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Quantifying the driving factors of particulate matter variabilities in the Beijing-Tianjin-Hebei and Yangtze River Delta regions from 2015 to 2022 by machine learning approach

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Supplement

Tables

Table S1. The information of each city over BTH and YRD regions in this study. TaizhouJS denotes Taizhou City in Jiangsu Province, while TaizhouZJ refers to Taizhou City in Zhejiang Province. The altitude data represent the average elevation of the urban areas, with population and area statistics sourced from the Ministry of Civil Affairs of the People's Republic of China

Name	Latitude	Longitude	Altitude (m)	Number of site	Population （million）	Area （thousand km2）
Beijing	40.0° N	116.4° E	455	12	13.92	1.6
Tianjin	39.1	117.3	64	15	11.05	1.2
Baoding	38.9	115.5	338	6	10.9	2.2
Tangshan	39.6	118.1	90	6	7.56	1.3
Langfang	39.5	116.7	45	4	4.83	0.6
Shijiazhuang	38.0	114.5	337	8	9.89	1.4
Qinhuangdao	39.5	119.6	143	5	3.01	0.8
Zhangjiakou	40.8	114.9	1203	5	4.65	3.6
Chengde	41.0	117.9	829	5	3.83	4.0
Cangzhou	38.3	116.9	11	3	7.87	1.3
Hengshui	37.7	115.7	27	3	4.58	0.9
Xingtai	37.1	114.5	356	4	8.01	1.2
Handan	36.6	114.5	310	4	10.61	1.2
Shanghai	31.2	121.5	13	10	14.69	0.6
Nanjing	32.1	118.8	28	9	7.1	0.7
Wuxi	31.6	120.3	8	8	5.03	0.5
Changzhou	31.8	120.0	5.3	6	3.85	0.4
Suzhou	32.1	119.4	6	8	7.23	0.8
Nantong	32.0	120.9	3	5	7.6	0.8
Yancheng	33.4	120.2	3	4	8.21	1.7
Yangzhou	32.4	119.4	10	4	4.57	0.7
Zhenjiang	32.2	119.5	20	4	2.7	0.4

TaizhouJS	32.4	120.0	7	4	5.01	0.6
Hangzhou	30.2	120.1	186	11	7.59	1.7
Ningbo	29.9	121.6	37	8	6.08	0.9
Wenzhou	28.0	120.7	217	4	8.32	1.2
Jiaxing	30.7	120.7	5	3	3.64	0.4
Huzhou	30.9	120.1	65	3	2.68	0.6
Shaoxing	30.0	120.6	180	3	4.48	0.8
Jinhua	29.1	119.7	316	3	4.92	1.1
Zhoushan	30.0	122.2	10	3	0.97	0.1
TaizhouZJ	28.6	121.4	141	3	6.07	0.9
Hefei	31.8	117.2	71	10	7.7	1.1
Wuhu	31.4	118.4	57	4	3.9	0.6
Maanshan	31.7	118.5	23	5	2.29	0.4
Tongling	30.9	117.8	100	6	1.71	0.3
Anqing	30.5	117.0	210	4	5.92	1.4
Chuzhou	32.3	118.3	36	3	4.55	1.3
Chizhou	30.7	117.5	216	3	1.62	0.8
Xuancheng	31.0	118.7	226	3	2.79	1.2

Table S2. The input variables for LightGBM model in this study.

Type	Abbreviation	Description	Source
/	month_sin month_cos season	Cyclical month encoding (sine term, cosine term), Seasonal index (four-category seasonal regime)	/
meteorogloy	CLDTOT PRECTOT QV2M T2M SLP SWGDN U10M V10M	Total Cloud Cover Total Precipitation Specific Humidity at 2 Meters Temperature at 2 Meters Sea Level Pressure Downward Shortwave Radiation 10 Meter U-Wind Component 10 Meter V-Wind Component	0.25° × 0.3125°GEOS FP
	CO_total, NH3_total, NOx_total, BC_total, SO2_total,		

	emission	OC_total, PRPE_total CO_total_sdiff, NH3_total_sdiff, NOx_total_sdiff, BC_total_sdiff, SO2_total_sdiff, OC_total_sdiff, PRPE_total_sdiff, CO_total_detr, NH3_total_detr, NOx_total_detr, BC_total_detr, SO2_total_detr, OC_total_detr, PRPE_total_detr	eight species-level aggregated emission totals (e.g., NO_total, SO_2_total, BC_total), and two derived indicators (sdiff and detr) for each emission species	0.5x0.5 CEDS
Target	observation	$PM_{2.5}$ PM_{10}	Average observation data per hour of near-surface observation	CNEMC

Table S3. Ranges of optimized LightGBM hyperparameters used across all city–pollutant models in this study.The full set of fold-wise hyperparameter configurations, including all individual parameter values and seeds, is supplied in the train/seeds directory of the associated code release.

