PM2.5-GNN: A Domain Knowledge Enhanced Graph Neural Network For PM2.5 Forecasting

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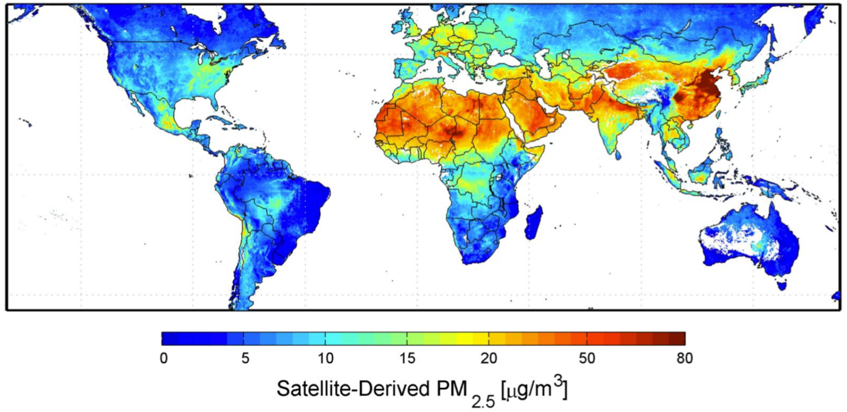
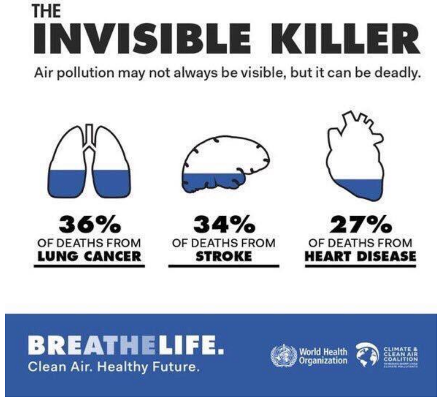
Background

What is PM2.5

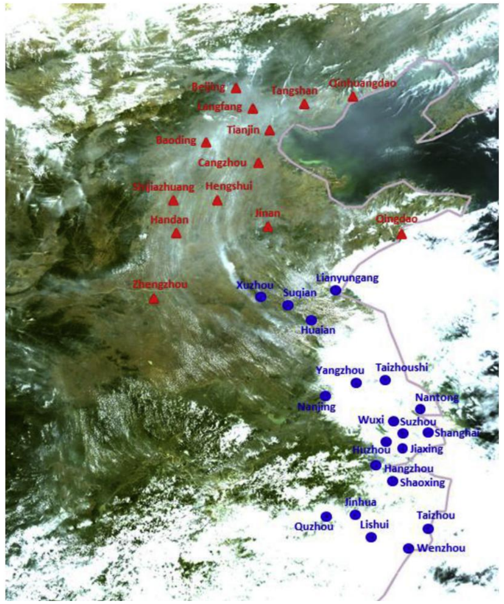
- Particles Matters smaller than 2.5μm
- One of the six major air contaminants (SO2, NO2, PM2.5, PM10, CO, O3), among which PM2.5 is the most harmful one for human body. Long exposure may cause cardiopulmonary diseases.
- Global issue, especially severe in China

