

Supporting Information

Incorporating Low-Cost Sensor Measurements into High-Resolution PM_{2.5} Modeling at A Large Spatial Scale

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1. Quality Control for PurpleAir PM_{2.5} Measurements

Each PurpleAir sensor consists of two identical laser particle counters providing two sets of PM readings (Channel A & Channel B). PurpleAir PM_{2.5} data were cleaned based on the dual-channel readings. We first discarded all hourly records with only one channel's reading since the outliers were hard to identify based on a single channel. Additionally, there were apparent outliers with PM_{2.5} levels greater than 3,000 µg/m³ in both channels which were also discarded. The discarded records accounted for ~3% of the total records. The remaining records (N = 5,658,772) still had a large dual-channel discrepancy with an R² of 0.32 and a slope of 0.60. We then used the absolute percentage bias (APB) computed from dual-channel readings (Eq. S1) to further filter out the outliers. In Eq. S1, PM_{2.5A} denotes Channel A's reading and PM_{2.5B} denotes Channel B's reading. A percentage threshold of APB was determined according to the improvement of overall dual-channel agreement. When setting the threshold to be 5%, *i.e.*, removing the records with top-5% largest APB values, all apparent outliers disappeared (Fig. S6). The remaining data (N = 5,375,833) had an excellent dual-channel agreement with an R² of 0.98 and a slope of 0.997. The final PurpleAir PM_{2.5} measurements were the average of the dual-channel readings.

Eq. S1

$$APB = \left| \frac{PM_{2.5B} - PM_{2.5A}}{PM_{2.5A}} \right| \times 100\%$$

2. Evaluation of PurpleAir PM_{2.5} Measurements

The evaluation of PurpleAir was performed based on the paired hourly PM_{2.5} measurements (N = 137,068). The hourly AQS measurements averaged 11.1 µg/m³ with an interquartile range (IQR) of 9.8 µg/m³ (25th, 75th percentiles: [5.0 µg/m³, 14.8 µg/m³], maximum: 369.0 µg/m³), while the corresponding PurpleAir measurements averaged 13.0 µg/m³ with an IQR of 14.8 µg/m³ (25th, 75th percentiles: [2.8 µg/m³, 17.6 µg/m³], maximum: 448.5 µg/m³). Compared to AQS, PurpleAir measured a higher overall PM_{2.5} level by 1.9 µg/m³ and significantly higher peak values. Previous low-cost sensor evaluation studies based on the same sensor (Plantower PMS, Beijing Plantower Co., Ltd) also found that the sensor tended to overestimate PM_{2.5} compared to reference-grade monitors ^{1, 2}. For example, Kelly, et al. ¹ reported that PMS overestimated PM_{2.5} concentrations when exceeding 10 µg/m³ during several cold-air pools (CAPs) in winter. Badura, et al. ² reported that the raw outputs from PMS overestimated collocated tapered element oscillating microbalance (TEOM) data by a factor of 3.5 during a half-year field campaign.

3. Nonlinearity of PurpleAir Systematic Bias

The nonlinearity of PurpleAir systematic bias was examined by locally weighted scatterplot smoothing (LOWESS). LOWESS fits a low-degree polynomial at each point of the data set where the data near the point are given higher weights ³. LOWESS is a non-parametric strategy for finding a curve of best fit without assuming the distribution of data. An important hyperparameter of LOWESS is the smoothing span controlling the degree of smoothing. This hyperparameter was tuned with 10-fold cross-validation (CV). A smoothing span of 10% was the

optimal value in this analysis. The LOWESS showed an almost linear curve coinciding with the curve of linear regression (Fig. S7), indicating that linear calibration was satisfactory for PurpleAir data.

