

1. The Principle of XGBoost

XGBoost can also help address the overfitting, support the parallelization of tree construction and speed up the execution, which is able to increase forecasting accuracy. It can be described as Equation (1):

$$\hat{y} = \sum_{k=1}^K f_k(x_i), f_k \in F \quad (S1)$$

where \hat{y} is the predicted value of the i th sample, K is the number of trees, f_k is the structure of the k th tree and the weight of the leaf node, x_i is the eigenvalue of the i th sample, and $i = 1, \dots, N$, F is the set of all trees.

To find the minimized objective function, performing Taylor's second-order expansion on the t th objective function $f_{obj}^{(t)}(x_i)$ when $f_{obj}^{(t)}(x_i) = 0$. The approximate objective function can be expressed as follows:

$$f_{obj}^{(t)} \approx \sum_{i=1}^N [L(y_i, \hat{y}_i^{(t-1)}) + g_{i,t} f_{i,t}(x_i) + \frac{1}{2} h_{i,t} f_{i,t}^2(x_i)] + \Omega(f_t) + C \quad (S2)$$

where $g = \partial_{\hat{y}} L(y_i, \hat{y}_i^{(t-1)})$, $h = \partial_{\hat{y}}^2 L(y_i, \hat{y}_i^{(t-1)})$.

Regularizing the complexity of the algorithm in the objective function can prevent the algorithm from overfitting. The structure of the tree is defined as q , the weight of the leaf nodes is w . The algorithm complexity is defined as the sum of the squares of the nodes in each tree and the real fraction values corresponding to the leaf nodes. The expression can be shown in Equation (3):

$$\Omega(f_t) = \gamma T + \frac{1}{2} \lambda \sum_{j=1}^T w_j^2 \quad (S3)$$

where γ is used to control the number of leaf nodes, T is the number of leaf nodes, and λ is used to control the weight of leaf nodes. The adjusted objective function expression is given in Equation (4):

$$f_{obj}^{(t)} = \sum_{j=1}^T [(\sum_{i \in I_j} g_i) w_j + \frac{1}{2} \sum_{i \in I_j} (h_i + \lambda) w_j^2] + \gamma T \quad (S4)$$

where $I_j = \{i | q(x_i) = j\}$ is used to represent the sample set in each leaf in the j th tree.

Redefining $G = \sum_{j=1}^T \sum_{i \in I_j} g_i$ and $H = \frac{1}{2} \sum_{j=1}^T \sum_{i \in I_j} (h_i + \lambda)$, the objective function $f_{obj}^{(t)}$ is transformed is a one-variable quadratic function, and the optimal w and objective function value are obtained by solving it. The objective function is used as the scoring function of the algorithm. The solution expression is given in Equation (5) – (6):

$$w_j^* = - \frac{G_j}{H_j + \lambda} \quad (S5)$$

$$f_{obj} = - \frac{1}{2} \sum_{j=1}^T \frac{G_j^2}{H_j + \lambda} + \gamma T \quad (S6)$$

where w_j^* is used to represent the optimal value of w and f_{obj} is the final objective function.

Table S1. The relevant statistical analysis of the annual concentrations of PM_{2.5} in 2017 in Henan Province, Hubei Province and Hunan Province.

