remote sensing

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Supplementary Materials

A High-Performance Convolutional Neural Network for Ground-Level Ozone Estimation in Eastern China

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The Supplementary Material Includes the Following (Pages 1–16):

1. Supporting Figures S1–S9 (Pages 1–12)
2. Supporting Table S1–S4 (Pages 13–16)

Supplementary Figures

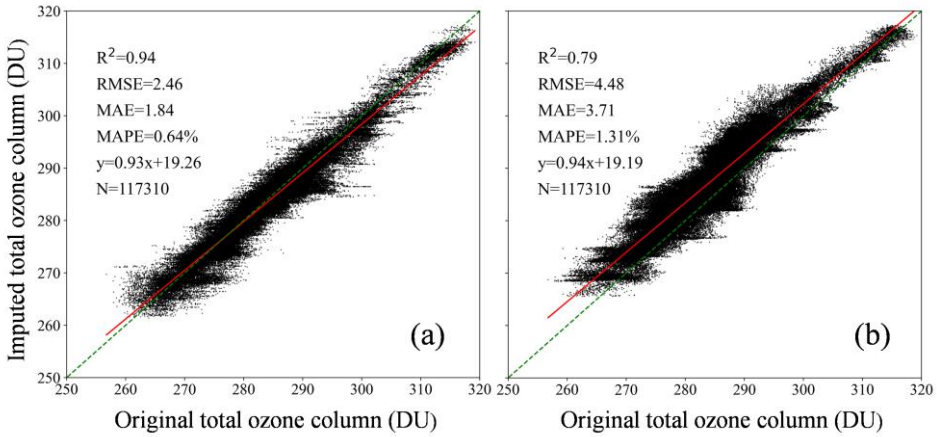


Figure S1. Scatter plot of impute total ozone column: (**a**) Kriging; (**b**) ERA5.

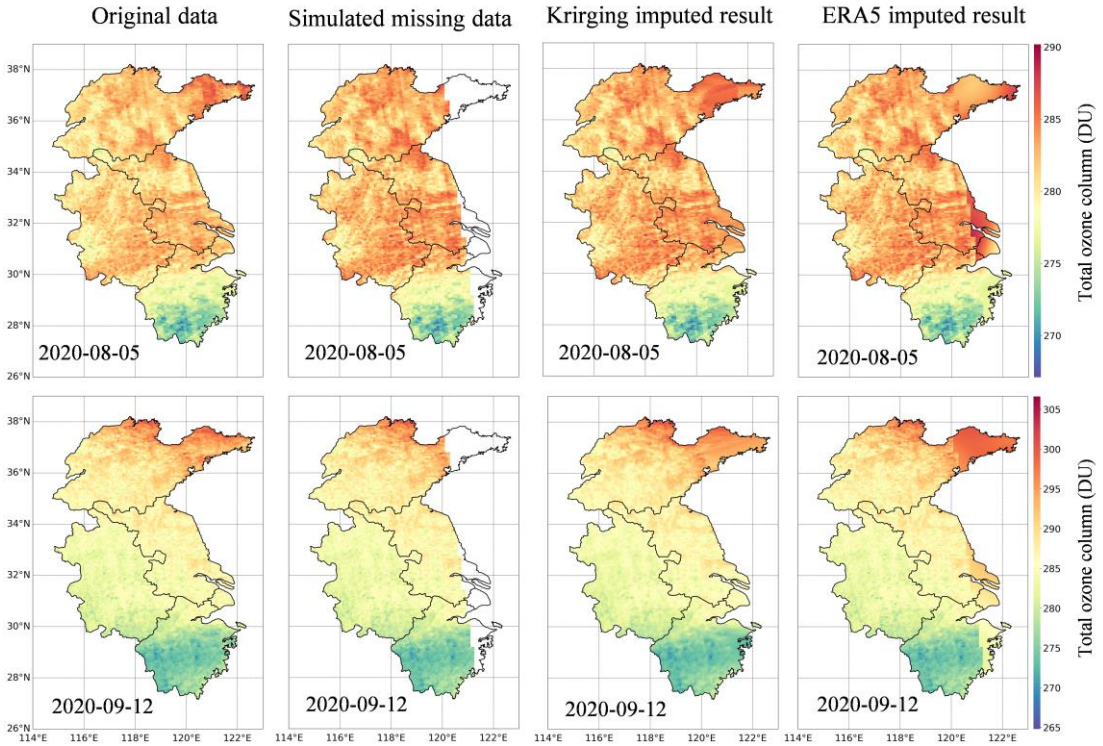


Figure S2. Imputed samples.