4. Validation of Scale Factor ρ

The scale factor ρ was mainly used as a proxy of implicit factors which may impact the prediction quality and further reduce the relative importance of PurpleAir in the model. This factor was set to be a multiplicative term within a range (0, 1). Intuitively, for a set of perfect measurements, *i.e.*, the data quality is identical to reference-grade data, this data-driven scale factor should be close to 1. In order to validate this assumption, we pretended the PurpleAir measurements had a perfect quality and used them as ground truth with AQS measurements in the prediction model. The trend of CV RMSPE with different ρ values is shown in Fig. S8(a). We can see that CV RMSPE reaches its minimum when ρ is closer to 1. This result indicates the reasonability of our assumption, *i.e.*, ρ is a physically meaningful parameter with the value closer to 1 for a perfect data set such as reference-grade data and closer to 0 for a data set with large uncertainty such as low-cost sensor measurements. The optimal ρ value of the weighted prediction model was also tuned based on the 10-fold CV (Fig. S8(b)). The CV RMSPE shows a U-curve with a minimum at a ρ value of ~ 0.23 . The range of CV RMSPE is as large as $0.2 \mu\text{g}/\text{m}^3$, indicating the large influence of this scale factor on the model performance.

References

1. Kelly, K. E.; Whitaker, J.; Petty, A.; Widmer, C.; Dybwad, A.; Sleeth, D.; Martin, R.; Butterfield, A., Ambient and laboratory evaluation of a low-cost particulate matter sensor. *Environ Pollut* **2017**, *221*, 491-500.
2. Badura, M.; Batog, P.; Drzeniecka-Osiadacz, A.; Modzel, P., Evaluation of Low-Cost Sensors for Ambient PM_{2.5} Monitoring. *Journal of Sensors* **2018**, 2018.
3. Cleveland, W. S.; Devlin, S. J., Locally weighted regression: an approach to regression analysis by local fitting. *Journal of the American statistical association* **1988**, *83*, (403), 596-610.

Table S1 Summary statistics of the absolute differences between fully calibrated PurpleAir data and the calibrated data based on subsets of collocated AQS/PurpleAir sites. The total number of collocated AQS/PurpleAir sites is 26 and the subsets are randomly selected from these 26 sites with different proportions from 90% to 10%. This analysis is based on a subset of 10,000 randomly selected PurpleAir measurements.

Proportion*	Mean ($\mu\text{g}/\text{m}^3$)	Q1** ($\mu\text{g}/\text{m}^3$)	Median ($\mu\text{g}/\text{m}^3$)	Q3** ($\mu\text{g}/\text{m}^3$)	Max ($\mu\text{g}/\text{m}^3$)
90%	0.02	0.00	0.01	0.02	0.77
80%	0.35	0.02	0.08	0.44	11.51
70%	0.47	0.07	0.20	0.52	12.58
60%	0.84	0.32	0.65	1.10	13.39
50%	1.06	0.37	0.76	1.34	20.26
40%	1.75	0.72	1.43	2.29	20.70
30%	1.87	0.83	1.62	2.50	20.40
20%	2.26	1.04	2.03	3.11	19.59
10%	2.35	1.01	2.02	3.22	23.49
Raw***	4.59	1.13	2.51	4.89	158.62

* The (gross) proportion of collocated AQS sites being kept.

** The 25th and 75th percentiles

*** Uncalibrated PurpleAir data

Table S2 The ten-most important variables of the AQS-based model based on which the HAC was performed.

PM_{2.5}-Related Variables Used in HAC	
1	PM _{2.5} /PM ₁₀ ratio
2	Elevation
3	Visibility
4	Gap-filled Aqua AOD
5	10-meter meridional wind speed
6	Gap-filled Terra AOD
7	Percentage of shrublands
8	2-meter specific humidity
9	Population
10	Nearest distance to roads

Table S3 Numbers and densities of continuous AQS stations (capable of providing hourly PM_{2.5} measurements) in 47 states of the Contiguous United States (CONUS) (without California). The rows in green are the states with densities of continuous AQS stations greater than 5 per 100,000 km².

Rank	CONUS State	N of AQS	State Area (km²)	N of AQS per 100,000 km²
1	Rhode Island	5	4,001	124.97
2	Delaware	5	6,446	77.57
3	Massachusetts	16	27,336	58.53
4	Connecticut	8	14,357	55.72
5	New Jersey	12	22,591	53.12
6	Maryland	11	32,131	34.24
7	Washington	61	184,661	33.03
8	Pennsylvania	39	119,280	32.70
9	New Hampshire	6	24,214	24.78
10	Florida	39	170,312	22.90
11	Ohio	26	116,098	22.40
12	New York	30	141,297	21.23
13	Indiana	19	94,326	20.14
14	Vermont	4	24,906	16.06
15	Tennessee	16	109,153	14.66
16	North Carolina	20	139,391	14.35