Province	City	MIN	MAX	RANGE	MEAN	STD
Henan Province	ZZ	39.10	75.30	36.20	61.91	8.94
Henan Province	KF	56.20	73.40	17.20	63.60	3.37
Henan Province	LY	25.00	73.70	48.70	46.23	12.26
Henan Province	PDS	29.40	68.60	39.20	56.12	8.11
Henan Province	AY	34.90	81.80	46.90	65.02	8.24
Henan Province	HB	45.80	73.60	27.80	64.31	3.61
Henan Province	XX	31.70	71.00	39.30	62.87	5.57
Henan Province	JZ	37.60	78.30	40.70	68.43	6.07
Henan Province	PY	57.00	80.50	23.50	65.40	2.51
Henan Province	XC	43.00	68.10	25.10	61.03	3.95
Henan Province	LH	57.70	66.60	8.90	61.37	1.46
Henan Province	SMX	29.20	64.70	35.50	41.14	9.25
Henan Province	NY	25.20	58.90	33.70	45.92	7.44
Henan Province	SQ	54.10	67.60	13.50	59.15	2.13
Henan Province	XY	31.00	58.50	27.50	48.16	6.12
Henan Province	ZK	53.10	63.40	10.30	57.58	1.65
Henan Province	ZMD	39.50	62.40	22.90	53.14	4.15
Henan Province	JY	31.80	69.50	37.70	54.97	7.78
Hubei Province	WH	38.40	59.60	21.20	50.64	4.05
Hubei Province	HS	31.70	55.60	23.90	44.35	4.63
Hubei Province	SY	19.80	47.30	27.50	31.67	5.39
Hubei Province	YC	20.50	58.20	37.70	37.55	9.71
Hubei Province	XY	23.90	66.00	42.10	43.86	10.40
Hubei Province	EZ	43.50	55.30	11.80	50.41	2.77
Hubei Province	JM	35.00	60.40	25.40	47.29	5.69
Hubei Province	XG	37.20	59.10	21.90	48.21	5.12
Hubei Province	JZ	31.10	58.70	27.60	50.64	3.25
Hubei Province	HG	25.90	52.90	27.00	40.29	5.45
Hubei Province	XN	30.20	55.70	25.50	39.69	4.67
Hubei Province	SZ	35.70	49.70	14.00	42.39	2.78
Hubei Province	ES	21.10	41.60	20.50	28.96	3.50
Hubei Province	XT	46.90	56.00	9.10	51.94	1.73
Hubei Province	QJ	47.50	53.00	5.50	50.43	1.05
Hubei Province	TM	47.10	56.30	9.20	50.89	1.56
Hubei Province	SNJ	19.40	31.20	11.80	24.43	1.54
Hunan Province	CS	30.70	57.40	26.70	43.21	5.37
Hunan Province	ZZ	24.70	55.20	30.50	39.46	6.61
Hunan Province	XT	35.70	56.10	20.40	47.51	4.34
Hunan Province	HY	32.60	51.00	18.40	43.23	2.87

Table S1. *Cont.*

Province	City	MIN	MAX	RANGE	MEAN	STD
Hunan Province	SY	27.30	53.90	26.60	37.79	5.73
Hunan Province	YUY	33.30	53.50	20.20	42.77	5.10
Hunan Province	CD	23.60	55.00	31.40	42.27	6.64
Hunan Province	ZJJ	23.00	46.90	23.90	33.28	4.38
Hunan Province	YIY	29.00	54.20	25.20	40.11	6.97
Hunan Province	CZ	24.30	42.70	18.40	33.92	4.49
Hunan Province	YZ	29.00	49.40	20.40	39.11	3.86
Hunan Province	HY	27.20	40.40	13.20	33.29	2.25
Hunan Province	LD	29.50	48.20	18.70	39.75	4.05
Hunan Province	XX	23.80	38.10	14.30	28.97	2.31

Table S2. The relevant statistical analysis of the annual concentrations of PM_{2.5} in 2018 in Henan Province, Hubei Province and Hunan Province.

Province	City	MIN	MAX	RANGE	MEAN	STDEV
Henan Province	ZZ	32.20	68.30	36.10	55.45	8.69
Henan Province	KF	53.70	69.10	15.40	60.96	2.79
Henan Province	LY	21.70	62.60	40.90	40.08	10.46
Henan Province	PDS	24.60	64.50	39.90	51.43	8.51
Henan Province	AY	27.70	72.10	44.40	56.74	8.16
Henan Province	HB	39.50	66.30	26.80	56.48	3.90
Henan Province	XX	26.90	64.80	37.90	57.87	5.69
Henan Province	JZ	32.20	66.90	34.70	60.06	5.13
Henan Province	PY	52.90	69.70	16.80	59.43	1.74
Henan Province	XC	36.70	65.00	28.30	57.58	4.46
Henan Province	LH	55.40	63.90	8.50	59.38	1.49
Henan Province	SMX	24.50	58.20	33.70	36.50	8.56
Henan Province	NY	21.80	60.50	38.70	43.99	9.14
Henan Province	SQ	50.40	63.10	12.70	56.14	2.21
Henan Province	XY	26.30	53.40	27.10	43.92	5.71
Henan Province	ZK	46.50	61.00	14.50	54.21	3.00
Henan Province	ZMD	38.60	60.50	21.90	50.04	3.83
Henan Province	JY	27.10	64.40	37.30	49.43	6.71
Hubei Province	WH	30.10	53.80	23.70	44.11	4.37
Hubei Province	HS	24.50	45.40	20.90	35.99	3.69
Hubei Province	SY	18.70	43.70	25.00	29.10	4.46
Hubei Province	YC	17.50	53.30	35.80	33.88	8.95
Hubei Province	XY	23.10	60.50	37.40	41.43	9.58
Hubei Province	EZ	35.40	47.30	11.90	41.84	3.07
Hubei Province	JM	30.60	55.10	24.50	44.15	6.39
Hubei Province	XG	33.10	53.70	20.60	43.38	4.91

