A model framework to reduce bias in ground-level $PM_{2.5}$ concentrations inferred from satellite-retrieved AOD

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Original method

Observed AOD → $AOD:PM_{2.5}$ + correlative variables → $PM_{2.5}$ inferred from AOD

Statistical regression → $AOD:PM_{2.5}$ + correlative variables

Machine learning → $AOD:PM_{2.5}$ + correlative variables

Model of atmospheric chemistry and transport → $AOD:PM_{2.5}$ + correlative variables

Revised method

Data clustering

- GEOS-Chem model AOD for individual chemical components sampled at Chinese $PM_{2.5}$ monitoring locations.
- Clustering algorithm to identify locations where $PM_{2.5}$:AOD varies coherently.

Data suitability

- Within identified monthly data clusters calculate $AOD_{PBL}:AOD_{TOTAL}$.
- Identify threshold below which data are discarded.

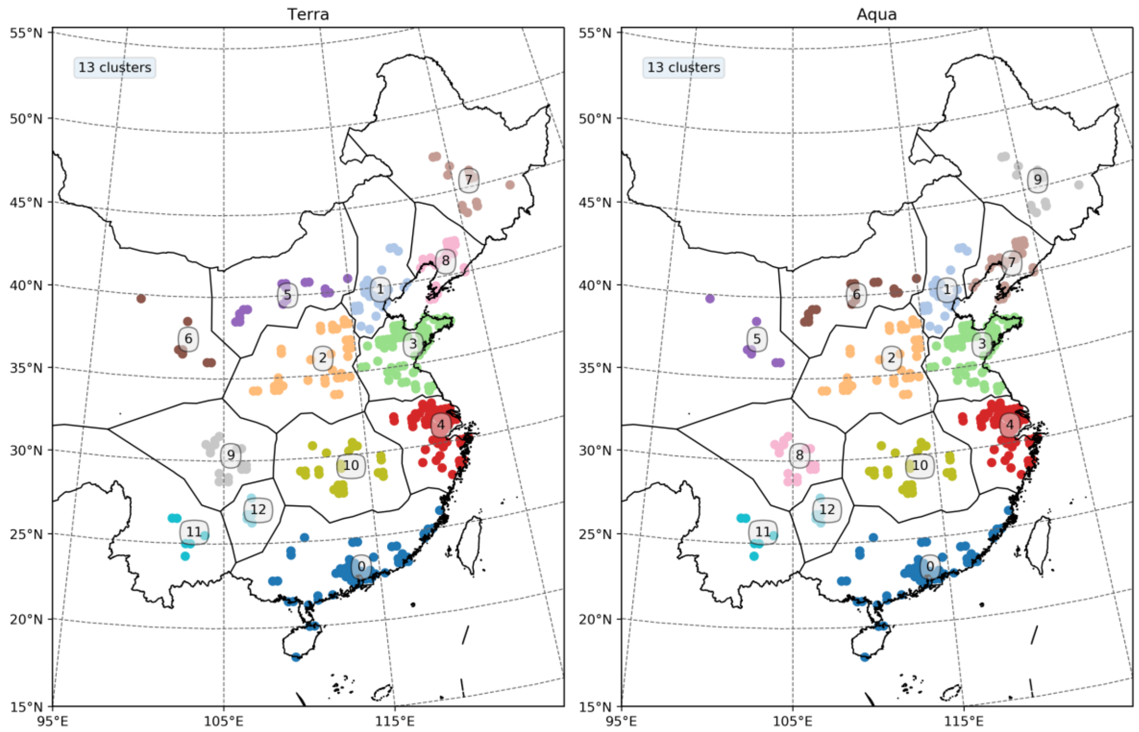
Data-driven $PM_{2.5}$:AOD model development