17	Illinois	21	149,995	14.00
18	Kentucky	14	104,656	13.38
19	South Carolina	11	82,933	13.26
20	Wisconsin	18	169,635	10.61
21	Alabama	14	135,767	10.31
22	Idaho	22	216,443	10.16
23	Oklahoma	18	181,037	9.94
24	Minnesota	22	225,163	9.77
25	Georgia	15	153,910	9.75
26	Maine	8	91,633	8.73
27	Virginia	9	110,787	8.12
28	Louisiana	10	135,659	7.37
29	Missouri	13	180,540	7.20
30	Arizona	21	295,234	7.11
31	Iowa	10	145,746	6.86
32	Utah	15	219,882	6.82
33	Michigan	17	250,487	6.79
34	Mississippi	8	125,438	6.38
35	Texas	44	695,662	6.33
36	Colorado	17	269,601	6.31
37	North Dakota	11	183,108	6.01

38	Montana	19	380,831	4.99
39	Wyoming	12	253,335	4.74
40	Nevada	13	286,380	4.54
41	South Dakota	8	199,729	4.01
42	Arkansas	5	137,732	3.63
43	West Virginia	2	62,756	3.19
44	New Mexico	9	314,917	2.86
45	Oregon	6	254,799	2.35
46	Kansas	5	213,100	2.35
47	Nebraska	2	200,330	1.00

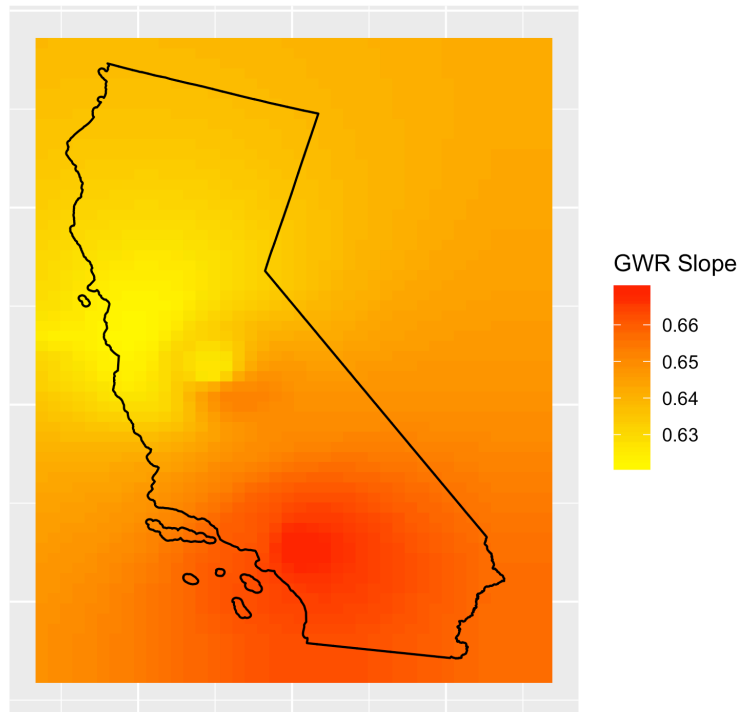


Fig. S1 The spatial distribution of GWR slopes.