Hyperparameter	Min	Max
learning_rate	0.0676	0.2857
n_estimators	130	267
num_leaves	17	43
max_depth	5	9
min_child_samples	7	22
subsample	0.6232	0.8909
colsample_bytree	0.6488	0.9089
reg_alpha	0.1560	0.7290
reg_lambda	0.1560	0.9267
subsample_freq	1	1
bagging_seed	42	42
data_random_seed	42	42
feature_fraction_seed	42	42
deterministic	true	true
early_stopping_rounds	20	20

Table S4. Linear trend slopes, corresponding 1-σ uncertainties, relative (% yr^{-1}) trends with uncertainties, and p-values for annual mean $PM_{2.5}$ and PM_{10} concentrations in all cities from 2015 to 2022. Trend estimates include absolute trends (μg m^{-3} yr^{-1}), relative trends (% yr^{-1}), and their associated uncertainties. TaizhouJS denotes Taizhou City in Jiangsu Province, while TaizhouZJ refers to Taizhou City in Zhejiang Province.

city	25_trend	25_trend_err	25_reltrend_%	25_reltrend_err_%	10_trend	10_trend_err	10_reltrend_%	10_reltrend_err_%	10_pvalue	2.5_pvalue
Anqing	3.3983	0.7671	-7.6115	1.7182	-3.9633	1.0477	-6.2525	1.6529	0.0092	0.0044
Baoding	-9.4582	0.7421	-13.9148	1.0918	13.0678	1.4594	-11.1494	1.2451	0.0001	0.0000
Beijing	-7.1168	0.6514	-14.1909	1.2990	-7.5035	0.9996	-9.6159	1.2810	0.0003	0.0000
Cangzhou	-5.1604	0.3471	-9.4390	0.6349	-7.2555	0.5567	-7.5933	0.5827	0.0000	0.0000
Changzhou	-2.9619	0.5008	-6.7848	1.1471	-5.1896	1.1999	-7.2187	1.6690	0.0050	0.0010
Chengde	-1.9808	0.3475	-6.1331	1.0759	-4.9551	1.0341	-7.1462	1.4914	0.0030	0.0013
Chizhou	-1.5253	1.5745	-3.6565	3.7743	-1.8358	2.0336	-2.9023	3.2151	0.4015	0.3701
Chuzhou	-4.2812	1.1209	-8.6680	2.2694	-4.1781	1.6955	-5.3563	2.1736	0.0488	0.0088
Handan	-6.4607	0.6468	-9.4392	0.9449	12.1742	0.9925	-9.5269	0.7767	0.0000	0.0001
Hangzhou	-3.5669	0.4246	-9.3057	1.1078	-4.0655	0.3304	-6.2661	0.5092	0.0000	0.0002
Hefei	-4.8250	0.3327	-10.4358	0.7196	-4.6190	0.8855	-6.1319	1.1756	0.0020	0.0000
Hengshui	-8.3632	0.6693	-12.9384	1.0354	13.7939	1.8179	-12.1935	1.6069	0.0003	0.0000
Huzhou	-5.6852	1.2180	-12.8548	2.7540	-5.4936	1.0600	-7.8470	1.5141	0.0020	0.0034
Jiaxing	-3.6855	0.3694	-10.0369	1.0059	-4.5766	0.4980	-7.7136	0.8394	0.0001	0.0001
Jinhua	-3.8504	0.5275	-10.5930	1.4513	-3.5175	0.4607	-6.1865	0.8102	0.0003	0.0003
Langfang	-6.4373	0.7907	-12.1520	1.4926	-8.8456	1.0815	-9.2034	1.1253	0.0002	0.0002
Maanshan	-3.4061	0.7181	-7.4615	1.5730	-4.6606	0.9821	-6.3858	1.3456	0.0032	0.0032
Nanjing	-3.6979	0.4796	-9.2912	1.2049	-5.8893	0.6359	-8.1153	0.8762	0.0001	0.0002
Nantong	-3.6112	0.4596	-9.2248	1.1741	-5.5371	0.6159	-9.1855	1.0217	0.0001	0.0002
Ningbo	-3.3387	0.3306	-10.8340	1.0729	-4.6377	0.4507	-9.1112	0.8854	0.0000	0.0001
Qinhuangdao	-2.5499	0.3656	-6.5147	0.9340	-5.4983	0.6103	-7.2156	0.8009	0.0001	0.0004
Shanghai	-3.6972	0.3830	-10.0904	1.0452	-4.7012	0.5427	-8.9540	1.0336	0.0001	0.0001
Shaoxing	-3.5070	0.4942	-9.3036	1.3111	-7.3633	2.8905	-9.5716	3.7573	0.0436	0.0004
Shijiazhuang	-7.1995	0.7383	-10.5791	1.0849	10.5974	1.4399	-8.4759	1.1517	0.0003	0.0001
Suzhou	-3.7795	0.4237	-9.5653	1.0724	-5.2528	0.5457	-8.4970	0.8828	0.0001	0.0001

