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Long-term trends of ambient nitrate (NO_3^-) concentrations across China based on ensemble machine-learning models

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Table S1 The basic information and data sources of predictors for NO_3^- estimation in this study. A total of 1636 NO_2 column data during 2011-2015 was applied to develop the ensemble model to estimate the national NO_3^- concentrations. A total of 1554236 useable NO_2 column data during 2005-2015 was applied to predict the gridded monthly NO_3^- concentrations across China.

Dataset	Variable	Unit	Spatial resolution	Time resolution	Data source
NO_3^-	NO_3^-	μg N m^{-3}	--	Monthly	NNDMN
NO_2 tropospheric column	NO_2 column	mole/cm^2	0.25°	Daily	NASA
Meteorology	D_{2m}	℃	0.25°	6-hour	ERA-Interim reanalysis product
	T_{2m}	℃	0.25°	6-hour	
	U_{10}	m/s	0.25°	6-hour	
	V_{10}	m/s	0.25°	6-hour	
	BLH	m	0.25°	3-hour	
	Sund	s	0.25°	6-hour	
	Sp	hPa	0.25°	6-hour	
	Tp	mm	0.25°	6-hour	
Land use types	Waters	m^2	30 m	Annually	CRESDC
	Grassland	m^2	30 m	Annually	
	Urban	m^2	30 m	Annually	
	Forest	m^2	30 m	Annually	
	Agricultural land	m^2	30 m	Annually	
Elevation	DEM	m	30 m	--	SRTM
Socioeconomic factors	Population	--	1 km	5-year	CRESDC
	GDP	Dollars	1 km	5-year	

Table S2 The basic information and data sources of samples used to validate the transferability of NO_3^- estimates.

Site	Latitude	Longitude	Sampling period
1	30.61	104.06	2014.6-2015.4
2	30.60	108.00	2014.6-2015.4
3	31.10	104.15	2015.5-2015.12
4	28.60	113.30	2010.9-2011.8
5	28.50	113.40	2010.9-2011.8
6	28.53	113.33	2010.9-2011.8
7	34.26	108.66	2010-2012
8	36.86	115.00	2006.8-2008.10
9	40.05	116.30	2006.8-2008.10
10	29.66	94.34	2015

Table S3 The annual mean NO_3^- concentrations (μg N m^{-3}) in different provinces (autonomous region, municipality) over China.