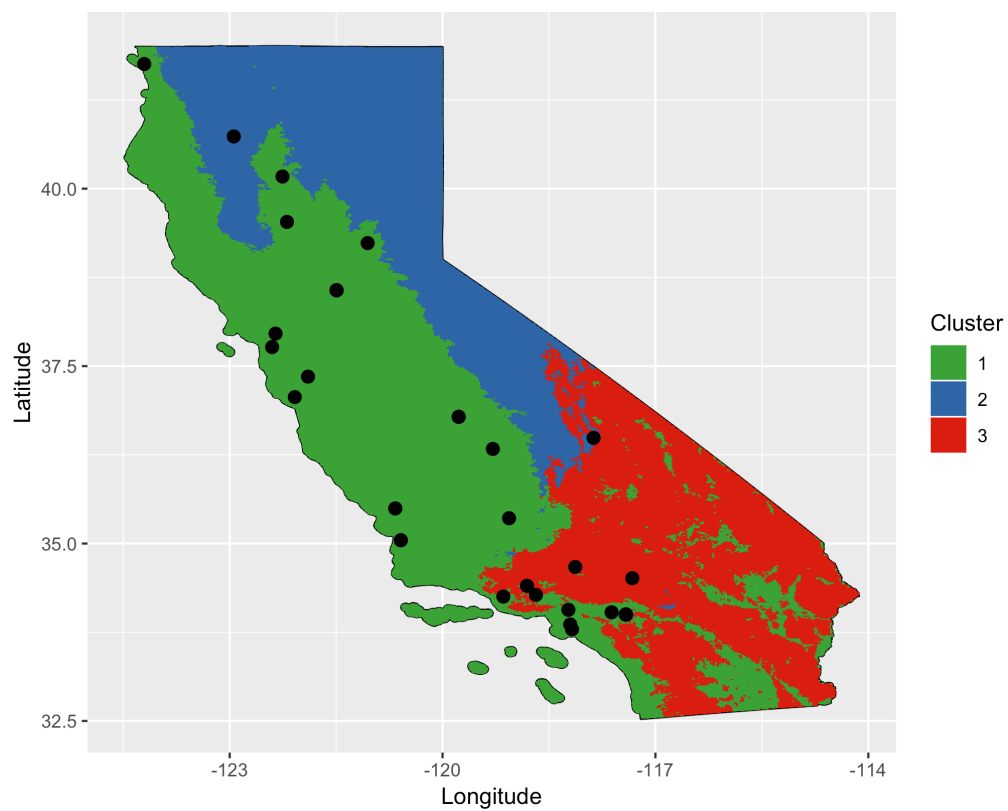


Fig. S2 Three clustered sub-domains with the locations of AQS/PurpleAir pairs (black points): 1 - agricultural/developed areas; 2 - mountainous areas; 3 - arid areas.

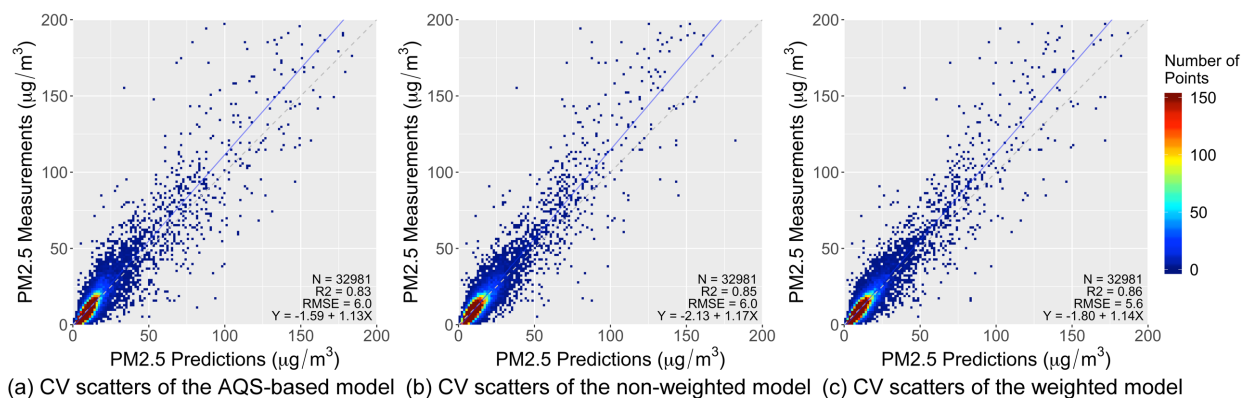


Fig. S3 10-fold CV scatter plots of (a) the AQS-based model, (b) the non-weighted model, and (c) the weighted model.