TaizhouJS	-4.0047	0.2671	-8.7936	0.5866	-7.1152	0.6978	-9.4391	0.9257	0.0001	0.0000
TaizhouZJ	-2.7186	0.2566	-9.2832	0.8761	-3.4839	0.2146	-6.7301	0.4145	0.0000	0.0000
Tangshan	-6.4196	0.3074	-10.9611	0.5249	-9.5901	0.6057	-8.9741	0.5668	0.0000	0.0000
Tianjin	-5.0378	0.4788	-9.4498	0.8981	-7.4306	0.9184	-8.3804	1.0358	0.0002	0.0000
Tongling	-3.5793	1.2085	-7.5729	2.5570	-3.8398	1.0910	-5.0328	1.4300	0.0125	0.0252
Wenzhou	-2.8331	0.3271	-8.9914	1.0381	-3.6385	0.3295	-6.2645	0.5673	0.0000	0.0001
Wuhu	-3.2490	0.9208	-7.0767	2.0055	-4.5983	0.9085	-6.7057	1.3249	0.0023	0.0124
Wuxi	-4.5422	0.3632	-10.9716	0.8772	-5.9502	0.5444	-8.3945	0.7680	0.0000	0.0000
Xingtai	-8.0177	0.5599	-11.7159	0.8182	12.7585	1.2946	-10.2946	1.0446	0.0001	0.0000
Xuancheng	-3.0473	0.8993	-7.1770	2.1181	-5.0424	1.0584	-8.2257	1.7266	0.0031	0.0147
Yancheng	-2.8740	0.2944	-7.5643	0.7750	-4.9486	0.4839	-7.4602	0.7295	0.0001	0.0001
Yangzhou	-3.4277	0.4217	-7.8603	0.9671	-6.0637	0.9556	-7.5957	1.1971	0.0007	0.0002
Zhangjiakou	-1.9981	0.4184	-7.0884	1.4843	-5.0129	1.6771	-7.2176	2.4147	0.0244	0.0031
Zhenjiang	-3.3792	0.5744	-7.2105	1.2256	-5.3458	0.8955	-7.2924	1.2216	0.0010	0.0011
Zhoushan	-2.1100	0.1445	-10.1085	0.6920	-2.7698	0.3012	-7.4022	0.8051	0.0001	0.0000

Table S5. The performance of LightGBM model of $PM_{2.5}$ and PM_{10}, respectively. TaizhouJS denotes Taizhou City in Jiangsu Province, while TaizhouZJ refers to Taizhou City in Zhejiang Province.

