopje and (d) Ulaanbaatar cities

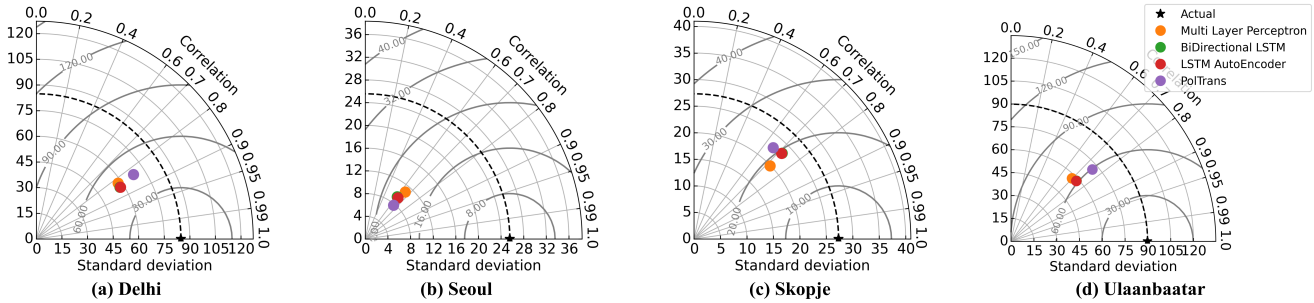


Fig. 3. Taylor diagrams comparing various deep learning methods vs PolTrans for (a) Delhi, (b) Seoul, (c) Skopje and (d) Ulaanbaatar cities

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, correlation of predicted values in comparison to actual values can be found to similar without much deviation.

2) Comparison with Machine Learning Methods: In this comparison, as evident from Table II, 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 over all 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 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.

TABLE II
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

3) Comparison with Statistical Methods: Analysis of the performance metric in Table III shows that econometric methods such as AR and ARIMA consistently performed well in all stations experimented on. With RMSE deviations in the range

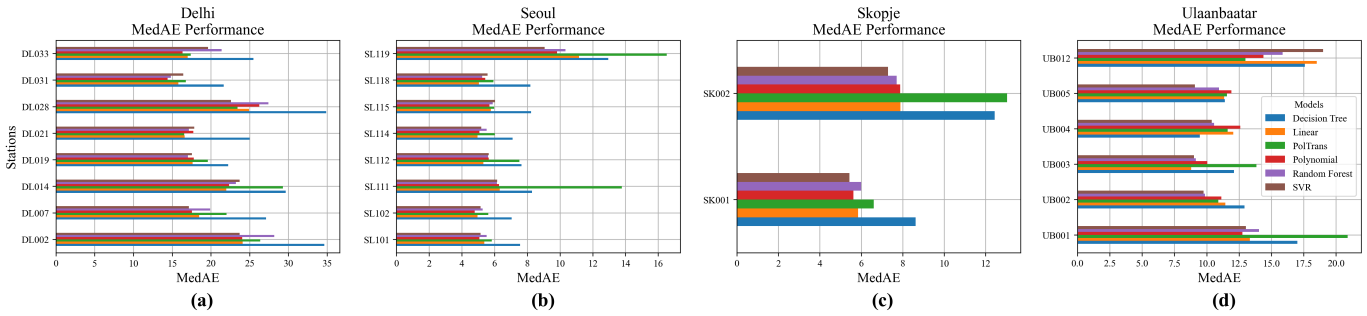


Fig. 4. MedAE performance of PolTrans (indicated in green) vs other machine learning models (in $\mu g/m^3$) for different stations in (a) Delhi, (b) Seoul, (c) Skopje and (d) Ulaanbaatar cities