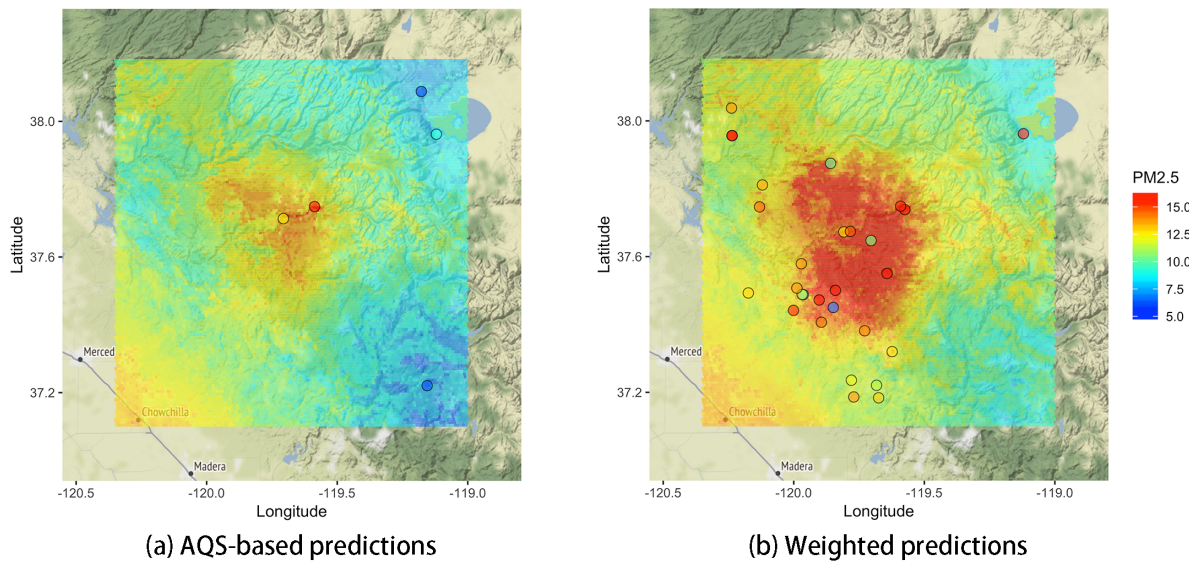


Fig. S4 Locations (with annual mean PM_{2.5} levels) of (a) AQS and (b) PurpleAir sites and the annual mean PM_{2.5} distributions derived by the (a) AQS-based and (b) weighted models in the region of Ferguson Fire in 2018.

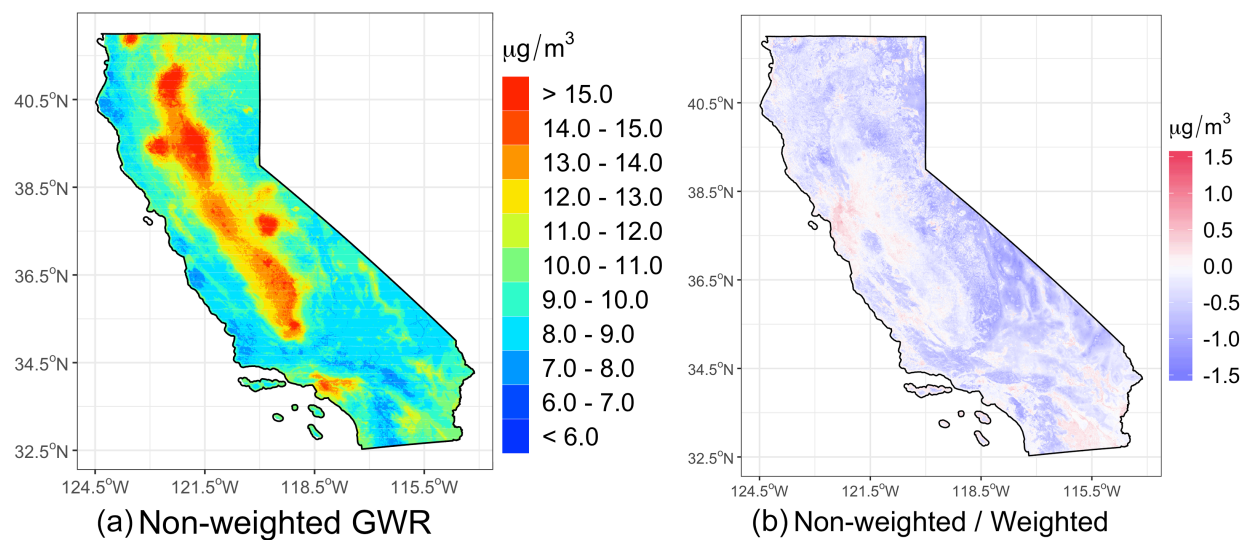


Fig. S5 (a): Annual mean PM_{2.5} distribution for 2018 from the non-weighted model. (b): Annual mean PM_{2.5} differences between the non-weighted and weighted predictions (non-weighted minus weighted).