city	PM2.5_r	PM10_r	PM2.5_RMSE	PM10_RMSE	PM2.5_MAE	PM10_MAE
Beijing	0.5644	0.5718	20.6706	26.6527	14.4762	19.8407
Tianjin	0.6921	0.6506	15.6387	23.8791	11.0815	17.0144
Baoding	0.8272	0.7767	24.0149	34.9302	16.9075	24.3295
Tangshan	0.5321	0.5480	20.9724	30.5558	15.5568	23.6637
Langfang	0.7237	0.7083	18.51454	25.5347	12.2293	18.6210
Shijiazhuang	0.7794	0.5854	24.5459	44.7494	17.3812	31.3860
Qinhuangdao	0.7011	0.6276	11.2524	20.1793	8.6251	15.3492
Zhangjiakou	0.5500	0.4491	7.9217	27.5828	5.9925	17.7796
Chengde	0.7144	0.6448	7.5943	18.6286	5.6171	13.6455
Cangzhou	0.8475	0.8461	13.5138	19.5238	10.0303	14.5251
Hengshui	0.8444	0.7810	18.7663	33.8730	12.4934	22.9780
Xingtai	0.6747	0.6381	28.3779	41.3640	21.3908	31.8897
Handan	0.7116	0.5325	25.7263	46.7850	18.4948	36.8554
Shanghai	0.8062	0.6959	8.9958	12.6902	7.0622	9.8051
Nanjing	0.6616	0.7646	13.9181	17.7208	10.4673	13.5751
Wuxi	0.5760	0.7580	14.5735	16.4633	10.2702	12.6619
Changzhou	0.8164	0.8292	10.1111	14.3833	7.4144	10.5479
Suzhou	0.8560	0.6876	9.0761	15.5955	6.8452	12.4429
Nantong	0.7061	0.4730	11.5009	18.4416	8.7388	14.6917
Yancheng	0.8982	0.8064	7.3902	14.4755	5.5103	11.4200
Yangzhou	0.8540	0.8170	9.6491	16.4180	7.7381	12.3822
Zhenjiang	0.6686	0.7201	14.0041	17.5832	11.1591	14.5593
TaizhouJS	0.7802	0.6517	11.6168	22.2128	9.4414	17.7950
Hangzhou	0.8874	0.8827	7.5883	10.9447	5.5673	8.2949
Ningbo	0.7471	0.7475	9.4954	13.9908	6.6607	10.4041
Wenzhou	0.8137	0.7777	6.5513	11.0396	4.6793	8.3051
Jiaxing	0.6404	0.8196	11.7675	12.4162	8.0015	9.1972

Huzhou	0.5938	0.6861	15.7273	15.3358	12.5205	12.4943
Shaoxing	0.8407	0.7143	8.2785	22.6327	6.1060	19.4315
Jinhua	0.7593	0.6948	10.3149	13.2076	6.6223	9.9251
Zhoushan	0.5642	0.6720	7.0846	9.5627	5.5608	7.4310
TaizhouZJ	0.8367	0.7543	6.4091	10.9694	4.6700	8.2166
Hefei	0.8776	0.7970	10.4666	14.6836	7.6459	11.4373
Wuhu	0.8404	0.7236	11.3914	17.3035	8.7330	13.3670
Maanshan	0.8696	0.7880	9.6970	14.4269	7.2498	10.9133
Tongling	0.8480	0.7748	10.7971	15.6917	8.4124	11.9264
Anqing	0.8896	0.8374	9.9570	13.5580	8.2567	10.6048
Chuzhou	0.8427	0.7694	11.2695	16.7653	8.8733	12.8443
Chizhou	0.8381	0.7932	11.4400	16.3194	9.2961	13.209
Xuancheng	0.8149	0.6723	11.2669	16.8123	9.3296	12.6950