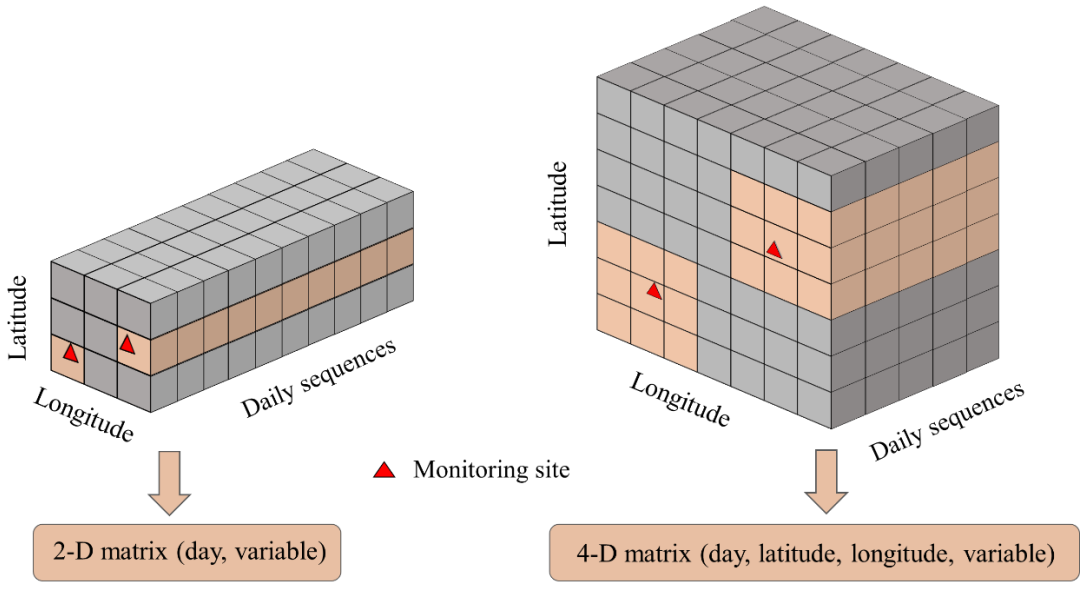


Figure S3. Spatiotemporal match methods: (**a**) 10-day single-point data; (**b**) 5-day spatiotemporal data.