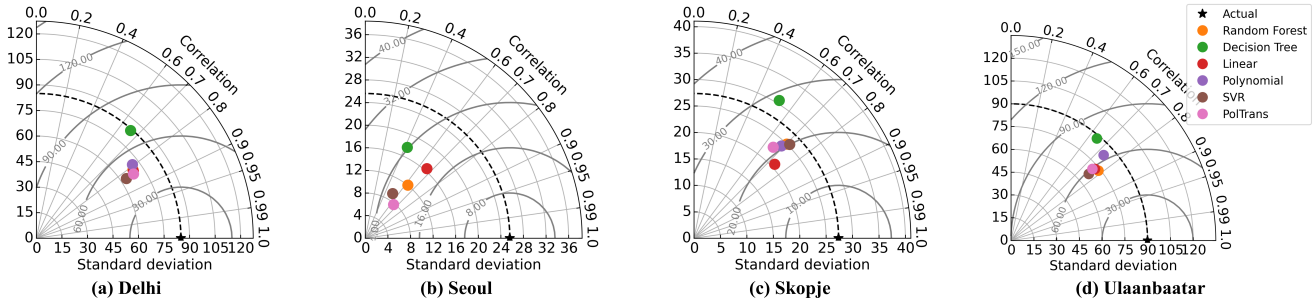


Fig. 5. Taylor diagrams comparing various machine learning methods vs PolTrans for (a) Delhi, (b) Seoul, (c) Skopje and (d) Ulaanbaatar cities

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.

TABLE III
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
Seoul	AR	**10.452**	**21.431**	**6.187**
	ARIMA	10.549	21.562	6.575
	Holt-Winters	12.102	26.199	6.711
	PolTrans	11.855	22.597	8.398
Skopje	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
Ulaanbaatar	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

Even though in most stations, PolTrans (as evident from Fig. 6) has been found to show 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 proportial amounts, for most of the Ulaanbaatar statiions specifically UB012, UB005 and UB004, AR was found to show disproportionaly 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 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.

C. Performance in Mutivariate Time-Series Datasets

TABLE IV
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**

1) Comparison with Deep Learning Models: In case of Beijing PM_{10} and Beijing $PM_{2.5}$ multivariate datasets, as evident from Table IV, 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

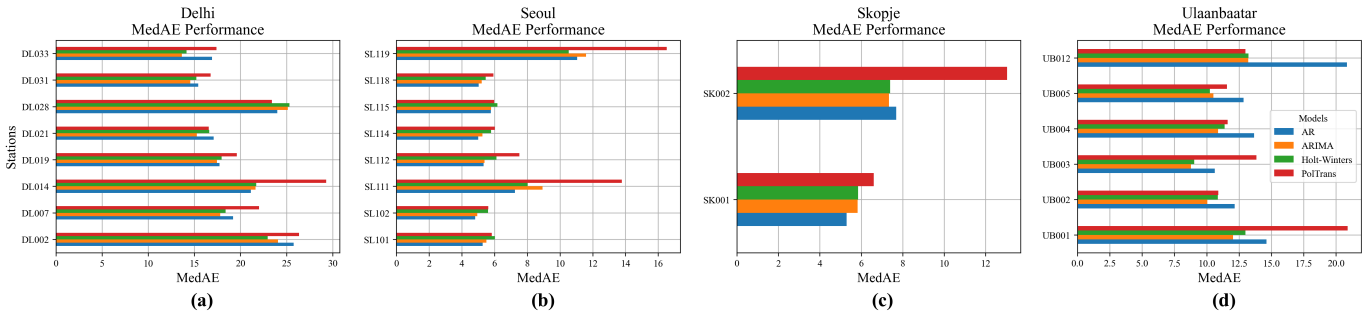


Fig. 6. MedAE performance of PolTrans (indicated in red) vs other statistical models (in $\mu g/m^3$) for different stations in (a) Delhi, (b) Seoul, (c) Skopje and (d) Ulaanbaatar cities