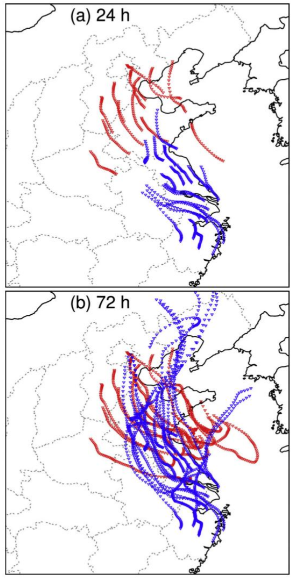




Purpose of PM2.5 forecasting

- governments' policy-making
- people's decision making



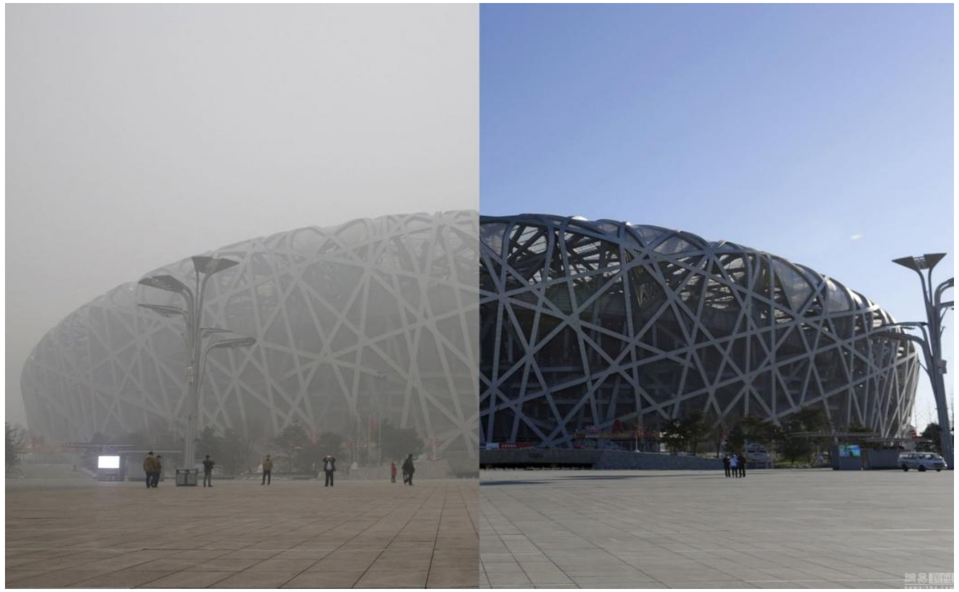


Challenges

- Air pollution is a complex dynamic system
- Long-term spatio-temporal dependency
- Incorporate domain knowledge

[1] J. Hu, et al., Spatial and temporal variability of PM 2.5 and PM 10 over the North China Plain and the Yangtze River Delta, China.
[2] http://www.mee.gov.cn/ http://106.37.208.228:8082/
[3] https://www.who.int/airpollution/news-and-events/how-air-pollution-is-destroying-our-health

Background



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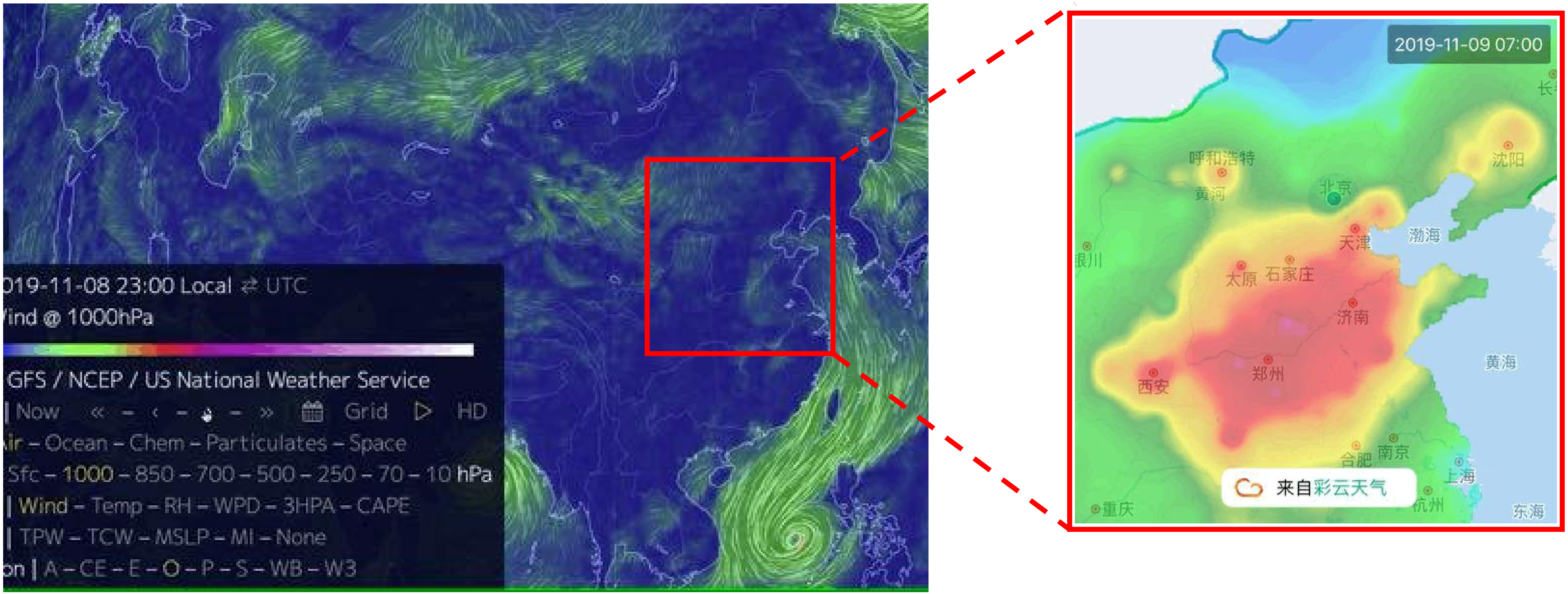
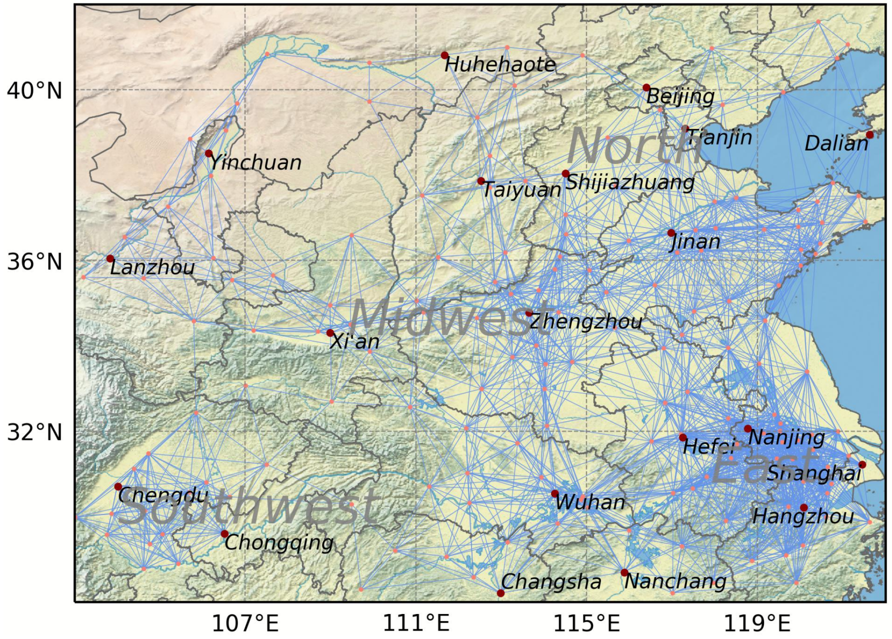