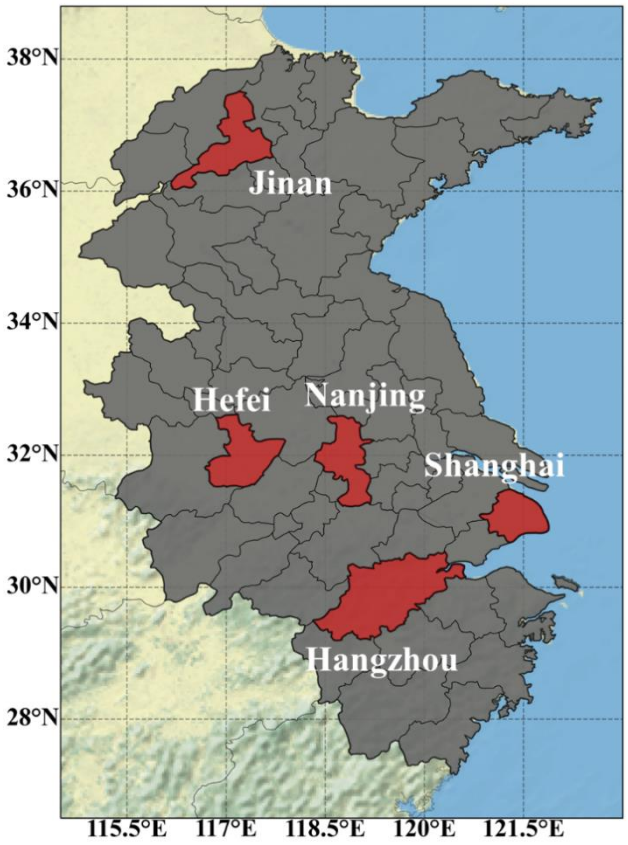


Figure S4. Geographical location of provincial capital cities (Jinan, Nanjing, Hangzhou, and Hefei) and Shanghai.

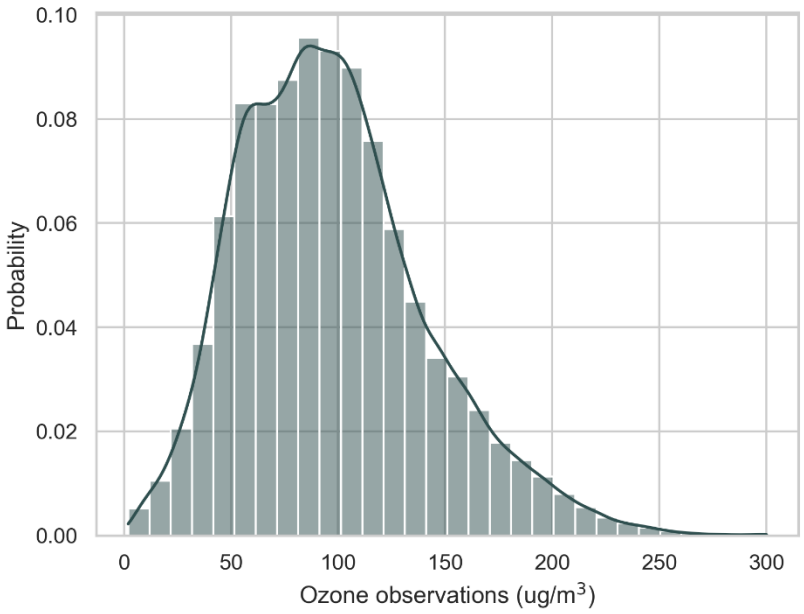
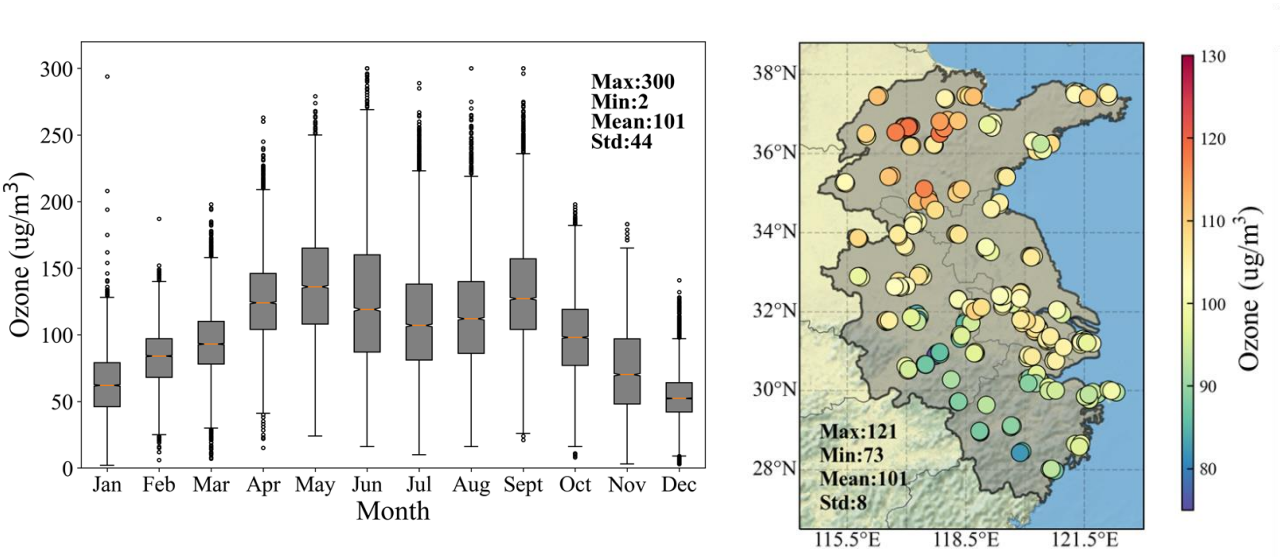


