

## Supporting Information

### **XIS-PM<sub>2.5</sub>: A daily spatiotemporal machine-learning model for PM<sub>2.5</sub> in the contiguous United States**

Allan C. Just<sup>1,2,3\*</sup>, Kodi B. Arfer<sup>1,3</sup>, Johnathan Rush<sup>3</sup>, Alexei Lyapustin<sup>4</sup>, Itai Kloog<sup>3,5</sup>

<sup>1</sup>Department of Epidemiology, Brown University School of Public Health, Providence, RI, USA

<sup>2</sup>Institute at Brown for Environment and Society, Brown University, Providence, RI, USA

<sup>3</sup>Department of Environmental Medicine and Public Health, Icahn School of Medicine at Mount Sinai, New York, NY, USA

<sup>4</sup>NASA Goddard Space Flight Center, Greenbelt, MD, USA

<sup>5</sup>The Department of Geography and Environmental Development, Ben-Gurion University of the Negev, Beer Sheva, Israel

Corresponding Author: [allan\\_just@brown.edu](mailto:allan_just@brown.edu)

Address: Allan Just, Box G-S121-2, Providence, RI 02912 USA

Cross-validation results stratified by meteorological season and for isolated sites by year, as well as scatterplots showing the association of relative topography and isolation with a summary of the contribution to predicted PM<sub>2.5</sub>

Table S1: 2019 cross-validation results ( $\mu\text{g}/\text{m}^3$ ) broken down by meteorological season. Results for December are taken from the 2018 model so that a contiguous winter is analyzed.

| Season | Observations | Sites | MAD  | MAE  | Bias  |
|--------|--------------|-------|------|------|-------|
| all    | 350,051      | 1,284 | 3.09 | 1.69 | -0.19 |
| Spring | 88,942       | 1,257 | 2.92 | 1.52 | -0.20 |
| Summer | 88,946       | 1,254 | 2.80 | 1.48 | -0.13 |
| Fall   | 87,022       | 1,246 | 3.06 | 1.65 | -0.19 |
| Winter | 85,141       | 1,284 | 3.55 | 2.12 | -0.25 |

Table [S1](#) shows cross-validation results by season for one year. Compared to the whole one-year period, MAD and MAE are lower in spring and summer and higher in winter.

Table S2: Results from each yearly cross-validation among isolated sites, in  $\mu\text{g}/\text{m}^3$ .

| Year | Observations | Sites | MAD  | MAE  | Bias  |
|------|--------------|-------|------|------|-------|
| 2003 | 25,913       | 236   | 4.67 | 1.92 | -0.03 |
| 2004 | 29,202       | 231   | 4.43 | 2.01 | 0.10  |
| 2005 | 30,520       | 225   | 5.02 | 2.09 | -0.00 |
| 2006 | 34,457       | 233   | 4.38 | 2.07 | 0.00  |
| 2007 | 37,396       | 225   | 4.78 | 2.21 | -0.08 |
| 2008 | 38,129       | 226   | 4.24 | 2.04 | -0.20 |
| 2009 | 40,172       | 223   | 3.83 | 1.94 | -0.19 |
| 2010 | 44,479       | 230   | 3.98 | 1.98 | -0.06 |
| 2011 | 45,310       | 223   | 4.20 | 2.22 | -0.26 |
| 2012 | 47,121       | 222   | 3.86 | 2.17 | -0.28 |
| 2013 | 49,856       | 224   | 3.71 | 2.12 | -0.16 |
| 2014 | 54,379       | 238   | 3.59 | 2.05 | -0.27 |
| 2015 | 55,638       | 242   | 3.58 | 2.04 | -0.17 |
| 2016 | 57,603       | 241   | 3.03 | 1.86 | -0.18 |
| 2017 | 60,450       | 239   | 3.49 | 1.99 | -0.15 |
| 2018 | 62,863       | 239   | 3.54 | 1.91 | -0.26 |
| 2019 | 63,539       | 242   | 3.00 | 1.68 | -0.18 |
| 2020 | 66,022       | 239   | 3.39 | 1.91 | -0.21 |
| 2021 | 67,509       | 243   | 3.86 | 1.95 | -0.27 |
| 2022 | 69,192       | 247   | 3.04 | 1.71 | -0.23 |
| 2023 | 71,329       | 251   | 3.97 | 1.92 | -0.18 |

In addition to the weighted analyses using all stations, we wished to evaluate performance where ground networks were especially sparse. Thus, Table [S2](#) shows unweighted MAE from cross-validation among the sites that were particularly isolated, defined as being more than 50 km from all other sites available in the same year.

