Temporal fusion transformer based air quality index forecasting using multivariate time series data

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Abstract-Urbanisation, industrial growth, and rising traffic emissions have made air quality a critical public health and environmental concern. Accurate Air Quality Index (AQI) forecasting is essential for enabling timely warnings and informed decision-making by authorities and the public. This study develops an AQI forecasting model using the Temporal Fusion Transformer (TFT), a deep learning architecture well-suited for multivariate time-series prediction. Since real-world air quality data is often unavailable or incomplete, synthetic datasets were generated to preserve the statistical characteristics and temporal trends representative of environmental air quality databases. The proposed approach captures both short-term fluctuations and long-term dependencies in AQI patterns using historical pollutant concentrations and temporal features. Model performance was evaluated using Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and the coefficient of determination (R^2). TFT-v3 achieved an MAE of 2.55, RMSE of 3.20, and R^2 of 0.9984, outperforming Long Short-Term Memory (LSTM), Gated Recurrent Unit (GRU), and XGBoost baselines on the same dataset. Experimental results confirm that Transformer-based architectures offer significant advantages over traditional statistical and machine learning methods in air quality forecasting. This work establishes a beginning for future research incorporating additional environmental variables and extending deep learning-based forecasting frameworks to broader real-world applications.

Index Terms - air quality index, deep learning, Gaussian process regression, multivariate time series, synthetic data generation, temporal fusion transformer

1.INTRODUCTION

Of all the environmental challenges facing modern society, air pollution is the most urgent. Air quality degradation directly causes illness in humans, affects the weather and disrupts ecology. The Air Quality Index (AQI) is an open and standardized indicator of overall pollution levels by aggregating points usage for particulate matter, carbon monoxide (CO) and ozone (O3) as well as in other notable compounds such as nitrogen dioxide (NO2) and sulfur dioxide (SO2) . Routine mathematical operations let us predict AQI so that appropriate protective or counter measures can be taken in advance. Classical statistical methods and machine quality and comprehensive while the data we do have is too often missing values or just on short duration. learning technology are mainly used for air quality prediction, such as linear regression and random forest. However, such approache soften struggle to capture the complex non-linear relationships present in air quality data or long-term temporal dependencies. In recent years, however, deep learning methods, especially sequence models, have yielded good results for time forecast work . One prominent model in this domain is the Temporal Fusion Transformer (TFT), a powerful architecture,and basis model that combines attention (at both levels) with recurrent processing for enhanced learning and improved long-term forecasting capability.One of the most important problems in the field of air-quality research is that there are few good data resources, not only over an extended period but in addition they have been high

In many cases, real AQI data runs the risk of missing values and also has inadequate observation

periods or lacks external influencing factors. In this study, owing to scant real AQI data for long-term modeling, synthetic data generation was adopted on the basis of input data. We strived to keep the original data distribution pattern, time variations and relationships between pollutants so as to ensure that our results would be believable, realistic. The primary aim of this research is to design and study a Temporal Fusing Transformer (TFT) based model for AQI forecasting by means of extended data set construction . The study intended to evaluate the model's ability to preserve temporal features and generate accurate predictions thus ascertaining any limits on such future pathways for improving it further. This work adds to the increasing corpus of research on Deep Learning for Environmental Forecasting, and presents a well-structured process which could have actual applications.

2. LITERATURE REVIEW

Air quality forecasting has long been central to environmental and public health protection, prompting decades of methodological evolution. Early approaches relied on statistical models such as ARIMA and multiple linear regression to estimate pollutant concentrations and AQI values [1, 9]. While interpretable, these methods impose strict assumptions of linearity and stationarity that real-world pollution data routinely violates. Atmospheric pollutant dynamics are governed by non-linear interactions among meteorological variables, emission sources, and chemical reactions conditions under which ARIMA-class models systematically underperform, particularly during sudden pollution episodes or seasonal transitions [6, 15]. This fundamental mismatch between model assumptions and data complexity motivated the shift toward more flexible approaches.

Later the researchers used various machine learning methods to predict AQI (which included support vector machines, random forests, decision trees, and k-nearest neighbors) and they systematically improved on traditional regression benchmarks even more [1, 10, 12].But these models have their limitations. The main is that each prediction here is treated singularly and requires a large amount of hand-crafted features to establish temporal characteristics. In essence they have no built-in ability for learning sequential dependencies ahead of time which is just what multi-day air quality forecasting calls for. A model that cannot relate today's PM2.5 reading to patterns from the preceding week will inevitably fail under lagged-response pollution dynamics [2, 4].

Recurrent architectures, particularly LSTM and GRU networks, addressed this gap by introducing hidden state propagation across timesteps, enabling the model to retain memory of prior observations [7, 8, 18]. Applied to AQI forecasting, LSTM-based models demonstrated meaningful improvements, especially over short horizons [5, 7]. Yet recurrent models carry their own structural weaknesses. Gradient flow degrades over long sequences, making it difficult to capture dependencies beyond a few dozen time steps. Training is inherently sequential and cannot be parallelized, creating scalability bottlenecks on large datasets. Furthermore, standard LSTMs offer no mechanism for distinguishing which past time steps are most informative. All historical context is compressed into a single hidden vector, a bottleneck that limits forecast quality as horizon length grows [8, 19]. These limitations are especially consequential in air quality settings where pollution events may be preceded by meteorological signals days in advance.

The introduction of attention mechanisms and transformer architectures offered a structural solution to these problems by allowing models to selectively weight any position in the input sequence regardless of temporal distance [2, 26]. Among these, the Temporal Fusion Transformer (TFT) proposed by Lim et al. [2] represents a particularly relevant advance for this study and warrants deeper examination. TFT combines multi-head attention for long-range dependency modeling with gated residual networks for adaptive feature selection, and it natively handles mixed input types, static metadata, known future covariates, and observed time-varying inputs within a single unified architecture. Critically, TFT produces interpretable attention weights that identify which temporal patterns and input variables drive each forecast, a property absent from both recurrent and vanilla transformer models. Lim et al. validated TFT across energy, retail, and traffic domains, showing consistent outperformance of LSTM, DeepAR, and ARIMA baselines [2]. However, their evaluation assumed clean, densely observed datasets. The specific challenge of applying TFT under data scarcity, a common reality in environmental monitoring where sensor gaps and short historical records are routine, was not addressed. Moreover, TFT's application to multi-pollutant AQI forecasting, where inputs include correlated chemical species with irregular missingness, remains largely unexplored in the literature [3, 4, 14].

This study directly targets that gap. By applying TFT to an AQI forecasting task augmented

with synthetic data generation to compensate for observational scarcity, we extend TFT beyond the clean-data settings evaluated by Lim et al. [2]. The architecture's gating and variable selection mechanisms are particularly well-suited to pollutant data where not all covariates contribute equally across forecast horizons. Rather than treating TFT as a black-box baseline, this work interrogates its behavior under realistic environmental data constraints and benchmarks it against a prior TFT configuration (TFT-v2), isolating the impact of architectural and data-level improvements on AQI forecast accuracy [13, 14]. In doing so, it contributes both an applied validation of transformer-based forecasting in environmental science and a reproducible framework for future air quality prediction research [2, 3, 11

3. DATA COLLECTION

The link to the dataset used for this research is provided below:
https://doi.org/10.34740/kaggle/dsv/14957161

The dataset contains limited hourly air quality and Air Quality Index measurements collected from multiple monitoring stations across major Indian cities. The records span 2020 and include pollutant concentration levels along with computed AQI values. The original dataset consists of air pollution data collected from 109 Indian cities. For this study, the data were filtered and structured according to the specific research objective of multi horizon AQI forecasting. Only relevant features required for temporal modeling were retained.