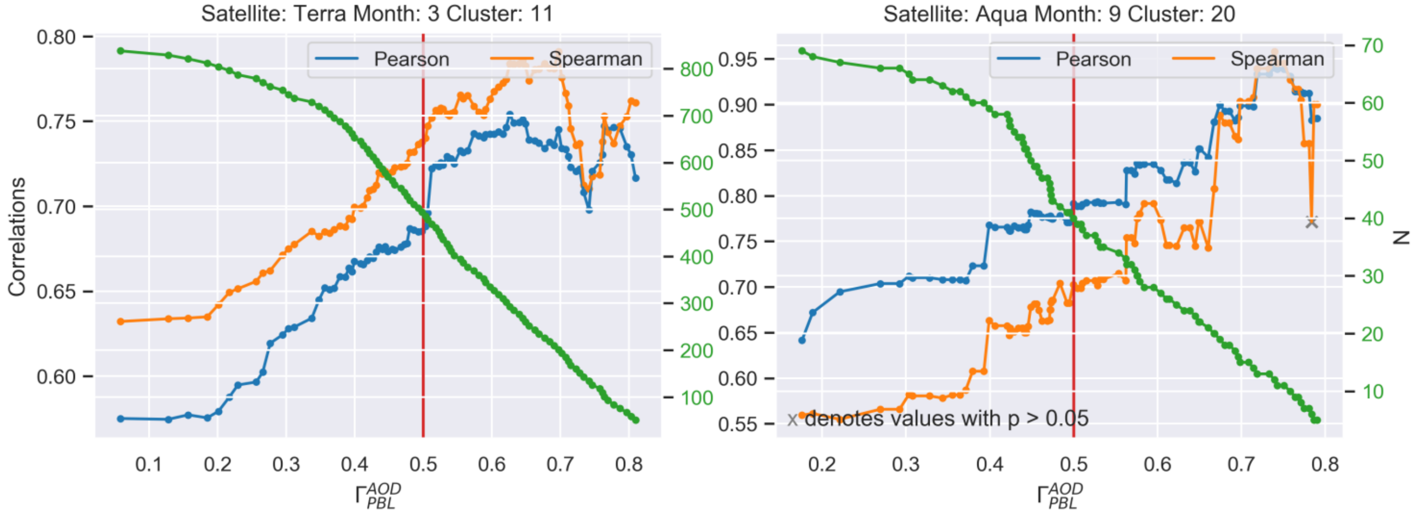
- Fit $PM_{2.5}$:AOD data using (2x) statistical models and (2x) machine learning models.
- Use Monte Carlo method to determine improvement in this approach with traditional approach.

Mapping $PM_{2.5}$ from AOD

- Map $PM_{2.5}$ inferred from AOD.

Results of data clustering and suitability





- We determine a total of 13 spatial clusters with similar extent across China. Among them the majority correspond to urban agglomerations.

- We define $\Gamma_{PBL}^{AOD} = \frac{AOD_{PBL}}{AOD_{TOTAL}}$ and determine 0.5 as the threshold, above which we retain the data to develop physically-meaningful $PM_{2.5}$:AOD relationships.

Results of data-driven model development

Benefiting from the improved representiveness of AOD for ground-level $PM_{2.5}$, the revised method:

1. reduces bias in inferred estimates of ground-level $PM_{2.5}$ by 9-15%;
2. captures more variations in ground-level $PM_{2.5}$ by up to 8%.

Model structure: $PM_{2.5}{}_g^d = f(AOD_g^d + PBLH_g^d + RH_{PBL}{}_g^d + TS_g^d + PRECTOT_g^d + U10M_g^d + V10M_g^d + SLP_g^d + DOY_g^d)$

Satellite	Model	N	N'	R^2	$R^{2\prime}$	$R^2{}_p$	MPE	MPE'	MPE_p
Terra	PooledOLS	57819.0	36692.0	0.36	0.39	0.0	-0.48	-0.41	0.0
	PanelOLS	57819.0	36692.0	0.58	0.58	0.0	-0.27	-0.24	0.0
	RF1	57819.0	36692.0	0.63	0.63	0.0	-0.32	-0.28	0.0
	RF2	57819.0	36692.0	0.68	0.66	0.0	-0.29	-0.26	0.0
Aqua	PooledOLS	55939.0	46961.0	0.43	0.45	0.0	-0.45	-0.41	0.0
	PanelOLS	55939.0	46961.0	0.64	0.66	0.0	-0.26	-0.23	0.0
	RF1	55939.0	46961.0	0.67	0.69	0.0	-0.31	-0.28	0.0
	RF2	55939.0	46961.0	0.73	0.73	0.0	-0.28	-0.25	0.0

- PBLH: Planetary boundary layer (PBL) height; RH_PBL: mean relative humidity in PBL; TS: surface temperature; PRECTOT: total precipitation; U10M: 10-metre eastward wind; V10M: 10-metre northward wind; SLP: sea level pressure; DOY: day of year (only included in PanelOLS and RF2).
- X and X' denote statistics trained by the full (ignoring the step of data suitability) and suitable data. X_p denotes the possibility of achieving the performance no worse than ours by chance determined from a Monte Carlo simulation.
- RF: Random Forest; MPE: mean percentage error.

Results of ground-level $PM_{2.5}$ mapping

Accordingly, we improve the seasonal ground-level $PM_{2.5}$ maps, e.g. the bias of the autumn (winter) mean of ground-level $PM_{2.5}$ estimates over Qinghai and Gansu (Shaaxi, Shanxi, and Henan) provinces reduces from -8% to -5% (11% to 6%).