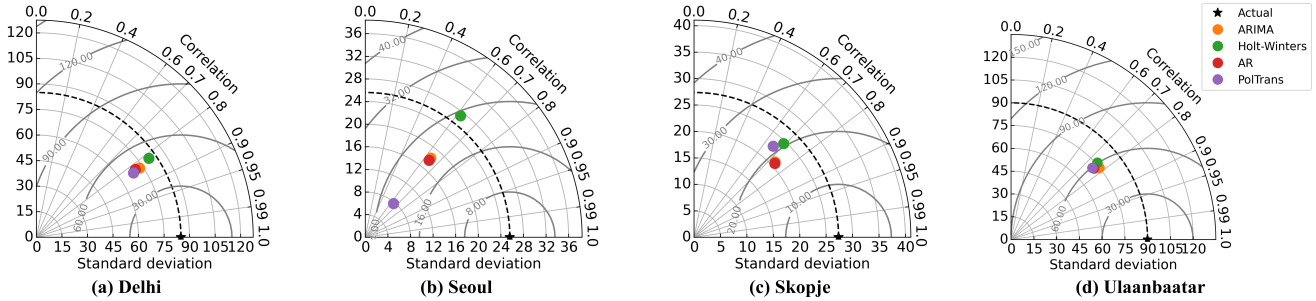


Fig. 7. Taylor diagrams comparing various statistical methods vs PolTrans for (a) Delhi, (b) Seoul, (c) Skopje and (d) Ulaanbaatar cities

multivariate Beijing datasets was found to perform consistently worse with RMSE values 83.391 and 75.782 respectively.

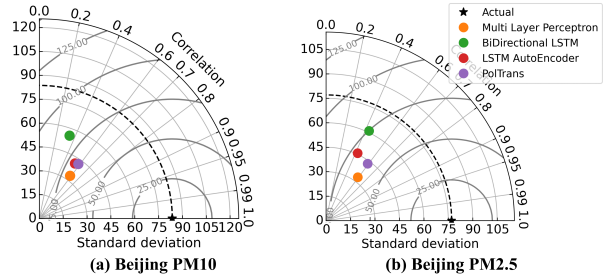


Fig. 8. Taylor diagrams comparing various deep learning methods vs PolTrans for (a) Beijing PM_{10} and (b) Beijing $PM_{2.5}$

For Taylor diagrams in Fig. 8, even though most correlation valuess were in the range 0.6 - 0.7, the correlation for BiDirectional LSTM was found to 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.

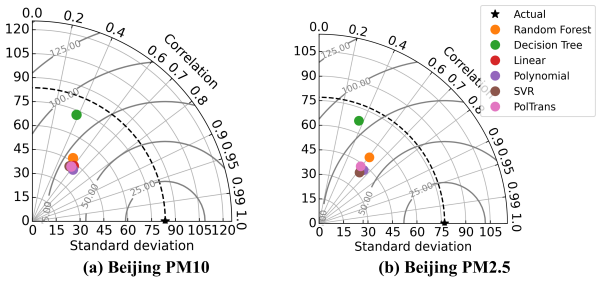
2) Comparison with Machine Learning Models: Similar to the scenario for univariate datasets mentioned in Section IV-B2, PolTrans as evident from Table V was unsuccesful in faring better than its machine learning counterparts. With SVR and Polynomial Regression dominating in terms of MAE and RMSE respectively, 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.

TABLE V
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**

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

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 VI. 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



(a) Beijing PM10 (b) Beijing PM2.5

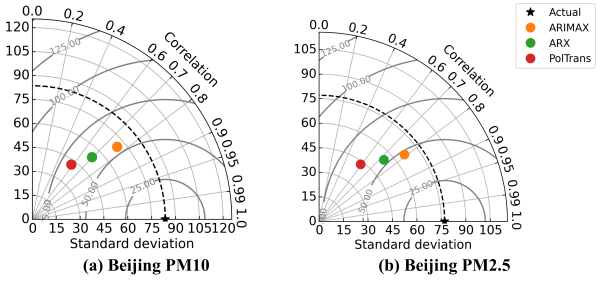
Fig. 9. Taylor diagrams comparing various machine learning methods vs PolTrans for (a) Beijing PM_{10} and (b) Beijing $PM_{2.5}$

experiments, the difference in the performance metrics for ARX was lower compared to PolTrans and were close in the 5 - 6 units interval for MAE and RMSE.