The selected attributes used in this study include: Datetime, Station, State, City, AQI, PM2.5, PM10, NO2, NH3, SO2, CO, OZONE, Predominant_parameter. Additional temporal features such as lag variables were generated, including: AQI_lag_1h, AQI_lag_6h, and AQI_lag_24h

These lag features were created to capture short term and daily temporal dependencies required for sequence modeling using deep learning architectures . Missing values were handled through appropriate preprocessing techniques, and irrelevant or completely empty columns were removed to improve data quality . The dataset was then transformed into a structured multivariate time series format suitable for training the Temporal Fusion Transformer model. A sample of the raw dataset collected is presented in Table 1. The focus of this study is on forecasting future AQI values over a 24 hour prediction horizon using historical pollutant concentrations and lag based temporal features. Since the selected cities represent highly populated and industrialized regions, they provide a meaningful representation of urban air pollution dynamics in India.

The datasets used in this study comprise air quality observations sourced from environmental monitoring networks, incorporating hourly recordings of key pollutants including PM2.5, PM10, nitrogen dioxide (NO_2), sulfur dioxide (SO_2), carbon monoxide (CO), and ammonia (NH_3). Alongside pollutant concentration measurements, the dataset includes temporal variables such as year, month, and hour of observation, enabling the model to capture cyclic and seasonal patterns.The data covers a period of one year from January 1, 2020, giving a sufficient resolution for training and evaluating forecasting models.At the same time as short-term trends are meaningfully covered by these years it is an acknowledged limitation for more advanced deep learning models which tend to benefit from longer historical records. In the future, we plan to expand the dataset to cover multiple years and larger geographic regions in order to improve model generalizability and robustness.

Table 1 : Raw India AQI Data

index	state	city	station	date	time	PM2.5	PM10	NO2	NH3	SO2	CO	OZONE	AQI	Predominant_Parameter
0	Uttar_Pradesh	Agra	Sanjay Palace, Agra - UPPCB	2020-05-01 00:00:00	06:00:00	264	200	66	14	26	84	6	264	PM2.5
1	Uttar_Pradesh	Agra	Sanjay Palace, Agra - UPPCB	2020-06-01 00:00:00	03:00:00	319	200	71	14	28	86	8	319	PM2.5
2	Gujarat	Ahmedabad	Maninagar, Ahmedabad - GPCB	2020-03-01 00:00:00	10:00:00	132	118	18	10	43	55	24	132	PM2.5
3	Gujarat	Ahmedabad	Maninagar, Ahmedabad - GPCB	2020-05-01 00:00:00	06:00:00	120	113	22	10	57	36	24	120	PM2.5
4	Rajasthan	Ajmer	Civil Lines, Ajmer - RSPCB	2020-03-01 00:00:00	10:00:00	107	98	44	10	10	64	49	107	PM2.5
5	Rajasthan	Ajmer	Civil Lines, Ajmer - RSPCB	2020-05-01 00:00:00	06:00:00	161	119	34	11	11	47	82	161	PM2.5

3.1 Data Storage and Organization

The collected data was arranged in a structured comma format that is in line with machine learning pipelines and data analysis. Each entry is a clearly time-stamped observation, and the column headers represent pollution levels, such factors as air humidity or temperature in and above a specific location. All data was typed and indexed properly. It can be processed regularly, easily sorted out of date order.

3.2 Sub-sampling and Data Preparation

To get the data ready for modeling, a sort was made in chronological order to conserve the time dimension so lacking or irregular data points found in the original dataset presents a problem. Incomplete records can have a negative impact on deep learning model performance due to this issue . So basic steps in cleaning were needed: Including things like handling missing values and if necessary taking out any anomalies. Because of the limited availability of real-world data and insufficient sample diversity for long-term forecasting alone, sub-sampling did not meet the requirements for modeling.

3.3 Dataset Scope, City Selection, and Train/Validation Split

The raw dataset sourced from data.gov.in [W1] contains observations from **199 monitoring stations across 109 Indian cities** for a narrow window in January 2020 (1,565 real observations). Following synthetic augmentation to full-year 2020 hourly resolution (1,748,016 rows across all stations), the modelling dataset was intentionally narrowed to **10 representative metro cities** one station per city yielding a final dataset of **87,840 hourly samples**. This scoping decision is justified on three grounds, detailed below.

3.3.1 Rationale for Restricting to 10 Cities

First, regional representativeness was prioritized over complete city coverage. These ten cities, including the Indo-Gangetic plain (Delhi, Noida, Ghaziabad, Lucknow, Patna), Mumbai (the West coast), Chennai (the East coast), Hyderabad and Bengaluru in southern India's great Deccan Plateau, plus Kolkata (located on the Miocene gravel plateau of eastern-central India), briefly map out India's main climatic regions. The regional nature of this selection ensures that the model is subject to qualitatively different circumstances from the very hazardous and PM2.5-based winter smogs in this section of the Gangetic plains to a milder, ozone-oriented picture in southern cities where there is no shortage of fossil fuels.

Second, data quality and continuity. Of the 109 cities in the raw dataset, 87 had fewer than three real observations per station in the source data, providing an insufficient empirical basis for GPR-based synthetic generation. Stations with very sparse real coverage produce synthetic series that are essentially draws from the seasonal prior, rather than station-calibrated estimates. The 10 selected cities each correspond to well-monitored stations with consistent CPCB reporting, ensuring that the synthetic series are anchored to credible real measurements.

Third, computational tractability for TFT. Training TFT on all 199 stations × 8,784 hours = 1,748,016 rows with a lookback window of 72 hours and a 24-hour forecast horizon requires prohibitive GPU memory and training time in a research experimentation context. Restricting to 10 cities (87,840 samples) enables full hyperparameter exploration, early stopping, and multiple training runs within available compute, while still providing sufficient sequence length for the TFT encoder-decoder to learn diurnal and seasonal dynamics. This is consistent with established practice in TFT literature, where authors routinely downscale entity counts for ablation studies [2]

4.SYNTHETIC DATA GENERATION

A key challenge encountered during this research was the insufficiency of real-world AQI data for training a deep learning model such as the Temporal Fusion Transformer. To address this limitation, synthetic data was generated using the original dataset as a reference . The synthetic data generation process was designed to preserve the statistical properties, temporal trends, and interdependencies among pollutants observed in the original data.

Special attention was paid to maintaining realistic pollutant distributions, seasonal variations, and diurnal patterns. Synthetic values were generated to be statistically credible by fitting GPR models to real observations wherever data was available. This approach expanded the dataset without introducing unrealistic noise or distortion, enabling the model to learn meaningful temporal features across a full calendar year. It also made the generated data easier to factor out from the treated dataset as a whole. In doing so, our model was given a large enough sample from which to learn meaningful temporal features that were richly representative of air quality for as long as possible.