Province	2005	2007	2010	2013	2014	2015
Anhui	2.27 ± 1.41	2.36 ± 1.44	2.47 ± 1.33	3.46 ± 1.77	3.09 ± 1.76	2.28 ± 1.42
Beijing	2.32 ± 1.51	2.80 ± 1.79	2.62 ± 1.64	3.76 ± 1.96	3.31 ± 1.81	2.69 ± 1.61
Fujian	0.91 ± 0.47	0.85 ± 0.49	1.00 ± 0.47	1.30 ± 0.60	1.24 ± 0.57	0.89 ± 0.46
Gansu	0.30 ± 0.26	0.32 ± 0.28	0.30 ± 0.26	0.95 ± 0.38	1.05 ± 0.49	0.77 ± 0.41
Guangdong	1.17 ± 0.74	1.14 ± 0.76	1.23 ± 0.68	1.61 ± 0.75	1.54 ± 0.65	1.07 ± 0.55
Guangxi	0.75 ± 0.28	0.66 ± 0.27	0.78 ± 0.27	1.15 ± 0.33	1.15 ± 0.32	0.83 ± 0.30
Guizhou	0.90 ± 0.27	0.85 ± 0.24	0.93 ± 0.27	1.32 ± 0.37	1.24 ± 0.35	0.96 ± 0.28
Hainan	1.14 ± 0.19	1.13 ± 0.18	1.14 ± 0.20	1.71 ± 0.28	1.78 ± 0.36	1.23 ± 0.22
Hebei	2.19 ± 1.81	2.59 ± 2.02	2.50 ± 1.87	3.74 ± 2.57	3.34 ± 2.40	2.61 ± 1.88
Henan	3.14 ± 1.83	3.36 ± 1.93	3.21 ± 1.72	4.77 ± 2.35	4.20 ± 2.03	3.24 ± 1.66
Heilongjiang	0.62 ± 0.22	0.67 ± 0.25	0.70 ± 0.25	1.36 ± 0.31	1.16 ± 0.32	0.87 ± 0.24
Hubei	1.19 ± 0.48	1.20 ± 0.47	1.33 ± 0.55	1.91 ± 0.57	1.76 ± 0.49	1.34 ± 0.39
Hunan	0.93 ± 0.26	0.88 ± 0.28	0.97 ± 0.28	1.33 ± 0.34	1.27 ± 0.33	1.02 ± 0.30
Jilin	0.75 ± 0.32	0.86 ± 0.41	0.92 ± 0.44	1.40 ± 0.47	1.30 ± 0.47	1.00 ± 0.37
Jiangsu	3.07 ± 0.81	3.23 ± 0.87	3.28 ± 0.77	4.21 ± 0.97	4.04 ± 0.89	3.02 ± 0.78
Jiangxi	0.78 ± 0.26	0.80 ± 0.28	0.95 ± 0.28	1.23 ± 0.37	1.16 ± 0.33	0.87 ± 0.29
Liaoning	1.27 ± 0.73	1.50 ± 0.78	1.66 ± 0.80	2.29 ± 0.94	2.15 ± 0.85	1.58 ± 0.69