Figure S5. Probability histogram of ozone observations.



(**a**) (**b**)

Figure S6. (**a**) Monthly and (**b**) spatial variations of ozone measurements.

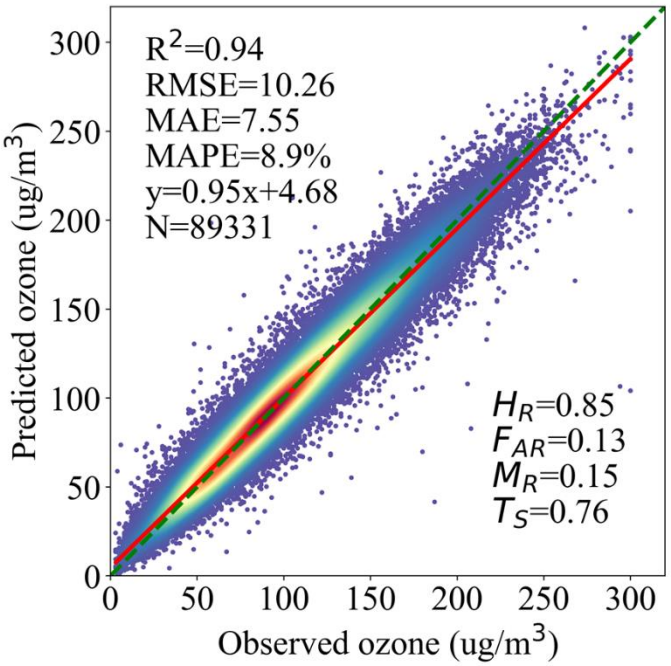


Figure S7. Model fitting results.