TABLE VI
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
Beijing $PM_{2.5}$	ARIMAX	**32.750**	**47.804**	**22.407**
	ARX	37.428	52.983	27.033
	PolTrans	45.161	62.305	34.179

The Taylor diagrams in Fig. 10 show a noticable 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.



(a) Beijing PM10 (b) Beijing PM2.5

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

D. 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 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 $>= 10^6$), statistical methods such as ARIMA, Holt-Winters, etc. take higher training times due to their inherent modelling characteristics.

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.

Although the pollutants in focus were $PM_{2.5}$ and PM_{10}, similar results could be expected in case of other major pollutants for different cities. In the experiments, 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.

V. CONCLUSION

In this paper, a transformer based deep learning approach (termed 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. The experiments ran on both univariate and multivariate datasets belonging to different major cities all round the world. Thre results show that although PolTrans show 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.

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 can be found in https://github.com/nathzi1505/PolTrans-Comparative-Study (permission through email needs to be sought from the author).

ACKNOWLEDGMENT

The research work of Asif Iqbal Middya is supported by UGC-NET Junior Research Fellowship (UGC-Ref. No.:3684 / (NET-JULY 2018)) provided by the University Grants Commission, Government of India. This research work is also supported by the project entitled “Participatory and Real-time Pollution Monitoring System For Smart City, funded by Higher Education, Science & Technology and Biotechnology, Department of Science & Technology, Government of West Bengal, India”.