Inner Mongolia	0.37 ± 0.26	0.44 ± 0.28	0.42 ± 0.29	1.03 ± 0.39	1.17 ± 0.52	0.81 ± 0.40
Ningxia	0.52 ± 0.40	0.62 ± 0.46	0.49 ± 0.45	1.04 ± 0.57	1.01 ± 0.58	0.81 ± 0.47
Qinghai	0.03 ± 0.19	0.02 ± 0.20	0.01 ± 0.19	0.78 ± 0.32	1.01 ± 0.48	0.68 ± 0.38
Shandong	3.57 ± 1.42	3.83 ± 1.53	3.82 ± 1.40	5.43 ± 1.70	4.79 ± 1.53	3.83 ± 1.41
Shanxi	1.22 ± 0.83	1.52 ± 0.92	1.30 ± 0.80	2.35 ± 1.19	2.01 ± 1.03	1.65 ± 0.81
Shaanxi	0.80 ± 0.70	0.93 ± 0.73	0.78 ± 0.78	1.44 ± 1.00	1.45 ± 0.93	1.24 ± 0.71
Shanghai	3.08 ± 0.52	3.26 ± 0.55	3.23 ± 0.56	3.72 ± 0.49	3.72 ± 0.52	2.82 ± 0.43
Sichuan	0.55 ± 0.48	0.56 ± 0.50	0.57 ± 0.53	1.08 ± 0.48	1.05 ± 0.47	0.78 ± 0.38
Tianjin	3.70 ± 1.01	4.46 ± 1.16	4.28 ± 1.12	5.72 ± 1.20	5.23 ± 1.18	4.30 ± 1.14
Tibet	0.08 ± 0.28	0.08 ± 0.31	0.12 ± 0.29	0.89 ± 0.26	1.16 ± 0.31	0.82 ± 0.26
Xinjiang	0.48 ± 0.37	0.45 ± 0.38	0.48 ± 0.38	1.31 ± 0.55	1.56 ± 0.70	1.22 ± 0.54
Yunnan	0.58 ± 0.18	0.58 ± 0.18	0.54 ± 0.16	1.03 ± 0.21	1.02 ± 0.22	0.81 ± 0.20
Zhejiang	1.44 ± 0.72	1.41 ± 0.78	1.55 ± 0.75	2.04 ± 0.85	1.89 ± 0.89	1.38 ± 0.68
Chongqing	1.29 ± 0.32	1.29 ± 0.36	1.27 ± 0.44	1.85 ± 0.44	1.83 ± 0.45	1.34 ± 0.28
Nation	0.72 ± 0.93	0.76 ± 1.01	0.77 ± 0.98	1.48 ± 1.20	1.52 ± 1.08	1.14 ± 0.87

Table S4 The seasonally average NO_3^- concentrations (μg N m^{-3}) in different provinces (autonomous region, municipality) over China.