Figures

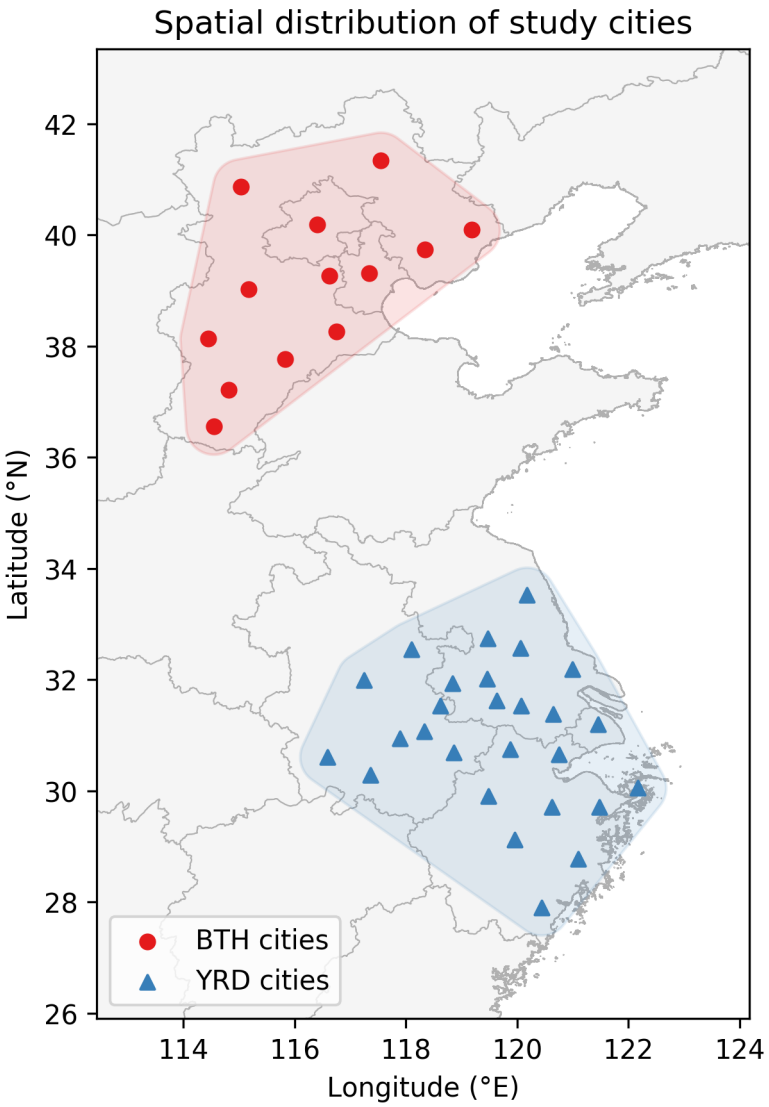

Fig.S1. Beijing-Tianjin-Hebei Yangtze River Delta city distribution map

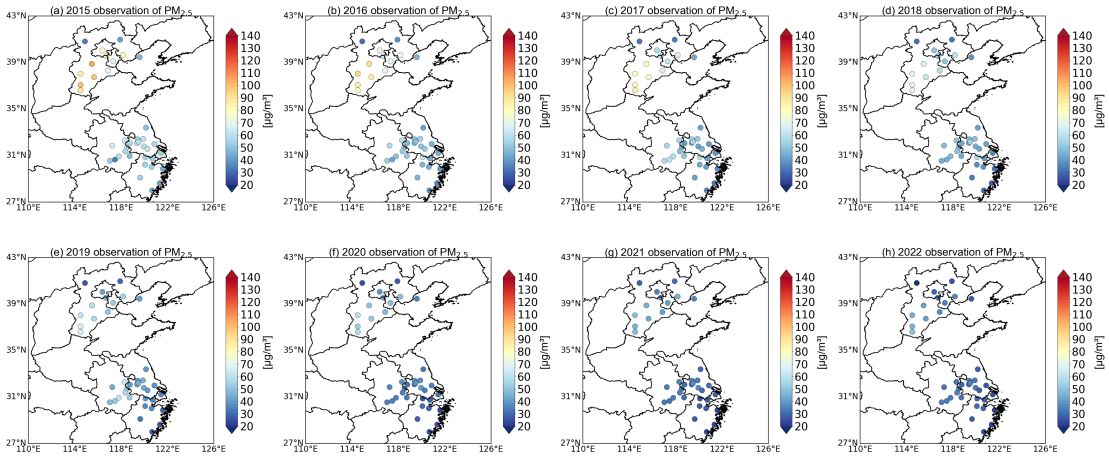

Fig. S2. The average concentrations of $PM_{2.5}$ over BTH and YRD regions during 2015 to 2022.

