



Machine learning-derived daily wildfire and non-wildfire $PM_{2.5}$ concentration estimates over the western US, 2008-2018

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Abstract

Fine particulate matter $(PM_{2.5})$ levels are declining in many areas of the US due to policies and enforcement of the Clean Air Act. However, in much of the western US, PM_{2.5} concentrations have been increasing, likely due to the increased presence of wildfires in this region. There is growing evidence of various health impacts of $PM_{2.5}$ exposures, even at levels below the federal standard. Health studies of $PM_{2.5}$ in the western US are limited by spatial sparseness of monitoring data. To improve population exposure assessment of PM_{2.5}, researchers are increasingly using statistical methods to "blend" information from multiple data sources to better estimate PM_{2.5} in space and time. Some studies have created daily fine-resolution estimates of PM_{2.5} for the whole US, but they perform poorly in the western US. We have tailored a machine learning model to the western US, combining satellite, meteorological, monitoring, land use and other spatiotemporal data to estimate daily PM_{2.5} estimates at the census tract, ZIP code, and county levels during 2008-2018. Our methods improve upon previous models by: use of a more extensive monitoring station network, which captures more spatial locations and proximity to wildfires; use of ensembles of machine learning algorithms, which have been shown to improve model performance; and coverage of a longer period of time. We are making our data publicly available for use in future studies of the health impacts of fine particulate air pollution in the western US.

Background & Summary

Fine particulate matter (PM_{2.5}) air pollution is increasingly associated with numerous adverse health outcomes including, but not limited to, mortality [1],





respiratory and cardiovascular morbidity [34, 23], negative birth outcomes [15], and lung cancer [10]. Although PM_{2.5} concentrations have been declining in many parts of the United States due to policies to limit emissions of air pollutants [7], PM_{2.5} levels have been increasing in parts of the northwestern US [21]. This increase has been shown to be associated with wildfire smoke [21, 22], which can cause PM_{2.5} concentrations that are several times higher than the Environmental Protection Agency's (EPA's) daily PM_{2.5} National Ambient Air Quality Standard (NAAQS) in areas downwind of the wildfires for several days at a time [25].

Estimates of PM_{2.5} concentrations for health studies have traditionally been derived from data from stationary air quality monitors placed in and around populated areas for regulatory purposes. In the US, the EPA's Federal Reference Method (FRM) monitors often only measure every third or sixth day and do not provide enough spatial coverage to obtain a good estimate of the air pollution exposures where every person lives. In fact, most US counties do not contain a regulatory air pollution monitor [3]. Using solely monitoring data in health studies leads to exposure misclassification, which often, but not always, drives effect estimates of the association between air pollution and health towards the null [35].

To improve population exposure assessment of $PM_{2.5}$, epidemiological researchers have increasingly been using methods to estimate $PM_{2.5}$ exposures in the temporal and spatial gaps between regulatory monitors using data from satellites (such as aerosol optical depth (AOD) or polygons of smoke plumes) or air pollution models [3, 19]) over the past two decades. Each of these data sources has its own benefits and limitations, and researchers are increasingly statistically "blending" information from a combination of data sources to better estimate $PM_{2.5}$ in space and time. Various methods of blending have been used including spatiotemporal regression kriging (e.g., [13]), geographically-weighted regression (e.g., [16]), and machine learning methods (e.g., [24, 14, 5]).

Machine learning methods train large auxiliary datasets, often including satellite AOD, meteorological data, chemical transport model output, and land cover and land use data to provide optimal estimates of PM_{2.5} where people breathe. These models have been implemented in various locations around the world at city, regional, and national scales [2]. Some epidemiological questions can only be addressed in longitudinal studies with large sample sizes. Exposure models with large spatial and temporal domains will help enable such studies. Within the US, Di et al. [5, 6] and Hu et al. [14] have separately used machine learning algorithms to create fine-resolution daily PM_{2.5} estimates for the continental US. These models, however, have performed poorly in the western US [5, 14] and particularly the mountain west [6] compared to the rest of the country. Given the increasing trends in PM_{2.5} concentrations in parts of the western US and the importance of wildfires as a source of PM_{2.5} there, it is important to have a model that is tailored to this region to capture the variability in space and time in this region.