Province	Spring	Summer	Autumn	Winter	Average
Anhui	2.15 ± 1.19	1.57 ± 1.08	2.60 ± 1.51	4.07 ± 2.17	2.60 ± 1.48
Beijing	2.51 ± 1.37	2.01 ± 1.05	3.08 ± 1.66	3.73 ± 2.68	2.83 ± 1.68
Fujian	0.98 ± 0.50	0.62 ± 0.40	0.89 ± 0.52	1.54 ± 0.63	1.01 ± 0.50
Gansu	0.34 ± 0.25	0.32 ± 0.20	0.67 ± 0.32	0.84 ± 0.44	0.54 ± 0.28
Guangdong	1.25 ± 0.66	0.85 ± 0.58	1.15 ± 0.71	1.84 ± 0.84	1.27 ± 0.68
Guangxi	0.75 ± 0.29	0.59 ± 0.23	0.76 ± 0.27	1.34 ± 0.38	0.86 ± 0.28
Guizhou	0.76 ± 0.20	0.56 ± 0.15	1.09 ± 0.36	1.78 ± 0.52	1.05 ± 0.28
Hainan	1.31 ± 0.25	1.00 ± 0.23	1.27 ± 0.23	1.62 ± 0.22	1.30 ± 0.22
Hebei	2.28 ± 1.65	1.77 ± 1.14	2.95 ± 2.06	3.99 ± 3.28	2.75 ± 2.01
Henan	2.73 ± 1.40	2.05 ± 1.12	3.71 ± 1.95	5.82 ± 3.11	3.58 ± 1.88
Heilongjiang	0.65 ± 0.23	0.65 ± 0.17	1.05 ± 0.27	1.56 ± 0.50	0.98 ± 0.24
Hubei	1.14 ± 0.44	0.75 ± 0.37	1.45 ± 0.46	2.40 ± 0.69	1.43 ± 0.48
Hunan	0.89 ± 0.23	0.49 ± 0.21	0.96 ± 0.32	1.88 ± 0.43	1.06 ± 0.29
Jilin	0.80 ± 0.42	0.77 ± 0.28	1.18 ± 0.46	1.37 ± 0.62	1.03 ± 0.41
Jiangsu	3.23 ± 0.75	2.33 ± 0.68	3.37 ± 0.87	4.75 ± 1.22	3.42 ± 0.84
Jiangxi	0.82 ± 0.24	0.46 ± 0.18	0.79 ± 0.33	1.65 ± 0.48	0.93 ± 0.29
Liaoning	1.64 ± 0.86	1.22 ± 0.61	1.87 ± 0.77	1.99 ± 0.95	1.69 ± 0.78
Inner Mongolia	0.42 ± 0.29	0.47 ± 0.22	0.78 ± 0.34	1.06 ± 0.55	0.68 ± 0.30
Ningxia	0.55 ± 0.48	0.45 ± 0.36	0.85 ± 0.51	1.11 ± 0.61	0.74 ± 0.48
Qinghai	0.13 ± 0.21	0.27 ± 0.18	0.37 ± 0.25	0.44 ± 0.36	0.30 ± 0.22
Shandong	3.45 ± 1.08	2.56 ± 0.91	4.25 ± 1.54	6.11 ± 2.54	4.09 ± 1.47
Shanxi	1.30 ± 0.70	1.01 ± 0.53	1.95 ± 0.96	2.39 ± 1.44	1.66 ± 0.89
Shaanxi	0.77 ± 0.59	0.63 ± 0.39	1.27 ± 0.83	1.66 ± 1.39	1.08 ± 0.79
Shanghai	3.69 ± 0.47	2.47 ± 0.44	2.98 ± 0.57	3.88 ± 0.68	3.26 ± 0.52
Sichuan	0.58 ± 0.40	0.48 ± 0.23	0.82 ± 0.50	0.99 ± 0.91	0.72 ± 0.48
Tianjin	4.07 ± 1.01	2.98 ± 0.77	4.68 ± 1.11	6.28 ± 1.64	4.50 ± 1.11
Tibet	0.25 ± 0.27	0.36 ± 0.23	0.43 ± 0.26	0.50 ± 0.37	0.38 ± 0.26
Xinjiang	0.53 ± 0.39	0.36 ± 0.31	1.01 ± 0.49	1.57 ± 0.89	0.86 ± 0.42
Yunnan	0.53 ± 0.14	0.67 ± 0.20	0.75 ± 0.19	0.93 ± 0.25	0.72 ± 0.17
Zhejiang	1.54 ± 0.85	0.97 ± 0.68	1.49 ± 0.73	2.35 ± 0.81	1.59 ± 0.75
Chongqing	1.10 ±0.40	0.71 ± 0.27	1.58 ± 0.36	2.56 ± 0.53	1.49 ± 0.37
Nation	0.78 ± 0.50	0.63 ± 0.40	1.09 ± 0.52	1.57 ± 0.63	1.01 ± 0.28

