

Supplementary materials

Table S1 Numerical statistics of PM_{2.5} concentration at the target monitoring site $\mu\text{g}/\text{m}^3$

Season	Mean	Median	Max	Min	SD	Skewness	Kurtosis
Spring	37.3771	23	203	2	37.7039	1.5338	1.8655
Summer	29.5619	23	205	1	25.9882	1.8085	3.9504
Autumn	24.1832	18	138	1	21.1828	1.7250	3.8372
Winter	38.7412	20	347	1	44.8917	1.9992	5.3272

Table S2 Statistics of interval prediction evaluation indicators of the comparison models for testing dataset (Spring)

Model	Probabilistic forecasting			
	PICP	PINAW	CWC	ACE
KNN-GNN-SBR-KDE	0.7763	0.1577	0.9713	0.2790
KNN-graph RNN-SBR-KDE	0.3973	0.2719	1.6747	0.5822
KNN-GCN-SBR-KDE	0.7489	0.1500	0.9240	0.3009
KNN-spatial temporal GCN-SBR-KDE	0.7626	0.1290	0.7942	0.2900
KNN-GIN-SBR-KDE	0.9475	0.0665	0.4098	0.1420
KNN-GaAN-SBR-KDE	0.8758	0.0923	0.5685	0.3594
KNN-graph U-netsGGN-SBR-KDE	0.9653	0.0509	0.3133	0.6078

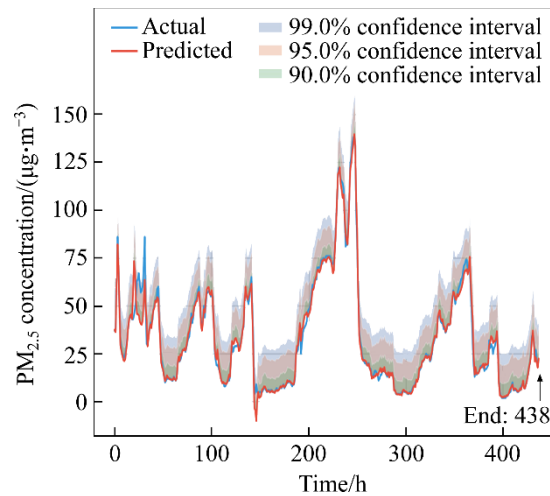


Figure S1 PM_{2.5} concentration interval prediction results of the proposed model (Spring)

Table S3 Statistics of interval prediction evaluation indicators of the comparison models for testing dataset (Summer)

Model	Probabilistic forecasting			
	PICP	PINAW	CWC	ACE
KNN-GNN-SBR-KDE	0.8288	0.1492	1.2645	0.2370
KNN-graph RNN-SBR-KDE	0.3721	0.2678	2.2704	0.6023
KNN-GCN-SBR-KDE	0.7922	0.1396	1.1835	0.2662
KNN-spatial temporal GCN-SBR-KDE	0.7237	0.0873	0.7405	0.3210
KNN-GIN-SBR-KDE	0.9351	0.0653	0.5536	0.4799
KNN-GaAN-SBR-KDE	0.9247	0.0719	0.6093	0.1603
KNN-graph U-nets GGN-SBR-KDE	0.9411	0.0479	0.4063	0.5712

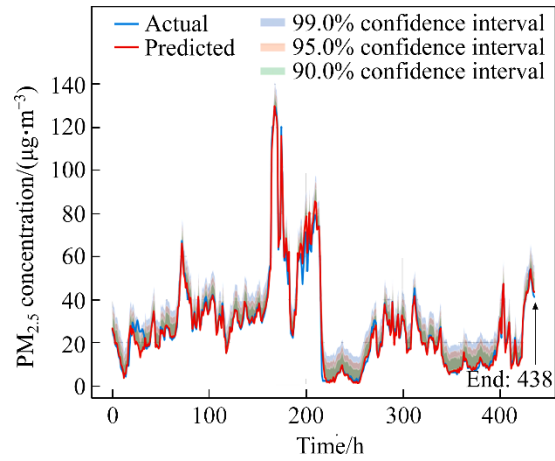


Figure S2 PM_{2.5} concentration interval prediction results of the proposed model (Summer)

Table S4 Statistics of interval prediction evaluation indicators of the comparison models for testing dataset (Autumn)