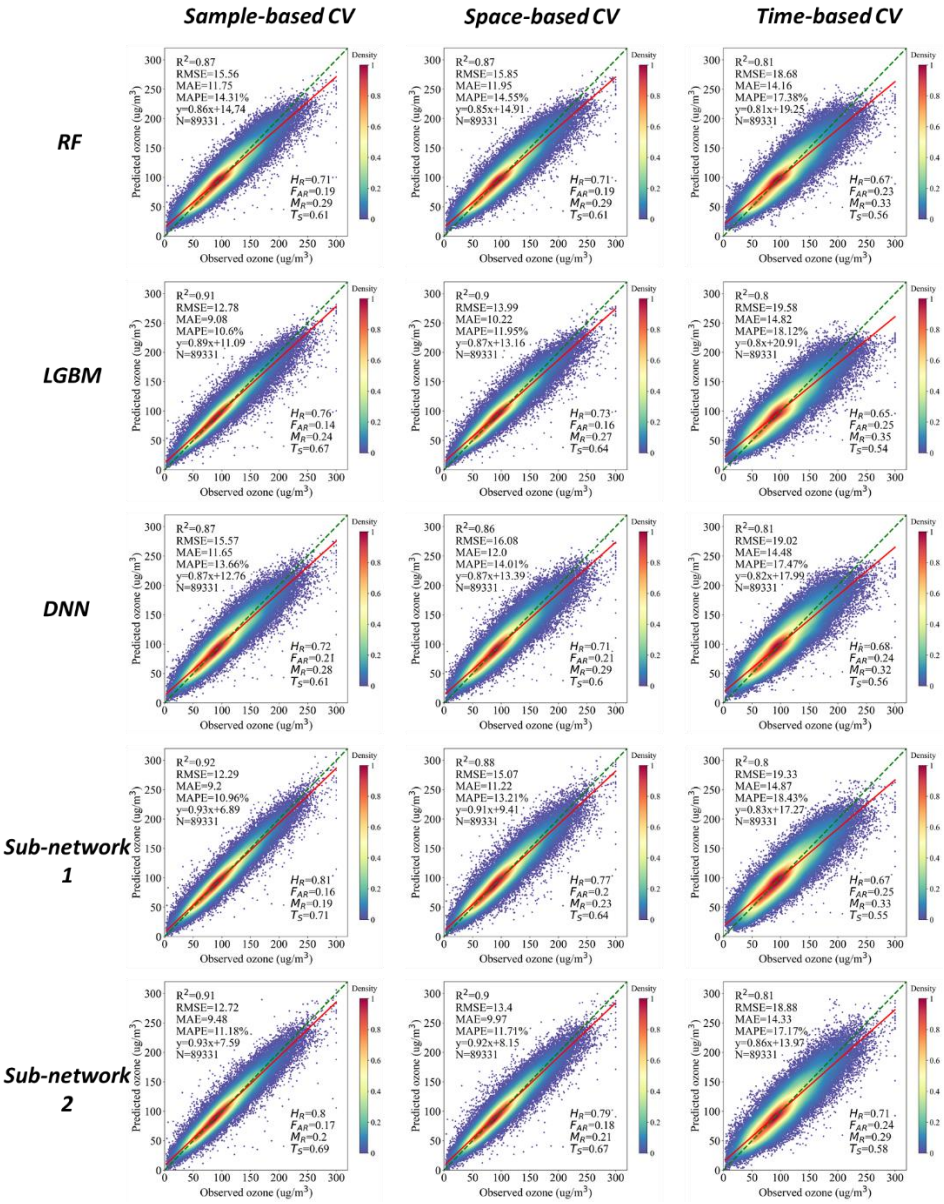


Figure S8. Density scatter plots of models' CV results.