Table S5 The validation of gridded air temperature and precipitation datasets against ground-level datasets in China during 2005-2015.

Variable	Unit	R^2	RMSE	MAE
T_{2m}	℃	0.98	1.20	0.96
Tp	mm	0.83	35.20	17.21

Fig. S1 The geographical locations of major study regions across China including BTH (green), YRD (yellow), and PRD (purple).

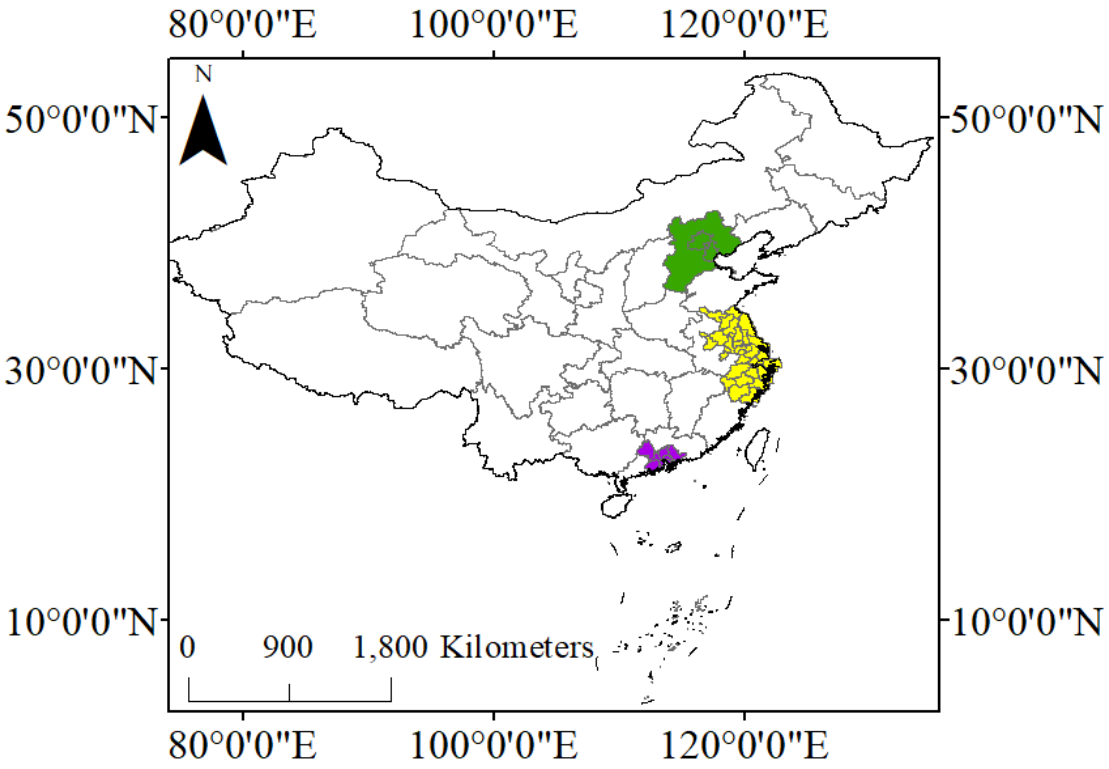

Figure S2 Spatial distributions of annual mean ground-measured NO_3^- concentrations over China from 2010 to 2015.

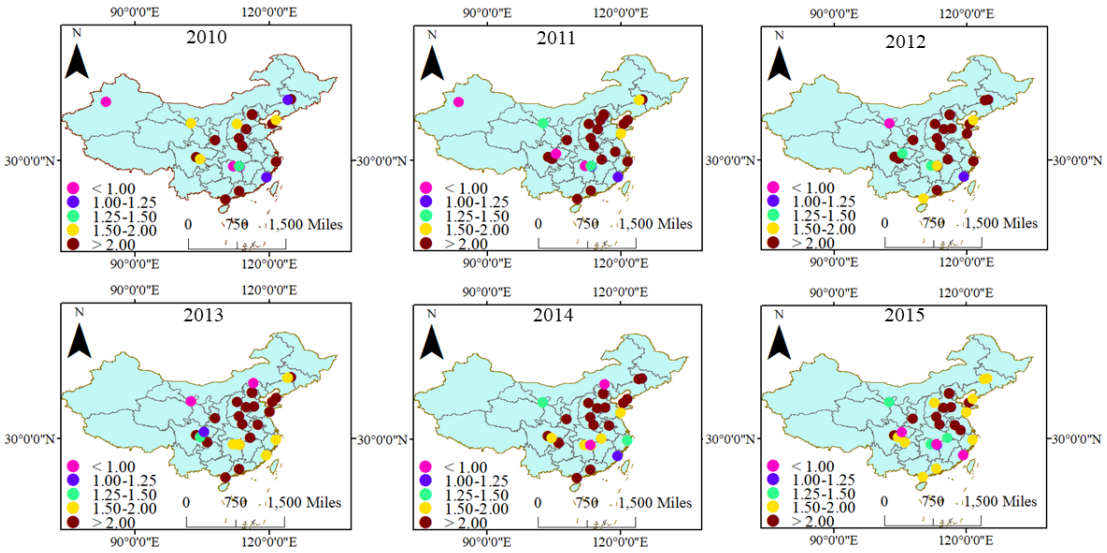

Fig. S3 The tropospheric NO_2 column amount (Unit: 10^{15} mole/cm^2) in 2005 (a), 2010 (b), 2015 (c), and the mean values during 2005-2015 (d).