[1] https://earth.nullschool.net/
[2] http://caiyunapp.com/map/

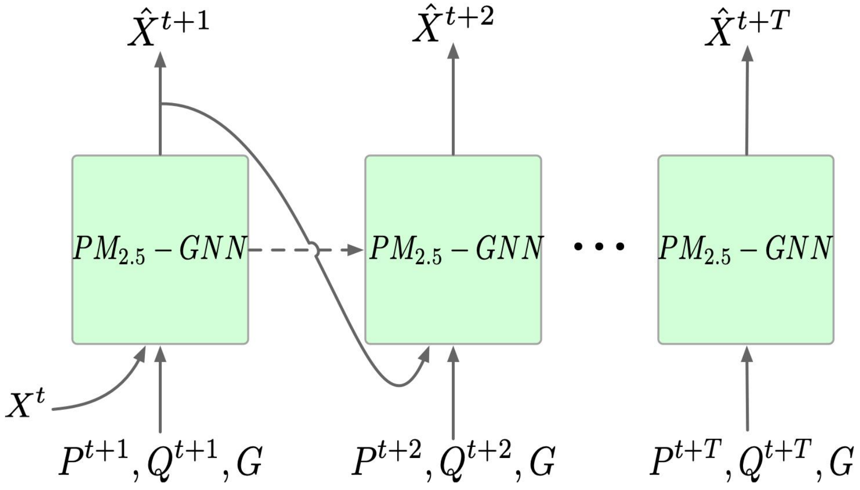
PM2.5-GNN

Graph Construction

- Nodes are cities, node state $X^t \in \mathbb{R}^{N\times 1}$ is PM2.5 concentrations
- Edges are possible PM2.5 transport paths between nodes
- Meteorological data are used as nodes' attributes $P^t \in \mathbb{R}^{N\times p}$ and edges' attributes $Q^t \in \mathbb{R}^{M\times \breve{q}}$



Algorithm Frame Work



Output: PM2.5 prediction at t+1, ..., t+T

Model

Input: PM2.5 at t;
Meteorological data at t+1, ..., t+T

Compared model: GC-LSTM

GC–LSTM[1]