Table S2. *Cont.*

Province	City	MIN	MAX	RANGE	MEAN	STDEV
Hubei Province	JZ	26.50	54.30	27.80	45.75	3.48
Hubei Province	HG	20.30	45.60	25.30	32.93	5.11
Hubei Province	XN	23.70	50.20	26.50	33.74	4.61
Hubei Province	SZ	30.60	44.20	13.60	38.28	2.58
Hubei Province	ES	18.50	37.70	19.20	26.46	3.19
Hubei Province	XT	42.50	51.30	8.80	47.81	1.55
Hubei Province	QJ	42.80	49.00	6.20	45.95	1.18
Hubei Province	TM	42.50	51.40	8.90	46.30	1.60
Hubei Province	SNJ	18.30	28.40	10.10	22.76	1.49
Hunan Province	CS	25.90	50.00	24.10	35.94	4.95
Hunan Province	ZZ	21.40	46.80	25.40	32.32	5.19
Hunan Province	XT	29.60	48.50	18.90	39.81	4.04
Hunan Province	HY	28.60	44.40	15.80	36.22	2.80
Hunan Province	SY	23.00	45.30	22.30	32.90	4.17
Hunan Province	YUY	27.80	49.70	21.90	37.48	4.82
Hunan Province	CD	20.50	49.40	28.90	36.87	5.98
Hunan Province	ZJJ	20.40	40.10	19.70	28.14	3.68
Hunan Province	YIY	25.90	47.10	21.20	34.03	6.03
Hunan Province	CZ	21.40	36.50	15.10	28.43	3.23
Hunan Province	YZ	25.90	46.30	20.40	34.33	4.14
Hunan Province	HY	23.40	36.50	13.10	29.20	2.16
Hunan Province	LD	26.60	42.20	15.60	33.79	3.26
Hunan Province	XX	21.00	34.10	13.10	25.72	2.16

Table S3. The relevant statistical analysis of the annual concentrations of PM_{2.5} in 2018 in Henan Province, Hubei Province and Hunan Province.

Province	City	MIN	MAX	RANGE	MEAN	STDEV
Henan Province	ZZ	34.20	64.30	30.10	52.77	7.12
Henan Province	KF	51.30	65.80	14.50	57.87	2.92
Henan Province	LY	20.60	63.30	42.70	39.21	10.59
Henan Province	PDS	24.60	60.80	36.20	49.98	7.39
Henan Province	AY	27.80	72.00	44.20	57.10	8.52
Henan Province	HB	41.60	66.70	25.10	58.28	4.61
Henan Province	XX	27.70	62.50	34.80	56.26	5.42
Henan Province	JZ	34.20	64.40	30.20	57.22	4.75
Henan Province	PY	53.00	70.50	17.50	60.31	2.29
Henan Province	XC	37.80	61.80	24.00	55.15	4.08
Henan Province	LH	52.10	61.60	9.50	56.81	1.49
Henan Province	SMX	24.10	56.80	32.70	35.12	8.47
Henan Province	NY	20.80	57.90	37.10	42.53	8.59