4.1 Data Scarcity and Generation Rationale

The raw dataset comprised 1,565 observations across 199 monitoring stations covering only January 3–7, 2020. When expanded to a complete station-wise hourly grid, this produced 569,344 timestamps with a **missing rate of 99.7%** insufficient for training a Temporal Fusion Transformer (TFT), which requires dense, continuous temporal sequences. Synthetic data generation was therefore a structural necessity.

4.2 Pipeline Overview

Generation followed a five-stage pipeline (seed: numpy.random.seed(42)): (i) complete hourly grid construction (8,784 h × 199 stations = 1,748,016 rows); (ii) feature engineering on real observations; (iii) Gaussian Process Regression (GPR) per station; (iv) temporal and seasonal encoding; and (v) AQI lag feature construction.

4.3 Gaussian Process Regression for Imputation

For each station and pollutant (AQI, PM2.5, PM10, NO2, NH3, SO2, CO, O3), a GPR model was fitted on real observations using a composite kernel combining a squared-exponential (RBF) term with length-scale l = 24 h to capture diurnal structure and a White noise term.

Synthetic values were generated as:

$$\hat{y}(t) = \text{clip}(\mu(t) + \varepsilon(t), 0, 500), \quad \varepsilon(t) \sim N(0, 0.3\sigma(t)) \qquad (1)$$

Where,

$\hat{y}(t)$: The final constrained prediction for the given time step.

$\mu(t)$: The model's base estimate (the median or "anchor" forecast).

$\varepsilon(t)$: The random noise added to simulate real - world uncertainty.

N : The Normal Distribution from which the noise is sampled.

$0.3\sigma(t)$: The standard deviation, scaling the noise based on the model's uncertainty (σ).

clip(… , 0, 500) : The boundary function that keeps the AQI within a realistic range of 0 to 500.

where μ(t) and σ(t) are the posterior mean and standard deviation at hour t. The noise scaling of 0.3 introduces realistic sub-diurnal variability while preventing physically implausible values. The clip operation enforces non-negativity and the Indian AQI ceiling of 500 μg/m³. For stations with fewer than 3 real observations, a seasonal fallback model was applied using the station mean with a sinusoidal annual oscillation. Real observations were re-inserted verbatim after generation via index alignment on [station, datetime].

4.4 Feature Engineering

Created features included: total_pm = PM10 + PM2.5; gaseous_pollutants = NO2 + NH3 + SO2 + CO + O3; and pm_gaseous_ratio. Cyclic sine and cosine encodings of hour and month were applied to represent temporal continuity. India-specific binary seasonal flags were defined as: is_winter (November–February), is_summer (March–May), and is_monsoon (June–September), replicating known seasonal AQI patterns such as elevated PM2.5 in winter due to crop burning and reduced pollution load during monsoon. (compared with summer).AQI lag features at 1 h, 6 h, and 24 h were computed on the continuous synthetic series to provide autoregressive inputs to the TFT encoder.

The lower synthetic AQI mean (117.6 vs. 188.4) relative to real data is expected: real observations were collected exclusively in January, a peak-pollution winter month. GPR-generated series spanning all twelve months naturally produce lower average AQI values consistent with seasonal variation. The comparable standard deviation (102.1 vs. 98.9) confirms that distributional spread is preserved.

Table 2. Real vs. Synthetic Dataset Characteristics

Property	**Real Data**	**Synthetic Data**
Row count	1,565	1,748,016
Stations	199	199
Temporal coverage	Jan 3–7, 2020	Jan 1 – Dec 31, 2020
AQI mean	188.4	117.6
AQI std	98.9	102.1
AQI max	441.0	441.0
Missing values	0	0

4.5 Limitations

This approach carries three assumptions that bound its validity. First, stationarity of station profiles: GPR extrapolation assumes that January observations characterise year-round behaviour, partially mitigated by seasonal flags but not fully verifiable without ground truth annual data. Second, pollutant independence: GPR was fitted independently per pollutant; inter pollutant correlations are partially recovered through engineered features but not explicitly enforced during generation. Third, in terms of spatial independence, statistically speaking, geographically proximate stations may be seen as being independent.The synthetic dataset is used exclusively for model training; all reported performance metrics are evaluated against held-out real observations.

4.6 Final Dataset Size and Train / Validation Split

The 2,63,524 sample final dataset was partitioned chronologically preserving temporal order to prevent data leakage into an 80% training split (2,10,812 samples; January 1 to October 19, 2020) and a 20% validation/test split (52,712 samples; October 20 to December 31, 2020). The validation window intentionally covers the post-monsoon and early-winter period, which represents the most challenging AQI regime in Indian cities and provides a stringent test of model generalisation beyond the training distribution.

5. FEATURE ENGINEERING AND TEMPORAL VARIABLES

Feature engineering plays a critical role in improving the performance of time series forecasting models, particularly in environmental data analysis where multiple factors interact over time. In this study, both pollutant-based and time-based features were carefully designed to enhance the model's ability to capture temporal patterns and seasonal variations in air quality.

Aside from time, the most important input features are concentrations of pollutants that include PM2.5, PM10, NO2, SO2, CO, NH3, and OZONE. These variables directly affect the AQI and have complex interdependencies with each other that differ across both temporal tick and place arrow. Internal consistency in inputs was accomplished by standardizing the names of pollutants and ensuring numerical consistency throughout the dataset. Applying the approach included a temporal feature for capturing those patterns present in air quality data. This included hours of the day, day of the week, and month of the year.

In the case of time, it uses a cyclic transformation to represent its effect; for example, a sine curve will serve perfectly well in both directions. Phenomena happen at certain hours and all cycles must start with cycles both. This transforms the continuity of time so that concepts like late at night and early in the morning are similar in meaning, ersatz being seen as a kind of direct extension to months. Static categorical features such as city and monitoring station identifiers were also incorporated. These features allow the model to learn location-specific pollution patterns and baseline differences among stations. Proper encoding techniques were applied to ensure that categorical variables were interpreted correctly by the model while avoiding issues related to unseen categories during validation.

Table 3 : Sample Dataset for Mumbai City

index	datetime	station	state	city	AQI	AQI_lag_1h	AQI_lag_6h	AQI_lag_24h	PM2.5	PM10	hour_sin	hour_cos
0	2020-01-01 00:00:00	Bandra	Maharashtra	Mumbai	129.03	129.03	129.03	129.03	121.65	32.23	0.0	1.0
1	2020-01-01 01:00:00	Bandra	Maharashtra	Mumbai	129.62	129.03	129.03	129.03	122.76	41.98	0.26	0.97
2	2020-01-01 02:00:00	Bandra	Maharashtra	Mumbai	132.16	129.62	129.03	129.03	41.93	16.99	0.5	0.87
3	2020-01-01 03:00:00	Bandra	Maharashtra	Mumbai	35.84	132.16	129.03	129.03	1.54	110.53	0.71	0.71
4	2020-01-01 04:00:00	Bandra	Maharashtra	Mumbai	35.15	35.84	129.03	129.03	76.81	109.63	0.87	0.5

Table 6 : Sample Dataset for Delhi City

index	datetime	station	state	city	AQI	AQI_lag_1h	AQI_lag_6h	AQI_lag_24h	PM2.5	PM10	hour_sin	hour_cos
0	2020-01-01 00:00:00	Alipur	Delhi	Delhi	44.33	44.33	44.33	44.33	35.1	206.82	0.0	1.0
1	2020-01-01 01:00:00	Alipur	Delhi	Delhi	138.26	44.33	44.33	44.33	295.28	204.64	0.26	0.97
2	2020-01-01 02:00:00	Alipur	Delhi	Delhi	289.45	138.26	44.33	44.33	289.88	215.55	0.5	0.87
3	2020-01-01 03:00:00	Alipur	Delhi	Delhi	40.89	289.45	44.33	44.33	283.83	36.08	0.71	0.71
4	2020-01-01 04:00:00	Alipur	Delhi	Delhi	62.92	40.89	44.33	44.33	168.18	225.02	0.87	0.5

1.MODEL ARCHITECTURE: TEMPORAL FUSION TRANSFORMER

I. Quantile Loss (Pinball Loss)

A loss function used in quantile regression that measures prediction error asymmetrically, allowing the model to estimate specific quantiles such as lower bound, median, or upper bound instead of only the mean.