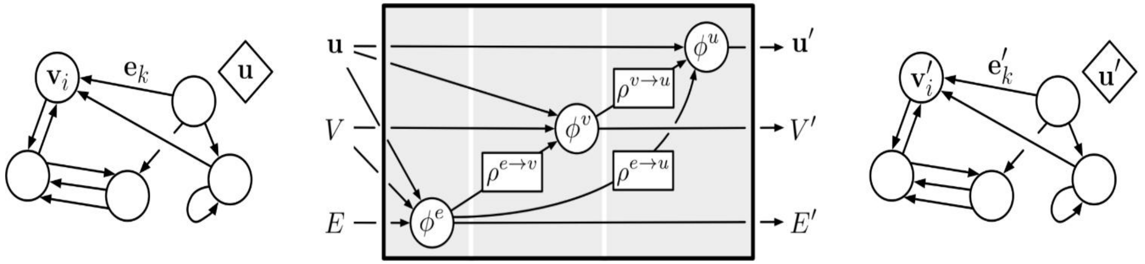
- the previous state–of–the–art graph–based model in PM2.5 forecasting
- Graph Convolutional Networks (GCN) + LSTM

GCN[2] vs. GNN proposed by DeepMind[3]

GCN

$$f(H^{(l)}, A) = \sigma\left(\hat{D}^{-\frac{1}{2}}\hat{A}\hat{D}^{-\frac{1}{2}}H^{(l)}W^{(l)}\right)$$

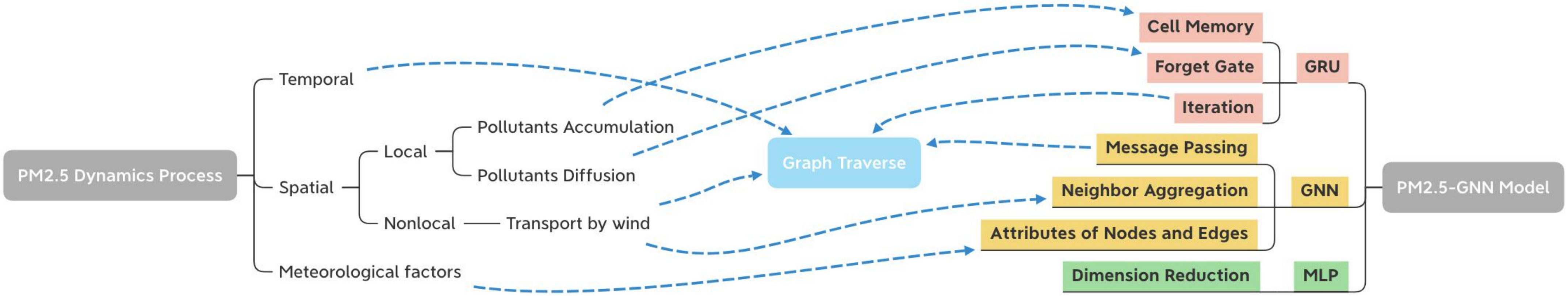
GNN (Basic block used in our model)



	GCN	GNN
Pass and aggregate Information on graphs	✓	✓
Work on directed graphs, feed in edge Attributes, and run MLPs on edges	✗	✓

[1] Y. Qi, Q. Li, H. Karimian, and D. Liu, A hybrid model for spatiotemporal forecasting of PM 2.5 based on graph convolutional neural network and long short–term memory, 2019.
[2] T. N. Kipf and M. Welling, Semi-supervised classification with graph convolutional networks, 2017
[3] P. W. Battaglia et al., Relational inductive biases, deep learning, and graph networks, 2018.