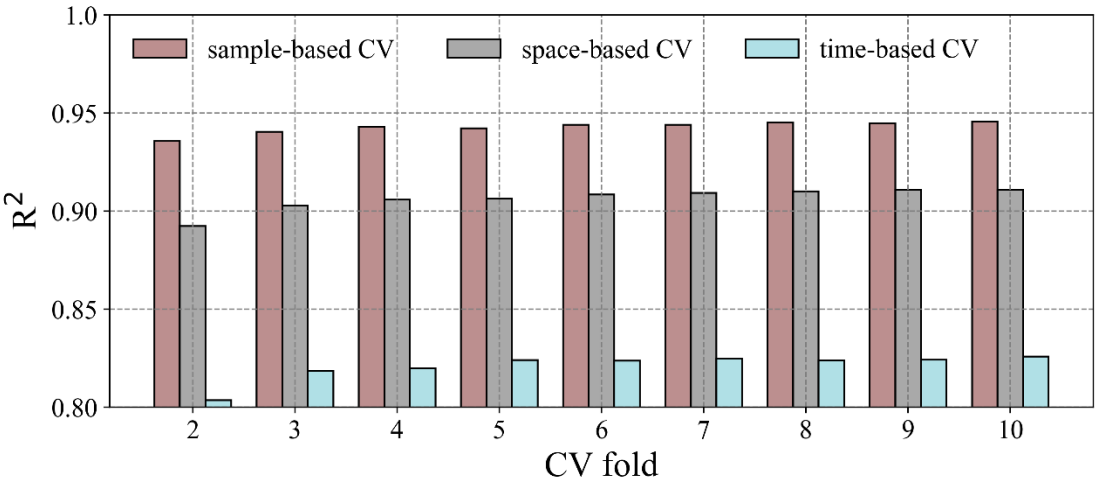
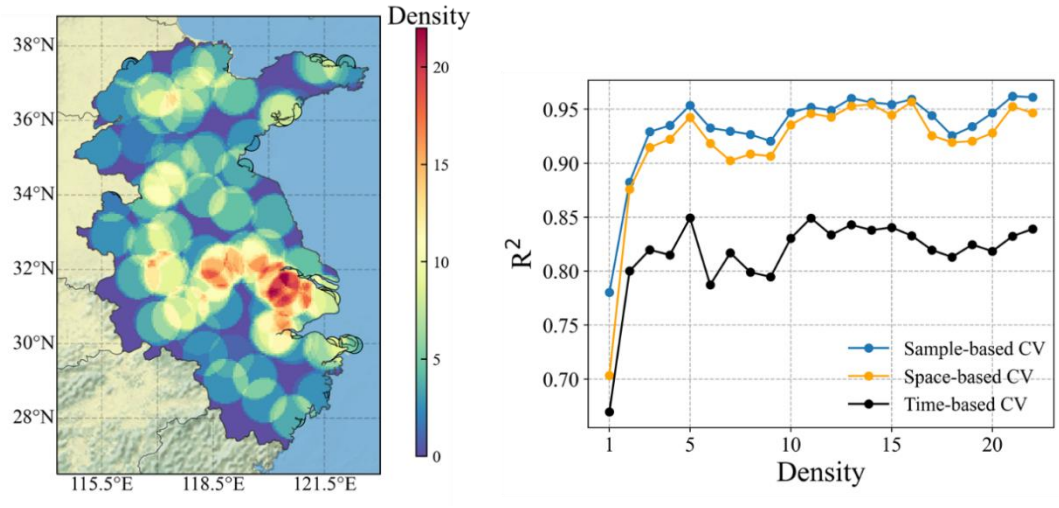
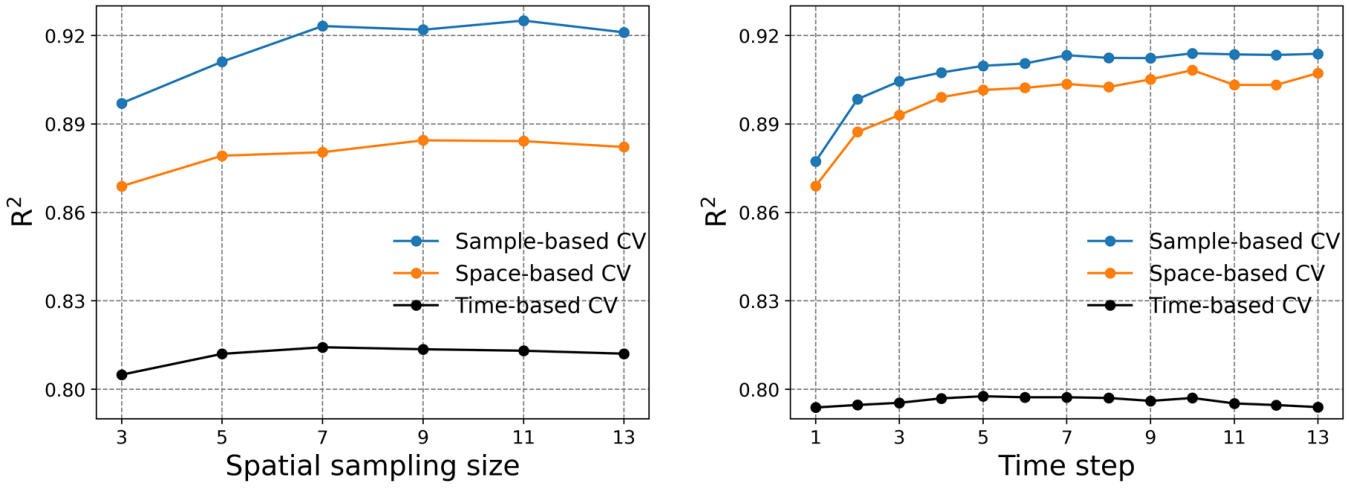


Figure S9. Validation results of different CV fold values.



(**a**) (**b**)

Figure S10. (**a**) Spatial density of ground-level monitoring sites and (**b**) CV results of sites with different densities.



(**a**) (**b**)

Figure S11. Variations of CV R^2 values: (**a**) time steps; (**b**) spatial sampling sizes.

