Urban Surface Ozone Concentration in Mainland China during 2015–2020: Spatial Clustering and Temporal Dynamics

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Summary

Number of figures:6; Number of tables:5.

Table S1. Data Types and Sources

Type	Data	Data description	Year	Source
Ground-level air pollutant	$PM_{2.5}$、PM_{10}、NO_2、SO_2、CO、$O3$	Hourly-average Observations	2015-2020	http://106.37.208.233:20036/
Land cover-related	Digital elevation model (DEM)	Spatial resolution (1 km)	2018	http://www.resdc.cn/
	Normalized difference vegetation index (NDVI)	Spatial resolution (1 km)	2018	http://www.resdc.cn/
Meteorological elements	Basic Meteorological Data	Precipitation; pressure; wind speed; temperature; relative humidity; sunshine hours	2018	http://data.cma.cn

Table S2. Statistics of the ground-level O_3 concentration in different cities/countries

Regions	Types	Year	O_3 concentration ($\mu g/m^3$)	References
Russian Territory	Urban stations	2020 first half	40	(Andreev et al. 2020)
Iran	Control stations	2015	2-126	(Ezimand and Kakroodi 2019)
Pune, India	Urban stations	2017	10-92	(Anand et al. 2020)
Silesia Region, Poland	Urban stations	2015	Max 160	(Kobza et al. 2021)
Hamburg, German	Urban stations	2000-2017	Mean 56.3, Max 192.1	(Krug et al. 2020)
Leipzig, German	Urban stations	2000-2017	Mean 65.3, Max 198.3	(Krug et al. 2020)
France	Urban sites	1999-2012	98th percentile 46.2	(Sicard et al. 2016)
China	Urban stations	2018	25-230	This study

Table S3. Standard deviation elliptic parameters of urban O$_3$ in mainland China from 2015 to 2020

Year	Xcoord	Ycoord	Long axis/km	Short axis/km	Rotation	Area/km²	North-South distances/km	East-West distances/km
2015	111.973288	33.36638	2727.82	1841.10	79.965774	3944147.97	0	0
2016	111.964956	33.364238	2697.48	1828.38	81.429260	3873060.80	-30.34	-12.72
2017	112.005505	33.377605	2671.06	1828.28	81.919845	3835207.67	-26.42	-0.10
2018	112.086342	33.408489	2682.62	1826.60	80.320602	3848261.55	11.56	-1.68
2019	111.961225	33.169184	2660.72	1854.44	81.130302	3875054.93	-21.90	27.84
2020	111.936832	33.243016	2691.02	1855.62	81.043078	3921629.37	30.30	1.18
							-36.80	14.52

Table S4. Fitting parameters of the OLS, GWR and MGWR models

Model indicators	OLS	GWR	MGWR
Residual sum of squares	216.299	125.966	124.541
Log-likelihood	-397.130	-308.464	-306.597
AICc	821.420	732.506	712.531
R^2	0.341	0.616	0.620
Adj. R^2	0.318	0.550	0.564
Bandwidth	None	170	326 (Intercept)
			314 (NO_2)
			150 (SO_2)
			56 ($PM_{2.5}$)
			298 (DEM)
			326 (Air pressure)
			326 (Wind speed)
			326 (Temperature)
			217 (Relative humidity)
			318 (Sunshine hours)
			108 (Precipitation)
			132 (NDVI)

Table S5. Fitting parameters for the interaction of multi-factors on O_3 concentration variation based on multi-factor generalized additive model (GAM)