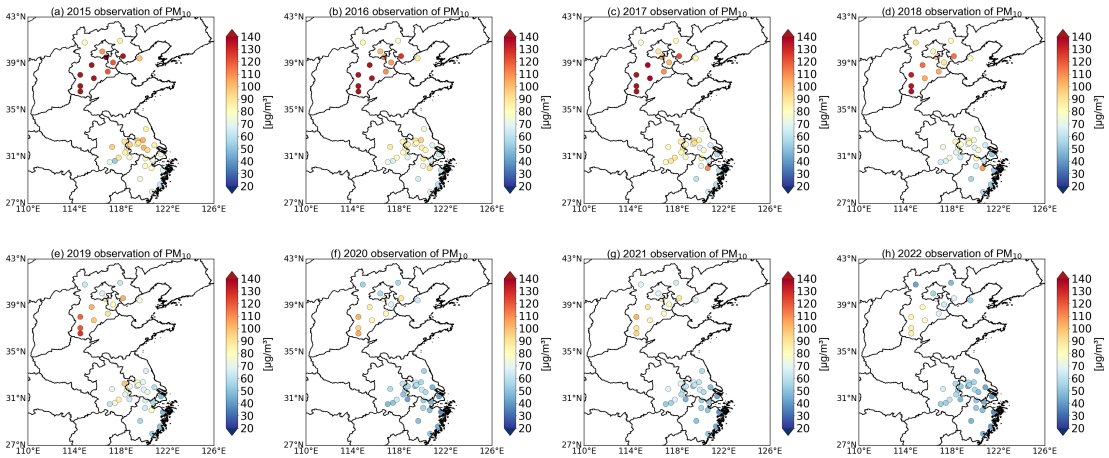

Fig. S3. The average concentrations of PM_{10} over BTH and YRD regions during 2015 to 2022.

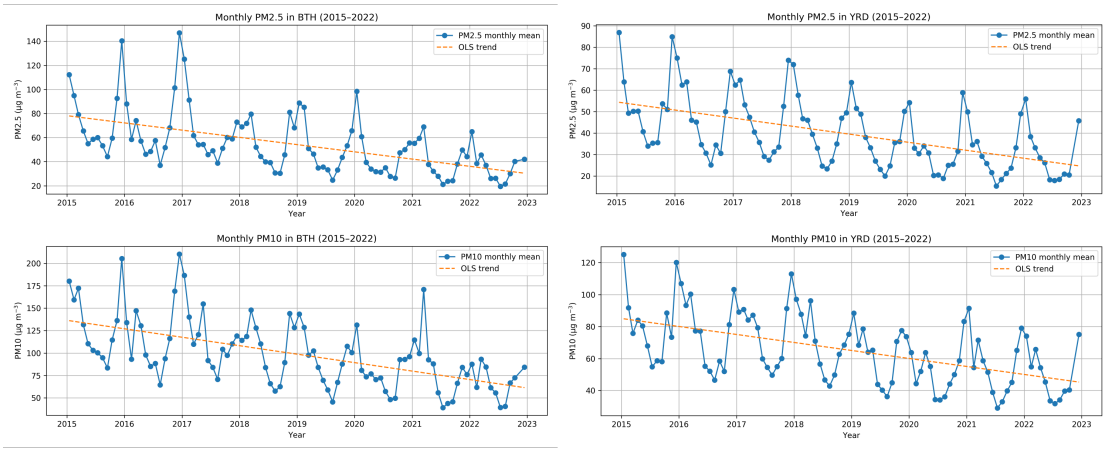

Fig.S4. Monthly mean $PM_{2.5}$ and PM_{10} time series for the BTH and YRD regions from 2015 to 2022, with corresponding OLS fitted trend lines.