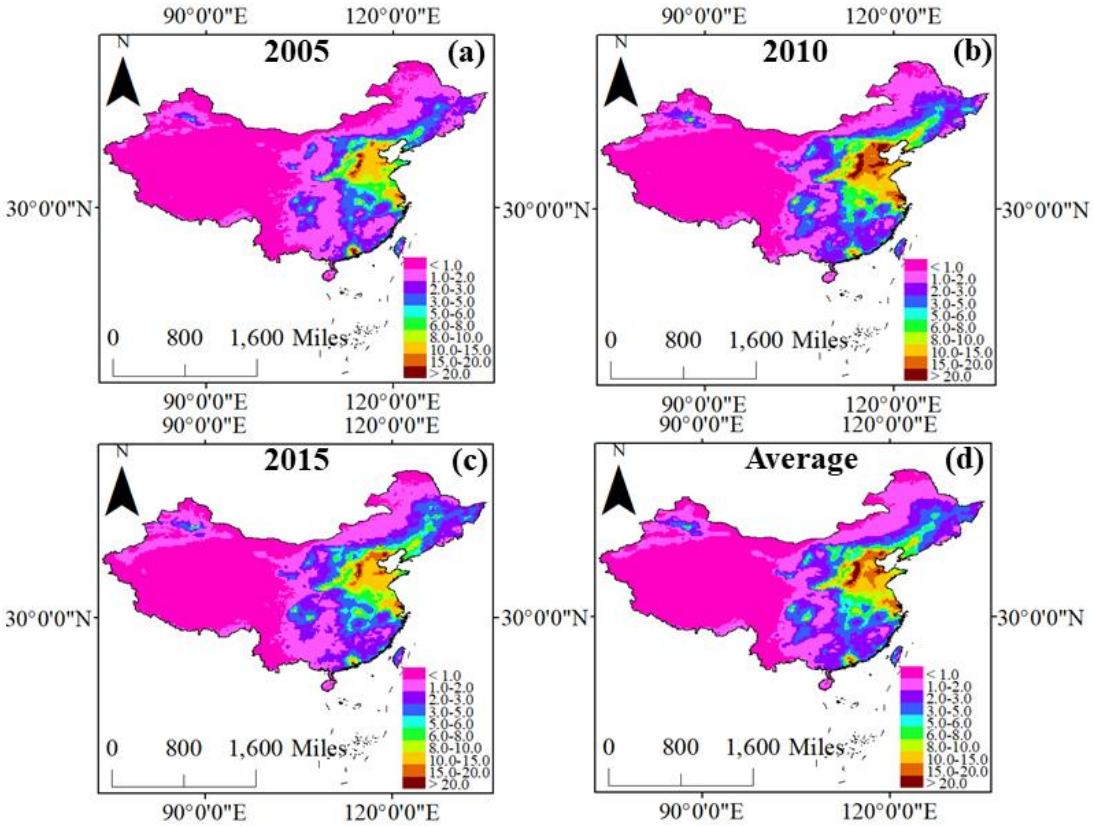

Figure S4 Correlation coefficient matrix between ambient NO_3^- concentration and all explanatory variables in China. The full names of Lon, NO3., NO2.column, U10, Lat, DEM, BLH, Sund, V10, T2m, D2m, Tp, Agr, GDP, and Sp are longitude, NO_3^- level, NO_2 column, 10-m latitudinal wind component, latitude, elevation, boundary layer height, sunshine duration, 10-m meridional wind component, 2-m air temperature, 2-m dewpoint temperature, agricultural land area, gross domestic production, and surface pressure, respectively.