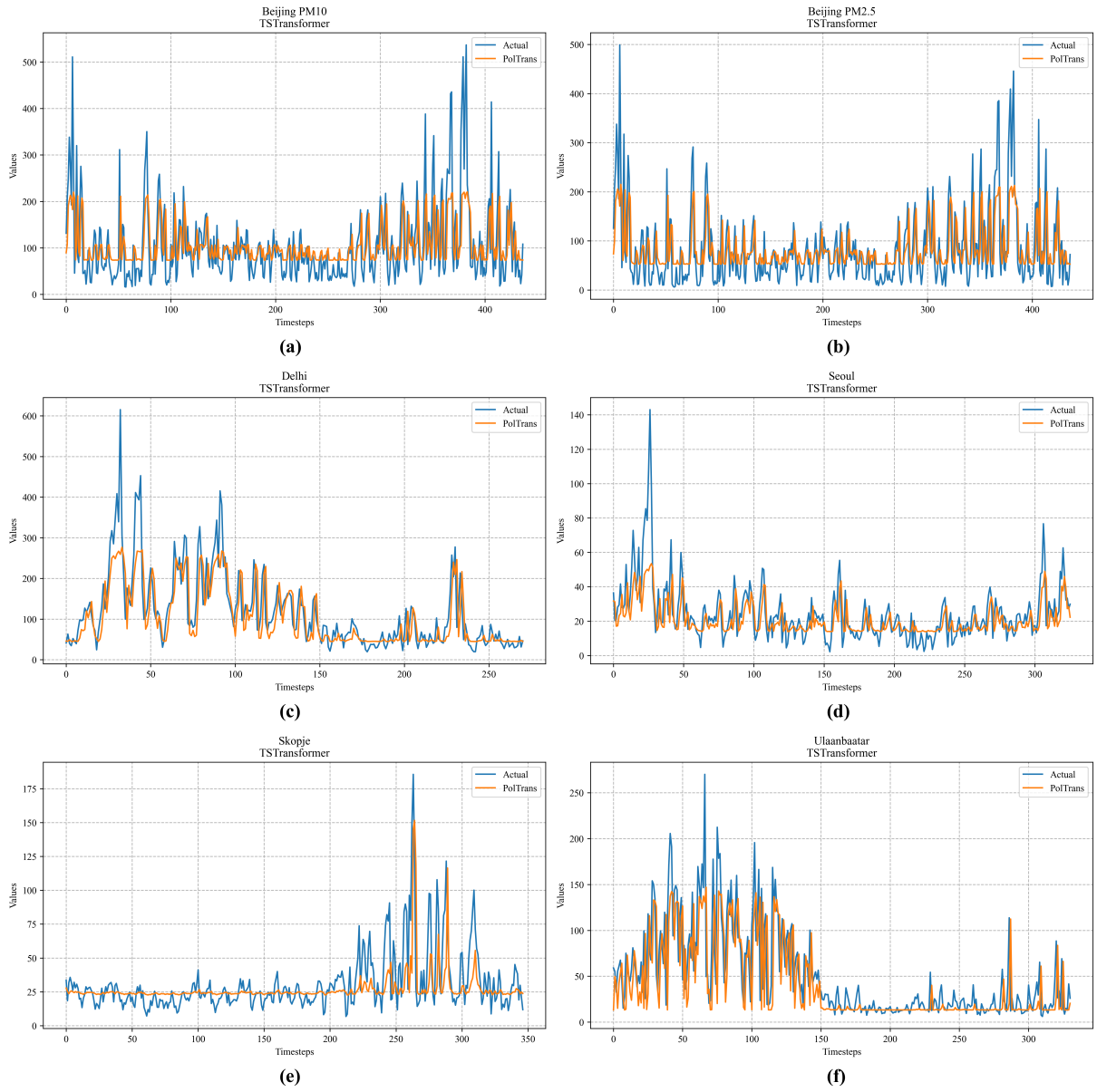


Fig. 11. Line plots demonstrating predictions made by PolTrans (indicated in orange) vs actual $PM_{2.5}$ / PM_{10} count as reported (in $\mu g/m^3$) for (a) Beijing PM_{10}, (b) Beijing $PM_{2.5}$ and a sample station in each of (c) Delhi, (d) Seoul, (e) Skopje and (f) Ulaanbaatar datasets

REFERENCES

[1] R. N. Jones, "An environmental risk assessment/management framework for climate change impact assessments," *Natural hazards*, vol. 23, no. 2, pp. 197–230, 2001. [Online]. Available: https://doi.org/10.1023/A:1011148019213

[2] "Climate change – united nations sustainable development." [Online]. Available: https://www.un.org/sustainabledevelopment/climate-change/

[3] C. Gomes, T. Dietterich, C. Barrett, J. Conrad, B. Dilkina, S. Ermon, F. Fang, A. Farnsworth, A. Fern, X. Fern *et al.*, "Computational sustainability: Computing for a better world and a sustainable future," *Communications of the ACM*, vol. 62, no. 9, pp. 56–65, 2019. [Online]. Available: https://doi.org/10.1145/3339399

[4] P. Nath, P. Saha, A. I. Middya, and S. Roy, "Long-term time-series pollution forecast using statistical and deep learning methods," *Neural Computing and Applications*, vol. 33, no. 19, pp. 12 551—-12 570, 2021. [Online]. Available: https://doi.org/10.1007/s00521-021-05901-2

[5] A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. N. Gomez, Ł. Kaiser, and I. Polosukhin, "Attention is all you need," in *Advances in neural information processing systems*, 2017, pp. 5998–6008. [Online]. Available: https://arxiv.org/abs/1706.03762