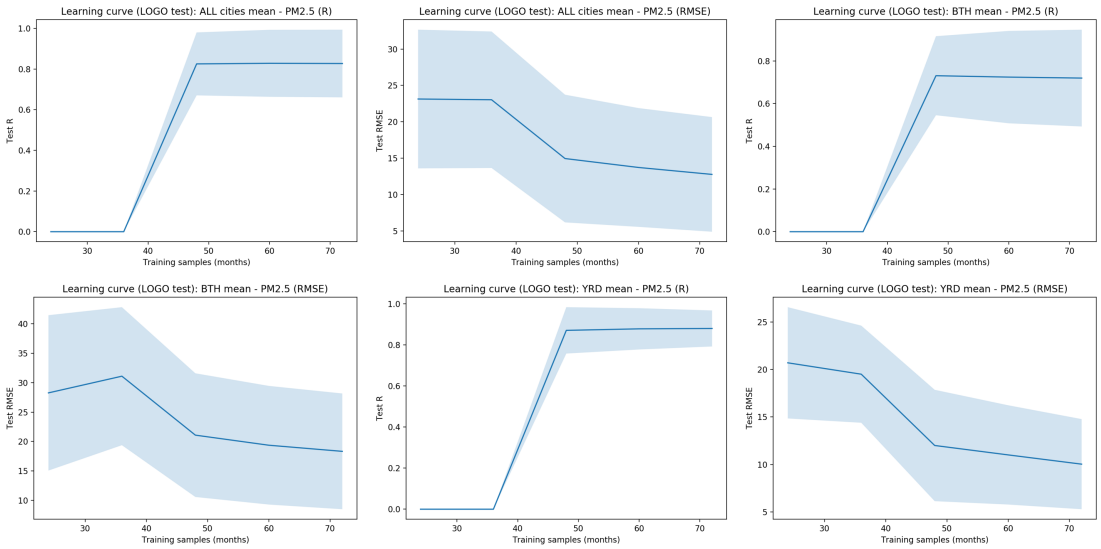

Fig.S5. Learning curves for $PM_{2.5}$ prediction under the leave-one-year-out (LOGO) cross-validation framework. The panels show test performance as a function of training sample size (months) for the all-city mean, the Beijing–Tianjin–Hebei (BTH) region, and the Yangtze River Delta (YRD) region. For each domain, the learning curve is reported using the test correlation coefficient (R) and the test root mean square error (RMSE), shown in separate panels. Solid lines denote the mean across LOGO folds, and the shaded areas indicate variability among folds.

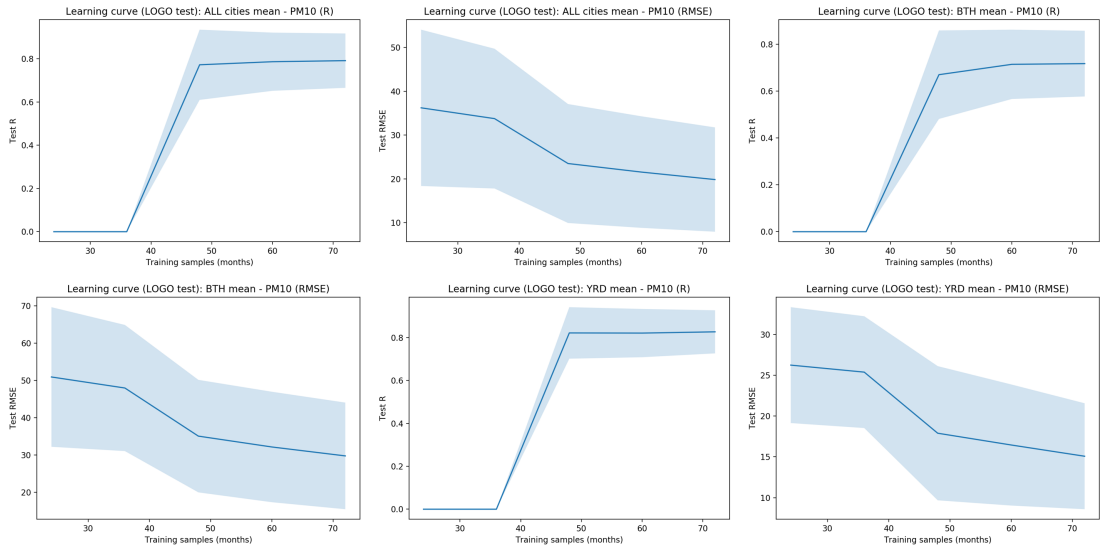

Fig.S6. Learning curves for PM_{10} prediction under the leave-one-year-out (LOGO) cross-validation framework. The panels show test performance as a function of training sample size (months) for the all-city mean, the Beijing–Tianjin–Hebei (BTH) region, and the Yangtze River Delta (YRD) region. For each domain, the learning curve is reported using the test correlation coefficient (R) and the test root mean square error (RMSE), shown in separate panels. Solid lines denote the mean across LOGO folds, and the shaded areas indicate variability among folds.