Factors	edf Ref	df	F-Value	P-Value	R-sq.(adj)	Deviance explained(%)	n
NO_2	8.745	8.963	340.8	2e-16***	0.0535	5.37	122739
SO_2	8.864	8.990	355.4	2e-16***			
NO_2	8.757	8.966	107.2	2e-16***	0.0711	7.12	122739
$PM_{2.5}$	8.856	8.988	620.9	2e-16***			
NO_2	8.593	8.909	456.1	2e-16***	0.0455	4.56	122014
DEM	8.924	8.998	240.8	2e-16***			
NO_2	8.491	8.862	559.9	2e-16***	0.3140	31.40	122739
SH	8.889	8.996	5673.7	2e-16***			
NO_2	8.502	8.867	618.9	2e-16***	0.0820	8.21	122739
PREC	8.960	8.999	788.7	2e-16***			
NO_2	8.761	8.967	287.0	2e-16***	0.0695	6.96	122379
NDVI	8.904	8.997	598.1	2e-16***			
SO_2	8.853	8.988	287.0	2e-16***	0.0831	8.33	122739
$PM_{2.5}$	8.829	8.983	791.9	2e-16***			
SO_2	8.879	8.992	413.6	2e-16***	0.0429	4.30	122014
DEM	8.853	8.994	175.8	2e-16***			
SO_2	8.860	8.989	455.7	2e-16***	0.309	31.00	122739
SH	8.859	8.994	5522.0	2e-16***			
SO_2	8.851	8.988	436.0	2e-16***	0.0706	7.07	122739
PREC	8.946	8.999	595.6	2e-16***			
SO_2	8.831	8.985	390.6	2e-16***	0.0764	7.66	122379
NDVI	8.940	8.999	681.5	2e-16***			
$PM_{2.5}$	8.876	8.991	933.5	2e-16***	0.0772	7.73	122014
DEM	8.940	8.999	204.4	2e-16***			
$PM_{2.5}$	8.894	8.994	921.2	2e-16***	0.332	33.20	122739
SH	8.878	8.996	5462.2	2e-16***			
$PM_{2.5}$	8.891	8.993	998.6	2e-16***	0.106	10.60	122739
PREC	8.948	8.999	647.8	2e-16***			
$PM_{2.5}$	8.802	8.978	689.2	2e-16***	0.0957	9.58	122379
NDVI	8.884	8.996	483.3	2e-16***			
DEM	8.892	8.997	274.6	2e-16***	0.3010	30.10	122014
SH	8.871	8.995	5567.8	2e-16***			
DEM	8.884	8.996	194.3	2e-16***	0.0546	5.47	122014
PREC	8.909	8.997	586.4	2e-16***			
DEM	8.837	8.992	240.9	2e-16***	0.0669	6.70	122014
NDVI	8.865	8.995	774.2	2e-16***			
SH	8.883	8.996	4851.8	2e-16***	0.2930	29.30	122739
PREC	8.973	9.000	118.2	2e-16***			
SH	8.816	8.990	5988.0	2e-16***	0.3400	34.00	122379

NDVI	8.719	8.977	1109.0	2e-16***			
PREC	8.974	9.000	1132.0	2e-16***	0.1230	12.30	122379
NDVI	8.915	8.998	1270.0	2e-16***			