[6] N. Parmar, A. Vaswani, J. Uszkoreit, L. Kaiser, N. Shazeer, A. Ku, and D. Tran, "Image transformer," in *Proceedings of the 35th International Conference on Machine Learning*, ser. Proceedings of Machine Learning Research, J. Dy and A. Krause, Eds., vol. 80. PMLR, 10–15 Jul 2018, pp. 4055–4064. [Online]. Available: https://proceedings.mlr.press/v80/parmar18a.html

[7] R. D. Peng, F. Dominici, and T. A. Louis, "Model choice in time series studies of air pollution and mortality," *Journal of the Royal Statistical Society: Series A (Statistics in Society)*, vol. 169, no. 2, pp. 179–203, 2006. [Online]. Available: https://doi.org/10.1111/j.1467-985X.2006.00410.x

[8] J. W. Koo, S. W. Wong, G. Selvachandran, H. V. Long, and L. H. Son, "Prediction of air pollution index in kuala lumpur using fuzzy time series and statistical models," *Air Quality, Atmosphere & Health*, vol. 13, no. 1, pp. 77–88, 2020. [Online]. Available: https://doi.org/10.1007/s11869-019-00772-y

[9] F. Dominici, A. McDermott, S. L. Zeger, and J. M. Samet, "On the Use of Generalized Additive Models in Time-Series Studies of Air Pollution and Health," *American Journal of Epidemiology*, vol. 156, no. 3, pp. 193–203, 08 2002. [Online]. Available:

https://doi.org/10.1093/aje/kwf062

[10] G. Reikard, "Volcanic emissions and air pollution: Forecasts from time series models," *Atmospheric Environment: X*, vol. 1, p. 100001, 2019. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S2590162118300017

[11] X. Fang, R. Li, H. Kan, M. Bottai, F. Fang, and Y. Cao, "Bayesian model averaging method for evaluating associations between air pollution and respiratory mortality: a time-series study," *BMJ Open*, vol. 6, no. 8, 2016. [Online]. Available: https://bmjopen.bmj.com/content/6/8/e011487

[12] N. Güler Dincer and Özge Akkuş, "A new fuzzy time series model based on robust clustering for forecasting of air pollution," *Ecological Informatics*, vol. 43, pp. 157–164, 2018. [Online]. Available: https://doi.org/10.1016/j.ecoinf.2017.12.001

[13] S. A. Shahriar, I. Kayes, K. Hasan, M. A. Salam, and S. Chowdhury, "Applicability of machine learning in modeling of atmospheric particle pollution in bangladesh," *Air Quality, Atmosphere & Health*, vol. 13, no. 10, pp. 1247–1256, 2020. [Online]. Available: https://doi.org/10.1007/s11869-020-00878-8

[14] S. Chen, K. Mihara, and J. Wen, "Time series prediction of co2, tvoc and hcho based on machine learning at different sampling points," *Building and Environment*, vol. 146, pp. 238–246, 2018. [Online]. Available: https://doi.org/10.1016/j.buildenv.2018.09.054

[15] W. Wang, C. Men, and W. Lu, "Online prediction model based on support vector machine," *Neurocomputing*, vol. 71, no. 4, pp. 550–558, 2008, neural Networks: Algorithms and Applications 50 Years of Artificial Intelligence: a Neuronal Approach. [Online]. Available: https://doi.org/10.1016/j.neucom.2007.07.020

[16] M. Stafoggia, T. Bellander, S. Bucci, M. Davoli, K. de Hoogh, F. de' Donato, C. Gariazzo, A. Lyapustin, P. Michelozzi, M. Renzi, M. Scortichini, A. Shtein, G. Viegi, I. Kloog, and J. Schwartz, "Estimation of daily pm10 and pm2.5 concentrations in italy, 2013–2015, using a spatiotemporal land-use random-forest model," *Environment International*, vol. 124, pp. 170–179, 2019. [Online]. Available: https://doi.org/10.1016/j.envint.2019.01.016