PM2.5-GNN



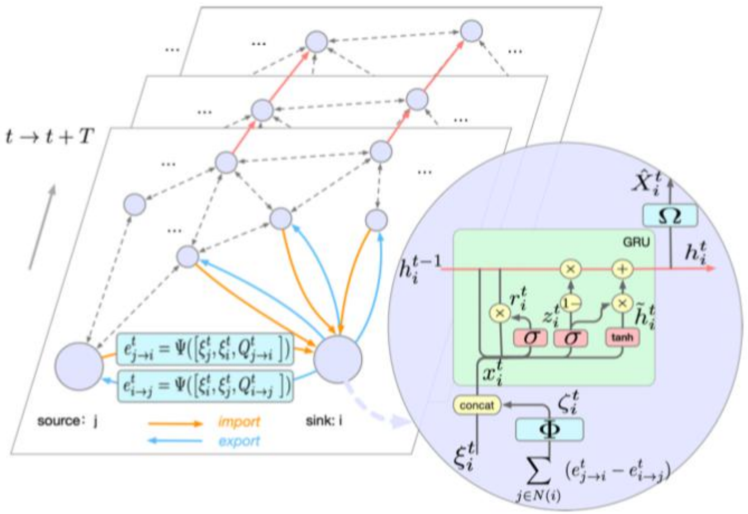


Figure 5: The proposed PM$_{2.5}$-GNN model consisting of a knowledge-enhanced GNN and a spatio-tempo RNN.

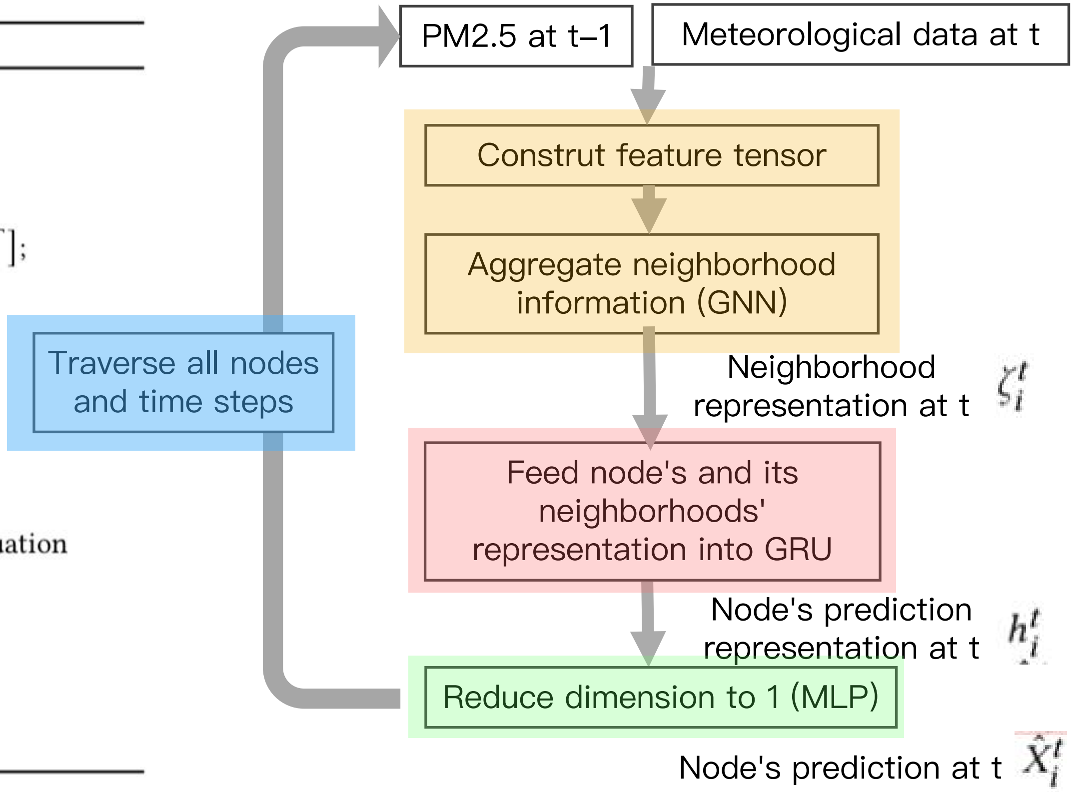
Algorithm 1: PM$_{2.5}$-GNN model

Input : PM$_{2.5}$ observed concentrations X^0 ;
nodes' attributes $[P^1, ..., P^T]$;
edges' attributes $[Q^1, ..., Q^T]$;
$G = (V, E)$;

Output: PM$_{2.5}$ predicted concentrations $[\hat{X}^1, ..., \hat{X}^T]$;

#Initialize:
$h^0 \leftarrow 0$;
$\hat{X}^0 \leftarrow X^0$;
$Output\_list = [\ \ ]$;

for $t = 1, ..., T$ **do**
  for $i \in V$ **do**
    ζ_i^t = **GNN**$(\xi_i^t, \{\xi_j^t, Q_{i\to j}^t, Q_{j\to i}^t\}_{j\in N(i)})$ (Equation 7);
    h_i^t = **GRUcell**$([\xi_i^t, \zeta_i^t], h_i^{t-1})$ (Equation 8);
    $\hat{X}_i^t$ = **MLP**(h_i^t) (Equation 9);
    Append $\hat{X}_i^t$ into $Output\_list$;



