DEEP SPATIO-TEMPORAL NEURAL NETWORK FOR AIR QUALITY REANALYSIS

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AQ-Net

ABSTRACT

Background

Air pollution affects 99% of the global population, posing a major threat to public health, with PM2.5 recognized as one of the most harmful pollutants due to its ability to penetrate deep into the lungs and bloodstream. While traditional models have advanced our understanding of pollution dynamics, they often lack spatial resolution or rely on computationally expensive simulations. To overcome these limitations, AQ-Net introduces a hybrid deep learning framework that combines temporal modeling and spatial interpolation for accurate, efficient air quality reanalysis.

Key Contributions

- We propose a hybrid neural network combining LSTM [1], multi-head attention [3] and neural kNN for spatiotemporal modeling.
- We introduce a cyclic time encoding to ensure smooth and continuous temporal representation.
- We perform spatiotemporal reanalysis across 584 stations in northern China, including unmonitored areas.

Experiments

AQ-Net consistently outperforms baseline models: such as LSTM, PatchTST [2] and linear regression: in both short- and long-term PM2.5 reanalysis tasks. In short-term predictions (6h–24h), it achieves higher R^2 scores and lower MAE/RMSE, demonstrating better capture of temporal fluctuations. Over longer horizons (2 to 7 days), AQ-Net maintains robust performance, whereas others degrade significantly. Importantly, its neural kNN module enables accurate spatial interpolation at unmonitored locations, achieving low error across 584 stations in northern China. These results confirm AQ-Net's strength in handling both temporal dynamics and spatial gaps, making it highly effective for real-world air quality monitoring and forecasting .

Conclusion

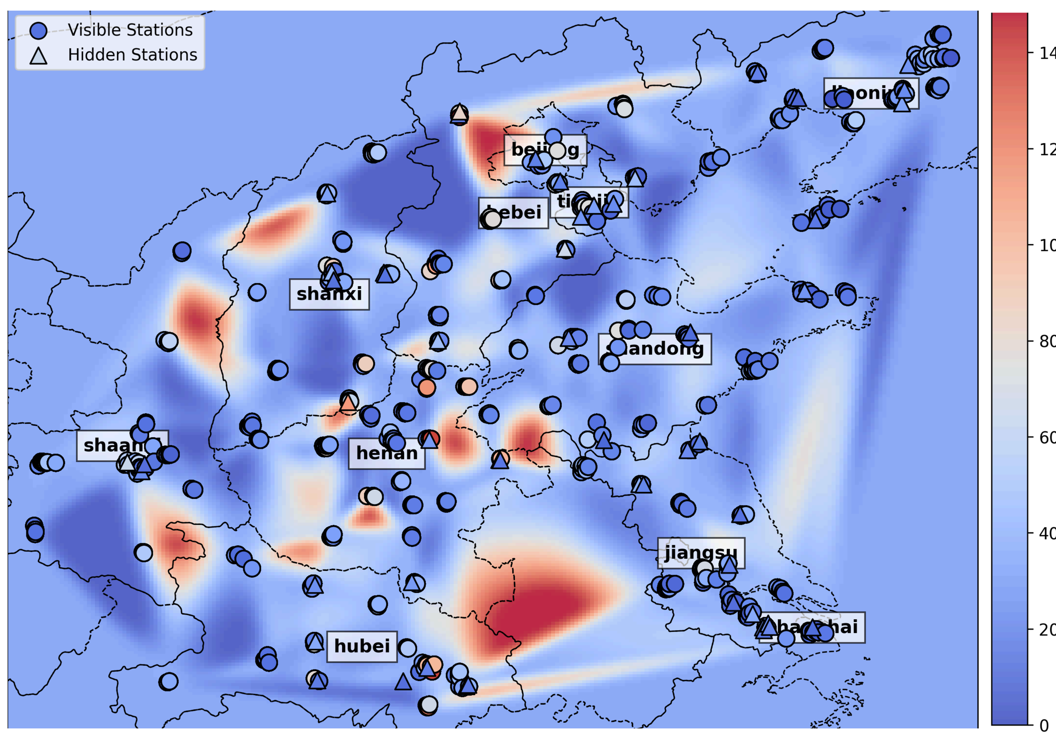
AQ-Net effectively combines temporal modeling and spatial interpolation to reanalyze air quality across both observed and unobserved locations. Its strong performance and generalization ability make it a promising tool for supporting health alerts and environmental policy, with potential extensions to other pollutants and urban contexts.