Note: DEM, Digital Elevation Model; SH, sunshine hours; PREC, precipitation; f. NDVI, normalized difference vegetation index; ***, significant at the 99.9% confidence level.
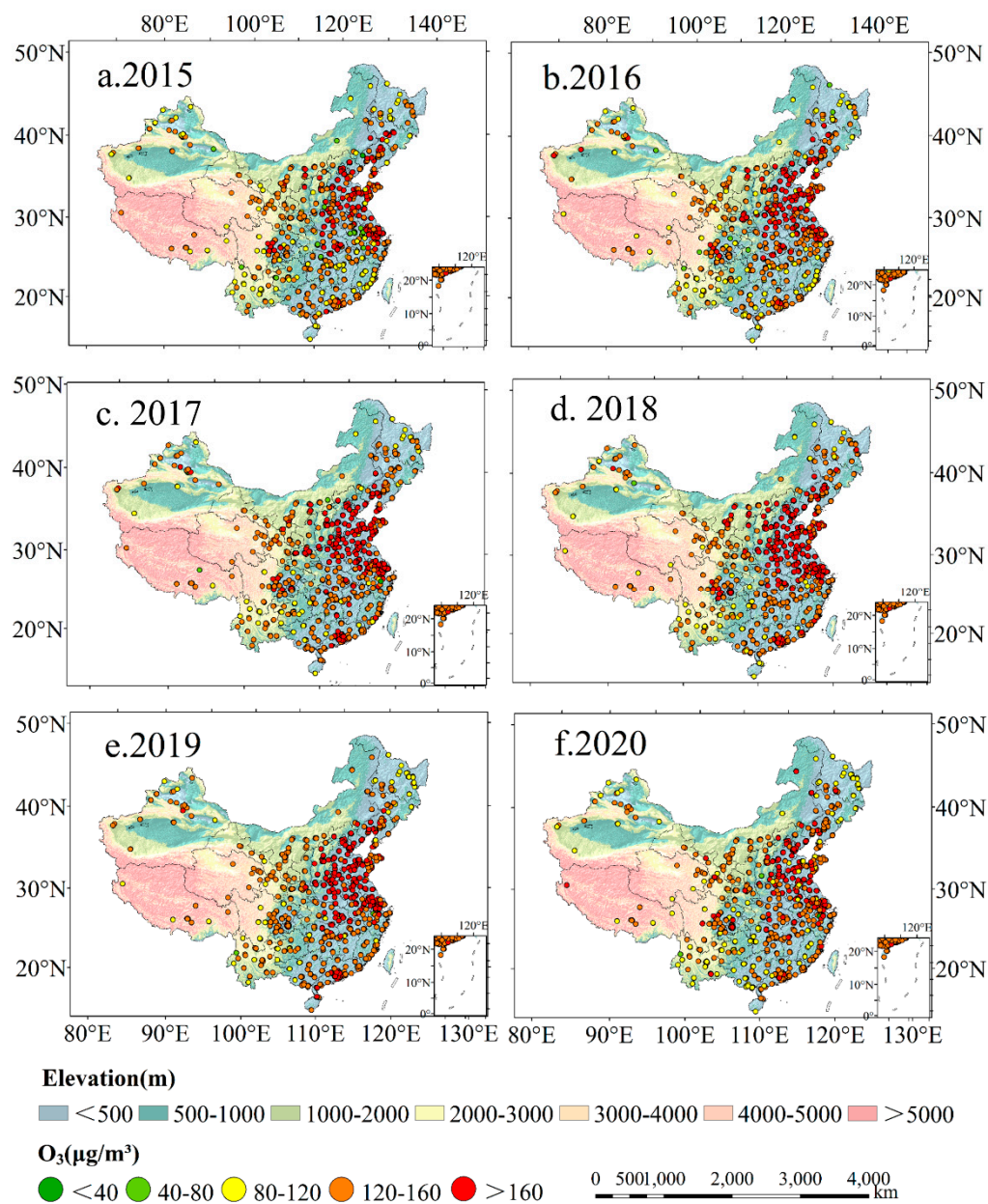