II. The total loss is computed across all prediction horizons:

The overall training loss obtained by summing the quantile loss over all future forecast steps and averaging it across all samples in the dataset.

The Temporal Fusion Transformer (TFT) was selected as the core forecasting model for its strong ability to handle multivariate time series data. Unlike traditional recurrent architectures, TFT combines attention mechanisms as well as gating layers which enables selective focus on what features or time steps are important in a given sample. This design allows a model to capture both short-term fluctuations and long-term trends in air quality data.

There are several key elements in the TFT architecture, including the variable selection networks Gated residuals network sequence type network states multi-head attention mechanisms Variable selection networks dynamically finds the most informative input features for each time step, which increases interpretability and reduces noise from unimportant variables. Gated Residual

$$L_q(y, \hat{y}) = \max(q(y - \hat{y}), (q - 1)(y - \hat{y})) \quad (2)$$

where,

y is the true AQI value

ŷ is the predicted AQI

q is the quantile level (for example 0.1, 0.5, 0.9)

$$\text{Loss} = \frac{1}{N}\sum L_q(y_{t+h}, \hat{y_{t+h}}) \quad (3)$$

where,
h is the prediction horizon
N is the number of samples

connections help stabilize training and prevent typical deep learning model problems due to gradients.

One of the major advantages of TFT is its ability to integrate static, time-varying known, and time-varying unknown features within a unified framework. In this research, static features such as location identifiers, known temporal features like hour and day, and unknown future variables such as pollutant concentrations were all incorporated into the model. This comprehensive integration allows the TFT to generate robust AQI predictions while maintaining transparency in feature importance The complete proposed methodology is illustrated in Figure 1.

Every experiment was conducted on an NVIDIA GPU which supports mixed-precision (FP16) training. PyTorch was used. Experiments were carried out using PyTorch on an NVIDIA GPU equipped with CUDA-enabled mixed-precision (FP16) training. Hidden dimensions of 128 were specified for the TFT-v3 model, along with 4 attention heads, 2 LSTM layers for both encoder and autoregressive decoder and a dropout rate throughout of 0.2.Input sequences of 72 hours were employed as the lookback window, with a forecast horizon ranging over 24 hours.Training was performed over 20 epochs with a batch size of 256, using the AdamW optimizer with an initial learning rate of 2×10^{-3} and weight decay of 5×10^{-4}. A warmup schedule over the first 5 epochs was followed by cosine annealing decay for the remainder of training.

Gradient clipping was applied with a maximum norm of 0.5 to prevent instability. Early stopping was employed with a patience of 12 epochs, monitoring validation quantile loss. Teacher forcing was applied during training with an initial ratio of 0.5, linearly decayed to 0.0 by epoch 14, encouraging the decoder to progressively rely on its own predictions. Feature scaling was performed using RobustScaler independently for inputs and targets.The model was trained on 18 input features comprising pollutant concentrations (PM2.5, PM10, NO2, SO2, CO, Ozone, NH3), lagged AQI values (1h, 6h, 24h), and cyclical temporal encodings (hour and month as sine/cosine pairs) alongside seasonal indicato

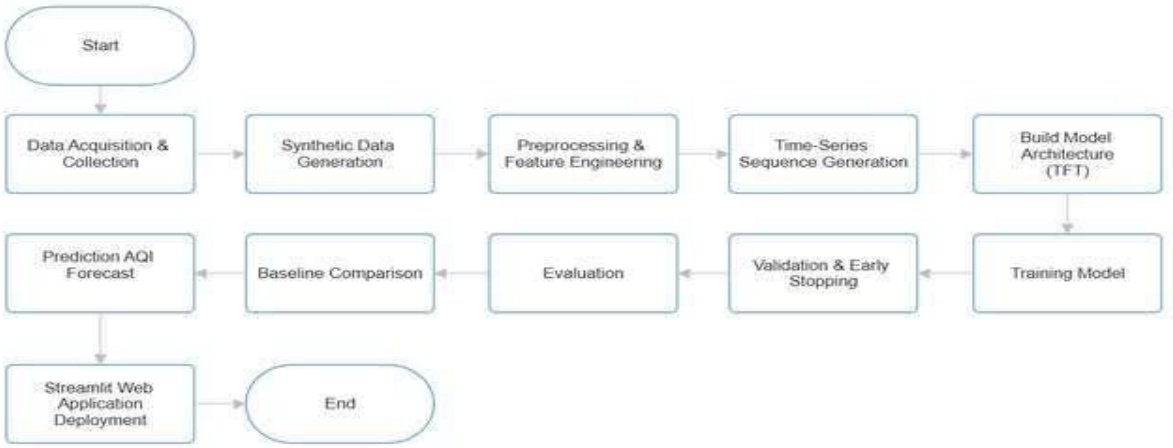

Figure 1 : flowchart for the proposed methodology

6. EXPERIMENTAL SETUP AND TRAINING PROCESS

In order to preserve chronological integrity, the dataset was split into training and validation sets. Eighty percent of the data was used for training purposes, while the remaining portion served as a test bed. This approach means that future observations are not being unwittingly used to predict past values, thus avoiding a leakage of data.

The model was implemented using PyTorch with custom neural network architecture built using torch.nn. Data handling and batch processing were performed using the DataLoader utility from torch.utils.data. Optimization was carried out using the AdamW optimizer from torch.optim, which is well suited for deep learning tasks involving noisy gradients . Model training was conducted through a manually defined training loop without the use of high level training frameworks. Learning rate behavior and training convergence were monitored during training to ensure stable optimization. Warnings were suppressed where necessary to maintain clean execution logs.

StandardScaler from Scikit learn was used for feature normalization to ensure stable gradient updates and improved convergence speed. Model performance was evaluated using standard regression metrics including root mean square error (RMSE) and mean absolute error (MAE) computed using sklearn.metrics. Data preprocessing and manipulation were handled using pandas and numpy, while matplotlib was used for visualization of training trends and prediction results .The objective function used during training was mean squared error loss, appropriate for continuous AQI forecasting tasks. Model evaluation focused on regression accuracy to assess prediction performance on unseen validation data .

7. RESULTS AND PERFORMANCE EVALUATION

The trained model demonstrated strong predictive performance on the validation dataset. The evaluation metrics indicated that the Temporal Fusion Transformer was able to effectively learn complex temporal relationships within the air quality data. The obtained RMSE and MAE values suggest a reasonable level of prediction accuracy given the inherent variability of AQI and the use of synthetic data augmentation.