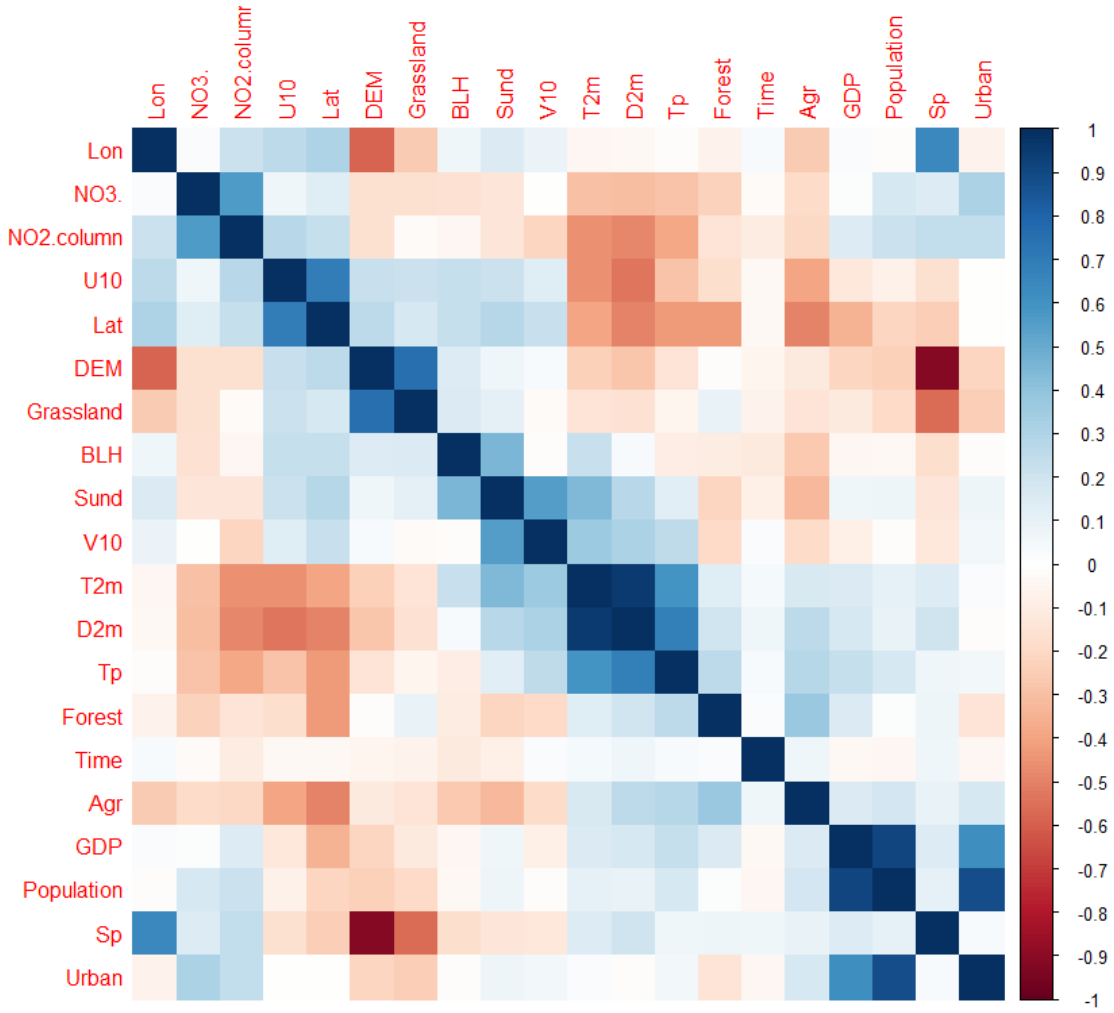

Fig. S5 Density scatterplots of 10-fold cross-validation results for annual NO_3^- estimation over China for the ensemble decision trees model. The linear regression relationship is also given in the panel. The red dashed line represents the best-fit lines through the data points.

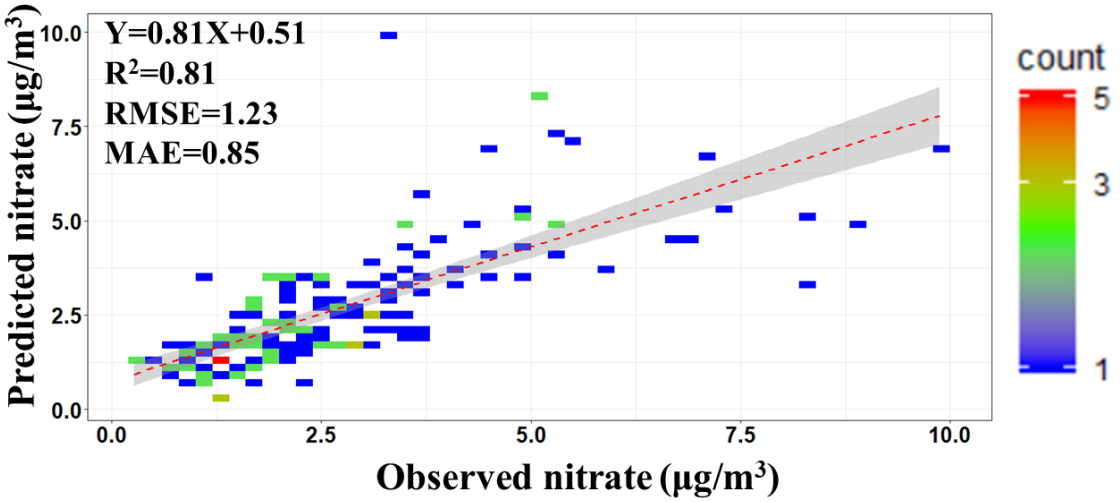

Fig. S6 The site-based cross-validation for the NO_3^- estimates across China.