References

[1] Hochreiter & Schmidhuber, 1997
[2] Nie et al., 2023
[3] Vaswani et al., 2017

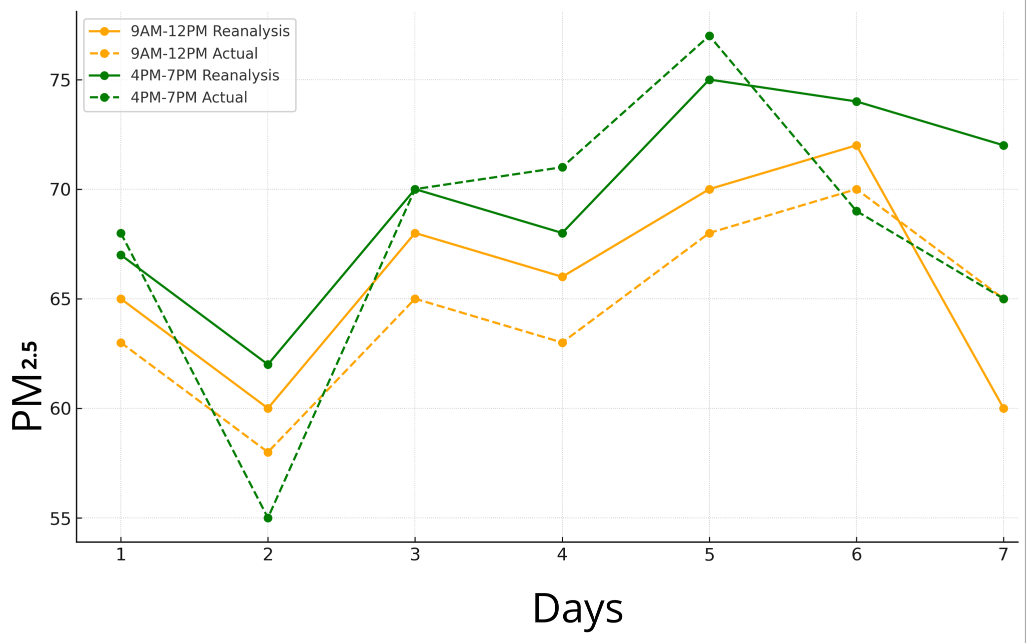
RESULTS

Daily mean PM2.5 reanalysis over northern



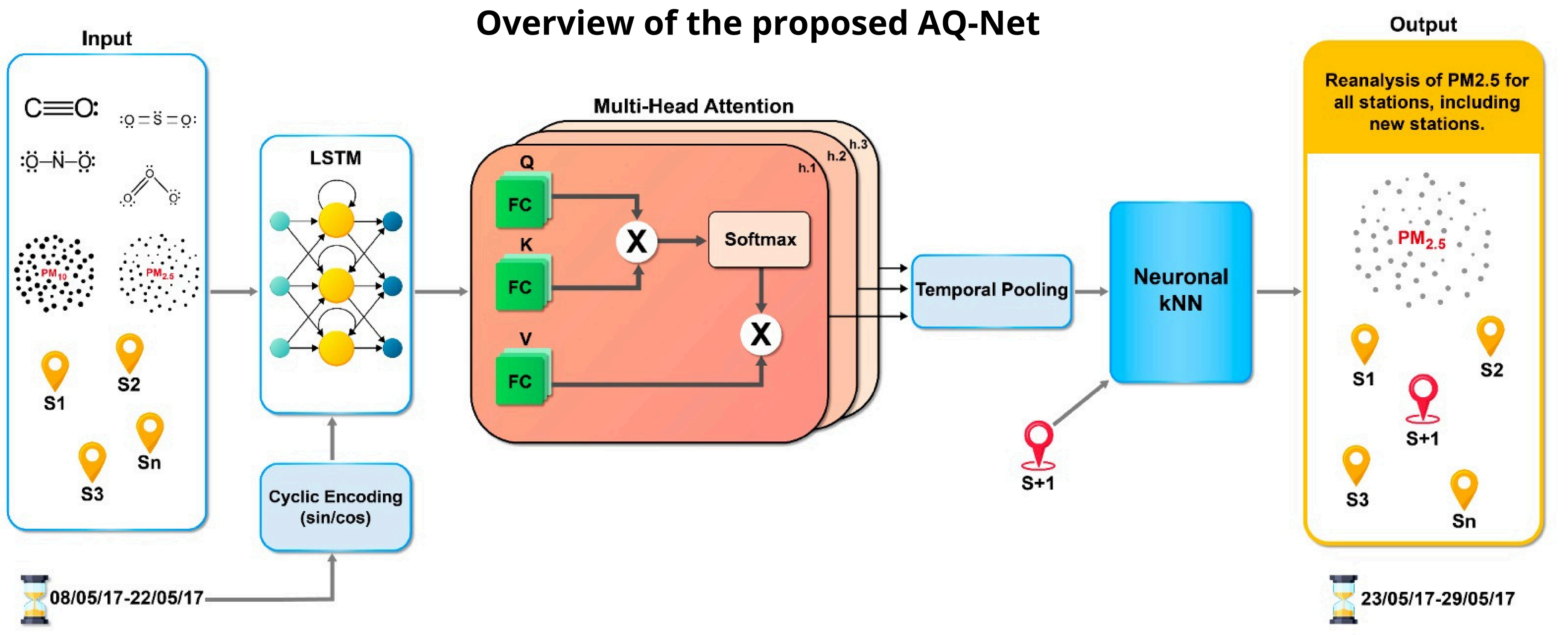
Daily mean PM2.5 reanalysis over northern China using AQ-Net. ● indicates "visible" stations, which provided historical data for training, △ whereas represents "hidden" stations for which only geographic coordinates were available (handled by our neural kNN module).