[17] R. Espinosa, J. Palma, F. Jiménez, J. Kamińska, G. Sciavicco, and E. Lucena-Sánchez, "A time series forecasting based multi-criteria methodology for air quality prediction," *Applied Soft Computing*, vol. 113, p. 107850, 2021. [Online]. Available: https://doi.org/10.1016/j.asoc.2021.107850

[18] H. Niska, T. Hiltunen, A. Karppinen, J. Ruuskanen, and M. Kolehmainen, "Evolving the neural network model for forecasting air pollution time series," *Engineering Applications of Artificial Intelligence*, vol. 17, no. 2, pp. 159–167, 2004, intelligent Control and Signal Processing. [Online]. Available: https://doi.org/10.1016/j.engappai.2004.02.002

[19] D. Dunea, A. Pohoata, and S. Iordache, "Using wavelet–feedforward neural networks to improve air pollution forecasting in urban environments," *Environmental monitoring and assessment*, vol. 187, no. 7, pp. 1–16, 2015. [Online]. Available: https://doi.org/10.1007/s10661-015-4697-x

[20] P. Soh, J. Chang, and J. Huang, "Adaptive deep learning-based air quality prediction model using the most relevant spatial-temporal relations," *IEEE Access*, vol. 6, pp. 38 186–38 199, 2018. [Online]. Available: https://ieeexplore.ieee.org/document/8392677

[21] F. Lei, X. Dong, and X. Ma, "Prediction of pm2. 5 concentration considering temporal and spatial features: A case study of fushun, liaoning province," *Journal of Intelligent & Fuzzy Systems*, no. Preprint, pp. 1–11, 2020. [Online]. Available: https://doi.org/10.3233/JIFS-201515

[22] S. M. Kazemi, R. Goel, S. Eghbali, J. Ramanan, J. Sahota, S. Thakur, S. Wu, C. Smyth, P. Poupart, and M. Brubaker, "Time2vec: Learning a vector representation of time," 2019. [Online]. Available: https://arxiv.org/abs/1907.05321

[23] Vopani, "Air quality data in india (2015 - 2020)," Jul 2020. [Online]. Available: https://www.kaggle.com/rohanrao/air-quality-data-in-india

[24] Bappe, "Air pollution in seoul," Apr 2020. [Online]. Available: https://www.kaggle.com/bappekim/air-pollution-in-seoul

[25] S. Petrushevski, "Air pollution in skopje from 2008 to 2018," Mar 2018. [Online]. Available: https://www.kaggle.com/cokastefan/pm10-pollution-data-in-skopje-from-2008-to-2018

[26] R. Ritz, "Ulaanbaatar particulate matter pollution 2015-2018," Nov 2018. [Online]. Available: https://www.kaggle.com/robertritz/ulaanbaatar-particulate-matter

[27] Ministry of Environment, Forest and Climate Change, "Central control room for air quality management," https://cpcb.nic.in/.

[28] US Department of State, *Air Now International US Embassies and Consulates*. [Online]. Available: https://www.airnow.gov/international/us-embassies-and-consulates/

[29] D. Dua and C. Graff, "UCI machine learning repository," 2017. [Online]. Available: http://archive.ics.uci.edu/ml

[30] S. Zhang, B. Guo, A. Dong, J. He, Z. Xu, and S. X. Chen, "Cautionary tales on air-quality improvement in beijing," *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 473, no. 2205, p. 20170457, 2017.

[31] K. He, X. Zhang, S. Ren, and J. Sun, "Delving deep into rectifiers: Surpassing human-level performance on imagenet classification," in *Proceedings of the IEEE international conference on computer vision*, 2015, pp. 1026–1034. [Online]. Available: https://openaccess.thecvf.com/content_iccv_2015/html/He_Delving_Deep_into_ICCV_2015_paper.html

[32] D. P. Kingma and J. Ba, "Adam: A method for stochastic optimization," *arXiv preprint arXiv:1412.6980*, 2014. [Online]. Available: https://arxiv.org/abs/1412.6980