Model	Probabilistic forecasting			
	PICP	PINAW	CWC	ACE
KNN-GNN-SBR-KDE	0.7900	0.2296	1.2154	0.2680
KNN-graph RNN-SBR-KDE	0.4635	0.5026	2.6602	0.5292
KNN-GCN-SBR-KDE	0.8082	0.2288	1.2110	0.2534
KNN-spatial temporal GCN-SBR-KDE	0.7215	0.1922	1.0174	0.3228
KNN-GIN-SBR-KDE	0.8758	0.1665	0.8814	0.3594
KNN-GaAN-SBR-KDE	0.9301	0.1126	0.5961	0.3959
KNN-graph U-nets GGN-SBR-KDE	0.9405	0.0816	0.4319	0.4836

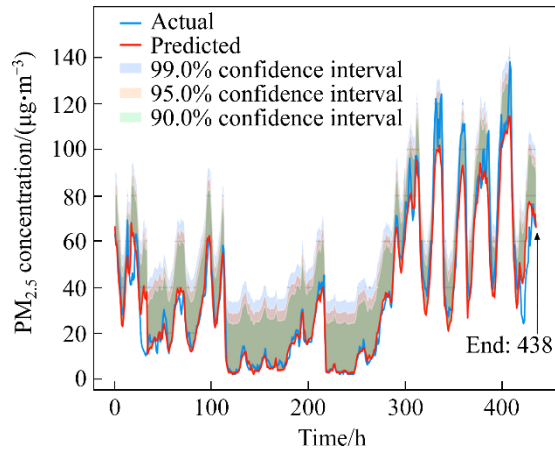


Figure S3 PM_{2.5} concentration interval prediction results of the proposed model (Autumn)

Table S5 Statistics of interval prediction evaluation indicators of the comparison models for testing dataset (Winter)

Model	Probabilistic forecasting			
	PICP	PINAW	CWC	ACE
KNN-GNN-SBR-KDE	0.5652	0.2172	1.3275	0.4478
KNN-graph RNN-SBR-KDE	0.1945	0.2155	1.3169	0.7444
KNN-GCN-SBR-KDE	0.5240	0.2285	1.3964	0.4808
KNN-spatial temporal GCN-SBR-KDE	0.4394	0.1980	1.2097	0.5485
KNN-GIN-SBR-KDE	0.0297	0.1532	0.9359	0.8762
KNN-GaAN-SBR-KDE	0.8357	0.1386	0.8468	0.7114
KNN-graph U-nets GGN-SBR-KDE	0.8808	0.0967	0.5909	0.6346

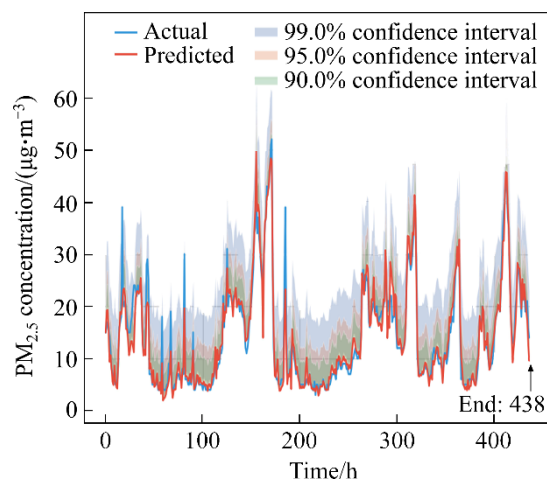


Figure S4 PM_{2.5} concentration interval prediction results of the proposed model (Winter)