Comparison of PM2.5 reanalysis



The figure illustrates the predicted and actual PM2.5 levels over a one-week period in Beijing for two time slots: 9-12 PM and 4-7 PM. Our model effectively captures the overall temporal trends of PM2.5 concentrations, with reanalysis generally following the fluctuations observed in real measurements.

Overview of the proposed AQ-Net



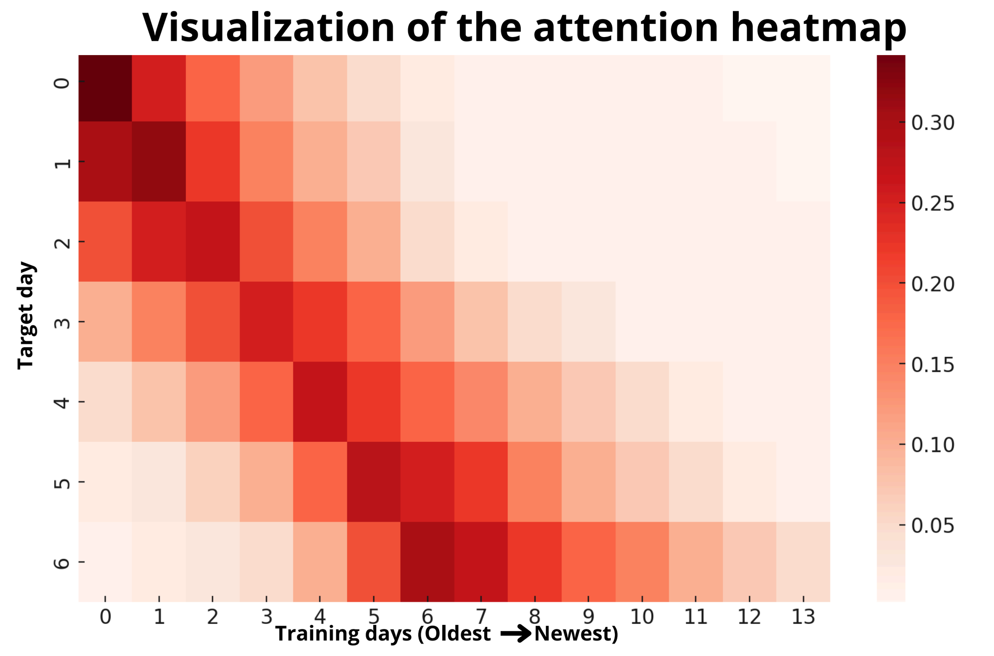
The input includes historical pollutant concentrations, and visible station coordinates. An LSTM extracts temporal dependencies, enhanced by Multi-Head Attention to highlight critical time steps. After temporal pooling, a neural kNN module performs spatial interpolation for unobserved stations (red markers).

The evaluation of long-term PM2.5 reanalysis

Model	2-Day reanalysis		4-Day reanalysis		1-Week reanalysis	
	MAE↓	RMSE↓	MAE↓	RMSE↓	MAE↓	RMSE↓
AQ-Net	13.57	16.80	17.44	21.29	21.29	25.17
AQ-Net wo CE	17.12	21.77	18.12	24.63	24.23	28.37
PatchTST	41.42	55.64	35.31	39.22	28.01	34.70
LSTM	24.04	28.37	25.11	31.21	22.87	28.81
Linear Regression	25.00	29.00	26.00	32.00	23.50	29.50