Figure S1 Distribution characteristics of the O₃ concentration (the 90th percentile of daily maximum 8-hour average) (90th MDA8) at various urban monitoring sites in mainland China from 2015 to 2020.
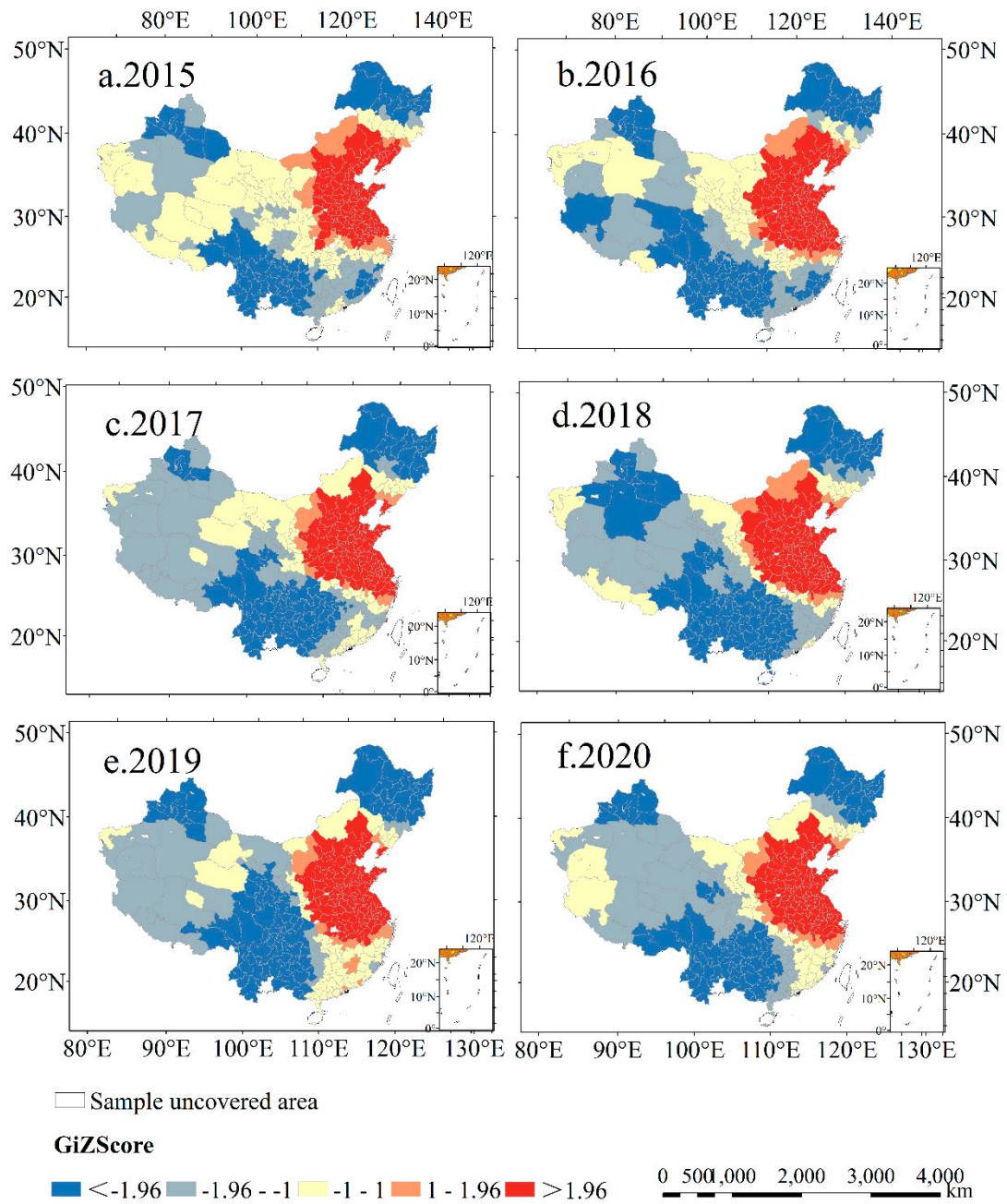