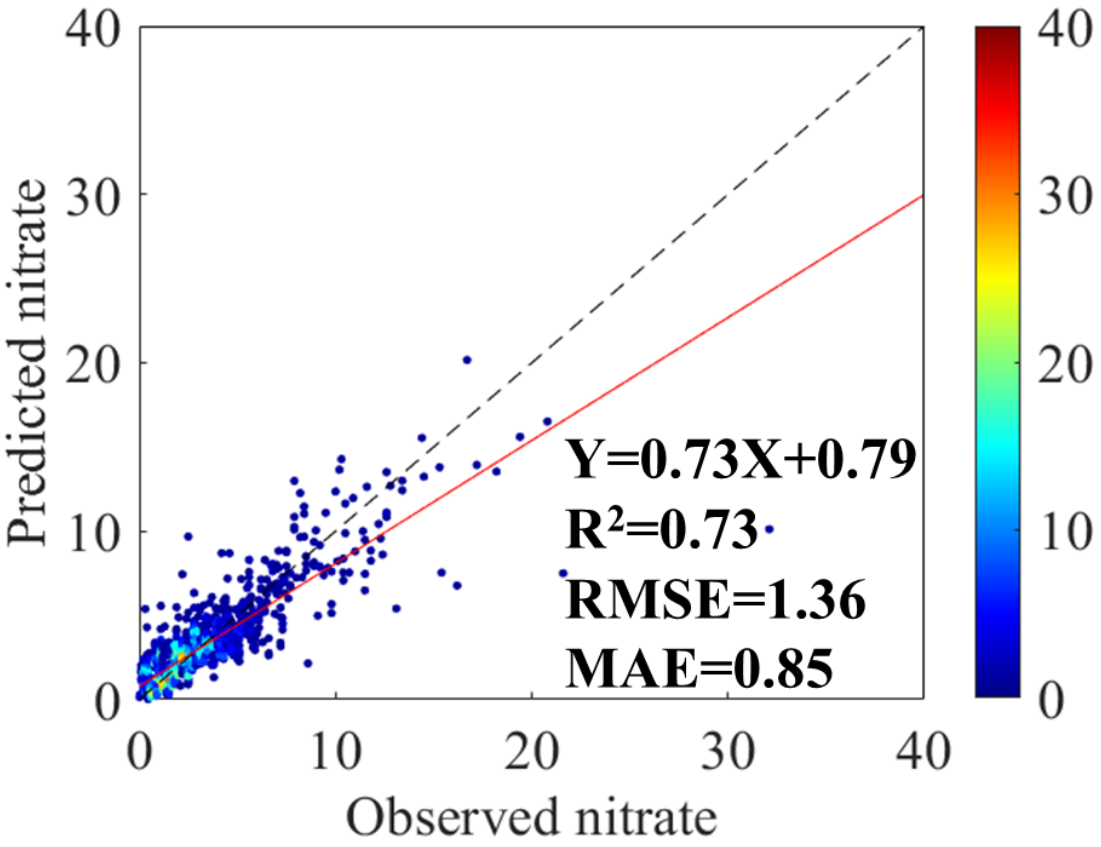

Fig. S7 The ranking of variable importance (%) in the ensemble model for the NO_3^- estimates in China. NO_2 column, Urban, BLH, T2m, D2m, Tp, V10, Time, U10, Sund, Sp, Agr, Forest, and DEM denote tropospheric NO_2 column, urban area, boundary layer height, 2-m air temperature, 2-m dewpoint temperature, total precipitation, 10-m meridional wind, month of year, 10-m latitudinal wind, sunshine duration, surface pressure, agricultural land area, forest area, and elevation, respectively.