Experiment

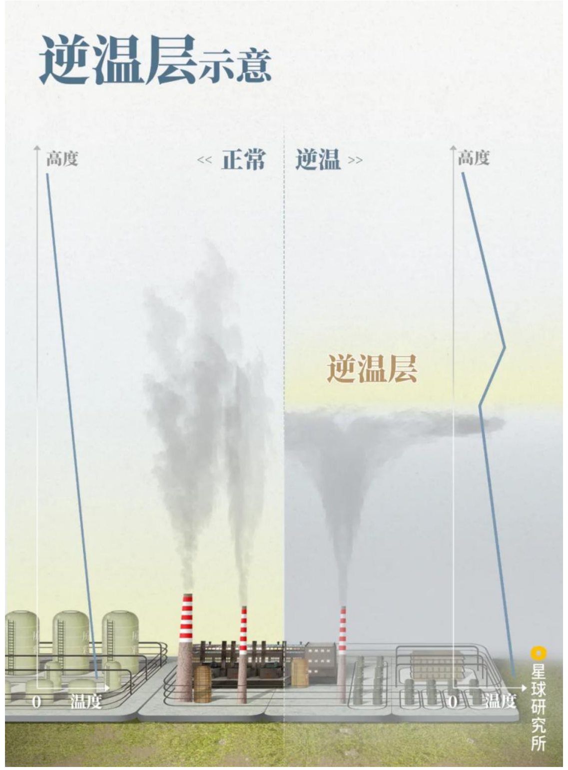
Dataset

- A 4–year dataset (2015–2018)
- PM2.5 concentrations from Ministry of Ecology and Environment
- Meteorological data from European Centre for Medium–Range Weather Forecasts (ECMWF)

Table 3: Dataset is spilt into 3 sub-datasets.

Dataset	Train	Validate	Test
1	2015/1/1 - 2016/12/31	2017/1/1 - 2017/12/31	2018/1/1 - 2018/12/31
2	2015/11/1 - 2016/2/28	2016/11/1 - 2017/2/28	2017/11/1 - 2018/2/28
3	2016/9/1 - 2016/11/30	2016/12/1 - 2016/12/31	2017/1/1 - 2017/1/31

Planetary Boundary Layer height (PBL)



[1] M. R. Perrone and S. Romano, Relationship between the planetary boundary layer height and the particle scattering coefficient at the surface, 2018.
[2] 中国雾霾说明书. 微信公众号 星球研究所

Results

Table 2: Experimental results of $PM_{2.5}$-GNN's compared models, and its different configurations for ablation study. Lack of PBL feature or subtraction (export) component worsens $PM_{2.5}$-GNN's performance.

	Sub-dataset 1		Sub-dataset 2		Sub-dataset 3	
	RMSE	CSI (%)	RMSE	CSI (%)	RMSE	CSI (%)
GRU	21.00 ± 0.17	45.38 ± 0.52	32.59 ± 0.16	51.07 ± 0.81	45.25 ± 0.85	59.40 ± 0.01
GC-LSTM	20.84 ± 0.11	45.83 ± 0.43	32.10 ± 0.29	51.24 ± 0.13	45.01 ± 0.81	60.58 ± 0.14
$PM_{2.5}$-GNN	**19.93 ± 0.11**	**48.52 ± 0.48**	**31.37 ± 0.34**	**52.33 ± 1.06**	**43.29 ± 0.79**	**61.91 ± 0.78**
$PM_{2.5}$-GNN no PBL	20.46 ± 0.18	47.43 ± 0.37	32.44 ± 0.36	51.05 ± 1.15	44.71 ± 1.02	60.64 ± 0.84
$PM_{2.5}$-GNN no export	20.54 ± 0.16	45.73 ± 0.58	31.91 ± 0.32	51.54 ± 1.27	43.72 ± 1.03	61.52 ± 0.95