The dataset we describe here improves upon previous daily estimates of $PM_{2.5}$ concentrations from machine learning models in the following ways: (1)





use of a more extensive monitoring station network than used in previous models that captures more spatial locations and also proximity to wildfires, a key driver of $PM_{2.5}$ in the western US, (2) use of an ensemble of machine learning algorithms which have been shown to improve model performance [6], (3) better temporal prediction through the use of a nonlinear function (cosine) on day of year, (4) allowance for different prediction models for fire-affected and non-fire affected days to better capture and predict high $PM_{2.5}$ levels during wildfires, and (5) incorporation of errors in prediction back into daily estimates through spatial interpolation. We are making these data available as daily estimates of $PM_{2.5}$ exposures at census tract, ZIP-code, county scales in a public repository, which the above cited papers have not done, to be used in future studies of the societal impacts of air pollution exposure in the western US, where wildfires are a significant contributor to $PM_{2.5}$ concentrations.

[insert Figure 1: monitor locations (points) and state boundaries]

[insert Table 1: list variables]

Methods

Study Area

Our study area includes 11 western US states: Arizona, California, Colorado, Idaho, Montana, Nevada, New Mexico, Oregon, Utah, Washington, and Wyoming. Our temporal domain were all days between January 1, 2008 and ***, 2018. We predicted daily estimates of $PM_{2.5}$ at the ZIP code and county levels from machine learning ensembles trained on observed daily $PM_{2.5}$ values from monitoring stations from a variety of sources (**put in all $PM_{2.5}$ data sources). The predictor variables for the machine learning ensemble included (**put in all variables here) More information on the sources of these data can be found in Table 1.

PM_{2.5} Measurements

To get a more comprehensive set of locations and time points of $PM_{2.5}$ measurement throughout the western US, we did an extensive search for as many $PM_{2.5}$ monitoring data within our spatial and temporal study area as we could find. We downloaded $PM_{2.5}$ data from the US EPA AQS Air Data Query Tool [28] for the 11-state region (Figure ??) including any of the following parameter codes: 88101, 88500, 88502, 81104 [27, 29, 31]. These data include the IMPROVE monitors that capture air quality information in more rural areas [30]. We also retrieved all available $PM_{2.5}$ data in the Fire Cache Smoke Monitor Archive (https://wrcc.dri.edu/cgi-bin/smoke.pl), which includes U.S. Forest Service monitors that were deployed to capture air quality impacts during wild-fire events.

Some states have additional $PM_{2.5}$ monitors beyond those required by the U.S. EPA. We reached out to the department charged with air quality in every





state within our study domain and obtained additional $PM_{2.5}$ data from California Air Resources Board and the Utah Department of Environmental Quality. We only included data that was in addition to the monitors in those states that was part of the U.S. EPA's AQS and IMPROVE data.

We also reached out to researchers who may have had their own monitoring networks of $PM_{2.5}$ throughout the region. We were able to obtain data from the Uintah Basin, Utah from Seth Lyman at Utah State University, and $PM_{2.5}$ measurements from the Persistent Cold Air Pool Study (PCAPS) [26] conducted in the Salt Lake Valley, Utah in January–February, 2011 from Dr. Geoff Silcox at the University of Utah.

All of this yielded a total of XX daily $\mathrm{PM}_{2.5}$ observations, which represent XX locations.

Predictor Variables

[Write short description of each predictor data set and refer to Table 1]

Satellite Aerosol Optical Depth (AOD) is a measure of particle loading in the atmosphere from the ground to the satellite, which can be used as a proxy measure of PM_{2.5} when combined with other variables such as ... We obtained daily estimates of AOD from the MODIS Terra and Aqua combined Multi-angle Implementation of Atmospheric Correction (MAIAC) dataset https://ladsweb.modaps.eosdis.nasa.gov/archive/allData/6/MCD19A2/. This is the finest resolution (1 km) AOD dataset currently available and was available for our whole time period and spatial domain. After downloading each Hierarchical Data Format (HDF) file from the online repository, we calculated the average daily AOD values at each location, and took the nearest neighbor value at each PM_{2.5} monitoring location. MAIAC AOD has been shown to better predict PM_{2.5} than coarser resolution AOD [4] and has been used in many studies in various geographic regions in blended models to predict daily PM_{2.5} [17, 8, 18].