Figure S2 The hot point analysis of urban O$_3$ distribution in mainland China from 2015 to 2020.
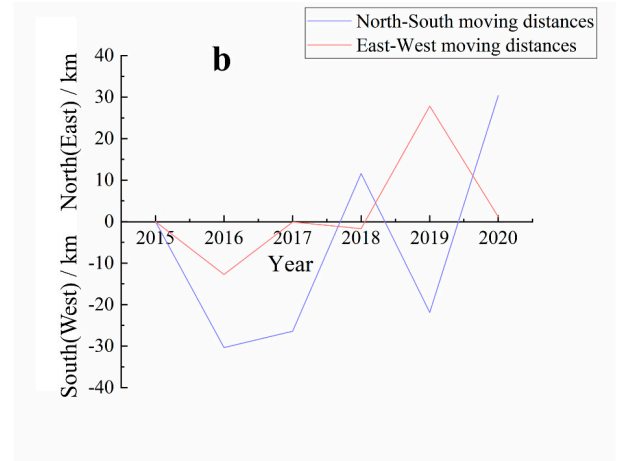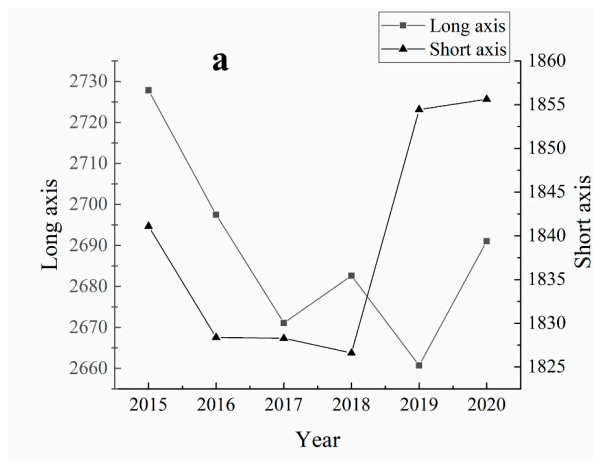
Figure S3 Long and short axes variation characteristics (a) and