Results

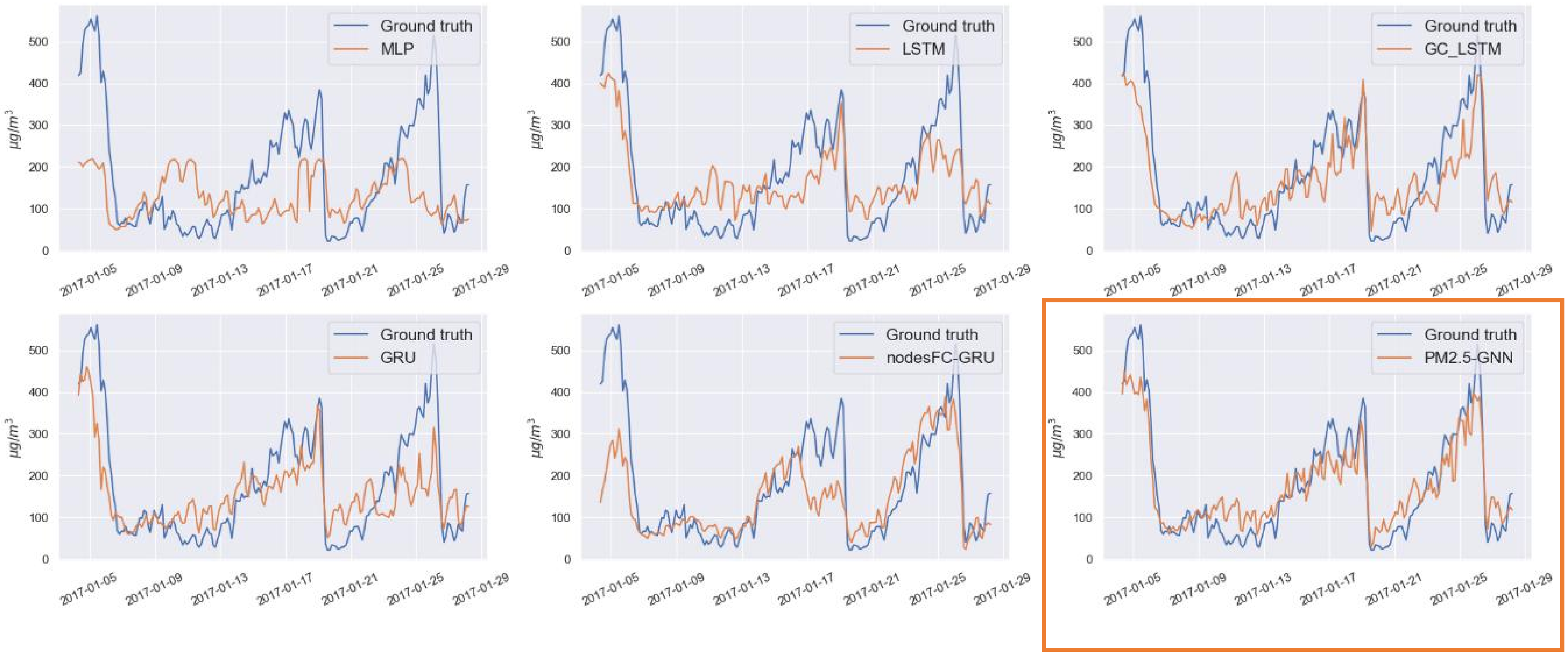


Figure 11: Comparison of prediction curves between $PM_{2.5}$-GNN and its baselines for 72 hours ahead prediction at Xi'an node of testset of Dataset 3.

Deployment

彩云科技
ColorfulClouds Tech.

http://caiyunapp.com/map/

Figure 2: Online website (http://caiyunapp.com/map/) that provides 72-hour real-time $PM_{2.5}$ concentration prediction using $PM_{2.5}$-GNN model proposed in this paper.