We obtained meteorological data from the North American Mesoscale (NAM), Analysis meteorological model https://www.ncdc.noaa.gov/data-access/model-data/model-datasets/north-american-mesoscale-forecast-system-nam because it includes all of the standard meteorological variables, including planetary boundary layer height, which are important for converting AOD to PM_{2.5} [20]. We calculated 24-hour averages from 6-hourly data for temperature, relative humidity, sea level pressure, surface pressure, planetary boundary layer height, dew point temperature, precipitation, snow coverage, and the U and V components of wind speed. NAM has 12 km resolution and is available from 2004 onward.

Because one of the reasons that $PM_{2.5}$ concentrations have been increasing in the western US is the increasing number and magnitude of wildfires, we wanted to have variables about the proximity of a location to an active fire. We collected daily data about fire detection locations and size from the MODIS Thermal Anomalies/Fire Daily L3 Global 1km product (MOD14 and MYD14) [9, 11]. As fires in closer proximity are likely to influence $PM_{2.5}$ more than fires





further away, we calculated the number of active fires in radial buffers of 25, 50, 100, and 500 km radii around each monitoring location.

Elevation can influence $PM_{2.5}$ concentrations. For example, $PM_{2.5}$ can accumulate in mountain valleys during persistent cold air pools (commonly referred to as inversions) during winter [33]. We obtained elevation data from the 3D Elevation Program, which has a resolution of 1 arc-second, which is approximately 30 m north/south and varies east/west with latitude [32].

Surrounding land cover can be a proxy for air pollution emissions. We used the land cover class information from the Landsat-derived National Land Cover Dataset (NLCD) [12] to calculate the percentage of urban development (codes 22, 23, and 24), agriculture (codes 81 and 82), and vegetated area other than agricultural land (codes 21, 41, 42, 43, 52, and 71) within buffer radii of 1 km, 5 km, and 10 km around each monitor. NLCD 2011 has a spatial resolution of 30 m and uses circa 2011 Landsat satellite data. We obtained the Normalized Difference Vegetation Index (NDVI) from the MODIS satellite product MOD13A3 https://lpdaac.usgs.gov/products/mod13a3v006/ at 1 km resolution by month as another measure of vegetation that was not just a measure of agricultural vegetation but all vegetation.

As a proxy indicator of emissions from vehicles, we calculated the sum of all road lengths of type Arterial and Collector within 100, 250, 500, 1000 m buffers of each monitoring location. Arterial roads are high-capacity urban roads. Collector roads are low-to-moderate capacity roads. The road data came from the National Highways Planning Network https://www.fhwa.dot.gov/planning/processes/tools/nhpn/index.cfm which contains spatial information on over 450,000 miles of highways in the United States.

We included population density as an additional proxy for emisions as areas with higher population have more sources of air pollution emissions. Population density was obtained from the American Community Survey at the XXX (spatial resolution) for each year or five year averages?

To account for seasonality in $PM_{2.5}$ data, we created the following predictor variables: cosine of day-of-year and cosine of month. We also created dummy variables for each state and month in our study domain to allow for spatial and temporal variation in the data that could not be explained by any of the other spatial, temporal, or spatiotemporal variables.

Data merging

We created three datasets: one dataset to train the model and two prediction datasets. The training dataset merged all predictor variables to each 24-hour average $PM_{2.5}$ monitoring observation by linking the data temporally (using date) and spatially (by selecting the nearest observation for each predictor variable). Similarly, the prediction datasets were created by spatially and temporally linking all predictor variables to the population-weighted centroid of each ZIP code and county for each day in the study domain.





Machine learning modeling and mapping

Finally, we created an indicator variable for whether there were one or more fires within 500 km of a monitor in the last week.

Code availability

[Insert brief description of how to access code on GitHub.] The code was written and annotated in R [version number] and Python [version number] and is available from GitHub [doi citation link]. The key package for implementing the ML model was [caretEnsemble?].

Data Records

All data are freely available from [repository name, data doi citation]. We provide ... [reference Figure 2]

[insert Figure 2: choropleths at zip code level - 4-panel: a) highest year $PM_{2.5}$, Aug or Sept, b) highest year $PM_{2.5}$, Jan/Feb, c) lowest year $PM_{2.5}$, Aug or Sept, d) lowest year $PM_{2.5}$, Jan/Feb.]

[insert Figure 3: Time series of select cities]

[Insert Table 3: list of files]

Technical Validation

[Write description of goodness of fit methods/metrics - out-of-bag data, RMSE, \mathbb{R}^2 , models run on subsets of data, etc.]