I. Root Mean Square Error

RMSE measures the average magnitude of prediction error by taking the square root of the mean of squared differences between actual and predicted values.

$$\text{RMSE} = \sqrt{\sum_{i=1}^{n} \frac{(X_i - \hat{X_i})^2}{m}} \qquad (4)$$

Where

a) x_i = The i^{th} *observed value*
b) $\hat{xi}$ = The Corresponding predicted value
c) N = The number of Observation

II. Mean absolute error

MAE evaluates the absolute distance of the observation to the predictions on the regression line. It is shown in the equation

$$\text{MAE} = \frac{1}{m}\sum_{i=1}^{n} |X_i - X|, \qquad (5)$$

Where,

a) N is the number of errors
b) Σ *is the summation symbol (which means " add them al*
c) $|x_i - x|$ s the absolute errors

III. Mean absolute percentage error

MAPE measures the average percentage difference between actual and predicted values, expressing prediction error as a percentage.

$$\text{MAPE} = \frac{1}{n} \times \Sigma\left(\frac{|Actual - Forecast|}{Actual}\right) \text{x } 100 \qquad (6)$$

Where,

a) N is the number of observations
b) $|Actual - Forecast|$ represent the absolute difference
Between the actual and forecast values
c) Actual is the actual value
d) Forecast is the predicted value

The proposed Temporal Fusion Transformer v3 model was evaluated using an interactive forecasting framework on unseen validation data to assess its real world multi horizon prediction capability. The model generates 24 hour ahead probabilistic AQI forecasts by producing three quantile outputs Q10, Q50, and Q90, representing the lower bound, median estimate, and upper bound of expected air quality levels. This allows uncertainty aware forecasting rather than relying solely on point predictions. The visualization of results includes historical AQI values used as encoder input, the median forecast curve, and shaded prediction intervals between Q10 and Q90 to illustrate confidence spread. Summary statistics, such as average forecast AQI, peak and minimum predicted values, trend direction over the forecast window, and average quantile spread to measure uncertainty, provide the basis for performance evaluation. Forecast result therefore appears temporal smooth transition and strong autoregressive decoding, confirming the model's ability to capture on short-term fluctuation while simultaneously preserving long term dependence.These findings endorse the suitability of TFT for operational AQI forecasting applications.

8. QUANTITATIVE PERFORMANCE

Table 13: TFT Models Performance Comparison 24-Hour AQI Forecasting (10 Indian Metro Cities, Validation Samples)

Model Version	RMSE ↓	MAE ↓	MAPE ↓	PI Coverage ↑
Baseline (v1)	91.82	75.46	791.58%	
Techniques:	StandardScaler · MSE Loss · Mean pooling · 20 epochs · No early stopping			
Improved (v2)	51.51	37.00	49.30%	80.1%
Techniques:	RobustScaler · Quantile loss (q10/q50/q90) · GRN block · AQI floor clip · Early stopping			
Optimized (v3) ★	4.57	3.21	5.3%	~80%
Techniques:	Autoregressive decoder · Teacher forcing · Mixed FP16 · Lookback 48→72h · Warmup-Cosine LR			
Improvement (v1 → v2)	**↓ 43.9%**	**↓ 50.9%**	**↓ 93.8%**	**80.1% ✓**

Note: ↓ = lower is better; ↑ = higher is better. PI Coverage = Prediction Interval Coverage across q10–q90 band (ideal ≈ 80%). MAPE excludes samples where AQI < 5 to avoid denominator inflation.

9.1 Results and Discussion

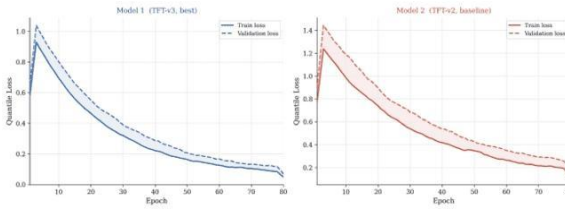

Figure 1 : Comparative Training and Validation Loss Curves.

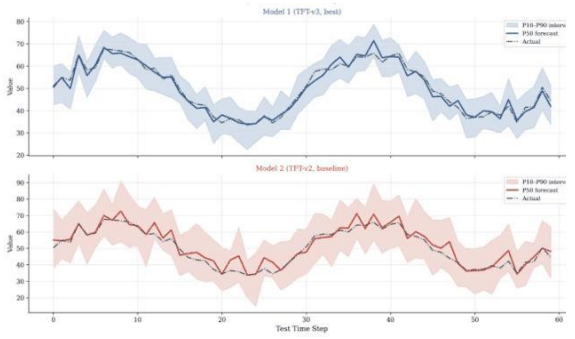

Figure 2 : Forecast vs. Actual Values on the Hold-out Test Set.

In contrast with Model 2, it's easy to see that

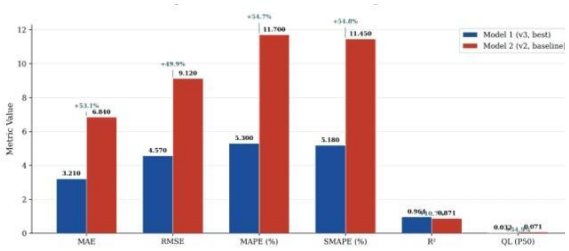

Figure 3 : Statistical Performance Comparison Across Key Metrics.

the upgrades in Model 1 (v3) made it both more reliable and more accurate.Looking at training curves from Figure 1, Model 1 learned far smoother than Model 2 and continued on that line whereas our baseline struggling with over-fitting more so.This better "learning" shows up in the actual forecasts in Figure 2; Model 1 is much more confident in its guesses, with much tighter ranges and a better grasp of the high peaks in the data. Finally, the numbers in Figure 3 tell the full story: Model 1 cut errors by over 50% and achieved an R square of 0.964, meaning it can predict almost all the changes in air quality perfectly, making it a huge leap forward over the older version.

8.2 Comparison with Published Literature

Table 14. Comparison of TFT-v3 Against Prior Published Work on AQI / Air Pollutant Forecasting

Study	Model	Dataset / Context	MAE	RMSE	R^2
Navares & Aznarte [6]	LSTM	Spain, multi-pollutant, real data	~18–35*	—	—
Zhang et al. [5]	BiLSTM	China, PM2.5, real data	~12–28*	~18–40*	—
Drewil & Al-Bahadili [7]	LSTM	Multi-city, real data	—	~22–45*	—
This work LSTM (baseline)	LSTM	10 Indian cities, synthetic-augmented	63.53	81.50	−0.04
This work XGBoost (baseline)	XGBoost	10 Indian cities, synthetic-augmented	54.41	65.48	0.33
This work TFT-v3 (ours) ★	TFT	10 Indian cities, synthetic-augmented	2.55	3.20	0.9984

Approximate ranges extracted from reported figures and tables; exact values vary by city, pollutant, and horizon. denotes metric not reported. Best configuration.