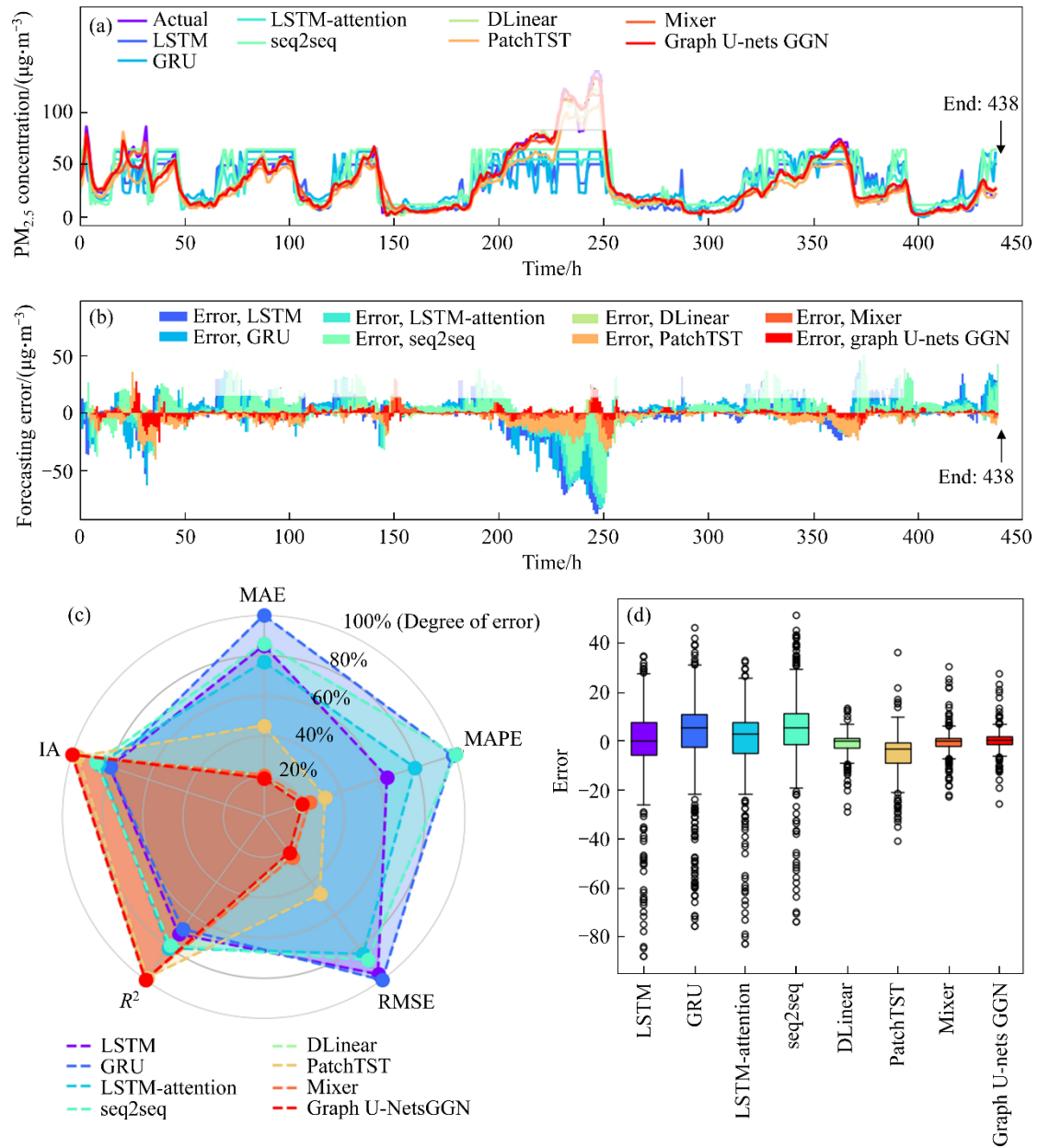


Figure S5 Comprehensive error evaluation of different network models (Spring): (a) Trend plots; (b) Error plots; (c) Radar plots; (d) Boxplots

Table S6 Statistics of deterministic/probabilistic prediction of different network models in four seasons (for testing dataset)