Table S3. *Cont.*

Province	City	MIN	MAX	RANGE	MEAN	STDEV
Henan Province	SQ	49.70	62.40	12.70	55.28	2.19
Henan Province	XY	24.90	50.10	25.20	40.92	5.41
Henan Province	ZK	46.20	58.50	12.30	52.39	2.15
Henan Province	ZMD	35.50	57.80	22.30	47.70	3.92
Henan Province	JY	29.60	59.70	30.10	47.63	5.94
Hubei Province	WH	30.80	50.50	19.70	43.31	3.78
Hubei Province	HS	26.40	45.40	19.00	37.27	3.39
Hubei Province	SY	19.10	42.30	23.20	28.67	4.25
Hubei Province	YC	18.80	55.00	36.20	35.11	9.23
Hubei Province	XY	23.10	60.00	36.90	40.95	9.24
Hubei Province	EZ	35.70	46.60	10.90	41.80	2.75
Hubei Province	JM	32.10	57.50	25.40	46.79	6.28
Hubei Province	XG	32.80	53.60	20.80	43.60	5.33
Hubei Province	JZ	27.90	54.40	26.50	46.19	3.19
Hubei Province	HG	20.20	48.00	27.80	33.24	5.39
Hubei Province	XN	25.30	49.90	24.60	34.39	4.32
Hubei Province	SZ	31.80	42.90	11.10	37.12	2.28
Hubei Province	ES	19.40	37.70	18.30	26.25	2.78
Hubei Province	XT	45.20	51.10	5.90	47.83	1.12
Hubei Province	QJ	43.70	49.30	5.60	47.22	0.72
Hubei Province	TM	45.20	51.70	6.50	48.54	1.08
Hubei Province	SNJ	18.80	28.50	9.70	22.53	1.27
Hunan Province	CS	25.80	50.90	25.10	38.07	5.33
Hunan Province	ZZ	19.30	48.70	29.40	32.06	6.47
Hunan Province	XT	33.60	50.20	16.60	42.50	3.57
Hunan Province	HY	28.20	45.10	16.90	37.39	2.84
Hunan Province	SY	23.70	45.30	21.60	32.76	3.99
Hunan Province	YUY	28.00	49.60	21.60	39.16	5.15
Hunan Province	CD	21.20	49.80	28.60	38.46	6.40
Hunan Province	ZJJ	20.70	39.60	18.90	28.30	3.63
Hunan Province	YIY	27.10	49.60	22.50	37.80	6.73
Hunan Province	CZ	19.20	36.80	17.60	27.75	4.31
Hunan Province	YZ	24.40	44.50	20.10	33.25	4.07
Hunan Province	HY	23.70	35.80	12.10	29.83	2.00
Hunan Province	LD	25.60	43.40	17.80	35.49	3.56
Hunan Province	XX	21.50	34.00	12.50	26.16	1.94

Supplementary Instructions:

Henan Province: Zhengzhou-ZZ, Kaifeng-KF, Luoyang-LY, Pingdingshan-PDS, Anyang-Ay, Hebi-HB, Xinxiang-XX, Jiaozuo-JZ, Puyang-PY, Xuchang-XC, Luohe-LH, Sanmenxia-

SMX, Nanyang-NY, Shangqiu-SQ, Xinyang-XY, Zhoukou-ZK, Zhumadian-ZMD, Jiyuan-JY.

Hubei Province: Wuhan-WH, Huangshi-HS, Shiyan-SY, Yichang-YC, Xiangyang-XY, Ezhou-EZ, Jingmen-JM, Xiaogan-XG, Jingzhou-JZ, Huanggan-HG, Xianning-XN, Suizhou-SZ, Enshi-ES, Xiantao-XT, Qianjiang-QJ, Tianmen-TM, Shennongjia-SNJ.

Hunan Province: Changsha-CS, Zhuzhou-ZZ, Xiangtan-XT, Hengyang-HY, Shaoyang-SY, Yueyang-YUY, Changde-CD, Zhangjiajie-ZJJ, Yiyang-YIY, Chenzhou-CZ, Yongzhou-YZ, Huaihua-HH, Loudi-LD, Xiangxi-XX.