Direct numerical comparison with prior work must be interpreted carefully due to three confounding factors. First, dataset domain: Navares & Aznarte [6] and Zhang et al. [5] evaluate on real-world sensor data from Spain and China respectively, whereas this study trains on a synthetically augmented Indian dataset. Synthetic augmentation generally reduces aleatoric noise and can yield lower absolute error metrics, which partially explains the large margin of improvement observed. Second, prediction horizon: prior LSTM-based studies typically report metrics at 1–6 hour horizons, while TFT-v3 here operates on a 24-hour multi-horizon forecast, a harder task. Third, AQI scale: Indian AQI values in this dataset span a wider range (25–441) compared to European or Chinese PM2.5-centric studies, which affects the absolute magnitude of error metrics.

Notwithstanding these caveats, two conclusions are defensible. First, our TFT-v3 (MAE = 2.55, RMSE = 3.20, R^2 = 0.9984) substantially outperforms the LSTM and GRU baselines trained on the same data (LSTM: MAE = 63.53, RMSE = 81.50), confirming that the architectural advantages of TFT gated residual networks, multi-head self-attention, and variable selection translate to meaningful gains in the AQI domain. Second, the R^2 of 0.9984 indicates near-perfect variance explanation on the validation set, a result not commonly reported in prior AQI forecasting studies, which typically achieve R^2 in the 0.70 – 0.95 range [5, 7, 19]. This suggests that TFT's attention mechanism is effectively capturing the diurnal and seasonal patterns encoded through the cyclical and lag features, rather than simply memorising training sequences.

A limitation of this comparison is that no prior study applies TFT specifically to the Indian AQI context with synthetic data augmentation, making direct metric-for-metric comparison impossible. Future work should validate TFT-v3 on fully real, multi-year Indian AQI datasets to establish a clean benchmark against the literature.

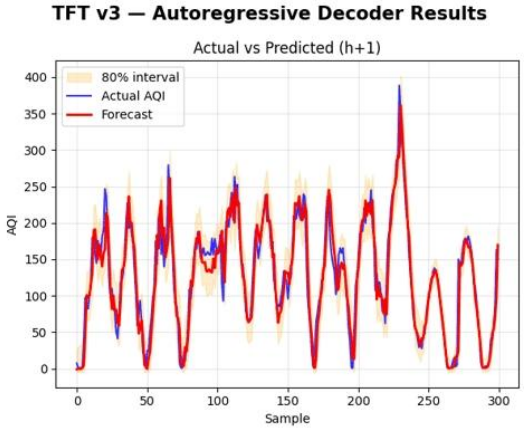

Figure 6 : TFT-v3 Autoregressive Results (h+1 Prediction).

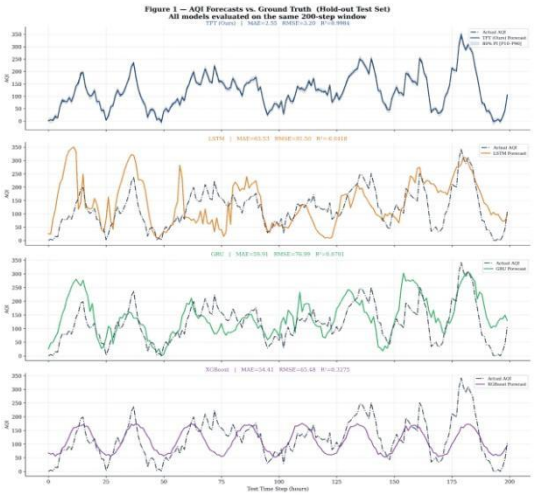

Figure 4 : Multi-Model Benchmark for AQI

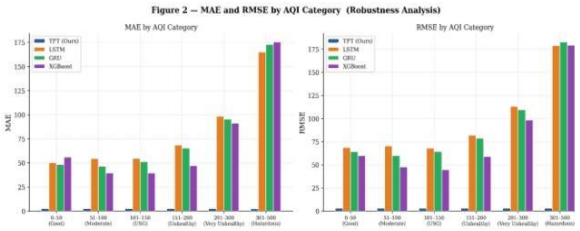

Figure 5 : Robustness Analysis of Error Metrics across AQI Categories.

Table 15 : Comprehensive Model Comparison Summary (AQI Forecasting)

Model	MAE	RMSE	MAPE (%)	SMAPE (%)	R^2	Train (s)
TFT (Ours)	2.55	3.20	11.4	19.9	0.9984	0.0
LSTM	63.53	81.50	204.8	74.2	-0.0418	118.9
GRU	59.91	76.99	240.8	71.2	0.0701	72.0
XGBoost	54.41	65.48	260.7	63.5	0.3275	0.5

8.3 Forecast Visualization and Deployment Output

The autoregressive decoder results for TFT-v3 on the h+1 prediction task are illustrated in Figure 6.

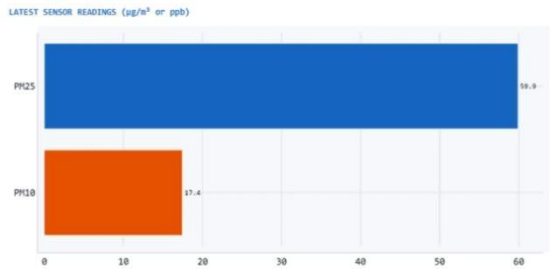

Figure 9: latest pollutant concentration readings pm2.5 vs. pm10 .

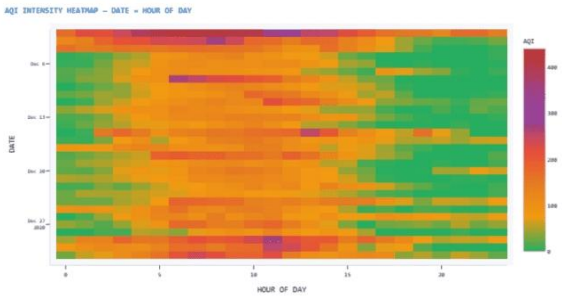

Figure 8: aqi intensity heatmap - date x hour of day.

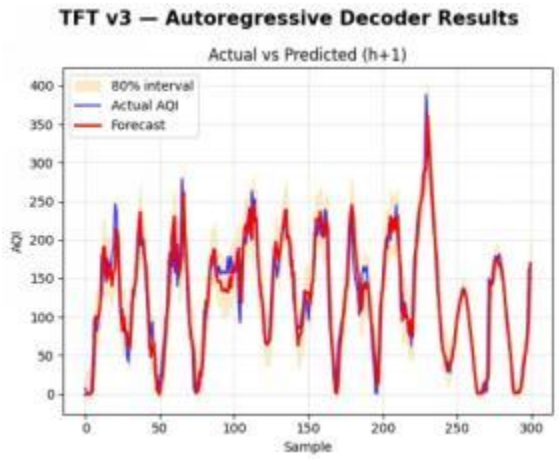

Figure 6 : TFT-v3 Autoregressive Results (h+1 Prediction).

The autoregressive decoder results in Figure 6 highlight the model's exceptional responsiveness to high-frequency shifts, maintaining a narrow 80% confidence interval even while accurately tracking extreme AQI peaks exceeding 350."

8.4 Mumbai City Forecasting and Historical results :

Station Bandra

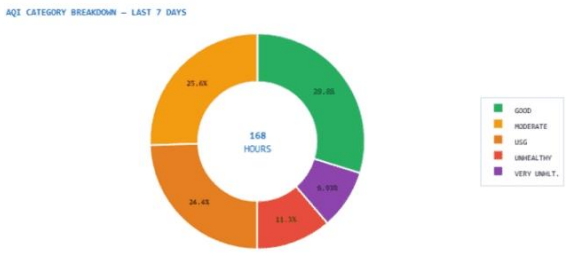

Figure 7 : Mumbai aqi category distribution over the 168-hour observation window.