Season	Model	Deterministic forecasting (without KNN-*-SBR-KDE)			Probabilistic forecasting (with KNN-*-SBR-KDE)		
		MAE	MAPE	RMSE	PICP	PINAW	CWC
Spring	LSTM	12.2540	38.4922	19.8059	0.4772	0.3496	2.1528
	GRU	14.4154	59.0141	20.5448	0.2763	0.3768	2.3203
	LSTM-attention	11.0918	47.2456	17.2461	0.3333	0.2456	1.5124
	seq2seq	12.4152	59.8540	17.9956	0.2877	0.3121	1.9220
	DLinear	2.9582	11.7369	4.6003	0.4635	0.0721	0.4442
	PatchTST	6.5413	19.1614	9.7252	0.8174	0.1562	0.9617
	Mixer	2.9968	14.3540	5.0591	0.4406	0.0724	0.4457
	Graph U-nets GGN	2.7793	12.0284	4.4760	0.9653	0.0509	0.3133
Summer	LSTM	4.8502	20.2408	7.7258	0.6233	0.1132	0.9596
	GRU	7.3419	31.6294	11.5864	0.6210	0.1934	1.6396
	LSTM-attention	4.0984	21.4677	7.0885	0.3721	0.1025	0.8686
	seq2seq	6.1862	26.2183	9.7180	0.6872	0.1739	1.4743
	DLinear	2.8235	15.7447	4.7378	0.3516	0.0670	0.5683
	PatchTST	2.6103	13.3952	4.2830	0.5731	0.0720	0.6105
	Mixer	3.4414	13.8478	6.2305	0.5160	0.0905	0.7673
	Graph U-nets GGN	1.0107	5.2661	2.0863	0.9411	0.0479	0.4063
Autumn	LSTM	7.5735	14.0730	15.8488	0.4429	0.3202	1.6948
	GRU	8.2320	15.3874	15.3969	0.6644	0.2977	1.5757
	LSTM-attention	6.5937	12.4037	14.5152	0.5091	0.3006	1.5913
	seq2seq	7.2110	15.5800	15.8956	0.5251	0.3331	1.7630
	DLinear	5.7707	15.4884	9.2756	0.6073	0.1614	0.8544
	PatchTST	5.5128	17.1815	8.8226	0.7603	0.1520	0.8048
	Mixer	4.9403	16.5214	7.9585	0.3813	0.1393	0.7373
	Graph U-nets GGN	4.3097	15.4907	6.9811	0.9405	0.0816	0.4319
Winter	LSTM	4.7654	36.1316	8.8571	0.1785	0.2657	1.6236
	GRU	4.0961	31.6253	5.8116	0.3570	0.2855	1.7447
	LSTM-attention	2.7041	17.9168	4.4602	0.5103	0.1750	1.0696
	seq2seq	4.2042	35.9451	5.9203	0.2540	0.2377	1.4523
	DLinear	2.2014	19.3064	3.2532	0.1808	0.1298	0.7933
	PatchTST	2.3986	18.8968	3.8200	0.3295	0.1494	0.9130
	Mixer	1.6421	12.1375	2.8788	0.2494	0.1137	0.6948
	Graph U-nets GGN	1.3780	10.9445	2.2175	0.8808	0.0967	0.5909

Table S7 Interval prediction result indicators of each comparison model (for testing dataset)

Season	Model	Probabilistic forecasting			
		PICP	PINAW	CWC	ACE
Spring	MLP	0.9840	0.8990	0.6280	0.8402
	CNN	0.9977	0.4985	0.3622	0.9772
	Dlinear	0.9977	0.9056	0.6580	0.9772
	LSTM	0.9585	0.7134	0.4582	0.8525
	LSTM- attention	0.9686	0.6783	0.3873	0.6857
	KNN-Graph	0.9653	0.0509	0.3133	0.6078
	U-nets GGN-SBR-KDE				
Summer	MLP	0.9954	0.7316	0.5282	0.9541
	CNN	0.9886	0.4404	0.3118	0.8865
	Dlinear	0.9954	0.7093	0.5121	0.9543
	LSTM	0.8410	0.9727	0.6028	-0.0590
	LSTM- attention	0.8318	0.3177	0.5674	-0.0682
	KNN-Graph	0.9411	0.0479	0.4063	0.5712
	U-nets GGN-SBR-KDE				
Autumn	MLP	1.0000	0.7546	0.5517	0.1000
	CNN	1.0000	0.8089	0.5914	0.1000
	Dlinear	0.9932	0.7325	0.5254	0.9321
	LSTM	0.6751	0.2032	0.4940	-0.2249
	LSTM- attention	0.6244	0.2357	0.4887	-0.2756
	KNN-Graph	0.9405	0.0816	0.4319	0.4836
	U-nets GGN-SBR-KDE				
Winter	MLP	0.9931	2.0350	1.4598	0.9314
	CNN	0.9725	0.5789	0.6901	0.7254
	Dlinear	0.9954	1.2372	0.8932	0.9542
	LSTM	0.8938	0.3739	0.8811	-0.0062
	LSTM- attention	0.9399	0.1371	0.7194	0.7993
	KNN-Graph	0.8808	0.0967	0.5909	0.6346
	U-nets GGN-SBR-KDE				