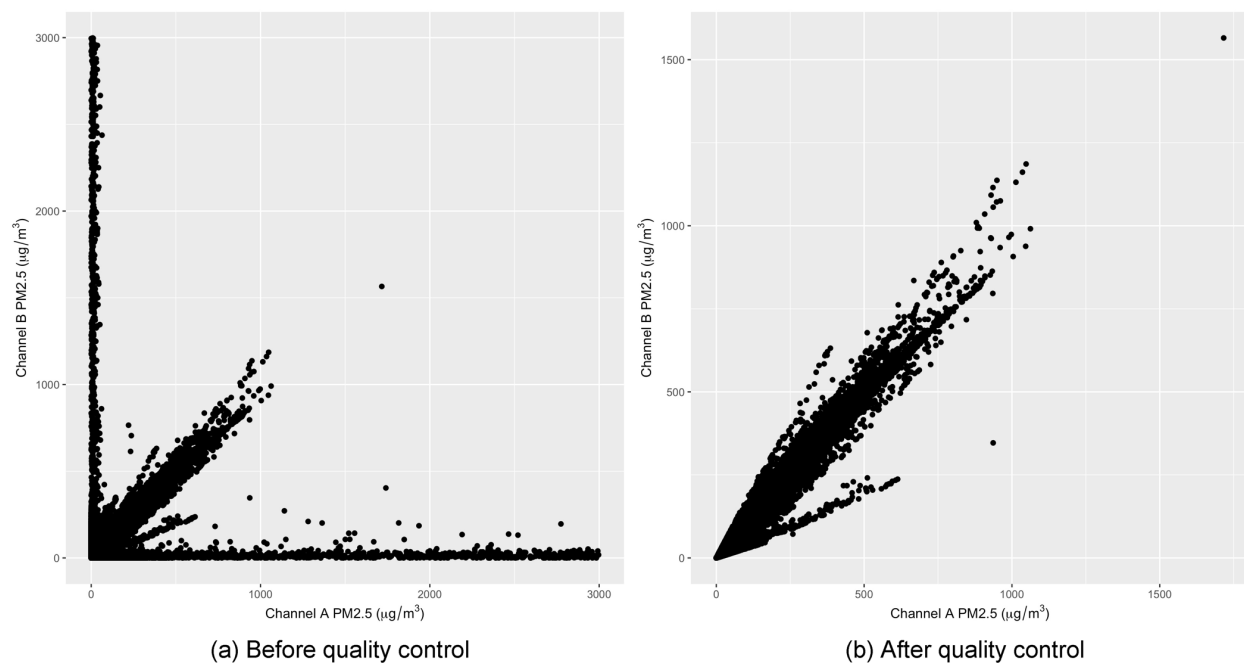


Fig. S6 Scatter plots of PurpleAir dual-channel hourly measurements (a) before and (b) after removing the 5% largest absolute percentage biases (APBs).