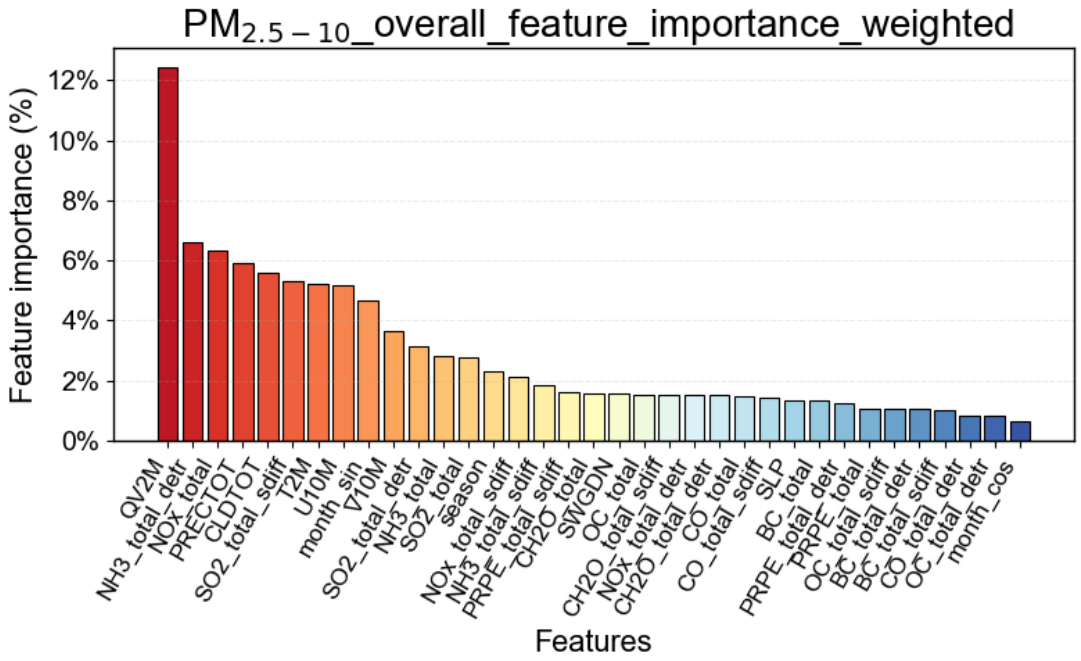

Fig.S7. Overall SHAP-based feature importance for the coarse-mode mass $PM_{2.5}$–10 (PM_{10} minus $PM_{2.5}$), derived from the LightGBM models under the leave-one-year-out cross-validation framework. Bars show the weighted mean contribution of each predictor across all cities and years, expressed as a percentage of total importance. Features include emission-related variables, meteorological variables, and their temporal descriptors (sdiff and detr), ranked in descending order of importance.

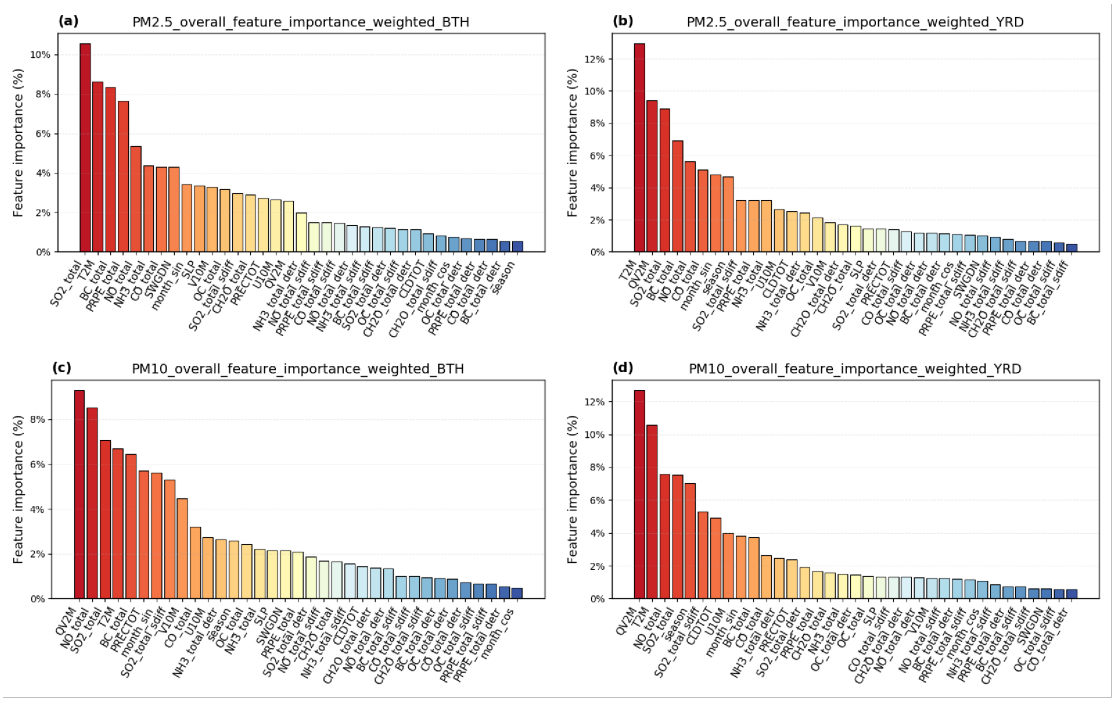

Fig. S8. The feature importance of $PM_{2.5}$ and PM_{10} over BTH and YRD regions.