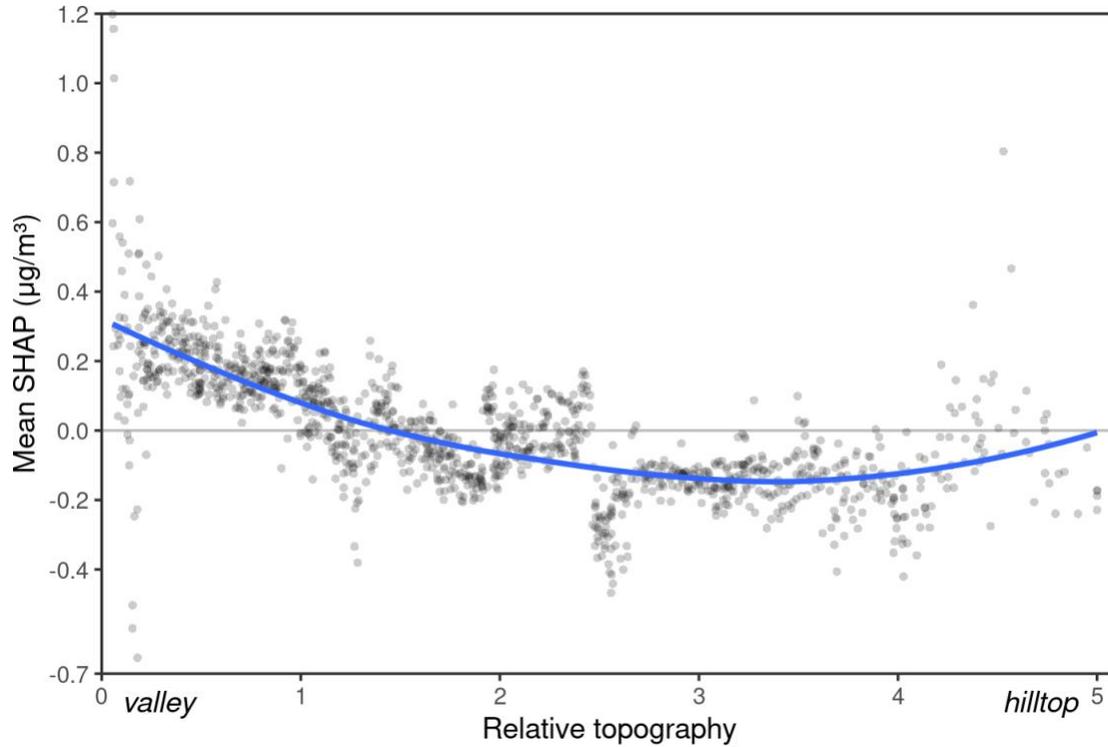


Figure S1: SHAP of hilliness as a function of hilliness.

Figure [S1](#), similar to Figure [3](#), plots the mean SHAP of the hilliness feature for each site. We see higher average predicted  $\text{PM}_{2.5}$  at sites in a valley versus on a hill.

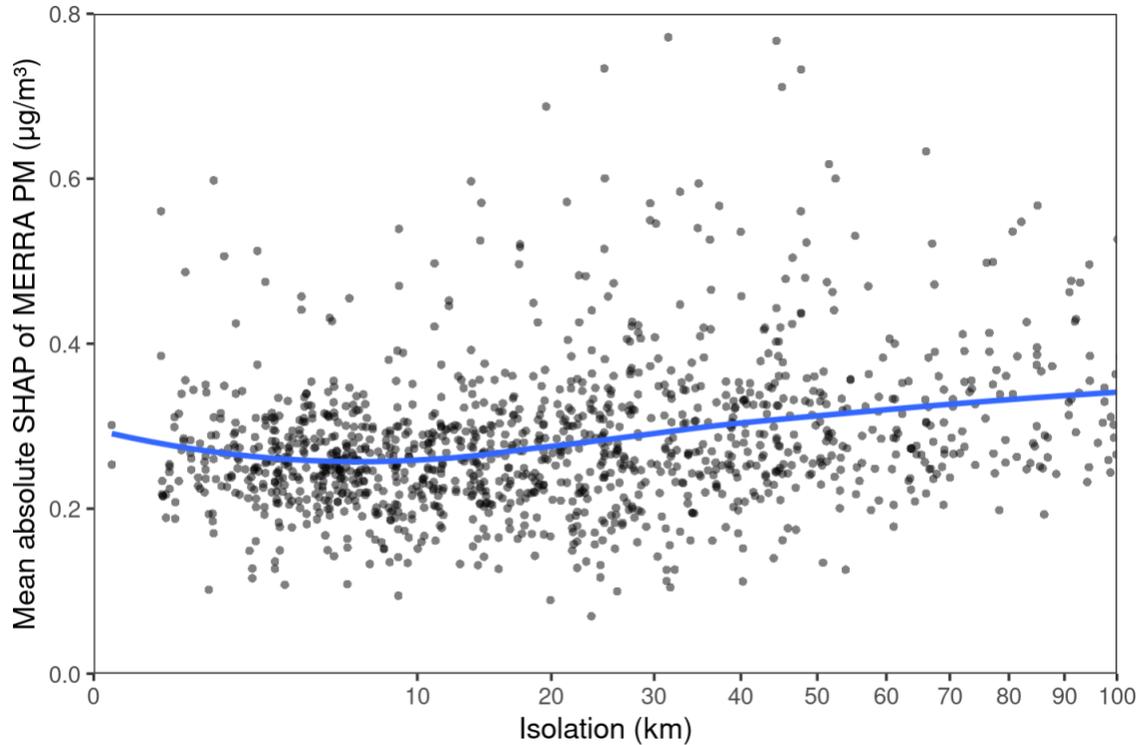


Figure S2: SHAP of modeled surface PM<sub>2.5</sub> concentrations from MERRA-2 as a function of site isolation. The  $x$ -axis is on a square-root scale.

Figure [S2](#) is an example of the relationship between the SHAP of one variable and a different quantity. The  $y$ -axis shows the per-site mean absolute SHAP of MERRA-2 modeled PM<sub>2.5</sub>, but the  $x$ -axis shows the site's distance from its nearest neighbor; that is, its degree of isolation. Similarly, we examined how the SHAP of the IDW feature varied according to isolation. The per-site mean absolute SHAP for IDW in 2010 was Kendall-correlated -0.17 with the distance to the nearest other site, meaning that the IDW is less influential on predictions for more isolated sites.