mean center movement characteristics (b) of standard deviation ellipse.
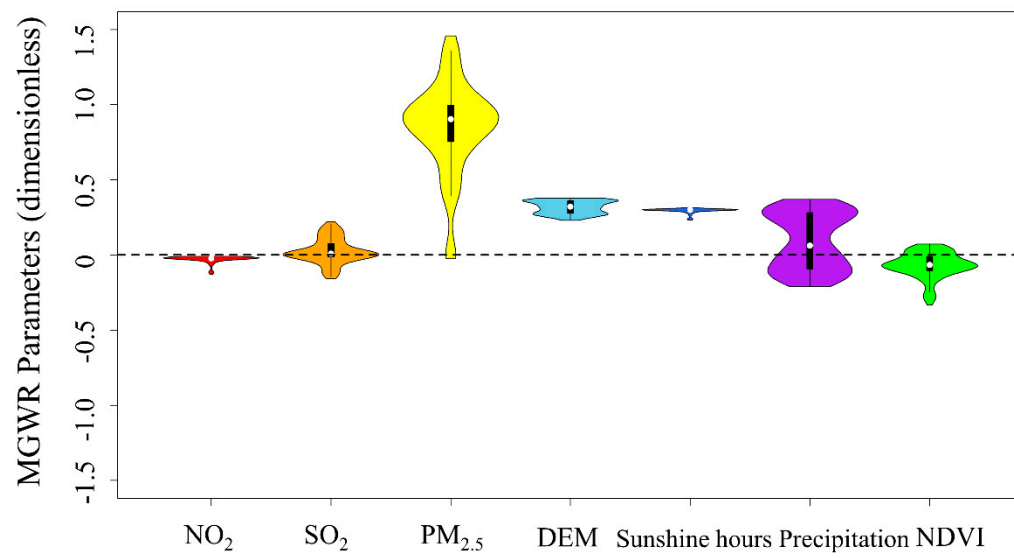
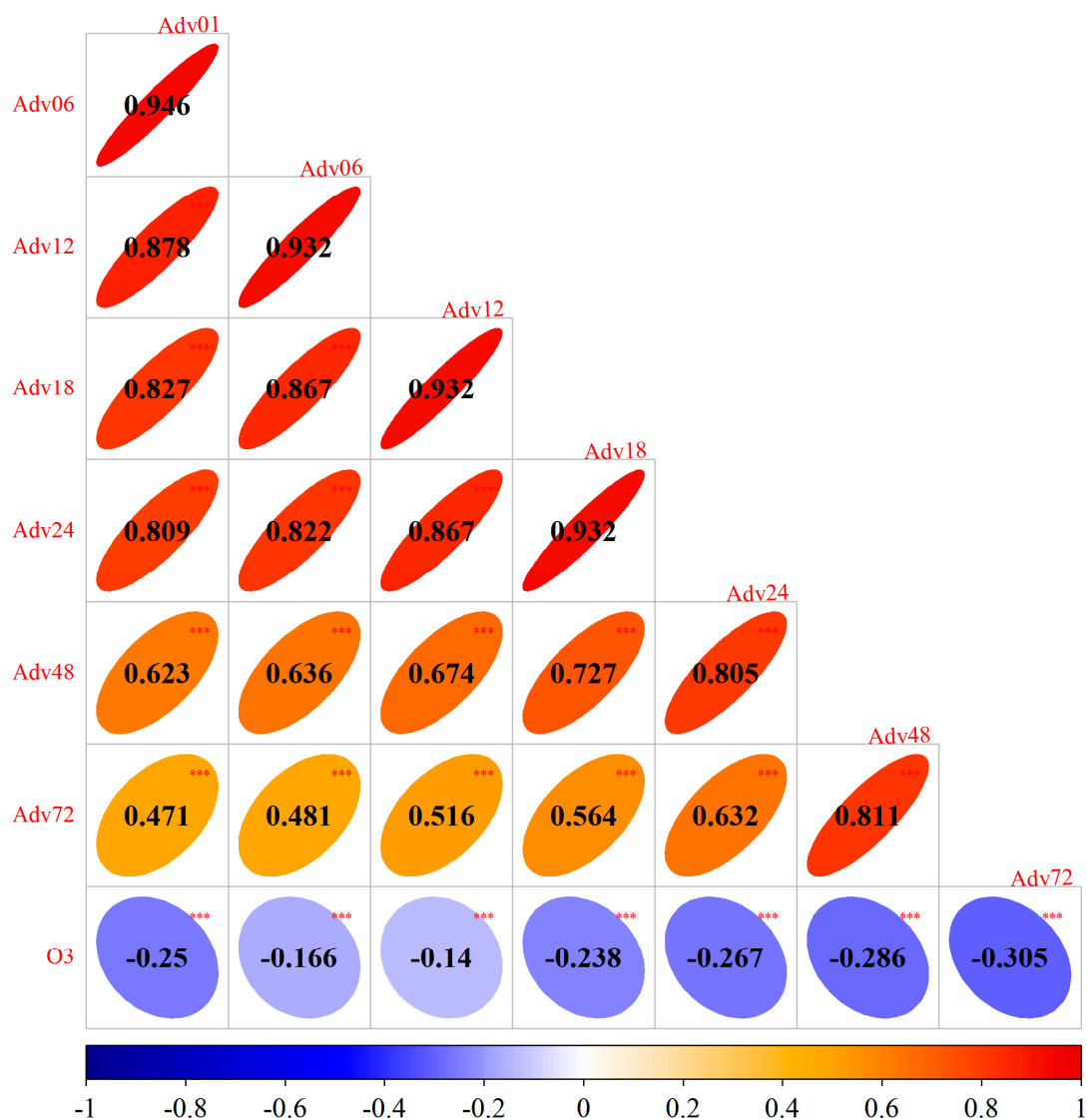Figure S4 Vioplot of multi-scale geographic weighted regression coefficients