[Insert Figure 4: a) out-of bag observed $PM_{2.5}$ vs predicted, b) full model observed $PM_{2.5}$ vs predicted, c-j) various subsets of data - oob and full model plots (see figure 5 of example paper)]

[Write discussion about variable importance, possibly referring to the suggested figure of variable importance panel figure. Could make an observation or two about the complexity of the variables, e.g., $PM_{2.5}$ can be highest at highest and lowest temperatures (summer fire season and winter inversions), etc.]

[Thoughts - insert figure of predicted $PM_{2.5}$ vs predictor variable for the 8 (or so) most important variables (panel figure)]

Thoughts: compare to $PM_{2.5}$. Concerned comparing to HMS will take too long?

Usage Notes

[Write brief description of things the provided code can be adapted to do, such as making plots of specific years, use in health/pollution studies.]





Acknowledgements

[Write acknowledgements text here.]

Author contributions

[Write brief description of contribution from each author.]

Competing interests

The authors declare not competing interests.

Figures and figures legends

[All figures go here and are referred to in the text]

Tables

Table 1: Variables used in the machine learning models.

| Variables | Type | Source |
|---|----------------|--|
| Coordinates in degrees (Latitude | Spatial | PM2.5 monitoring |
| and Longitude) | | data |
| Count of Active Fire Points within each of the following radial buffers (25 km, 50 km, 100 km, and 500 km) for same day and up to 7 lag days for each radial buffer | Spatiotemporal | MODIS Thermal Anomalies/Fire Daily L3 Global 1km product |
| Binary Fire indicator (0 for no active fire points in any buffer radii or lag for given point; 1 otherwise) | Spatiotemporal | MODIS Thermal Anomalies/Fire Daily L3 Global 1km product |
| Summed length (in meters) of arterial (A) and collector (C) roads and both $(A + C)$ within 100, 250, 500, and 1000 m buffer radii | Spatial | National Highways Planning Network |
| Population Density | Spatial | **Ellen, can you provide this information? |





| AOD (unitless) | Spatiotemporal | MODIS Terra and Aqua combined Multi-angle Implementation of Atmospheric Correction (MAIAC) dataset |
|---|----------------|--|
| Planetary Boundary Layer Height (m) | Spatiotemporal | NAM |
| Temperature at 2 m above ground (K) | Spatiotemporal | NAM |
| Relative humidity at 2 m above ground (%) | Spatiotemporal | NAM |
| Dew point temperature at 2 m above ground (K) | Spatiotemporal | NAM |
| Snow Cover (%) | Spatiotemporal | NAM |
| U-component (east/west) of wind at 10 m above ground (m/s) | Spatiotemporal | NAM |
| V-component (north/south) of wind at 10 m above ground (m/s) | Spatiotemporal | NAM |
| mean sea level pressure (Pa) | Spatiotemporal | NAM |
| surface pressure (Pa) | Spatiotemporal | NAM |
| Vertical Velocity (Geometric) at 850 mb (m/s) | Spatiotemporal | NAM |
| Vertical Velocity (Geometric) at 700 mb (m/s) | Spatiotemporal | NAM |
| % of urban development within each of the following radial buffers (1 km, 5 km, and 10 km) | Spatial | National Land Cover Database |
| Normalized Difference Vegetation Index (NDVI) | Spatiotemporal | MODIS |
| Season (Winter = December-February; Spring = March-May; Summer = June-August; Fall = September-November) | Temporal | derived from date |
| indicator variables for state | Spatial | derived from latitude and longitude |
| Indicator variable for year | Temporal | derived from date |
| Month | Temporal | derived from date |
| Cosine of Day of Week | Temporal | derived from date |
| Cosine of Day of Year | Temporal | derived from date |
| elevation | Spatial | NED |
| CONSIDER REMOVING VARIABLES BELOW | | |
| FROM LIST - Are any of these | | |
| actually used as predictors? | | |





| Date | Temporal | PM2.5 monitoring data |
|---|----------------|--|
| TimeZone | Spatial | **are we using this as a predictor variable??? |
| APCP.surface | Spatiotemporal | NAM (Total Precipitation - had no variation in the data, not sure why) |
| WEASD.surface Water Equivalent of Accumulated Snow Depth | Spatiotemporal | NAM (data looks time series) |
| Day of Week | Temporal | derived from date |

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