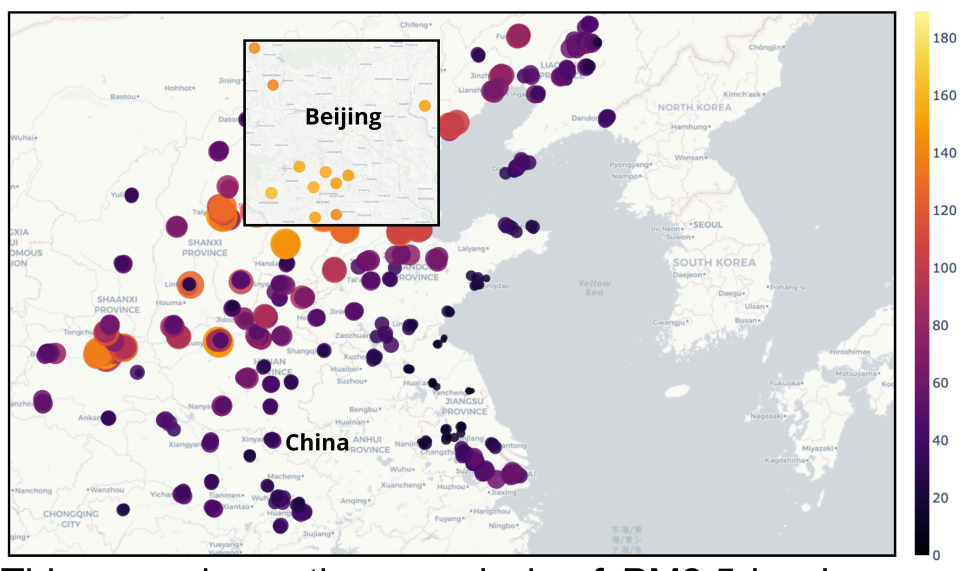
The table presents long-term reanalysis performance on MAE and RMSE over 2-day, 4-day, and 1- week horizons, using a 2-week (336-hour) historical input.Therefore, the evaluation metrics in The table reflect the aggregated daily errors rather than step-by-step hourly deviations. For long-term estimation, AQ-Net retains the lowest RMSE across all horizons, effectively modeling extended dependencies.

Visualization of the attention heatmap



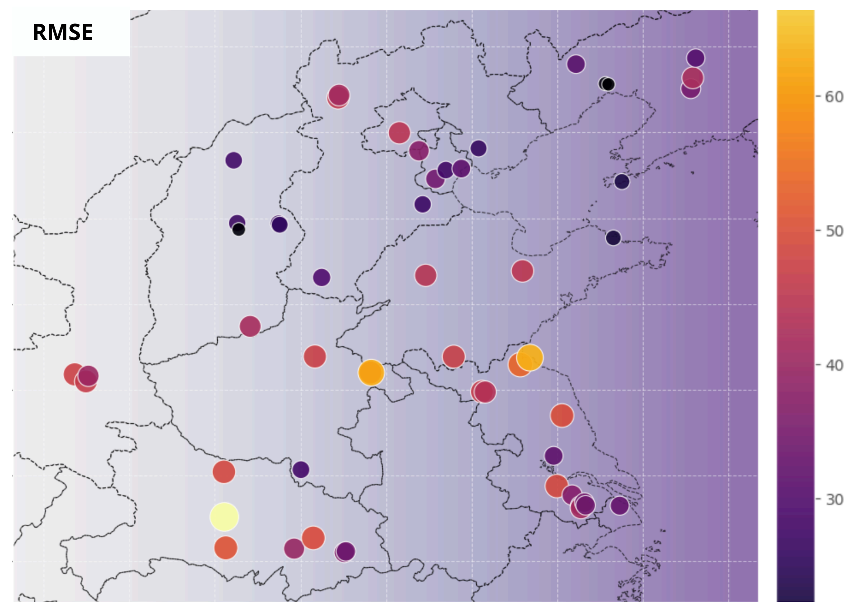
This figure shows which past days of the reanalsys the model focuses on to predict future values. Each row represents a prediction day, and each column corresponds to a reanalsys day. Darker colors indicate higher attention. We use this heatmap to understand how the model connects past reanalsys data with future outcomes. The diagonal pattern reveals that the model captures temporal dependencies, such as delays in pollution transport.

Spatial Reanalysis of PM2.5 Levels Across China



This map shows the reanalysis of PM2.5 levels across all stations used in our study, whether visible or hidden. The color indicates the PM2.5 concentration (from dark purple for low values to yellow for high values), and the size of the circles reflects the relative measured intensity. The zoom on the Beijing area highlights a crucial aspect: some stations are extremely close to each other.

Visualization of prediction errors for hidden stations



The bubbles indicate the RMSE. The bubbles are proportional to the magnitude of the error.

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