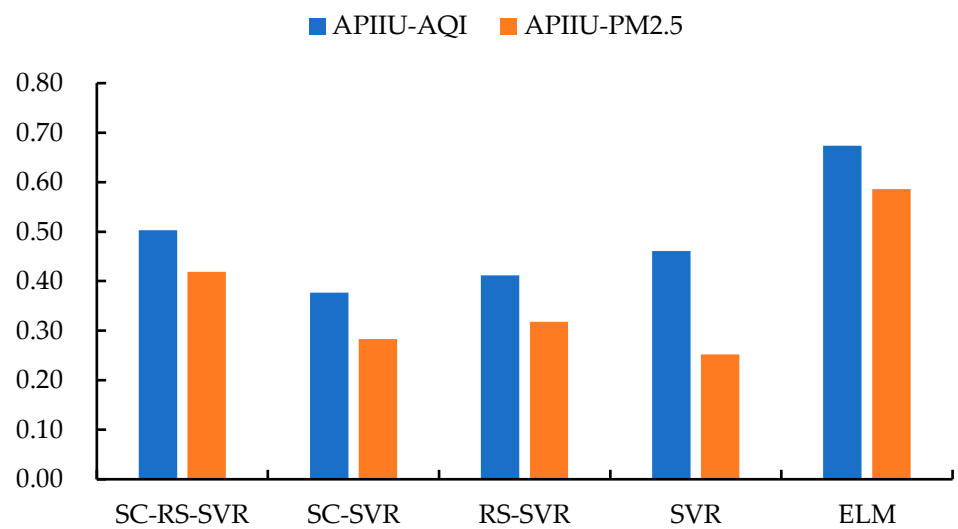


Figure S1. Comparison of R^2 of SC-RS-SVR model, SC-SVR model, RS-SVR model, SVR model and ELM model.

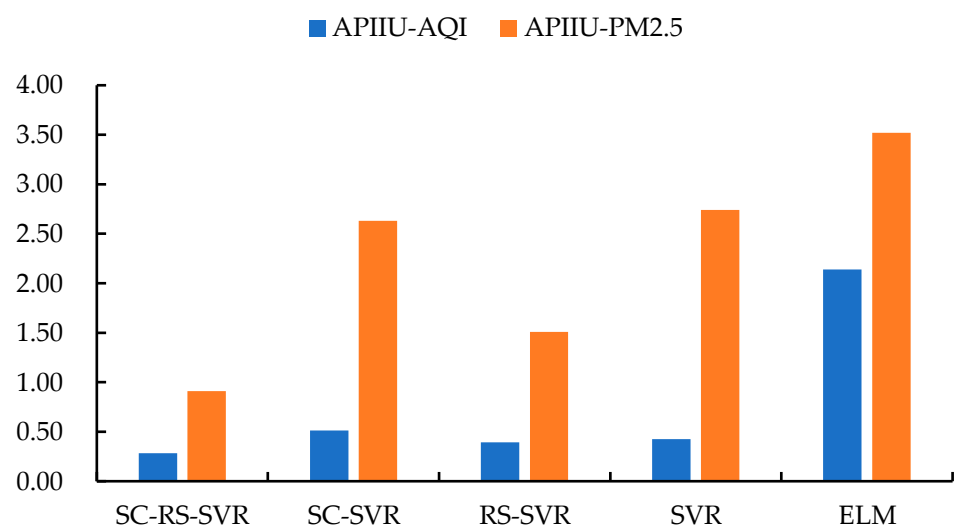


Figure S2. Comparison of RMSE of SC-RS-SVR model, SC-SVR model, RS-SVR model, SVR model and ELM model.

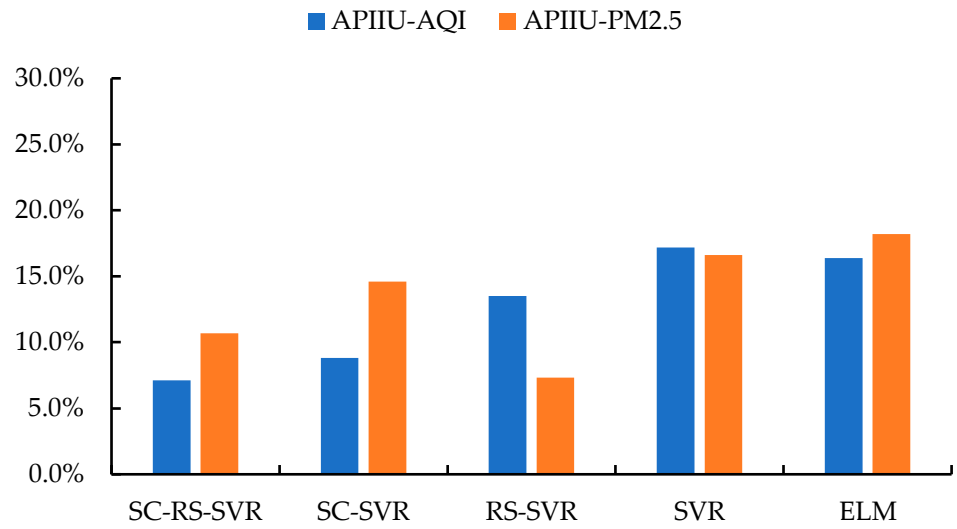


Figure S3. Comparison of MAPE of SC-RS-SVR model, SC-SVR model, RS-SVR model, SVR model and ELM model.