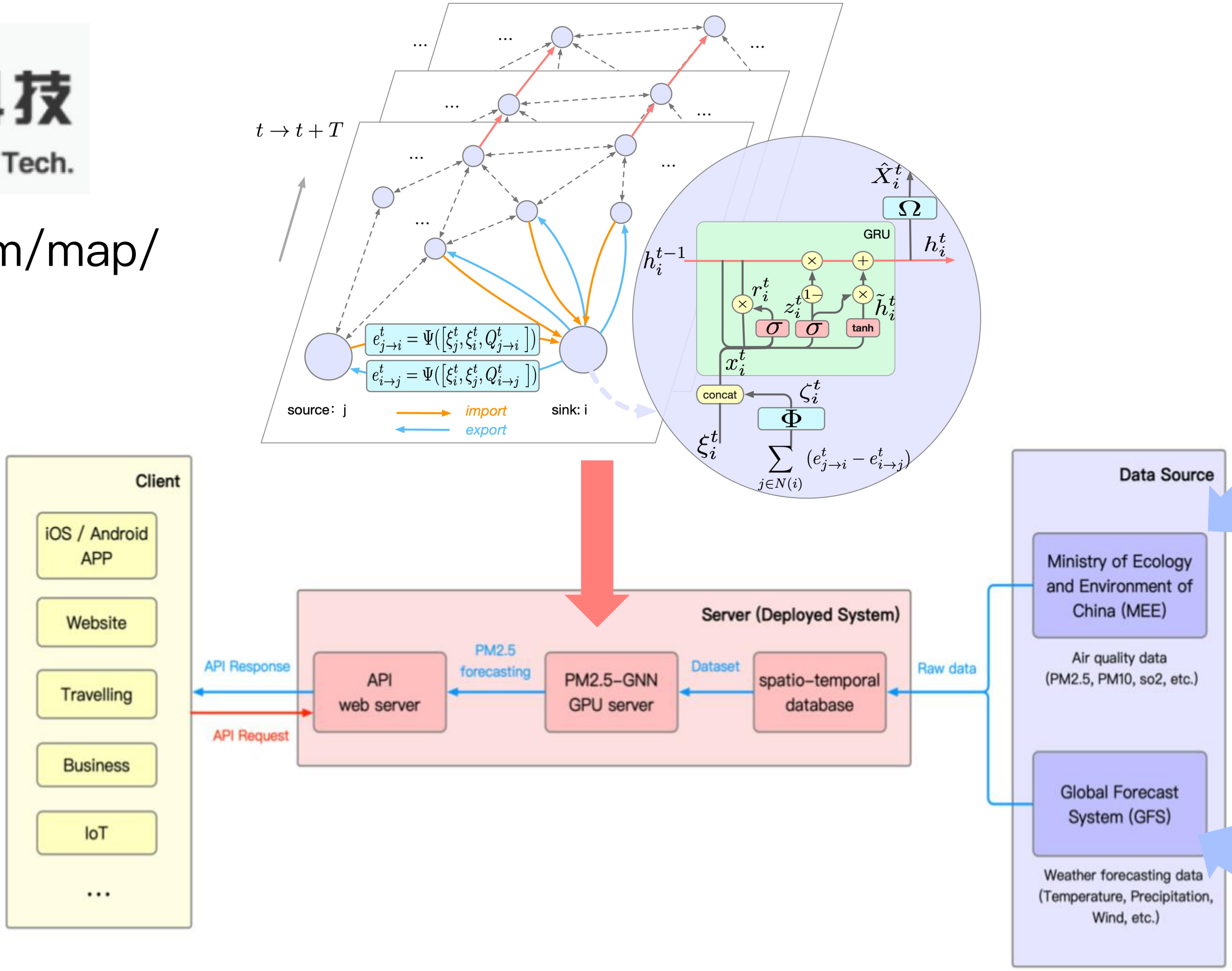
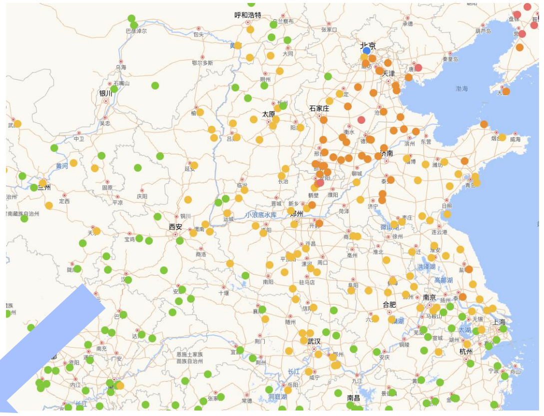
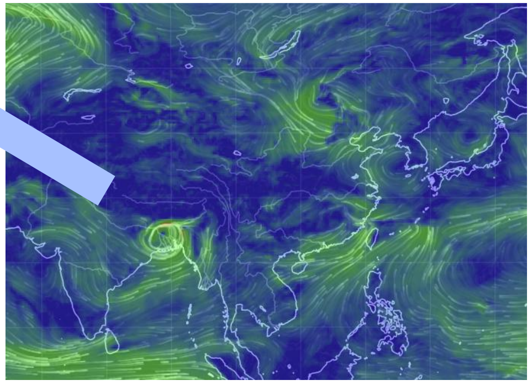


Figure 10: Deployment Framework





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Code: https://github.com/shawnwang-tech/PM2.5-GNN