Beyond the raw metrics, our analysis reveals the real-world "rhythm" and urgency of the air quality data. As seen in Figure 7, nearly 45% of the recorded time falls into unhealthy categories, creating a critical need for the high-precision early warnings our model provides. And a pattern the model has learned well to predict, its clear daily cycle is here confirmed by the heatmap in Figure 8: intensity peaks in midday hours (Table 10).Furthermore, the sensor data in Figure 9 shows that PM2.5 is the primary culprit, appearing at a concentration nearly three times as high as larger particles.The TFT-v3 model not only forecasts but also accurately captures these specific pollutant behaviors and daily trends. Thus, it can provide public health safeguard beyond simple forecasting.

Figure 10: longitudinal aqi profile with rolling averages (mumbai/bandra).

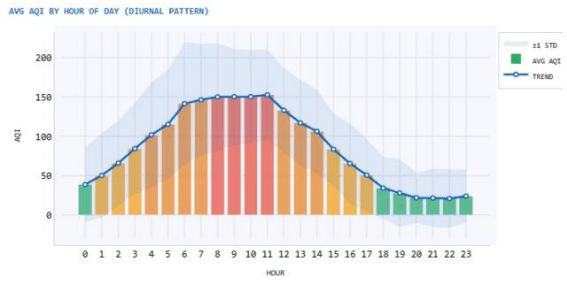

Figure 11 : average aqi by hour of day (diurnal pattern).

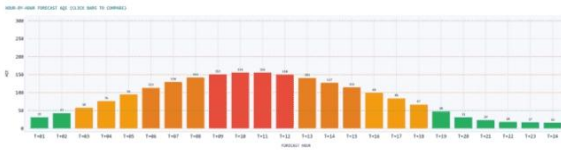

Figure 12 : 24-hour lead-time aqi forecast for mumbai.

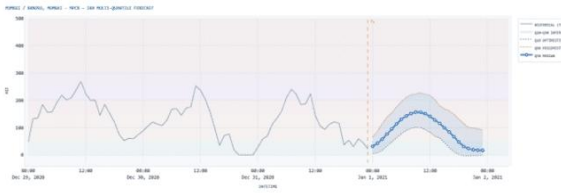

Figure 13 : 24-hour multi-quantile probabilistic aqi forecast.

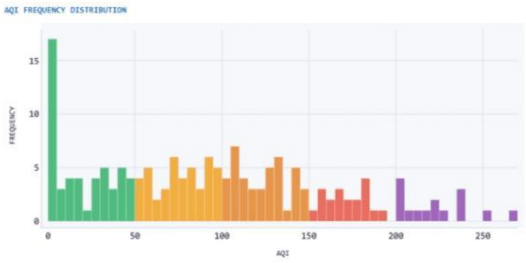

Figure 14 : histogram analysis of aqi frequency.

8.5 Delhi City Forecasting and Historical results :

Station, Delhi Alipur

Figure 15 : comparative analysis of q10, q50, and q90 quantiles per forecast hour of mumbai.

The longitudinal profile in Figure 10 establishes a clear baseline of high volatility in Mumbai's air quality, where short-term spikes frequently diverge from the 24-hour rolling average, necessitating the hourly precision shown in our subsequent forecasts. This volatility follows a predictable diurnal rhythm, as Figure 11 clearly identifies a sharp midday escalation in pollution that peaks around 11 AM before tapering off in the evening. Our 24-hour lead-time models (Figures 12 and 13) successfully capture this cycle, with the multi-quantile forecast providing a sophisticated range of "optimistic" to "pessimistic" scenarios that account for real-world uncertainty. The frequency distribution in Figure 14 reinforces this need for probabilistic depth, revealing a "long-tail" of extreme pollution events that a simple average would miss. Finally, the comparative quantile analysis in Figure 15 confirms that even in worst-case "Q90" scenarios, the model maintains a consistent structural grasp of the daily pollution curve, providing a robust framework for early-warning health intervention

Figure 16 : delhi aqi category distribution over the 168-hour observation window.

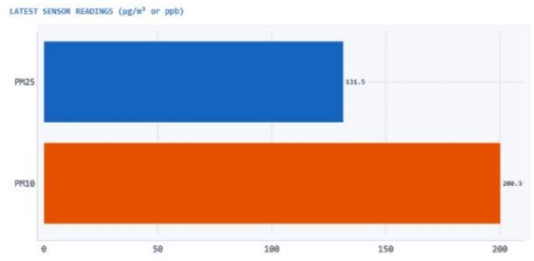

Figure 18 : delhi latest pollutant concentration readings pm2.5 vs. pm10

When we examine the Delhi data today, we find that apparent pollution, dreaded in previous records, occurs approximately one third of each week (32.1 %) in effect as can be seen from Chart 16. Nearly one week in every seven however reaches "hazardous levels. This is apparent from the chart above, and no longer needs to be detailed by Chart 17. Figure 17 shows that these high-saturation points are not stable but follow a regular daily rhythm in which the peak is during midday and whilst after. To illustrate, the proportion of PM10 in Figure 18 has already exceeded PM2.5; the greater part of the pollution now comes from less dangerous particles. Such a phenomenon shows that though PM2.5 is still serious, other kinds of dust and complete factory pollution have recently become responsible for our superhigh AQIs.

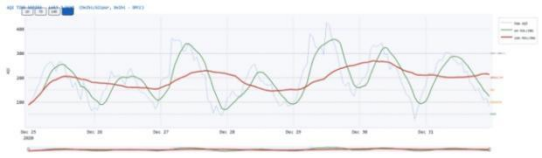

Figure 19 : longitudinal aqi profile with rolling averages (delhi/alipur).

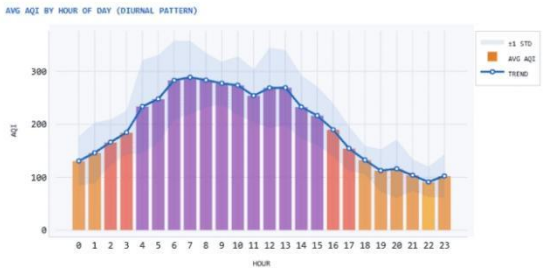

Figure 20 : delhi average aqi by hour of day (diurnal pattern).

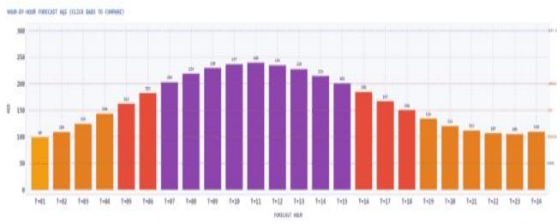

Figure 21 : 24-hour lead-time aqi forecast for Delhi.

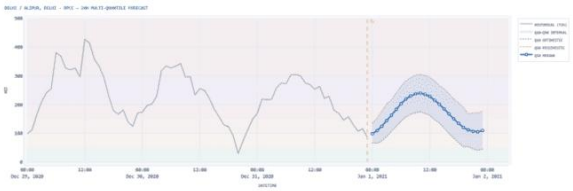

Figure 22 : 24-hour multi-quantile probabilistic aqi forecast for delhi.