Supplementary Tables

Table S1. Data descriptions.

Variable	Description	Unit	Spatial Resolution	Temporal Resolution	Source
Ozone	Ground-level measurement	ug/m^3	-	Hourly	CNEMC
TROPMI-ozone	Tropospheric Monitoring Instrument's total ozone	mol/m^2	5.5 × 3.5 km	Daily	Copernicus Open Access Hub
PRE	1 hour precipitation	mm/h	0.0625° × 0.0625°	Hourly	China Meteorological Administration Land Data Assimilation System
SP	Surface pressure	Pa			
SH	Specific humidity	kg/kg			
DSR	Downward shortwave radiation flux	W/m^2			
TMP	2 m temperature	K			
WIN	10 m wind speed	m/s			
DPT	2 m dew point temperature	K	0.25° × 0.25°	Hourly	ERA5
BLH	Boundary layer height	m			
WRF-ozone	WRF-Chem ozone simulation	ug/m^3	6 × 6 km	Hourly	Regional Atmospheric Environmental Modeling System
WRF-PM_{25}	WRF-Chem PM_{25} simulation	ug/m^3			
WRF-NO_2	WRF-Chem NO_2 simulation	ug/m^3			
NDVI	Normalized difference vegetation index		250 × 250 m	16 day	MODIS
DEM	Surface elevation	m	90 × 90 m	-	SRTM
DOY	Day of year	-	-	-	-

Table S2. Statistical descriptions of input variables.

Variable	Unit	Model Building			Data Grid Generation		
		Min	Max	Mean	Min	Max	Mean
TROPMI-ozone	mol/m^2	0.102	0.198	0.132	0.100	0.201	0.131
PRE	mm/h	0.0	28.2	0.14	0.0	31.6	0.71
SP	Pa	88645.1	103803.7	101139.3	78771.4	103896.5	100177.3
SH	kg/kg	0.00039	0.02788	0.01005	0.00032	0.03016	0.00995
DSR	W/m^2	34.4	1109.9	447.7	25.6	1114.6	458.5
TMP	K	252.2	313.0	293.2	250.6	313.9	293.0
WIN	m/s	0.06	15.15	2.08	0.02	16.86	2.00
DPT	K	247.2	301.9	283.8	245.7	302.3	283.3
BLH	m	58.4	3758.8	997.3	27.3	3912.0	1028.6
WRF-ozone	ug/m^3	0.0	327.2	102.5	0.0	345.2	109.2
WRF-PM_{25}	ug/m^3	0.0	330.2	34.0	0.0	334.7	25.0
WRF-NO_2	ug/m^3	0.0	181.2	30.0	0.0	184.1	11.6
NDVI	-	-0.36	0.90	0.32	-0.49	1.01	0.49
DEM	m	1.0	556.0	50.75	1.0	1508.0	125.18
DOY	-	10	366	188	10	366	188

Table S3. Comparison between 2-D CNN and sub-network 2.

Model	Total Parameters	Sample-Based R^2	Space-Based R^2	Time-Based R^2
2-D CNN	58608	0.892	0.855	0.785
Sub-network 2	59958	0.921	0.884	0.811

Table S4. Comparison between 1-D CNN, GRU and LSTM.

Model	Configuration[1]	Total Parameters	Sample-Based R^2	Space-Based R^2	Time-Based R^2
1-D CNN	32/16/8/32/1	8281	0.894	0.883	0.773
	64/32/16/32/1	20849	0.912	0.901	0.801
	80/40/20/32/1	32605	0.916	0.905	0.803
GRU	32/16/10/32/1	8329	0.891	0.885	0.788
	60/20/10/32/1	20125	0.916	0.909	0.806
	70/30/25/32/1	32590	0.918	0.904	0.802
LSTM	25/16/10/32/1	8253	0.898	0.882	0.785
	50/20/10/32/1	20505	0.911	0.902	0.803
	60/30/15/32/1	32465	0.915	0.903	0.807

[1] The number of neurons/filters in each layer, and the last two layers are fully connected layers.