Figure S5 Correlation analysis of O₃ concentrations with PM₂.₅ at 1, 6, 12, 18, 24, 48 and 72 hours in advance in the Yangtze River Delta region in 2018.(Note: Adv01, Adv06, Adv012, Adv018, Adv24, Adv48 and Adv72 represent urban PM₂.₅ concentration at 1, 6, 12, 18, 24, 48 and 72 hours in advance, respectively.)
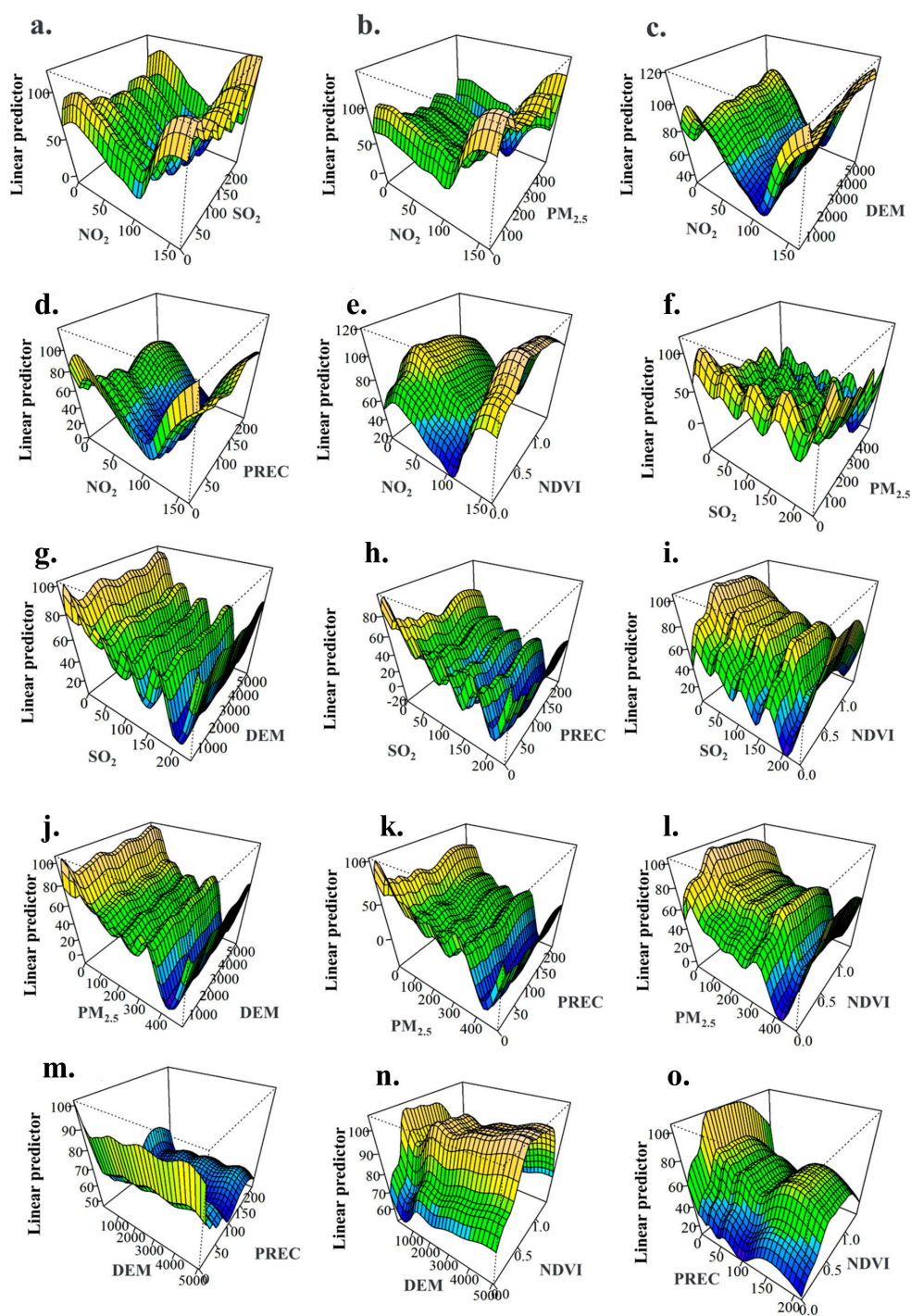
Figure S6. Interaction of different factors on the variation of urban O_3 concentration three-dimensional effect plots. a. NO_2 and SO_2; b. NO_2 and $PM_{2.5}$; c. NO_2 and Digital Elevation Model (DEM); d. NO_2 and precipitation (PREC); e. NO_2 and normalized difference vegetation index (NDVI); f. SO_2 and $PM_{2.5}$; g. SO_2 and DEM; h. SO_2 and PREC; i. SO_2 and NDVI; j. $PM_{2.5}$ and DEM; k. $PM_{2.5}$ and PREC; l. $PM_{2.5}$ and NDVI; m. DEM and PREC; n. DEM and NDVI; o. PREC and NDVI.

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