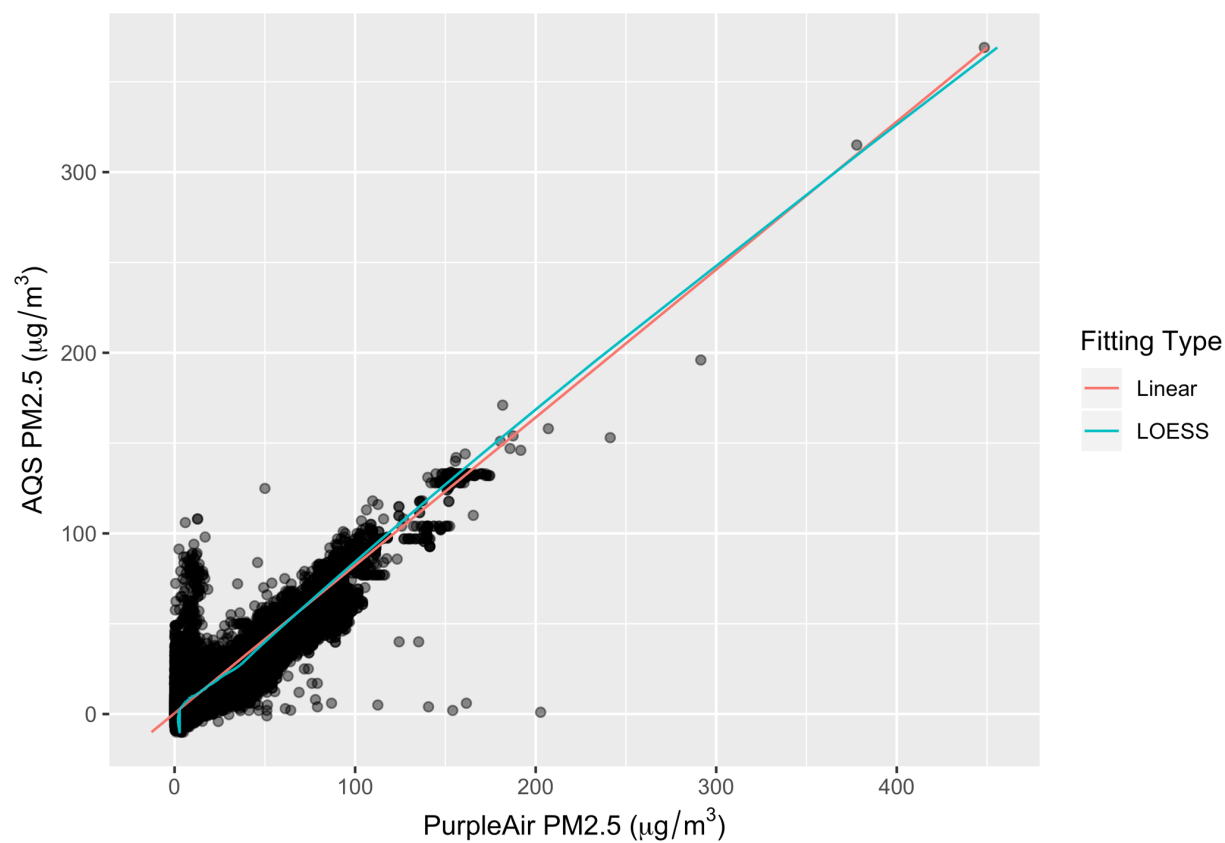


Fig. S7 LOWESS (green) and linear (red) fitting curves of the paired AQS/PurpleAir hourly measurements (black scatters).

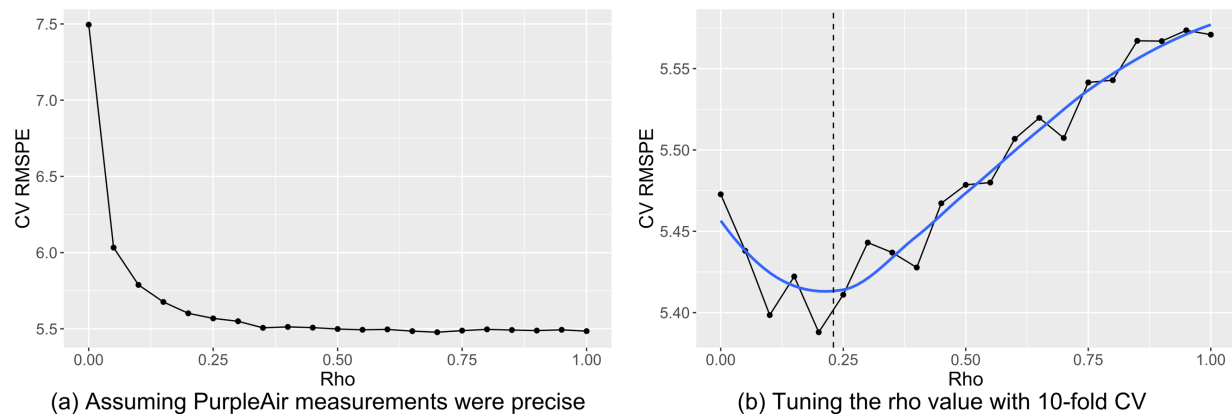


Fig. S8 (a): The trend of the 10-fold CV RMSPE with ρ within a range [0, 1] when assuming PurpleAir measurements were precise. (b): The trend of the 10-fold CV RMSPE with ρ within the range [0, 1] in the real case. The blue curve is the smoothed fitting curve, showing the minimum of CV RMSPE at a ρ value of ~ 0.23 .