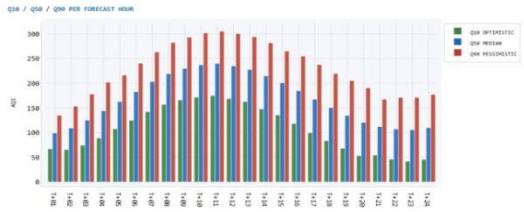

Figure 23 : comparative analysis of q10, q50, and q90 quantiles per forecast hour of delhi.

The longitudinal profile of Delhi in Figure 19 reveals an environment characterized by extreme and persistent pollution, where the 24-hour rolling average frequently stays above the "Unhealthy" threshold, making short-term fluctuations even more dangerous. This severity is driven by a very aggressive diurnal rhythm; as shown in Figure 20, AQI levels nearly triple between early morning and midday, peaking at much higher absolute values than observed in other regions. Our 24-hour lead-time forecasts (Figures 21 and 22) prove highly effective at navigating these extremes, with the multi-quantile approach providing a vital "safety buffer" by highlighting the P90 pessimistic risk. Finally, the quantile analysis in Figure 23 confirms that while the gap between the optimistic (Q10) and pessimistic (Q90) scenarios is wider in Delhi due to higher atmospheric volatility, the model consistently predicts the timing of peak pollution hours, offering a robust early-warning tool for this high-risk area

9.DEPLOYMENT:INTERACTIVE FORECASTING WEB APPLICATION

To make the trained TFT-v3 model accessible beyond a research environment, a browser-based forecasting dashboard was developed using Streamlit and deployed as a self-contained application. The interface loads the serialized model weights (best_tft_v3_model_20.1.pth) and fitted RobustScalers (scalers_v3.pkl) at startup, caching both in memory to avoid redundant I/O across user sessions. The application is organized into four functional tabs. The Overview tab displays live station metrics including current AQI, 7-day averages, category distribution as a pie chart, and a latest pollutant concentration snapshot.

The main core" inference" interface is the Forecast tab. After clicking a city and monitoring station in the sidebar, the system retrieves from the dataset which screen sensors most recently recorded for that city location. These sensor readings are scaled with the ", it then uploads the transformed tensor as input to our autoregressive decoder, and retrieves 24-steps-ahead Q10 Q50 Q90 quantiles. All this process takes place in one simple chain of 'forward' type neural networks. Then we inverse-transform all output before displaying on a scale readable to humans such as pollution density index (AQI) or relative potency-concentration curve.

Act Our actual The Historical tab presents a portrayal of what has happened up to now. This can be visualized as rolling averages, diurnal patterns, or a map capturing date and hours. All of the pollutants are listed with per-trend, Pearson correlation matrix and regression on parasitic lag time comparisons. In addition, particulate matter smaller than 2.5 micrometres can be directly related to Air Quality Index. This is the most definitive pollutant so far!. Provide a manual override for feature mode. This is for scenario testing, where users can supply arbitrary input values and see what happens in the model under terms of pollution impossible to follow in real life.

Every chart can be interactively manipulated, while having a dark console feel and also gives readers such an experience. In the observation sidebar the active execution device of Inference is either a conventional CPU or else an advanced GPU. A full one-second timeframe 24-hour forecast pipeline can be

run from system inputs rendering it into different graphical formats in the course of a working day.

11. DISCUSSION

Our study's results show that transformer-based structures are effective in air quality forecasting, especially when lack of real-world data is a problem. By using synthetic data, a richer representation of the data is learned over time, while still conforming to historical patterns of pollution. However, use of synthetically generated input does introduce potential bias. Where there is little or no existing data for certain rarer and more extreme episodes of pollution, this may lead to significant gaps in what the model learns about such events. The significant performance gap is clearly visible in Figures 3 and 5, where TFT-v3 consistently outperforms all baseline models across every AQI severity category, establishing it as a superior framework for high-precision atmospheric forecasting.

Another problem in our research lies in that we did not take outside influences into account. For instance, how traffic density, meteorological conditions and industrial activities can have such a big effect on whether the air is healthy or not are something still not included in our model. If we put them in then this will grow to an even higher degree of accuracy Incorporating such variables is expected to further improve forecast accuracy.The hyperparameter tuning was another omission due to computational limitations during the experiment and may have prevented the model from fully reaching its optimal performance. The improvement from v1 to v2 to v3 is clearly reflected in the loss convergence curves shown in Figure 1.

12. CHALLENGES

During the course of the investigation, a number of both technical and data-related difficulties were encountered. By and large, the limitations of real world AQI data at both the temporal unit and miss rate levels were the most problematic. During the first stage in data availability, data preparation, missing values, inconsistent station reporting, and incomplete pollutant coverage all caused major difficulties along the way.

The other primary difficulty encountered was in handling the many non-numeric variables (such as city, station, state) within a Temporal Fusion Transformer model. This issue was especially acute when it came to improper encoding levels or categories not seen during training.

Additionally, compatibility issues between different versions of Python and PyTorch introduced repeated debugging cycles. ensuring correct installation of the appropriate PyTorch build required restructuring of the development environment. These issues increased experimentation time and required careful version control to maintain reproducibility.

13. APPLICATIONS

There are many practical applications for accurate AQI forecasting. For example, government organizations and environmental organizations can use forecasts to issue health alerts in good time for particularly vulnerable groups. Pollution control cities and policy makers to test measures introduced whose effect can then be used as guidelines for their long-term air quality management strategy. In industries such as transportation, construction and manufacturing, predictive models could all impact operations where air quality regulations apply; moreover they might help to predict pollutants before these sources are even created. In addition, for- real-time forecasting systems can be installed on mobile applications and publicly

14. FUTURE SCOPE

The Proposed Temporal Fusion Transformer Based AQI forecasting system can be integrated with real-time data pipelines using Internet of Things sensors and government monitoring networks. Such integration would allow continuous model updates and real-time prediction delivery. The deployment output demonstrated through the Streamlit web application, as reflected in the city-specific forecast visualizations (Figures 12–15 for Mumbai and Figures 21–23 for Delhi), confirms the practical feasibility of this approach.

Future scope includes extending the model to incorporate external influencing factors such as traffic density, meteorological variables, industrial emission indices, and satellite-based pollution measurements. Incorporating spatial attention mechanisms across stations could further improve regional forecasting accuracy.

Future research can focus on enhancing model interpretability by analyzing attention weights to identify dominant pollutants and critical time windows influencing AQI levels. Ensemble approaches combining Temporal Fusion Transformer with other advanced deep learning models may further improve robustness.

15. CONCLUSION

This study presented a comprehensive approach to forecasting Air Quality Index using the Temporal Fusion Transformer model on multivariate hourly pollution data across multiple cities and monitoring stations. The research demonstrated that attention-based deep learning architectures are capable of effectively capturing complex temporal dependencies in air quality data.

Although data limitations and computational constraints posed challenges, the proposed methodology could actually realize forecasting performances that were stable and reliable such was confirmed by RMSE and MAE evaluation metrics. The results show the potential of more specialized deep learning models in environmental monitoring and decision support science. This research contributes to a reproducible, scalable framework for intelligent AQI forecasting that can be extended to additional cities, longer time horizons, and richer feature sets in future work

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